Supporting Information for

ADME prediction with KNIME: *In silico* aqueous solubility consensus model based on supervised recursive random forest approaches

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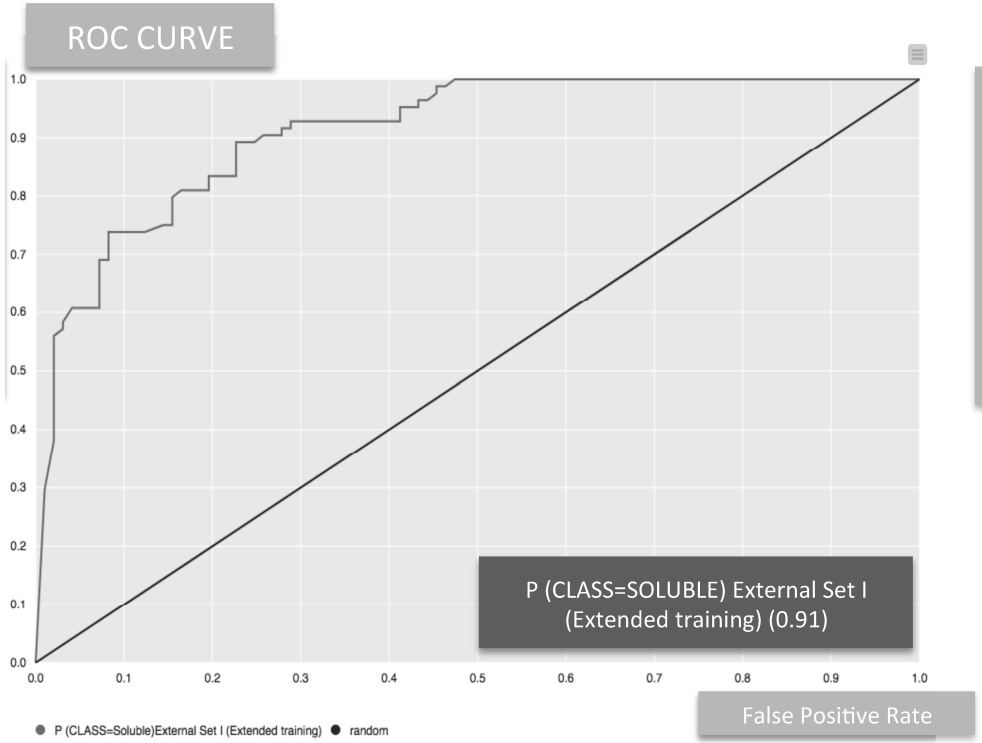
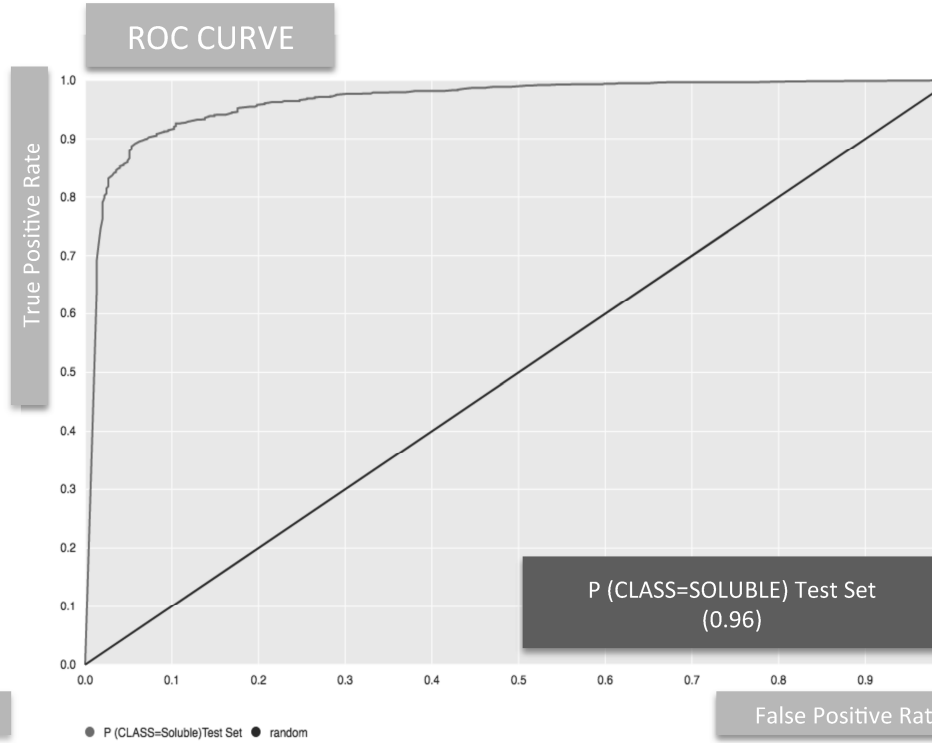
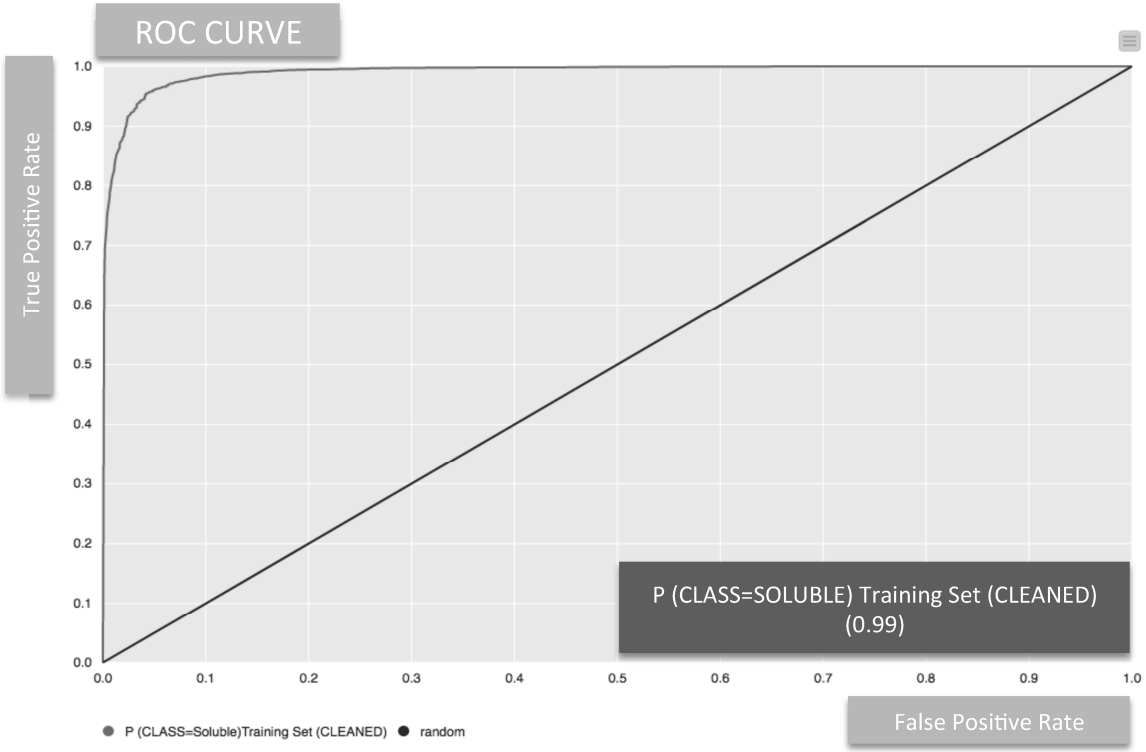

ROC CURVE
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
P (CLASS=SOLUBLE) External Set I (Extended training) (0.91)
False Positive Rate
P (CLASS=Soluble)External Set I (Extended training)
random


ROC CURVE
True Positive Rate
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
P (CLASS=SOLUBLE) Test Set (0.96)
False Positive Rat
P (CLASS=Soluble)Test Set
random


ROC CURVE
True Positive Rate
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
P (CLASS=SOLUBLE) Training Set (CLEANED) (0.99)
False Positive Rate
P (CLASS=Soluble)Training Set (CLEANED)
random

Supporting Information
Table S1

Training Set (CLEANED)(Unknown STD OR STD >= 1)

"InChi"	"logS(M)"
InChI=1S/C10H12N6/c11-1-5-15(6-2-12)9-10-16(7-3-13)8-4-14/h5-10H2	-2.82
InChI=1S/C4H12N2/c1-4(2,6)3-5/h3,5-6H2,1-2H3	1.055
InChI=1S/C15H29NO/c17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-15/h1-14H2,(H,16,17)	-2.874
InChI=1S/C20H41NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(23)21-18-19-22/h22H,2-19H2,1H3,(H,21,23)	-5.515
InChI=1S/C18H23N9O4S3/c1-25(2)3-4-26-18(22-23-24-26)34-7-9-6-32-15-12(14(29)27(15)13(9)h8,12,15H,3-7H2,1-2H3,(H2,19,20)(H,21,28)(H,30,31)	-3.149
InChI=1S/C6H5ClO2S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H	-1.885
InChI=1S/C16H17NO4/c17-13(8-12-6-7-14(18)15(19)9-12)16(20)21-10-11-4-2-1-3-5-11/h1-7,9,13,18-19H,8,10,17H2	-1.81
InChI=1S/C9H8N4OS/c14-9(12-8-6-10-13-15-8)11-7-4-2-1-3-5-7/h1-6H,(H2,11,12,14)	-3.85
InChI=1S/C14H15O2P/c1-16-12-17(15,13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-11H,12H2,1H3	-1.949
InChI=1S/C10H10O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7+	-2.734
InChI=1S/C4H7N3S/c1-3-5-6-4(8)7(3)2/h1-2H3,(H,6,8)	-1.431
InChI=1S/C10H12N4O3/c1-14-4-9(16)5-2-6(12-13-10(11)17)8(15)3-7(5)14/h2-3,9,16H,4H2,1H3,(H3,11,13,17)/b12-6+	-2.72
InChI=1S/C7H6ClN3O/c8-4-1-2-6-5(3-4)10-7(11-9)12-6/h1-3H,9H2,(H,10,11)	-2.062
InChI=1S/C16H17N3O5S/c1-7-6-25-15-11(14(22)19(15)12(7)16(23)24)18-13(21)10(17)8-2-4-9(h2-5,10-11,15,20H,6,17H2,1H3,(H,18,21)(H,23,24)	-2.515
InChI=1S/C10H12O4/c1-3-14-10(12)8-6-7(13-2)4-5-9(8)11/h4-6,11H,3H2,1-2H3	-2.764
InChI=1S/C18H41N7/c19-17(20)24-15-11-7-3-1-5-9-13-23-14-10-6-2-4-8-12-16-25-18(21)2h23H,1-16H2,(H4,19,20,24)(H4,21,22,25)	0.332
InChI=1S/C35H58O12/c1-4-5-11-16-29(41)32-30(42)20-26(38)18-24(36)17-25(37)19-27(39)h6-10,12-15,23-34,36-45H,4-5,11,16-21H2,1-3H3/b7-6-,10-8-,12-9-,15-13-,22-14-	-2.586
InChI=1S/C17H18N2O2/c1-3-21-17(20)14-9-11-15(12-10-14)18-13-19(2)16-7-5-4-6-8-16/h4-13H,3H2,1-2H3/b18-13+	-5.451
InChI=1S/C14H19IN2O6/c1-2-3-4-12(19)22-7-10-9(18)5-11(23-10)17-6-8(15)13(20)16-14(17)2h6,9-11,18H,2-5,7H2,1H3,(H,16,20,21)	-3.4

RELIABLE SET_TEST SET (STD < 1)

"InChi"	"logS(M)"
InChI=1S/C13H16F3N3O4/c1-3-5-17(6-4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(22)23/h7-8H,3-6H2,1-2H3	-6.05
InChI=1S/C11H22O/c1-3-5-7-9-11(12)10-8-6-4-2/h3-10H2,1-2H3	-3.532
InChI=1S/C11H12ClNO3S/c1-13-10(14)6-7-17(15,16)11(13)8-2-4-9(12)5-3-8/h2-5,11H,6-7H2,1H3	-2.039
InChI=1S/C8H15NO3/c1-3-9(4-2)7(10)5-6-8(11)12/h3-6H2,1-2H3,(H,11,12)	-0.794
InChI=1S/C12H3Cl7/c13-5-2-1-4(9(16)10(5)17)8-6(14)3-7(15)11(18)12(8)19/h1-3H	-8.261
InChI=1S/C12H6Cl4/c13-7-1-3-9(11(15)5-7)10-4-2-8(14)6-12(10)16/h1-6H	-6.51
InChI=1S/C18H21NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18)9-12(19)3-6,11-13,17,20H,7-9H2,1-2H3	-1.522
InChI=1S/C10H12/c1-2-6-10-8-4-3-7-9(10)5-1/h1-2,5-6H,3-4,7-8H2	-3.567
InChI=1S/C3H7ClO2/c4-1-3(6)2-5/h3,5-6H,1-2H2	0.957
InChI=1S/C12H8N2/c1-3-9-5-6-10-4-2-8-14-12(10)11(9)13-7-1/h1-8H	-1.826
InChI=1S/C7H13N3O3S/c1-8-7(12)13-9-5(14-4)6(11)10(2)3/h1-4H3,(H,8,12)/b9-5-	0.106
InChI=1S/C10H8N2/c1-5-11-6-2-9(1)10-3-7-12-8-4-10/h1-8H	-1.538
InChI=1S/C27H38N2O4/c1-20(2)27(19-28,22-10-12-24(31-5)26(18-22)33-7)14-8-15-29(3)16-17-9-12,17-18,20H,8,13-16H2,1-7H3	-3.98
InChI=1S/C10H14N2O/c1-3-12(10(11)13)9-7-5-4-6-8(9)2/h4-7H,3H2,1-2H3,(H2,11,13)	-0.21
InChI=1S/C4H8O2/c1-2-3-6-4-5/h4H,2-3H2,1H3	-0.49
InChI=1S/C7H8/c1-2-4-6-7-5-3-1/h1-6H,7H2	-2.172
InChI=1S/C3H5Br2Cl/c4-1-3(5)2-6/h3H,1-2H2	-2.374
InChI=1S/C16H12ClF4N3O4/c1-2-22(8-10-11(17)4-3-5-12(10)18)15-13(23(25)26)6-9(16(19,20)21)h3-7H,2,8H2,1H3	-6.625
InChI=1S/C4H10O/c1-3-5-4-2/h3-4H2,1-2H3	-0.089
InChI=1S/C27H42O3/c1-16-7-12-27(29-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19(28)h5,16-17,19-24,28H,6-15H2,1-4H3	-7.317
InChI=1S/C13H11N3/c14-10-3-1-8-5-9-2-4-11(15)7-13(9)16-12(8)6-10/h1-7H,14-15H2	0.378
InChI=1S/C5H11NO2/c1-4(2)3-8-5(6)7/h4H,3H2,1-2H3,(H2,6,7)	-0.3
InChI=1S/C2H5NO/c1-2(3)4/h1H3,(H2,3,4)	1.581
InChI=1S/C15H23NO4/c1-8-3-9(2)15(20)11(4-8)12(17)5-10-6-13(18)16-14(19)7-10/h8-12,17H,3-7H2,1-2H3,(H,16,18,19)	-1.127
InChI=1S/C3H6N2O2/c4-2-1-7-5-3(2)6/h2H,1,4H2,(H,5,6)	-0.01

"InChi"	"logS(M)"
InChI=1S/C20H26N2O2/ c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6-8-21-18-5-4-15(24-2)1 h4-6,8,11,13-14,19-20,23H,3,7,9-10,12H2,1-2H3	-3.051
InChI=1S/C16H22O4/ c1-11(2)9-19-15(17)13-7-5-6-8-14(13)16(18)20-10-12(3)4/ h5-8,11-12H,9-10H2,1-4H3	-4.384
InChI=1S/C18H20NO3PS/ c1-3-21-23(20,22-4-2)13-14-9-11-15(12-10-14)18-19-16-7-5-6-8-17(1 h5-12H,3-4,13H2,1-2H3	-4.002
InChI=1S/C6H10O/c1-4-6(3,7)5-2/h1,7H,5H2,2-3H3	0.017
InChI=1S/C8H11NO/c9-6-8(10)7-4-2-1-3-5-7/h1-5,8,10H,6,9H2	-0.476
InChI=1S/C12H15Cl2NO5S/ c1-21(19,20)8-4-2-7(3-5-8)10(17)9(6-16)15-12(18)11(13)14/ h2-5,9-11,16-17H,6H2,1H3,(H,15,18)	-2.15
InChI=1S/C5H10N2O/c8-6-7-4-2-1-3-5-7/h1-5H2	-0.174
InChI=1S/C23H32O6/ c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14,2) h10,16-18,20,26,28H,4-9,11-12H2,1-3H3	-4.458
InChI=1S/C12H16O3/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/ h3-6,9,13H,7-8H2,1-2H3	-3.157
InChI=1S/C6H13NS2/c1-4-7-5(2)9-6(3)8-4/h4-7H,1-3H3	-1.368
InChI=1S/C27H40O6/ c1-24(2,3)14-22(31)33-15-21(30)27(32)11-9-19-18-7-6-16-12-17(28)8 h12,18-20,23,29,32H,6-11,13-15H2,1-5H3	-5.511
InChI=1S/C20H13N/ c1-3-7-15-13(5-1)9-11-17-18-12-10-14-6-2-4-8-16(14)20(18)21-19(15 h1-12,21H	-7.41
InChI=1S/C6H10/c1-3-5-6-4-2/h1H,4-6H2,2H3	-2.36
InChI=1S/C12H4Cl6/ c13-6-3-1-2-5(10(6)16)9-11(17)7(14)4-8(15)12(9)18/h1-4H	-8.604
InChI=1S/C6H12O2/c1-3-4-5-6(7)8-2/h3-5H2,1-2H3	-1.361
InChI=1S/C11H26NO2PS/c1-7-14-15(6,13)16-9-8-12(10(2)3)11(4)5/ h10-11H,7-9H2,1-6H3	-0.95
InChI=1S/C11H14N4O2S2/ c1-7(2)10-13-14-11(18-10)15-19(16,17)9-5-3-8(12)4-6-9/h3-7H, 12H2,1-2H3,(H,14,15)	-3.414
InChI=1S/C10H9N/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,11H2	-1.925
InChI=1S/C10H10O3/c1-13-9-5-2-8(3-6-9)4-7-10(11)12/h2-7H,1H3, (H,11,12)/b7-4+	-2.398
InChI=1S/C15H15ClN2O2/ c1-18(2)15(19)17-12-5-9-14(10-6-12)20-13-7-3-11(16)4-8-13/ h3-10H,1-2H3,(H,17,19)	-4.895
InChI=1S/C20H26O2/ c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(18, h1,12,15-18,22H,4-11H2,2H3	-4.627
InChI=1S/C7H7ClO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3	-2.464
InChI=1S/C14H12N4O2S/ c15-10-5-7-11(8-6-10)21(19,20)18-14-9-16-12-3-1-2-4-13(12)17-14/ h1-9H,15H2,(H,17,18)	-4.603

"InChi"	"logS(M)"
InChI=1S/C12H12N4O3/c17-11(14-8-10-4-2-1-3-5-10)9-15-7-6-13-12(15)16(18)19/h1-7H,8-9H2,(H,14,17)	-2.813
InChI=1S/C11H14O2/c1-2-3-9-13-11(12)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3	-3.48
InChI=1S/C6H3ClN4/c7-5-2-9-4-1-8-3-10-6(4)11-5/h1-3H	-0.875
InChI=1S/C33H36N4O6/c1-7-20-19(6)32(42)37-27(20)14-25-18(5)23(10-12-31(40)41)29(35-25)h7-8,13-14,34-35H,1-2,9-12,15H2,3-6H3,(H,36,43)(H,37,42)(H,38,39)(H,40,41)/b26-13-,27-14-	-4.813
InChI=1S/C10H4Cl2O2/c11-7-8(12)10(14)6-4-2-1-3-5(6)9(7)13/h1-4H	-5.024
InChI=1S/C6H12O/c1-4-5(2)6(3)7/h5H,4H2,1-3H3	-0.68
InChI=1S/C3H7NO2/c1-2-6-3(4)5/h2H2,1H3,(H2,4,5)	0.731
InChI=1S/C5H12O/c1-4(2)5(3)6/h4-6H,1-3H3	-0.18
InChI=1S/C8H8N4O4/c13-8-9-3-4-11(8)10-5-6-1-2-7(16-6)12(14)15/h1-2,5H,3-4H2,(H,9,13)/b10-5+	-3.357
InChI=1S/C14H13ClN6O5S/c1-25-9-7-10(26-2)18-13(17-9)19-14(22)20-27(23,24)12-11(15)16-8-5h3-7H,1-2H3,(H2,17,18,19,20,22)	-4.789
InChI=1S/C4H10NO3PS/c1-4(6)5-9(7,8-2)10-3/h1-3H3,(H,5,6,7)	0.54
InChI=1S/C5H6N2O2/c1-7-3-2-4(8)6-5(7)9/h2-3H,1H3,(H,6,8,9)	-0.8
InChI=1S/C12H8N2/c1-3-9-5-6-11-10(4-2-7-13-11)12(9)14-8-1/h1-8H	-2.681
InChI=1S/C8H6Cl2O3/c9-5-1-2-7(6(10)3-5)13-4-8(11)12/h1-3H,4H2,(H,11,12)	-2.514
InChI=1S/C13H12N2S/c16-13(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10H,(H2,14,15,16)	-3.972
InChI=1S/C8H15NO/c1-7(10)6-8-4-2-3-5-9-8/h8-9H,2-6H2,1H3	-0.451
InChI=1S/C8H10O8/c9-5(10)1-3-7(13)15-16-8(14)4-2-6(11)12/h1-4H2,(H,9,10)(H,11,12)	-0.847
InChI=1S/C8H8O2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3,(H,9,10)	-2.062
InChI=1S/C13H17N3O3/c1-10(17)15(4)16(11-8-6-5-7-9-11)13(19)12(18)14(2)3/h5-9H,1-4H3	-0.534
InChI=1S/C14H16ClO5PS/c1-4-17-21(22,18-5-2)20-10-6-7-12-11(8-10)9(3)13(15)14(16)19-12/h6-8H,4-5H2,1-3H3	-5.382
InChI=1S/C10H14N2/c1-2-7-12-10(5-1)9-4-3-6-11-8-9/h3-4,6,8,10,12H,1-2,5,7H2	0.79
InChI=1S/C2H2Cl2/c3-1-2-4/h1-2H/b2-1+	-1.187
InChI=1S/C8H18O/c1-3-5-6-8(4-2)7-9/h8-9H,3-7H2,1-2H3	-2.16
InChI=1S/C10H11NO2/c1-2-7-13-9-6-4-3-5-8(9)10(11)12/h2-6H,1,7H2,(H2,11,12)	-2.227
InChI=1S/C8H15NO/c1-9-6-2-3-7(9)5-8(10)4-6/h6-8,10H,2-5H2,1H3	0.083
InChI=1S/C6H9N3O3/c1-5-7-4-6(9(11)12)8(5)2-3-10/h4,10H,2-3H2,1H3	-1.21
InChI=1S/C9H13NO/c1-7(10)9(11)8-5-3-2-4-6-8/h2-7,9,11H,10H2,1H3	-0.879

"InChi"	"logS(M)"
InChI=1S/C12H4Cl6/c13-7-2-1-5(3-8(7)14)6-4-9(15)11(17)12(18)10(6)16/h1-4H	-7.831
InChI=1S/C3H6O3/c4-1-3(6)2-5/h4-5H,1-2H2	1.014
InChI=1S/C9H8O2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H,(H,10,11)/b7-6+	-2.433
InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h1H,4-9H2,2H3	-4.094
InChI=1S/C13H18O5S/c1-5-16-12-13(2,3)10-8-9(18-19(4,14)15)6-7-11(10)17-12/h6-8,12H,5H2,1-4H3	-3.42
InChI=1S/C7H9N/c1-6-3-4-8-5-7(6)2/h3-5H,1-2H3	-0.314
InChI=1S/C6H14O/c1-5(2)4-6(3)7/h5-7H,4H2,1-3H3	-0.794
InChI=1S/C7H6O5/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,8-10H,(H,11,12)	-1.155
InChI=1S/C22H29FO4/c1-12-9-17-15-6-8-21(27,13(2)24)20(15,4)11-18(26)22(17,23)19(3)7-5h5,7,10,12,15,17-18,26-27H,6,8-9,11H2,1-4H3	-4.099
InChI=1S/C8H7ClO3/c9-6-3-1-2-4-7(6)12-5-8(10)11/h1-4H,5H2,(H,10,11)	-2.164
InChI=1S/C14H9Cl5O/c15-11-5-1-9(2-6-11)13(20,14(17,18)19)10-3-7-12(16)8-4-10/h1-8,20H	-5.666
InChI=1S/C2HBrClF3/c3-1(4)2(5,6)7/h1H	-1.704
InChI=1S/C15H23NO2/c1-4-7-13-8-5-6-9-15(13)18-11-14(17)10-16-12(2)3/h4-6,8-9,12,14,16-17H,1,7,10-11H2,2-3H3	-2.88
InChI=1S/C7H5NO3S/c9-7-5-3-1-2-4-6(5)12(10,11)8-7/h1-4H,(H,8,9)	-1.672
InChI=1S/C13H16N2O6/c1-7-10(14(17)18)6-9(13(3,4)5)12(21-8(2)16)11(7)15(19)20/h6H,1-5H3	-4.47
InChI=1S/C17H18F3N3O3/c1-21-4-6-22(7-5-21)15-12(19)8-10-14(13(15)20)23(3-2-18)9-11(16(1h8-9H,2-7H2,1H3,(H,25,26)	-2.73
InChI=1S/C11H13F3N4O4/c1-3-16(4-2)9-7(17(19)20)5-6(11(12,13)14)8(15)10(9)18(21)22/h5H,3-4,15H2,1-2H3	-5.467
InChI=1S/C18H19Cl2NO4/c1-5-25-18(23)14-10(3)21-9(2)13(17(22)24-4)15(14)11-7-6-8-12(19)1h6-8,15,21H,5H2,1-4H3	-5.68
InChI=1S/C9H13N3O5/c10-5-1-2-12(9(16)11-5)8-7(15)6(14)4(3-13)17-8/h1-2,4,6-8,13-15H,3H2,(H2,10,11,16)	-0.141
InChI=1S/C13H13Cl2N3O3/c1-7(2)16-12(20)17-6-11(19)18(13(17)21)10-4-8(14)3-9(15)5-10/h3-5,7H,6H2,1-2H3,(H,16,20)	-4.376
InChI=1S/C9H7BrO4/c1-5(11)14-8-3-2-6(10)4-7(8)9(12)13/h2-4H,1H3,(H,12,13)	-2.59
InChI=1S/C6H13Cl/c1-2-3-4-5-6-7/h2-6H2,1H3	-3.122
InChI=1S/C21H30O3/c1-13(22)24-15-8-10-20(2)14(12-15)4-5-16-17-6-7-19(23)21(17,3)11-h4,15-18H,5-12H2,1-3H3	-4.458

"InChi"	"logS(M)"
InChI=1S/C6H4Cl2/c7-5-1-2-6(8)4-3-5/h1-4H	-3.35
InChI=1S/C7H6N2/c8-5-6-1-3-7(9)4-2-6/h1-4H,9H2	-1.143
InChI=1S/C6H3Br3/c7-4-1-5(8)3-6(9)2-4/h1-3H	-5.6
InChI=1S/C11H16N2O3/c1-4-6-11(7(3)5-2)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3H3,(H2,12,13,14,15,16)	-2.02
InChI=1S/C11H15BrN2O3/c1-4-6(2)11(5-7(3)12)8(15)13-10(17)14-9(11)16/h6H,3-5H2,1-2H3,(H2,13,14,15,16,17)	-2.65
InChI=1S/C13H15N3O2/c1-10-9-12(18-13(17)15(2)3)16(14-10)11-7-5-4-6-8-11/h4-9H,1-3H3	-2.089
InChI=1S/C14H18N4O3/c1-19-10-5-8(6-11(20-2)12(10)21-3)4-9-7-17-14(16)18-13(9)15/h5-7H,4H2,1-3H3,(H4,15,16,17,18)	-2.861
InChI=1S/C12H6Cl4/c13-8-2-4-10(14)9(6-8)7-1-3-11(15)12(16)5-7/h1-6H	-6.853
InChI=1S/C11H16/c1-2-3-5-8-11-9-6-4-7-10-11/h4,6-7,9-10H,2-3,5,8H2,1H3	-4.643
InChI=1S/C14H12N2O4/c17-15(18)13-7-3-11(4-8-13)1-2-12-5-9-14(10-6-12)16(19)20/h3-10H,1-2H2	-4.59
InChI=1S/C5H10O2/c1-3-5(6)7-4-2/h3-4H2,1-2H3	-0.66
InChI=1S/C7H7ClN4O2/c1-11-4-3(9-6(8)10-4)5(13)12(2)7(11)14/h1-2H3,(H,9,10)	-1.508
InChI=1S/C21H26N2S2/c1-22-13-6-5-7-16(22)12-14-23-18-8-3-4-9-20(18)25-21-11-10-17(24-h3-4,8-11,15-16H,5-7,12-14H2,1-2H3	-5.82
InChI=1S/C7H5ClO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,(H,10,11)	-1.237
InChI=1S/C8H16/c1-2-4-6-8-7-5-3-1/h1-8H2	-4.152
InChI=1S/C6H14O/c1-5(2)6(3,4)7/h5,7H,1-4H3	-0.411
InChI=1S/C6H14O/c1-2-3-4-5-6-7/h7H,2-6H2,1H3	-1.383
InChI=1S/C5H12O/c1-5(2,3)4-6/h6H,4H2,1-3H3	-0.401
InChI=1S/C11H17N3O3/c1-2-11(14-6-4-3-5-7-14)8(15)12-10(17)13-9(11)16/h2-7H2,1H3,(H2,12,13,15,16,17)	-2.156
InChI=1S/C7H16O/c1-4-6-7(3,8)5-2/h8H,4-6H2,1-3H3	-1.001
InChI=1S/C6H4Br2/c7-5-2-1-3-6(8)4-5/h1-4H	-3.543
InChI=1S/C12H8O4/c1-14-12-10-8(4-5-15-10)6-7-2-3-9(13)16-11(7)12/h2-6H,1H3	-3.52
InChI=1S/C7H13BrN2O2/c1-3-7(8,4-2)5(11)10-6(9)12/h3-4H2,1-2H3,(H3,9,10,11,12)	-2.68
InChI=1S/C16H16N2O/c1-3-18-13-9-5-4-8-12(13)16(19)17(2)14-10-6-7-11-15(14)18/h4-11H,3H2,1-2H3	-4.749
InChI=1S/C6H6O2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H	0.612
InChI=1S/C10H12O3/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h3-6,11H,2,7H2,1H3	-2.68
InChI=1S/C4H8O2/c1-4(2)6-3-5/h3-4H,1-2H3	-0.63

"InChi"	"logS(M)"
InChI=1S/C13H10N2O4/c16-10-6-5-9(11(17)14-10)15-12(18)7-3-1-2-4-8(7)13(15)19/h1-4,9H,5-6H2,(H,14,16,17)	-2.676
InChI=1S/C13H18O3/c1-2-3-4-5-10-16-13(15)11-6-8-12(14)9-7-11/h6-9,14H,2-5,10H2,1H3	-3.949
InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,7,11H,4,6,8H2,1-3H3/b10-7+	-2.321
InChI=1S/C11H12Cl2N2O5/c12-10(13)11(18)14-8(5-16)9(17)6-1-3-7(4-2-6)15(19)20/h1-4,8-10,16-17H,5H2,(H,14,18)	-2.111
InChI=1S/C21H28O2/c1-3-20-11-9-17-16-8-6-15(22)13-14(16)5-7-18(17)19(20)10-12-21(2(h2,13,16-19,23H,3,5-12H2,1H3	-5.257
InChI=1S/C8H13NO2/c1-9-5-3-4-7(6-9)8(10)11-2/h4H,3,5-6H2,1-2H3	0.809
InChI=1S/C5H12N2O/c1-6(2)5(8)7(3)4/h1-4H3	0.935
InChI=1S/C6H4Cl2/c7-5-3-1-2-4-6(5)8/h1-4H	-3.053
InChI=1S/C13H26N2O4/c1-4-6-8-15-12(17)19-10-13(3,7-5-2)9-18-11(14)16/h4-10H2,1-3H3,(H2,14,16)(H,15,17)	-2.74
InChI=1S/C12H16O3/c1-2-3-4-9-15-12(14)10-5-7-11(13)8-6-10/h5-8,13H,2-4,9H2,1H3	-3.813
InChI=1S/C10H15N/c1-9(8-11-2)10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3	-1.095
InChI=1S/C25H28O3/c1-4-27-22-15-13-21(14-16-22)25(2,3)19-26-18-20-9-8-12-24(17-20)2 h5-17H,4,18-19H2,1-3H3	-8.576
InChI=1S/C15H14N4O2S/c16-12-6-8-14(9-7-12)22(20,21)18-15-10-11-17-19(15)13-4-2-1-3-5-1 h1-11,18H,16H2	-2.321
InChI=1S/C8H18O2/c1-3-5-8(10)7(4-2)6-9/h7-10H,3-6H2,1-2H3	-0.542
InChI=1S/C26H22ClF3N2O3/c1-16(2)24(32-22-12-11-18(14-21(22)27)26(28,29)30)25(33)35-23(15 h3-14,16,23-24,32H,1-2H3	-8.002
InChI=1S/C14H11N/c15-14-6-5-12-7-10-3-1-2-4-11(10)8-13(12)9-14/h1-9H,15H2	-5.172
InChI=1S/C10H12O2/c1-7(2)8-3-5-9(6-4-8)10(11)12/h3-7H,1-2H3,(H,11,12)	-3.036
InChI=1S/C24H31FO6/c1-20(2)30-19-10-16-15-6-5-13-9-14(27)7-8-21(13,3)23(15,25)17(28) h7-9,15-17,19,26,28H,5-6,10-12H2,1-4H3	-4.316
InChI=1S/C13H16N4O6/c18-13-16(14-7-10-1-2-12(22-10)17(19)20)9-11(23-13)8-15-3-5-21-6-4-h1-2,7,11H,3-6,8-9H2/b14-7+	-2.636
InChI=1S/C18H19F3N2S/c1-22(2)10-5-11-23-14-6-3-4-7-16(14)24-17-9-8-13(12-15(17)23)18(1 h3-4,6-9,12H,5,10-11H2,1-2H3	-5.3
InChI=1S/C3H4N2O2/c6-2-1-4-3(7)5-2/h1H2,(H2,4,5,6,7)	-0.402
InChI=1S/C9H11Cl2N3O4S2/c1-14-9(4-10)13-6-2-5(11)7(19(12,15)16)3-8(6)20(14,17)18/h2-3,9,13H,4H2,1H3,(H2,12,15,16)	-3.78

"InChi"	"logS(M)"
InChI=1S/C3H7N3O2/c1-2-6(5-8)3(4)7/h2H2,1H3,(H2,4,7)	-0.955
InChI=1S/C15H20N2O4S/c1-11(18)12-7-9-14(10-8-12)22(20,21)17-15(19)16-13-5-3-2-4-6-13/h7-10,13H,2-6H2,1H3,(H2,16,17,19)	-2.06
InChI=1S/C15H12O6/c16-8-4-11(19)15-12(20)6-13(21-14(15)5-8)7-1-2-9(17)10(18)3-7/h1-5,13,16-19H,6H2	-3.615
InChI=1S/C7H4Cl2O2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H,10,11)	-1.131
InChI=1S/C8H16O2/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)	-1.858
InChI=1S/C8H14N4OS/c1-8(2,3)5-6(13)12(9)7(14-4)11-10-5/h9H2,1-4H3	-2.245
InChI=1S/C10H14N2O3/c13-7-10(5-3-1-2-4-6-10)8(14)12-9(15)11-7/h1-6H2,(H2,11,12,13,14,15)	-2.98
InChI=1S/C8H10N2O3/c11-5-8(3-1-2-4-8)6(12)10-7(13)9-5/h1-4H2,(H2,9,10,11,12,13)	-2.349
InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2	0.569
InChI=1S/C7H12O2/c8-7(9)6-4-2-1-3-5-6/h6H,1-5H2,(H,8,9)	-1.445
InChI=1S/C7H14O/c1-3-4-5-6-7(2)8/h3-6H2,1-2H3	-1.433
InChI=1S/C9H9N3O3/c1-6(9(14)15)11-12-8(13)7-2-4-10-5-3-7/h2-5H,1H3,(H,12,13)(H,14,15)/b11-6-	-3.31
InChI=1S/C18H15OP/c19-20(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H	-2.877
InChI=1S/C4H10O/c1-3-4-5-2/h3-4H2,1-2H3	-0.386
InChI=1S/C9H18O3/c1-7(2)4-9(3)11-6-8(5-10)12-9/h7-8,10H,4-6H2,1-3H3	-0.706
InChI=1S/C15H16O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h3-10,16-17H,1-2H3	-2.88
InChI=1S/C15H10O7/c16-6-1-2-8(9(18)3-6)15-14(21)13(20)12-10(19)4-7(17)5-11(12)22-15h1-5,16-19,21H	-3.082
InChI=1S/C6H5Br/c7-6-4-2-1-3-5-6/h1-5H	-2.569
InChI=1S/C18H18ClN3O/c1-21-8-10-22(11-9-21)18-14-12-13(19)6-7-16(14)23-17-5-3-2-4-15(18h2-7,12H,8-11H2,1H3	-4.42
InChI=1S/C3H4ClN/c4-2-1-3-5/h1-2H2	-0.29
InChI=1S/C23H22O6/c1-11(2)16-8-14-15(28-16)6-5-12-22(24)21-13-7-18(25-3)19(26-4)9-18h5-7,9,16,20-21H,1,8,10H2,2-4H3	-6.295
InChI=1S/C7H16O/c1-7(2,3)5-4-6-8/h8H,4-6H2,1-3H3	-1.54
InChI=1S/C10H14/c1-10(2,3)9-7-5-4-6-8-9/h4-8H,1-3H3	-3.658
InChI=1S/C9H6O2/c10-9-6-5-7-3-1-2-4-8(7)11-9/h1-6H	-1.886
InChI=1S/C12H12/c1-9-7-8-10(2)12-6-4-3-5-11(9)12/h3-8H,1-2H3	-4.137
InChI=1S/C11H10/c1-9-5-4-7-10-6-2-3-8-11(9)10/h2-8H,1H3	-3.741
InChI=1S/C17H14ClF7O2/c1-6-11(19)13(21)7(14(22)12(6)20)5-27-15(26)10-8(16(10,2)3)4-9(18h4,8,10H,5H2,1-3H3/b9-4-	-7.321
InChI=1S/C5H11NO2/c1-2-3-4-8-5(6)7/h2-4H2,1H3,(H2,6,7)	-0.657

"InChi"	"logS(M)"
InChI=1S/C6H10O/c7-6-4-2-1-3-5-6/h1-5H2	-0.057
InChI=1S/C15H17Cl2N3O2/c1-2-3-12-7-21-15(22-12,8-20-10-18-9-19-20)13-5-4-11(16)6-14(13)1h4-6,9-10,12H,2-3,7-8H2,1H3	-3.493
InChI=1S/C9H11ClO3/c10-7-1-3-9(4-2-7)13-6-8(12)5-11/h1-4,8,11-12H,5-6H2	-1.307
InChI=1S/C12H2Cl8/c13-3-1-4(14)10(18)7(9(3)17)8-11(19)5(15)2-6(16)12(8)20/h1-2H	-9.38
InChI=1S/C22H26F3N3OS/c23-22(24,25)17-6-7-21-19(16-17)28(18-4-1-2-5-20(18)30-21)9-3-8-2h1-2,4-7,16,29H,3,8-15H2	-4.149
InChI=1S/C11H16N2O2/c1-8-7-9(15-11(14)12-2)5-6-10(8)13(3)4/h5-7H,1-4H3,(H,12,14)	-2.357
InChI=1S/C7H5NO/c1-2-4-7-6(3-1)8-5-9-7/h1-5H	-1.155
InChI=1S/C6H12/c1-4-5-6(2)3/h2,4-5H2,1,3H3	-3.033
InChI=1S/C14H12/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-12H/b12-11+	-5.79
InChI=1S/C7H6N2O/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H2,8,9,10)	-2.393
InChI=1S/C12H12/c1-9-7-10(2)12-6-4-3-5-11(12)8-9/h3-8H,1-2H3	-4.291
InChI=1S/C8H18O/c1-3-5-6-7-8(9)4-2/h8-9H,3-7H2,1-2H3	-2.017
InChI=1S/C11H15NO2/c1-8(2)9-6-4-5-7-10(9)14-11(13)12-3/h4-8H,1-3H3,(H,12,13)	-2.684
InChI=1S/C21H26O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2)1(h5,7,9,14-15,18,22,26H,3-4,6,8,10-11H2,1-2H3	-3.48
InChI=1S/C13H28/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-13H2,1-2H3	-7.594
InChI=1S/C20H14/c1-2-7-16-13(4-1)8-10-17-18-11-9-14-5-3-6-15(20(14)18)12-19(16)17h1-8,10,12H,9,11H2	-7.861
InChI=1S/C7H7Br/c1-6-2-4-7(8)5-3-6/h2-5H,1H3	-3.192
InChI=1S/C14H10O4/c15-13(16)11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(17)18/h1-8H,(H,15,16)(H,17,18)	-2.284
InChI=1S/C14H20N2O/c1-11-7-5-6-10-13(11)16-14(17)15-12-8-3-2-4-9-12/h2-4,8-9,11,13H,5-7,10H2,1H3,(H2,15,16,17)	-4.111
InChI=1S/C3H3NOS2/c5-2-1-7-3(6)4-2/h1H2,(H,4,5,6)	-1.772
InChI=1S/C6H2Cl4/c7-3-1-2-4(8)6(10)5(3)9/h1-2H	-4.562
InChI=1S/C9H6ClNO3S/c10-5-2-1-3-6-8(5)11(4-7(12)13)9(14)15-6/h1-3H,4H2,(H,12,13)	-2.609
InChI=1S/C12H2Cl8/c13-5-1-3(7(15)11(19)9(5)17)4-2-6(14)10(18)12(20)8(4)16/h1-2H	-9.16
InChI=1S/C16H12N2O3/c19-13-16(11-7-3-1-4-8-11,12-9-5-2-6-10-12)14(20)18-15(21)17-13/h1-10H,(H2,17,18,19,20,21)	-4.2
InChI=1S/CHCl3/c2-1(3)4/h1H	-1.174
InChI=1S/C4H8O2S/c5-7(6)3-1-2-4-7/h1-4H2	-0.08
InChI=1S/C8H9NO2/c1-6(10)9-7-4-2-3-5-8(7)11/h2-5,11H,1H3,(H,9,10)	-2.13
InChI=1S/C4H10O/c1-4(2)3-5/h4-5H,3H2,1-2H3	0.04

"InChi"	"logS(M)"
InChI=1S/C9H8N2OS/c12-8-6-10-9(13)11(8)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)	-3.243
InChI=1S/C5H8/c1-2-4-5-3-1/h1-2H,3-5H2	-2.105
InChI=1S/C15H12I3NO4/c16-9-6-8(1-2-13(9)20)23-14-10(17)3-7(4-11(14)18)5-12(19)15(21)22h1-4,6,12,20H,5,19H2,(H,21,22)	-5.22
InChI=1S/C2H6S2/c1-3-4-2/h1-2H3	-1.497
InChI=1S/C4H10N2/c1-2-6-4-3-5-1/h5-6H,1-4H2	1.065
InChI=1S/C7H9N/c1-6-2-4-7(8)5-3-6/h2-5H,8H2,1H3	-1.048
InChI=1S/C12H5Cl5/c13-6-1-2-7(10(16)5-6)11-8(14)3-4-9(15)12(11)17/h1-5H	-7.43
InChI=1S/C6H2Cl4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H	-5.47
InChI=1S/C6H12N2O3/c1-8(2)7-5(9)3-4-6(10)11/h3-4H2,1-2H3,(H,7,9)(H,10,11)	-0.205
InChI=1S/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H	-4.32
InChI=1S/C8H8O2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3,(H,9,10)	-2.143
InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)	-2.737
InChI=1S/C15H22ClNO2/c1-5-13-8-6-7-11(2)15(13)17(14(18)9-16)12(3)10-19-4/h6-8,12H,5,9-10H2,1-4H3	-2.729
InChI=1S/C8H18/c1-4-5-6-7-8(2)3/h8H,4-7H2,1-3H3	-5.08
InChI=1S/C6H7NO/c7-5-1-3-6(8)4-2-5/h1-4,8H,7H2	-0.8
InChI=1S/C15H12ClNO2/c1-8(15(18)19)9-2-4-11-12-7-10(16)3-5-13(12)17-14(11)6-9/h2-8,17H,1H3,(H,18,19)	-4.7
InChI=1S/C6H7NO2S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H2,7,8,9)	-1.563
InChI=1S/C7H12ClN5/c1-3-9-6-11-5(8)12-7(13-6)10-4-2/h3-4H2,1-2H3,(H2,9,10,11,12,13)	-4.55
InChI=1S/C6H4Cl2O/c7-4-2-1-3-5(9)6(4)8/h1-3,9H	-1.656
InChI=1S/C8H10O/c1-6-4-3-5-7(2)8(6)9/h3-5,9H,1-2H3	-1.292
InChI=1S/C11H17N5O3/c1-13(5-6-17)10-12-8-7(14(10)2)9(18)16(4)11(19)15(8)3/h17H,5-6H2,1-4H3	-0.649
InChI=1S/C6H4N4S/c11-6-9-3-4-5(10-6)8-2-1-7-4/h1-3H,(H,8,9,10,11)	-2.68
InChI=1S/C12H20O7/c1-4-17-9(13)7-12(16,11(15)19-6-3)8-10(14)18-5-2/h16H,4-8H2,1-3H3	-0.628
InChI=1S/C15H24NO4PS/c1-6-18-21(22,16-11(2)3)20-14-10-8-7-9-13(14)15(17)19-12(4)5/h7-12H,6H2,1-5H3,(H,16,22)	-4.194
InChI=1S/C4H7Br2Cl2O4P/c1-10-13(9,11-2)12-3(5)4(6,7)8/h3H,1-2H3	-2.28
InChI=1S/C15H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h16H,2-15H2,1H3	-6.348
InChI=1S/C8H5F3O2/c9-8(10,11)6-4-2-1-3-5(6)7(12)13/h1-4H,(H,12,13)	-1.598

"InChi"	"logS(M)"
InChI=1S/C14H18N2O3/c1-2-14(11(17)15-13(19)16-12(14)18)10-6-8-3-4-9(5-8)7-10/h6,8-9H,2-5,7H2,1H3,(H2,15,16,17,18,19)	-2.77
InChI=1S/C5H10N2O3/c6-3(5(9)10)1-2-4(7)8/h3H,1-2,6H2,(H2,7,8)(H,9,10)	-0.548
InChI=1S/C13H11NO2/c15-12-9-5-4-8-11(12)13(16)14-10-6-2-1-3-7-10/h1-9,15H,(H,14,16)	-3.588
InChI=1S/C9H18O2/c1-3-5-6-7-8-9(10)11-4-2/h3-8H2,1-2H3	-2.737
InChI=1S/C6H11NO2/c7-6(5(8)9)3-1-2-4-6/h1-4,7H2,(H,8,9)	-0.412
InChI=1S/C21H28O5/c1-20-7-6-13(24)8-12(20)2-3-14-15-4-5-16(18(26)10-22)21(15,11-23)h8,11,14-17,19,22,25H,2-7,9-10H2,1H3	-3.85
InChI=1S/C12H22O11/c13-1-3-5(15)6(16)9(19)12(22-3)23-10-4(2-14)21-11(20)8(18)7(10)17h3-20H,1-2H2	0.358
InChI=1S/C12H16Cl2N2O/c1-3-4-7-16(2)12(17)15-9-5-6-10(13)11(14)8-9/h5-6,8H,3-4,7H2,1-2H3,(H,15,17)	-4.758
InChI=1S/C6H12/c1-6-4-2-3-5-6/h6H,2-5H2,1H3	-3.302
InChI=1S/C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H	-1.21
InChI=1S/C9H10O2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,11)	-1.406
InChI=1S/C10H16N4O2S/c1-10(2,3)7-11-12-8(17-7)14-6(15)5-13(4)9(14)16/h6,15H,5H2,1-4H3	-1.877
InChI=1S/C19H26O12/c1-27-17(26)8-4-2-3-5-10(8)30-19-16(25)14(23)13(22)11(31-19)7-29-h2-5,9,11-16,18-25H,6-7H2,1H3	-0.742
InChI=1S/C10H9NO/c1-7-6-10(12)8-4-2-3-5-9(8)11-7/h2-6H,1H3,(H,11,12)	-1.202
InChI=1S/C5H8O2/c1-4(2)5(6)7-3/h1H2,2-3H3	-0.8
InChI=1S/C12H10ClNO6/c13-7-1-2-9-8(5-7)14(12(18)20-9)6-19-11(17)4-3-10(15)16/h1-2,5H,3-4,6H2,(H,15,16)	-3.41
InChI=1S/C9H12/c1-2-6-9-7-4-3-5-8-9/h3-5,7-8H,2,6H2,1H3	-3.362
InChI=1S/C8H18NO4PS2/c1-7(8(10)9-2)15-5-6-16-14(11,12-3)13-4/h7H,5-6H2,1-4H3,(H,9,10)	0.54
InChI=1S/C6H3Br3/c7-4-1-2-5(8)6(9)3-4/h1-3H	-4.808
InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4-7,11H,1-3H3	-2.08
InChI=1S/C12HCl9/c13-2-1-3(14)7(16)4(6(2)15)5-8(17)10(19)12(21)11(20)9(5)18/h1H	-10.412
InChI=1S/C7H8N2O3/c10-4-7(2-1-3-7)5(11)9-6(12)8-4/h1-3H2,(H2,8,9,10,11,12)	-1.66
InChI=1S/C14H21N3O3S/c1-12-6-8-13(9-7-12)21(19,20)16-14(18)15-17-10-4-2-3-5-11-17/h6-9H,2-5,10-11H2,1H3,(H2,15,16,18)	-3.678
InChI=1S/C14H24NO4PS3/c1-12(2)18-20(21,19-13(3)4)22-11-10-15-23(16,17)14-8-6-5-7-9-14/h5-9,12-13,15H,10-11H2,1-4H3	-4.201
InChI=1S/C4H6N4O3/c5-3(10)6-1-2(9)8-4(11)7-1/h1H,(H3,5,6,10)(H2,7,8,9,11)	-1.509

"InChi"	"logS(M)"
InChI=1S/C16H22N4O4/c1-21-4-5-24-14-12(22-2)7-10(8-13(14)23-3)6-11-9-19-16(18)20-15(1h7-9H,4-6H2,1-3H3,(H4,17,18,19,20)	-2.101
InChI=1S/C5H12/c1-3-5-4-2/h3-5H2,1-2H3	-3.007
InChI=1S/C7H8O/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H3	-0.663
InChI=1S/C7H7NO3/c1-5-2-3-6(8(10)11)7(9)4-5/h2-4,9H,1H3	-2.751
InChI=1S/C8H18/c1-3-5-7-8-6-4-2/h3-8H2,1-2H3	-5.238
InChI=1S/C7H7Cl/c1-6-4-2-3-5-7(6)8/h2-5H,1H3	-2.53
InChI=1S/C12H8N2/c1-2-4-10-9(3-1)5-6-11-12(10)14-8-7-13-11/h1-8H	-2.68
InChI=1S/C13H19ClNO3PS2/c1-10(2)15(12-7-5-11(14)6-8-12)13(16)9-21-19(20,17-3)18-4/h5-8,10H,9H2,1-4H3	-4.432
InChI=1S/C22H24N2O4/c1-2-3-6-15-19(25)28-16-24-20(26)22(23-21(24)27,17-11-7-4-8-12-17h4-5,7-14H,2-3,6,15-16H2,1H3,(H,23,27)	-5.886
InChI=1S/C18H12/c1-2-6-14-10-18-12-16-8-4-3-7-15(16)11-17(18)9-13(14)5-1/h1-12H	-8.6
InChI=1S/C4H10O2S2/c5-3(1-7)4(6)2-8/h3-8H,1-2H2	0.081
InChI=1S/C7H10N2O2S/c1-6-2-4-7(5-3-6)12(10,11)9-8/h2-5,9H,8H2,1H3	-1.48
InChI=1S/C7H6O4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,8-9H,(H,10,11)	-1.207
InChI=1S/C10H23N/c1-2-3-4-5-6-7-8-9-10-11/h2-11H2,1H3	-2.456
InChI=1S/C11H10ClNO2/c1-3-8(2)15-11(14)13-10-6-4-5-9(12)7-10/h1,4-8H,2H3,(H,13,14)	-2.617
InChI=1S/C13H22N4O3S/c1-14-13(9-17(18)19)15-6-7-21-10-12-5-4-11(20-12)8-16(2)3/h4-5,9,14-15H,6-8,10H2,1-3H3/b13-9+	-2.5
InChI=1S/C12H11NO2/c1-13-12(14)15-11-8-4-6-9-5-2-3-7-10(9)11/h2-8H,1H3,(H,13,14)	-3.224
InChI=1S/C11H13F3N2O3S/c1-6-4-7(2)10(5-9(6)15-8(3)17)16-20(18,19)11(12,13)14/h4-5,16H,1-3H3,(H,15,17)	-3.236
InChI=1S/C17H12/c1-2-6-13-11-17-15(9-12(13)5-1)10-14-7-3-4-8-16(14)17/h1-9,11H,10H2	-7.733
InChI=1S/C5H10O5/c6-2-1-10-5(9)4(8)3(2)7/h2-9H,1H2	0.578
InChI=1S/C11H12N2O2/c12-9(11(14)15)5-7-6-13-10-4-2-1-3-8(7)10/h1-4,6,9,13H,5,12H2,(H,14,15)	-1.77
InChI=1S/C11H14O3/c1-2-3-8-14-11(13)9-4-6-10(12)7-5-9/h4-7,12H,2-3,8H2,1H3	-2.972
InChI=1S/C10H5Cl7/c11-4-2-1-3-5(4)9(15)7(13)6(12)8(3,14)10(9,16)17/h1-5H	-6.317
InChI=1S/C11H22O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-10H2,1-2H3	-4.627
InChI=1S/C9H16N2O2/c1-4-5-7(6(2)3)8(12)11-9(10)13/h4,6-7H,1,5H2,2-3H3,(H3,10,11,12,13)	-2.747
InChI=1S/C17H16Cl2O3/c1-11(2)22-16(20)17(21,12-6-8-14(18)9-7-12)13-4-3-5-15(19)10-13/h3-11,21H,1-2H3	-4.53

"InChi"	"logS(M)"
InChI=1S/C9H13N/c1-8(10)7-9-5-3-2-4-6-9/h2-6,8H,7,10H2,1H3	-0.683
InChI=1S/C4H6/c1-3-4-2/h1H,4H2,2H3	-1.275
InChI=1S/C10H12N2O3S/ c1-7(2)12-10(13)8-5-3-4-6-9(8)11-16(12,14)15/h3-7,11H,1-2H3	-2.682
InChI=1S/C15H15ClN4O6S/ c1-3-26-14(22)10-6-4-5-7-11(10)27(23,24)19-20(9-21)15-17-12(16)8- h4-9,19H,3H2,1-2H3	-4.576
InChI=1S/C8H17N/c1-2-5-8-6-3-4-7-9-8/h8-9H,2-7H2,1H3	-0.849
InChI=1S/C6H14S/c1-3-5-7-6-4-2/h3-6H2,1-2H3	-2.58
InChI=1S/C10H16N5O13P3/ c11-8-5-9(13-2-12-8)15(3-14-5)10-7(17)6(16)4(26-10)1-25-30(21,22)2 h2-4,6-7,10,16-17H,1H2,(H,21,22)(H,23,24)(H2,11,12,13) (H2,18,19,20)	0.295
InChI=1S/C9H10O4/c1-13-9-4-6(8(12)5-10)2-3-7(9)11/h2-4,10-11H, 5H2,1H3	-1.78
InChI=1S/C8H15NO2/c9-5-6-1-3-7(4-2-6)8(10)11/h6-7H,1-5,9H2,(H, 10,11)	0.025
InChI=1S/C14H8Cl4/ c15-10-7-5-9(6-8-10)13(14(17)18)11-3-1-2-4-12(11)16/h1-8H	-6.356
InChI=1S/C11H18ClN3O4/ c1-8(16)19-10-5-3-2-4-9(10)13-11(17)15(14-18)7-6-12/h9-10H, 2-7H2,1H3,(H,13,17)	-3.019
InChI=1S/C12H16N2O3/ c1-12(8-6-4-3-5-7-8)9(15)13-11(17)14(2)10(12)16/h6H, 3-5,7H2,1-2H3,(H,13,15,17)	-2.91
InChI=1S/C2H2Cl2/c1-2(3)4/h1H2	-1.589
InChI=1S/C22H43N5O13/ c23-2-1-8(29)20(36)27-7-3-6(25)18(39-22-16(34)15(33)13(31)9(4-24) h6-19,21-22,28-35H,1-5,23-26H2,(H,27,36)	-0.5
InChI=1S/C12H7Cl3/c13-9-3-1-2-8(6-9)11-7-10(14)4-5-12(11)15/ h1-7H	-6.008
InChI=1S/C6H12O2/c1-3-5-6(7)8-4-2/h3-5H2,1-2H3	-1.36
InChI=1S/C16H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/ h17H,2-16H2,1H3	-6.77
InChI=1S/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H, 4-6H2,1-3H3	-2.488
InChI=1S/C7H7NO2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3	-2.324
InChI=1S/C19H21NO/ c1-20(2)13-7-11-17-16-9-4-3-8-15(16)14-21-19-12-6-5-10-18(17)19/ h3-6,8-12H,7,13-14H2,1-2H3/b17-11-	-3.947
InChI=1S/C6H4BrF/c7-5-3-1-2-4-6(5)8/h1-4H	-2.696
InChI=1S/C12H16F3N/c1-3-16-9(2)7-10-5-4-6-11(8-10)12(13,14)15/ h4-6,8-9,16H,3,7H2,1-2H3	-2.749
InChI=1S/C4H10O/c1-3-4(2)5/h4-5H,3H2,1-2H3	0.388
InChI=1S/C17H19ClN2S/ c1-19(2)10-5-11-20-14-6-3-4-7-16(14)21-17-9-8-13(18)12-15(17)20/ h3-4,6-9,12H,5,10-11H2,1-2H3	-5.07
InChI=1S/C14H14O5/ c1-18-8-5-10(16)13-12(6-8)19-11-3-2-7(15)4-9(11)14(13)17/ h2-6,9,11-13,15-16H,1H3	-2.943

"InChi"	"logS(M)"
InChI=1S/C11H16ClO2PS3/c1-3-13-15(16,14-4-2)18-9-17-11-7-5-10(12)6-8-11/h5-8H,3-4,9H2,1-2H3	-6.05
InChI=1S/C10H12ClN3O2/c1-13-10(15)16-14-9-7-3-5(8(9)11)2-6(7)4-12/h5-8H,2-3H2,1H3,(H,13,15)/b14-9-	-2.082
InChI=1S/C9H14O6/c1-6(10)13-4-9(15-8(3)12)5-14-7(2)11/h9H,4-5H2,1-3H3	-0.575
InChI=1S/C3H5Cl3/c4-1-3(6)2-5/h3H,1-2H2	-1.925
InChI=1S/C17H20FN3O3/c1-3-20-10-12(17(23)24)16(22)11-8-13(18)15(9-14(11)20)21-6-4-19(2h8-10H,3-7H2,1-2H3,(H,23,24)	-1.47
InChI=1S/C9H11NO2/c1-7-4-3-5-8(6-7)12-9(11)10-2/h3-6H,1-2H3,(H,10,11)	-1.803
InChI=1S/C5H4N2O4/c8-3-1-2(4(9)10)6-5(11)7-3/h1H,(H,9,10)(H2,6,7,8,11)	-1.93
InChI=1S/C6H5I/c7-6-4-2-1-3-5-6/h1-5H	-3.01
InChI=1S/C9H12/c1-7-4-8(2)6-9(3)5-7/h4-6H,1-3H3	-3.383
InChI=1S/C11H16N2O3/c1-4-5-11(6-7(2)3)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3H3,(H2,12,13,14,15,16)	-2.119
InChI=1S/C16H15Cl3O2/c1-20-13-7-3-11(4-8-13)15(16(17,18)19)12-5-9-14(21-2)10-6-12/h3-10,15H,1-2H3	-6.539
InChI=1S/C11H12N2O/c1-8-3-5-10(6-4-8)13-11(14)7-9(2)12-13/h3-6H,7H2,1-2H3	-2.366
InChI=1S/C22H30O5/c1-12-8-14-15-5-7-22(27,18(26)11-23)21(15,3)10-17(25)19(14)20(2)6h4,6,9,12,14-15,17,19,23,25,27H,5,7-8,10-11H2,1-3H3	-3.494
InChI=1S/C8H7NS/c10-7-9-6-8-4-2-1-3-5-8/h1-5H,6H2	-3.136
InChI=1S/C9H16O4/c10-8(11)6-4-2-1-3-5-7-9(12)13/h1-7H2,(H,10,11)(H,12,13)	-1.894
InChI=1S/C4H9NO2/c5-3-1-2-4(6)7/h1-3,5H2,(H,6,7)	1.101
InChI=1S/C16H16N4/c17-15(18)13-7-3-11(4-8-13)1-2-12-5-9-14(10-6-12)16(19)20/h1-10H,(H3,17,18)(H3,19,20)/b2-1+	-2.868
InChI=1S/C4H9Br/c1-4(2)3-5/h4H,3H2,1-2H3	-2.432
InChI=1S/C10H8BrN3O/c11-9-8(12)6-13-14(10(9)15)7-4-2-1-3-5-7/h1-6H,12H2	-3.124
InChI=1S/C6H3Cl2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H	-3.201
InChI=1S/C9H11NO2/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-5,8H,6,10H2,(H,11,12)	-1.066
InChI=1S/C6H10O3/c1-5(2)6(8)9-4-3-7/h7H,1,3-4H2,2H3	-0.114
InChI=1S/C14H20N2O3S/c1-11-7-9-13(10-8-11)20(18,19)16-14(17)15-12-5-3-2-4-6-12/h7-10,12H,2-6H2,1H3,(H2,15,16,17)	-4.207
InChI=1S/C7H5NS/c1-2-4-7-6(3-1)8-5-9-7/h1-5H	-1.654
InChI=1S/CH3NO2/c1-2(3)4/h1H3	0.234
InChI=1S/C13H17N3O/c1-10-12(14(2)3)13(17)16(15(10)4)11-8-6-5-7-9-11/h5-9H,1-4H3	-0.629

"InChi"	"logS(M)"
InChI=1S/C13H11NO3/c15-10-5-3-4-9(8-10)14-12-7-2-1-6-11(12)13(16)17/h1-8,14-15H,(H,16,17)	-3.54
InChI=1S/C8H19O3PS2/c1-4-10-12(9,11-5-2)14-8-7-13-6-3/h4-8H2,1-3H3	-2.111
InChI=1S/C5H8O/c1-4-5(2,3)6/h1,6H,2-3H3	1.075
InChI=1S/C8H5Cl3O3/c9-4-1-5(10)8(6(11)2-4)14-3-7(12)13/h1-2H,3H2,(H,12,13)	-3.23
InChI=1S/C6H8N2/c7-5-1-2-6(8)4-3-5/h1-4H,7-8H2	-0.466
InChI=1S/C11H24/c1-3-5-7-9-11-10-8-6-4-2/h3-11H2,1-2H3	-7.551
InChI=1S/C7H7Cl/c8-6-7-4-2-1-3-5-7/h1-5H,6H2	-2.382
InChI=1S/C4H10/c1-3-4-2/h3-4H2,1-2H3	-2.978
InChI=1S/C8H20O7P2/c1-5-11-16(9,12-6-2)15-17(10,13-7-3)14-8-4/h5-8H2,1-4H3	0.537
InChI=1S/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h12,14-17,21H,3-11H2,1-2H3	-4.919
InChI=1S/C9H17ClN3O3PS/c1-5-14-17(18,15-6-2)16-9-11-8(10)13(12-9)7(3)4/h7H,5-6H2,1-4H3	-3.658
InChI=1S/C16H18N2O5S/c1-16(2)12(15(21)22)18-13(20)11(14(18)24-16)17-10(19)8-23-9-6-4-3h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)	-2.81
InChI=1S/C5H10O2/c1-3-4-5(6)7-2/h3-4H2,1-2H3	-0.833
InChI=1S/C21H29FO5/c1-18-7-5-13(24)9-12(18)3-4-15-14-6-8-20(27,17(26)11-23)19(14,2)1h9,14-16,23,25,27H,3-8,10-11H2,1-2H3	-3.434
InChI=1S/C8H10N2O/c9-8(11)10-6-7-4-2-1-3-5-7/h1-5H,6H2,(H3,9,10,11)	-0.946
InChI=1S/C15H21NO2/c1-11-9-13(10-15(2,3)16-11)18-14(17)12-7-5-4-6-8-12/h4-8,11,13,16H,9-10H2,1-3H3	-1.922
InChI=1S/C10H8O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7,11H	-2.062
InChI=1S/C6H12O3/c1-4-7-5(2)9-6(3)8-4/h4-6H,1-3H3	-0.072
InChI=1S/C4H7Cl2O4P/c1-8-11(7,9-2)10-3-4(5)6/h3H,1-2H3	-1.344
InChI=1S/C15H10O2/c16-15(17)14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H,(H,16,17)	-3.417
InChI=1S/C6H10O2/c1-4-8-6(7)5(2)3/h2,4H2,1,3H3	-1.325
InChI=1S/C12H24O2/c1-3-5-6-7-8-9-10-11-12(13)14-4-2/h3-11H2,1-2H3	-4.101
InChI=1S/C6H12N3PS/c11-10(7-1-2-7,8-3-4-8)9-5-6-9/h1-6H2	0.002
InChI=1S/C21H34O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-21(h14-19,23H,4-12H2,1-3H3	-5.258
InChI=1S/C17H20N2O5S/c1-2-3-9-19-14-10-12(17(20)21)11-15(25(18,22)23)16(14)24-13-7-5-4h4-8,10-11,19H,2-3,9H2,1H3,(H,20,21)(H2,18,22,23)	-3.56
InChI=1S/C17H21NO3/c1-3-11-6-5-7-12-13-8-9-21-17(4-2,10-14(19)20)16(13)18-15(11)12/h5-7,18H,3-4,8-10H2,1-2H3,(H,19,20)	-3.31

"InChi"	"logS(M)"
InChI=1S/C10H10O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-8H,1H3/b8-7+	-2.051
InChI=1S/C12H4Cl6/c13-7-2-1-5(11(17)12(7)18)6-3-9(15)10(16)4-8(6)14/h1-4H	-8.381
InChI=1S/C10H18N2O4/c1-3-15-9(13)11-5-7-12(8-6-11)10(14)16-4-2/h3-8H2,1-2H3	-0.729
InChI=1S/C21H28O5/c1-20-7-6-12(23)8-11(20)2-3-13-14-4-5-15(16(24)10-22)21(14)9-17(1h8,13-15,17-19,22,25H,2-7,9-10H2,1H3	-3.85
InChI=1S/C11H16/c1-11(2,3)9-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3	-4.15
InChI=1S/C17H16Cl2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6-13/h3-11,21H,1-2H3	-5.354
InChI=1S/C6H5Cl/c7-6-4-2-1-3-5-6/h1-5H	-2.449
InChI=1S/C2H3ClO2/c3-1-2(4)5/h1H2,(H,4,5)	0.928
InChI=1S/C4H6N2O2/c7-3-1-5-4(8)2-6-3/h1-2H2,(H,5,8)(H,6,7)	-0.831
InChI=1S/C8H9NO2/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3,(H2,9,10)	-1.72
InChI=1S/C8H16O2/c1-3-5-6-7-10-8(9)4-2/h3-7H2,1-2H3	-2.251
InChI=1S/C8H10O/c1-7-2-4-8(6-9)5-3-7/h2-5,9H,6H2,1H3	-1.2
InChI=1S/C10H9NO2/c12-10(13)5-7-6-11-9-4-2-1-3-8(7)9/h1-4,6,11H,5H2,(H,12,13)	-2.067
InChI=1S/C6H4ClI/c7-5-1-3-6(8)4-2-5/h1-4H	-4.03
InChI=1S/C7H12/c1-2-4-6-7-5-3-1/h1-2H,3-7H2	-3.18
InChI=1S/C14H9Cl5/c15-10-7-5-9(6-8-10)13(14(17,18)19)11-3-1-2-4-12(11)16/h1-8,13H	-7.13
InChI=1S/C6H14O/c1-6(2,3)4-5-7/h7H,4-5H2,1-3H3	-1.131
InChI=1S/C8H10O/c1-2-9-8-6-4-3-5-7-8/h3-7H,2H2,1H3	-2.332
InChI=1S/C15H19NO2/c1-16-12-7-8-13(16)10-14(9-12)18-15(17)11-5-3-2-4-6-11/h2-6,12-14H,7-10H2,1H3	-2.369
InChI=1S/C20H25NO4/c1-11(22)24-16-7-5-13-14-10-12-4-6-15(23-3)18-17(12)20(13,19(16)2h4,6,13-14,16,19H,5,7-10H2,1-3H3	-1.75
InChI=1S/C9H14O6/c1-8(2,6(12)13)9(3,7(14)15)4-5(10)11/h4H2,1-3H3,(H,10,11)(H,12,13)(H,14,15)	-0.29
InChI=1S/C13H11N3O4S2/c1-16-10(13(18)15-9-4-2-3-6-14-9)11(17)12-8(5-7-21-12)22(16,19)20h2-7,17H,1H3,(H,14,15,18)	-3.88
InChI=1S/C12H7Cl3/c13-9-3-1-8(2-4-9)11-7-10(14)5-6-12(11)15/h1-7H	-6.27
InChI=1S/C8H8O2/c1-10-8-4-2-7(6-9)3-5-8/h2-6H,1H3	-1.502
InChI=1S/C11H16N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h6H,4-5H2,1-3H3,(H2,12,13,14,15,16)/b7-6+	-2.31
InChI=1S/C6H3Cl3O/c7-3-1-5(9)6(10)2-4(3)8/h1-2,10H	-2.216
InChI=1S/C14H17ClNO4PS2/c1-3-19-21(22,20-4-2)23-12(9-15)16-13(17)10-7-5-6-8-11(10)14(16)1h5-8,12H,3-4,9H2,1-2H3	-5.85
InChI=1S/C12H4Cl6/c13-5-1-3-7(15)11(17)9(5)10-6(14)2-4-8(16)12(10)18/h1-4H	-7.903

"InChi"	"logS(M)"
InChI=1S/C11H7NO/c13-11-8-5-1-3-7-4-2-6-9(12-11)10(7)8/h1-6H,(H,12,13)	-3.255
InChI=1S/C23H19ClF3NO3/c1-22(2)17(12-19(24)23(25,26)27)20(22)21(29)31-18(13-28)14-7-6-16h3-12,17-18,20H,1-2H3/b19-12-	-7.954
InChI=1S/C5H11N2O2P/c1-4-9-10(8,5-6)7(2)3/h4H2,1-3H3	-0.219
InChI=1S/C6H6O2/c7-5-1-2-6(8)4-3-5/h1-4,7-8H	-0.197
InChI=1S/C12H5Cl5/c13-8-2-1-6(3-10(8)15)7-4-11(16)12(17)5-9(7)14/h1-5H	-7.387
InChI=1S/C7H7Br/c1-6-3-2-4-7(8)5-6/h2-5H,1H3	-3.523
InChI=1S/C14H16ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h4-9,13H,1-3H3	-3.614
InChI=1S/C6H12O5/c7-2-1-3(8)5(10)6(11)4(2)9/h2-11H,1H2	-0.174
InChI=1S/C9H11NO3/c10-8(9(12)13)5-6-1-3-7(11)4-2-6/h1-4,8,11H,5,10H2,(H,12,13)	-2.605
InChI=1S/C14H11NO2/c16-13(11-7-3-1-4-8-11)15-14(17)12-9-5-2-6-10-12/h1-10H,(H,15,16,17)	-2.273
InChI=1S/C6H3Cl3/c7-4-2-1-3-5(8)6(4)9/h1-3H	-4.003
InChI=1S/C6H6N4O4/c7-6(11)9-8-3-4-1-2-5(14-4)10(12)13/h1-3H,(H3,7,9,11)/b8-3+	-2.98
InChI=1S/C6H11NO/c8-7-6-4-2-1-3-5-6/h8H,1-5H2	-0.85
InChI=1S/C6H7NO/c8-7-6-4-2-1-3-5-6/h1-5,7-8H	-0.436
InChI=1S/C11H22O2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h2-10H2,1H3,(H,12,13)	-3.553
InChI=1S/C4H8Cl2/c1-2-3-4(5)6/h4H,2-3H2,1H3	-2.404
InChI=1S/C8H6O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H,(H,9,10)(H,11,12)	-4.044
InChI=1S/C8H6O5/c9-6-2-1-4(7(10)11)3-5(6)8(12)13/h1-3,9H,(H,10,11)(H,12,13)	-1.78
InChI=1S/C5H6N2/c6-5-2-1-3-7-4-5/h1-4H,6H2	1.026
InChI=1S/C6H3Cl3O/c7-3-1-2-4(8)6(10)5(3)9/h1-2,10H	-2.642
InChI=1S/C12H7Cl3/c13-9-6-4-8(5-7-9)10-2-1-3-11(14)12(10)15/h1-7H	-6.29
InChI=1S/C8H14O/c1-3-5-6-8(4-2)7-9/h6-7H,3-5H2,1-2H3/b8-6-	-2.256
InChI=1S/C4H7NO/c6-4-2-1-3-5-4/h1-3H2,(H,5,6)	1.07
InChI=1S/C10H12Cl3O2PS/c1-3-14-16(17,4-2)15-10-6-8(12)7(11)5-9(10)13/h5-6H,3-4H2,1-2H3	-5.752
InChI=1S/C9H10Cl2N2O2/c1-13(15-2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	-3.521
InChI=1S/C10H20O2/c1-3-5-6-7-8-9-10(11)12-4-2/h3-9H2,1-2H3	-3.391
InChI=1S/C3H8O3/c4-1-3(6)2-5/h3-6H,1-2H2	1.036
InChI=1S/C9H9ClO3/c1-6-4-7(10)2-3-8(6)13-5-9(11)12/h2-4H,5H2,1H3,(H,11,12)	-2.503
InChI=1S/C17H12Cl2N4/c1-10-21-22-16-9-20-17(12-4-2-3-5-14(12)19)13-8-11(18)6-7-15(13)22h2-8H,9H2,1H3	-4.08
InChI=1S/C9H10O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3	-2.049

"InChi"	"logS(M)"
InChI=1S/C14H8O2/c15-13-9-5-1-2-6-10(9)14(16)12-8-4-3-7-11(12)13/h1-8H	-6.04
InChI=1S/C16H14ClN3O/c1-18-15-10-20(21)16(11-5-3-2-4-6-11)13-9-12(17)7-8-14(13)19-15/h2-9,21H,10H2,1H3/b18-15-	-2.176
InChI=1S/C8H16/c1-7-3-5-8(2)6-4-7/h7-8H,3-6H2,1-2H3	-4.466
InChI=1S/C7H8O/c8-6-7-4-2-1-3-5-7/h1-5,8H,6H2	-0.432
InChI=1S/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H	-2.12
InChI=1S/C6H4N4O/c11-6-9-3-4-5(10-6)8-2-1-7-4/h1-3H,(H,8,9,10,11)	-2
InChI=1S/C9H7NO/c11-8-3-4-9-7(6-8)2-1-5-10-9/h1-6,11H	-2.162
InChI=1S/C11H20O2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h2H,1,3-10H2,(H,12,13)	-3.553
InChI=1S/C9H12N2O/c1-7-5-3-4-6-8(7)11(2)9(10)12/h3-6H,1-2H3,(H2,10,12)	-0.403
InChI=1S/C11H17NO3/c1-11(2)6-8(13)5-9(7-11)15-10(14)12(3)4/h5H,6-7H2,1-4H3	-0.848
InChI=1S/C5H6N2OS/c1-3-2-6-5(9)7-4(3)8/h2H,1H3,(H2,6,7,8,9)	-2.446
InChI=1S/C7H9N/c1-2-7-5-3-4-6-8-7/h3-6H,2H2,1H3	0.501
InChI=1S/C17H22I3N3O8/c1-6(28)15(29)23-14-12(19)9(16(30)21-7(2-24)3-25)11(18)10(13(14)2h6-8,24-28H,2-5H2,1H3,(H,21,30)(H,22,31)(H,23,29)	-0.744
InChI=1S/C3H7Br/c1-3(2)4/h3H,1-2H3	-1.599
InChI=1S/C6HCl5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H	-4.279
InChI=1S/C14H14NO4PS/c1-2-18-20(21,14-6-4-3-5-7-14)19-13-10-8-12(9-11-13)15(16)17/h3-11H,2H2,1H3	-5.017
InChI=1S/C20H22N8O5/c1-28(9-11-8-23-17-15(24-11)16(21)26-20(22)27-17)12-4-2-10(3-5-12h2-5,8,13H,6-7,9H2,1H3,(H,25,31)(H,29,30)(H,32,33)(H4,21,22,23,26,27)	-4
InChI=1S/C22H19Cl2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-1h3-12,17-18,20H,1-2H3	-7.619
InChI=1S/C7H8O/c1-6-2-4-7(8)5-3-6/h2-5,8H,1H3	-0.702
InChI=1S/C23H29N3O2S2/c1-24(2)30(27,28)18-10-11-23-21(17-18)19(20-7-4-5-9-22(20)29-23)8h4-5,7-11,17H,6,12-16H2,1-3H3/b19-8-	-5.766
InChI=1S/C7H7Cl3NO3PS/c1-12-15(16,13-2)14-7-5(9)3-4(8)6(10)11-7/h3H,1-2H3	-4.831
InChI=1S/C8H16O/c1-3-4-5-6-7-8(2)9/h3-7H2,1-2H3	-2.154
InChI=1S/C20H26N2O2/c1-3-10-11-8-14-17-20(12-6-4-5-7-13(12)21(17)2)9-15(16(11)18(20)2h4-7,10-11,14-19,23-24H,3,8-9H2,1-2H3	-2.827
InChI=1S/C6H3Br3/c7-4-2-1-3-5(8)6(4)9/h1-3H	-5.04
InChI=1S/C15H32/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h3-15H2,1-2H3	-9.446
InChI=1S/C7H3I2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H	-3.61
InChI=1S/C10H13NO2/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h3-6H,2,7,11H2,1H3	-2.452

"InChi"	"logS(M)"
InChI=1S/C4H9NO3/c1-2(6)3(5)4(7)8/h2-3,6H,5H2,1H3,(H,7,8)	0.067
InChI=1S/C8H8ClNO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)	-2.84
InChI=1S/C11H8ClFN2O2/c12-8-3-1-7(2-4-8)5-15-6-9(13)10(16)14-11(15)17/h1-4,6H,5H2,(H,14,16,17)	-3.49
InChI=1S/C15H12/c1-11-6-9-15-13(10-11)8-7-12-4-2-3-5-14(12)15/h2-10H,1H3	-5.837
InChI=1S/C24H38O4/c1-19(2)13-7-5-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-18-12-h9-10,15-16,19-20H,5-8,11-14,17-18H2,1-4H3	-6.638
InChI=1S/C20H12/c1-2-8-15-13(5-1)11-12-17-16-9-3-6-14-7-4-10-18(19(14)16)20(15)17h1-12H	-8.004
InChI=1S/C8H10N4O5/c9-8(14)11(3-4-13)10-5-6-1-2-7(17-6)12(15)16/h1-2,5,13H,3-4H2,(H2,9,14)/b10-5+	-2.685
InChI=1S/C14H12O5/c1-7-6-9(15)10-11(16-2)8-4-5-18-12(8)14(17-3)13(10)19-7/h4-6H,1-3H3	-3.021
InChI=1S/C10H10Cl2O3/c11-7-3-4-9(8(12)6-7)15-5-1-2-10(13)14/h3-4,6H,1-2,5H2,(H,13,14)	-3.57
InChI=1S/C3H6O2/c1-2-5-3-4/h3H,2H2,1H3	0.151
InChI=1S/C6H14/c1-4-6(3)5-2/h6H,4-5H2,1-3H3	-3.683
InChI=1S/C7H15Br/c1-2-3-4-5-6-7-8/h2-7H2,1H3	-4.431
InChI=1S/C5H10/c1-4-5(2)3/h4H,1-3H3	-2.233
InChI=1S/C15H13NO3/c17-14(10-4-2-1-3-5-10)13-7-6-12-11(15(18)19)8-9-16(12)13/h1-7,11H,8-9H2,(H,18,19)	-3.26
InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)6-10(9)11/h4-7,11H,1-3H3	-2.19
InChI=1S/C4H4N2O/c7-4-1-2-5-3-6-4/h2-3H,1H2	0.586
InChI=1S/C12H27N/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-13H2,1H3	-3.376
InChI=1S/C8H18O/c1-4-5-6-7-8(2,3)9/h9H,4-7H2,1-3H3	-1.717
InChI=1S/C15H13NO2/c1-2-16-12-8-4-6-10-14(12)18-13-9-5-3-7-11(13)15(16)17/h3-10H,2H2,1H3	-3.68
InChI=1S/CH4N2O/c2-1(3)4/h(H4,2,3,4)	0.958
InChI=1S/C8H10O4/c1-5(2)8(11)6(12-3)4-7(9)10/h4H,1H2,2-3H3,(H,9,10)/b6-4-	-0.93
InChI=1S/C5H11NO3/c1-4(8)5(9)6-2-3-7/h4,7-8H,2-3H2,1H3,(H,6,9)	1.307
InChI=1S/C8H6N4O8/c13-1-7(19,2(14)10-5(17)9-1)8(20)3(15)11-6(18)12-4(8)16/h19-20H,(H2,9,10,13,14,17)(H2,11,12,15,16,18)	-1.994
InChI=1S/C12H9Cl2NO3/c1-3-12(2)10(16)15(11(17)18-12)9-5-7(13)4-8(14)6-9/h3-6H,1H2,2H3	-4.925
InChI=1S/C7H7NO/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H2,8,9)	-0.953
InChI=1S/CHI3/c2-1(3)4/h1H	-3.595
InChI=1S/C10H16O/c1-9(2)7-4-5-10(3,6-7)8(9)11/h7H,4-6H2,1-3H3	-1.851

"InChi"	"logS(M)"
InChI=1S/C13H8Cl2N2O4/c14-7-1-4-12(18)9(5-7)13(19)16-11-3-2-8(17(20)21)6-10(11)15/h1-6,18H,(H,16,19)	-5.311
InChI=1S/C7H10N4O2S/c8-5-1-3-6(4-2-5)14(12,13)11-7(9)10/h1-4H,8H2,(H4,9,10,11)	-1.988
InChI=1S/C6H6N4O/c1-4-2-5(11)10-6(9-4)7-3-8-10/h2-3H,1H3,(H,7,8,9)	-1.347
InChI=1S/C11H11N/c1-8-7-9(2)12-11-6-4-3-5-10(8)11/h3-7H,1-2H3	-1.942
InChI=1S/C7H16/c1-5-6-7(2,3)4/h5-6H2,1-4H3	-4.357
InChI=1S/C8H17NO2/c1-2-3-4-5-6-7-11-8(9)10/h2-7H2,1H3,(H2,9,10)	-2.62
InChI=1S/C8H6F3N3O4S2/c9-8(10,11)4-1-5-7(2-6(4)19(12,15)16)20(17,18)14-3-13-5/h1-3H,(H,13,14)(H2,12,15,16)	-0.819
InChI=1S/C8H2Cl4N2/c9-3-4(10)6(12)8-7(5(3)11)13-1-2-14-8/h1-2H	-5.428
InChI=1S/C9H9ClO3/c1-6(9(11)12)13-8-5-3-2-4-7(8)10/h2-6H,1H3,(H,11,12)	-2.223
InChI=1S/C11H12O2/c1-2-13-11(12)9-8-10-6-4-3-5-7-10/h3-9H,2H2,1H3/b9-8+	-3.013
InChI=1S/C9H12N2O3/c12-6-9(4-2-1-3-5-9)7(13)11-8(14)10-6/h1-5H2,(H2,10,11,12,13,14)	-3.06
InChI=1S/C6H5BrO/c7-5-1-3-6(8)4-2-5/h1-4,8H	-1.092
InChI=1S/C5H12O/c1-5(2)3-4-6/h5-6H,3-4H2,1-2H3	-0.468
InChI=1S/C7H5IO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)	-3.271
InChI=1S/C7H15N/c1-2-7-5-3-4-6-8-7/h7-8H,2-6H2,1H3	-0.346
InChI=1S/C21H26O2/c1-4-21(22)12-10-19-18-7-5-14-13-15(23-3)6-8-16(14)17(18)9-11-20(1,6,8,13,17-19,22H,5,7,9-12H2,2-3H3	-5.49
InChI=1S/C8H10O2/c9-6-7-10-8-4-2-1-3-5-8/h1-5,9H,6-7H2	-0.742
InChI=1S/C5H8/c1-3-5-4-2/h1H,4-5H2,2H3	-1.637
InChI=1S/C24H40O4/c1-14(4-7-21(27)28)17-5-6-18-22-19(9-11-24(17,18)3)23(2)10-8-16(2h14-20,22,25-26H,4-13H2,1-3H3,(H,27,28)	-4.293
InChI=1S/C10H12ClNO/c11-7-6-10(13)12-8-9-4-2-1-3-5-9/h1-5H,6-8H2,(H,12,13)	-3.296
InChI=1S/C7H7NO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,8H2,(H,9,10)	-1.351
InChI=1S/C14H12ClNO2/c1-9-11(15)6-4-8-12(9)16-13-7-3-2-5-10(13)14(17)18/h2-8,16H,1H3,(H,17,18)	-5.06
InChI=1S/C6H5NO2/c8-6-3-1-5(7-9)2-4-6/h1-4,8H	-1.546
InChI=1S/C8H8O3/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5,9H,1H3	-1.827
InChI=1S/C8H8Cl3O3PS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3	-5.507
InChI=1S/C6H13Br/c1-2-3-4-5-6-7/h2-6H2,1H3	-3.808
InChI=1S/C17H19NO4/c1-2-20-17(19)18-12-13-21-14-8-10-16(11-9-14)22-15-6-4-3-5-7-15/h3-11H,2,12-13H2,1H3,(H,18,19)	-4.701
InChI=1S/C6H13NO2/c1-6(2,3)4-9-5(7)8/h4H2,1-3H3,(H2,7,8)	-0.8
InChI=1S/C6H5ClO/c7-5-3-1-2-4-6(5)8/h1-4,8H	-0.754

"InChi"	"logS(M)"
InChI=1S/C9H9NO2/c1-7(12)10-9-4-2-8(6-11)3-5-9/h2-6H,1H3,(H,10,12)	-1.63
InChI=1S/C9H5N5O2/c10-5-7(6-11)12-13-8-3-1-2-4-9(8)14(15)16/h1-4,13H	-3.93
InChI=1S/C19H22N2S/c1-20-12-6-7-15(13-20)14-21-16-8-2-4-10-18(16)22-19-11-5-3-9-17(1h2-5,8-11,15H,6-7,12-14H2,1H3	-4.74
InChI=1S/C6H5ClO/c7-5-1-3-6(8)4-2-5/h1-4,8H	-0.688
InChI=1S/C6H4Cl2O/c7-4-1-2-6(9)5(8)3-4/h1-3,9H	-1.559
InChI=1S/C10H10Cl6N4O2/c11-9(12,13)7(17-5-21)19-1-2-20(4-3-19)8(18-6-22)10(14,15)16/h1-8H,(H,17,21)(H,18,22)	-4.19
InChI=1S/C10H12N2O/c11-4-3-7-6-12-10-2-1-8(13)5-9(7)10/h1-2,5-6,12-13H,3-4,11H2	-0.945
InChI=1S/C4H11NO3/c5-4(1-6,2-7)3-8/h6-8H,1-3,5H2	0.791
InChI=1S/C4H10O4/c5-1-3(7)4(8)2-6/h3-8H,1-2H2	0.699
InChI=1S/C4H10O2S/c1-3-7(5,6)4-2/h3-4H2,1-2H3	0.043
InChI=1S/C9H13NO2/c1-2-9(12-8(10)11)6-4-3-5-7-9/h1H,3-7H2,(H2,10,11)	-1.825
InChI=1S/C6H9N3/c1-4-3-6(7)9-5(2)8-4/h3H,1-2H3,(H2,7,8,9)	-1.284
InChI=1S/C16H25NO2/c1-15(2,3)11-8-12(16(4,5)6)10-13(9-11)19-14(18)17-7/h8-10H,1-7H3,(H,17,18)	-4.245
InChI=1S/C6H12O/c1-3-4-5-6(2)7/h3-5H2,1-2H3	-0.8
InChI=1S/C7H9N/c1-6-3-4-7(2)8-5-6/h3-5H,1-2H3	-0.03
InChI=1S/C18H22I3N3O8/c1-5(26)22-12-9(19)8(10(20)14(11(12)21)24(3)6(2)27)17(30)23-13-16h7,13,15-16,18,25,28-29,31H,4H2,1-3H3,(H,22,26)(H,23,30)	-0.198
InChI=1S/C18H12/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1-12H	-8.057
InChI=1S/C14H16N2O2/c1-3-18-14(17)13-9-15-10-16(13)11(2)12-7-5-4-6-8-12/h4-11H,3H2,1-2H3	-4.73
InChI=1S/C6H12O6/c7-2-6(11)5(10)4(9)3(8)1-12-6/h3-5,7-11H,1-2H2	0.64
InChI=1S/C5H12O/c1-3-4-5(2)6/h5-6H,3-4H2,1-2H3	-0.254
InChI=1S/C7H14/c1-3-5-7-6-4-2/h3,5H,4,6-7H2,1-2H3/b5-3+	-3.816
InChI=1S/C13H6Cl6O2/c14-6-2-8(16)12(20)4(10(6)18)1-5-11(19)7(15)3-9(17)13(5)21/h2-3,20-21H,1H2	-3.463
InChI=1S/C10H12O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h5-7,11H,1-4H2	-1.995
InChI=1S/C23H34O4/c1-21-8-5-16(24)12-15(21)3-4-19-18(21)6-9-22(2)17(7-10-23(19,22)2h11,15-19,24,26H,3-10,12-13H2,1-2H3	-4.57
InChI=1S/C10H13NO4/c1-15-10(14)7(11)4-6-2-3-8(12)9(13)5-6/h2-3,5,7,12-13H,4,11H2,1H3	0.48
InChI=1S/C3H6Cl2O/c4-1-3(6)2-5/h3,6H,1-2H2	-0.115
InChI=1S/C5H12/c1-4-5(2)3/h5H,4H2,1-3H3	-3.163
InChI=1S/C6H12O2/c1-3-4-5-8-6(2)7/h3-5H2,1-2H3	-1.22

"InChi"	"logS(M)"
InChI=1S/C9H19NO4/c1-9(2,6-12)7(13)8(14)10-4-3-5-11/h7,11-13H,3-6H2,1-2H3,(H,10,14)	0.438
InChI=1S/C4H4N2OS/c7-3-1-2-5-4(8)6-3/h1-2H,(H2,5,6,7,8)	-2.257
InChI=1S/C4H5N/c1-2-4-5-3-1/h1-5H	-0.173
InChI=1S/C9H7NO/c11-9-5-1-4-8-7(9)3-2-6-10-8/h1-6,11H	-2.542
InChI=1S/C21H32O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-21(h4,15-19,23H,5-12H2,1-3H3	-4.652
InChI=1S/C13H15NO2/c1-2-13(10-6-4-3-5-7-10)9-8-11(15)14-12(13)16/h3-7H,2,8-9H2,1H3,(H,14,15,16)	-2.337
InChI=1S/C6H10N2O2/c1-3-5(9)8-4(2)6(10)7-3/h3-4H,1-2H3,(H,7,10)(H,8,9)	-0.153
InChI=1S/C17H19N3/c1-3-7-15(8-4-1)13-20(14-17-18-11-12-19-17)16-9-5-2-6-10-16/h1-10H,11-14H2,(H,18,19)	-2.6
InChI=1S/C2H5N3O2/c1-5(4-7)2(3)6/h1H3,(H2,3,6)	-0.855
InChI=1S/C4H10O/c1-2-3-4-5/h5H,2-4H2,1H3	-0.05
InChI=1S/C7H5NOS/c9-7-5-3-1-2-4-6(5)10-8-7/h1-4H,(H,8,9)	-1.947
InChI=1S/C14H28NO3PS2/c1-4-10-17-19(20,18-11-5-2)21-12-14(16)15-9-7-6-8-13(15)3/h13H,4-12H2,1-3H3	-4.15
InChI=1S/C8H6O3/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-4H,5H2	-1.632
InChI=1S/C11H12N2O3/c12-9(11(15)16)3-6-5-13-10-2-1-7(14)4-8(6)10/h1-2,4-5,9,13-14H,3,12H2,(H,15,16)	-1.343
InChI=1S/C16H14N2O2S/c1-18(12-7-3-2-4-8-12)15(19)11-20-16-17-13-9-5-6-10-14(13)21-16/h2-10H,11H2,1H3	-4.873
InChI=1S/C19H30O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17(1h11-15,17,20-21H,3-10H2,1-2H3	-3.593
InChI=1S/C12H26O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3	-4.985
InChI=1S/C7H16/c1-6(2)5-7(3)4/h6-7H,5H2,1-4H3	-4.261
InChI=1S/C8H8O2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3,(H,9,10)	-2.53
InChI=1S/C14H18N4O3/c1-3-4-9-15-13(19)18-11-8-6-5-7-10(11)16-12(18)17-14(20)21-2/h5-8H,3-4,9H2,1-2H3,(H,15,19)(H,16,17,20)	-4.86
InChI=1S/C14H12O2/c15-14(13-9-5-2-6-10-13)16-11-12-7-3-1-4-8-12/h1-10H,11H2	-4.178
InChI=1S/C13H14F3N3O4/c1-4-17(7-8(2)3)12-10(18(20)21)5-9(13(14,15)16)6-11(12)19(22)23/h5-6H,2,4,7H2,1,3H3	-6.124
InChI=1S/C6H9N3O2/c7-5(6(10)11)1-4-2-8-3-9-4/h2-3,5H,1,7H2,(H,8,9)(H,10,11)	-0.531
InChI=1S/C16H34/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-16H2,1-2H3	-8.401
InChI=1S/C19H30OS/c1-18-8-7-14-12(13(18)5-6-17(18)20)4-3-11-9-15-16(21-15)10-19(11,h11-17,20H,3-10H2,1-2H3	-5.407

"InChi"	"logS(M)"
InChI=1S/C13H10O2/c14-13(11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10H	-2.85
InChI=1S/C13H18Cl2N2O2/c14-5-7-17(8-6-15)11-3-1-10(2-4-11)9-12(16)13(18)19/h1-4,12H,5-9,16H2,(H,18,19)	-3.49
InChI=1S/C8H8Cl2IO3PS/c1-12-15(16,13-2)14-8-4-5(9)7(11)3-6(8)10/h3-4H,1-2H3	-6.616
InChI=1S/C8H10N2O/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,9H2,1H3,(H,10,11)	-0.98
InChI=1S/C5H11NO2S/c1-9-3-2-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)	-0.659
InChI=1S/C13H11NO5/c1-2-14-5-8(13(16)17)12(15)7-3-10-11(4-9(7)14)19-6-18-10/h3-5H,2,6H2,1H3,(H,16,17)	-4.38
InChI=1S/C6H6O2/c7-5-2-1-3-6(8)4-5/h1-4,7-8H	1.003
InChI=1S/C13H12O/c14-13-8-6-12(7-9-13)10-11-4-2-1-3-5-11/h1-9,14H,10H2	-3.401
InChI=1S/C12H6Cl4O2S/c13-5-1-7(15)11(17)9(3-5)19-10-4-6(14)2-8(16)12(10)18/h1-4,17-18H	-4.949
InChI=1S/C6H9N3O2/c1-8-4(7)3-5(10)9(2)6(8)11/h3H,7H2,1-2H3	-1.454
InChI=1S/C9H17N5O/c1-5-10-7-12-8(11-6(2)3)14-9(13-7)15-4/h6H,5H2,1-4H3,(H2,10,11,12,13,14)	-2.07
InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2	-2.687
InChI=1S/C9H17N5S/c1-5-10-7-12-8(11-6(2)3)14-9(13-7)15-4/h6H,5H2,1-4H3,(H2,10,11,12,13,14)	-3.047
InChI=1S/C12H8Cl6/c13-8-9(14)11(16)7-5-2-1-4(3-5)6(7)10(8,15)12(11,17)18/h1-2,4-7H,3H2	-6.31
InChI=1S/C14H19N3S/c1-16(2)9-10-17(12-13-6-5-11-18-13)14-7-3-4-8-15-14/h3-8,11H,9-10,12H2,1-2H3	-2.638
InChI=1S/C27H42O3/c1-16-9-22-23(29-15-16)14-27(4)24(30-22)12-21-20-11-18-10-19(28)(h11,16-17,19-24,28H,5-10,12-15H2,1-4H3	-7.32
InChI=1S/C2H5NO2/c1-5-2(3)4/h1H3,(H2,3,4)	0.964
InChI=1S/C19H22FN3O3/c1-2-21-5-7-22(8-6-21)17-10-16-13(9-15(17)20)18(24)14(19(25)26)11 h9-12H,2-8H2,1H3,(H,25,26)	-3.18
InChI=1S/C17H17Cl2N/c1-20-17-9-7-12(13-4-2-3-5-14(13)17)11-6-8-15(18)16(19)10-11/h2-6,8,10,12,17,20H,7,9H2,1H3	-5.23
InChI=1S/C6H4N4S/c11-6-4-5(9-3-10-6)8-2-1-7-4/h1-3H,(H,8,9,10,11)	-2.647
InChI=1S/C6H14O/c1-3-5-7-6-4-2/h3-6H2,1-2H3	-1.319
InChI=1S/C6H12/c1-3-5-6-4-2/h3H,1,4-6H2,2H3	-3.226
InChI=1S/C10H12O2/c1-8-4-2-3-5-10(8)12-7-9-6-11-9/h2-5,9H,6-7H2,1H3	-2.291
InChI=1S/C3H8O2/c1-4-3-5-2/h3H2,1-2H3	0.506
InChI=1S/C10H18O/c1-8(2)10(11)6-4-9(3)5-7-10/h4,8,11H,5-7H2,1-3H3	-1.941

"InChi"	"logS(M)"
InChI=1S/C9H10O2/c1-6-3-4-8(9(10)11)5-7(6)2/h3-5H,1-2H3,(H,10,11)	-3.16
InChI=1S/C5H4N4O/c10-5-6-1-3-4(9-5)8-2-7-3/h1-2H,(H2,6,7,8,9,10)	-1.714
InChI=1S/C11H9N3O/c15-11(9-4-3-6-12-8-9)14-10-5-1-2-7-13-10/h1-8H,(H,13,14,15)	-2.977
InChI=1S/C8H12N2O2S/c1-3-8(4-2)5(11)9-7(13)10-6(8)12/h3-4H2,1-2H3,(H2,9,10,11,12,13)	-2.32
InChI=1S/C18H16N2O4/c1-13(21)24-12-20-16(22)18(19-17(20)23,14-8-4-2-5-9-14)15-10-6-3-h2-11H,12H2,1H3,(H,19,23)	-4.47
InChI=1S/C10H15N/c1-3-11(4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3	-3.028
InChI=1S/C19H28O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h3,13-16,20H,4-11H2,1-2H3	-4.122
InChI=1S/C10H20O2/c1-3-4-5-6-7-8-9-10(11)12-2/h3-9H2,1-2H3	-3.38
InChI=1S/C6H2F4/c7-3-1-4(8)6(10)5(9)2-3/h1-2H	-2.306
InChI=1S/C7H15I/c1-2-3-4-5-6-7-8/h2-7H2,1H3	-4.81
InChI=1S/C8H8O2/c1-6(9)7-2-4-8(10)5-3-7/h2-5,10H,1H3	-1.138
InChI=1S/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3,5-7,11H,1,4H2,2H3	-2.153
InChI=1S/C7H9N/c1-6-3-4-8-7(2)5-6/h3-5H,1-2H3	0.447
InChI=1S/C8H18O/c1-4-6-7-8(3,9)5-2/h9H,4-7H2,1-3H3	-1.736
InChI=1S/C6H2F4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H	-2.376
InChI=1S/C10H9Cl4NO2S/c11-9(12)10(13,14)18-15-7(16)5-3-1-2-4-6(5)8(15)17/h1-2,5-6,9H,3-4H2	-5.397
InChI=1S/C4H8O2/c1-3-4(5)6-2/h3H2,1-2H3	-0.15
InChI=1S/C6H6N4/c1-4-5-6(9-2-7-4)10-3-8-5/h2-3H,1H3,(H,7,8,9,10)	0.173
InChI=1S/C16H22N4O/c1-19(2)11-12-20(16-17-9-4-10-18-16)13-14-5-7-15(21-3)8-6-14/h4-10H,11-13H2,1-3H3	-2.99
InChI=1S/C5H4N4O2/c10-4-2-3(6-1-7-4)9-5(11)8-2/h1H,(H3,6,7,8,9,10,11)	-2.96
InChI=1S/C20H42/c1-3-5-7-9-11-13-15-17-19-20-18-16-14-12-10-8-6-4-2/h3-20H2,1-2H3	-8.172
InChI=1S/C11H20ClN5/c1-5-16(6-2)10-13-9(12)14-11(15-10)17(7-3)8-4/h5-8H2,1-4H3	-4.411
InChI=1S/C14H10/c1-2-6-12-10-14-8-4-3-7-13(14)9-11(12)5-1/h1-10H	-6.445
InChI=1S/C13H9N/c1-2-5-11-10(4-1)7-8-13-12(11)6-3-9-14-13/h1-9H	-3.357
InChI=1S/C19H22N2O/c1-2-13-12-21-10-8-14(13)11-18(21)19(22)16-7-9-20-17-6-4-3-5-15(1h2-7,9,13-14,18-19,22H,1,8,10-12H2	-3.089

"InChi"	"logS(M)"
InChI=1S/C22H32O3/c1-4-20(24)25-19-8-7-17-16-6-5-14-13-15(23)9-11-21(14,2)18(16)10-h13,16-19H,4-12H2,1-3H3	-5.367
InChI=1S/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H	-0.89
InChI=1S/C6H8N2O8/c9-7(10)15-3-1-13-6-4(16-8(11)12)2-14-5(3)6/h3-6H,1-2H2	-2.633
InChI=1S/C7H9N/c1-6-4-3-5-8-7(6)2/h3-5H,1-2H3	0.094
InChI=1S/C9H18O/c1-3-5-7-9(10)8-6-4-2/h3-8H2,1-2H3	-2.58
InChI=1S/C20H19NO3/c1-20(2)10-9-13-15(24-20)11-16(23-4)17-18(13)21(3)14-8-6-5-7-12(1h5-11H,1-4H3	-5.21
InChI=1S/C10H12ClNO2/c1-7(2)14-10(13)12-9-5-3-4-8(11)6-9/h3-7H,1-2H3,(H,12,13)	-3.38
InChI=1S/C12H5Cl5/c13-6-1-2-7(10(15)5-6)8-3-4-9(14)12(17)11(8)16/h1-5H	-7.62
InChI=1S/C10H10Cl2O2/c1-14-10(13)9(12)6-7-2-4-8(11)5-3-7/h2-5,9H,6H2,1H3	-3.765
InChI=1S/C8H7NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-6H,(H,9,10,11)	-2.932
InChI=1S/C12H5Cl5/c13-8-4-2-1-3-6(8)7-5-9(14)11(16)12(17)10(7)15/h1-5H	-7.523
InChI=1S/C8H6ClNO3/c9-5-1-2-7-6(3-5)10(4-11)8(12)13-7/h1-3,11H,4H2	-2.7
InChI=1S/C9H13BrN2O2/c1-4-5(2)12-8(13)7(10)6(3)11-9(12)14/h5H,4H2,1-3H3,(H,11,14)	-2.506
InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h1H,4-8H2,2H3	-3.662
InChI=1S/C4H10/c1-4(2)3/h4H,1-3H3	-2.978
InChI=1S/C6H14O/c1-4-5-7-6(2)3/h6H,4-5H2,1-3H3	-1.337
InChI=1S/C24H40O5/c1-13(4-7-21(28)29)16-5-6-17-22-18(12-20(27)24(16,17)3)23(2)9-8-1h13-20,22,25-27H,4-12H2,1-3H3,(H,28,29)	-3.368
InChI=1S/C5H10O2/c1-5(2)3-7-4-6/h4-5H,3H2,1-2H3	-1.001
InChI=1S/C5H11Br/c1-2-3-4-5-6/h2-5H2,1H3	-3.075
InChI=1S/C10H13N5O4/c1-5-3-15(10(18)12-9(5)17)8-2-6(13-14-11)7(4-16)19-8/h3,6-8,16H,2,4H2,1H3,(H,12,17,18)	-1.122
InChI=1S/C5H5N5O/c6-3-2-4(8-1-7-2)10-5(11)9-3/h1H,(H4,6,7,8,9,10,11)	-3.38
InChI=1S/C9H12/c1-8(2)9-6-4-3-5-7-9/h3-8H,1-2H3	-3.292
InChI=1S/C10H10O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-6H,1-2H3	-1.686
InChI=1S/C4H7NO4/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H,6,7)(H,8,9)	-1.229
InChI=1S/C14H9NO2/c16-14-11-8-4-5-9-12(11)15-13(17-14)10-6-2-1-3-7-10/h1-9H	-4.608
InChI=1S/C9H6I3NO3/c1-3(14)13-8-5(11)2-4(10)6(7(8)12)9(15)16/h2H,1H3,(H,13,14)(H,15,16)	-2.64
InChI=1S/C6H6N4O3S/c11-5-7-1-2-9(5)6-8-3-4(14-6)10(12)13/h3H,1-2H2,(H,7,11)	-3.217
InChI=1S/C10H14/c1-9(2)8-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3	-4.123

"InChi"	"logS(M)"
InChI=1S/C6H9NO3/c1-6(2)4(8)7(3)5(9)10-6/h1-3H3	-0.457
InChI=1S/C8H19N/c1-3-5-6-8(4-2)7-9/h8H,3-7,9H2,1-2H3	-1.713
InChI=1S/C13H26O2/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h3-12H2,1-2H3	-4.69
InChI=1S/C7H7NO/c9-6-8-7-4-2-1-3-5-7/h1-6H,(H,8,9)	-0.678
InChI=1S/C11H22N2O/c1-13(2)11(14)12-10-8-6-4-3-5-7-9-10/h10H,3-9H2,1-2H3,(H,12,14)	-2.26
InChI=1S/CH4N4O2/c2-1(3)4-5(6)7/h(H4,2,3,4)	-1.486
InChI=1S/C26H23F2NO4/c1-17(2)24(18-11-13-21(14-12-18)32-26(27)28)25(30)33-23(16-29)19h3-15,17,23-24,26H,1-2H3	-6.877
InChI=1S/C7H6ClF/c8-5-6-1-3-7(9)4-2-6/h1-4H,5H2	-2.544
InChI=1S/C10H12O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3	-1.716
InChI=1S/C8H10/c1-7-5-3-4-6-8(7)2/h3-6H,1-2H3	-2.819
InChI=1S/C7H7NO2/c1-10-7(9)6-3-2-4-8-5-6/h2-5H,1H3	-0.46
InChI=1S/C16H13N3O3/c1-22-16(21)19-15-17-12-8-7-11(9-13(12)18-15)14(20)10-5-3-2-4-6-1h2-9H,1H3,(H2,17,18,19,21)	-3.88
InChI=1S/C6H5NO2/c8-6(9)5-1-3-7-4-2-5/h1-4H,(H,8,9)	-1.376
InChI=1S/C12H12N2/c1-3-7-11(8-4-1)13-14-12-9-5-2-6-10-12/h1-10,13-14H	-2.921
InChI=1S/C7H14O/c1-3-5-7(8)6-4-2/h3-6H2,1-2H3	-1.48
InChI=1S/C7H6ClN3O4S2/c8-4-1-5-7(2-6(4)16(9,12)13)17(14,15)11-3-10-5/h1-3H,(H,10,11)(H2,9,12,13)	-2.92
InChI=1S/C12H8Cl2/c13-11-5-1-3-9(7-11)10-4-2-6-12(14)8-10/h1-8H	-5.798
InChI=1S/C13H14N2/c14-12-5-1-10(2-6-12)9-11-3-7-13(15)8-4-11/h1-8H,9,14-15H2	-2.293
InChI=1S/C7H5NS2/c9-7-8-5-3-1-2-4-6(5)10-7/h1-4H,(H,8,9)	-3.152
InChI=1S/C9H7N/c1-2-4-9-7-10-6-5-8(9)3-1/h1-7H	-1.456
InChI=1S/C7H12O2/c1-4-7(8)9-5-6(2)3/h4,6H,1,5H2,2-3H3	-1.807
InChI=1S/C14H17NO2/c1-4-15(5-2)11-6-7-12-10(3)8-14(16)17-13(12)9-11/h6-9H,4-5H2,1-3H3	-4
InChI=1S/C16H19N3O5S/c1-24-9-7-25-15-11(14(21)19(15)12(9)16(22)23)18-13(20)10(17)8-5-3h2-3,6,10-11,15H,4-5,7,17H2,1H3,(H,18,20)(H,22,23)	-1.89
InChI=1S/C12H10O2/c13-12(14)8-10-6-3-5-9-4-1-2-7-11(9)10/h1-7H,8H2,(H,13,14)	-2.647
InChI=1S/C12H8Cl2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H	-6.556
InChI=1S/C7H7ClO/c1-9-7-4-2-3-6(8)5-7/h2-5H,1H3	-2.783
InChI=1S/C7H14NO5P/c1-6(5-7(9)8-2)13-14(10,11-3)12-4/h5H,1-4H3,(H,8,9)/b6-5-	0.651
InChI=1S/C10H19N5S/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,12,13,14,15)	-3.864
InChI=1S/C9H6INO4S/c10-6-4-7(16(13,14)15)5-2-1-3-11-8(5)9(6)12/h1-4,12H,(H,13,14,15)	-2.2

"InChi"	"logS(M)"
InChI=1S/C5H8O2/c1-4(6)3-5(2)7/h3H2,1-2H3	0.186
InChI=1S/C5H10/c1-2-4-5-3-1/h1-5H2	-2.64
InChI=1S/C4H7Cl3O/c1-3(2,8)4(5,6)7/h8H,1-2H3	-1.346
InChI=1S/C10H12N4O2S2/c1-2-9-12-13-10(17-9)14-18(15,16)8-5-3-7(11)4-6-8/h3-6H,2,11H2,1H3,(H,13,14)	-3.12
InChI=1S/C12H5Cl5/c13-6-1-3-9(14)8(5-6)7-2-4-10(15)12(17)11(7)16/h1-5H	-7.91
InChI=1S/C2HCl5/c3-1(4)2(5,6)7/h1H	-2.625
InChI=1S/C9H12N4O2/c1-4-13-8(14)6-7(10-5-11(6)2)12(3)9(13)15/h5H,4H2,1-3H3	-0.719
InChI=1S/C10H12ClN3O3S/c1-2-9-13-7-4-6(11)8(18(12,16)17)3-5(7)10(15)14-9/h3-4,9,13H,2H2,1H3,(H,14,15)(H2,12,16,17)	-3.286
InChI=1S/C4H6O6/c5-1(3(7)8)2(6)4(9)10/h1-2,5-6H,(H,7,8)(H,9,10)	0.572
InChI=1S/C7H16O/c1-3-5-6-7(8)4-2/h7-8H,3-6H2,1-2H3	-1.463
InChI=1S/C5H5NO/c7-5-3-1-2-4-6-5/h1-4H,(H,6,7)	1.022
InChI=1S/C17H26ClNO2/c1-4-7-11-21-13-19(16(20)12-18)17-14(5-2)9-8-10-15(17)6-3/h8-10H,4-7,11-13H2,1-3H3	-4.193
InChI=1S/C17H34O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-17(18)19-16(2)3/h16H,4-15H2,1-3H3	-6.733
InChI=1S/C8H10O/c1-6-3-7(2)5-8(9)4-6/h3-5,9H,1-2H3	-1.388
InChI=1S/C19H23NO3/c1-3-22-15-7-4-11-10-13-12-5-6-14(21)18-19(12,8-9-20(13)2)16(11)1h4-7,12-14,18,21H,3,8-10H2,1-2H3	-2.079
InChI=1S/C15H15NO3/c1-10-3-5-11(6-4-10)15(19)13-8-7-12(16(13)2)9-14(17)18/h3-8H,9H2,1-2H3,(H,17,18)	-4.09
InChI=1S/C13H18N2O2/c16-12-10-7-4-8-11(10)14-13(17)15(12)9-5-2-1-3-6-9/h9H,1-8H2,(H,14,17)	-4.592
InChI=1S/C9H20/c1-3-5-7-9-8-6-4-2/h3-9H2,1-2H3	-5.766
InChI=1S/C16H10/c1-2-8-13-12(7-1)14-9-3-5-11-6-4-10-15(13)16(11)14/h1-10H	-5.93
InChI=1S/C14H8Cl4/c15-11-5-1-9(2-6-11)13(14(17)18)10-3-7-12(16)8-4-10/h1-8H	-6.9
InChI=1S/C12H11I3N2O4/c1-4(18)16-3-6-8(13)7(12(20)21)10(15)11(9(6)14)17-5(2)19/h3H2,1-2H3,(H,16,18)(H,17,19)(H,20,21)	-2.321
InChI=1S/C17H23NO/c1-18-9-8-17-7-3-2-4-14(17)16(18)10-12-5-6-13(19)11-15(12)17/h5-6,11,14,16,19H,2-4,7-10H2,1H3	-2.72
InChI=1S/C16H21N3/c1-18(2)12-13-19(16-10-6-7-11-17-16)14-15-8-4-3-5-9-15/h3-11H,12-14H2,1-2H3	-2.64
InChI=1S/C11H11N3O/c1-8-11(13-15)9(2)14(12-8)10-6-4-3-5-7-10/h3-7H,1-2H3	-3.736
InChI=1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H	-6.179

"InChi"	"logS(M)"
InChI=1S/C9H18O/c1-3-4-5-6-7-8-9(2)10/h3-8H2,1-2H3	-2.93
InChI=1S/C7H14O/c1-6-2-4-7(8)5-3-6/h6-8H,2-5H2,1H3	-0.881
InChI=1S/C17H13ClO3/c1-11(17(20)21)10-16(19)13-8-6-12(7-9-13)14-4-2-3-5-15(14)18/h2-9H,1,10H2,(H,20,21)	-3.2
InChI=1S/C13H19NO2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(15)14-16/h4-7,9-10,16H,8H2,1-3H3,(H,14,15)	-3.044
InChI=1S/C8H8O2/c1-10-8(9)7-5-3-2-4-6-7/h2-6H,1H3	-1.812
InChI=1S/C15H16O3/c1-10(2)4-7-12-13(17-3)8-5-11-6-9-14(16)18-15(11)12/h4-6,8-9H,7H2,1-3H3	-4.309
InChI=1S/C10H17Cl2NOS/c1-7(2)13(8(3)4)10(14)15-6-9(12)5-11/h5,7-8H,6H2,1-4H3/b9-5-	-4.286
InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3	-3.944
InChI=1S/C7H5N/c8-6-7-4-2-1-3-5-7/h1-5H	-1.712
InChI=1S/C13H21NO3/c1-13(2,3)14-7-12(17)9-4-5-11(16)10(6-9)8-15/h4-6,12,14-17H,7-8H2,1-3H3	-1.23
InChI=1S/C6H12N2O4S2/c7-3(5(9)10)1-13-14-2-4(8)6(11)12/h3-4H,1-2,7-8H2,(H,9,10)(H,11,12)	-3.16
InChI=1S/C19H23N3/c1-14-6-8-18(16(3)10-14)20-12-22(5)13-21-19-9-7-15(2)11-17(19)4/h6-13H,1-5H3/b20-12+,21-13+	-5.468
InChI=1S/C19H18N2O3/c1-14(22)12-13-17-18(23)20(15-8-4-2-5-9-15)21(19(17)24)16-10-6-3-h2-11,17H,12-13H2,1H3	-3.268
InChI=1S/C10H20NO4PS/c1-6-11-16(17,13-5)15-9(4)7-10(12)14-8(2)3/h7-8H,6H2,1-5H3,(H,11,17)/b9-7+	-3.408
InChI=1S/C10H13NO4/c1-10(11,9(14)15)5-6-2-3-7(12)8(13)4-6/h2-4,12-13H,5,11H2,1H3,(H,14,15)	-1.325
InChI=1S/C8H9NO2/c9-8(10)11-6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,9,10)	-0.35
InChI=1S/C15H23N3O4/c1-5-7-16(8-6-2)15-13(17(19)20)9-12(11(3)4)10-14(15)18(21)22/h9-11H,5-8H2,1-4H3	-6.449
InChI=1S/C6H4ClNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H	-2.812
InChI=1S/C6H7NO/c8-5-6-2-1-3-7-4-6/h1-4,8H,5H2	0.962
InChI=1S/C18H18O2/c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11-16(20)12-8-14/h3-12,17-20H,1-2H2	-4.95
InChI=1S/C11H18N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(H2,12,13,14,15,16)	-2.39
InChI=1S/C21H21O4P/c1-16-11-13-19(14-12-16)23-26(22,24-20-9-6-7-17(2)15-20)25-21-10-h4-15H,1-3H3	-6.01
InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H	-4.311
InChI=1S/C9H13N3O3/c10-7-3-4-12(9(14)11-7)8-2-1-6(5-13)15-8/h3-4,6,8,13H,1-2,5H2,(H2,10,11,14)	-0.442
InChI=1S/C8H8O4/c1-4(9)5-2-3-6(10)8(12)7(5)11/h2-3,10-12H,1H3	-2.022

"InChi"	"logS(M)"
InChI=1S/C7H16O/c1-4-5-6-7(2,3)8/h8H,4-6H2,1-3H3	-1.078
InChI=1S/C13H10Cl2O2/c14-10-1-3-12(16)8(6-10)5-9-7-11(15)2-4-13(9)17/h1-4,6-7,16-17H,5H2	-3.953
InChI=1S/C11H14O2/c12-11(13)9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2,(H,12,13)	-2.466
InChI=1S/C21H30O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2)10h9,14-16,18,22,24,26H,3-8,10-11H2,1-2H3	-3.112
InChI=1S/C11H19NOS/c1-2-3-4-5-6-7-9-12-11(13)8-10-14-12/h8,10H,2-7,9H2,1H3	-2.63
InChI=1S/C8H8N2O2/c9-7(11)5-3-1-2-4-6(5)8(10)12/h1-4H,(H2,9,11)(H2,10,12)	-2.437
InChI=1S/C6H6ClN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2	-1.358
InChI=1S/C14H14Cl2N2O/c1-2-7-19-14(9-18-6-5-17-10-18)12-4-3-11(15)8-13(12)16/h2-6,8,10,14H,1,7,9H2	-3.218
InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3	-0.91
InChI=1S/C5H4N4O/c10-5-3-4(7-1-6-3)8-2-9-5/h1-2H,(H2,6,7,8,9,10)	-2.289
InChI=1S/C8H11NO2/c1-10-6-3-4-8(11-2)7(9)5-6/h3-5H,9H2,1-2H3	-1.859
InChI=1S/C20H28O2/c1-15(8-6-9-16(2)14-19(21)22)11-12-18-17(3)10-7-13-20(18,4)5/h6,8-9,11-12,14H,7,10,13H2,1-5H3,(H,21,22)/b9-6+,12-11+,15-8+,16-14+	-6.377
InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-2,5-6H,3-4H2	-2.059
InChI=1S/C21H23BrFNO2/c22-18-7-5-17(6-8-18)21(26)11-14-24(15-12-21)13-1-2-20(25)16-3-9-h3-10,26H,1-2,11-15H2	-3.669
InChI=1S/C11H12NO4PS2/c1-15-17(18,16-2)19-7-12-10(13)8-5-3-4-6-9(8)11(12)14/h3-6H,7H2,1-2H3	-4.1
InChI=1S/C10H20N2O4/c1-4-7(2)10(3,5-15-8(11)13)6-16-9(12)14/h7H,4-6H2,1-3H3,(H2,11,13)(H2,12,14)	-2.366
InChI=1S/C5H9N3O4/c1-2-12-4(9)3-8(7-11)5(6)10/h2-3H2,1H3,(H2,6,10)	0.757
InChI=1S/C7H13NO3S/c1-5(9)8-6(7(10)11)3-4-12-2/h6H,3-4H2,1-2H3,(H,8,9)(H,10,11)	0.03
InChI=1S/C6H5Cl2N/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2	-2.446
InChI=1S/C14H22N2O3/c1-10(2)16-8-12(17)9-19-13-5-3-11(4-6-13)7-14(15)18/h3-6,10,12,16-17H,7-9H2,1-2H3,(H2,15,18)	-1.302
InChI=1S/C8H14O2/c1-4-5-6-10-8(9)7(2)3/h2,4-6H2,1,3H3	-2.544
InChI=1S/C10H15O3PS2/c1-8-7-9(5-6-10(8)16-4)13-14(15,11-2)12-3/h5-7H,1-4H3	-4.569
InChI=1S/C8H8Cl3N3O4S2/c9-3-1-4-6(2-5(3)19(12,15)16)20(17,18)14-8(13-4)7(10)11/h1-2,7-8,13-14H,(H2,12,15,16)	-3.18

"InChi"	"logS(M)"
InChI=1S/C33H25N3O3/c37-31-28-22-19-23(33(39,21-13-5-2-6-14-21)25-16-8-10-18-35-25)29-h1-19,22,28-30,39H,(H,36,37,38)/b27-26+	-3.931
InChI=1S/C20H24ClN3S/c1-22-11-13-23(14-12-22)9-4-10-24-17-5-2-3-6-19(17)25-20-8-7-16(2-h2-3,5-8,15H,4,9-14H2,1H3	-4.398
InChI=1S/C12H18N2O3/c1-7(2)5-6-12(8(3)4)9(15)13-11(17)14-10(12)16/h5,8H,6H2,1-4H3,(H2,13,14,15,16,17)	-2.59
InChI=1S/C13H10INO/c14-12-9-5-4-8-11(12)13(16)15-10-6-2-1-3-7-10/h1-9H,(H,15,16)	-4.208
InChI=1S/C11H18N2O3/c1-3-5-6-7-11(4-2)8(14)12-10(16)13-9(11)15/h3-7H2,1-2H3,(H2,12,13,14,15,16)	-2.51
InChI=1S/C23H27ClO4/c1-13(25)23(28-14(2)26)10-7-18-16-12-20(24)19-11-15(27)5-8-21(19,-h5,8,11-12,16-18H,6-7,9-10H2,1-4H3	-4.945
InChI=1S/CH3Br/c1-2/h1H3	-0.796
InChI=1S/C15H23NO2/c1-2-3-4-5-6-7-12-18-15(17)13-8-10-14(16)11-9-13/h8-11H,2-7,12,16H2,1H3	-5.4
InChI=1S/C7H6N2O4/c1-5-6(8(10)11)3-2-4-7(5)9(12)13/h2-4H,1H3	-3
InChI=1S/C5H10O2/c1-2-3-4-7-5-6/h5H,2-4H2,1H3	-1.131
InChI=1S/C10H10O4/c1-12-7-4-3-6-5-14-10(11)8(6)9(7)13-2/h3-4H,5H2,1-2H3	-1.89
InChI=1S/C7H5IO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)	-2.731
InChI=1S/C11H14ClNO/c1-9(2)13(11(14)8-12)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3	-2.481
InChI=1S/C10H16N2O3/c1-3-5-6-10(4-2)7(13)11-9(15)12-8(10)14/h3-6H2,1-2H3,(H2,11,12,13,14,15)	-1.67
InChI=1S/C12H23NO/c1-2-3-4-5-6-7-10-13-11-8-9-12(13)14/h2-11H2,1H3	-2.258
InChI=1S/C3H5N3O9/c7-4(8)13-1-3(15-6(11)12)2-14-5(9)10/h3H,1-2H2	-2.152
InChI=1S/C2H3FO2/c3-1-2(4)5/h1H2,(H,4,5)	1.108
InChI=1S/C6H4N2O5/c9-6-2-1-4(7(10)11)3-5(6)8(12)13/h1-3,9H	-2.598
InChI=1S/C5H11Cl/c1-3-4-5(2)6/h5H,3-4H2,1-2H3	-2.63
InChI=1S/C7H9N/c1-8-7-5-3-2-4-6-7/h2-6,8H,1H3	-1.28
InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3	-2.206
InChI=1S/C10H14N4O4/c1-12-8-7(9(17)13(2)10(12)18)14(5-11-8)3-6(16)4-15/h5-6,15-16H,3-4H2,1-2H3	-0.17
InChI=1S/C12H5Cl5/c13-8-3-1-6(5-10(8)15)7-2-4-9(14)12(17)11(7)16/h1-5H	-7.982
InChI=1S/C6H7NO/c8-5-6-1-3-7-4-2-6/h1-4,8H,5H2	0.962
InChI=1S/C18H12/c1-2-8-14-13(7-1)15-9-3-4-11-17(15)18-12-6-5-10-16(14)18/h1-12H	-6.745
InChI=1S/C11H15NO2S/c1-3-15-8-9-6-4-5-7-10(9)14-11(13)12-2/h4-7H,3,8H2,1-2H3,(H,12,13)	-2.093
InChI=1S/C8H4N2/c9-5-7-3-1-2-4-8(7)6-10/h1-4H	-2.38

"InChi"	"logS(M)"
InChI=1S/C8H11Cl2NO/c1-3-5-11(6-4-2)8(12)7(9)10/h3-4,7H,1-2,5-6H2	-1.619
InChI=1S/C6H14O/c1-6(2)4-3-5-7/h6-7H,3-5H2,1-2H3	-1.129
InChI=1S/C12H24O2/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h2-11H2,1H3,(H,13,14)	-4.62
InChI=1S/C13H16F3N3O4/c1-3-5-6-17(4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(22)23/h7-8H,3-6H2,1-2H3	-5.53
InChI=1S/C14H18O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h5-8H,3-4,9-10H2,1-2H3	-3.82
InChI=1S/C4H6O2/c1-3(2)4(5)6/h1H2,2H3,(H,5,6)	0.056
InChI=1S/C16H15ClN2/c1-19-10-9-18-16(12-5-3-2-4-6-12)14-11-13(17)7-8-15(14)19/h2-8,11H,9-10H2,1H3	-4.43
InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2	0.443
InChI=1S/C6H8S/c1-2-6-4-3-5-7-6/h3-5H,2H2,1H3	-2.585
InChI=1S/C6H14O/c1-3-4-5-6(2)7/h6-7H,3-5H2,1-2H3	-0.873
InChI=1S/C8H15N3O2/c1-6(2)5-10-8(13)11-4-3-9-7(11)12/h6H,3-5H2,1-2H3,(H,9,12)(H,10,13)	-2.154
InChI=1S/C17H27NO3/c1-4-7-13-20-16-10-8-15(9-11-16)17(19)21-14-12-18(5-2)6-3/h8-11H,4-7,12-14H2,1-3H3	-3.84
InChI=1S/C13H10N2/c14-11-5-3-7-13-10(11)8-9-4-1-2-6-12(9)15-13/h1-8H,14H2	-4.222
InChI=1S/C22H18Cl2FNO3/c1-22(2)15(11-19(23)24)20(22)21(27)29-18(12-26)13-8-9-16(25)17(1(h3-11,15,18,20H,1-2H3	-7.337
InChI=1S/C12H16N2O/c1-13-6-9-5-10(8-13)11-3-2-4-12(15)14(11)7-9/h2-4,9-10H,5-8H2,1H3	0.648
InChI=1S/C25H31FO8/c1-13(27)33-12-20(31)25(32)21(34-14(2)28)10-18-17-6-5-15-9-16(29) h7-9,17-19,21,30,32H,5-6,10-12H2,1-4H3	-4.13
InChI=1S/C6H15O4P/c1-4-8-11(7,9-5-2)10-6-3/h4-6H2,1-3H3	0.439
InChI=1S/C6H14O/c1-5(2)7-6(3)4/h5-6H,1-4H3	-1.517
InChI=1S/C6H12NO4PS2/c1-7(5-8)6(9)4-14-12(13,10-2)11-3/h5H,4H2,1-3H3	-1.995
InChI=1S/C20H12/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14 h1-12H	-8.192
InChI=1S/C13H9N/c1-2-6-11-10(5-1)9-14-13-8-4-3-7-12(11)13/h1-9H	-2.776
InChI=1S/C9H18O/c1-2-3-4-5-6-7-8-9-10/h9H,2-8H2,1H3	-3.149
InChI=1S/C12H17NO2/c1-2-3-4-9-15-12(14)10-5-7-11(13)8-6-10/h5-8H,2-4,9,13H2,1H3	-3.35
InChI=1S/C11H10/c1-9-6-7-10-4-2-3-5-11(10)8-9/h2-8H,1H3	-3.762
InChI=1S/C20H24O6/c1-2-6-18-17(5-1)23-13-9-21-11-15-25-19-7-3-4-8-20(19)26-16-12-22 h1-8H,9-16H2	-4.694

"InChi"	"logS(M)"
InChI=1S/C5H10Cl2/c1-4(6)5(2,3)7/h4H,1-3H3	-2.69
InChI=1S/C11H12N4O3S/c1-18-9-6-13-11(14-7-9)15-19(16,17)10-4-2-8(12)3-5-10/h2-7H,12H2,1H3,(H,13,14,15)	-2.584
InChI=1S/C14H17N5O3/c1-2-18-8-10(13(21)22)11(20)9-7-16-14(17-12(9)18)19-5-3-15-4-6-19h7-8,15H,2-6H2,1H3,(H,21,22)	-2.974
InChI=1S/C10H22O/c1-2-3-4-5-6-7-8-9-10-11/h11H,2-10H2,1H3	-3.631
InChI=1S/C2H3Cl3/c3-1-2(4)5/h2H,1H2	-1.581
InChI=1S/C9H11ClN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	-2.47
InChI=1S/C8H10/c1-7-3-5-8(2)6-4-7/h3-6H,1-2H3	-2.819
InChI=1S/C8H8O5/c1-13-8(12)4-2-5(9)7(11)6(10)3-4/h2-3,9-11H,1H3	-1.24
InChI=1S/C6H4FI/c7-5-1-3-6(8)4-2-5/h1-4H	-3.126
InChI=1S/C12H14ClNO2/c1-12(2)8-16-14(11(12)15)7-9-5-3-4-6-10(9)13/h3-6H,7-8H2,1-2H3	-2.338
InChI=1S/C13H12/c1-11-7-9-13(10-8-11)12-5-3-2-4-6-12/h2-10H,1H3	-4.619
InChI=1S/C7H6N4S/c1-12-7-5-6(10-4-11-7)9-3-2-8-5/h2-4H,1H3	-1.76
InChI=1S/C2H4Cl2/c3-1-2-4/h1-2H2	-1.08
InChI=1S/C8H12N2O3/c1-3-8(4-2)5(11)9-7(13)10-6(8)12/h3-4H2,1-2H3,(H2,9,10,11,12,13)	-1.42
InChI=1S/C16H21NO2/c1-12(2)17-10-14(18)11-19-16-9-5-7-13-6-3-4-8-15(13)16/h3-9,12,14,17-18H,10-11H2,1-2H3	-3.62
InChI=1S/C24H32O4/c1-14-12-18-19(22(4)9-6-17(27)13-21(14)22)7-10-23(5)20(18)8-11-24h12-13,18-20H,6-11H2,1-5H3	-5.284
InChI=1S/C9H16N2O2/c1-3-5-6-7(4-2)8(12)11-9(10)13/h4H,3,5-6H2,1-2H3,(H3,10,11,12,13)/b7-4-	-2.788
InChI=1S/C6H5NO2/c8-6(9)5-2-1-3-7-4-5/h1-4H,(H,8,9)	-0.835
InChI=1S/C11H8O2/c1-7-6-10(12)8-4-2-3-5-9(8)11(7)13/h2-6H,1H3	-3.032
InChI=1S/C6H12O2/c1-2-3-4-5-6(7)8/h2-5H2,1H3,(H,7,8)	-1.052
InChI=1S/C6H12O/c1-3-5-6(7)4-2/h3-5H2,1-2H3	-0.833
InChI=1S/C9H10O3/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6,10H,2H2,1H3	-2.2
InChI=1S/C6HCl5/c7-2-1-3(8)5(10)6(11)4(2)9/h1H	-5.65
InChI=1S/C8H12N4O5/c9-6(16)7-10-2-12(11-7)8-5(15)4(14)3(1-13)17-8/h2-5,8,13-15H,1H2,(H2,9,16)	-0.235
InChI=1S/C10H14/c1-8(2)10-7-5-4-6-9(10)3/h4-8H,1-3H3	-3.761
InChI=1S/C15H18Cl2N2O3/c1-8(2)21-12-7-11(9(16)6-10(12)17)19-14(20)22-13(18-19)15(3,4)5/h6-8H,1-5H3	-5.54
InChI=1S/C10H8N2/c1-3-7-11-9(5-1)10-6-2-4-8-12-10/h1-8H	-1.421
InChI=1S/C14H12N2S/c1-9-2-7-12-13(8-9)17-14(16-12)10-3-5-11(15)6-4-10/h2-8H,15H2,1H3	-3.68

"InChi"	"logS(M)"
InChI=1S/C3H3N/c1-2-3-4/h2H,1H2	0.147
InChI=1S/C8H10O/c1-6-3-4-8(9)7(2)5-6/h3-5,9H,1-2H3	-1.191
InChI=1S/C21H20Cl2O3/ c1-21(2)17(12-18(22)23)19(21)20(24)25-13-14-7-6-10-16(11-14)26-1 h3-12,17,19H,13H2,1-2H3	-6.99
InChI=1S/C8H14O2/c1-3-4-5-8(10)6-7(2)9/h3-6H2,1-2H3	-1.56
InChI=1S/C6H10O/c1-3-5-6(7)4-2/h4H,2-3,5H2,1H3	-0.83
InChI=1S/C8H18/c1-4-6-7-8(3)5-2/h8H,4-7H2,1-3H3	-5.159
InChI=1S/C12H12/c1-9-7-11-5-3-4-6-12(11)8-10(9)2/h3-8H,1-2H3	-4.72
InChI=1S/C17H20N2O2/ c1-2-19(12-14-8-10-18-11-9-14)17(21)16(13-20)15-6-4-3-5-7-15/ h3-11,16,20H,2,12-13H2,1H3	-1.7
InChI=1S/C14H10Cl4/ c15-11-5-1-9(2-6-11)13(14(17)18)10-3-7-12(16)8-4-10/h1-8,13-14H	-7.2
InChI=1S/C22H28N2O/ c1-2-22(25)24(20-11-7-4-8-12-20)21-14-17-23(18-15-21)16-13-19-9-5 h3-12,21H,2,13-18H2,1H3	-3.82
InChI=1S/C9H12/c1-7-4-5-8(2)9(3)6-7/h4-6H,1-3H3	-3.31
InChI=1S/C7H9N/c1-6-3-7(2)5-8-4-6/h3-5H,1-2H3	-0.511
InChI=1S/C2H6O3S/c1-5-6(2,3)4/h1-2H3	-0.042
InChI=1S/C7H14O2/c1-3-4-5-6-7(8)9-2/h3-6H2,1-2H3	-1.87
InChI=1S/C4H8O2/c1-2-3-4(5)6/h2-3H2,1H3,(H,5,6)	-0.167
InChI=1S/C8H8O/c1-2-4-7(5-3-1)8-6-9-8/h1-5,8H,6H2	-1.907
InChI=1S/C10H7Cl/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H	-4.143
InChI=1S/C10H14N2/c1-12-7-3-5-10(12)9-4-2-6-11-8-9/ h2,4,6,8,10H,3,5,7H2,1H3	0.79
InChI=1S/C29H42N6O9/ c1-15-19(44-26-24(38)23(37)22(34(4)5)16(2)43-26)10-11-21(42-15)35 h6-9,12-13,15-16,19,21-24,26,36-38H,10-11,14,30H2,1-5H3,(H, 31,40)(H,32,33,39,41)	-2.49
InChI=1S/C6H4F2/c7-5-2-1-3-6(8)4-5/h1-4H	-2
InChI=1S/C12H3Cl7/ c13-4-1-2-5(6(14)3-4)7-8(15)10(17)12(19)11(18)9(7)16/h1-3H	-8.971
InChI=1S/C10H14/c1-3-9(2)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3	-3.759
InChI=1S/C25H48N6O8/ c1-21(32)29(37)18-9-3-6-16-27-22(33)12-14-25(36)31(39)20-10-4-7-1 h37-39H,2-20,26H2,1H3,(H,27,33)(H,28,34)	-1.669
InChI=1S/C7H7N5O2/c1-11-5-4(8-3-9-10-5)6(13)12(2)7(11)14/h3H, 1-2H3	-1.985
InChI=1S/C5H6N2O4/c6-5(11)7-3(8)1-2-4(9)10/h1-2H,(H,9,10) (H3,6,7,8,11)/b2-1+	-1.92
InChI=1S/C6H13ClO/c7-5-3-1-2-4-6-8/h8H,1-6H2	-1.082
InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H	-0.04
InChI=1S/C20H12/ c1-2-8-16-15(7-1)17-9-3-5-13-11-12-14-6-4-10-18(16)20(14)19(13)17 h1-12H	-7.66
InChI=1S/C8H18O/c1-2-3-4-5-6-7-8-9/h9H,2-8H2,1H3	-2.638

"InChi"	"logS(M)"
InChI=1S/C13H14N2O4S2/c1-14-10(18)12-5-7-3-2-4-8(17)9(7)15(12)11(19)13(14,6-16)21-20-12/h2-4,8-9,16-17H,5-6H2,1H3	-3.669
InChI=1S/C12H7Cl3O2/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6,16H	-4.462
InChI=1S/C17H27NO3/c1-5-9-12-21-14-10-11-15(17(19)20-8-4)16(13-14)18(6-2)7-3/h10-11,13H,5-9,12H2,1-4H3	-3.84
InChI=1S/C13H12N2O/c16-13(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10H,(H2,14,15,16)	-3.151
InChI=1S/C11H24O/c1-3-4-5-6-7-8-9-10-11(2)12/h11-12H,3-10H2,1-2H3	-2.942
InChI=1S/C21H19NO4/c1-14-17(13-21(24)25)18-12-16(26-2)9-10-19(18)22(14)20(23)11-8-15-3-12H,13H2,1-2H3,(H,24,25)/b11-8+	-5.543
InChI=1S/C21H16/c1-13-6-7-15-12-20-17-5-3-2-4-14(17)8-9-18(20)19-11-10-16(13)21(15)12-9,12H,10-11H2,1H3	-7.966
InChI=1S/C10H12O4/c1-9-5-3-4-6(13-5)10(9,2)8(12)14-7(9)11/h5-6H,3-4H2,1-2H3	-3.816
InChI=1S/C12H13ClN2O/c1-4-9(2)15(3)12(16)14-11-7-5-10(13)6-8-11/h1,5-9H,2-3H3,(H,14,16)	-3.897
InChI=1S/C2H4N4/c3-1-6-2(4)5/h(H4,4,5,6)	-0.309
InChI=1S/C3H6Br2/c1-3(5)2-4/h3H,2H2,1H3	-2.15
InChI=1S/C5H11Cl/c1-2-3-4-5-6/h2-5H2,1H3	-2.732
InChI=1S/C11H14O3/c1-6(2)8-5-4-7(3)9(10(8)12)11(13)14/h4-6,12H,1-3H3,(H,13,14)	-3.288
InChI=1S/C10H20N2S4/c1-5-11(6-2)9(13)15-16-10(14)12(7-3)8-4/h5-8H2,1-4H3	-4.86
InChI=1S/C6H3Cl3O/c7-3-1-2-4(10)6(9)5(3)8/h1-2,10H	-2.67
InChI=1S/C6H6N2O2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H,7H2	-2.278
InChI=1S/C11H13NO3/c1-8(13)7-11(14)12-9-3-5-10(15-2)6-4-9/h3-6H,7H2,1-2H3,(H,12,14)	-1.901
InChI=1S/C12H24O2/c1-3-5-7-8-10-11(12(13)14)9-6-4-2/h11H,3-10H2,1-2H3,(H,13,14)	-4.959
InChI=1S/C7H8N2O/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,8H2,(H2,9,10)	-0.914
InChI=1S/C2H3Cl/c1-2-3/h2H,1H2	-1.36
InChI=1S/C19H21N5O4/c1-26-15-10-12-13(11-16(15)27-2)21-19(22-17(12)20)24-7-5-23(6-8-24)18(25)4-3-14-9-11H,5-8H2,1-2H3,(H2,20,21,22)	-5.09
InChI=1S/C2H3F3O/c3-2(4,5)1-6/h6H,1H2	1
InChI=1S/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3-8H,1-2H3/b4-3+	-3.126
InChI=1S/C12H4Cl6/c13-5-1-2-7(14)6(3-5)10-11(17)8(15)4-9(16)12(10)18/h1-4H	-7.425
InChI=1S/C8H5NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-4H,(H,9,10,11)	-2.611
InChI=1S/C10H20O/c1-3-4-5-6-7-8-9-10(2)11/h3-9H2,1-2H3	-3.308

"InChi"	"logS(M)"
InChI=1S/C7H4F3NO3/c8-7(9,10)4-1-2-6(12)5(3-4)11(13)14/h1-3,12H	-2.503
InChI=1S/C5H12O/c1-4-6-5(2)3/h5H,4H2,1-3H3	-0.561
InChI=1S/C5H11Br/c1-5(2)3-4-6/h5H,3-4H2,1-2H3	-2.886
InChI=1S/C7H8S/c1-8-7-5-3-2-4-6-7/h2-6H,1H3	-2.39
InChI=1S/C6H14O2/c1-2-3-5-8-6-4-7/h7H,2-6H2,1H3	-0.42
InChI=1S/C7H8O2/c8-5-6-3-1-2-4-7(6)9/h1-4,8-9H,5H2	-0.295
InChI=1S/C9H14N2O3/c1-4-9(5(2)3)6(12)10-8(14)11-7(9)13/h5H,4H2,1-3H3,(H2,10,11,12,13,14)	-2.148
InChI=1S/C12H18N2O7/c1-6-3-4-21-12(7(16)10(2,19)5-15)9(18)13-11(6,20)8(17)14-12/h7,15-16,19-20H,1,3-5H2,2H3,(H,13,18)(H,14,17)	-0.197
InChI=1S/C18H34O4/c1-3-5-15-21-17(19)13-11-9-7-8-10-12-14-18(20)22-16-6-4-2/h3-16H2,1-2H3	-3.896
InChI=1S/C7H6N4/c1-5-10-4-6-7(11-5)9-3-2-8-6/h2-4H,1H3	-0.119
InChI=1S/C9H21O2PS3/c1-6-10-12(13,11-7-2)15-8-14-9(3,4)5/h6-8H2,1-5H3	-4.755
InChI=1S/C16H34O/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3-16H2,1-2H3	-6.385
InChI=1S/C14H22ClN3O2/c1-4-18(5-2)7-6-17-14(19)10-8-11(15)12(16)9-13(10)20-3/h8-9H,4-7,16H2,1-3H3,(H,17,19)	-3.18
InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3	-0.159
InChI=1S/C8H15N5S/c1-12(2)6-9-7(13(3)4)11-8(10-6)14-5/h1-5H3	-2.676
InChI=1S/C2H6S/c1-2-3/h3H,2H2,1H3	-0.846
InChI=1S/C8H16O2/c1-3-4-5-6-7-10-8(2)9/h3-7H2,1-2H3	-2.451
InChI=1S/C8H11N/c1-9(2)8-6-4-3-5-7-8/h3-7H,1-2H3	-1.922
InChI=1S/C6H5NO3/c8-6-3-1-2-5(4-6)7(9)10/h1-4,8H	-1.07
InChI=1S/C27H37FO6/c1-5-6-7-23(33)34-27(22(32)15-29)16(2)12-20-19-9-8-17-13-18(30)10h10-11,13,16,19-21,29,31H,5-9,12,14-15H2,1-4H3	-4.71
InChI=1S/C11H13NO4/c1-12-11(13)16-9-5-3-2-4-8(9)10-14-6-7-15-10/h2-5,10H,6-7H2,1H3,(H,12,13)	-1.571
InChI=1S/C14H19NO4/c1-9(16)19-14-12(15-8-13(14)17)7-10-3-5-11(18-2)6-4-10/h3-6,12-15,17H,7-8H2,1-2H3	-1.607
InChI=1S/C19H24O5/c1-5-6-16(21)24-14-8-15-19(10-22-19)18(14,4)17(3)9-12(20)11(2)7-1h5-7,13-15H,8-10H2,1-4H3/b6-5+	-2.92
InChI=1S/C9H10BrClN2O2/c1-13(15-2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H,1-2H3,(H,12,14)	-3.924
InChI=1S/C6H6NO5P/c8-7(9)5-2-1-3-6(4-5)13(10,11)12/h1-4H,(H2,10,11,12)	0.683
InChI=1S/C11H8O3/c12-10-6-8-4-2-1-3-7(8)5-9(10)11(13)14/h1-6,12H,(H,13,14)	-3.417
InChI=1S/C5H10O/c1-4(2)5(3)6/h4H,1-3H3	-0.151
InChI=1S/C11H22O2/c1-3-5-6-7-8-9-10-11(12)13-4-2/h3-10H2,1-2H3	-3.801

"InChi"	"logS(M)"
InChI=1S/C23H28ClN3O2S/c1-18(28)29-16-15-26-13-11-25(12-14-26)9-4-10-27-20-5-2-3-6-22(20)h2-3,5-8,17H,4,9-16H2,1H3	-4.7
InChI=1S/C21H36O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-21(h13-19,22-23H,4-12H2,1-3H3	-7.02
InChI=1S/C8H8N2/c1-6-9-7-4-2-3-5-8(7)10-6/h2-5H,1H3,(H,9,10)	-1.96
InChI=1S/C7H3Cl3O2/c8-3-1-2-4(9)6(10)5(3)7(11)12/h1-2H,(H,11,12)	-1.467
InChI=1S/C2H6N2O/c1-4-2(3)5/h1H3,(H3,3,4,5)	1.13
InChI=1S/C20H12/c1-5-13-6-2-11-17-18-12-4-8-14-7-3-10-16(20(14)18)15(9-1)19(13)17h1-12H	-8.7
InChI=1S/C3H7Cl/c1-3(2)4/h3H,1-2H3	-1.404
InChI=1S/C25H38O5/c1-6-25(4,5)24(28)30-21-12-15(2)11-17-8-7-16(3)20(23(17)21)10-9-1h7-8,11,15-16,18-21,23,26H,6,9-10,12-14H2,1-5H3	-7.145
InChI=1S/C13H16O3/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h4-5,8-10,14H,1-3,6-7H2	-4.554
InChI=1S/C12H4Cl6/c13-5-1-7(12(18)11(17)2-5)6-3-9(15)10(16)4-8(6)14/h1-4H	-8.58
InChI=1S/C12H6Cl4/c13-7-2-4-11(15)10(5-7)9-3-1-8(14)6-12(9)16/h1-6H	-7.26
InChI=1S/C10H18/c1-2-6-10-8-4-3-7-9(10)5-1/h9-10H,1-8H2	-4.141
InChI=1S/C14H12O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10,13,15H	-2.85
InChI=1S/C18H16O7/c1-6-14(22)12(8(3)20)16-13(15(6)23)18(4)10(25-16)5-9(21)11(7(2)19h5,11,22-23H,1-4H3	-3.537
InChI=1S/CH2Br2/c2-1-3/h1H2	-1.286
InChI=1S/C7H14O2/c1-3-4-5-6-9-7(2)8/h3-6H2,1-2H3	-1.884
InChI=1S/C2H4BrCl/c3-1-2-4/h1-2H2	-1.318
InChI=1S/C5H8N4O3S2/c1-3(10)7-4-9(2)8-5(13-4)14(6,11)12/h1-2H3,(H2,6,11,12)/b7-4-	-1.92
InChI=1S/C7H16/c1-3-5-7-6-4-2/h3-7H2,1-2H3	-4.469
InChI=1S/C8H10NO5PS/c1-12-15(16,13-2)14-8-5-3-7(4-6-8)9(10)11/h3-6H,1-2H3	-3.68
InChI=1S/C22H16F3N3/c23-22(24,25)20-13-7-12-19(14-20)21(28-16-26-15-27-28,17-8-3-1-4-h1-16H	-8.403
InChI=1S/C10H7NO2/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H	-3.71
InChI=1S/C19H17ClN2O/c20-15-8-9-17-16(10-15)19(14-4-2-1-3-5-14)21-11-18(23)22(17)12-13h1-5,8-10,13H,6-7,11-12H2	-4.91
InChI=1S/C18H18O2/c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11-16(20)12-8-14/h3-12,19-20H,1-2H3/b17-3-,18-4+	-4.948
InChI=1S/C8H10N2O3S/c1-6(11)10-7-2-4-8(5-3-7)14(9,12)13/h2-5H,1H3,(H,10,11)(H2,9,12,13)	-1.607

"InChi"	"logS(M)"
InChI=1S/C4H6N2/c1-4-2-3-5-6-4/h2-3H,1H3,(H,5,6)	1.086
InChI=1S/C3H6N2O3/c4-3(8)5-1-2(6)7/h1H2,(H,6,7)(H3,4,5,8)	-0.581
InChI=1S/C7H8O2/c1-9-7-5-3-2-4-6(7)8/h2-5,8H,1H3	-0.822
InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3	-2.026
InChI=1S/C7H14O/c1-6-4-2-3-5-7(6)8/h6-8H,2-5H2,1H3	-0.864
InChI=1S/C18H12N2/ c1-3-7-15-13(5-1)9-11-17(19-15)18-12-10-14-6-2-4-8-16(14)20-18/ h1-12H	-5.4
InChI=1S/C16H16N2O4/ c1-2-21-15(19)18-13-9-6-10-14(11-13)22-16(20)17-12-7-4-3-5-8-12/ h3-11H,2H2,1H3,(H,17,20)(H,18,19)	-4.52
InChI=1S/C18H28N2O/ c1-4-5-12-20-13-7-6-11-16(20)18(21)19-17-14(2)9-8-10-15(17)3/ h8-10,16H,4-7,11-13H2,1-3H3,(H,19,21)	-3.22
InChI=1S/C9H18O2/c1-3-4-5-6-7-8-9(10)11-2/h3-8H2,1-2H3	-3.17
InChI=1S/C12H8Cl2/c13-10-6-7-11(12(14)8-10)9-4-2-1-3-5-9/h1-8H	-5.288
InChI=1S/C8H7Cl2NO2/c1-13-8(12)5-2-4(9)3-6(11)7(5)10/h2-3H, 11H2,1H3	-3.263
InChI=1S/C12H14O4/c1-3-15-11(13)9-7-5-6-8-10(9)12(14)16-4-2/ h5-8H,3-4H2,1-2H3	-2.35
InChI=1S/C26H36O6/ c1-23(2,3)22(30)32-14-20(29)26(31)11-9-18-17-7-6-15-12-16(27)8-10 h8,10,12,17-19,21,28,31H,6-7,9,11,13-14H2,1-5H3	-4.583
InChI=1S/C3H8O3S/c1-3-6-7(2,4)5/h3H2,1-2H3	0.402
InChI=1S/C7H3Cl2N/c8-6-2-1-3-7(9)5(6)4-10/h1-3H	-3.98
InChI=1S/C6H12O6/c7-1-3-4(9)5(10)6(11,2-8)12-3/h3-5,7-11H, 1-2H2	0.64
InChI=1S/C8H9NO3/c1-5-8(12)7(4-11)6(3-10)2-9-5/h2,4,10,12H, 3H2,1H3	0.476
InChI=1S/C9H6Cl2N2O3/ c1-12-8(14)13(16-9(12)15)5-2-3-6(10)7(11)4-5/h2-4H,1H3	-2.82
InChI=1S/C6H11NO/c1-2-7-5-3-4-6(7)8/h2-5H2,1H3	0.946
InChI=1S/C5H12N2O/c1-5(2,3)7-4(6)8/h1-3H3,(H3,6,7,8)	-0.731
InChI=1S/C12H15NO3/ c1-12(2)7-8-5-4-6-9(10(8)16-12)15-11(14)13-3/h4-6H,7H2,1-3H3,(H, 13,14)	-2.42
InChI=1S/C10H10N2O/c1-8-7-10(13)12(11-8)9-5-3-2-4-6-9/h2-6H, 7H2,1H3	-1.925
InChI=1S/C5H4N4O3/c10-3-1-2(7-4(11)6-1)8-5(12)9-3/ h(H4,6,7,8,9,10,11,12)	-3.62
InChI=1S/C13H18N4O3/ c1-9(18)6-4-5-7-17-12(19)10-11(14-8-15(10)2)16(3)13(17)20/h8H, 4-7H2,1-3H3	-0.558
InChI=1S/C6H4N2O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H	-2.499
InChI=1S/C6H2Cl4O/c7-2-1-3(11)5(9)6(10)4(2)8/h1,11H	-3.15
InChI=1S/C8H16/c1-7-5-3-4-6-8(7)2/h7-8H,3-6H2,1-2H3	-4.272
InChI=1S/C10H12O4/c1-12-7-4-3-6-5-14-10(11)8(6)9(7)13-2/ h3-4,6,8H,5H2,1-2H3	-1.899
InChI=1S/C9H9NS/c11-8-10-7-6-9-4-2-1-3-5-9/h1-5H,6-7H2	-3.171

"InChi"	"logS(M)"
InChI=1S/C6H13Cl2N/c1-2-9(5-3-7)6-4-8/h2-6H2,1H3	-3.026
InChI=1S/C14H18N2O3/c1-2-14(11(17)15-13(19)16-12(14)18)10-6-4-8-3-5-9(10)7-8/h6,8-9H,2-5,7H2,1H3,(H2,15,16,17,18,19)	-2.696
InChI=1S/C5H8/c1-3-5-4-2/h3-4H,1-2,5H2	-2.087
InChI=1S/C12H5Cl5/c13-8-7(6-4-2-1-3-5-6)9(14)11(16)12(17)10(8)15/h1-5H	-7.911
InChI=1S/C2H6S/c1-3-2/h1-2H3	-0.931
InChI=1S/C8H19O2PS3/c1-4-9-11(12,10-5-2)14-8-7-13-6-3/h4-8H2,1-3H3	-4.226
InChI=1S/C7H10O3/c1-5(2)7(8)10-4-6-3-9-6/h6H,1,3-4H2,2H3	-0.454
InChI=1S/C8H16O2/c1-3-5-6-7-8(9)10-4-2/h3-7H2,1-2H3	-2.35
InChI=1S/C3H6Cl2/c1-3(5)2-4/h3H,2H2,1H3	-1.622
InChI=1S/C12H14NO4PS/c1-3-16-18(19,17-4-2)13-11(14)9-7-5-6-8-10(9)12(13)15/h5-8H,3-4H2,1-2H3	-3.352
InChI=1S/C14H12F3NO4S2/c1-10-9-12(23(19,20)11-5-3-2-4-6-11)7-8-13(10)18-24(21,22)14(15,16)h2-9,18H,1H3	-3.801
InChI=1S/C3H6O/c1-2-3-4/h3H,2H2,1H3	0.58
InChI=1S/C22H14/c1-3-7-19-15(5-1)9-11-17-14-22-18(13-21(17)19)12-10-16-6-2-4-8-20h1-14H	-8.668
InChI=1S/C11H16N2O/c1-2-3-9-13(11(12)14)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3,(H2,12,14)	-1.297
InChI=1S/C11H23NOS/c1-6-14-11(13)12(7-9(2)3)8-10(4)5/h9-10H,6-8H2,1-5H3	-3.684
InChI=1S/C14H22O7/c1-7(15)17-10-9(8-6-16-13(2,3)19-8)18-12-11(10)20-14(4,5)21-12/h8-12H,6H2,1-5H3	-1.523
InChI=1S/C12HCl9/c13-3-1-2(5(14)9(18)6(3)15)4-7(16)10(19)12(21)11(20)8(4)17/h1H	-9.62
InChI=1S/C3H5F3O/c1-2(7)3(4,5)6/h2,7H,1H3	0.309
InChI=1S/C15H27N3O/c1-16(2)9-12-7-13(10-17(3)4)15(19)14(8-12)11-18(5)6/h7-8,19H,9-11H2,1-6H3	0.506
InChI=1S/C14H10Cl4/c15-10-7-5-9(6-8-10)13(14(17)18)11-3-1-2-4-12(11)16/h1-8,13-14H	-6.505
InChI=1S/C23H15ClO3/c24-16-12-10-15(11-13-16)19(14-6-2-1-3-7-14)23(27)20-21(25)17-8-4h1-13,19-20H	-3.574
InChI=1S/C6H12O2/c1-6(2)3-4-8-5-7/h5-6H,3-4H2,1-2H3	-1.521
InChI=1S/C21H21NO6/c1-22-7-6-11-8-15-16(27-10-26-15)9-13(11)18(22)19-12-4-5-14(24-2)h4-5,8-9,18-19H,6-7,10H2,1-3H3	-4.106
InChI=1S/C6H14O/c1-3-5-6(7)4-2/h6-7H,3-5H2,1-2H3	-0.802
InChI=1S/C21H21O7P/c1-13-7-8-17(23)12-20(13)27-29(25,26-19-10-9-16(22)11-15(19)3)28-h4-12,22-24H,1-3H3	-6.7

"InChi"	"logS(M)"
InChI=1S/C17H16Cl2N2O5/c18-16(19)17(23)20(9-10-22)11-12-1-5-14(6-2-12)26-15-7-3-13(4-8-1h1-8,16,22H,9-11H2	-5.124
InChI=1S/C11H13N3O3S/c1-7-8(2)17-11(13-7)14-18(15,16)10-5-3-9(12)4-6-10/h3-6H,12H2,1-2H3,(H,13,14)	-2.22
InChI=1S/C15H23NO3/c1-4-16(5-2)11-12-19-15(17)13-7-9-14(10-8-13)18-6-3/h7-10H,4-6,11-12H2,1-3H3	-2.715
InChI=1S/C4H8O/c1-3-4(2)5/h3H2,1-2H3	0.52
InChI=1S/C19H24N2OS/c1-14(12-20(2)3)13-21-16-7-5-6-8-18(16)23-19-10-9-15(22-4)11-17(1h5-11,14H,12-13H2,1-4H3	-4.215
InChI=1S/C5H4O3/c6-5(7)4-2-1-3-8-4/h1-3H,(H,6,7)	-0.48
InChI=1S/C7H14/c1-7-5-3-2-4-6-7/h7H,2-6H2,1H3	-3.846
InChI=1S/C4H9NO/c1-4(6)5(2)3/h1-3H3	1.06
InChI=1S/C11H15N3O2/c1-12-11(15)16-10-6-4-5-9(7-10)13-8-14(2)3/h4-8H,1-3H3,(H,12,15)/b13-8+	-2.34
InChI=1S/C13H15NO2/c1-10-12(8-5-9-16-10)13(15)14-11-6-3-2-4-7-11/h2-4,6-7H,5,8-9H2,1H3,(H,14,15)	-2.56
InChI=1S/C7H7Cl2NO/c1-3-5(8)7(11)6(9)4(2)10-3/h1-2H3,(H,10,11)	-4.283
InChI=1S/C8H16O/c1-3-5-6-8(4-2)7-9/h7-8H,3-6H2,1-2H3	-2.263
InChI=1S/C20H30O2/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(16,3)10-5-11-20(17,4)18(21)2h7,12-13,16-17H,5-6,8-11H2,1-4H3,(H,21,22)	-3.796
InChI=1S/C9H10O3/c1-6(10)7-3-4-8(11)9(5-7)12-2/h3-5,11H,1-2H3	-1.522
InChI=1S/C11H16N8O8/c20-2-18-4(6(22)16-10(18)26)14-8(24)12-1-13-9(25)15-5-7(23)17-11(h4-5,20-21H,1-3H2,(H2,12,14,24)(H2,13,15,25)(H,16,22,26)(H,17,23,27)	0.411
InChI=1S/C14H14O3/c1-14(2,3)13(17)10-11(15)8-6-4-5-7-9(8)12(10)16/h4-7,10H,1-3H3	-4.107
InChI=1S/C8H16/c1-2-5-8-6-3-4-7-8/h8H,2-7H2,1H3	-4.74
InChI=1S/C7H9NO2S/c1-6-4-2-3-5-7(6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)	-1.526
InChI=1S/C5H6N2O2/c1-3-2-6-5(9)7-4(3)8/h2H,1H3,(H2,6,7,8,9)	-1.519
InChI=1S/C21H26N2O3/c1-26-21(25)19-15-10-17-20-14(13-4-2-3-5-16(13)22-20)8-9-23(17)11h2-5,12,15,17-19,22,24H,6-11H2,1H3	-4.031
InChI=1S/C16H11NO2/c18-16(19)13-10-15(11-6-2-1-3-7-11)17-14-9-5-4-8-12(13)14/h1-10H,(H,18,19)	-3.193
InChI=1S/C15H14ClN3O4S/c16-8-6-24-14-10(13(21)19(14)11(8)15(22)23)18-12(20)9(17)7-4-2-1-h1-5,9-10,14H,6,17H2,(H,18,20)(H,22,23)	-1.566
InChI=1S/C10H12O3/c1-2-13-10(12)9(11)8-6-4-3-5-7-8/h3-7,9,11H,2H2,1H3	-1.26
InChI=1S/C7H14O2/c1-6(2)4-5-9-7(3)8/h6H,4-5H2,1-3H3	-1.813

"InChi"	"logS(M)"
InChI=1S/C10H11F3N2O/c1-15(2)9(16)14-8-5-3-4-7(6-8)10(11,12)13/h3-6H,1-2H3,(H,14,16)	-3.437
InChI=1S/C5H6S/c1-5-2-3-6-4-5/h2-4H,1H3	-2.39
InChI=1S/C9H21N/c1-4-7-10(8-5-2)9-6-3/h4-9H2,1-3H3	-2.472
InChI=1S/C6H15O2PS3/c1-4-11-5-6-12-9(10,7-2)8-3/h4-6H2,1-3H3	-3.091
InChI=1S/C24H25NO3/c1-25-12-11-24-17-8-9-19(26)23(24)28-22-20(27-14-15-5-3-2-4-6-15)h2-10,17-19,23,26H,11-14H2,1H3	-2.973
InChI=1S/C9H15N5O/c10-7-6-8(12-9(11)14(7)15)13-4-2-1-3-5-13/h6H,1-5,10H2,(H2,11,12)	-1.94
InChI=1S/C14H9NO2/c16-13-11-8-4-5-9-12(11)17-14(15-13)10-6-2-1-3-7-10/h1-9H	-4.61
InChI=1S/C12H24N2O4/c1-5-6-12(4,7-17-10(13)15)8-18-11(16)14-9(2)3/h9H,5-8H2,1-4H3,(H2,13,15)(H,14,16)	-2.938
InChI=1S/C22H30O3/c1-20-9-5-15(23)13-14(20)3-4-16-17(20)6-10-21(2)18(16)7-11-22(21)h13,16-18H,3-12H2,1-2H3	-4.225
InChI=1S/C5H7N3O/c1-3-2-7-5(9)8-4(3)6/h2H,1H3,(H3,6,7,8,9)	-1.44
InChI=1S/C6H14N2/c1-5-3-8-6(2)4-7-5/h5-8H,3-4H2,1-2H3	0.49
InChI=1S/C20H20N2O4/c1-2-9-17(23)26-14-22-18(24)20(21-19(22)25,15-10-5-3-6-11-15)16-1h3-8,10-13H,2,9,14H2,1H3,(H,21,25)	-4.68
InChI=1S/C3H6Cl2/c4-2-1-3-5/h1-3H2	-1.614
InChI=1S/C9H7NO/c11-8-5-1-3-7-4-2-6-10-9(7)8/h1-6,11H	-2.35
InChI=1S/C12H6Cl4/c13-7-4-5-10(14)9(6-7)8-2-1-3-11(15)12(8)16/h1-6H	-6.465
InChI=1S/C4H9Br/c1-2-3-4-5/h2-4H2,1H3	-2.198
InChI=1S/C12H15N3O2S/c1-3-6-18-8-4-5-9-10(7-8)14-11(13-9)15-12(16)17-2/h4-5,7H,3,6H2,1-2H3,(H2,13,14,15,16)	-4.22
InChI=1S/C16H16ClN3O3S/c1-10-8-11-4-2-3-5-14(11)20(10)19-16(21)12-6-7-13(17)15(9-12)24(1h2-7,9-10H,8H2,1H3,(H,19,21)(H2,18,22,23)	-3.79
InChI=1S/C5H12O/c1-4-5(2,3)6/h6H,4H2,1-3H3	0.127
InChI=1S/C9H9Cl2NO/c1-2-9(13)12-6-3-4-7(10)8(11)5-6/h3-5H,2H2,1H3,(H,12,13)	-2.986
InChI=1S/C4H8Cl3O4P/c1-10-12(9,11-2)3(8)4(5,6)7/h3,8H,1-2H3	-0.332
InChI=1S/C15H15ClN2O4S/c1-8-4-3-5-9(2)14(8)18-15(20)10-6-13(23(17,21)22)11(16)7-12(10)19h3-7,19H,1-2H3,(H,18,20)(H2,17,21,22)	-3.9
InChI=1S/C13H12O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13-14H	-2.549
InChI=1S/C8H9NO2/c1-9-7-5-3-2-4-6(7)8(10)11/h2-5,9H,1H3,(H,10,11)	-2.878
InChI=1S/C12H8Cl2/c13-10-7-5-9(6-8-10)11-3-1-2-4-12(11)14/h1-8H	-5.28
InChI=1S/C10H9NO3S/c1-2-7-14-10-8-5-3-4-6-9(8)15(12,13)11-10/h2-6H,1,7H2	-3.173

"InChi"	"logS(M)"
InChI=1S/C17H16Br2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6-13/h3-11,21H,1-2H3	-4.933
InChI=1S/C8H8O4/c1-4(9)5-2-6(10)8(12)7(11)3-5/h2-3,10-12H,1H3	-1.471
InChI=1S/C8H8N4S/c9-7(10)12-8-11-5-3-1-2-4-6(5)13-8/h1-4H,(H4,9,10,11,12)	-2.441
InChI=1S/C10H14N5O7P/c11-8-5-9(13-2-12-8)15(3-14-5)10-7(17)6(16)4(22-10)1-21-23(18,19)2h2-4,6-7,10,16-17H,1H2,(H2,11,12,13)(H2,18,19,20)	-1.995
InChI=1S/C8H8O3/c9-8(10)6-11-7-4-2-1-3-5-7/h1-5H,6H2,(H,9,10)	-1.103
InChI=1S/C4H9I/c1-2-3-4-5/h2-4H2,1H3	-2.959
InChI=1S/C6H6N2O2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H,7H2	-2.061
InChI=1S/C3H6O2/c1-3(4)5-2/h1-2H3	0.46
InChI=1S/C9H18O2/c1-2-3-4-5-6-7-8-9(10)11/h2-8H2,1H3,(H,10,11)	-2.722
InChI=1S/C11H15NO3/c1-2-11(14,8-15-10(12)13)9-6-4-3-5-7-9/h3-7,14H,2,8H2,1H3,(H2,12,13)	-0.923
InChI=1S/C11H19N3O/c1-4-6-7-9-8(3)13-11(12-5-2)14-10(9)15/h4-7H2,1-3H3,(H2,12,13,14,15)	-3.02
InChI=1S/C12H27N/c1-4-7-10-13(11-8-5-2)12-9-6-3/h4-12H2,1-3H3	-3.116
InChI=1S/C10H14N2O3/c1-6(2)4-5-10(3)7(13)11-9(15)12-8(10)14/h4H,5H2,1-3H3,(H2,11,12,13,14,15)	-2.6
InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h5H,2-4,6H2,1H3	-3.267
InChI=1S/C10H14/c1-2-3-7-10-8-5-4-6-9-10/h4-6,8-9H,2-3,7H2,1H3	-4.056
InChI=1S/C11H14N4O4/c12-9-5-1-2-15(10(5)14-4-13-9)11-8(18)7(17)6(3-16)19-11/h1-2,4,6-8,11,16-18H,3H2,(H2,12,13,14)	-1.952
InChI=1S/C12H7Cl3/c13-10-4-2-1-3-9(10)8-5-6-11(14)12(15)7-8/h1-7H	-6.287
InChI=1S/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)	-4.43
InChI=1S/C4H4FN3O/c5-2-1-7-4(9)8-3(2)6/h1H,(H3,6,7,8,9)	-0.972
InChI=1S/C22H22O8/c1-25-16-4-10(5-17(26-2)21(16)27-3)18-11-6-14-15(30-9-29-14)7-12(h4-7,13,18-20,23H,8-9H2,1-3H3	-3.617
InChI=1S/C20H38N4O4/c1-3-5-7-21(19(25)23-11-15-27-16-12-23)9-10-22(8-6-4-2)20(26)24-1h3-18H2,1-2H3	0.099
InChI=1S/C10H20NO5PS2/c1-5-14-10(13)11(4)9(12)8-19-17(18,15-6-2)16-7-3/h5-8H2,1-4H3	-2.518
InChI=1S/C10H6Cl6/c11-6-7(12)9(14)5-3-1-2-4(5)8(6,13)10(9,15)16/h1-2,4-5H,3H2	-5.64
InChI=1S/C5H11N/c1-2-4-6-5-3-1/h6H,1-5H2	1.07
InChI=1S/C23H32O4/c1-14(24)27-13-21(26)20-7-6-18-17-5-4-15-12-16(25)8-10-22(15,2)19h12,17-20H,4-11,13H2,1-3H3	-4.63
InChI=1S/C9H12/c1-3-9-6-4-8(2)5-7-9/h4-7H,3H2,1-2H3	-3.103
InChI=1S/C9H12N2O/c1-11(2)9(12)10-8-6-4-3-5-7-8/h3-7H,1-2H3,(H,10,12)	-1.61

"InChi"	"logS(M)"
InChI=1S/C10H14N4O3/c1-12-8-7(9(16)13(2)10(12)17)14(6-11-8)4-3-5-15/h6,15H,3-5H2,1-2H3	-0.155
InChI=1S/C7H16O/c1-6(2)4-5-7(3)8/h6-8H,4-5H2,1-3H3	-1.375
InChI=1S/C15H23N3O4S/c1-3-18-8-4-5-11(18)10-17-15(19)13-9-12(23(16,20)21)6-7-14(13)22-h6-7,9,11H,3-5,8,10H2,1-2H3,(H,17,19)(H2,16,20,21)	-2.88
InChI=1S/C2H2Cl4/c3-1(4)2(5)6/h1-2H	-1.754
InChI=1S/C5H4O2S/c6-5(7)4-1-2-8-3-4/h1-3H,(H,6,7)	-1.474
InChI=1S/C11H17N3O3S/c1-2-3-8-13-11(15)14-18(16,17)10-6-4-9(12)5-7-10/h4-7H,2-3,8,12H2,1H3,(H2,13,14,15)	-2.178
InChI=1S/C14H12O3/c15-13(16)14(17,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,17H,(H,15,16)	-2.209
InChI=1S/C9H8O2/c1-7(9(10)11)8-5-3-2-4-6-8/h2-6H,1H2,(H,10,11)	-2.057
InChI=1S/C18H21NO/c20-18(15-9-3-1-4-10-15,16-11-5-2-6-12-16)17-13-7-8-14-19-17/h1-6,9-12,17,19-20H,7-8,13-14H2	-1.9
InChI=1S/C13H10O3/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9,14H	-3.155
InChI=1S/C10H14N4O3/c1-6(15)4-14-5-11-8-7(14)9(16)13(3)10(17)12(8)2/h5-6,15H,4H2,1-3H3	0.623
InChI=1S/C9H13ClN2O2/c1-5-6(10)7(13)12(8(14)11-5)9(2,3)4/h1-4H3,(H,11,14)	-2.485
InChI=1S/C4H4S/c1-2-4-5-3-1/h1-4H	-1.445
InChI=1S/C11H23NO2/c12-10-8-6-4-2-1-3-5-7-9-11(13)14/h1-10,12H2,(H,13,14)	-2.401
InChI=1S/C7H5ClO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)	-2.542
InChI=1S/C8H18/c1-7(2)6-8(3,4)5/h7H,6H2,1-5H3	-4.67
InChI=1S/C9H7N7O2S/c1-15-4-14-7(16(17)18)9(15)19-8-5-6(11-2-10-5)12-3-13-8/h2-4H,1H3,(H,10,11,12,13)	-3.21
InChI=1S/C10H11ClO3/c1-6-5-8(11)3-4-9(6)14-7(2)10(12)13/h3-5,7H,1-2H3,(H,12,13)	-2.466
InChI=1S/C8H9NO2/c1-6(10)9-7-3-2-4-8(11)5-7/h2-5,11H,1H3,(H,9,10)	-1.06
InChI=1S/C2H3Cl3O2/c3-2(4,5)1(6)7/h1,6-7H	1.037
InChI=1S/C8H7NS/c1-7-2-4-8(5-3-7)9-6-10/h2-5H,1H3	-4.721
InChI=1S/C10H14O3/c1-8-4-2-3-5-10(8)13-7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3	-1.189
InChI=1S/C2H2I2/c3-1-2-4/h1-2H/b2-1+	-2.781
InChI=1S/C19H22O6/c1-9-7-17-8-18(9,24)5-3-10(17)19-6-4-11(20)16(2,15(23)25-19)13(19)h4,6,10-13,20,24H,1,3,5,7-8H2,2H3,(H,21,22)	-1.841
InChI=1S/C7H6N2O4/c1-5-2-3-6(8(10)11)4-7(5)9(12)13/h2-4H,1H3	-3.04
InChI=1S/C23H26N2O4/c1-27-16-8-14-15(9-17(16)28-2)25-20(26)10-18-21-13-7-19-23(14,22(h3,8-9,13,18-19,21-22H,4-7,10-11H2,1-2H3	-2.091

"InChi"	"logS(M)"
InChI=1S/C11H14N2O/c14-11-3-1-2-10-9-4-8(5-12-6-9)7-13(10)11/h1-3,8-9,12H,4-7H2	0.363
InChI=1S/C12H5Cl5/c13-6-4-9(16)12(10(17)5-6)11-7(14)2-1-3-8(11)15/h1-5H	-7.316
InChI=1S/C6H5F/c7-6-4-2-1-3-5-6/h1-5H	-1.792
InChI=1S/C16H16N2O4/c1-11-5-3-6-12(9-11)18-16(20)22-14-8-4-7-13(10-14)17-15(19)21-2/h3-10H,1-2H3,(H,17,19)(H,18,20)	-4.779
InChI=1S/C7H4ClNO2/c8-4-1-2-6-5(3-4)9-7(10)11-6/h1-3H,(H,9,10)	-2.66
InChI=1S/C17H23NO3/c1-18-13-7-8-14(18)10-15(9-13)21-17(20)16(11-19)12-5-3-2-4-6-12/h2-6,13-16,19H,7-11H2,1H3	-1.91
InChI=1S/C6H4ClNO2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H	-2.761
InChI=1S/C7H5F3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H	-2.511
InChI=1S/C12H6Cl4/c13-9-6-8(7-4-2-1-3-5-7)10(14)12(16)11(9)15/h1-6H	-7.16
InChI=1S/C17H25N5O13/c18-6(8(25)5(24)3-34-16(19)32)13(29)20-7(15(30)31)11-9(26)10(27)1h1,5-11,14,23-27H,2-3,18H2,(H2,19,32)(H,20,29)(H,30,31)(H,21,28,33)	0.295
InChI=1S/C3H9N/c1-4(2)3/h1-3H3	1.178
InChI=1S/C21H30O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-10-h12,16-18,24H,4-11H2,1-3H3	-4.708
InChI=1S/C7H4Cl2O2/c8-5-1-4(7(10)11)2-6(9)3-5/h1-3H,(H,10,11)	-3.114
InChI=1S/C20H16/c1-13-14(2)20-17-9-4-3-7-15(17)11-12-19(20)18-10-6-5-8-16(13)18/h3-12H,1-2H3	-7.011
InChI=1S/C7H6N2/c1-2-4-7-6(3-1)5-8-9-7/h1-5H,(H,8,9)	-2.155
InChI=1S/C10H11NO3/c1-7(12)11-9-3-5-10(6-4-9)14-8(2)13/h3-6H,1-2H3,(H,11,12)	-1.908
InChI=1S/C14H18O4/c1-9(2)17-13(15)11-7-5-6-8-12(11)14(16)18-10(3)4/h5-10H,1-4H3	-2.877
InChI=1S/C21H22N2O3/c24-18-10-16-19-13-9-17-21(6-7-23(17,25)11-12(13)5-8-26-16)14-3-1h1-5,13,16-17,19-20H,6-11H2	-1.28
InChI=1S/C12H4Cl6/c13-5-1-2-8(14)6(3-5)7-4-9(15)11(17)12(18)10(7)16/h1-4H	-7.679
InChI=1S/C6H4N2O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H	-3.387
InChI=1S/C6H4F2/c7-5-1-2-6(8)4-3-5/h1-4H	-1.971
InChI=1S/C6H6O3/c7-4-2-1-3-5(8)6(4)9/h1-3,7-9H	0.604
InChI=1S/C4H6O4/c5-3(6)1-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)	-0.17
InChI=1S/C7H16O/c1-3-5-7(8)6-4-2/h7-8H,3-6H2,1-2H3	-1.393
InChI=1S/C10H21NOS/c1-4-7-8-11(6-3)10(12)13-9-5-2/h4-9H2,1-3H3	-3.41
InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H2,1-2H3	-2.167
InChI=1S/C8H8O3/c1-5-3-2-4-6(9)7(5)8(10)11/h2-4,9H,1H3,(H,10,11)	-2.04
InChI=1S/C10H8O2/c1-7(11)10-6-8-4-2-3-5-9(8)12-10/h2-6H,1H3	-2.548

"InChi"	"logS(M)"
InChI=1S/C16H19N3O4S/c1-16(2)11(15(22)23)19-13(21)10(14(19)24-16)18-12(20)9(17)8-6-4-3-7,9-11,14H,17H2,1-2H3,(H,18,20)(H,22,23)	-1.539
InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3	0.699
InChI=1S/C6H5N3/c1-2-4-6-5(3-1)7-9-8-6/h1-4H,(H,7,8,9)	-0.779
InChI=1S/C10H11N3O2S2/c1-7-6-16-10(12-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2,1H3,(H,12,13)	-2.91
InChI=1S/C7H7Cl/c1-6-2-4-7(8)5-3-6/h2-5H,1H3	-3.102
InChI=1S/C5H11NO2S/c1-5(2,9)3(6)4(7)8/h3,9H,6H2,1-2H3,(H,7,8)	-0.129
InChI=1S/C29H31F2N3O/c30-24-12-8-22(9-13-24)27(23-10-14-25(31)15-11-23)7-4-18-33-19-1(h1-3,5-6,8-15,27H,4,7,16-21H2,(H,32,35)	-4.677
InChI=1S/C7H8N2O2/c1-5-2-3-6(8)7(4-5)9(10)11/h2-4H,8H2,1H3	-1.86
InChI=1S/C12H15ClNO4PS2/c1-3-16-19(20,17-4-2)21-8-14-10-6-5-9(13)7-11(10)18-12(14)15/h5-7H,3-4,8H2,1-2H3	-5.081
InChI=1S/C19H26O6/c1-11-5-4-6-14(10-21)8-16-17(13(3)19(23)25-16)15(7-11)24-18(22)12h5,8,12,15-17,20-21H,3-4,6-7,9-10H2,1-2H3/b11-5-,14-8+	-2.244
InChI=1S/C22H24N2O9/c1-21(32)7-5-4-6-8(25)9(7)15(26)10-12(21)17(28)13-14(24(2)3)16(27h4-6,12-14,17,25,27-29,32-33H,1-3H3,(H2,23,31)	-3.15
InChI=1S/C2H4ClNO/c3-1-2(4)5/h1H2,(H2,4,5)	-0.017
InChI=1S/C7H6N4S/c1-12-7-10-4-5-6(11-7)9-3-2-8-5/h2-4H,1H3	-1.756
InChI=1S/C7H5ClO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)	-3.31
InChI=1S/C10H18ClN5/c1-5-16(6-2)10-14-8(11)13-9(15-10)12-7(3)4/h7H,5-6H2,1-4H3,(H,12,13,14,15)	-3.785
InChI=1S/C7H5NO4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)	-1.746
InChI=1S/C12H8Cl6O/c13-8-9(14)11(16)5-3-1-2(6-7(3)19-6)4(5)10(8,15)12(11,17)18/h2-7H,1H2	-6.291
InChI=1S/C10H19N5O/c1-6(2)11-8-13-9(12-7(3)4)15-10(14-8)16-5/h6-7H,1-5H3,(H2,11,12,13,14,15)	-2.56
InChI=1S/C3H7Br/c1-2-3-4/h2-3H2,1H3	-1.711
InChI=1S/C6H12O/c1-3-5-6(7)4-2/h4,6-7H,2-3,5H2,1H3	-0.599
InChI=1S/C10H14Cl6N4O2/c11-9(12,13)7(17-5-21)19-1-2-20(4-3-19)8(18-6-22)10(14,15)16/h5-8H,1-4H2,(H,17,21)(H,18,22)	-4.16
InChI=1S/C7H16/c1-5-7(3,4)6-2/h5-6H2,1-4H3	-4.229
InChI=1S/C41H64O13/c1-20-36(46)29(42)16-34(49-20)53-38-22(3)51-35(18-31(38)44)54-37h14,20-22,24-31,33-38,42-44,46-47H,6-13,15-19H2,1-5H3	-5.293
InChI=1S/C18H18O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h2-5,10,16,19H,6-9H2,1H3	-4.96
InChI=1S/C7H7NO2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3	-2.46

"InChi"	"logS(M)"
InChI=1S/C33H47NO13/ c1-18-10-8-6-4-3-5-7-9-11-21(45-32-30(39)28(34)29(38)19(2)44-32)1 h3-9,11-13,18-25,27-30,32,35-36,38-39,42H,10,14-17,34H2,1-2H3, (H,40,41)/b4-3-,7-5-,8-6-,11-9-,13-12-	-2.21
InChI=1S/C21H28O5/ c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2)1 h5,7,9,14-16,18,22,24,26H,3-4,6,8,10-11H2,1-2H3	-3.178
InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H	-1.642
InChI=1S/C10H19O7PS/ c1-5-16-9(11)7-8(10(12)17-6-2)19-18(13,14-3)15-4/h8H, 5-7H2,1-4H3	-1.622
InChI=1S/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3	-1.28
InChI=1S/C5H12O/c1-3-5(2)4-6/h5-6H,3-4H2,1-2H3	-0.468
InChI=1S/C14H21N3O3/ c1-9(2)15-7-12-4-3-10-5-11(8-18)14(17(19)20)6-13(10)16-12/ h5-6,9,12,15-16,18H,3-4,7-8H2,1-2H3	-2.97
InChI=1S/C7H6Cl2O/c8-6-2-1-3-7(9)5(6)4-10/h1-3,10H,4H2	-2.102
InChI=1S/C24H38O4/ c1-5-9-13-19(7-3)17-27-23(25)21-15-11-12-16-22(21)24(26)28-18-20(h11-12,15-16,19-20H,5-10,13-14,17-18H2,1-4H3	-6.979
InChI=1S/C4H5NO2/c6-3-1-2-4(7)5-3/h1-2H2,(H,5,6,7)	0.39
InChI=1S/C6H14O/c1-3-6(2)4-5-7/h6-7H,3-5H2,1-2H3	-0.72
InChI=1S/C10H14/c1-7-5-9(3)10(4)6-8(7)2/h5-6H,1-4H3	-3.84
InChI=1S/C16H14N2O/ c1-11-7-3-6-10-15(11)18-12(2)17-14-9-5-4-8-13(14)16(18)19/ h3-10H,1-2H3	-2.92
InChI=1S/C15H10Cl2N2O2/ c16-8-5-6-12-10(7-8)13(19-15(21)14(20)18-12)9-3-1-2-4-11(9)17/ h1-7,15,21H,(H,18,20)	-3.604
InChI=1S/C15H13NO2S/ c1-16-11-4-2-3-5-13(11)19-14-7-6-10(8-12(14)16)9-15(17)18/h2-8H, 9H2,1H3,(H,17,18)	-3.942
InChI=1S/C5H4O2S/c6-5(7)4-2-1-3-8-4/h1-3H,(H,6,7)	-1.233
InChI=1S/C7H16O/c1-6(2)5-7(3,4)8/h6,8H,5H2,1-4H3	-0.931
InChI=1S/C11H15NO5/ c1-15-9-4-2-3-5-10(9)16-6-8(13)7-17-11(12)14/h2-5,8,13H, 6-7H2,1H3,(H2,12,14)	-1.525
InChI=1S/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3,5-8H,1,4H2,2H3	-2.921
InChI=1S/C30H23BrO4/ c31-23-16-14-20(15-17-23)19-10-12-22(13-11-19)26(32)18-25(21-6-2 h1-17,25-26,32-33H,18H2	-4.45
InChI=1S/C6H4ClNO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H	-2.564
InChI=1S/C4H8Cl2OS/c5-1-3-8(7)4-2-6/h1-4H2/p+1	-1.164
InChI=1S/C8H18O/c1-4-5-6-7(2)8(3)9/h7-9H,4-6H2,1-3H3	-2.058
InChI=1S/C8H18O/c1-6-8(5,9)7(2,3)4/h9H,6H2,1-5H3	-1.271
InChI=1S/C2H7NO3S/c3-1-2-7(4,5)6/h1-3H2,(H,4,5,6)	-0.191
InChI=1S/C9H11ClN2O/c1-12(2)9(13)11-8-5-3-7(10)4-6-8/h3-6H, 1-2H3,(H,11,13)	-2.89
InChI=1S/C5H10O/c1-2-3-4-5-6/h2,6H,1,3-5H2	-0.179
InChI=1S/C9H10/c1-2-5-9-7-3-6-8(9)4-1/h1-2,4-5H,3,6-7H2	-3.035

"InChi"	"logS(M)"
InChI=1S/C4H3FN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9)	-1.069
InChI=1S/C6H14O2/c1-4-7-6(3)8-5-2/h6H,4-5H2,1-3H3	-0.429
InChI=1S/C6H12O2/c1-3-5(4-2)6(7)8/h5H,3-4H2,1-2H3,(H,7,8)	-0.81
InChI=1S/C11H12N4O2S/c1-8-6-13-11(14-7-8)15-18(16,17)10-4-2-9(12)3-5-10/h2-7H,12H2,1H3,(H,13,14,15)	-2.82
InChI=1S/C5H10O/c1-3-5(6)4-2/h3-4H2,1-2H3	-0.253
InChI=1S/C8H4O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-4H	-1.364
InChI=1S/C15H12/c1-11-5-4-8-15-13(11)10-9-12-6-2-3-7-14(12)15/h2-10H,1H3	-5.854
InChI=1S/C6H3Cl4N/c7-5-3-1-2-4(11-5)6(8,9)10/h1-3H	-3.506
InChI=1S/C21H30O3/c1-20-9-7-14(23)11-13(20)3-4-15-16-5-6-18(19(24)12-22)21(16,2)10-h11,15-18,22H,3-10,12H2,1-2H3	-3.745
InChI=1S/C8H18O/c1-3-4-5-6-7-8(2)9/h8-9H,3-7H2,1-2H3	-2.066
InChI=1S/C9H10O3/c1-11-8-5-3-7(4-6-8)9(10)12-2/h3-6H,1-2H3	-2.34
InChI=1S/C6H3N3O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H	-2.885
InChI=1S/C7H4ClNS/c8-6-2-1-3-7(4-6)9-5-10/h1-4H	-3.951
InChI=1S/C17H27NO4/c1-17(2,3)18-9-12(19)10-22-16-6-4-5-11-7-14(20)15(21)8-13(11)16/h4-6,12,14-15,18-21H,7-10H2,1-3H3	-1.57
InChI=1S/C12H6Cl3NO3/c13-7-8(16-12(19)11(14)15)10(18)6-4-2-1-3-5(6)9(7)17/h1-4,11H,(H,16,19)	-5.026
InChI=1S/C5H11NO/c1-6-2-4-7-5-3-6/h2-5H2,1H3	0.995
InChI=1S/C6H15N/c1-3-5-7-6-4-2/h7H,3-6H2,1-2H3	-0.461
InChI=1S/C11H15NO3/c1-8(2)14-9-6-4-5-7-10(9)15-11(13)12-3/h4-8H,1-3H3,(H,12,13)	-2.051
InChI=1S/C16H16N2O6S2/c1-8(19)24-6-9-7-26-15-12(14(21)18(15)13(9)16(22)23)17-11(20)5-10h2-4,12,15H,5-7H2,1H3,(H,17,20)(H,22,23)	-2.94
InChI=1S/C6H8N2/c7-5-3-1-2-4-6(5)8/h1-4H,7-8H2	-0.44
InChI=1S/C9H13N3O2/c1-6(2)5-12-7(10)4-8(13)11(3)9(12)14/h4H,1,5,10H2,2-3H3	-0.99
InChI=1S/C5H5N3O/c6-5(9)4-3-7-1-2-8-4/h1-3H,(H2,6,9)	-0.667
InChI=1S/C9H8Cl2O3/c1-5(9(12)13)14-8-3-2-6(10)4-7(8)11/h2-5H,1H3,(H,12,13)	-2.6
InChI=1S/C10H14O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9H,1,5-6H2,2-3H3	-1.903
InChI=1S/C9H16ClN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h8H,1-7H2,(H,11,14)	-3.37
InChI=1S/C8H17Br/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3	-5.063
InChI=1S/C23H30N2O4/c1-24-7-6-23-16-3-4-18(26)22(23)29-21-19(5-2-15(20(21)23)14-17(16h2-5,16-18,22,26H,6-14H2,1H3	-1.299
InChI=1S/C12H6Cl4/c13-9-5-1-3-7(11(9)15)8-4-2-6-10(14)12(8)16/h1-6H	-7.272

"InChi"	"logS(M)"
InChI=1S/C12H10Cl2F3NO/c13-5-7-6-18(11(19)10(7)14)9-3-1-2-8(4-9)12(15,16)17/h1-4,7,10H,5-6H2	-4.05
InChI=1S/C6H5ClO/c7-5-2-1-3-6(8)4-5/h1-4,8H	-0.71
InChI=1S/C12H5Cl5/c13-7-4-2-1-3-6(7)10-8(14)5-9(15)11(16)12(10)17/h1-5H	-7.435
InChI=1S/C7H4I2O3/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2,10H,(H,11,12)	-3.307
InChI=1S/C14H12O2/c15-14(16)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H,(H,15,16)	-3.223
InChI=1S/C7H8N2S/c8-7(10)9-6-4-2-1-3-5-6/h1-5H,(H3,8,9,10)	-1.79
InChI=1S/C14H9ClF2N2O2/c15-8-4-6-9(7-5-8)18-14(21)19-13(20)12-10(16)2-1-3-11(12)17/h1-7H,(H2,18,19,20,21)	-6.54
InChI=1S/C7H6F3N/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4H,11H2	-1.508
InChI=1S/C7H12O/c1-6-3-2-4-7(8)5-6/h6H,2-5H2,1H3	-1.874
InChI=1S/C10H8O2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1-6,11-12H	-2.92
InChI=1S/C6H12O/c1-5(7)6(2,3)4/h1-4H3	-0.722
InChI=1S/C7H16FO2P/c1-6(7(2,3)4)10-11(5,8)9/h6H,1-5H3	-0.938
InChI=1S/C5H10/c1-3-5-4-2/h3H,1,4-5H2,2H3	-2.676
InChI=1S/C10H12N2O3/c1-3-5-10(6-4-2)7(13)11-9(15)12-8(10)14/h3-4H,1-2,5-6H2,(H2,11,12,13,14,15)	-2.061
InChI=1S/C7H16O/c1-3-4-5-6-7(2)8/h7-8H,3-6H2,1-2H3	-1.551
InChI=1S/C4H10S/c1-2-3-4-5/h5H,2-4H2,1H3	-2.179
InChI=1S/C6H12O2/c1-5(2)4-8-6(3)7/h5H,4H2,1-3H3	-1.266
InChI=1S/C4H11NO2/c6-3-1-5-2-4-7/h5-7H,1-4H2	0.958
InChI=1S/C11H10Cl2N2O/c12-8-1-2-9(10(13)5-8)11(16)6-15-4-3-14-7-15/h1-5,7,11,16H,6H2	-3.264
InChI=1S/C11H9Cl2NO2/c12-6-1-2-7-16-11(15)14-10-5-3-4-9(13)8-10/h3-5,8H,6-7H2,(H,14,15)	-4.24
InChI=1S/C6H12N2S4/c1-7(2)5(9)11-12-6(10)8(3)4/h1-4H3	-4.116
InChI=1S/C8H9ClNO5PS/c1-13-16(17,14-2)15-8-4-3-6(10(11)12)5-7(8)9/h3-5H,1-2H3	-4.68
InChI=1S/C2HCl3O2/c3-2(4,5)1(6)7/h(H,6,7)	0.519
InChI=1S/C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3	-0.138
InChI=1S/C9H7N3S/c1-6-3-2-4-7-8(6)12-5-10-11-9(12)13-7/h2-5H,1H3	-2.073
InChI=1S/C13H19NO2S/c1-14(2)13(15)17-11-7-6-10-16-12-8-4-3-5-9-12/h3-5,8-9H,6-7,10-11H2,1-2H3	-3.927
InChI=1S/C3H5Cl/c1-2-3-4/h2H,1,3H2	-1.356
InChI=1S/C6H14O/c1-4-5(2)6(3)7/h5-7H,4H2,1-3H3	-0.722
InChI=1S/C2H2Cl4/c3-1-2(4,5)6/h1H2	-2.196
InChI=1S/C9H20O/c1-3-4-5-6-7-8-9(2)10/h9-10H,3-8H2,1-2H3	-2.744
InChI=1S/C19H12O6/c20-16-10-5-1-3-7-14(10)24-18(22)12(16)9-13-17(21)11-6-2-4-8-15(11)8-21H,9H2	-4.27

"InChi"	"logS(M)"
InChI=1S/C10H11N3/c1-8-7-10(11)13(12-8)9-5-3-2-4-6-9/h2-7H,11H2,1H3	-0.938
InChI=1S/C12H8/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-8H	-3.976
InChI=1S/C18H14/c1-3-7-15(8-4-1)17-11-13-18(14-12-17)16-9-5-2-6-10-16/h1-14H	-6.183
InChI=1S/C9H11NO/c1-8(11)10(2)9-6-4-3-5-7-9/h3-7H,1-2H3	-0.951
InChI=1S/C3H5Br/c1-2-3-4/h2H,1,3H2	-1.5
InChI=1S/C6H2Cl4O/c7-2-1-3(8)5(10)6(11)4(2)9/h1,11H	-3.37
InChI=1S/C10H19N5S/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,12,13,14,15)	-3.985
InChI=1S/C15H13N3O4S/c1-18-13(15(20)17-12-8-4-5-9-16-12)14(19)10-6-2-3-7-11(10)23(18,22)9,19H,1H3,(H,16,17,20)	-4.5
InChI=1S/C12H10N2/c1-3-7-11(8-4-1)13-14-12-9-5-2-6-10-12/h1-10H/b14-13+	-4.454
InChI=1S/C21H22N2O4/c1-2-3-14-18(24)27-15-23-19(25)21(22-20(23)26,16-10-6-4-7-11-16)14H,2-3,14-15H2,1H3,(H,22,26)	-4.68
InChI=1S/C4H8Cl2O2S/c5-1-3-9(7,8)4-2-6/h1-4H2	-1.503
InChI=1S/C8H8O3/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3,(H,9,10)	-2.458
InChI=1S/C6H5NO3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H	-1.803
InChI=1S/C5H8N2/c1-4-3-5(2)7-6-4/h3H,1-2H3,(H,6,7)	-0.52
InChI=1S/C17H13ClN4/c1-11-20-21-16-10-19-17(12-5-3-2-4-6-12)14-9-13(18)7-8-15(14)22(1)h2-9H,10H2,1H3	-3.6
InChI=1S/C8H8N2O3/c1-6(11)9-7-4-2-3-5-8(7)10(12)13/h2-5H,1H3,(H,9,11)	-1.909
InChI=1S/C4H9NO2/c1-3(5)2-4(6)7/h3H,2,5H2,1H3,(H,6,7)	0.987
InChI=1S/C22H30N2O2S/c1-3-21(25)24(19-8-5-4-6-9-19)22(18-26-2)12-15-23(16-13-22)14-11-h4-10,17H,3,11-16,18H2,1-2H3	-3.706
InChI=1S/C16H13F2N3O/c17-13-7-5-12(6-8-13)16(22,9-21-11-19-10-20-21)14-3-1-2-4-15(14)1h1-8,10-11,22H,9H2	-3.365
InChI=1S/C6H7N/c7-6-4-2-1-3-5-6/h1-5H,7H2	-0.425
InChI=1S/C2H3N3/c1-3-2-5-4-1/h1-2H,(H,3,4,5)	1.006
InChI=1S/C12H3Cl7/c13-4-1-2-6(14)5(3-4)7-8(15)10(17)12(19)11(18)9(7)16/h1-3H	-8.46
InChI=1S/C2H2O4/c3-1(4)2(5)6/h(H,3,4)(H,5,6)	0.079
InChI=1S/C10H7I/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H	-4.55
InChI=1S/C10H16Cl3NOS/c1-6(2)14(7(3)4)10(15)16-5-8(11)9(12)13/h6-7H,5H2,1-4H3	-4.882
InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)	1.002
InChI=1S/C5H10O/c1-2-4-6-5-3-1/h1-5H2	-0.031
InChI=1S/C7H8O/c1-6-4-2-3-5-7(6)8/h2-5,8H,1H3	-0.619
InChI=1S/C13H19N3O5S2/c1-8-10(12(19)16-13(20)14-8)3-4-11(18)15-9(5-17)6-23(21)7-22-2/h3-4,9,17H,5-7H2,1-2H3,(H,15,18)(H2,14,16,19,20)/p+1/b4-3+	-1.981

"InChi"	"logS(M)"
InChI=1S/C15H18N4O5/c1-5-9(16)12(21)8-6(4-24-14(17)22)15(23-2)13-7(18-13)3-19(15)10(8)6-7,13,18H,3-4,16H2,1-2H3,(H2,17,22)	-2.56
InChI=1S/C11H12N2O2/c14-9-5-6-13-10(9)12-8-4-2-1-3-7(8)11(13)15/h1-4,9,11,14-15H,5-6H2	-2.07
InChI=1S/C7H17O2PS3/c1-4-8-10(11,9-5-2)13-7-12-6-3/h4-7H2,1-3H3	-3.717
InChI=1S/C8H10O2/c1-9-7-3-5-8(10-2)6-4-7/h3-6H,1-2H3	-2.246
InChI=1S/C10H16O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7H,4-6H2,1-3H3	-1.978
InChI=1S/C6H4BrF/c7-5-2-1-3-6(8)4-5/h1-4H	-2.666
InChI=1S/C13H24N4O3S/c1-6-8-9-11-10(3)15-13(14-7-2)16-12(11)20-21(18,19)17(4)5/h6-9H2,1-5H3,(H,14,15,16)	-4.158
InChI=1S/C9H16ClN5/c1-4-11-8-12-7(10)13-9(14-8)15(5-2)6-3/h4-6H2,1-3H3,(H,11,12,13,14)	-4.06
InChI=1S/C7H15Cl2N2O2P/c8-2-5-11(6-3-9)14(12)10-4-1-7-13-14/h1-7H2,(H,10,12)	-0.815
InChI=1S/C3H6N2S/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)	-0.708
InChI=1S/C16H22O4/c1-3-5-11-19-15(17)13-9-7-8-10-14(13)16(18)20-12-6-4-2/h7-10H,3-6,11-12H2,1-2H3	-4.388
InChI=1S/C15H23N3O3S/c1-15(2)11(14(20)21)18-12(19)10(13(18)22-15)16-9-17-7-5-3-4-6-8-17h9-11,13H,3-8H2,1-2H3,(H,20,21)/b16-9+	-4.5
InChI=1S/C20H23N/c1-21(2)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(17)20/h3-6,8-12H,7,13-15H2,1-2H3	-4.55
InChI=1S/C6H8N4O3S/c1-2-7-5(11)9-6-8-3-4(14-6)10(12)13/h3H,2H2,1H3,(H2,7,8,9,11)	-2.858
InChI=1S/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h12-16,20H,3-11H2,1-2H3	-4.158
InChI=1S/C14H13N3O2/c1-8-3-4-11-12(5-8)19-13-10(14(18)17(11)2)6-9(15)7-16-13/h3-7H,15H2,1-2H3	-3.043
InChI=1S/C6H4Cl2O/c7-4-1-5(8)3-6(9)2-4/h1-3,9H	-1.559
InChI=1S/C14H10Cl2O3/c15-10-5-6-13(11(16)8-10)19-12-4-2-1-3-9(12)7-14(17)18/h1-6,8H,7H2,(H,17,18)	-4.86
InChI=1S/C8H15NO2/c1-7(2)8(10)11-6-5-9(3)4/h1,5-6H2,2-4H3	0.502
InChI=1S/C9H12O/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,10H,4,7-8H2	-1.38
InChI=1S/C10H5Cl7O/c11-3-1-2(4-5(3)18-4)9(15)7(13)6(12)8(1,14)10(9,16)17/h1-5H	-6.289
InChI=1S/C5H6N2OS/c1-3-2-4(8)7-5(9)6-3/h2H,1H3,(H2,6,7,8,9)	-2.426
InChI=1S/C6H14FO3P/c1-5(2)9-11(7,8)10-6(3)4/h5-6H,1-4H3	-1.078
InChI=1S/C10H12O5/c1-2-3-15-10(14)6-4-7(11)9(13)8(12)5-6/h4-5,11-13H,2-3H2,1H3	-1.783
InChI=1S/C8H16/c1-7-4-5-8(2,3)6-7/h7H,4-6H2,1-3H3	-4.478

"InChi"	"logS(M)"
InChI=1S/C18H36O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-17H2,1H3,(H,19,20)	-4.98
InChI=1S/CH2BrCl/c2-1-3/h1H2	-0.889
InChI=1S/C10H14N2O/c1-3-12(4-2)10(13)9-6-5-7-11-8-9/h5-8H,3-4H2,1-2H3	0.749
InChI=1S/C14H21NO2/c1-2-3-4-5-6-11-17-14(16)12-7-9-13(15)10-8-12/h7-10H,2-6,11,15H2,1H3	-4.6
InChI=1S/C8H10N4O2/c1-4-9-5-6(10-4)11(2)8(14)12(3)7(5)13/h1-3H3,(H,9,10)	-0.728
InChI=1S/C26H43NO6/c1-14(4-7-22(31)27-13-23(32)33)17-5-6-18-24-19(12-21(30)26(17,18)h14-21,24,28-30H,4-13H2,1-3H3,(H,27,31)(H,32,33)	-5.149
InChI=1S/C27H38O3/c1-4-6-7-8-9-25(29)30-27(5-2)17-15-24-23-12-10-19-18-20(28)11-13-h2,18,21-24H,4,6-17H2,1,3H3	-6.89
InChI=1S/C3H7NO2/c1-3(2)4(5)6/h3H,1-2H3	-0.615
InChI=1S/C4H4N2/c1-2-5-4-6-3-1/h1-4H	1.096
InChI=1S/C12H12/c1-9-3-5-12-8-10(2)4-6-11(12)7-9/h3-8H,1-2H3	-4.893
InChI=1S/C10H12N2O5/c1-3-6(2)8-4-7(11(14)15)5-9(10(8)13)12(16)17/h4-6,13H,3H2,1-2H3	-3.665
InChI=1S/C10H18O/c1-5-10(4,11)8-6-7-9(2)3/h5,7,11H,1,6,8H2,2-4H3	-1.987
InChI=1S/C13H10N2O2/c1-15-10-6-2-3-7-11(10)17-12-9(13(15)16)5-4-8-14-12/h2-8H,1H3	-3.672
InChI=1S/C6H7NO/c7-5-3-1-2-4-6(5)8/h1-4,8H,7H2	-0.737
InChI=1S/C9H18N2O4/c1-3-4-9(2,5-14-7(10)12)6-15-8(11)13/h3-6H2,1-2H3,(H2,10,12)(H2,11,13)	-1.74
InChI=1S/C8H10N2O3S/c1-6(11)10-14(12,13)8-4-2-7(9)3-5-8/h2-5H,9H2,1H3,(H,10,11)	-1.41
InChI=1S/C7H9N3O/c8-10-7(11)9-6-4-2-1-3-5-6/h1-5H,8H2,(H2,9,10,11)	-2.33
InChI=1S/C10H10N4O2S/c11-8-2-4-9(5-3-8)17(15,16)14-10-12-6-1-7-13-10/h1-7H,11H2,(H,12,13,14)	-2.16
InChI=1S/C9H9I2NO3/c10-5-1-4(2-6(11)8(5)13)3-7(12)9(14)15/h1-2,7,13H,3,12H2,(H,14,15)	-2.858
InChI=1S/C9H20/c1-8(2)6-7-9(3,4)5/h8H,6-7H2,1-5H3	-5.047
InChI=1S/C5H10O/c1-5-3-2-4-6-5/h5H,2-4H2,1H3	0.207
InChI=1S/C4H5NO2/c1-3-2-4(6)5-7-3/h2H,1H3,(H,5,6)	-0.067
InChI=1S/C9H5ClN4/c10-7-1-3-8(4-2-7)13-14-9(5-11)6-12/h1-4,13H	-4.36
InChI=1S/C19H21ClN2O/c20-16-12-10-15(11-13-16)14-22(18-8-4-5-9-18)19(23)21-17-6-2-1-3-h1-3,6-7,10-13,18H,4-5,8-9,14H2,(H,21,23)	-5.915
InChI=1S/C10H15NO2/c12-8-6-11(7-9-13)10-4-2-1-3-5-10/h1-5,12-13H,6-9H2	-0.583
InChI=1S/C7H5IO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)	-3.963
InChI=1S/C12H10/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-6H,7-8H2	-4.63

"InChi"	"logS(M)"
InChI=1S/C13H14N2O3/c1-8(16)15-12(13(17)18)6-9-7-14-11-5-3-2-4-10(9)11/h2-5,7,12,14H,6H2,1H3,(H,15,16)(H,17,18)	-2.31
InChI=1S/C6H14/c1-5(2)6(3)4/h5-6H,1-4H3	-3.583
InChI=1S/C14H21N3O3/c1-14(2,3)16-13(19)20-11-8-6-7-10(9-11)15-12(18)17(4)5/h6-9H,1-5H3,(H,15,18)(H,16,19)	-2.934
InChI=1S/C15H14N2O2/c1-9-3-5-13-11(7-9)15(18)17(2)12-8-10(16)4-6-14(12)19-13/h3-8H,16H2,1-2H3	-3.928
InChI=1S/C8H9NO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,9H2,1H3	-1.606
InChI=1S/C14H20O3/c1-2-3-4-5-6-11-17-14(16)12-7-9-13(15)10-8-12/h7-10,15H,2-6,11H2,1H3	-4.072
InChI=1S/C14H28O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14(15)16/h2-13H2,1H3,(H,15,16)	-5.329
InChI=1S/C10H20O2/c1-2-3-4-5-6-7-8-9-10(11)12/h2-9H2,1H3,(H,11,12)	-3.445
InChI=1S/C7H6N4/c1-5-2-9-6-3-8-4-10-7(6)11-5/h2-4H,1H3	-0.01
InChI=1S/C19H24O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17(1h9,13-14,17H,3-8,10H2,1-2H3	-3.484
InChI=1S/C6H7N3O/c7-9-6(10)5-1-3-8-4-2-5/h1-4H,7H2,(H,9,10)	-0.04
InChI=1S/C11H7NS/c13-8-12-11-7-3-5-9-4-1-2-6-10(9)11/h1-7H	-4.602
InChI=1S/C8H11N5O3/c9-8-11-6-5(7(15)12-8)10-3-13(6)4-16-2-1-14/h3,14H,1-2,4H2,(H3,9,11,12,15)	-2.12
InChI=1S/C8H9NO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,9H2,1H3	-1.597
InChI=1S/C7H16O/c1-6(2)4-7(3)5-8/h6-8H,4-5H2,1-3H3	-1.601
InChI=1S/C8H14ClNS2/c1-4-10(5-2)8(11)12-6-7(3)9/h3-6H2,1-2H3	-3.39
InChI=1S/C8H16/c1-2-8-6-4-3-5-7-8/h8H,2-7H2,1H3	-4.251
InChI=1S/C20H24O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(18,h1,5,7,12,16-18,21-22H,4,6,8-11H2,2H3	-4.419
InChI=1S/C41H64O14/c1-19-36(47)28(42)15-34(50-19)54-38-21(3)52-35(17-30(38)44)55-37h12,19-21,23-31,33-38,42-45,47-48H,6-11,13-18H2,1-5H3	-4.081
InChI=1S/C7H12/c1-3-5-7-6-4-2/h1H,4-7H2,2H3	-3.01
InChI=1S/C12H12/c1-2-10-7-5-8-11-6-3-4-9-12(10)11/h3-9H,2H2,1H3	-4.164
InChI=1S/C5H5N5/c6-4-3-5(9-1-7-3)10-2-8-4/h1-2H,(H3,6,7,8,9,10)	-2.118
InChI=1S/C24H12/c1-2-14-5-6-16-9-11-18-12-10-17-8-7-15-4-3-13(1)19-20(14)22(16)24h1-12H	-8.83
InChI=1S/C8H10O/c1-6-3-4-8(9)5-7(6)2/h3-5,9H,1-2H3	-1.38
InChI=1S/C11H14N2O2/c1-8(14)12-11(13-9(2)15)10-6-4-3-5-7-10/h3-7,11H,1-2H3,(H,12,14)(H,13,15)	-1.314
InChI=1S/C7H5N3O6/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10(15)16/h2-3H,1H3	-3.242
InChI=1S/C7H14/c1-2-4-6-7-5-3-1/h1-7H2	-3.515

"InChi"	"logS(M)"
InChI=1S/C13H12N2O3/c1-2-8-13(9-6-4-3-5-7-9)10(16)14-12(18)15-11(13)17/h2-7H,1,8H2,(H2,14,15,16,17,18)	-2.18
InChI=1S/C12H4Cl6/c13-7-3-1-2-5(9(7)15)6-4-8(14)11(17)12(18)10(6)16/h1-4H	-8.421
InChI=1S/C16H20O6P2S3/c1-17-23(25,18-2)21-13-5-9-15(10-6-13)27-16-11-7-14(8-12-16)22-24(26,19-3)20-4/h5-12H,1-4H3	-6.237
InChI=1S/C14H14/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-10H,11-12H2	-4.627
InChI=1S/C6H4BrI/c7-5-1-3-6(8)4-2-5/h1-4H	-4.452
InChI=1S/C3H8N4O2/c4-6-2(8)1-3(9)7-5/h1,4-5H2,(H,6,8)(H,7,9)	-0.121
InChI=1S/C10H13NO2/c1-7-4-8(2)6-9(5-7)13-10(12)11-3/h4-6H,1-3H3,(H,11,12)	-2.581
InChI=1S/C12H11FN2O3/c1-18-9-4-2-8(3-5-9)6-15-7-10(13)11(16)14-12(15)17/h2-5,7H,6H2,1H3,(H,14,16,17)	-2.75
InChI=1S/C22H23NO3/c1-21(2)19(22(21,3)4)20(24)26-18(14-23)15-9-8-12-17(13-15)25-16-10-6-5-11-18/h5-13,18-19H,1-4H3	-6.025
InChI=1S/C22H16O8/c1-2-28-20(25)15(16-18(23)11-7-3-5-9-13(11)29-21(16)26)17-19(24)12-8-4-6-10-14(12)30-22(17)27/h3-10,15,23-24H,2H2,1H3	-3.66
InChI=1S/C7H7NO3/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3	-2.414
InChI=1S/C6H3Cl3N2O2/c7-1-3(10)2(8)5(9)11-4(1)6(12)13/h(H2,10,11)(H,12,13)	-2.749
InChI=1S/C4H7NO2S/c6-4(7)3-1-8-2-5-3/h3,5H,1-2H2,(H,6,7)	0.354
InChI=1S/C14H17ClN2O3S/c15-12-6-9-8-17(10-4-2-1-3-5-10)14(18)11(9)7-13(12)21(16,19)20/h6-7,10H,1-5,8H2,(H2,16,19,20)	-4.313
InChI=1S/C24H36O5/c1-5-15(3)24(27)29-21-11-14(2)10-17-7-6-16(4)20(23(17)21)9-8-19-12-18(25)13-22(26)28-19/h6-7,10,14-16,18-21,23,25H,5,8-9,11-13H2,1-4H3	-6.01
InChI=1S/C5H10N2S2/c1-6-3-7(2)5(8)9-4-6/h3-4H2,1-2H3	-1.733
InChI=1S/C12H6Cl4/c13-7-4-5-9(14)8(6-7)12-10(15)2-1-3-11(12)16/h1-6H	-6.8
InChI=1S/C5H11Cl/c1-3-5(6)4-2/h5H,3-4H2,1-2H3	-2.631
InChI=1S/C6H4Cl2/c7-5-2-1-3-6(8)4-5/h1-4H	-3.072
InChI=1S/C20H29N5O6/c1-20(2,27)11-31-19(26)25-8-6-24(7-9-25)18-22-14-12(17(21)23-18)10-27H,6-9,11H2,1-5H3,(H2,21,22,23)	-3.64
InChI=1S/C8H8O4/c1-12-7-4-5(8(10)11)2-3-6(7)9/h2-4,9H,1H3,(H,10,11)	-2.05
InChI=1S/C9H5Br2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H	-4.194
InChI=1S/C12H12N2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H,13-14H2	-3.094
InChI=1S/C9H11IN2O5/c10-4-2-12(9(16)11-8(4)15)7-1-5(14)6(3-13)17-7/h2,5-7,13-14H,1,3H2,(H,11,15,16)	-2.248
InChI=1S/C2H6OS/c1-4(2)3/h1-2H3/p+1	1.107

"InChi"	"logS(M)"
InChI=1S/C22H28F2O5/ c1-11-6-13-14-8-16(23)15-7-12(26)4-5-19(15,2)21(14,24)17(27)9-20(h4-5,7,11,13-14,16-17,25,27,29H,6,8-10H2,1-3H3	-5.613
InChI=1S/C6H11Br/c7-6-4-2-1-3-5-6/h6H,1-5H2	-2.294
InChI=1S/C19H14/ c1-13-12-15-7-3-4-8-16(15)18-11-10-14-6-2-5-9-17(14)19(13)18/ h2-12H,1H3	-6.592
InChI=1S/C16H14/ c1-2-12-7-8-15-10-13-5-3-4-6-14(13)11-16(15)9-12/h3-11H,2H2,1H3	-6.886
InChI=1S/C10H24N2O2/c1-3-9(7-13)11-5-6-12-10(4-2)8-14/h9-14H, 3-8H2,1-2H3	0.57
InChI=1S/C3H6BrCl/c4-2-1-3-5/h1-3H2	-1.94
InChI=1S/C10H11N3O3S/ c1-7-6-10(12-16-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2,1H3, (H,12,13)	-2.618
InChI=1S/C15H22N2O/ c1-11-7-6-8-12(2)14(11)16-15(18)13-9-4-5-10-17(13)3/h6-8,13H, 4-5,9-10H2,1-3H3,(H,16,18)	-1.99
InChI=1S/C7H16O/c1-5(2)7(8)6(3)4/h5-8H,1-4H3	-1.22
InChI=1S/C18H25NO/ c1-19-10-9-18-8-4-3-5-15(18)17(19)11-13-6-7-14(20-2)12-16(13)18/ h6-7,12,15,17H,3-5,8-11H2,1-2H3	-3.48
InChI=1S/C11H15NO2/c1-8(2)7-14-11(13)9-3-5-10(12)6-4-9/ h3-6,8H,7,12H2,1-2H3	-2.944
InChI=1S/C12H5Cl5/ c13-8-3-1-2-6(10(8)15)7-4-5-9(14)12(17)11(7)16/h1-5H	-7.05
InChI=1S/C8H14O2/c1-6(2)7(9)10-8(3,4)5/h1H2,2-5H3	-2.486
InChI=1S/C14H12O2/ c15-14(16)10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-9H,10H2,(H, 15,16)	-3.73
InChI=1S/C16H12O6/ c17-10-2-1-8-13-9-4-12(19)11(18)3-7(9)5-16(13,21)6-22-15(8)14(10)2 h1-4,17,19-21H,5-6H2	-2.699
InChI=1S/C11H11N/c1-8-3-5-10-6-4-9(2)12-11(10)7-8/h3-7H,1-2H3	-1.942
InChI=1S/C4H8Cl2/c1-3(5)4(2)6/h3-4H,1-2H3	-2.354
InChI=1S/C7H3Br2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H	-3.328
InChI=1S/C5H12O/c1-3-4-5-6-2/h3-5H2,1-2H3	-0.991
InChI=1S/C2H4Cl2/c1-2(3)4/h2H,1H3	-1.291
InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2	-2.555
InChI=1S/C12H18N2O3/ c1-4-6-8(3)12(7-5-2)9(15)13-11(17)14-10(12)16/h5,8H, 2,4,6-7H2,1,3H3,(H2,13,14,15,16,17)	-2.36
InChI=1S/C23H26N2O4/ c1-2-3-4-11-16-20(26)29-17-25-21(27)23(24-22(25)28,18-12-7-5-8-13 h5-10,12-15H,2-4,11,16-17H2,1H3,(H,24,28)	-6.301
InChI=1S/C20H35NO13/ c22-3-6-1-8(12(26)15(29)11(6)25)21-9-2-7(4-23)19(17(31)13(9)27)34 h1,7-32H,2-5H2	0.303
InChI=1S/C23H28ClN3O5S/ c1-32-21-12-9-17(24)15-20(21)22(28)25-14-13-16-7-10-19(11-8-16)33 h7-12,15,18H,2-6,13-14H2,1H3,(H,25,28)(H2,26,27,29)	-5.092

"InChi"	"logS(M)"
InChI=1S/C6H6N2O2/c9-6(10)2-1-5-3-7-4-8-5/h1-4H,(H,7,8)(H,9,10)/b2-1+	-1.964
InChI=1S/C20H30O4/c1-3-5-7-11-15-23-19(21)17-13-9-10-14-18(17)20(22)24-16-12-8-6-4-h9-10,13-14H,3-8,11-12,15-16H2,1-2H3	-6.144
InChI=1S/C9H15N5O/c10-7-6-8(12-9(11)14(7)15)13-4-2-1-3-5-13/h6,11,15H,1-5,10H2/b11-9+	-1.978
InChI=1S/CH2I2/c2-1-3/h1H2	-2.334
InChI=1S/C12H6Cl4/c13-7-1-3-11(15)9(5-7)10-6-8(14)2-4-12(10)16/h1-6H	-7.04
InChI=1S/C24H40O4/c1-14(4-7-22(27)28)17-5-6-18-16-13-21(26)20-12-15(25)8-10-24(20,3h14-21,25-26H,4-13H2,1-3H3,(H,27,28)	-4.82
InChI=1S/C3H6BrNO4/c4-3(1-6,2-7)5(8)9/h6-7H,1-2H2	0.127
InChI=1S/C10H13ClN2O/c1-7-4-5-8(6-9(7)11)12-10(14)13(2)3/h4-6H,1-3H3,(H,12,14)	-3.483
InChI=1S/C13H12N2O/c1-8-13-11(5-6-14-8)10-4-3-9(16-2)7-12(10)15-13/h3-7,15H,1-2H3	-4.48
InChI=1S/C20H26O3/c1-3-19(22)10-8-16-15-5-4-13-12-14(21)6-11-20(13,23)17(15)7-9-18(h1,12,15-17,22-23H,4-11H2,2H3	-4.57
InChI=1S/C19H20O4/c1-2-3-13-22-18(20)16-11-7-8-12-17(16)19(21)23-14-15-9-5-4-6-10-1h4-12H,2-3,13-14H2,1H3	-5.64
InChI=1S/C9H22O4P2S4/c1-5-10-14(16,11-6-2)18-9-19-15(17,12-7-3)13-8-4/h5-9H2,1-4H3	-5.284
InChI=1S/C12H16N2/c1-2-10(13)7-9-8-14-12-6-4-3-5-11(9)12/h3-6,8,10,14H,2,7,13H2,1H3	-2.57
InChI=1S/C8H11NO2/c9-4-3-6-1-2-7(10)8(11)5-6/h1-2,5,10-11H,3-4,9H2	0.12
InChI=1S/C6H6ClN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2	-1.629
InChI=1S/C8H9NO2/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3,(H2,9,10)	-1.72
InChI=1S/C9H10O4/c1-12-7-5-3-4-6(9(10)11)8(7)13-2/h3-5H,1-2H3,(H,10,11)	-2.14
InChI=1S/C12H4Cl6/c13-7-3-1-5(9(15)11(7)17)6-2-4-8(14)12(18)10(6)16/h1-4H	-8.78
InChI=1S/C8H8ClNO/c1-6(11)10-8-5-3-2-4-7(8)9/h2-5H,1H3,(H,10,11)	-1.4
InChI=1S/C7H7NO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3	-2.515
InChI=1S/C11H14O4/c1-14-10(12)8-6-3-4-7(5-6)9(8)11(13)15-2/h3-4,6-9H,5H2,1-2H3	-1.202
InChI=1S/C2HCl3O/c3-2(4,5)1-6/h1H	-0.691
InChI=1S/C4H3N3O5/c8-2-1(7(11)12)3(9)6-4(10)5-2/h1H,(H2,5,6,8,9,10)	-2.284
InChI=1S/C12H6Cl4/c13-8-2-3-9(11(15)6-8)7-1-4-10(14)12(16)5-7/h1-6H	-6.899
InChI=1S/C5H4N4O/c10-5-3-1-8-9-4(3)6-2-7-5/h1-2H,(H2,6,7,8,9,10)	-2.379
InChI=1S/C5H12O/c1-5(2,3)6-4/h1-4H3	-0.324

"InChi"	"logS(M)"
InChI=1S/C14H9ClO3/c15-8-5-6-10-9-3-1-2-4-11(9)14(18,13(16)17)12(10)7-8/h1-7,18H,(H,16,17)	-4.161
InChI=1S/C7H9NO2S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)	-1.742
InChI=1S/C4H9NO/c1-3-6-4-2-5-1/h5H,1-4H2	1.06
InChI=1S/C3H5N3O3/c4-2(7)1(6-9)3(5)8/h9H,(H2,4,7)(H2,5,8)	-0.038
InChI=1S/C19H14/c1-13-12-19-16-8-3-2-6-14(16)10-11-18(19)17-9-5-4-7-15(13)17/h2-12H,1H3	-6.572
InChI=1S/C4H4N2O/c7-4-1-2-5-3-6-4/h1-3H,(H,5,6,7)	0.586
InChI=1S/C20H12/c1-2-6-15-12-19-17-10-4-8-13-7-3-9-16(20(13)17)18(19)11-14(15)5-1h1-12H	-8.499
InChI=1S/C7H7NO3/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3	-1.957
InChI=1S/C12H18O2/c1-2-3-4-5-6-10-7-8-11(13)9-12(10)14/h7-9,13-14H,2-6H2,1H3	-2.59
InChI=1S/C10H7Br/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H	-4.347
InChI=1S/C12H18N4O6S/c1-3-5-14(6-4-2)12-10(15(17)18)7-9(23(13,21)22)8-11(12)16(19)20/h7-8H,3-6H2,1-2H3,(H2,13,21,22)	-5.13
InChI=1S/C2H5Cl/c1-2-3/h2H2,1H3	-1.051
InChI=1S/C5H4O2/c6-4-5-2-1-3-7-5/h1-4H	-0.096
InChI=1S/C10H14N2O3/c1-4-5-10(6(2)3)7(13)11-9(15)12-8(10)14/h4,6H,1,5H2,2-3H3,(H2,11,12,13,14,15)	-1.712
InChI=1S/C7H5BrO2/c8-5-3-1-2-4-6(9)7(5)10/h1-4H,(H,9,10)	-2.435
InChI=1S/C7H6N2S/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H2,8,9,10)	-2.177
InChI=1S/C8H5Cl3O2/c9-5-1-2-6(10)8(11)4(5)3-7(12)13/h1-2H,3H2,(H,12,13)	-3.08
InChI=1S/C4H8O2/c5-4-1-2-6-3-4/h4-5H,1-3H2	1.055
InChI=1S/C8H9FN2O3/c9-5-4-11(6-2-1-3-14-6)8(13)10-7(5)12/h4,6H,1-3H2,(H,10,12,13)	-1.01
InChI=1S/C9H12/c1-7-5-4-6-8(2)9(7)3/h4-6H,1-3H3	-3.204
InChI=1S/C6H2Cl4/c7-3-1-4(8)6(10)5(9)2-3/h1-2H	-4.68
InChI=1S/CH4N2S/c2-1(3)4/h(H4,2,3,4)	0.189
InChI=1S/C7H14/c1-3-5-7-6-4-2/h3H,1,4-7H2,2H3	-3.732
InChI=1S/CHBr3/c2-1(3)4/h1H	-1.911
InChI=1S/C12H8S/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H	-5.098
InChI=1S/C18H24O3/c1-18-7-6-13-12-5-3-11(19)8-10(12)2-4-14(13)15(18)9-16(20)17(18)2h3,5,8,13-17,19-21H,2,4,6-7,9H2,1H3	-4
InChI=1S/C19H21NO4/c1-2-8-20-9-7-18-15-11-3-4-12(21)16(15)24-17(18)13(22)5-6-19(18,2h2-4,14,17,21,23H,1,5-10H2	-3.39
InChI=1S/C19H14F3NO/c1-23-11-16(13-6-3-2-4-7-13)18(24)17(12-23)14-8-5-9-15(10-14)19(2h2-12H,1H3	-4.438

"InChi"	"logS(M)"
InChI=1S/C17H20N2O/c1-17(2,14-10-6-4-7-11-14)18-16(20)19(3)15-12-8-5-9-13-15/h4-13H,1-3H3,(H,18,20)	-3.349
InChI=1S/C6H12O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-12H	-0.1
InChI=1S/C8H9N/c1-2-4-8-7(3-1)5-6-9-8/h1-4,9H,5-6H2	-1.043
InChI=1S/C22H24N2O8/c1-21(31)8-5-4-6-11(25)12(8)16(26)13-9(21)7-10-15(24(2)3)17(27)14h4-6,9-10,15,25-26,29,31-32H,7H2,1-3H3,(H2,23,30)	-3.284
InChI=1S/C19H18N2O4/c1-2-16(22)25-13-21-17(23)19(20-18(21)24,14-9-5-3-6-10-14)15-11-7h3-12H,2,13H2,1H3,(H,20,24)	-4.91
InChI=1S/C12H4Cl6/c13-6-1-2-7(14)12(18)11(6)5-3-9(16)10(17)4-8(5)15/h1-4H	-7.93
InChI=1S/C7H6N4/c1-5-6-7(11-4-10-5)9-3-2-8-6/h2-4H,1H3	-0.466
InChI=1S/C14H10O9/c15-7-2-6(3-8(16)11(7)18)14(22)23-10-4-5(13(20)21)1-9(17)12(10)19h1-4,15-19H,(H,20,21)	-2.809
InChI=1S/C4H6O/c1-3-5-4-2/h3-4H,1-2H2	-1.261
InChI=1S/C15H16N2O2/c1-19-14-6-4-12(5-7-14)15(18,11-2-3-11)13-8-16-10-17-9-13/h4-11,18H,2-3H2,1H3	-2.596
InChI=1S/C23H30O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14,2)h6,8,10,16-18,20,26,28H,4-5,7,9,11-12H2,1-3H3	-4.369
InChI=1S/C10H15N/c1-3-8-6-5-7-9(4-2)10(8)11/h5-7H,3-4,11H2,1-2H3	-2.348
InChI=1S/C8H12N4O5/c9-7-10-2-12(8(16)11-7)6-5(15)4(14)3(1-13)17-6/h2-6,13-15H,1H2,(H2,9,11,16)	-0.439
InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h8-9H,1,4-6H2,2-3H3	-2.18
InChI=1S/C10H14O4/c1-13-9-4-2-3-5-10(9)14-7-8(12)6-11/h2-5,8,11-12H,6-7H2,1H3	-0.73
InChI=1S/C12H12/c1-9-5-3-8-12-10(2)6-4-7-11(9)12/h3-8H,1-2H3	-4.74
InChI=1S/C8H18/c1-6(2)8(5)7(3)4/h6-8H,1-5H3	-4.696
InChI=1S/C13H10O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	-3.882
InChI=1S/C11H12N4O3S/c1-18-11-7-6-10(13-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H,12H2,1H3,(H,13,15)	-2.68
InChI=1S/C18H13N/c19-18-11-17-13-6-2-1-5-12(13)9-10-15(17)14-7-3-4-8-16(14)18/h1-11H,19H2	-6.196
InChI=1S/C8H7N/c1-2-4-8-7(3-1)5-6-9-8/h1-6,9H	-1.21
InChI=1S/C20H30O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(19,h12,15-17,22H,4-11H2,1-3H3	-3.95
InChI=1S/C7H16/c1-6(2)7(3,4)5/h6H,1-5H3	-4.36
InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)	-1.62

"InChi"	"logS(M)"
InChI=1S/C10H16N2O8/c13-7(14)3-11(4-8(15)16)1-2-12(5-9(17)18)6-10(19)20/h1-6H2,(H,13,14)(H,15,16)(H,17,18)(H,19,20)	-2.767
InChI=1S/C7H7NO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,8H2,(H,10,11)	-2.26
InChI=1S/C7H5Cl2NO2/c8-3-1-4(7(11)12)6(9)5(10)2-3/h1-2H,10H2,(H,11,12)	-2.469
InChI=1S/C5H12O/c1-3-5(6)4-2/h5-6H,3-4H2,1-2H3	-0.233
InChI=1S/C6H3Cl3/c7-4-1-2-5(8)6(9)3-4/h1-3H	-3.702
InChI=1S/C7H6N4O/c1-12-7-5-6(10-4-11-7)9-3-2-8-5/h2-4H,1H3	-1.113
InChI=1S/C24H40O5/c1-13(4-7-19(26)27)15-5-6-16-20-17(9-11-23(15,16)2)24(3)10-8-14(2h13-18,20-22,25,28-29H,4-12H2,1-3H3,(H,26,27)	-4.346
InChI=1S/C21H30O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-21(h12,16-19H,4-11H2,1-3H3	-4.553
InChI=1S/C8H15NO/c10-8-6-4-2-1-3-5-7-9-8/h1-7H2,(H,9,10)	0.633
InChI=1S/C12H10O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9,13H	-2.507
InChI=1S/C15H21NO2/c1-3-18-14(17)15(9-11-16(2)12-10-15)13-7-5-4-6-8-13/h4-8H,3,9-12H2,1-2H3	-1.886
InChI=1S/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-14-12(10-13)11-8-6-5-7-9-11/h5-9H,3-4H2,1-2H3/b14-12+	-4.63
InChI=1S/C9H14N2O3/c1-4-9(5-2)6(12)10-8(14)11(3)7(9)13/h4-5H2,1-3H3,(H,10,12,14)	-2.1
InChI=1S/C15H26N2/c1-3-7-16-11-13-9-12(14(16)5-1)10-17-8-4-2-6-15(13)17/h12-15H,1-11H2	-1.887
InChI=1S/C12H20N2O3/c1-3-5-7-12(8-6-4-2)9(15)13-11(17)14-10(12)16/h3-8H2,1-2H3,(H2,13,14,15,16,17)	-2.876
InChI=1S/C4H6O2/c5-4-2-1-3-6-4/h1-3H2	1.065
InChI=1S/C2H2ClN/c3-1-2-4/h1H2	-0.092
InChI=1S/C16H14/c1-11-13-7-3-5-9-15(13)12(2)16-10-6-4-8-14(11)16/h3-10H,1-2H3	-6.566
InChI=1S/C20H30N2O5S/c1-7-25-17(23)11-12-22(14(2)3)28-21(6)19(24)26-16-10-8-9-15-13-2(h8-10,14H,7,11-13H2,1-6H3	-4.71
InChI=1S/C7H6N4O/c1-12-7-10-4-5-6(11-7)9-3-2-8-5/h2-4H,1H3	-1.113
InChI=1S/C5H9N3O10/c9-1-5(2-16-6(10)11,3-17-7(12)13)4-18-8(14)15/h9H,1-4H2	-1.585
InChI=1S/C7H16/c1-5-7(4)6(2)3/h6-7H,5H2,1-4H3	-4.281
InChI=1S/C9H9N/c1-7-6-10-9-5-3-2-4-8(7)9/h2-6,10H,1H3	-2.421
InChI=1S/C7H7ClO/c1-5-4-6(9)2-3-7(5)8/h2-4,9H,1H3	-1.57
InChI=1S/C5H9NO/c1-6-4-2-3-5(6)7/h2-4H2,1H3	1.004
InChI=1S/C17H19NO3/c19-17(18-10-4-1-5-11-18)7-3-2-6-14-8-9-15-16(12-14)21-13-20-15/h2-3,6-9,12H,1,4-5,10-11,13H2/b6-2+,7-3+	-3.853

"InChi"	"logS(M)"
InChI=1S/C11H13N3O/c1-8-10(12)11(15)14(13(8)2)9-6-4-3-5-7-9/h3-7H,12H2,1-2H3	0.31
InChI=1S/C10H14/c1-3-9-7-5-6-8-10(9)4-2/h5-8H,3-4H2,1-2H3	-3.276
InChI=1S/C11H18N2O3/c1-4-11(6-5-7(2)3)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(H2,12,13,14,15,16)	-2.574
InChI=1S/C17H25ClN2O2/c1-3-4-10-20-11-6-8-14(12-20)22-17(21)19-16-13(2)7-5-9-15(16)18/h5,7,9,14H,3-4,6,8,10-12H2,1-2H3,(H,19,21)	-5.211
InChI=1S/C15H15NO2/c1-10-6-5-9-13(11(10)2)16-14-8-4-3-7-12(14)15(17)18/h3-9,16H,1-2H3,(H,17,18)	-4.082
InChI=1S/C12H14N4O2S/c1-8-7-9(2)15-12(14-8)16-19(17,18)11-5-3-10(13)4-6-11/h3-7H,13H2,1-2H3,(H,14,15,16)	-2.73
InChI=1S/C19H24N2O/c1-2-13-12-21-10-8-14(13)11-18(21)19(22)16-7-9-20-17-6-4-3-5-15(16)h3-7,9,13-14,18-19,22H,2,8,10-12H2,1H3	-2.63
InChI=1S/C12H18/c1-2-3-4-6-9-12-10-7-5-8-11-12/h5,7-8,10-11H,2-4,6,9H2,1H3	-5.255
InChI=1S/C2H2Br2/c3-1-2-4/h1-2H/b2-1+	-1.319
InChI=1S/C2H3Cl3/c1-2(3,4)5/h1H3	-2.14
InChI=1S/C22H25NO6/c1-12(24)23-16-8-6-13-10-19(27-3)21(28-4)22(29-5)20(13)14-7-9-18(h7,9-11,16H,6,8H2,1-5H3,(H,23,24)	-0.948
InChI=1S/C5H6N2O2/c1-3-2-4(8)7-5(9)6-3/h2H,1H3,(H2,6,7,8,9)	-1.256
InChI=1S/C5H8O2/c1-3-5(6)7-4-2/h3H,1,4H2,2H3	-0.74
InChI=1S/C12H10N2/c1-8-12-10(6-7-13-8)9-4-2-3-5-11(9)14-12/h2-7,14H,1H3	-3.79
InChI=1S/C9H18/c1-3-5-7-9-8-6-4-2/h3H,1,4-9H2,2H3	-5.052
InChI=1S/C10H19N5O/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,12,13,14,15)	-3.239
InChI=1S/C12H7Cl3/c13-9-6-10(14)12(11(15)7-9)8-4-2-1-3-5-8/h1-7H	-6.06
InChI=1S/C3H7NO2S/c4-2(1-7)3(5)6/h2,7H,1,4H2,(H,5,6)	0.36
InChI=1S/C13H20O8/c1-9(14)18-5-13(6-19-10(2)15,7-20-11(3)16)8-21-12(4)17/h5-8H2,1-4H3	-1.569
InChI=1S/C16H13ClN2O2/c1-19-13-8-7-11(17)9-12(13)14(18-15(20)16(19)21)10-5-3-2-4-6-10/h2-9,15,20H,1H3	-2.7
InChI=1S/C18H22N2/c1-19-12-14-20(15-13-19)18(16-8-4-2-5-9-16)17-10-6-3-7-11-17/h2-11,18H,12-15H2,1H3	-2.425
InChI=1S/C10H7Cl/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H	-3.971
InChI=1S/C11H9NO4/c1-2-16-11(15)12-9(13)7-5-3-4-6-8(7)10(12)14/h3-6H,2H2,1H3	-2.739
InChI=1S/C9H18N6/c1-13(2)7-10-8(14(3)4)12-9(11-7)15(5)6/h1-6H3	-3.364
InChI=1S/C8H19N/c1-3-5-7-9-8-6-4-2/h9H,3-8H2,1-2H3	-1.504
InChI=1S/C4H10S2/c1-3-5-6-4-2/h3-4H2,1-2H3	-2.42

"InChi"	"logS(M)"
InChI=1S/C18H23NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18)9-12-11-13,17,20H,4-5,7-9H2,1-2H3	-1
InChI=1S/C11H18N4O2/c1-7-8(2)12-10(14(3)4)13-9(7)17-11(16)15(5)6/h1-6H3	-1.946
InChI=1S/C14H12/c1-10-5-4-8-13-12-7-3-2-6-11(12)9-14(10)13/h2-8H,9H2,1H3	-5.218
InChI=1S/C22H32O3/c1-14(23)25-22(4)12-9-19-17-6-5-15-13-16(24)7-10-20(15,2)18(17)8-h13,17-19H,5-12H2,1-4H3	-5.28
InChI=1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-2-4-h2-6,11-16,19H,7-9H2,1H3	-1.24
InChI=1S/C21H30O3/c1-13(22)24-19-7-6-17-16-5-4-14-12-15(23)8-10-20(14,2)18(16)9-11-h12,16-19H,4-11H2,1-3H3	-5.184
InChI=1S/C10H18O3/c1-10(2,9(11)12)13-8-6-4-3-5-7-8/h8H,3-7H2,1-2H3,(H,11,12)	-1.08
InChI=1S/C9H10O3/c10-6-8(9(11)12)7-4-2-1-3-5-7/h1-5,8,10H,6H2,(H,11,12)	-0.93
InChI=1S/C22H28O3/c1-4-22(25-14(2)23)12-10-20-19-7-5-15-13-16(24)6-8-17(15)18(19)9-h1,13,17-20H,5-12H2,2-3H3	-4.804
InChI=1S/C22H23ClN6O/c1-2-3-8-20-24-21(23)19(14-30)29(20)13-15-9-11-16(12-10-15)17-6-4-h4-7,9-12,30H,2-3,8,13-14H2,1H3,(H,25,26,27,28)	-4.945
InChI=1S/C17H20N4O6/c1-7-3-9-10(4-8(7)2)21(5-11(23)14(25)12(24)6-22)15-13(18-9)16(26)h3-4,11-12,14,22-25H,5-6H2,1-2H3,(H,20,26,27)	-3.648
InChI=1S/C14H12O3S/c1-9(14(16)17)10-4-6-11(7-5-10)13(15)12-3-2-8-18-12/h2-9H,1H3,(H,16,17)	-2
InChI=1S/C27H29NO11/c1-10-22(31)13(28)6-17(38-10)39-15-8-27(36,16(30)9-29)7-12-19(15)h3-5,10,13,15,17,22,29,31,33,35-36H,6-9,28H2,1-2H3	-3.767
InChI=1S/C3H8OS2/c4-1-3(6)2-5/h3-6H,1-2H2	-0.155
InChI=1S/C8H9NO2/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3,(H2,9,10)	-1.782
InChI=1S/C9H10O3/c1-7-4-2-3-5-8(7)12-6-9(10)11/h2-5H,6H2,1H3,(H,10,11)	-2.442
InChI=1S/C12H9Cl/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H	-5.2
InChI=1S/C21H28O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2)1h9,14-15,18,22,26H,3-8,10-11H2,1-2H3	-3.11
InChI=1S/C4H4N2/c1-2-4-6-5-3-1/h1-4H	1.096
InChI=1S/C22H12/c1-3-13-7-9-15-11-12-16-10-8-14-4-2-6-18-17(5-1)19(13)21(15)22(16h1-12H	-9.027
InChI=1S/C14H30/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-14H2,1-2H3	-7.456
InChI=1S/C9H13ClN6/c1-4-12-7-13-6(10)14-8(15-7)16-9(2,3)5-11/h4H2,1-3H3,(H2,12,13,14,15,16)	-3.151

"InChi"	"logS(M)"
InChI=1S/C10H12O2/c1-6-4-7(2)9(10(11)12)8(3)5-6/h4-5H,1-3H3,(H,11,12)	-2.357
InChI=1S/C6H14O/c1-5(7)6(2,3)4/h5,7H,1-4H3	-0.624
InChI=1S/C8H9ClO/c1-5-3-7(10)4-6(2)8(5)9/h3-4,10H,1-2H3	-2.67
InChI=1S/C15H11ClO3/c1-19-14(17)15(18)12-5-3-2-4-10(12)11-7-6-9(16)8-13(11)15/h2-8,18H,1H3	-4.184
InChI=1S/C3H4N2S/c4-3-5-1-2-6-3/h1-2H,(H2,4,5)	-0.36
InChI=1S/C5H11Cl/c1-4-5(2,3)6/h4H2,1-3H3	-2.511
InChI=1S/C13H10/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)12/h1-8H,9H2	-4.91
InChI=1S/C4H9Cl/c1-3-4(2)5/h4H,3H2,1-2H3	-2.001
InChI=1S/C15H20O3/c1-12(2)10-11-18-15(16)9-6-13-4-7-14(17-3)8-5-13/h4-9,12H,10-11H2,1-3H3/b9-6+	-5.492
InChI=1S/C11H16/c1-4-11(2,3)10-8-6-5-7-9-10/h5-9H,4H2,1-3H3	-4.501
InChI=1S/C7H16O/c1-4-5-7(2,3)6-8/h8H,4-6H2,1-3H3	-1.439
InChI=1S/C7H14O2/c1-3-5-6-7(8)9-4-2/h3-6H2,1-2H3	-1.771
InChI=1S/C8H18O/c1-3-5-7-9-8-6-4-2/h3-8H2,1-2H3	-2.638
InChI=1S/C22H24N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(h4-7,10,14-15,17,25,27-29,32H,1-3H3,(H2,23,31)	-2.87
InChI=1S/C13H9F3N2O2/c14-13(15,16)8-3-1-4-9(7-8)18-11-10(12(19)20)5-2-6-17-11/h1-7H,(H,17,18)(H,19,20)	-4.172
InChI=1S/C10H19ClNO5P/c1-5-12(6-2)10(13)9(11)7-8-17-18(14,15-3)16-4/h7H,5-6,8H2,1-4H3/b9-7-	0.523
InChI=1S/C6H3Cl3O/c7-3-1-4(8)6(9)5(10)2-3/h1-2,10H	-2.67
InChI=1S/C9H12N2O2S/c12-6-9(4-2-1-3-5-9)7(13)11-8(14)10-6/h1-5H2,(H2,10,11,12,13,14)	-3.46
InChI=1S/C23H34O5/c1-4-14(2)23(26)28-20-7-5-6-16-9-8-15(3)19(22(16)20)11-10-18-12-1h6,8-9,14-15,17-20,22,24H,4-5,7,10-13H2,1-3H3	-5.42
InChI=1S/C3H6N2O2/c1-2(6)5-3(4)7/h1H3,(H3,4,5,6,7)	-0.9
InChI=1S/C5H5NO/c7-5-1-3-6-4-2-5/h1-4H,(H,6,7)	1.022
InChI=1S/C16H18NO4P/c18-22(17-11-13-19-14-12-17,20-15-7-3-1-4-8-15)21-16-9-5-2-6-10-1h1-10H,11-14H2	-2.143
InChI=1S/C6H6O3/c7-4-1-5(8)3-6(9)2-4/h1-3,7-9H	-1.05
InChI=1S/C14H10O5/c1-18-8-5-10(16)13-12(6-8)19-11-3-2-7(15)4-9(11)14(13)17/h2-6,15-16H,1H3	-2.93
InChI=1S/C6H8N2O2S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,7H2,(H2,8,9,10)	-1.34
InChI=1S/C8H11NO/c1-2-10-8-5-3-7(9)4-6-8/h3-6H,2,9H2,1H3	-0.861
InChI=1S/C15H19ClN4O3/c1-15(2,3)12-18-20(14(22)23-12)11-7-6-9(8-10(11)16)17-13(21)19(4)h6-8H,1-5H3,(H,17,21)	-4.326

"InChi"	"logS(M)"
InChI=1S/C10H13ClN2O2/c1-13(2)10(14)12-7-4-5-9(15-3)8(11)6-7/h4-6H,1-3H3,(H,12,14)	-2.564
InChI=1S/C4H11N/c1-3-4(2)5/h4H,3,5H2,1-2H3	0.185
InChI=1S/C9H15NO3/c1-10-5-2-3-6(10)8(9(12)13)7(11)4-5/h5-8,11H,2-4H2,1H3,(H,12,13)	-0.017
InChI=1S/C6H4N4O2/c11-5-3-4(8-2-1-7-3)9-6(12)10-5/h1-2H,(H2,8,9,10,11,12)	-2.118
InChI=1S/C19H24N2O2/c22-18-13-20(19(23)15-7-2-1-3-8-15)12-17-16-9-5-4-6-14(16)10-11-21(17)18/h4-6,9,15,17H,1-3,7-8,10-13H2	-2.893
InChI=1S/C8H5Cl3O3/c9-4-1-6(11)7(2-5(4)10)14-3-8(12)13/h1-2H,3H2,(H,12,13)	-2.98
InChI=1S/C16H12O5/c17-14(12-7-3-4-8-13(12)16(20)21)9-10-5-1-2-6-11(10)15(18)19/h1-8H,9H2,(H,18,19)(H,20,21)	-2.791
InChI=1S/C8H10O/c1-6-4-3-5-8(9)7(6)2/h3-5,9H,1-2H3	-1.424
InChI=1S/C7H10N2OS/c1-2-3-5-4-6(10)9-7(11)8-5/h4H,2-3H2,1H3,(H2,8,9,10,11)	-2.15
InChI=1S/C11H15NO2/c1-2-3-8-14-11(13)9-4-6-10(12)7-5-9/h4-7H,2-3,8,12H2,1H3	-3.06
InChI=1S/C6H4BrCl/c7-5-3-1-2-4-6(5)8/h1-4H	-3.203
InChI=1S/C8H10O/c1-6-3-4-7(2)8(9)5-6/h3-5,9H,1-2H3	-1.538
InChI=1S/C9H12/c1-3-9-7-5-4-6-8(9)2/h4-7H,3H2,1-2H3	-3.207
InChI=1S/C7H6N4O/c1-12-6-3-9-5-2-8-4-10-7(5)11-6/h2-4H,1H3	-0.91
InChI=1S/C9H11NO/c1-2-9(11)7-3-5-8(10)6-4-7/h3-6H,2,10H2,1H3	-2.627
InChI=1S/C9H9ClO3/c1-6(9(11)12)13-8-4-2-3-7(10)5-8/h2-6H,1H3,(H,11,12)	-2.223
InChI=1S/C10H10O2/c1-8(11)7-10(12)9-5-3-2-4-6-9/h2-6H,7H2,1H3	-2.627
InChI=1S/C20H12/c1-2-7-14-13(6-1)12-19-16-9-4-3-8-15(16)18-11-5-10-17(14)20(18)19/h1-12H	-8.226
InChI=1S/C7H12O2/c1-3-7(8-5-1)4-2-6-9-7/h1-6H2	-0.108
InChI=1S/C9H20O/c1-2-3-4-5-6-7-8-9-10/h10H,2-9H2,1H3	-3.013
InChI=1S/C9H12N2O2/c1-2-13-8-5-3-7(4-6-8)11-9(10)12/h3-6H,2H2,1H3,(H3,10,11,12)	-2.173
InChI=1S/C19H26O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h11,14-16H,3-10H2,1-2H3	-3.695
InChI=1S/C7H14O/c1-6(2)4-5-7(3)8/h6H,4-5H2,1-3H3	-1.325
InChI=1S/C6H6N4O3/c1-10-4(11)2-3(9-6(10)13)8-5(12)7-2/h1H3,(H,9,13)(H2,7,8,12)	-1.561
InChI=1S/C8H10O5/c9-7(10)5-3-1-2-4(13-3)6(5)8(11)12/h3-6H,1-2H2,(H,9,10)(H,11,12)	-0.27
InChI=1S/C10H13ClN2/c1-8-6-9(11)4-5-10(8)12-7-13(2)3/h4-7H,1-3H3/b12-7+	-2.88
InChI=1S/C12H12/c1-2-10-7-8-11-5-3-4-6-12(11)9-10/h3-9H,2H2,1H3	-4.29
InChI=1S/C4H10FO2P/c1-4(2)7-8(3,5)6/h4H,1-3H3	0.854

"InChi"	"logS(M)"
InChI=1S/C10H18O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7-8,11H,4-6H2,1-3H3	-2.421
InChI=1S/C12H9Cl/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H	-4.592
InChI=1S/C5H10O2/c1-4(2)7-5(3)6/h4H,1-3H3	-0.547
InChI=1S/C2H4N4/c3-2-4-1-5-6-2/h1H,(H3,3,4,5,6)	0.833
InChI=1S/C23H32O2/c1-14-12-17-18(21(3)9-6-16(25)13-20(14)21)7-11-23(5)19(17)8-10-22h12-13,17-19H,6-11H2,1-5H3	-5.272
InChI=1S/C5H4N4O2/c10-4-6-1-2-3(8-4)9-5(11)7-2/h1H,(H3,6,7,8,9,10,11)	-3.6
InChI=1S/C17H21NO4/c1-18-12-8-9-13(18)15(17(20)21-2)14(10-12)22-16(19)11-6-4-3-5-7-1h3-7,12-15H,8-10H2,1-2H3	-2.227
InChI=1S/C14H16ClO5PS/c1-4-17-21(22,18-5-2)20-10-6-7-11-9(3)13(15)14(16)19-12(11)8-10/h6-8H,4-5H2,1-3H3	-5.383
InChI=1S/C19H34O3/c1-15(2)22-18(20)14-17(4)11-8-10-16(3)12-9-13-19(5,6)21-7/h8,11,14-16H,9-10,12-13H2,1-7H3/b11-8+,17-14+	-5.346
InChI=1S/C6H12O/c1-5(2)4-6(3)7/h5H,4H2,1-3H3	-0.851
InChI=1S/C7H16O2/c1-3-7(4-2,5-8)6-9/h8-9H,3-6H2,1-2H3	0.18
InChI=1S/C5H4N2O4/c8-6-3-4-1-2-5(11-4)7(9)10/h1-3,8H/b6-3+	-2.193
InChI=1S/C9H16ClN5/c1-5(2)11-8-13-7(10)14-9(15-8)12-6(3)4/h5-6H,1-4H3,(H2,11,12,13,14,15)	-4.46
InChI=1S/C5H8N4O12/c10-6(11)18-1-5(2-19-7(12)13,3-20-8(14)15)4-21-9(16)17/h1-4H2	-3.866
InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3	-2.329
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)	-0.74
InChI=1S/C17H19NO3/c1-18-7-6-17-10-3-5-13(20)16(17)21-15-12(19)4-2-9(14(15)17)8-11(1h2-5,10-11,13,16,19-20H,6-8H2,1H3	-3.15
InChI=1S/C13H11N3O2/c17-12-4-2-1-3-11(12)9-15-16-13(18)10-5-7-14-8-6-10/h1-9,15H,(H,16,18)/b11-9+	-3.683
InChI=1S/C8H10/c1-7-4-3-5-8(2)6-7/h3-6H,1-2H3	-2.833
InChI=1S/C8H10N2O4S/c1-14-8(11)10-15(12,13)7-4-2-6(9)3-5-7/h2-5H,9H2,1H3,(H,10,11)	-1.76
InChI=1S/C3H7NO2/c1-2-3-4(5)6/h2-3H2,1H3	-0.8
InChI=1S/C6H10OS2/c1-3-5-8-9(7)6-4-2/h3-4H,1-2,5-6H2/p+1	-0.83
InChI=1S/C10H9Cl4O4P/c1-16-19(15,17-2)18-10(5-11)6-3-8(13)9(14)4-7(6)12/h3-5H,1-2H3/b10-5-	-4.522
InChI=1S/C3H7Cl/c1-2-3-4/h2-3H2,1H3	-1.453
InChI=1S/C12H7Cl3/c13-9-3-1-8(2-4-9)11-6-5-10(14)7-12(11)15/h1-7H	-6
InChI=1S/C12H10O/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9,13H	-3.481
InChI=1S/C2H3Cl3O/c3-2(4,5)1-6/h6H,1H2	-0.254
InChI=1S/C21H28O2/c1-4-21(23)12-9-18-16-6-5-14-13-15(22)7-10-19(14,2)17(16)8-11-20(h1,13,16-18,23H,5-12H2,2-3H3	-5.658

"InChi"	"logS(M)"
InChI=1S/C2H4Br2/c3-1-2-4/h1-2H2	-1.68
InChI=1S/C19H20N2O2/c1-2-3-14-17-18(22)20(15-10-6-4-7-11-15)21(19(17)23)16-12-8-5-9-1h4-13,17H,2-3,14H2,1H3	-3.812
InChI=1S/C30H44O9/c1-16-24(33)26(36-3)25(34)27(38-16)39-19-6-10-29(15-31)18(13-19)h12,15-16,18-22,24-27,33-35H,4-11,13-14H2,1-3H3	-3.137
InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-9H,4-6H2,1-3H3	-2.492
InChI=1S/C11H21NOS/c1-3-12(11(13)14-4-2)10-8-6-5-7-9-10/h10H,3-9H2,1-2H3	-3.404
InChI=1S/C7H9N/c1-6-4-3-5-7(2)8-6/h3-5H,1-2H3	0.447
InChI=1S/C8H10O/c1-2-7-5-3-4-6-8(7)9/h3-6,9H,2H2,1H3	-1.359
InChI=1S/C25H32N2O2/c1-21(20-26-16-18-29-19-17-26)25(22-10-4-2-5-11-22,23-12-6-3-7-13h2-7,10-13,21H,8-9,14-20H2,1H3	-5.145
InChI=1S/C2HCl2F3/c3-1(4)2(5,6)7/h1H	-1.862
InChI=1S/C12H16N2O3/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(12)16/h6H,2-5,7H2,1H3,(H2,13,14,15,16,17)	-2.169
InChI=1S/C4H8O2/c1-3-6-4(2)5/h3H2,1-2H3	-0.025
InChI=1S/C14H10O/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9,15H	-4.733
InChI=1S/C3H7I/c1-3(2)4/h3H,1-2H3	-2.084
InChI=1S/C4H8O2/c1-3(2)4(5)6/h3H,1-2H3,(H,5,6)	0.278
InChI=1S/C12H4Cl6/c13-6-2-1-5(3-7(6)14)10-8(15)4-9(16)11(17)12(10)18/h1-4H	-7.651
InChI=1S/C16H18N2O3/c1-18(2)16(19)17-12-4-6-14(7-5-12)21-15-10-8-13(20-3)9-11-15/h4-11H,1-3H3,(H,17,19)	-4.156
InChI=1S/C9H12N2O/c1-7-3-5-8(6-4-7)11(2)9(10)12/h3-6H,1-2H3,(H2,10,12)	-0.423
InChI=1S/C5H5N5/c6-5-7-1-3-4(10-5)9-2-8-3/h1-2H,(H3,6,7,8,9,10)	-1.21
InChI=1S/C8H8O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7,9H,(H,10,11)	-0.032
InChI=1S/C7H16O/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3	-1.843
InChI=1S/C7H5NS/c9-6-8-7-4-2-1-3-5-7/h1-5H	-3.177
InChI=1S/C6H12/c1-4-5-6(2)3/h4,6H,1,5H2,2-3H3	-3.244
InChI=1S/C7H6O3/c8-6-3-1-2-5(4-6)7(9)10/h1-4,8H,(H,9,10)	-1.24
InChI=1S/C13H18O2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(14)15/h4-7,9-10H,8H2,1-3H3,(H,14,15)	-3.992
InChI=1S/C7H9N/c1-6-3-2-4-7(8)5-6/h2-5H,8H2,1H3	-0.951
InChI=1S/C6H10/c1-5(2)6(3)4/h1,3H2,2,4H3	-2.401
InChI=1S/C6H4N2O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H	-3.102
InChI=1S/C5H9Cl2N3O2/c6-1-3-8-5(11)10(9-12)4-2-7/h1-4H2,(H,8,11)	-1.728
InChI=1S/C8H11N/c1-2-9-8-6-4-3-5-7-8/h3-7,9H,2H2,1H3	-1.652
InChI=1S/C12H10Cl2N2/c13-9-5-7(1-3-11(9)15)8-2-4-12(16)10(14)6-8/h1-6H,15-16H2	-4.912

"InChi"	"logS(M)"
InChI=1S/C18H18F3NO4/c19-18(20,21)13-4-3-5-14(12-13)22-16-7-2-1-6-15(16)17(24)26-11-10h1-7,12,22-23H,8-11H2	-5.363
InChI=1S/C18H20O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h3-5,10,14,16,19H,2,6-9H2,1H3	-5.279
InChI=1S/C12H8Cl2/c13-11-7-6-10(8-12(11)14)9-4-2-1-3-5-9/h1-8H	-6.39
InChI=1S/C7H6Cl2O/c8-6-2-1-5(4-10)7(9)3-6/h1-3,10H,4H2	-2.248
InChI=1S/C12H9ClF3N3O/c1-17-9-6-18-19(11(20)10(9)13)8-4-2-3-7(5-8)12(14,15)16/h2-6,17H,1H3	-3.955
InChI=1S/C15H22O3/c1-2-3-4-5-6-7-12-18-15(17)13-8-10-14(16)11-9-13/h8-11,16H,2-7,12H2,1H3	-4.222
InChI=1S/C22H23ClN2O8/c1-21(32)7-6-8-15(25(2)3)17(28)13(20(24)31)19(30)22(8,33)18(29)11h4-5,7-8,15,26,28-29,32-33H,6H2,1-3H3,(H2,24,31)	-2.88
InChI=1S/C6H14O/c1-4-5-6(2,3)7/h7H,4-5H2,1-3H3	-0.499
InChI=1S/C11H21N5OS/c1-8(2)13-10-14-9(12-6-5-7-17-3)15-11(16-10)18-4/h8H,5-7H2,1-4H3,(H2,12,13,14,15,16)	-2.928
InChI=1S/C12H8O2/c1-2-6-10-9(5-1)13-11-7-3-4-8-12(11)14-10/h1-8H	-5.311
InChI=1S/C18H32O16/c19-1-5-8(22)11(25)13(27)16(31-5)30-3-7-9(23)12(26)14(28)17(32-7)h5-17,19-29H,1-4H2	-0.396
InChI=1S/C20H14I6N2O6/c21-7-5-9(23)17(15(25)13(7)19(31)32)27-11(29)3-1-2-4-12(30)28-18-h5-6H,1-4H2,(H,27,29)(H,28,30)(H,31,32)(H,33,34)	-3.39
InChI=1S/C12H20N2O3/c1-3-5-6-7-8-12(4-2)9(15)13-11(17)14-10(12)16/h3-8H2,1-2H3,(H2,13,14,15,16,17)	-3.05
InChI=1S/C8H8N4/c9-11-8-7-4-2-1-3-6(7)5-10-12-8/h1-5H,9H2,(H,11,12)	-2.6
InChI=1S/C17H15NO5/c1-11(19)18-13-7-9-14(10-8-13)23-17(21)15-5-3-4-6-16(15)22-12(2)2h3-10H,1-2H3,(H,18,19)	-4.195
InChI=1S/C2H5I/c1-2-3/h2H2,1H3	-1.601
InChI=1S/C14H14O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10,13-16H	-1.933
InChI=1S/C14H14N8O4S3/c1-6-17-18-14(29-6)28-4-7-3-27-12-9(11(24)22(12)10(7)13(25)26)16-h5,9,12H,2-4H2,1H3,(H,16,23)(H,25,26)	-2.62
InChI=1S/C12H4Cl6/c13-5-1-2-6(8(14)3-5)7-4-9(15)11(17)12(18)10(7)16/h1-4H	-8.32
InChI=1S/C12H11NO2/c1-9-11(7-8-15-9)12(14)13-10-5-3-2-4-6-10/h2-8H,1H3,(H,13,14)	-3.304
InChI=1S/CH3I/c1-2/h1H3	-1.215
InChI=1S/C13H10BrCl2O2PS/c1-17-19(20,9-5-3-2-4-6-9)18-13-8-11(15)10(14)7-12(13)16/h2-8H,1H3	-7.138

"InChi"	"logS(M)"
InChI=1S/C5H5NO/c7-5-2-1-3-6-4-5/h1-4,7H	-0.456
InChI=1S/C12H9NS/c1-3-7-11-9(5-1)13-10-6-2-4-8-12(10)14-11/h1-8,13H	-5.59
InChI=1S/C10H14O/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7,11H,1-3H3	-2.391
InChI=1S/C10H18ClN3O7/c1-20-9-8(17)7(16)6(15)5(21-9)4-12-10(18)14(13-19)3-2-11/h5-9,15-17H,2-4H2,1H3,(H,12,18)	-1.561
InChI=1S/C14H11ClN2O4S/c15-11-6-5-8(7-12(11)22(16,20)21)14(19)10-4-2-1-3-9(10)13(18)17-1h1-7,19H,(H,17,18)(H2,16,20,21)	-3.451
InChI=1S/C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3/b5-3+	-2.545
InChI=1S/C12H5Cl5/c13-6-1-2-9(14)7(3-6)8-4-11(16)12(17)5-10(8)15/h1-5H	-7.326
InChI=1S/C11H16O2/c1-2-3-4-5-9-6-7-10(12)8-11(9)13/h6-8,12-13H,2-5H2,1H3	-1.955
InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2+	0.412
InChI=1S/C15H10ClN3O3/c16-12-4-2-1-3-10(12)15-11-7-9(19(21)22)5-6-13(11)18-14(20)8-17-1h1-7H,8H2,(H,18,20)	-4.41
InChI=1S/C4H10O/c1-4(2)5-3/h4H,1-3H3	-0.057
InChI=1S/C8H6O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H,(H,9,10)(H,11,12)	-1.425
InChI=1S/C18H22O2/c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11-16(20)12-8-14/h5-12,17-20H,3-4H2,1-2H3	-4.353
InChI=1S/C6H3Cl3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H	-2.392
InChI=1S/C15H13NO3/c1-10(17)11-5-4-6-12(9-11)16-14-8-3-2-7-13(14)15(18)19/h2-9,16H,1H3,(H,18,19)	-4.86
InChI=1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)	-1.69
InChI=1S/C17H21NO2/c1-4-18(5-2)17(19)13(3)20-16-12-8-10-14-9-6-7-11-15(14)16/h6-13H,4-5H2,1-3H3	-3.57
InChI=1S/C12H8O/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H	-4.6
InChI=1S/C12H18N2O/c1-9(2)10-5-7-11(8-6-10)13-12(15)14(3)4/h5-9H,1-4H3,(H,13,15)	-3.5
InChI=1S/C8H8N2O3/c1-6(11)9-7-2-4-8(5-3-7)10(12)13/h2-5H,1H3,(H,9,11)	-2.69
InChI=1S/C30H42O8/c1-16-24(32)25(33)26(34)27(37-16)38-19-8-11-28(2)18(14-19)5-6-22-h4,7,14-16,19-22,24-27,32-35H,5-6,8-13H2,1-3H3	-3.955
InChI=1S/C12H12N2O3/c1-3-14-6-9(12(16)17)10(15)8-5-4-7(2)13-11(8)14/h4-6H,3H2,1-2H3,(H,16,17)	-3.61
InChI=1S/C7H9NO/c1-9-7-4-2-6(8)3-5-7/h2-5H,8H2,1H3	-0.748
InChI=1S/C15H28N4O4/c1-3-22-14(20)18-9-5-16(6-10-18)13-17-7-11-19(12-8-17)15(21)23-4-h3-13H2,1-2H3	-0.844
InChI=1S/C10H14O/c1-3-8(2)9-4-6-10(11)7-5-9/h4-8,11H,3H2,1-2H3	-2.195

"InChi"	"logS(M)"
InChI=1S/C8H8BrCl2O3PS/c1-12-15(16,13-2)14-8-4-6(10)5(9)3-7(8)11/h3-4H,1-2H3	-6.086
InChI=1S/C11H18N2O2S/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(H2,12,13,14,15,16)	-3.6
InChI=1S/CH4N2O2/c2-1(4)3-5/h5H,(H3,2,3,4)	1.119
InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,10H,1,5-7H2,2-3H3	-3.846
InChI=1S/C10H14NO6P/c1-3-15-18(14,16-4-2)17-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3	-2.059
InChI=1S/C12H9Cl/c13-12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-9H	-4.88
InChI=1S/C12H18N2O2S/c1-4-6-8(3)12(7-5-2)9(15)13-11(17)14-10(12)16/h5,8H,2,4,6-7H2,1,3H3,(H2,13,14,15,16,17)	-3.458
InChI=1S/C11H16N4O2/c1-4-5-6-15-10(16)8-9(12-7-13(8)2)14(3)11(15)17/h7H,4-6H2,1-3H3	-1.625
InChI=1S/C8H11Cl3O6/c9-8(10,11)7-16-5-3(14)4(2(13)1-12)15-6(5)17-7/h2-7,12-14H,1H2	-1.843
InChI=1S/C10H16O3/c1-6(11)8-4-7(5-9(12)13)10(8,2)3/h7-8H,4-5H2,1-3H3,(H,12,13)	-0.575
InChI=1S/C4H9NO2/c1-2-3(5)4(6)7/h3H,2,5H2,1H3,(H,6,7)	0.287
InChI=1S/C8H11NO/c9-6-5-7-1-3-8(10)4-2-7/h1-4,10H,5-6,9H2	-1.116
InChI=1S/C10H12N4O5/c15-1-4-6(16)7(17)10(19-4)14-3-13-5-8(14)11-2-12-9(5)18/h2-4,6-7,10,15-17H,1H2,(H,11,12,18)	-1.23
InChI=1S/C8H10O/c1-7(9)8-5-3-2-4-6-8/h2-7,9H,1H3	-1.797
InChI=1S/C8H9NO2/c1-9-8(10)11-7-5-3-2-4-6-7/h2-6H,1H3,(H,9,10)	-1.803
InChI=1S/C9H18N2O2S/c1-9(2,3)7(6-14-5)11-13-8(12)10-4/h6H2,1-5H3,(H,10,12)/b11-7+	-1.623
InChI=1S/C12H22O11/c13-1-4-6(16)8(18)9(19)11(21-4)23-12(3-15)10(20)7(17)5(2-14)22-12h4-11,13-20H,1-3H2	0.788
InChI=1S/C11H19N3O/c1-5-6-7-9-8(2)12-11(14(3)4)13-10(9)15/h5-7H2,1-4H3,(H,12,13,15)	-2.242
InChI=1S/C17H12Cl2N2O/c18-14-7-5-12(6-8-14)17(22,13-9-20-11-21-10-13)15-3-1-2-4-16(15)1h1-11,22H	-4.374
InChI=1S/C8H8BrNO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)	-3.08
InChI=1S/C2H5Br/c1-2-3/h2H2,1H3	-1.086
InChI=1S/C12H7Cl3/c13-9-6-4-8(5-7-9)12-10(14)2-1-3-11(12)15/h1-7H	-6.21
InChI=1S/C9H10O2/c1-2-11-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3	-2.4
InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3	0.838
InChI=1S/C6H3Cl3/c7-4-1-5(8)3-6(9)2-4/h1-3H	-4.6
InChI=1S/C6H6ClN/c7-5-2-1-3-6(8)4-5/h1-4H,8H2	-1.373
InChI=1S/C10H12O2/c1-2-8-12-10(11)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3	-2.67

"InChi"	"logS(M)"
InChI=1S/C12H13NO4S/c1-9-11(18(15,16)8-7-17-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3,(H,13,14)	-2.43
InChI=1S/C16H22O4/c1-3-5-11-19-15(17)13-7-9-14(10-8-13)16(18)20-12-6-4-2/h7-10H,3-6,11-12H2,1-2H3	-6.403
InChI=1S/C14H12O/c1-11(15)12-7-9-14(10-8-12)13-5-3-2-4-6-13/h2-10H,1H3	-3.31
InChI=1S/C4H10S/c1-3-5-4-2/h3-4H2,1-2H3	-1.468
InChI=1S/C5H12O/c1-2-3-4-5-6/h6H,2-5H2,1H3	-0.603
InChI=1S/C6H12O/c7-6-4-2-1-3-5-6/h6-7H,1-5H2	-0.377
InChI=1S/C3H5NO/c1-2-3(4)5/h2H,1H2,(H2,4,5)	0.954
InChI=1S/C13H9N/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-9H	-3.669
InChI=1S/C13H14N2O3/c1-3-13(9-7-5-4-6-8-9)10(16)14-12(18)15(2)11(13)17/h4-8H,3H2,1-2H3,(H,14,16,18)	-3.68
InChI=1S/C14H12N2/c1-9-5-7-15-13-11(9)3-4-12-10(2)6-8-16-14(12)13/h3-8H,1-2H3	-3.969
InChI=1S/C7H6F3N/c8-7(9,10)5-1-3-6(11)4-2-5/h1-4H,11H2	-2.847
InChI=1S/C15H12/c1-11-6-7-14-9-12-4-2-3-5-13(12)10-15(14)8-11/h2-10H,1H3	-6.955
InChI=1S/C6H7NO/c1-7-5-3-2-4-6(7)8/h2-5H,1H3	0.962
InChI=1S/C14H20ClNO2/c1-4-11-7-6-8-12(5-2)14(11)16(10-18-3)13(17)9-15/h6-8H,4-5,9-10H2,1-3H3	-3.17
InChI=1S/C7H14O/c1-5(2)7(8)6(3)4/h5-6H,1-4H3	-1.302
InChI=1S/C6H14O/c1-5(2)6(3)4-7/h5-7H,4H2,1-3H3	-0.39
InChI=1S/C8H10N2O2/c1-12-7-4-2-6(3-5-7)10-8(9)11/h2-5H,1H3,(H3,9,10,11)	-1.592
InChI=1S/C12H7Cl2NO3/c13-8-1-6-12(11(14)7-8)18-10-4-2-9(3-5-10)15(16)17/h1-7H	-5.454
InChI=1S/C6H4BrCl/c7-5-1-3-6(8)4-2-5/h1-4H	-3.63
InChI=1S/C6H2Cl4O/c7-2-1-3(8)6(11)5(10)4(2)9/h1,11H	-3.1
InChI=1S/C10H17NO2/c1-4-10(5-2)8(12)7(3)6-11-9(10)13/h7H,4-6H2,1-3H3,(H,11,13)	-0.38
InChI=1S/C8H16O/c1-2-3-4-5-6-7-8-9/h8H,2-7H2,1H3	-2.36
InChI=1S/C19H15ClO4/c1-11(21)10-15(12-6-8-13(20)9-7-12)17-18(22)14-4-2-3-5-16(14)24-1h2-9,15,22H,10H2,1H3	-5.839
InChI=1S/C5H10O2/c1-3-4-7-5(2)6/h3-4H2,1-2H3	-0.72
InChI=1S/C6H8O7/c7-3(8)1-6(13,5(11)12)2-4(9)10/h13H,1-2H2,(H,7,8)(H,9,10)(H,11,12)	0.477
InChI=1S/C5H11NO3/c1-5(2)3-4-9-6(7)8/h5H,3-4H2,1-2H3	-2.481
InChI=1S/C6H6N2O/c7-6(9)5-2-1-3-8-4-5/h1-4H,(H2,7,9)	0.612
InChI=1S/C8H8O3/c1-11-8(10)6-4-2-3-5-7(6)9/h2-5,9H,1H3	-1.313
InChI=1S/C7H14O2/c1-3-5-7(8)9-6-4-2/h3-6H2,1-2H3	-1.905

"InChi"	"logS(M)"
InChI=1S/C14H10F3NO2/c15-14(16,17)9-4-3-5-10(8-9)18-12-7-2-1-6-11(12)13(19)20/h1-8,18H,(H,19,20)	-4.4
InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)	-1.033
InChI=1S/C13H18O7/c14-5-7-3-1-2-4-8(7)19-13-12(18)11(17)10(16)9(6-15)20-13/h1-4,9-18H,5-6H2	-0.855
InChI=1S/C14H14O/c1-11-5-3-7-13(9-11)15-14-8-4-6-12(2)10-14/h3-10H,1-2H3	-4.85
InChI=1S/C9H11NO/c1-2-9(11)10-8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H,10,11)	-1.55
InChI=1S/C14H8O4/c15-10-6-5-9-11(14(10)18)13(17)8-4-2-1-3-7(8)12(9)16/h1-6,15,18H	-2.779
InChI=1S/C13H8Cl3NO3/c14-8(15)5-9(18)17-11-10(16)12(19)6-3-1-2-4-7(6)13(11)20/h1-4,8H,5H2,(H,17,18)	-5.03
InChI=1S/C19H24N2O3/c1-13(7-8-14-5-3-2-4-6-14)21-12-18(23)15-9-10-17(22)16(11-15)19(2h2-6,9-11,13,18,21-23H,7-8,12H2,1H3,(H2,20,24)	-3.448
InChI=1S/C3H5N/c1-2-3-4/h2H2,1H3	0.272
InChI=1S/C5H10/c1-4-5(2)3/h2,4H2,1,3H3	-2.731
InChI=1S/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5,7-8H,4,6H2,1-3H3/b10-7+	-2.412
InChI=1S/C4H6/c1-3-4-2/h3-4H,1-2H2	-1.867
InChI=1S/C6H3Cl2NO2/c7-4-2-1-3-5(6(4)8)9(10)11/h1-3H	-3.488
InChI=1S/C10H12N4O4/c15-2-6-7(16)8(17)10(18-6)14-4-13-5-1-11-3-12-9(5)14/h1,3-4,6-8,10,15-17H,2H2	-0.402
InChI=1S/C16H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3,(H,17,18)	-6.807
InChI=1S/C17H12/c1-3-7-14-12(5-1)9-10-16-15-8-4-2-6-13(15)11-17(14)16/h1-10H,11H2	-6.678
InChI=1S/C11H16/c1-7-6-8(2)10(4)11(5)9(7)3/h6H,1-5H3	-3.981
InChI=1S/C4H5N3O/c5-3-1-2-6-4(8)7-3/h1-2H,(H3,5,6,7,8)	-1.143
InChI=1S/C21H24F3N3S/c1-25-11-13-26(14-12-25)9-4-10-27-17-5-2-3-6-19(17)28-20-8-7-16(1h2-3,5-8,15H,4,9-14H2,1H3	-4.524
InChI=1S/C7H16/c1-4-5-6-7(2)3/h7H,4-6H2,1-3H3	-4.596
InChI=1S/C10H14ClN3OS/c1-3-14(4-2)10(15)7-16-9-6-5-8(11)12-13-9/h5-6H,3-4,7H2,1-2H3	-1.716
InChI=1S/C6H4Br2/c7-5-1-2-6(8)4-3-5/h1-4H	-4.072
InChI=1S/C12H8Cl2/c13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14/h1-8H	-5.081
InChI=1S/C23H26O3/c1-16(2)13-20-21(23(20,3)4)22(24)25-15-17-9-8-12-19(14-17)26-18-1h5-14,20-21H,15H2,1-4H3	-5.24
InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3	-1.94

"InChi"	"logS(M)"
InChI=1S/C12H22O11/c13-1-4-6(16)7(17)8(18)11(21-4)22-9-5(2-14)23-12(20,3-15)10(9)19/h4-11,13-20H,1-3H2	0.349
InChI=1S/C22H19Br2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-16(11-1 h3-12,17-18,20H,1-2H3	-8.402
InChI=1S/C3H6Br2/c4-2-1-3-5/h1-3H2	-2.075
InChI=1S/C5H10/c1-4-5(2)3/h4-5H,1H2,2-3H3	-2.732
InChI=1S/C9H7NO/c11-9-6-5-7-3-1-2-4-8(7)10-9/h1-6H,(H,10,11)	-2.139
InChI=1S/C26H54/c1-3-5-7-9-11-13-15-17-19-21-23-25-26-24-22-20-18-16-14-12-10-8-(h3-26H2,1-2H3	-8.334
InChI=1S/C9H12O/c1-6-4-7(2)9(10)8(3)5-6/h4-5,10H,1-3H3	-2.055
InChI=1S/C15H12F4N4O7S/c1-28-11(24)7-4-2-3-5-8(7)31(26,27)23-15(25)22-14-20-9(29-12(16)1 h2-6,12-13H,1H3,(H2,20,21,22,23,25)	-5.152
InChI=1S/C12H6Cl4/c13-7-3-1-4-8(14)11(7)12-9(15)5-2-6-10(12)16/h1-6H	-7.39
InChI=1S/C9H14O/c1-7-4-8(10)6-9(2,3)5-7/h4H,5-6H2,1-3H3	-1.061
InChI=1S/C15H22N4O3/c1-4-8-18-10-16-13-12(18)14(21)19(15(22)17(13)3)9-6-5-7-11(2)20/h10H,4-9H2,1-3H3	-0.981
InChI=1S/C9H11NO/c1-7-4-3-5-9(6-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)	-2.091
InChI=1S/C6H5NO3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H	-0.94
InChI=1S/C6H14O/c1-4-6(7)5(2)3/h5-7H,4H2,1-3H3	-0.706
InChI=1S/C6H4Cl2O/c7-5-2-1-4(9)3-6(5)8/h1-3,9H	-1.246
InChI=1S/C7H16O/c1-6(2,3)7(4,5)8/h8H,1-5H3	-0.723
InChI=1S/C20H16/c1-13-16-8-5-6-9-17(16)14(2)20-18(13)12-11-15-7-3-4-10-19(15)20/h3-12H,1-2H3	-6.78
InChI=1S/C8H16/c1-3-5-7-8-6-4-2/h3H,1,4-8H2,2H3	-4.437
InChI=1S/C12H16N2O3/c1-3-13-11(15)9(2)17-12(16)14-10-7-5-4-6-8-10/h4-9H,3H2,1-2H3,(H,13,15)(H,14,16)	-1.829
InChI=1S/C17H19NO3/c1-18-7-6-17-10-3-5-13(20)16(17)21-15-12(19)4-2-9(14(15)17)8-11(1 h2,4,10-11,16,19H,3,5-8H2,1H3	-2.1
InChI=1S/C6H2Br2ClNO/c7-4-1-3(10-9)2-5(8)6(4)11/h1-2H	-3.707
InChI=1S/C10H13N5O4/c11-8-5-9(13-2-12-8)15(3-14-5)10-7(18)6(17)4(1-16)19-10/h2-4,6-7,10,16-18H,1H2,(H2,11,12,13)	-1.73
InChI=1S/C8H8O3/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3,(H,9,10)	-1.6
InChI=1S/C15H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15(16)17/h2-14H2,1H3,(H,16,17)	-4.31
InChI=1S/C5H12N2/c1-5-4-6-2-3-7-5/h5-7H,2-4H2,1H3	0.638
InChI=1S/C7H7NO4/c9-6(10)4-8-7(11)5-2-1-3-12-5/h1-3H,4H2,(H,8,11)(H,9,10)	-0.727
InChI=1S/C10H8ClN3O/c11-9-8(12)6-13-14(10(9)15)7-4-2-1-3-5-7/h1-6H,12H2	-2.744

"InChi"	"logS(M)"
InChI=1S/C5H12O/c1-3-5-6-4-2/h3-5H2,1-2H3	-0.681
InChI=1S/C7H7N3O4/c1-5(11)9-8-4-6-2-3-7(14-6)10(12)13/h2-4H,1H3,(H,9,11)/b8-4+	-2.596
InChI=1S/C10H7Br/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H	-4.4
InChI=1S/C9H7N/c1-2-6-9-8(4-1)5-3-7-10-9/h1-7H	-1.325
InChI=1S/C6H10/c1-2-4-6-5-3-1/h1-2H,3-6H2	-2.71
InChI=1S/C4H8O/c1-3-5-4-2/h3H,1,4H2,2H3	-0.858
InChI=1S/C14H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h15H,2-14H2,1H3	-5.787
InChI=1S/C10H14N4O2/c1-4-5-14-9(15)7-8(11-6-12(7)2)13(3)10(14)16/h6H,4-5H2,1-3H3	-1.208
InChI=1S/C3H2N2O3/c6-1-2(7)5-3(8)4-1/h(H2,4,5,6,7,8)	-0.4
InChI=1S/C14H6Cl2F4N2O2/c15-5-4-8(12(20)10(16)11(5)19)21-14(24)22-13(23)9-6(17)2-1-3-7(9)h1-4H,(H2,21,22,23,24)	-7.302
InChI=1S/C12H14N4O3S/c1-8-14-11(7-12(15-8)19-2)16-20(17,18)10-5-3-9(13)4-6-10/h3-7H,13H2,1-2H3,(H,14,15,16)	-2.543
InChI=1S/C8H14O2/c1-6(2)5-10-8(9)7(3)4/h6H,3,5H2,1-2,4H3	-2.039
InChI=1S/C14H14O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h3-8H,1-2,9-10H2	-3.221
InChI=1S/C7H16O/c1-5-7(4,8)6(2)3/h6,8H,5H2,1-4H3	-0.85
InChI=1S/C10H20/c1-3-5-7-9-10-8-6-4-2/h3H,1,4-10H2,2H3	-5.51
InChI=1S/C10H10O5/c1-14-7-4-3-6(5-11)8(10(12)13)9(7)15-2/h3-5H,1-2H3,(H,12,13)	-1.925
InChI=1S/C19H30O/c1-18-11-4-3-5-13(18)6-7-14-15-8-9-17(20)19(15,2)12-10-16(14)18/h13-16H,3-12H2,1-2H3	-6.7
InChI=1S/C17H19F2N3O3/c1-3-21-8-11(17(24)25)16(23)10-6-12(18)15(13(19)14(10)21)22-5-4-2h6,8-9,20H,3-5,7H2,1-2H3,(H,24,25)	-2.33
InChI=1S/C6H11NO4/c7-4(6(10)11)2-1-3-5(8)9/h4H,1-3,7H2,(H,8,9)(H,10,11)	-1.865
InChI=1S/C20H21N2O3PS/c1-2-25-26(24,22-13-5-8-19(22)23)14-15-9-11-16(12-10-15)20-21-17-h3-4,6-7,9-12H,2,5,8,13-14H2,1H3	-3.73
InChI=1S/C13H11Cl2NO2/c1-12-6-13(12,2)11(18)16(10(12)17)9-4-7(14)3-8(15)5-9/h3-5H,6H2,1-2H3	-4.8
InChI=1S/C7H15Cl/c1-2-3-4-5-6-7-8/h2-7H2,1H3	-3.996
InChI=1S/C5H11Cl2N/c1-8(4-2-6)5-3-7/h2-5H2,1H3	-1.114
InChI=1S/C20H26N2/c1-16(14-21(2)3)15-22-19-10-6-4-8-17(19)12-13-18-9-5-7-11-20(18)2h4-11,16H,12-15H2,1-3H3	-4.79
InChI=1S/C6H12/c1-2-4-6-5-3-1/h1-6H2	-3.1
InChI=1S/C7H16O/c1-5-6(8)7(2,3)4/h6,8H,5H2,1-4H3	-1.151
InChI=1S/C15H18O3/c1-8-10-4-6-15(3)7-5-11(16)9(2)12(15)13(10)18-14(8)17/h5,7-8,10,13H,4,6H2,1-3H3	-3.091

"InChi"	"logS(M)"
InChI=1S/C12H10N2O/c15-13-14(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	-3.753
InChI=1S/C16H14FNO/c17-9-10-18-15-8-4-2-6-13(15)11-12-5-1-3-7-14(12)16(18)19/h1-8H,9-11H2	-3.535
InChI=1S/C7H6O2/c8-5-6-1-3-7(9)4-2-6/h1-5,9H	-0.976
InChI=1S/C7H9N/c1-6-4-2-3-5-7(6)8/h2-5H,8H2,1H3	-0.854
InChI=1S/C10H15NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,10-12H,1-2H3	-1.405
InChI=1S/C10H20/c1-2-3-4-7-10-8-5-6-9-10/h10H,2-9H2,1H3	-6.086
InChI=1S/C11H15N5O5/c12-9-6-10(14-3-13-9)16(4-15-6)11(2-18)8(20)7(19)5(1-17)21-11/h3-5,7-8,17-20H,1-2H2,(H2,12,13,14)	-1.57
InChI=1S/C6H4BrCl/c7-5-2-1-3-6(8)4-5/h1-4H	-3.21
InChI=1S/C9H10O3/c1-11-8-3-4-9(12-2)7(5-8)6-10/h3-6H,1-2H3	-2.32
InChI=1S/C10H8O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7,11H	-2.281
InChI=1S/C10H12O4/c1-3-14-10(12)7-4-5-8(11)9(6-7)13-2/h4-6,11H,3H2,1-2H3	-1.72
InChI=1S/C5H6Cl2N2O2/c1-5(2)3(10)8(6)4(11)9(5)7/h1-2H3	-2.595
InChI=1S/C8H10O/c9-7-6-8-4-2-1-3-5-8/h1-5,9H,6-7H2	-0.786
InChI=1S/C6H10O2/c1-7-6-4-2-3-5-8-6/h3,5-6H,2,4H2,1H3	-0.853
InChI=1S/C7H7ClO/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3	-2.779
InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H	-5.19
InChI=1S/C7H14O/c1-2-3-4-5-6-7-8/h7H,2-6H2,1H3	-1.75

"InChi"	"logS(M)"
InChI=1S/C7H7N3O3S/c1-4(7(12)13)9-10-5(11)6-8-2-3-14-6/h2-3H,1H3,(H,10,11)(H,12,13)/b9-4-	-1.93
InChI=1S/C6H7O3P/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H2,7,8,9)	-1.027
InChI=1S/C18H10N2O/c21-18-13-8-2-1-7-12(13)17-19-14-9-3-5-11-6-4-10-15(16(11)14)20(1h1-10H	-7.256
InChI=1S/C2H3Cl2F/c1-2(3,4)5/h1H3	-2.445
InChI=1S/C14H24N2O4/c1-6-8-14(5,9-19-11(15)17)10-20-12(18)16-13(3,4)7-2/h2H,6,8-10H2,1,3-5H3,(H2,15,17)(H,16,18)	-3.433
InChI=1S/C22H24FN3OS/c23-17-9-7-16(8-10-17)21(27)6-3-13-25-14-11-18(12-15-25)26-20-5-2h1-2,4-5,7-10,18H,3,6,11-15H2,(H,24,28)	-5.679
InChI=1S/C16H26N2O3S/c1-5-6-7-8-9-16(19)18(4)22(20,21)15-12-10-14(11-13-15)17(2)3/h10-13H,5-9H2,1-4H3	-3.68
InChI=1S/C12H14O3/c1-3-14-11(13)10-12(2,15-10)9-7-5-4-6-8-9/h4-8,10H,3H2,1-2H3	-2.314
InChI=1S/C4H8S/c1-2-4-5-3-1/h1-4H2	-1.182
InChI=1S/C12H18O3/c13-11-8-5-7-10(11)6-3-1-2-4-9-12(14)15/h7H,1-6,8-9H2,(H,14,15)	-2.873
InChI=1S/C9H10O2/c1-6-3-7(2)5-8(4-6)9(10)11/h3-5H,1-2H3,(H,10,11)	-3.075
InChI=1S/C3H6O3S/c4-7(5)3-1-2-6-7/h1-3H2	-0.087
InChI=1S/C2H5N3S2/c3-1(6)5-2(4)7/h(H5,3,4,5,6,7)	-1.7
InChI=1S/C7H4Br2O2/c8-5-1-4(3-10)7(11)6(9)2-5/h1-3,11H	-3.422
InChI=1S/C12H25NO3/c1-5-6-12(4,8-14)9-16-11(15)13-7-10(2)3/h10,14H,5-9H2,1-4H3,(H,13,15)	-3.215
InChI=1S/C17H14Cl2N2O2/c18-11-5-6-15-13(9-11)17(12-3-1-2-4-14(12)19)21(7-8-23-17)10-16(2h1-6,9H,7-8,10H2,(H,20,22)	-5.796
InChI=1S/C13H15NO2S/c1-3-16-13(15)14-11-7-5-4-6-10(11)8-9-12(14)17-2/h4-9,12H,3H2,1-2H3	-4.19
InChI=1S/C16H22O11/c1-8(18)23-7-14(25-10(3)20)16(27-12(5)22)15(26-11(4)21)13(6-17)24h6,13-16H,7H2,1-5H3	-2.415
InChI=1S/C13H17NO3/c1-3-8-17-12-6-4-11(9-10(12)2)5-7-13(15)14-16/h4-7,9,16H,3,8H2,1-2H3,(H,14,15)/b7-5+	-3.342
InChI=1S/C17H22N2O/c1-2-7-16-15(5-1)6-3-8-17(16)18-9-4-10-19-11-13-20-14-12-19/h1-3,5-8,18H,4,9-14H2	-2.703
InChI=1S/C13H10O3/c14-11-7-6-10(8-12(11)15)13(16)9-4-2-1-3-5-9/h1-8,14-15H	-2.923
InChI=1S/C7H10O4/c1-5(7(9)11-3)4-6(8)10-2/h1,4H2,2-3H3	-0.654
InChI=1S/C6H8N2O3S/c7-12(10,11)6-3-1-5(8-9)2-4-6/h1-4,8-9H,(H2,7,10,11)	-0.84
InChI=1S/C5H6O/c1-5-3-2-4-6-5/h2-4H,1H3	-1.437
InChI=1S/C10H13ClN2S/c1-7-6-8(11)4-5-9(7)12-10(14)13(2)3/h4-6H,1-3H3,(H,12,14)	-3.66

"InChi"	"logS(M)"
InChI=1S/C18H29NO4/c1-7-22-18(21)16-13(4)8-9-15(12(2)3)17(16)23-11-14(20)10-19(5)6/h8-9,12,14,20H,7,10-11H2,1-6H3	-3.158
InChI=1S/C6H9N3O/c1-2-4-3-8-6(10)9-5(4)7/h3H,2H2,1H3,(H3,7,8,9,10)	-1.02
InChI=1S/C12H15NO/c14-10-12(6-8-13-9-7-12)11-4-2-1-3-5-11/h1-5,10,13H,6-9H2	-1.098
InChI=1S/C15H12F2N4O3/c1-8(13-12(14(22)23)3-2-4-18-13)20-21-15(24)19-11-6-9(16)5-10(17)h2-7H,1H3,(H,22,23)(H2,19,21,24)/b20-8+	-3.725
InChI=1S/C10H16O4/c11-8(12)6-10(7-9(13)14)4-2-1-3-5-10/h1-7H2,(H,11,12)(H,13,14)	-1.472
InChI=1S/C8H9NO2/c1-2-11-8(10)7-4-3-5-9-6-7/h3-6H,2H2,1H3	-0.431
InChI=1S/C6H4BrNO/c7-8-5-1-3-6(9)4-2-5/h1-4H	-1.515
InChI=1S/C7H15NO4S/c9-13(10,11)7-1-2-8-3-5-12-6-4-8/h1-7H2,(H,9,10,11)	0.456
InChI=1S/C10H12N4O3/c1-2-3-8(15)17-6-14-9-7(4-13-14)10(16)12-5-11-9/h4-5H,2-3,6H2,1H3,(H,11,12,16)	-2.83
InChI=1S/C17H23NO6/c1-10(2)18-17(24-13(5)21)8-14-6-15(22-11(3)19)9-16(7-14)23-12(4)2h6-7,9-10,17-18H,8H2,1-5H3	-3.064
InChI=1S/C10H11N3O3/c1-7(14)16-9-4-2-8(3-5-9)6-12-13-10(11)15/h2-6H,1H3,(H3,11,13,15)/b12-6+	-2.84
InChI=1S/C26H27NO9/c1-10-21(29)15(27)7-17(35-10)36-16-9-26(34,11(2)28)8-14-18(16)25(h3-6,10,15-17,21,29,32-34H,7-9,27H2,1-2H3	-4.145
InChI=1S/C12H8O2S/c13-15(14)11-7-3-1-5-9(11)10-6-2-4-8-12(10)15/h1-8H	-4.57
InChI=1S/C10H6O3/c11-8-5-9(12)10(13)7-4-2-1-3-6(7)8/h1-5,11H	-1.65
InChI=1S/C23H32N2O5/c1-3-30-23(29)18(13-12-16-8-5-4-6-9-16)24-15(2)21(26)25-19-11-7-1h4-6,8-9,15,17-20,24H,3,7,10-14H2,1-2H3,(H,27,28)	-4.572
InChI=1S/C4H8N2O2/c7-5-6-1-3-8-4-2-6/h1-4H2	0.935
InChI=1S/C5H10N2O2S/c1-4(10-3)7-9-5(8)6-2/h1-3H3,(H,6,8)/b7-4-	-0.447
InChI=1S/C5H10Br2O2/c6-1-5(2-7,3-8)4-9/h8-9H,1-4H2	-1.13
InChI=1S/C5H9BrO2/c1-3(2)4(6)5(7)8/h3-4H,1-2H3,(H,7,8)	-1.103
InChI=1S/C16H15N5O4S2/c17-26(22,23)13-8-6-12(7-9-13)19-15-10-11-18-16(20-15)21-27(24,25h1-11H,(H2,17,22,23)(H2,18,19,20,21)	-2.55
InChI=1S/C2HCl2F3/c3-1(5)2(4,6)7/h1H	-2.819
InChI=1S/C14H17N3O4S2/c1-17(2)23(20,21)14-9-5-12(6-10-14)16-22(18,19)13-7-3-11(15)4-8-1h3-10,16H,15H2,1-2H3	-2.447
InChI=1S/C2H8N2/c1-4(2)3/h3H2,1-2H3	1.221
InChI=1S/C14H10O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10H	-2.8
InChI=1S/C32H49NO9/c1-6-18(3)25(35)41-24-11-12-26(4)19-8-9-20-28(37)13-23(34)31(39)2h6,17,19-24,34,36-40H,7-16H2,1-5H3/b18-6+	-3.016

"InChi"	"logS(M)"
InChI=1S/C13H13N3O/c1-9-8-15-7-6-12(9)16-13(17)10-2-4-11(14)5-3-10/h2-8H,14H2,1H3,(H,15,16,17)	-1.831
InChI=1S/C14H10Cl4/c1-8-6-12(16)14(18)13(17)11(8)7-9-2-4-10(15)5-3-9/h2-6H,7H2,1H3	-7.44
InChI=1S/C4H8S2/c1-2-6-4-3-5-1/h1-4H2	-1.603
InChI=1S/C11H9ClN2O2S/c12-10-7-4-8-13-11(10)14-17(15,16)9-5-2-1-3-6-9/h1-8H,(H,13,14)	-3.17
InChI=1S/C17H26N2O4S/c1-3-5-10-24-14-8-6-13(7-9-14)17(4-2,11-22-15(18)20)12-23-16(19)2h6-9H,3-5,10-12H2,1-2H3,(H2,18,20)(H2,19,21)	-5.014
InChI=1S/C11H9Cl2NO3/c12-5-1-2-9(8(13)3-5)14-10(15)6-4-7(6)11(16)17/h1-3,6-7H,4H2,(H,14,15)(H,16,17)	-3.87
InChI=1S/C18H23ClN2O3/c19-15-5-3-14(4-6-15)16(22)2-1-11-21-12-8-18(9-13-21)7-10-20-17(2h3-6H,1-2,7-13H2,(H,20,23)	-3.532
InChI=1S/C20H20N2O/c1-4-10-16(11-5-1)18-19(17-12-6-2-7-13-17)23-20(21-18)22-14-8-3-9h1-2,4-7,10-13H,3,8-9,14-15H2	-6.458
InChI=1S/C17H13NO2/c19-17(18(20)14-9-2-1-3-10-14)16-12-6-8-13-7-4-5-11-15(13)16/h1-12,20H	-3.943
InChI=1S/C17H27NO4/c1-6-21-17(20)15-12(4)7-8-14(11(2)3)16(15)22-10-13(19)9-18-5/h7-8,11,13,18-19H,6,9-10H2,1-5H3	-2.876
InChI=1S/C19H34N2O/c1-6-7-10-16-13-18(2,3)21(19(4,5)14-16)17(22)15-20-11-8-9-12-20/h13H,6-12,14-15H2,1-5H3	-5.62
InChI=1S/C14H12O4/c1-17-13(15)11-5-3-10-8-12(14(16)18-2)6-4-9(10)7-11/h3-8H,1-2H3	-6.212
InChI=1S/C12H9F13O2/c1-5(2)6(26)27-4-3-7(13,14)8(15,16)9(17,18)10(19,20)11(21,22)12(23h1,3-4H2,2H3	-6.058
InChI=1S/C23H12OS/c24-23-17-7-2-1-5-13(17)15-11-12-20-22-16(9-10-18(23)21(15)22)14h1-12H	-7.983
InChI=1S/C6H15NO3S2/c1-6(2,3)7-4-5-11-12(8,9)10/h7H,4-5H2,1-3H3,(H,8,9,10)	0.365
InChI=1S/C8H18O2/c1-3-4-7(2)8(5-9)6-10/h7-10H,3-6H2,1-2H3	-1.635
InChI=1S/C13H26O2/c1-2-3-4-5-6-7-8-9-10-11-12-13(14)15/h2-12H2,1H3,(H,14,15)	-3.813
InChI=1S/C8H8N2O2S2/c1-4(11)9-6-7-5(3-13-14-7)10(2)8(6)12/h3H,1-2H3,(H,9,11)	-3.036
InChI=1S/C12H24N2O4/c1-5-12(6-2,7-17-10(13)15)8-18-11(16)14-9(3)4/h9H,5-8H2,1-4H3,(H2,13,15)(H,14,16)	-3.112
InChI=1S/C18H23N3O4/c1-5-20(6-2)15(22)11-25-18(24)14-10-21(7-3)17-13(16(14)23)9-8-12(h8-10H,5-7,11H2,1-4H3	-1.43

"InChi"	"logS(M)"
InChI=1S/C15H12N2O2/ c18-14-13(11-7-3-1-4-8-11)15(19)17(16-14)12-9-5-2-6-10-12/ h1-10,13H,(H,16,18)	-3.595
InChI=1S/C16H14Cl2O4/ c1-10(16(19)20-2)21-12-4-6-13(7-5-12)22-15-8-3-11(17)9-14(15)18/ h3-10H,1-2H3	-3.834
InChI=1S/C15H29NO3/ c1-13(2)9-5-3-6-10-14(17)16-12-8-4-7-11-15(18)19/h13H, 3-12H2,1-2H3,(H,16,17)(H,18,19)	-2.771
InChI=1S/C13H14N2O2/ c1-3-17-12-7-6-11(15-9(2)16)10-5-4-8-14-13(10)12/h4-8H, 3H2,1-2H3,(H,15,16)	-1.517
InChI=1S/C12H14N2/c1-2-5-11-9(4-1)10(8-14-11)12-6-3-7-13-12/ h1-2,4-5,8,12-14H,3,6-7H2	-1.292
InChI=1S/C16H20O3/ c17-15-9-13-11(6-7-12(13)16(18)19)8-14(15)10-4-2-1-3-5-10/ h8-10,12,17H,1-7H2,(H,18,19)	-4.067
InChI=1S/C16H23NO6/ c1-9-13(18)23-11-5-7-17-6-4-10(12(11)17)8-22-14(19)16(3,21)15(9,2 h4,9,11-12,20-21H,5-8H2,1-3H3	0.059
InChI=1S/C15H14N2O3/ c16-15(19)12-8-4-5-9-13(12)20-10-14(18)17-11-6-2-1-3-7-11/h1-9H, 10H2,(H2,16,19)(H,17,18)	-2.059
InChI=1S/C7H8O2S/c1-10-7-3-5(8)2-6(9)4-7/h2-4,8-9H,1H3	-1.796
InChI=1S/C10H28N2O12P4/ c13-25(14,15)7-11(8-26(16,17)18)5-3-1-2-4-6-12(9-27(19,20)21)10-2 h1-10H2,(H2,13,14,15)(H2,16,17,18)(H2,19,20,21)(H2,22,23,24)	-1.516
InChI=1S/C9H7NO2/c1-5-2-3-7-6(4-5)8(11)9(12)10-7/h2-4H,1H3, (H,10,11,12)	-1.231
InChI=1S/C9H11NO2/c1-6(9(11)12)7-2-4-8(10)5-3-7/h2-6H, 10H2,1H3,(H,11,12)	-0.805
InChI=1S/C12H15N/c1-2-3-7-12(10-13)11-8-5-4-6-9-11/ h4-6,8-9,12H,2-3,7H2,1H3	-3.662
InChI=1S/C6H11O3P/c1-2-6-3-7-10(8-4-6)9-5-6/h2-5H2,1H3	-0.144
InChI=1S/C15H24/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,9,12H, 1,4,7-8,10-11H2,2-3,5H3/b15-12-	-6.31
InChI=1S/C3H8S/c1-2-3-4/h4H,2-3H2,1H3	-1.602
InChI=1S/C6H4Cl2N4/c1-12-2-9-5-3(12)4(7)10-6(8)11-5/h2H,1H3	-1.152
InChI=1S/C18H26O2/ c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/ h10,13-17,20H,2-9H2,1H3	-1.948
InChI=1S/C9H13N3O4/c1-2-5-16-7-8(13)6-11-4-3-10-9(11)12(14)15/ h2-4,8,13H,1,5-7H2	-1.59
InChI=1S/C15H13NO3/ c1-10(17)19-14-12(11-6-3-2-4-7-11)8-5-9-13(14)15(16)18/h2-9H, 1H3,(H2,16,18)	-2.228
InChI=1S/C13H16N2/ c1-15-8-4-7-13(15)11-9-14-12-6-3-2-5-10(11)12/h2-3,5-6,9,13-14H, 4,7-8H2,1H3	-1.574
InChI=1S/C24H30F2O6/ c1-20(2)31-19-9-13-14-8-16(25)15-7-12(28)5-6-21(15,3)23(14,26)17(h5-7,13-14,16-17,19,27,29H,8-11H2,1-4H3	-4.616

"InChi"	"logS(M)"
InChI=1S/C7H11NO4/c1-4(9)8-3-5(10)2-6(8)7(11)12/h5-6,10H,2-3H2,1H3,(H,11,12)/p-1	0.345
InChI=1S/C10H8N4O3/c11-9-5-2-7(12-13-9)1-3-8-4-6-10(17-8)14(15)16/h1-6H,(H2,11,13)/b3-1+	-2.649
InChI=1S/C8H7NO5/c10-3-5-6(9(11)12)1-2-7-8(5)14-4-13-7/h1-2,10H,3-4H2	-3.064
InChI=1S/C9H12N2O6/c12-3-4-6(14)7(15)8(17-4)11-2-1-5(13)10-9(11)16/h1-2,4,6-8,12,14-15H,3H2,(H,10,13,16)	-0.601
InChI=1S/C7H13NO2S2/c1-7(2)11-4-5(12-7)3-10-6(8)9/h5H,3-4H2,1-2H3,(H2,8,9)	-2.22
InChI=1S/C8H8N2O3/c11-10(12)8-2-1-6-4-9-13-5-7(6)3-8/h1-3,9H,4-5H2	-2.214
InChI=1S/C12H11N3/c13-10-6-8-12(9-7-10)15-14-11-4-2-1-3-5-11/h1-9H,13H2/b15-14+	-3.76
InChI=1S/C12H14O4/c1-3-4-9-5-6-10(11(7-9)15-2)16-8-12(13)14/h3,5-7H,1,4,8H2,2H3,(H,13,14)/p-1	-2.279
InChI=1S/C12H10FNO2S/c13-10-6-8-12(9-7-10)17(15,16)14-11-4-2-1-3-5-11/h1-9,14H	-3.452
InChI=1S/C12H13ClO4S/c1-17-11(14)12(7-2-8-12)18(15,16)10-5-3-9(13)4-6-10/h3-6H,2,7-8H2,1H3	-3
InChI=1S/C14H19NO3/c1-3-4-9-18-13-7-5-12(10-11(13)2)6-8-14(16)15-17/h5-8,10,17H,3-4,9H2,1-2H3,(H,15,16)/b8-6+	-3.864
InChI=1S/C12H14N2O4S2/c1-12(2,3)10(15)18-7-4-5-8-9(6-7)19-11(14-8)20(13,16)17/h4-6H,1-3H3,(H2,13,16,17)	-3.73
InChI=1S/C12H18/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-10H,1-4H3	-6.603
InChI=1S/C16H17F3N2O6/c1-27-14(25)11(7-9-5-3-2-4-6-9)20-13(24)10(8-12(22)23)21-15(26)16(2-6,10-11H,7-8H2,1H3,(H,20,24)(H,21,26)(H,22,23)	-2.66
InChI=1S/C13H10N2/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1-8H,(H2,14,15)	-4.068
InChI=1S/C13H14N2O3S/c1-18-12-6-4-11(5-7-12)15-19(16,17)13-8-2-10(14)3-9-13/h2-9,15H,14H2,1H3	-4.23
InChI=1S/C15H22N2O2/c1-3-17-9-5-8-14(11-17)19-15(18)16-13-7-4-6-12(2)10-13/h4,6-7,10,14H,3,5,8-9,11H2,1-2H3,(H,16,18)	-3.366
InChI=1S/C3HBr2IO2/c4-1(2(5)6)3(7)8/h(H,7,8)/b2-1+	-1.02
InChI=1S/C14H14N2O5/c1-8(10-6-4-3-5-7-10)14(21-9(2)17)11(18)15-13(20)16-12(14)19/h3-8H,1-2H3,(H2,15,16,18,19,20)	-3.278
InChI=1S/C18H25N3O/c1-2-18(22)19-21-16-10-11-17(21)14-20(13-16)12-6-9-15-7-4-3-5-8-1h3-9,16-17H,2,10-14H2,1H3,(H,19,22)/b9-6+	-3.111
InChI=1S/C14H21NO3/c1-12-6-2-3-8-15(12)9-5-11-18-14(16)13-7-4-10-17-13/h4,7,10,12H,2-3,5-6,8-9,11H2,1H3	-2.517
InChI=1S/C5H13N/c1-4-6-5(2)3/h5-6H,4H2,1-3H3	1.06

"InChi"	"logS(M)"
InChI=1S/C7H4ClN/c8-7-3-1-2-6(4-7)5-9/h1-4H	-2.345
InChI=1S/C4H9NO3/c1-2-3-4-8-5(6)7/h2-4H2,1H3	-2.027
InChI=1S/C9H18O3/c1-3-5-12-8-9(4-2,6-10)7-11/h3,10-11H,1,4-8H2,2H3	-0.2
InChI=1S/C20H22N2O2/c1-3-19-10-22(2)16-11-9-24-15(8-13(11)19)20(17(16)19)12-6-4-5-7-1h3-7,11,13,15-17H,1,8-10H2,2H3,(H,21,23)	-3.032
InChI=1S/C6H7NO/c8-6-4-1-2-5(3-4)7-6/h1-2,4-5H,3H2,(H,7,8)	0.936
InChI=1S/C18H15NO2/c20-15-8-4-13(5-9-15)18(17-3-1-2-12-19-17)14-6-10-16(21)11-7-14/h1-12,18,20-21H	-4.524
InChI=1S/C11H12O4/c1-14-10-7-8(3-5-9(10)12)4-6-11(13)15-2/h3-7,12H,1-2H3/b6-4+	-2.172
InChI=1S/C8H16N2O2/c1-3-12-8(11)10-6-4-9(2)5-7-10/h3-7H2,1-2H3	1.13
InChI=1S/C23H29NO3/c1-3-21(19-10-6-4-7-11-19)23(25)27-17-15-24-14-16-26-22(18(24)2)2h4-13,18,21-22H,3,14-17H2,1-2H3	-4.588
InChI=1S/C10H14O3/c1-9-4-3-6(5-7(9)11)10(9,2)8(12)13/h6H,3-5H2,1-2H3,(H,12,13)	-1.78
InChI=1S/C11H17NO3S2/c13-17(14,15)16-10-9-12-8-4-7-11-5-2-1-3-6-11/h1-3,5-6,12H,4,7-10H2,(H,13,14,15)	-1.22
InChI=1S/C18H14N4O5S/c23-16-9-6-13(11-15(16)18(24)25)21-20-12-4-7-14(8-5-12)28(26,27)2h1-11,20H,(H,19,22)(H,24,25)/b21-13-	-4.495
InChI=1S/C10H20N2O2/c1-3-5-9(13)11-7-8-12-10(14)6-4-2/h3-8H2,1-2H3,(H,11,13)(H,12,14)	-0.622
InChI=1S/C12H18O3/c1-9-4-5-11(6-10(9)2)15-8-12(3,14)7-13/h4-6,13-14H,7-8H2,1-3H3	-2.449
InChI=1S/C42H62O16/c1-37(2)21-8-11-42(7)31(20(43)16-18-19-17-39(4,36(53)54)13-12-38(h16,19,21-31,34-35,44-48H,8-15,17H2,1-7H3,(H,49,50)(H,51,52)(H,53,54)	-7.191
InChI=1S/C3H6N2O/c1-3-5(2)4-6/h3H,1H2,2H3	-0.458
InChI=1S/C8H10BrNO2S/c1-10(2)13(11,12)8-5-3-7(9)4-6-8/h3-6H,1-2H3	-2.781
InChI=1S/C2H4F2/c1-2(3)4/h2H,1H3	-1.315
InChI=1S/C21H23N3O2/c22-12-1-2-15-14(7-12)21-4-5-23-10-11-3-6-26-16-9-18(25)24(15)20(h1-3,7,13,16-17,19-20H,4-6,8-10,22H2	-2.209
InChI=1S/C5H4INO/c6-4-1-2-5(8)7-3-4/h1-3H,(H,7,8)	-1.742
InChI=1S/C6H6N4/c7-1-4-10(5-2-8)6-3-9/h4-6H2	-1.648
InChI=1S/C12H18N2O/c1-4-14(5-2)12-8-6-7-11(9-12)13-10(3)15/h6-9H,4-5H2,1-3H3,(H,13,15)	-2.469
InChI=1S/C4H5ClO2/c1-3(5)2-4(6)7/h2H,1H3,(H,6,7)/b3-2-	-0.605
InChI=1S/C32H62O4/c1-29(2)23-17-13-9-5-7-11-15-21-27-35-31(33)25-19-20-26-32(34)36-h29-30H,5-28H2,1-4H3	-5.708

"InChi"	"logS(M)"
InChI=1S/C21H28N2O/c1-16(2)11-12-21(20(22)24,13-14-23(3)4)19-10-9-17-7-5-6-8-18(17)15h5-11,15H,12-14H2,1-4H3,(H2,22,24)	-5.064
InChI=1S/C10H10O4S/c11-8(12)6-15-9(10(13)14)7-4-2-1-3-5-7/h1-5,9H,6H2,(H,11,12)(H,13,14)	-1.23
InChI=1S/C16H12N2O2/c1-12(13-2-6-15(7-3-13)19-10-17)14-4-8-16(9-5-14)20-11-18/h2-9,12H,1H3	-5.218
InChI=1S/C20H25N3O/c1-19(2,3)13-20(4,5)14-10-11-18(24)17(12-14)23-21-15-8-6-7-9-16(15h6-12,24H,13H2,1-5H3	-5.51
InChI=1S/C14H29NO3S2/c1-4-13(14-7-5-6-11(2)8-14)9-15-12(3)10-19-20(16,17)18/h11-15H,4-10H2,1-3H3,(H,16,17,18)	-3.665
InChI=1S/C6H12N2O/c7-6(9)8-4-2-1-3-5-8/h1-5H2,(H2,7,9)	-0.549
InChI=1S/C8H9NO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5,9H2,(H,10,11)	-1.233
InChI=1S/C14H11N3O3S/c15-21(19,20)12-8-4-2-6-10(12)13-16-11-7-3-1-5-9(11)14(18)17-13/h1-8H,(H2,15,19,20)(H,16,17,18)	-3.08
InChI=1S/C12H18O/c1-8(2)10-5-6-12(13)11(7-10)9(3)4/h5-9,13H,1-4H3	-3.701
InChI=1S/C6HBr5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H	-6.6
InChI=1S/C9H15NO/c1-10-7-3-2-4-8(10)6-9(11)5-7/h7-8H,2-6H2,1H3	0.417
InChI=1S/C9H9N5O/c10-8-3-1-7(2-4-8)9(15)13-14-6-11-5-12-14/h1-6H,10H2,(H,13,15)	-1.42
InChI=1S/C14H31NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-15-13-14-19-20(16,17)18/h15H,2-14H2,1H3,(H,16,17,18)	-3.902
InChI=1S/C17H18O/c1-12(11-18)14-8-9-17-15(10-14)7-6-13-4-2-3-5-16(13)17/h2-5,8-10,12,18H,6-7,11H2,1H3	-5.579
InChI=1S/C19H20Cl2N2O5/c1-2-27-12-11-22(19(24)18(20)21)13-14-3-7-16(8-4-14)28-17-9-5-15(h3-10,18H,2,11-13H2,1H3	-6.449
InChI=1S/C17H17N3O2/c1-11(2)19-20-17(21)18-16-12-7-3-5-9-14(12)22-15-10-6-4-8-13(15)1h3-10,16H,1-2H3,(H2,18,20,21)	-4.17
InChI=1S/C9H16O/c1-7-4-8(10)6-9(2,3)5-7/h7H,4-6H2,1-3H3	-1.647
InChI=1S/C8H16N2O2/c1-3-7(11)9-5-6-10-8(12)4-2/h3-6H2,1-2H3,(H,9,11)(H,10,12)	0.375
InChI=1S/C9H9NO3/c1-10-4-9(13)5-2-7(11)8(12)3-6(5)10/h2-3,9,13H,4H2,1H3	0.747
InChI=1S/C35H62O3/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-38-32(36)25-3h27-28,37H,8-26H2,1-7H3	-8.27
InChI=1S/C12H21N5O2S2/c1-13-11(6-17(18)19)14-4-5-20-8-10-9-21-12(15-10)7-16(2)3/h6,9,13-14H,4-5,7-8H2,1-3H3/b11-6+	-0.566

"InChi"	"logS(M)"
InChI=1S/C19H17NO7/c1-2-25-19(24)27-8-7-26-13-9-12(21)14-15(16(13)20)18(23)11-6-4-3-h3-6,9,21H,2,7-8,20H2,1H3	-9.22
InChI=1S/C5H12FN/c6-4-2-1-3-5-7/h1-5,7H2	-0.043
InChI=1S/C17H18ClN3O/c1-10-7-12(17(2,3)4)16(22)15(8-10)21-19-13-6-5-11(18)9-14(13)20-2h5-9,22H,1-4H3	-5.499
InChI=1S/C16H32N4O2/c1-15(2)8-12(18-14(22)20(6)7)9-16(3,10-15)11-17-13(21)19(4)5/h12H,8-11H2,1-7H3,(H,17,21)(H,18,22)	-1.894
InChI=1S/C15H12ClNO3S/c16-9-1-4-13-12(7-9)17(6-5-15(19)20)11-3-2-10(18)8-14(11)21-13/h1-4,7-8,18H,5-6H2,(H,19,20)	-5.618
InChI=1S/C19H38O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21/h2-18H2,1H3,(H,20,21)	-3.776
InChI=1S/C3H2N4O4/c8-6(9)2-1-4-3(5-2)7(10)11/h1H,(H,4,5)	-0.916
InChI=1S/C10H11ClN2O/c11-6-3-7-13-9-5-2-1-4-8(9)12-10(13)14/h1-2,4-5H,3,6-7H2,(H,12,14)	-3.02
InChI=1S/C10H17N3O2/c1-7(2)13-9(6-8(3)11-13)15-10(14)12(4)5/h6-7H,1-5H3	0.675
InChI=1S/C9H15NO2/c1-6(2)9(3)4-7(11)10-8(12)5-9/h6H,4-5H2,1-3H3,(H,10,11,12)	-1.238
InChI=1S/C12H4Cl2F6N4OS/c13-5-1-4(11(15,16)17)2-6(14)8(5)24-10(22)9(7(3-21)23-24)26(25)12h1-2H,22H2/p+1	-5.362
InChI=1S/C17H35NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-17(20)16(2)19/h16,19H,3-15H2,1-2H3,(H,18,20)	-3.978
InChI=1S/C12H16N2O4/c1-12(7-17-10(13)15,8-18-11(14)16)9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H2,13,15)(H2,14,16)	-2.08
InChI=1S/C11H10N2O3/c1-11(7-5-3-2-4-6-7)8(14)12-10(16)13-9(11)15/h2-6H,1H3,(H2,12,13,14,15,16)	-2.458
InChI=1S/C22H35NO3/c1-4-5-10-19(3)26-21-13-11-20(12-14-21)22(24)25-17-8-16-23-15-7-6h11-14,18-19H,4-10,15-17H2,1-3H3	-6.173
InChI=1S/C8H15NO3/c10-8(11)2-1-3-9-4-6-12-7-5-9/h1-7H2,(H,10,11)	0.293
InChI=1S/C22H29FO4/c1-11-6-14-13-8-16(23)15-7-12(25)4-5-21(15,2)20(13)17(26)9-22(14,3h4-5,7,11,13-14,16-17,19-20,24,26H,6,8-10H2,1-3H3	-3.204
InChI=1S/C8H8O3/c1-5-3-7(10)8(11-2)4-6(5)9/h3-4H,1-2H3	-0.811
InChI=1S/C9H21NO3S2/c1-2-3-4-5-6-7-10-8-9-14-15(11,12)13/h10H,2-9H2,1H3,(H,11,12,13)	-1.293
InChI=1S/C8H18/c1-6-7(2)8(3,4)5/h7H,6H2,1-5H3	-4.678
InChI=1S/C10H14O6/c1-7(2)10(14)16-6-5-15-9(13)4-3-8(11)12/h1,3-6H2,2H3,(H,11,12)	-0.707
InChI=1S/C21H25NO/c1-22-18-12-13-19(22)15-20(14-18)23-21(16-8-4-2-5-9-16)17-10-6-3-h2-11,18-21H,12-15H2,1H3	-4.092

"InChi"	"logS(M)"
InChI=1S/C12H13NO2/c1-7-12(2,3)9-6-8(11(14)15)4-5-10(9)13-7/h4-6H,1-3H3,(H,14,15)	-2.663
InChI=1S/C5H12O4/c6-1-5(2-7,3-8)4-9/h6-9H,1-4H2	-0.342
InChI=1S/CH2F2/c2-1-3/h1H2	-1.437
InChI=1S/C10H21NO3S2/c12-16(13,14)15-9-8-11-10-6-4-2-1-3-5-7-10/h10-11H,1-9H2,(H,12,13,14)	-1.643
InChI=1S/C10H14N2O/c1-12(2)8-11-10(13)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H,11,13)	0.42
InChI=1S/C15H28O3/c16-15-11-7-5-3-1-2-4-6-8-12-17-13-9-10-14-18-15/h1-14H2	-4.018
InChI=1S/C8H10O/c1-2-7-3-5-8(9)6-4-7/h3-6,9H,2H2,1H3	-1.4
InChI=1S/C17H16F3NO2/c1-11(2)23-13-7-5-6-12(10-13)21-16(22)14-8-3-4-9-15(14)17(18,19)2h3-11H,1-2H3,(H,21,22)	-4.695
InChI=1S/C8H12O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)	-0.872
InChI=1S/C10H20O/c1-10(2,3)8-4-6-9(11)7-5-8/h8-9,11H,4-7H2,1-3H3	-3.103
InChI=1S/C35H37ClN2O11/c1-16(2)7-9-18-15-19(10-13-22(18)39)31(42)38-25-26(40)20-11-14-2h7-8,10-15,27,29-30,34,37,39-41H,9H2,1-6H3,(H,38,42)	-7.392
InChI=1S/C4H10O2/c5-3-1-2-4-6/h5-6H,1-4H2	1.045
InChI=1S/C17H28O8S4/c18-13(1-5-26)22-9-17(10-23-14(19)2-6-27,11-24-15(20)3-7-28)12-25h26-29H,1-12H2	-5.123
InChI=1S/C17H11ClN6O3/c1-9-15(21-20-13-7-6-10(18)8-14(13)24(26)27)16-19-12-5-3-2-4-11(1h2-8,20H,1H3/b21-15+	-7.583
InChI=1S/C16H22N2O2/c1-6-8-18(9-7-2)15-12(3)10-14(11-13(15)4)20-16(19)17-5/h6-7,10-11H,1-2,8-9H2,3-5H3,(H,17,19)	-3.593
InChI=1S/C16H24N2O/c1-16(15(17)19,14-8-4-2-5-9-14)10-13-18-11-6-3-7-12-18/h2,4-5,8-9H,3,6-7,10-13H2,1H3,(H2,17,19)	-3.214
InChI=1S/C17H10BrNO2/c1-19-13-7-6-12(18)16-15(13)11(8-14(19)20)9-4-2-3-5-10(9)17(16)21h2-8H,1H3	-6.68
InChI=1S/C16H24N2O2/c1-4-18-10-6-9-14(11-18)20-16(19)17-15-12(2)7-5-8-13(15)3/h5,7-8,14H,4,6,9-11H2,1-3H3,(H,17,19)	-3.936
InChI=1S/C13H11N3O3/c1-9-8-14-7-6-12(9)15-13(17)10-2-4-11(5-3-10)16(18)19/h2-8H,1H3,(H,14,15,17)	-3.066
InChI=1S/C27H42O3/c1-3-4-5-6-7-8-9-26(29)30-25-15-14-24-23-12-10-19-18-20(28)11-13-h18,21-25H,3-17H2,1-2H3	-5.72
InChI=1S/C6H10O2/c1-3-5(7-3)6-4(2)8-6/h3-6H,1-2H3	-0.058
InChI=1S/C12H16O2/c1-10(2)9-14-12(13)8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3	-3.271

"InChi"	"logS(M)"
InChI=1S/C8H15NO/c1-7(10)9-8-5-3-2-4-6-8/h8H,2-6H2,1H3,(H,9,10)	-1.576
InChI=1S/C7H5N3O7/c1-17-7-5(9(13)14)2-4(8(11)12)3-6(7)10(15)16/h2-3H,1H3	-3.085
InChI=1S/C9H7NO/c11-8-4-3-7-2-1-5-10-9(7)6-8/h1-6,11H	-2.504
InChI=1S/C6H12O/c1-4-6(7)5(2)3/h4-7H,1H2,2-3H3	-0.515
InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h2,8H,1,3-7H2	-1.997
InChI=1S/C8H14O2/c1-6(9)5-7(10)8(2,3)4/h5H2,1-4H3	-1.63
InChI=1S/C18H18N6O5S2/c1-23-18(20-21-22-23)31-8-10-7-30-16-11(15(27)24(16)12(10)17(28)2 h2-6,11,13,16,25H,7-8H2,1H3,(H,19,26)(H,28,29)	-0.14
InChI=1S/C23H30/c1-3-5-19-8-12-21(13-9-19)23-16-14-22(15-17-23)20-10-6-18(4-2)7-1 h6-7,10-11,14-17,19,21H,3-5,8-9,12-13H2,1-2H3	-7.185
InChI=1S/C2H2N2S3/c5-1-3-2(6)7-4-1/h(H2,3,4,5,6)	-1.762
InChI=1S/C7H7ClO/c1-5-4-6(8)2-3-7(5)9/h2-4,9H,1H3	-1.552
InChI=1S/C6H10O4/c1-4(6(8)9-3)10-5(2)7/h4H,1-3H3	-0.262
InChI=1S/C12H18O4/c1-2-16-12-6-4-3-5-10(12)8-15-9-11(14)7-13/h3-6,11,13-14H,2,7-9H2,1H3	-1.818
InChI=1S/C30H58O4/c1-27(2)21-15-9-7-13-19-25-33-29(31)23-17-11-5-6-12-18-24-30(32)3 h27-28H,5-26H2,1-4H3	-7.252
InChI=1S/C16H10N2O2/c19-15-9-5-1-3-7-11(9)17-13(15)14-16(20)10-6-2-4-8-12(10)18-14/h1-8,17-18H/b14-13-	-6.72
InChI=1S/C50H74O14/c1-27-13-12-16-34-26-57-47-42(51)30(4)21-37(50(34,47)54)48(53)60 h12-13,16-17,19-21,27,29,31-33,35-47,51-52,54H,9-11,14-15,18,22-26H2,1-8H3/b13-12-,28-17-,34-16-	-7.556
InChI=1S/C20H23ClN2/c1-22-16-11-12-17(22)14-23(13-16)20(15-7-3-2-4-8-15)18-9-5-6-10-1 h2-10,16-17,20H,11-14H2,1H3	-4.387
InChI=1S/C6H12O/c1-4-7-5-6(2)3/h4,6H,1,5H2,2-3H3	-1.524
InChI=1S/C21H30N2O2/c1-22-18-9-10-19(22)16-23(15-18)13-14-25-20(24)21(11-5-6-12-21)1 h2-4,7-8,18-19H,5-6,9-16H2,1H3	-3.957
InChI=1S/C14H23N5/c1-12-15-13(18-8-4-2-5-9-18)17-14(16-12)19-10-6-3-7-11-19/h2-11H2,1H3	-5.493
InChI=1S/C16H16FN3O3/c17-12-3-10-13(4-14(12)19-5-8(18)6-19)20(9-1-2-9)7-11(15(10)21)16 h3-4,7-9H,1-2,5-6,18H2,(H,22,23)	-5.32
InChI=1S/C20H25NO/c1-21(2)15-7-14-20(22)18-10-5-3-8-16(18)12-13-17-9-4-6-11-19(17)2 h3-6,8-11,22H,7,12-15H2,1-2H3	-5.159
InChI=1S/C9H9ClOS/c1-2-11-9(12)7-3-5-8(10)6-4-7/h3-6H,2H2,1H3	-3.633
InChI=1S/C23H38N2O8/c1-16(2)19(26)30-10-12-32-21(28)24-9-8-18(5)14-23(6,7)15-25-22(29 h18H,1,3,8-15H2,2,4-7H3,(H,24,28)(H,25,29)	-4.62

"InChi"	"logS(M)"
InChI=1S/C12H18Br2N2O4S2/c13-10-8-11(14)12(16-9-10)20-6-3-1-2-4-15-5-7-21-22(17,18)19/h8-9,15H,1-7H2,(H,17,18,19)	-4.031
InChI=1S/C13H19ClN2O5S2/c1-13(6-3-7-21-13)9-16(2)23(19,20)10-4-5-11(14)12(8-10)22(15,17)1 h4-5,8H,3,6-7,9H2,1-2H3,(H2,15,17,18)	-4.357
InChI=1S/C8H8O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-2,5-6H,3-4H2	-0.714
InChI=1S/C11H10N2O/c1-9-5-2-3-6-10(9)14-11-7-4-8-12-13-11/h2-8H,1H3	-1.969
InChI=1S/C15H14FN3O3/c1-3-22-15(21)13-12-7-18(2)14(20)10-6-9(16)4-5-11(10)19(12)8-17-1 h4-6,8H,3,7H2,1-2H3	-3.376
InChI=1S/C7H9NO5S3/c8-16(12,13)6-3-5-7(14-6)4(9)1-2-15(5,10)11/h3-4,9H,1-2H2,(H2,8,12,13)	-1.28
InChI=1S/C4H6O/c1-3-4(2)5/h1,4-5H,2H3	0.901
InChI=1S/C11H11NO6S/c1-18-11(13)9-6-10(9)19(16,17)8-4-2-7(3-5-8)12(14)15/h2-5,9-10H,6H2,1H3	-3.38
InChI=1S/C12H19NO2/c1-2-3-8-13-9-12(15)10-4-6-11(14)7-5-10/h4-7,12-15H,2-3,8-9H2,1H3	-0.284
InChI=1S/C29H31N5/c30-27-16-18-31-28(32-27)34-22-20-33(21-23-34)19-17-29(24-10-4-1 h1-16,18H,17,19-23H2,(H2,30,31,32)	-5.843
InChI=1S/C13H14N2O/c16-13-10-6-3-4-7-11(10)14-12-8-2-1-5-9-15(12)13/h3-4,6-7H,1-2,5,8-9H2	-2.472
InChI=1S/C8H12N4/c1-7(2,5-9)11-12-8(3,4)6-10/h1-4H3/b12-11+	-2.713
InChI=1S/C8H8F6O3/c1-3(15)5(4(2)16)6(17,7(9,10)11)8(12,13)14/h5,17H,1-2H3	-1.235
InChI=1S/C2H4O2S/c3-2(4)1-5/h5H,1H2,(H,3,4)	-1.964
InChI=1S/C4H7NO2/c5-4(1-2-4)3(6)7/h1-2,5H2,(H,6,7)	0.364
InChI=1S/C11H14O/c1-12-11-7-6-9-4-2-3-5-10(9)8-11/h6-8H,2-5H2,1H3	-2.748
InChI=1S/C14H13NO6/c1-9(16)21-11-5-3-2-4-10(11)14(19)20-8-15-12(17)6-7-13(15)18/h2-5H,6-8H2,1H3	-2.77
InChI=1S/C27H32O6/c1-19(2)25(28)32-17-15-30-23-11-7-21(8-12-23)27(5,6)22-9-13-24(14 h7-14H,1,3,15-18H2,2,4-6H3	-5.379
InChI=1S/C42H23N3O6/c46-37-24-14-7-8-15-25(24)38(47)34-33(37)30(44-42(51)22-12-5-2-6- h1-20,45H,(H,43,50)(H,44,51)	-5.647
InChI=1S/C12H15N/c1-9-8-12(2,3)13-11-7-5-4-6-10(9)11/h4-8,13H,1-3H3	-5.239
InChI=1S/C6H2Br4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H	-6.98
InChI=1S/C8H5ClO4/c9-5-3-1-2-4(7(10)11)6(5)8(12)13/h1-3H,(H,10,11)(H,12,13)	-0.976
InChI=1S/C12H16N2O2/c1-13(2)11(15)9-7-5-6-8-10(9)12(16)14(3)4/h5-8H,1-4H3	0.508

"InChi"	"logS(M)"
InChI=1S/C14H26O7/ c1-2-3-4-5-6-7-10(16)21-13-11(17)9(8-15)20-14(19)12(13)18/ h9,11-15,17-19H,2-8H2,1H3	-2.63
InChI=1S/C14H21NO3/ c1-4-14(10-16,11-18-13(17)15(2)3)12-8-6-5-7-9-12/h5-9,16H, 4,10-11H2,1-3H3	-3.135
InChI=1S/C6H13NO/c1-5(2)4-6(3)7-8/h5,8H,4H2,1-3H3/b7-6-	-2.265
InChI=1S/C22H30N2O/ c1-5-24(4)16-15-22(21(23)25,14-13-17(2)3)20-12-8-10-18-9-6-7-11-1 h6-13H,5,14-16H2,1-4H3,(H2,23,25)	-5.585
InChI=1S/C12H18N2O5/ c15-7-9(16)10(17)11(18)12(19)14-13-6-8-4-2-1-3-5-8/ h1-5,9-11,13,15-18H,6-7H2,(H,14,19)	-1.489
InChI=1S/C8H6ClN5O6S3/ c9-5-2-1-4(3-6(5)14(15)16)23(19,20)13-7-11-12-8(21-7)22(10,17)18/ h1-3H,(H,11,13)(H2,10,17,18)	-1.99
InChI=1S/C10H13NO2/c1-2-7-13-9-6-4-3-5-8(9)10(11)12/h3-6H, 2,7H2,1H3,(H2,11,12)	-1.59
InChI=1S/C9H9NO/c1-10-8-5-3-2-4-7(8)6-9(10)11/h2-5H,6H2,1H3	-1.019
InChI=1S/C8H13N3O2/c1-3-4-11-7(12)5-6(9)10(2)8(11)13/h5H, 3-4,9H2,1-2H3	-1.611
InChI=1S/C12H15N3O3/ c1-4-7-16-10-13-11(17-8-5-2)15-12(14-10)18-9-6-3/h4-6H,1-3,7-9H2	-2.874
InChI=1S/C6H6N2O2/c9-7-5-6-1-3-8(10)4-2-6/h1-5,10H	0.86
InChI=1S/C6H7NO2/c1-3-9-6(8)5(2)4-7/h2-3H2,1H3	-6.717
InChI=1S/C8H11N3O4/c1-3-15-8(12)5-10-6(2)9-4-7(10)11(13)14/ h4H,3,5H2,1-2H3	-2.002
InChI=1S/C12H7Cl3/c13-10-6-2-1-4-8(10)9-5-3-7-11(14)12(9)15/ h1-7H	-5.944
InChI=1S/C12H5Cl5O/ c13-7-2-1-6(5-10(7)16)18-12-9(15)4-3-8(14)11(12)17/h1-5H	-7.35
InChI=1S/C48H84O6/ c1-40(2)31-25-19-13-7-10-16-22-28-36-52-46(49)43-34-35-44(47(50) h34-35,39-42H,7-33,36-38H2,1-6H3	-7.18
InChI=1S/C18H24N2O/ c1-2-18(21)19-13-16-10-11-17(14-19)20(16)12-6-9-15-7-4-3-5-8-15/ h3-9,16-17H,2,10-14H2,1H3/b9-6+	-3.656
InChI=1S/C17H34N2O/ c1-2-3-4-5-6-7-8-12-15-18-17(20)19-16-13-10-9-11-14-16/h16H, 2-15H2,1H3,(H2,18,19,20)	-2.81
InChI=1S/C10H7NO2/c12-10(13)8-3-4-9-7(6-8)2-1-5-11-9/h1-6H,(H, 12,13)	-0.046
InChI=1S/C22H32N2O2/ c1-23-19-12-13-20(23)15-24(14-19)21(26)22(16-25,17-8-4-2-5-9-17)1 h2,4-5,8-9,18-20,25H,3,6-7,10-16H2,1H3	-4.122
InChI=1S/C2H5NO/c1-2-3-4/h2,4H,1H3/b3-2+	0.496
InChI=1S/C12H10O2/c13-11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/ h1-9,13H	-3.229
InChI=1S/C14H20ClNO2/ c1-4-12-8-6-7-11(3)14(12)16(10-18-5-2)13(17)9-15/h6-8H, 4-5,9-10H2,1-3H3	-3.083

"InChi"	"logS(M)"
InChI=1S/C40H53N9O6/c1-3-24(2)34-40(55)49-17-9-7-14-33(49)39(54)48-16-8-6-13-31(48)37h4-5,11-12,21-24,29-34,42H,3,6-10,13-20H2,1-2H3,(H,41,43)(H,44,51)(H,45,52)(H,46,50)	-2.58
InChI=1S/C10H11FN2O6/c1-6(14)18-4-12-3-8(11)9(16)13(10(12)17)5-19-7(2)15/h3H,4-5H2,1-2H3	-1.81
InChI=1S/C5H10O4S/c6-1-4(7)2-9-5(8)3-10/h4,6-7,10H,1-3H2	0.779
InChI=1S/C7H12N2O4/c1-7(2)5(12)8(3-10)6(13)9(7)4-11/h10-11H,3-4H2,1-2H3	0.142
InChI=1S/C3H3BrN2/c4-3-1-5-6-2-3/h1-2H,(H,5,6)	-1.084
InChI=1S/C10H15NO2/c1-2-6-10(13-9(11)12)7-4-3-5-8-10/h1H,3-8H2,(H2,11,12)	-2.883
InChI=1S/C2H7NO/c3-1-2-4/h4H,1-3H2	1.214
InChI=1S/C22H31O4P/c1-20(2)14-8-4-3-5-13-19-24-27(23,25-21-15-9-6-10-16-21)26-22-17-h6-7,9-12,15-18,20H,3-5,8,13-14,19H2,1-2H3	-5.716
InChI=1S/C14H12O3/c15-13-8-6-12(7-9-13)14(16)17-10-11-4-2-1-3-5-11/h1-9,15H,10H2	-3.325
InChI=1S/C14H14O3S/c1-11-7-9-13(10-8-11)18(15,16)17-14-6-4-3-5-12(14)2/h3-10H,1-2H3	-3.942
InChI=1S/C9H12O4/c10-5-7(11)6-13-9-4-2-1-3-8(9)12/h1-4,7,10-12H,5-6H2	-0.65
InChI=1S/C17H16N4O2/c1-12-15(19-16(22)13-7-6-10-18-11-13)17(23)21(20(12)2)14-8-4-3-5-h3-11H,1-2H3,(H,19,22)	-2.931
InChI=1S/C7H7NO3S3/c8-14(10,11)6-3-4-5(9)1-2-12-7(4)13-6/h3H,1-2H2,(H2,8,10,11)	-3.55
InChI=1S/C19H28ClN3/c1-5-23(6-2)11-7-8-15(4)22-19-14(3)13-21-18-12-16(20)9-10-17(18)1h9-10,12-13,15H,5-8,11H2,1-4H3,(H,21,22)	-4.935
InChI=1S/C9H21O4P/c1-4-6-8-12-14(10,11-3)13-9-7-5-2/h4-9H2,1-3H3	-1.5
InChI=1S/C8H10O/c1-7-4-3-5-8(6-7)9-2/h3-6H,1-2H3	-2.365
InChI=1S/C6H14O/c1-4-6(3,7)5-2/h7H,4-5H2,1-3H3	-0.38
InChI=1S/C22H27NO2/c24-21(25)13-3-1-2-8-16-23-22-19-11-6-4-9-17(19)14-15-18-10-5-7-1h4-7,9-12,22-23H,1-3,8,13-16H2,(H,24,25)	-7.114
InChI=1S/C14H21NO4/c1-2-3-4-7-19-14(18)11(15)8-10-5-6-12(16)13(17)9-10/h5-6,9,11,16-17H,2-4,7-8,15H2,1H3	-0.99
InChI=1S/C10H13N5O/c1-3-5-6(4-2)13-9-7(12-5)8(11)14-10(16)15-9/h3-4H2,1-2H3,(H3,11,13,14,15,16)	-3.55
InChI=1S/C9H18N2O4/c1-2-3-4-7(5-14-8(10)12)6-15-9(11)13/h7H,2-6H2,1H3,(H2,10,12)(H2,11,13)	-1.664
InChI=1S/C14H26O2/c1-12(2)10-8-6-5-7-9-11-16-14(15)13(3)4/h12H,3,5-11H2,1-2,4H3	-6.056
InChI=1S/C9H20O/c1-3-5-6-8-9(10)7-4-2/h9-10H,3-8H2,1-2H3	-2.591
InChI=1S/C6H8ClN3/c1-10(2)5-3-4-8-6(7)9-5/h3-4H,1-2H3	-1.002

"InChi"	"logS(M)"
InChI=1S/C13H9ClN2/c14-10-1-3-12-8(6-10)5-9-7-11(15)2-4-13(9)16-12/h1-7H,15H2	-4.58
InChI=1S/C15H19N5O7S/c1-24-8-9-27-10-6-4-5-7-11(10)28(22,23)20-13(21)16-12-17-14(25-2)h4-7H,8-9H2,1-3H3,(H2,16,17,18,19,20,21)	-3.537
InChI=1S/C17H30O7/c1-4-5-6-7-8-9-12(20)21-14-13(11(19)10-18)22-16-15(14)23-17(2,3)2h11,13-16,18-19H,4-10H2,1-3H3	-3.17
InChI=1S/C9H12N4O/c1-13(2)12-11-8-6-4-3-5-7(8)9(10)14/h3-6H,1-2H3,(H2,10,14)/b12-11+	-2.081
InChI=1S/C24H32O10/c1-13(2)7-19(27)33-22-21-17(16(11-30-22)10-29-14(3)25)8-18(24(21)h8,11,13,18,21-22H,7,9-10,12H2,1-6H3	-4.696
InChI=1S/C10H12O4/c1-6(11)7-4-8(13-2)10(12)9(5-7)14-3/h4-5,12H,1-3H3	-1.352
InChI=1S/C6H12O/c1-3-4-6(2)5-7/h5-6H,3-4H2,1-2H3	-1.377
InChI=1S/C15H19N3O3/c1-10-13(16(2)3)14(19)17(4)15(20)18(10)11-6-8-12(21-5)9-7-11/h6-9H,1-5H3	-2.165
InChI=1S/C14H19ClN4O/c15-11-1-3-12(4-2-11)19-7-5-18(6-8-19)10-13-9-17-14(16)20-13/h1-4,13H,5-10H2,(H2,16,17)	-2.81
InChI=1S/C21H44O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-24-20-21(23)19-22/h21-23H,2-20H2,1H3	-7.721
InChI=1S/C21H20N4O3/c1-28-19-7-6-17(20(26)24-13-15-4-2-8-22-11-15)10-18(19)21(27)25-1h2-12H,13-14H2,1H3,(H,24,26)(H,25,27)	-1.63
InChI=1S/C6H11N/c1-6-4-3-5-7(6)2/h4H,3,5H2,1-2H3	0.127
InChI=1S/C7H12O/c1-4-7(8,5-2)6-3/h1,8H,5-6H2,2-3H3	-0.733
InChI=1S/C21H34O3/c1-12(22)15-4-5-16-14-11-19(24)18-10-13(23)6-8-21(18,3)17(14)7-9-h13-19,23-24H,4-11H2,1-3H3	-4.067
InChI=1S/C11H10N2O2/c1-7-6-15-13-10(7)12-9-5-3-2-4-8(9)11(13)14/h2-5,7H,6H2,1H3	-2.394
InChI=1S/C8H5NO2/c10-7-5-3-1-2-4-6(5)9-8(7)11/h1-4H,(H,9,10,11)	-0.984
InChI=1S/C10H18/c1-8(2)10-6-4-9(3)5-7-10/h4,8,10H,5-7H2,1-3H3	-5.01
InChI=1S/C13H20/c1-2-3-4-5-7-10-13-11-8-6-9-12-13/h6,8-9,11-12H,2-5,7,10H2,1H3	-5.596
InChI=1S/C5H8O2/c1-3-4-7-5(2)6/h3H,1,4H2,2H3	-0.553
InChI=1S/C20H29ClO4/c1-4-18(22)16(19(23)5-2)10-8-6-7-9-13-25-20-12-11-15(24-3)14-17(2h11-12,14,16H,4-10,13H2,1-3H3	-5.27
InChI=1S/C8H9NO4/c1-12-6-3-4-8(13-2)7(5-6)9(10)11/h3-5H,1-2H3	-3.017
InChI=1S/C14H21NO3/c1-3-5-10-18-12-8-6-11(7-9-12)13(4-2)14(16)15-17/h6-9,13,17H,3-5,10H2,1-2H3,(H,15,16)	-3.497
InChI=1S/C7H6ClNO2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,9H2,(H,10,11)	-3.677
InChI=1S/C10H6Cl2/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h1-6H	-5.796

"InChi"	"logS(M)"
InChI=1S/C15H28O2/c1-3-5-6-7-8-9-10-11-12-13-14-17-15(16)4-2/h4H,2-3,5-14H2,1H3	-4.381
InChI=1S/C5H8N2O3/c1-3(8)6-5(10)7-4(2)9/h1-2H3,(H2,6,7,8,9,10)	-0.314
InChI=1S/C6H11Cl2O4P/c1-3-10-13(9,11-4-2)12-5-6(7)8/h5H,3-4H2,1-2H3	-2.371
InChI=1S/C12H5Cl5/c13-6-1-2-8(9(15)3-6)12-10(16)4-7(14)5-11(12)17/h1-5H	-7.66
InChI=1S/C11H18O2/c1-8-4-5-11(9(2)6-8)7-13-10(3)12/h6,9,11H,4-5,7H2,1-3H3	-3.25
InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,6,8H,5,7H2,1-3H3	-4.256
InChI=1S/C10H9NO4/c1-2-9-7-4-3-6(11(13)14)5-8(7)10(12)15-9/h3-5,9H,2H2,1H3	-2.55
InChI=1S/C10H16N2O2S/c1-3-5-6-10(4-2)7(13)11-9(15)12-8(10)14/h3-6H2,1-2H3,(H2,11,12,13,14,15)	-3.14
InChI=1S/C21H23O8P/c22-9-11-27-20(24)13-15(21(25)28-12-10-23)14-30(26)19-8-4-2-6-17(h1-8,15,22-23H,9-14H2	-4.462
InChI=1S/C12H8Cl2O2/c13-8-1-4-10(5-2-8)16-12-6-3-9(14)7-11(12)15/h1-7,15H	-4.239
InChI=1S/C11H13NO4/c1-7(13)12-10(11(15)16)6-8-2-4-9(14)5-3-8/h2-5,10,14H,6H2,1H3,(H,12,13)(H,15,16)	0.01
InChI=1S/C11H11NO5S3/c1-17-8-2-4-9(5-3-8)19(13,14)10-6-11(18-7-10)20(12,15)16/h2-7H,1H3,(H2,12,15,16)	-4.22
InChI=1S/C11H23N/c1-6-9-12-10(2,3)7-8-11(12,4)5/h6-9H2,1-5H3	-2.146
InChI=1S/C7H4Br2O2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H,10,11)	-3.682
InChI=1S/C6H15N/c1-4-6(3)7-5-2/h6-7H,4-5H2,1-3H3	-0.21
InChI=1S/C10H6Br2O3/c11-6-3-1-5(2-4-6)9-7(12)8(13)10(14)15-9/h1-4,7,9H	-3.05
InChI=1S/C19H26O3/c1-18-7-5-12(20)9-11(18)3-4-13-14(18)6-8-19(2)16(22)10-15(21)17(1 h9,13-15,17,21H,3-8,10H2,1-2H3	-2.213
InChI=1S/C10H20N2O3S3/c11-10(8-17-18(13,14)15)12-6-7-16-9-4-2-1-3-5-9/h9H,1-8H2,(H2,11,12)(H,13,14,15)	-3.113
InChI=1S/C8H9Br/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2	-3.676
InChI=1S/C13H19NO2/c1-2-3-4-5-10-16-13(15)11-6-8-12(14)9-7-11/h6-9H,2-5,10,14H2,1H3	-3.95
InChI=1S/C10H10O5/c1-2-14-10(13)15-8-6-4-3-5-7(8)9(11)12/h3-6H,2H2,1H3,(H,11,12)	-1.998
InChI=1S/C4H2N2O4/c7-1-2(8)5-4(10)6-3(1)9/h(H2,5,6,8,9,10)	-1.25
InChI=1S/C24H18N4O4/c1-15-11-12-18(28(31)32)14-21(15)26-27-22-19-10-6-5-7-16(19)13-2(h2-14,26H,1H3,(H,25,30)/b27-22-	-7.558
InChI=1S/C20H27NO11/c21-6-10(9-4-2-1-3-5-9)30-20-18(28)16(26)14(24)12(32-20)8-29-19-1 h1-5,10-20,22-28H,7-8H2	-0.77
InChI=1S/C13H14N2O4/c1-2-13(8-7-11(16)14-12(13)17)9-3-5-10(6-4-9)15(18)19/h3-6H,2,7-8H2,1H3,(H,14,16,17)	-2.832

"InChi"	"logS(M)"
InChI=1S/C14H22N2O3/c17-11-14(12(18)16-13(19)15-11)9-7-5-3-1-2-4-6-8-10-14/h1-10H2,(H2,15,16,17,18,19)	-4.59
InChI=1S/C10H14N2O4/c1-3-4-10(7(13)12-9(11)15)5-6(2)16-8(10)14/h3,6H,1,4-5H2,2H3,(H3,11,12,13,15)	-2.35
InChI=1S/C18H26ClN3/c1-4-22(5-2)12-6-7-14(3)21-17-10-11-20-18-13-15(19)8-9-16(17)18/h8-11,13-14H,4-7,12H2,1-3H3,(H,20,21)	-2.83
InChI=1S/C22H47NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23(19-21-24)20-22-2h24-25H,2-22H2,1H3	-5.775
InChI=1S/C8H6O2/c9-5-7-3-1-2-4-8(7)6-10/h1-6H	-1.34
InChI=1S/C12H4Cl6/c13-6-1-2-7(14)12(18)10(6)5-3-8(15)11(17)9(16)4-5/h1-4H	-8.27
InChI=1S/C8H14N2O2/c1-4-6(5(2)3)7(11)10-8(9)12/h4-5H,1-3H3,(H3,9,10,11,12)/b6-4-	-1.483
InChI=1S/C8H18O3/c1-3-9-5-7-11-8-6-10-4-2/h3-8H2,1-2H3	0.79
InChI=1S/C7H10O2/c8-7(9)6-4-2-1-3-5-6/h4H,1-3,5H2,(H,8,9)	-1.256
InChI=1S/C14H24N2O7/c1-5-4-6(17)14(20)13(21-5)22-12-10(19)7(15-2)9(18)8(16-3)11(12)23h5,7-13,15-16,18-20H,4H2,1-3H3	0.088
InChI=1S/C19H16O4/c1-12(20)11-15(13-7-3-2-4-8-13)17-18(21)14-9-5-6-10-16(14)23-19(1h2-10,15,22H,11H2,1H3	-3.063
InChI=1S/C20H20N6O9S/c1-25-19(22-23-24-25)36-8-10-7-35-18-20(34-2,17(33)26(18)13(10)1(h3-6,12,18,27H,7-8H2,1-2H3,(H,21,28)(H,29,30)(H,31,32)	-3.228
InChI=1S/C9H14N3O8P/c10-5-1-2-12(9(15)11-5)8-7(14)6(13)4(20-8)3-19-21(16,17)18/h1-2,4,6-8,13-14H,3H2,(H2,10,11,15)(H2,16,17,18)	-1.199
InChI=1S/C7H11BrN2O4/c1-4(8)7(14)10-2-5(11)9-3-6(12)13/h4H,2-3H2,1H3,(H,9,11)(H,10,14)(H,12,13)	-0.964
InChI=1S/C8H20N/c1-5-9(6-2,7-3)8-4/h5-8H2,1-4H3/q+1	0.885
InChI=1S/C20H22N6O2S/c1-5-26(6-2)17-7-8-18(19(11-17)25-29(4,27)28)23-24-20-15(12-21)9-h7-11,25H,5-6H2,1-4H3/b24-23+	-7.233
InChI=1S/C13H14N2O3/c1-8(16)15-12(13(17)18)6-9-7-14-11-5-3-2-4-10(9)11/h2-5,7,12,14H,6H2,1H3,(H,15,16)(H,17,18)/p-1	-2.312
InChI=1S/C16H26N2O3/c1-4-10-20-15-8-7-13(12-14(15)17)16(19)21-11-9-18(5-2)6-3/h7-8,12H,4-6,9-11,17H2,1-3H3	-2.943
InChI=1S/C14H8O8S2/c15-13-7-3-1-5-9(23(17,18)19)11(7)14(16)12-8(13)4-2-6-10(12)24(20h1-6H,(H,17,18,19)(H,20,21,22)	1.257
InChI=1S/C11H14O2/c1-9(7-8-11(12)13)10-5-3-2-4-6-10/h2-6,9H,7-8H2,1H3,(H,12,13)	-2.283
InChI=1S/C35H63NO2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-36-32(37)25-3h27-28,38H,8-26H2,1-7H3,(H,36,37)	-7.724

"InChi"	"logS(M)"
InChI=1S/C17H24N2O/c1-19-11-10-15-14(12-19)8-5-9-16(15)18-17(20)13-6-3-2-4-7-13/h5,8-9,13H,2-4,6-7,10-12H2,1H3,(H,18,20)	-3.554
InChI=1S/C13H11ClO3/c14-10-5-3-9(4-6-10)12(13(15)16)8-11-2-1-7-17-11/h1-7,12H,8H2,(H,15,16)	-3.681
InChI=1S/C26H21NO6/c1-16(28)27-24-7-5-4-6-23(24)26(25(27)31,19-8-12-21(13-9-19)32-17h4-15H,1-3H3	-4.058
InChI=1S/C16H21N3O2/c1-5-18(6-2)14-12(3)19(13-10-8-7-9-11-13)16(21)17(4)15(14)20/h7-11H,5-6H2,1-4H3	-3.166
InChI=1S/C9H11NO/c1-7-3-5-9(6-4-7)10-8(2)11/h3-6H,1-2H3,(H,10,11)	-2.095
InChI=1S/C11H13IO3/c1-2-3-6-15-11(14)8-4-5-10(13)9(12)7-8/h4-5,7,13H,2-3,6H2,1H3	-3.903
InChI=1S/C13H26O3/c1-10(9-12(2,3)4)8-11(14)15-16-13(5,6)7/h10H,8-9H2,1-7H3	-4.21
InChI=1S/C27H34N4O6S/c1-26(2,3)29-24(34)22-27(4,5)38-16-30(22)25(35)21(32)20(15-17-9-7h6-14,20-22,32H,15-16H2,1-5H3,(H,28,33)(H,29,34)	-3.98
InChI=1S/C13H26O3/c1-9(2)12-5-4-10(3)6-13(12)16-8-11(15)7-14/h9-15H,4-8H2,1-3H3	-2.006
InChI=1S/C12H18N2O2/c1-8-6-10(16-12(15)13-3)7-9(2)11(8)14(4)5/h6-7H,1-5H3,(H,13,15)	-3.347
InChI=1S/C10H9O3P/c11-14(12,13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H2,11,12,13)	-1.619
InChI=1S/C6H12O/c1-4-6(3,7)5-2/h4,7H,1,5H2,2-3H3	-0.768
InChI=1S/C16H34O/c1-3-5-6-7-8-9-10-11-12-13-15-16(17)14-4-2/h16-17H,3-15H2,1-2H3	-6.771
InChI=1S/C10H20N2O4S2/c11-10(7-17-18(14,15)16)12-5-8-1-3-9(6-13)4-2-8/h8-9,13H,1-7H2,(H2,11,12)(H,14,15,16)	-2.028
InChI=1S/C7H9N/c8-6-7-4-2-1-3-5-7/h1-5H,6,8H2	-1.53
InChI=1S/C23H32O5/c1-21-7-5-15(24)10-14(21)3-4-17-18(21)11-19(25)22(2)16(6-8-23(17,h9,14,16-19,25,27H,3-8,10-12H2,1-2H3	-2.963
InChI=1S/C8H18/c1-7(2,3)8(4,5)6/h1-6H3	-4.87
InChI=1S/C9H11N3O2/c1-12(2)11-10-8-5-3-4-7(6-8)9(13)14/h3-6H,1-2H3,(H,13,14)/b11-10+	-2.344
InChI=1S/C16H15N2O6P/c19-14-16(12-7-3-1-4-8-12,13-9-5-2-6-10-13)17-15(20)18(14)11-24-2h1-10H,11H2,(H,17,20)(H2,21,22,23)	-0.43
InChI=1S/C9H10O3/c1-5-2-3-6-7(4-5)9(11)12-8(6)10/h2,6-7H,3-4H2,1H3	-1.1
InChI=1S/C4H10O4S/c1-3-7-9(5,6)8-4-2/h3-4H2,1-2H3	-1.343
InChI=1S/C10H8O6S2/c11-17(12,13)8-4-5-9-7(6-8)2-1-3-10(9)18(14,15)16/h1-6H,(H,11,12,13)(H,14,15,16)	0.54

"InChi"	"logS(M)"
InChI=1S/C13H28O6S3/c1-4-7-10-20(14,15)13(21(16,17)11-8-5-2)22(18,19)12-9-6-3/h13H,4-12H2,1-3H3	-2.97
InChI=1S/C6H12Cl2O2/c7-1-3-9-5-6-10-4-2-8/h1-6H2	-0.996
InChI=1S/C15H21Cl2FN2O3/c1-3-4-5-6-7-9(2)23-10(21)8-22-15-12(17)13(19)11(16)14(18)20-15/h9H,3-8H2,1-2H3,(H2,19,20)	-6.43
InChI=1S/C15H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15(16)17-2/h3-14H2,1-2H3	-6.65
InChI=1S/C16H22O7S/c1-10-5-7-11(8-6-10)24(17,18)20-9-12-13-14(15(19-4)21-12)23-16(2,3)h5-8,12-15H,9H2,1-4H3	-4.156
InChI=1S/C11H16N2O/c1-13(2)9-8-12-11(14)10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3,(H,12,14)	-1.543
InChI=1S/C12H9N2O6P/c15-13(16)9-3-1-5-11(7-9)21(19,20)12-6-2-4-10(8-12)14(17)18/h1-8H,(H,19,20)	-3.071
InChI=1S/C18H25NO3/c1-12-3-5-13(6-4-12)17(11-20)18(21)22-16-9-14-7-8-15(10-16)19(14)2h3-6,14-17,20H,7-11H2,1-2H3	-2.502
InChI=1S/C8H2Cl4O4/c9-3-1(7(13)14)2(8(15)16)4(10)6(12)5(3)11/h(H,13,14)(H,15,16)	-1.926
InChI=1S/C16H20N2O4S2/c1-9-15(21)13(5-19)11(3-17-9)7-23-24-8-12-4-18-10(2)16(22)14(12)6h3-4,19-22H,5-8H2,1-2H3	-3.802
InChI=1S/C29H38N4O10/c1-28(42)13-7-6-9-17(34)18(13)22(35)19-14(28)11-15-21(33(2)3)23(3h6-7,9,14-16,21,31,34-35,38,42-43H,4-5,8,10-12,30H2,1-3H3,(H,32,39)(H,40,41)	-3.643
InChI=1S/C14H13N3O2/c1-10-4-2-3-5-12(10)14(19)17-16-13(18)11-6-8-15-9-7-11/h2-9H,1H3,(H,16,18)(H,17,19)	-2.73
InChI=1S/C15H26O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,11,16H,5-6,8,10,12H2,1-4H3/b14-9+,15-11+	-5.117
InChI=1S/C12H7Cl3O/c13-8-4-6-9(7-5-8)16-12-10(14)2-1-3-11(12)15/h1-7H	-5.91
InChI=1S/C23H32N2O3/c1-18(19-6-7-21-17-22(27-3)9-8-20(21)16-19)23(26)28-15-5-4-10-25-h6-9,16-18H,4-5,10-15H2,1-3H3	-1.29
InChI=1S/C8H6N6O8S3/c9-24(19,20)8-11-10-7(23-8)12-25(21,22)6-2-1-4(13(15)16)3-5(6)14(1h1-3H,(H,10,12)(H2,9,19,20)	-2.91
InChI=1S/C10H10N4O6S3/c1-14-9(21-10(12-14)22(11,17)18)13-23(19,20)7-5-3-2-4-6(7)8(15)16/h2-5H,1H3,(H,15,16)(H2,11,17,18)/b13-9-	-2.51
InChI=1S/C16H24N2O/c1-18(2)16(11-7-4-8-12-16)13-17-15(19)14-9-5-3-6-10-14/h3,5-6,9-10H,4,7-8,11-13H2,1-2H3,(H,17,19)	-3.775
InChI=1S/C11H16O4/c1-11(13,7-12)8-15-10-5-3-9(14-2)4-6-10/h3-6,12-13H,7-8H2,1-2H3	-1.598

"InChi"	"logS(M)"
InChI=1S/C15H16ClN3O4S3/c16-11-6-12-14(7-13(11)25(17,20)21)26(22,23)19-15(18-12)9-24-8-10h1-7,15,18-19H,8-9H2,(H2,17,20,21)	-5.044
InChI=1S/C6H5ClN2O2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H,8H2	-2.538
InChI=1S/C5H8N2O/c1-4-5(2-8)7-3-6-4/h3,8H,2H2,1H3,(H,6,7)	0.268
InChI=1S/C13H18ClNO2/c1-10-5-4-6-11(2)13(10)15(7-8-17-3)12(16)9-14/h4-6H,7-9H2,1-3H3	-2.09
InChI=1S/C8H7N3O6/c12-8(13)4-9-6-2-1-5(10(14)15)3-7(6)11(16)17/h1-3,9H,4H2,(H,12,13)	-1.496
InChI=1S/C14H19BrO3/c1-2-3-4-5-6-9-18-14(17)11-7-8-13(16)12(15)10-11/h7-8,10,16H,2-6,9H2,1H3	-4.42
InChI=1S/C8H11N5O2/c9-8-10-3-6-7(12-8)13(4-11-6)5-15-2-1-14/h3-4,14H,1-2,5H2,(H2,9,10,12)	-1.077
InChI=1S/C6H8N2/c1-2-6(5-8)3-4-7/h6H,2-3H2,1H3	-0.692
InChI=1S/C10H12ClNO2/c1-3-12-10(14)8-5-7(11)4-6(2)9(8)13/h4-5,13H,3H2,1-2H3,(H,12,14)	-3.211
InChI=1S/C5H14N2/c1-7(2)5-3-4-6/h3-6H2,1-2H3	0.991
InChI=1S/C12H19ClN2O4S2/c13-11-4-5-12(15-10-11)19-8-3-1-2-6-14-7-9-20-21(16,17)18/h4-5,10,14H,1-3,6-9H2,(H,16,17,18)	-2.164
InChI=1S/C13H13ClN2O2S/c1-9-8-10(15)6-7-13(9)19(17,18)16-12-5-3-2-4-11(12)14/h2-8,16H,15H2,1H3	-5.05
InChI=1S/C16H17BrFN3O4/c1-9-14(19-13-4-3-10(17)7-12(13)18)11(8-21(2)16(9)24)15(23)20-25-h3-4,7-8,19,22H,5-6H2,1-2H3,(H,20,23)	-2.96
InChI=1S/C14H14N4O/c1-3-18-12-10(6-4-8-15-12)14(19)17(2)11-7-5-9-16-13(11)18/h4-9H,3H2,1-2H3	-2.62
InChI=1S/C7H15N/c1-8-7-5-3-2-4-6-7/h7-8H,2-6H2,1H3	-0.321
InChI=1S/C8H9NO3/c9-4-8(12)5-1-2-6(10)7(11)3-5/h1-3,10-11H,4,9H2	0.777
InChI=1S/C12H20O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h5,11H,6-8H2,1-4H3	-3.931
InChI=1S/C14H23NO4S2/c1-12(20-21(16,17)18)11-15-10-4-3-5-13-6-8-14(19-2)9-7-13/h6-9,12,15H,3-5,10-11H2,1-2H3,(H,16,17,18)	-2.49
InChI=1S/C12H8Cl2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H	-5.524
InChI=1S/C5H6O2/c1-4-2-3-7-5(4)6/h1-3H2	0.184
InChI=1S/C10H11NO4/c1-14-9(12)6-3-4-7(8(11)5-6)10(13)15-2/h3-5H,11H2,1-2H3	-3.719
InChI=1S/C8H4BrNO2/c9-4-1-2-6-5(3-4)7(11)8(12)10-6/h1-3H,(H,10,11,12)	-1.996
InChI=1S/C8H12N2/c9-5-7-1-2-8(6-10)4-3-7/h1-4H,5-6,9-10H2	1.175
InChI=1S/C15H22N2O3/c1-4-17(5-2)10-11-20-15(19)13-6-8-14(9-7-13)16-12(3)18/h6-9H,4-5,10-11H2,1-3H3,(H,16,18)	-1.65

"InChi"	"logS(M)"
InChI=1S/C14H20O2/c1-11-10-14(2,3)16-13(15-11)9-12-7-5-4-6-8-12/h4-8,11,13H,9-10H2,1-3H3	-2.745
InChI=1S/C22H24N2O4/c1-13-9-17(5-7-19(13)23-21(27)11-15(3)25)18-6-8-20(14(2)10-18)24-h5-10H,11-12H2,1-4H3,(H,23,27)(H,24,28)	-5.325
InChI=1S/C9H11Br/c1-7(2)8-5-3-4-6-9(8)10/h3-7H,1-2H3	-4.19
InChI=1S/C24H17Cl2N3O3/c1-32-21-9-5-4-8-19(21)27-24(31)17-12-14-6-2-3-7-16(14)22(23(17)3h2-13,28H,1H3,(H,27,31)/b29-22-	-8.465
InChI=1S/C4H7Cl3O/c1-2-3(8)4(5,6)7/h3,8H,2H2,1H3	-0.948
InChI=1S/C12H12O3/c1-9(13)11(8-12(14)15)7-10-5-3-2-4-6-10/h2-7H,8H2,1H3,(H,14,15)/b11-7-	-1.611
InChI=1S/C11H23O4PS2/c1-6-13-11(12)7-8-18-16(17,14-9(2)3)15-10(4)5/h9-10H,6-8H2,1-5H3	-4.275
InChI=1S/C18H18N2O2/c1-20(12-13-21)18-19-16(14-8-4-2-5-9-14)17(22-18)15-10-6-3-7-11-1h2-11,21H,12-13H2,1H3	-4.39
InChI=1S/C15H21NO5/c1-19-12-7-9-5-4-6-10(16-15(18)21-3)8-11(9)13(17)14(12)20-2/h7,10,17H,4-6,8H2,1-3H3,(H,16,18)	-2.926
InChI=1S/C22H43NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24/h9-10H,2-8,11-21H2,1H3,(H2,23,24)/b10-9+	-6.528
InChI=1S/C12H6Cl4/c13-7-5-10(15)12(11(16)6-7)8-3-1-2-4-9(8)14/h1-6H	-6.65
InChI=1S/C13H24O2/c1-4-13(14)15-11-9-7-5-6-8-10-12(2)3/h4,12H,1,5-11H2,2-3H3	-5.2
InChI=1S/C19H21ClN6O6/c1-5-24(6-2)16-9-14(21-11(3)27)15(10-18(16)32-4)22-23-19-13(20)7-h7-10H,5-6H2,1-4H3,(H,21,27)/b23-22+	-4.667
InChI=1S/C17H13NO3/c19-15-17(21-16(20)18-15)13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)1h1-8H,9-10H2,(H,18,19,20)	-5.417
InChI=1S/C6H12BrNO/c1-3-6(7,4-2)5(8)9/h3-4H2,1-2H3,(H2,8,9)	-1.44
InChI=1S/C13H11N3O2/c17-12(10-5-4-8-14-9-10)16-13(18)15-11-6-2-1-3-7-11/h1-9H,(H2,15,16,17,18)	-3.382
InChI=1S/C22H25N3O/c26-22(17-6-2-1-3-7-17)24-19-11-14-25(15-12-19)13-10-18-16-23-21-h1-9,16,19,23H,10-15H2,(H,24,26)	-5.549
InChI=1S/C7H15N3O5/c1-3(11)5(13)6(14)4(12)2-9-10-7(8)15/h2-6,11-14H,1H3,(H3,8,10,15)/b9-2+	-0.7
InChI=1S/C14H14N2O/c1-14(2,12-6-4-8-16-10-12)13(17)11-5-3-7-15-9-11/h3-10H,1-2H3	-2.053
InChI=1S/C7H4Cl4O/c1-12-4-2-3(8)5(9)7(11)6(4)10/h2H,1H3	-5.261
InChI=1S/C7H6O3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H,(H,9,10)	-1.41
InChI=1S/C13H10O7/c14-7-2-1-6(11(18)13(7)20)10(17)5-3-8(15)12(19)9(16)4-5/h1-4,14-16,18-20H	-3.285

"InChi"	"logS(M)"
InChI=1S/C4H4N2O2/c7-3-1-4(8)6-2-5-3/h1-2H,(H2,5,6,7,8)	-1.587
InChI=1S/C13H12ClN5/c14-6-1-3-7(4-2-6)19-13-9-5-8(12(13)17-18-19)10-11(9)16-15-10/h1-4,8-13H,5H2	-4.87
InChI=1S/C8H7N3/c1-2-4-7(5-3-1)8-9-6-10-11-8/h1-6H,(H,9,10,11)	-1.576
InChI=1S/C20H14/c1-2-5-15-12-19-17(10-14(15)4-1)11-16-9-8-13-6-3-7-18(19)20(13)16h1-7,10-12H,8-9H2	-2.97
InChI=1S/C10H8ClN3O2/c11-7-1-3-8(4-2-7)13-9(15)14-10-12-5-6-16-10/h1-6H,(H2,12,13,14,15)	-3.028
InChI=1S/C11H7ClO2/c12-9-6-5-7-3-1-2-4-8(7)10(9)11(13)14/h1-6H,(H,13,14)	-2.315
InChI=1S/C16H20N2O/c1-17-14-8-9-15(17)12-18(11-14)16(19)10-7-13-5-3-2-4-6-13/h2-7,10,14-15H,8-9,11-12H2,1H3/b10-7+	-2.613
InChI=1S/C15H22O5/c1-2-3-4-5-6-7-8-20-15(19)11-9-12(16)14(18)13(17)10-11/h9-10,16-18H,2-8H2,1H3	-3.894
InChI=1S/C14H18ClN2O3PS/c1-3-9-22-21(18,19-4-2)20-14-10-16-17(11-14)13-7-5-12(15)6-8-13/h5-8,10-11H,3-4,9H2,1-2H3	-4.039
InChI=1S/C9H18O2/c1-7(5-8(10)11)6-9(2,3)4/h7H,5-6H2,1-4H3,(H,10,11)	-2.354
InChI=1S/C7H5Br3O2/c1-2-3(8)7(12)5(10)4(9)6(2)11/h11-12H,1H3	-4.881
InChI=1S/C9H10N2O/c1-12-9-5-3-2-4-8(9)11-7-6-10/h2-5,11H,7H2,1H3	-1.76
InChI=1S/C15H18O6/c1-5(2)6-7-12(17)20-8(6)9(16)13(3)14(4-19-14)10-11(21-10)15(7,13)1h6-11,16,18H,1,4H2,2-3H3	-1.19
InChI=1S/C16H35N/c1-5-9-11-15(7-3)13-17-14-16(8-4)12-10-6-2/h15-17H,5-14H2,1-4H3	-4.237
InChI=1S/C19H20ClNO4/c1-19(2,18(23)24)25-16-9-3-13(4-10-16)11-12-21-17(22)14-5-7-15(20h3-10H,11-12H2,1-2H3,(H,21,22)(H,23,24)	-6.008
InChI=1S/C20H22N2O/c1-20(2,3)16-10-8-15(9-11-16)12-13-23-19-17-6-4-5-7-18(17)21-14-2h4-11,14H,12-13H2,1-3H3	-6.144
InChI=1S/C10H14O4/c11-5-8-3-1-2-4-10(8)14-7-9(13)6-12/h1-4,9,11-13H,5-7H2	-0.256
InChI=1S/C12H12N4O5/c17-12(13-7-1-2-7)8-5-10(14-3-4-14)11(16(20)21)6-9(8)15(18)19/h5-7H,1-4H2,(H,13,17)	-3.39
InChI=1S/C21H29NS2/c1-4-5-16-23-20-13-11-19(12-14-20)21(24-17-15-22(2)3)18-9-7-6-8-1h6-14,21H,4-5,15-17H2,1-3H3	-5.966
InChI=1S/C12H6Cl4/c13-9-3-1-7(5-11(9)15)8-2-4-10(14)12(16)6-8/h1-6H	-8.53
InChI=1S/C10H15N3O6S2/c14-13(15)9-2-3-10(12-8-9)19-6-1-4-11-5-7-20-21(16,17)18/h2-3,8,11H,1,4-7H2,(H,16,17,18)	-0.882

"InChi"	"logS(M)"
InChI=1S/C13H9NO/c15-11-5-6-13-10(8-11)7-9-3-1-2-4-12(9)14-13/h1-8,15H	-3.58
InChI=1S/C7H6N2O3/c8-7(10)5-2-1-3-6(4-5)9(11)12/h1-4H,(H2,8,10)	-1.461
InChI=1S/C16H14Cl2N2O2/c1-19(2)16(22)20(12-8-9-13(17)14(18)10-12)15(21)11-6-4-3-5-7-11/h3-10H,1-2H3	-4.324
InChI=1S/C5H10O/c1-5(2)3-4-6/h3,6H,4H2,1-2H3	-0.129
InChI=1S/C13H9NS/c15-10-14-13-8-6-12(7-9-13)11-4-2-1-3-5-11/h1-9H	-4.85
InChI=1S/C20H25NO6/c1-14(20(25)27-13-19(24)21(7-9-22)8-10-23)15-3-4-17-12-18(26-2)6-h3-6,11-12,14,22-23H,7-10,13H2,1-2H3	-2.96
InChI=1S/C20H16N2O4/c23-19(24)15-12-18(22-14-9-5-2-6-10-14)16(20(25)26)11-17(15)21-1h1-12,21-22H,(H,23,24)(H,25,26)	-4.986
InChI=1S/C6H5IO2/c8-7(9)6-4-2-1-3-5-6/h1-5H	-1.842
InChI=1S/C10H23O2P/c1-4-7-9-13(11,12-6-3)10-8-5-2/h4-10H2,1-3H3	-1.2
InChI=1S/C2HClF4/c3-1(4)2(5,6)7/h1H	-1.959
InChI=1S/C23H30N2O3/c1-17-4-7-21(14-18(17)2)25-12-10-24(11-13-25)15-22(27)16-28-23-8h4-9,14,22,27H,10-13,15-16H2,1-3H3	-3.727
InChI=1S/C14H17NO6/c1-8(2)20-13(16)10-5-11(14(17)21-9(3)4)7-12(6-10)15(18)19/h5-9H,1-4H3	-5.039
InChI=1S/C11H23N/c1-6-12-10(2,3)8-7-9-11(12,4)5/h6-9H2,1-5H3	-2.146
InChI=1S/C24H30N2O5/c1-18(27)21-8-4-6-10-23(21)30-17-20(31-19(2)28)16-25-12-14-26(15h4-11,20H,12-17H2,1-3H3	-4.04
InChI=1S/C13H20O3/c1-9(2)11-5-4-10(3)13(6-11)16-8-12(15)7-14/h4-6,9,12,14-15H,7-8H2,1-3H3	-3.283
InChI=1S/C12H24N2O4S2/c13-9(11(15)16)7-19-5-3-1-2-4-6-20-8-10(14)12(17)18/h9-10H,1-8,13-14H2,(H,15,16)(H,17,18)	-2.77
InChI=1S/C6H11NO4S/c8-6(9)5-7-3-1-2-4-12(7,10)11/h1-5H2,(H,8,9)	-0.59
InChI=1S/C9H10N2O2/c1-6(12)11-8-5-3-2-4-7(8)9(10)13/h2-5H,1H3,(H2,10,13)(H,11,12)	-2.084
InChI=1S/C14H23N5O/c1-3-4-5-6-7-11(10(2)20)19-9-18-12-13(15)16-8-17-14(12)19/h8-11,20H,3-7H2,1-2H3,(H2,15,16,17)	-2.25
InChI=1S/C19H31NO4/c1-4-5-6-7-8-9-10-11-12-24-18-16(22-2)13-15(19(20)21)14-17(18)23-h13-14H,4-12H2,1-3H3,(H2,20,21)	-5.737
InChI=1S/C38H40O8P2/c1-25-14-9-15-26(2)35(25)43-47(39,44-36-27(3)16-10-17-28(36)4)41-h9-24H,1-8H3	-6.837
InChI=1S/C10H9NO2S/c1-2-13-10(12)8-3-5-9(6-4-8)11-7-14/h3-6H,2H2,1H3	-4.05

"InChi"	"logS(M)"
InChI=1S/C13H19N5O4/ c1-2-16-5-7-17(8-6-16)10-12(19)15-14-9-11-3-4-13(22-11)18(20)21/ h3-4,9H,2,5-8,10H2,1H3,(H,15,19)/b14-9+	-2.943
InChI=1S/C20H27NO5/ c1-5-21(6-2)11-10-17-14(4)16-9-8-15(12-18(16)26-20(17)23)25-13-19 h8-9,12H,5-7,10-11,13H2,1-4H3	-3.73
InChI=1S/C5H4N2O4/c8-3-2(4(9)10)1-6-5(11)7-3/h1H,(H,9,10) (H2,6,7,8,11)	-1.938
InChI=1S/C17H25NO2/ c1-15-8-5-6-11-18(15)12-7-13-20-17(19)14-16-9-3-2-4-10-16/ h2-4,9-10,15H,5-8,11-14H2,1H3	-3.657
InChI=1S/C23H27N5O7S/ c1-4-26-10-11-27(19(32)18(26)31)22(35)25-13(12-8-6-5-7-9-12)16(29 h5-9,13-15,20H,4,10-11H2,1-3H3,(H,24,29)(H,25,35)(H,33,34)	-3.399
InChI=1S/C21H30O2/ c1-5-6-7-8-15-10-12-18(22)19-16-13-14(2)9-11-17(16)21(3,4)23-20(1 h9-13,16-17,19-20,22H,5-8H2,1-4H3	-6.866
InChI=1S/C14H9NOS/ c16-14(11-5-2-1-3-6-11)12-7-4-8-13(9-12)15-10-17/h1-9H	-5.4
InChI=1S/C16H25NO4/ c1-10(2)17(11(3)4)16(18)12-8-13(19-5)15(21-7)14(9-12)20-6/ h8-11H,1-7H3	-3.111
InChI=1S/C9H8O2S/c1-7-2-3-9-8(6-7)4-5-12(9,10)11/h2-6H,1H3	-2.65
InChI=1S/C14H14N4O2/ c1-17-12-11(13(19)18(2)14(17)20)15-10(16-12)8-9-6-4-3-5-7-9/ h3-7H,8H2,1-2H3,(H,15,16)	-2.763
InChI=1S/C5H7NO/c1-4-3-5(2)7-6-4/h3H,1-2H3	-1.029
InChI=1S/C5H8N4O/c1-3-7-4(6)9-5(8-3)10-2/h1-2H3,(H2,6,7,8,9)	-1.303
InChI=1S/C11H9I3N2O4/ c1-3(17)15-9-6(12)5(11(19)20)7(13)10(8(9)14)16-4(2)18/h1-2H3,(H, 15,17)(H,16,18)(H,19,20)	-2.01
InChI=1S/C15H9ClO2/ c16-10-7-5-9(6-8-10)13-14(17)11-3-1-2-4-12(11)15(13)18/h1-8,13H	-4.156
InChI=1S/C32H30N2O2/ c1-5-21-13-9-11-19(3)29(21)33-25-17-18-26(34-30-20(4)12-10-14-22(h7-18,33-34H,5-6H2,1-4H3	-7.375
InChI=1S/C12H15NO2/c1-8-4-5-11(9(2)6-8)13-12(15)7-10(3)14/ h4-6H,7H2,1-3H3,(H,13,15)	-1.99
InChI=1S/C7H5NS/c1-3-8-5-6-2-4-9-7(1)6/h1-5H	-1.675
InChI=1S/C11H22N2O3S2/ c12-11(9-17-18(14,15)16)13-8-7-10-5-3-1-2-4-6-10/h10H,1-9H2, (H2,12,13)(H,14,15,16)	-1.244
InChI=1S/C18H38O2/ c1-2-3-4-12-15-18(20)16-13-10-8-6-5-7-9-11-14-17-19/h18-20H, 2-17H2,1H3	-5.156
InChI=1S/C5H12N2O6/c1-5(13-7(10)11)3-2-4-12-6(8)9/h5H, 2-4H2,1H3,(H,8,9)(H,10,11)/q+2	-2.44
InChI=1S/C4H9Cl/c1-2-3-4-5/h2-4H2,1H3	-2.03
InChI=1S/C16H24N2O2/ c1-11(2)18-9-8-14(10-18)20-16(19)17-15-12(3)6-5-7-13(15)4/ h5-7,11,14H,8-10H2,1-4H3,(H,17,19)	-3.873

"InChi"	"logS(M)"
InChI=1S/C12H15BrO3/c1-2-4-9-5-3-6-11(13)12(9)16-8-10(15)7-14/h2-3,5-6,10,14-15H,1,4,7-8H2	-3.978
InChI=1S/C14H12O4/c15-13(16)14(17-11-7-3-1-4-8-11)18-12-9-5-2-6-10-12/h1-10,14H,(H,15,16)	-3.15
InChI=1S/C9H20O3/c1-2-3-4-5-6-12-9(7-10)8-11/h9-11H,2-8H2,1H3	-1.056
InChI=1S/C13H18ClNO/c1-4-5-10(3)13(16)15-11-7-6-9(2)12(14)8-11/h6-8,10H,4-5H2,1-3H3,(H,15,16)	-4.45
InChI=1S/C22H19Br4NO3/c1-21(2)17(19(23)22(24,25)26)18(21)20(28)30-16(12-27)13-7-6-10-15h3-11,16-19H,1-2H3	-6.92
InChI=1S/C11H23NO3/c1-4-6-11(3,8-13)9-15-10(14)12-7-5-2/h13H,4-9H2,1-3H3,(H,12,14)	-2.757
InChI=1S/C15H33N/c1-4-7-10-13-16(14-11-8-5-2)15-12-9-6-3/h4-15H2,1-3H3	-4.033
InChI=1S/C11H14O3/c1-8(12)6-9-4-5-10(13-2)11(7-9)14-3/h4-5,7H,6H2,1-3H3	-1.572
InChI=1S/C6H14O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3-12H,1-2H2	1.09
InChI=1S/C18H36O2/c1-4-7-9-10-11-12-13-14-16-20-18(19)17(6-3)15-8-5-2/h17H,4-16H2,1-3H3	-8.194
InChI=1S/C7H14O3/c1-5(2)4-10-7(9)6(3)8/h5-6,8H,4H2,1-3H3	-0.413
InChI=1S/C17H27NO3/c1-12(2)14-9-8-13(3)15(17(19)20-6)16(14)21-11-7-10-18(4)5/h8-9,12H,7,10-11H2,1-6H3	-3.834
InChI=1S/C12H17BrO3/c1-2-4-9-5-3-6-11(13)12(9)16-8-10(15)7-14/h3,5-6,10,14-15H,2,4,7-8H2,1H3	-4.109
InChI=1S/C16H26N2O2/c1-15(2)8-6-9-16(3,4)18(15)14(19)12-17-11-13-7-5-10-20-13/h5,7,10,17H,6,8-9,11-12H2,1-4H3	-3.486
InChI=1S/C17H19NO/c1-18-11-12-19-17(14-7-3-2-4-8-14)16-10-6-5-9-15(16)13-18/h2-10,17H,11-13H2,1H3	-2.645
InChI=1S/C8H6N2O7/c11-8(12)4-17-7-2-1-5(9(13)14)3-6(7)10(15)16/h1-3H,4H2,(H,11,12)	-1.937
InChI=1S/C9H18NO3PS2/c1-4-8(3)16-14(12,13-5-2)10-6-7-15-9(10)11/h8H,4-7H2,1-3H3	-1.459
InChI=1S/C9H14N2O4S/c1-11-16(12,13)9-5-7(14-2)6(10)4-8(9)15-3/h4-5,11H,10H2,1-3H3	-3.651
InChI=1S/C19H23ClN2/c1-21-12-5-13-22(15-14-21)19(16-6-3-2-4-7-16)17-8-10-18(20)11-9-1h2-4,6-11,19H,5,12-15H2,1H3	-3.991
InChI=1S/C20H19NO3/c22-18-16-8-4-5-9-17(16)19(23)20(18,15-6-2-1-3-7-15)14-21-10-12-2h1-9H,10-14H2	-2.062
InChI=1S/C12H6N2O2/c15-11-9-7(3-1-5-13-9)8-4-2-6-14-10(8)12(11)16/h1-6H	-3.584
InChI=1S/C6H9N3O3S/c1-13(12)5-4-8-3-2-7-6(8)9(10)11/h2-3H,4-5H2,1H3/p+1	-0.031
InChI=1S/C5H4O2/c1-4-2-3-5(6)7-4/h2-3H,1H2	-0.983

"InChi"	"logS(M)"
InChI=1S/C19H31NO3/c1-7-20(8-2)12-13-23-18-16(14(4)5)11-10-15(6)17(18)19(21)22-9-3/h10-11,14H,7-9,12-13H2,1-6H3	-4.877
InChI=1S/C11H11NO4/c1-8(13)12-10(14)7-16-11(15)9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,12,13,14)	-2.4
InChI=1S/C14H21N2O4P/c17-21(15-6-10-18-11-7-15,16-8-12-19-13-9-16)20-14-4-2-1-3-5-14/h1-5H,6-13H2	0.393
InChI=1S/C9H11N5O3/c1-3(15)6(16)4-2-11-7-5(12-4)8(17)14-9(10)13-7/h2-3,6,15-16H,1H3,(H3,10,11,13,14,17)	-2.53
InChI=1S/C31H51NO9/c1-9-25-20(5)29-31(6,41-29)12-10-23(34)17(2)14-21(11-13-33)28(19(h10,12-13,17-22,24-25,27-30,35,37H,9,11,14-16H2,1-8H3/b12-10-	-4.301
InChI=1S/C16H10ClN3O3/c17-13-9-11(20(22)23)6-7-14(13)18-19-16-12-4-2-1-3-10(12)5-8-15(1h1-9,18H/b19-16-	-7.997
InChI=1S/C22H33NO2/c1-18-8-5-6-15-23(18)16-7-17-25-22(24)21-13-11-20(12-14-21)19-9-3h11-14,18-19H,2-10,15-17H2,1H3	-6.343
InChI=1S/C17H28N2O3/c1-4-7-12-21-16-14(9-8-10-15(16)18)17(20)22-13-11-19(5-2)6-3/h8-10H,4-7,11-13,18H2,1-3H3	-3.465
InChI=1S/C3H8S/c1-3-4-2/h3H2,1-2H3	-1.057
InChI=1S/C14H19BrN2O2/c1-2-17-9-3-4-13(10-17)19-14(18)16-12-7-5-11(15)6-8-12/h5-8,13H,2-4,9-10H2,1H3,(H,16,18)	-4.131
InChI=1S/C6H14O3/c1-7-3-5-9-6-4-8-2/h3-6H2,1-2H3	0.845
InChI=1S/C24H38O4/c1-3-5-7-9-11-15-19-27-23(25)21-17-13-14-18-22(21)24(26)28-20-16h13-14,17-18H,3-12,15-16,19-20H2,1-2H3	-7.249
InChI=1S/C9H7Cl2NO2/c10-5-1-2-6(7(11)3-5)9(4-14-9)8(12)13/h1-3H,4H2,(H2,12,13)	-2.886
InChI=1S/C5H8N2O2/c6-2-1-3-7-4-5(8)9/h7H,1,3-4H2,(H,8,9)	0.324
InChI=1S/C9H10O2/c1-2-3-7-4-5-8(10)9(11)6-7/h2,4-6,10-11H,1,3H2	-0.779
InChI=1S/C7H8ClN/c1-5-2-3-6(8)4-7(5)9/h2-4H,9H2,1H3	-2.072
InChI=1S/C22H22O3/c1-24-20-10-6-16(7-11-20)14-18-4-3-5-19(22(18)23)15-17-8-12-21(25h6-15H,3-5H2,1-2H3/b18-14-,19-15+	-6.467
InChI=1S/C9H5BrO2/c10-7-5-9(11)12-8-4-2-1-3-6(7)8/h1-5H	-1.653
InChI=1S/C12H27O4P/c1-10(2)7-14-17(13,15-8-11(3)4)16-9-12(5)6/h10-12H,7-9H2,1-6H3	-3.002
InChI=1S/C26H12N4O2/c31-25-15-12-10-14-22-16(26(32)30-20-8-4-2-6-18(20)28-24(14)30)1h1-12H	-7.758
InChI=1S/C7H4FNO4/c8-5-2-1-4(7(10)11)3-6(5)9(12)13/h1-3H,(H,10,11)	-1.581
InChI=1S/C10H18O/c1-8(2)6-10-7-9(3)4-5-11-10/h6,9-10H,4-5,7H2,1-3H3	-2.224

"InChi"	"logS(M)"
InChI=1S/C10H20N2O3S2/ c11-10(8-16-17(13,14)15)12-7-9-5-3-1-2-4-6-9/h9H,1-8H2, (H2,11,12)(H,13,14,15)	-3.225
InChI=1S/C17H25NO3/ c1-15-7-5-6-10-18(15)11-12-20-13-14-21-17(19)16-8-3-2-4-9-16/ h2-4,8-9,15H,5-7,10-14H2,1H3	-2.905
InChI=1S/C20H28N2O2/ c1-3-20(23)21-14-17-9-10-18(15-21)22(17)13-5-6-16-7-11-19(12-8-16 h5-8,11-12,17-18H,3-4,9-10,13-15H2,1-2H3/b6-5+	-4.463
InChI=1S/C2H6O2/c3-1-2-4/h3-4H,1-2H2	1.207
InChI=1S/C8H11NO2/c9-5-8(11)6-1-3-7(10)4-2-6/h1-4,8,10-11H, 5,9H2	0.815
InChI=1S/C17H15NO3/ c1-10-5-3-4-6-13(10)16-18-14-9-12(11(2)17(19)20)7-8-15(14)21-16/ h3-9,11H,1-2H3,(H,19,20)	-4.173
InChI=1S/C21H29NO3/ c23-20(16-25-21(24)17-10-4-1-5-11-17)22(18-12-6-2-7-13-18)19-14-8 h1,4-5,10-11,18-19H,2-3,6-9,12-16H2	-5.06
InChI=1S/C9H9N3/c10-9-6-7-11-12(9)8-4-2-1-3-5-8/h1-7H,10H2	-1.137
InChI=1S/C20H24O7/ c1-8-4-12(21)16(24)18(3)10(8)5-13-19-7-26-20(25,17(18)19)15(23)9(h4,10-11,13,15-17,23-25H,2,5-7H2,1,3H3	-2.154
InChI=1S/C19H21Cl2NO2/ c1-14-4-3-5-15(2)18(14)19(23)24-17-8-6-16(7-9-17)22(12-10-20)13-1 h3-9H,10-13H2,1-2H3	-6.83
InChI=1S/C6H6N6/c7-12-6-4-5(10-3-11-6)9-2-1-8-4/h1-3H,7H2,(H, 9,10,11,12)	-1.863
InChI=1S/C13H10O4/ c1-7-6-16-11-5-10-8(3-9(7)11)4-12(15-2)13(14)17-10/h3-6H,1-2H3	-5
InChI=1S/C24H34O9/ c1-7-19(25)30-15-23(11-5,16-31-20(26)8-2)13-29-14-24(12-6,17-32-2 h7-10H,1-4,11-18H2,5-6H3	-4.493
InChI=1S/C11H18O/c1-5-10(3)8-7-9-11(4,12)6-2/h2,8,12H, 5,7,9H2,1,3-4H3/b10-8-	-2.303
InChI=1S/C14H15N/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/ h1-10,15H,11-12H2	-2.688
InChI=1S/C7H14O3/c1-6(2)4-10-5-7(9)3-8/h7-9H,1,3-5H2,2H3	-0.478
InChI=1S/C9H10/c1-3-9-6-4-8(2)5-7-9/h3-7H,1H2,2H3	-3.123
InChI=1S/C11H15NO4/ c1-5(13)4-12-10(14)8-6-2-3-7(16-6)9(8)11(12)15/h5-9,13H, 2-4H2,1H3	0.601
InChI=1S/C11H22O3/c12-10-8-6-4-2-1-3-5-7-9-11(13)14/h12H, 1-10H2,(H,13,14)/p-1	-2.704
InChI=1S/C10H9NO/c1-12-10-6-4-9(5-7-10)3-2-8-11/h2-7H,1H3/ b3-2+	-2.267
InChI=1S/C9H17N/c1-8(2)6-5-7-9(3,4)10-8/h5-6,10H,7H2,1-4H3	-1.144
InChI=1S/C16H22N2O4S2/ c1-13-12-16(18-15-7-3-2-6-14(13)15)22-10-5-4-8-17-9-11-23-24(19,2 h2-3,6-7,12,17H,4-5,8-11H2,1H3,(H,19,20,21)	-2.917
InChI=1S/C13H10O4/ c14-10-7-6-9(12(16)13(10)17)11(15)8-4-2-1-3-5-8/h1-7,14,16-17H	-3.345

"InChi"	"logS(M)"
InChI=1S/C9H10N4O3/c1-11-4-10-5-6(8(11)15)12(2)9(16)13(3)7(5)14/h4H,1-3H3	-1.985
InChI=1S/C9H13NO3S2/c10-15(12,13)9-4-2-8(3-5-9)14-7-1-6-11/h2-5,11H,1,6-7H2,(H2,10,12,13)	-2.247
InChI=1S/C15H11N3S/c19-15-16-13(11-7-3-1-4-8-11)14(17-18-15)12-9-5-2-6-10-12/h1-10H,(H,16,18,19)	-7.545
InChI=1S/C13H9FN2/c14-9-5-3-7-11-12(9)13(15)8-4-1-2-6-10(8)16-11/h1-7H,(H2,15,16)	-0.95
InChI=1S/C9H12N2O4/c1-3-9(4-5(2)12)6(13)10-8(15)11-7(9)14/h3-4H2,1-2H3,(H2,10,11,13,14,15)	-0.766
InChI=1S/C9H9NO3/c10-8(11)6-13-9(12)7-4-2-1-3-5-7/h1-5H,6H2,(H2,10,11)	-1.641
InChI=1S/C15H22ClNO2/c1-5-13-8-6-7-12(4)15(13)17(14(18)9-16)10-19-11(2)3/h6-8,11H,5,9-10H2,1-4H3	-3.188
InChI=1S/C11H8O2/c12-11(13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H,12,13)	-3.564
InChI=1S/C8H11NO/c10-7-6-9-8-4-2-1-3-5-8/h1-5,9-10H,6-7H2	-0.474
InChI=1S/C11H16N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h5,7H,2,4,6H2,1,3H3,(H2,12,13,14,15,16)	-2.36
InChI=1S/C14H19N3O2/c1-19-12-6-5-10-8-17(14(15)16-18)7-9-3-2-4-11(12)13(9)10/h5-6,9,18H,2-4,7-8H2,1H3,(H2,15,16)	-1.78
InChI=1S/C17H20O6/c1-9(5-7-13(18)19)4-6-11-15(20)14-12(8-23-17(14)21)10(2)16(11)22-h4,20H,5-8H2,1-3H3,(H,18,19)/b9-4-	-3.817
InChI=1S/C12H22O3/c1-3-4-5-6-11-9-14-8-7-12(11)15-10(2)13/h11-12H,3-9H2,1-2H3	-2.999
InChI=1S/C13H10N2/c14-11-6-3-5-10-8-9-4-1-2-7-12(9)15-13(10)11/h1-8H,14H2	-4.512
InChI=1S/C28H36O3/c1-27-16-14-21(29)18-20(27)9-10-22-23-11-12-25(28(23,2)17-15-24(3h3-7,18,22-25H,8-17H2,1-2H3	-5.27
InChI=1S/C4H8Cl2/c5-3-1-2-4-6/h1-4H2	-0.92
InChI=1S/C8H14N2O2/c1-5-3-4-6(2)8(10-12)7(5)9-11/h5-6,11-12H,3-4H2,1-2H3/b9-7-,10-8+	-1.32
InChI=1S/C16H18N2O4S2/c17-24(20,21)15-9-14(11-23-15)16(19)13-3-1-12(2-4-13)10-18-5-7-22h1-4,9,11H,5-8,10H2,(H2,17,20,21)	-1.52
InChI=1S/C4H9N3O/c1-3(2)6-7-4(5)8/h1-2H3,(H3,5,7,8)	-0.267
InChI=1S/C15H16N2O5/c1-4-17-7-12(15(20)22-8-21-10(3)18)13(19)11-6-5-9(2)16-14(11)17/h5-7H,4,8H2,1-3H3	-2.49
InChI=1S/C8H15N5S/c1-5(2)10-7-11-6(9-3)12-8(13-7)14-4/h5H,1-4H3,(H2,9,10,11,12,13)	-2.566
InChI=1S/C4H5BrO2/c5-3-1-2-4(6)7/h1-2H,3H2,(H,6,7)/b2-1+	-0.74
InChI=1S/C12H22O5/c1-4-14-5-6-15-7-8-16-9-10-17-12(13)11(2)3/h2,4-10H2,1,3H3	-0.603

"InChi"	"logS(M)"
InChI=1S/C12H5Cl5/c13-8-3-1-2-7(11(8)16)6-4-9(14)12(17)10(15)5-6/h1-5H	-7.405
InChI=1S/C5H6N2O3/c1-2-3(8)6-5(10)7-4(2)9/h2H,1H3,(H2,6,7,8,9,10)	-1.13
InChI=1S/C6H3Br3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H	-3.675
InChI=1S/C11H19NO2/c1-3-5-6-10(4-2)9-14-11(13)7-8-12/h10H,3-7,9H2,1-2H3	-3.286
InChI=1S/C8H14O3/c1-4-10-5-6-11-8(9)7(2)3/h2,4-6H2,1,3H3	-0.967
InChI=1S/C18H20N2O4/c1-18(12-23-16(19)21,14-8-4-2-5-9-14)13-24-17(22)20-15-10-6-3-7-11-15/h2-11H,12-13H2,1H3,(H2,19,21)(H,20,22)	-4.566
InChI=1S/C10H14O4/c11-8(6-10(13)14)5-4-7-2-1-3-9(7)12/h2,8,11H,1,3-6H2,(H,13,14)	-0.4
InChI=1S/C13H28N2/c1-6-7-8-14-11-9-12(2,3)15-13(4,5)10-11/h11,14-15H,6-10H2,1-5H3	0.575
InChI=1S/C8H8N6O/c9-6-3-1-5(2-4-6)7(15)10-8-11-13-14-12-8/h1-4H,9H2,(H2,10,11,12,13,14,15)	-0.948
InChI=1S/C13H11NO2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10,16H	-2.73
InChI=1S/C19H15N3/c20-13-7-5-12(6-8-13)19-15-3-1-2-4-17(15)22-18-11-14(21)9-10-16(18)19/h1-11H,20-21H2	-5.165
InChI=1S/C14H19BrN2O2/c1-2-17-8-4-7-13(10-17)19-14(18)16-12-6-3-5-11(15)9-12/h3,5-6,9,13H,2,4,7-8,10H2,1H3,(H,16,18)	-4.131
InChI=1S/C11H22O/c1-2-3-4-5-6-7-8-9-10-11-12/h11H,2-10H2,1H3	-3.152
InChI=1S/C15H14O4/c1-15(2)7-6-10-12(19-15)8-11-9(14(10)17-3)4-5-13(16)18-11/h4-8H,1-3H3	-3.81
InChI=1S/C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)	1.13
InChI=1S/C5H5N/c1-2-4-6-5-3-1/h1-5H	0.76
InChI=1S/C18H27NO3/c1-3-12-18(21,15-9-6-5-7-10-15)17(20)22-16-11-8-13-19(4-2)14-16/h5-7,9-10,16,21H,3-4,8,11-14H2,1-2H3	-2.736
InChI=1S/C8H17NO2/c1-2-3-4-5-6-7-8(10)9-11/h11H,2-7H2,1H3,(H,9,10)	-1.895
InChI=1S/C8H8O4/c9-6-1-2-7(10)5(3-6)4-8(11)12/h1-3,9-10H,4H2,(H,11,12)	0.704
InChI=1S/C12H8N4O6S/c17-12(9-4-6-11(23-9)16(20)21)14-13-7-1-2-8-3-5-10(22-8)15(18)19/h1-7H,(H,14,17)/b2-1+,13-7+	-5.083
InChI=1S/C28H38N2O8/c31-11-15-37-19-17-35-13-3-9-29-23-7-8-24(30-10-4-14-36-18-20-38-h1-2,5-8,29-32H,3-4,9-20H2	0.057
InChI=1S/C30H58O4S/c1-3-5-7-9-11-13-15-17-19-21-25-33-29(31)23-27-35-28-24-30(32)34-h3-28H2,1-2H3	-5.712
InChI=1S/C22H35NO3/c1-3-4-5-8-17-25-21-13-11-20(12-14-21)22(24)26-18-9-16-23-15-7-6-h11-14,19H,3-10,15-18H2,1-2H3	-6.234

"InChi"	"logS(M)"
InChI=1S/C20H38N2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-21-18-19-22-20/h18-19H,2-17H2,1H3,(H,21,22)	-7.215
InChI=1S/C11H14O2/c1-6-5-7(2)9(4)10(8(6)3)11(12)13/h5H,1-4H3,(H,12,13)	-3.033
InChI=1S/C13H20N2O3/c1-8(2)6-7-13(12(3,4)5)9(16)14-11(18)15-10(13)17/h6H,7H2,1-5H3,(H2,14,15,16,17,18)	-3.55
InChI=1S/C8H14N6O10/c1-7(15)23-5-10(13(19)20)3-9(12(17)18)4-11(14(21)22)6-24-8(2)16/h3-6H2,1-2H3	-1.748
InChI=1S/C5H13N/c1-5(2)6(3)4/h5H,1-4H3	1.06
InChI=1S/C14H19NO/c1-9-13-7-10-3-4-11(16)8-12(10)14(9,2)5-6-15-13/h3-4,8-9,13,15-16H,5-7H2,1-2H3	-1.769
InChI=1S/C7H12O6/c8-3-1-7(13,6(11)12)2-4(9)5(3)10/h3-5,8-10,13H,1-2H2,(H,11,12)	0.179
InChI=1S/C14H20N3O5PS/c1-5-19-14(18)11-9-17-12(15-10(11)4)8-13(16-17)22-23(24,20-6-2)21h8-9H,5-7H2,1-4H3	-4.949
InChI=1S/C17H13N3O2/c1-2-20-12-7-9(8-18)15(19)14-13(12)16(21)10-5-3-4-6-11(10)17(14)2h3-7,20H,2,19H2,1H3	-7.638
InChI=1S/C13H18N2O/c16-13(12-7-3-1-4-8-12)14-11-15-9-5-2-6-10-15/h1,3-4,7-8H,2,5-6,9-11H2,(H,14,16)	-2.15
InChI=1S/C14H10Cl4/c1-8-12(16)5-3-10(14(8)18)6-9-2-4-11(15)7-13(9)17/h2-5,7H,6H2,1H3	-7.4
InChI=1S/C20H24N2O2/c1-3-12-22-13-11-18-16(14-22)5-4-6-19(18)21-20(23)15-7-9-17(24-2)h4-10H,3,11-14H2,1-2H3,(H,21,23)	-4.268
InChI=1S/C16H11NS/c1-2-6-12-11(5-1)9-10-14-16(12)18-15-8-4-3-7-13(15)17-14/h1-10,17H	-6.573
InChI=1S/C9H5Cl2N/c10-6-1-2-7-8(11)3-4-12-9(7)5-6/h1-5H	-2.803
InChI=1S/C18H22O5/c1-12-6-5-9-14(19)8-4-2-3-7-13-10-15(20)11-16(21)17(13)18(22)23-1h3,7,10-12,20-21H,2,4-6,8-9H2,1H3/b7-3-	-4.068
InChI=1S/C7H9N5O2S/c1-11-3-2-8-6(11)10-7-9-4-5(15-7)12(13)14/h4H,2-3H2,1H3,(H,8,9,10)	-2.785
InChI=1S/C6H11NO2/c1-5(2)6(8)7-4-9-3/h1,4H2,2-3H3,(H,7,8)	0.792
InChI=1S/C5H10O2/c1-3-4(2)5(6)7/h4H,3H2,1-2H3,(H,6,7)	-0.356
InChI=1S/C16H17NO3/c1-17-16(19)14-8-7-13(11-15(14)20-10-9-18)12-5-3-2-4-6-12/h2-8,11,18H,9-10H2,1H3,(H,17,19)	-2.952
InChI=1S/C19H25NO2/c1-13(21)12-20-9-8-19-7-3-2-4-16(19)18(20)10-14-5-6-15(22)11-17(14)h5-6,11,16,18,22H,2-4,7-10,12H2,1H3	-2.443
InChI=1S/C12H13N3O2/c1-9-7-11(15-17-9)12(16)14-13-8-10-5-3-2-4-6-10/h2-7,13H,8H2,1H3,(H,14,16)	-2.46

"InChi"	"logS(M)"
InChI=1S/C15H12O3/c16-14(10-11-6-2-1-3-7-11)12-8-4-5-9-13(12)15(17)18/h1-9H,10H2,(H,17,18)	-3.447
InChI=1S/C25H36O2/c1-9-16-11-18(22(26)20(13-16)24(3,4)5)15-19-12-17(10-2)14-21(23(1h11-14,26-27H,9-10,15H2,1-8H3	-5.567
InChI=1S/C3H3ClF4/c4-1(2(5)6)3(7)8/h1-3H	-2.417
InChI=1S/C5H12O2/c1-5(2,3-6)4-7/h6-7H,3-4H2,1-2H3	0.901
InChI=1S/C6HCl4NO2/c7-2-1-3(11(12)13)5(9)6(10)4(2)8/h1H	-4.553
InChI=1S/C14H24N2O6/c1-5-7-14(6-2,8-21-12(19)15-10(3)17)9-22-13(20)16-11(4)18/h5-9H2,1-4H3,(H,15,17,19)(H,16,18,20)	-2.667
InChI=1S/C6H11NO2S/c1-5(8)7-3-4-10-6(2)9/h3-4H2,1-2H3,(H,7,8)	0.318
InChI=1S/C10H12N4O3/c1-2-3-8(15)17-6-14-4-7-9(13-14)11-5-12-10(7)16/h4-5H,2-3,6H2,1H3,(H,11,12,13,16)	-2.2
InChI=1S/C5H7N3O/c1-3-2-4(9)5(6)8-7-3/h2H,1H3,(H2,6,8)(H,7,9)	0.611
InChI=1S/C38H42N2O6/c1-39-15-13-25-20-32(42-4)34-22-28(25)29(39)17-23-7-10-27(11-8-2h7-12,19-22,29-30H,13-18H2,1-6H3	-9.864
InChI=1S/C8H12O/c1-2-8(9)6-4-3-5-7-8/h1,9H,3-7H2	-0.705
InChI=1S/C14H12ClNO2/c1-10-2-4-11(5-3-10)14(17)16(18)13-8-6-12(15)7-9-13/h2-9,18H,1H3	-4.42
InChI=1S/C3H4O2/c1-2-3(4)5/h2H,1H2,(H,4,5)	0.006
InChI=1S/C18H19Br2NO3/c1-23-17-4-2-3-14(13-17)18(22)24-16-7-5-15(6-8-16)21(11-9-19)12-1h2-8,13H,9-12H2,1H3	-6.779
InChI=1S/C23H25ClN2O9/c1-22(34)8-6-9-16(26(2)3)18(30)14(21(33)25-7-27)20(32)23(9,35)19(h4-5,8-9,16,27-29,32,34-35H,6-7H2,1-3H3,(H,25,33)	-2.393
InChI=1S/C9H9N3O/c10-5-6-12-8-4-2-1-3-7(8)9(11)13/h1-4,12H,6H2,(H2,11,13)	-1.171
InChI=1S/C18H18N2O/c21-13-12-20(17-7-2-1-3-8-17)14-16-11-10-15-6-4-5-9-18(15)19-16/h1-11,21H,12-14H2	-3.582
InChI=1S/C17H19N3O5S2/c18-27(24,25)13-8-6-11(7-9-13)10-19-17(26)20-14(16(22)23)15(21)12h1-9,14-15,21H,10H2,(H,22,23)(H2,18,24,25)(H2,19,20,26)	-1.29
InChI=1S/C7H5BrN2O/c8-4-1-2-5-6(3-4)11-7(9)10-5/h1-3H,(H2,9,10)	-2.726
InChI=1S/C14H15N3/c1-17(2)14-10-8-13(9-11-14)16-15-12-6-4-3-5-7-12/h3-11H,1-2H3/b16-15+	-5.25
InChI=1S/C11H13NO5/c13-8-3-1-7(2-4-8)5-9(11(16)17)12-6-10(14)15/h1-4,9,12-13H,5-6H2,(H,14,15)(H,16,17)	-2.59
InChI=1S/C10H24N4/c1-3-11-7-9-13-5-2-6-14-10-8-12-4-1/h11-14H,1-10H2	0.698
InChI=1S/C10H15NO3/c1-3-10(4-2)8(13)7(6-12)5-11-9(10)14/h5,12H,3-4,6H2,1-2H3,(H,11,14)	-0.733

"InChi"	"logS(M)"
InChI=1S/C10H20N2O3S2/c11-10(8-16-17(13,14)15)12-9-6-4-2-1-3-5-7-9/h9H,1-8H2,(H2,11,12)(H,13,14,15)	-3.225
InChI=1S/C34H52N2O4/c1-31(2,3)23-17-21(18-24(29(23)39)32(4,5)6)13-15-27(37)35-36-28(3h17-20,39-40H,13-16H2,1-12H3,(H,35,37)(H,36,38)	-7.044
InChI=1S/C7H12N2O2/c10-8-6-4-2-1-3-5-7(6)9-11/h8,10H,1-5H2	-1.425
InChI=1S/C12H10OS/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9,13H	-2.775
InChI=1S/C7H4INS/c8-6-2-1-3-7(4-6)9-5-10/h1-4H	-4.68
InChI=1S/C18H19Cl2NO3/c1-23-16-6-2-14(3-7-16)18(22)24-17-8-4-15(5-9-17)21(12-10-19)13-1h2-9H,10-13H2,1H3	-5.978
InChI=1S/C23H28N2O5/c1-26-6-5-12-10-25-15-9-23-18(25)7-13(12)14(15)11-30-22(23)24-20-h5,8,13-15,18H,6-7,9-11H2,1-4H3/b12-5+	-3.108
InChI=1S/C13H17NO3/c1-14(2)12(15)9-6-10-17-13(16)11-7-4-3-5-8-11/h3-5,7-8H,6,9-10H2,1-2H3	-1.229
InChI=1S/C17H15ClN4O4/c1-10-3-8-14(15(9-10)22(25)26)20-21-16(11(2)23)17(24)19-13-6-4-12h3-9,16H,1-2H3,(H,19,24)/b21-20+	-7.605
InChI=1S/C10H12S2/c1-8-2-4-9(5-3-8)10-11-6-7-12-10/h2-5,10H,6-7H2,1H3	-3.937
InChI=1S/C8H7NO5/c1-14-7-3-5(4-10)2-6(8(7)11)9(12)13/h2-4,11H,1H3	-2.45
InChI=1S/C13H19NO4/c1-3-4-7-18-11-6-5-10(8-12(11)17-2)9-13(15)14-16/h5-6,8,16H,3-4,7,9H2,1-2H3,(H,14,15)	-2.362
InChI=1S/C9H11FN2O6/c10-3-1-12(9(17)11-7(3)16)8-6(15)5(14)4(2-13)18-8/h1,4-6,8,13-15H,2H2,(H,11,16,17)	-0.883
InChI=1S/C14H13N3O4S2/c1-8-7-15-14(22-8)16-13(19)11-12(18)9-5-3-4-6-10(9)23(20,21)17(11h3-7,18H,1-2H3,(H,15,16,19)	-1.92
InChI=1S/C15H11FO3/c16-12-7-5-10(6-8-12)14(17)9-11-3-1-2-4-13(11)15(18)19/h1-8H,9H2,(H,18,19)	-3.749
InChI=1S/C2H2Cl3F/c3-1-2(4,5)6/h1H2	-3.04
InChI=1S/C8H6Cl2O3/c9-5-2-1-3-6(10)8(5)13-4-7(11)12/h1-3H,4H2,(H,11,12)	-2.15
InChI=1S/C12H24N2O4/c1-4-6-8(3)10(18-12(14)16)9(5-2)7-17-11(13)15/h8-10H,4-7H2,1-3H3,(H2,13,15)(H2,14,16)	-3.134
InChI=1S/C6H7N3O2/c1-3-8-5(2)4-7-6(8)9(10)11/h3-4H,1H2,2H3	-1.841
InChI=1S/C7H4BrNO2/c8-4-1-2-6-5(3-4)9-7(10)11-6/h1-3H,(H,9,10)	-2.33
InChI=1S/C12H10O3/c1-2-9(13)10-11(14)7-5-3-4-6-8(7)12(10)15/h3-6,10H,2H2,1H3	-2.385
InChI=1S/C13H9NO2/c15-14(16)11-5-6-13-10(8-11)7-9-3-1-2-4-12(9)13/h1-6,8H,7H2	-4.72

"InChi"	"logS(M)"
InChI=1S/C13H29NO3S2/c1-3-4-5-6-7-8-9-10-13(2)14-11-12-18-19(15,16)17/h13-14H,3-12H2,1-2H3,(H,15,16,17)	-3.317
InChI=1S/C14H22O/c1-2-3-4-5-6-7-10-13-11-8-9-12-14(13)15/h8-9,11-12,15H,2-7,10H2,1H3	-4.822
InChI=1S/C17H14N2O2/c1-12(20)18-17-19-15(13-8-4-2-5-9-13)16(21-17)14-10-6-3-7-11-14/h2-11H,1H3,(H,18,19,20)	-4.189
InChI=1S/C8H18O2/c1-7(2)4-8(3,5-9)6-10/h7,9-10H,4-6H2,1-3H3	-1.603
InChI=1S/C19H20O10/c1-25-18-9-2-3-26-11(9)5-12-14(18)10(21)4-8(28-12)7-27-19-17(24)1h2-5,13,15-17,19-20,22-24H,6-7H2,1H3	-1.605
InChI=1S/C37H69NO5/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-35(39)38-32-33(31-34(38h33-34H,3-32H2,1-2H3,(H,41,42)	-5.784
InChI=1S/C24H33NO5/c1-5-16(2)22(25)24(27)30-13-7-6-12-29-23(26)17(3)18-8-9-20-15-21(h8-11,14-17,22H,5-7,12-13,25H2,1-4H3	-4.52
InChI=1S/C7H4N2O2S/c10-9(11)7-3-1-2-6(4-7)8-5-12/h1-4H	-3.55
InChI=1S/C19H21NS/c1-20(2)13-7-11-17-16-9-4-3-8-15(16)14-21-19-12-6-5-10-18(17)19/h3-6,8-12H,7,13-14H2,1-2H3/b17-11-	-5.291
InChI=1S/C7H9NO2S/c8-6(7(9)10)4-5-2-1-3-11-5/h1-3,6H,4,8H2,(H,9,10)	-0.836
InChI=1S/C11H12N2O4/c1-2-11(14)12-6-8-3-4-10(13(15)16)5-9(8)7-17-12/h3-5H,2,6-7H2,1H3	-2.775
InChI=1S/C16H25NO5S/c1-20-14-11-13(12-15(21-2)16(14)22-3)23(18,19)10-9-17-7-5-4-6-8-1h11-12H,4-10H2,1-3H3	-2.063
InChI=1S/C12H20O2/c1-6-14-11(13)10-9(7-8(2)3)12(10,4)5/h7,9-10H,6H2,1-5H3	-4.765
InChI=1S/C14H22O6/c1-11(2)13(15)19-9-7-17-5-6-18-8-10-20-14(16)12(3)4/h1,3,5-10H2,2,4H3	-1.901
InChI=1S/C8H12N2O3S3/c1-6-2-3-7(15-6)4-10-8(9)5-14-16(11,12)13/h2-3H,4-5H2,1H3,(H2,9,10)(H,11,12,13)	-2.22
InChI=1S/C3H9N3O3S/c4-3(5)6-1-2-10(7,8)9/h1-2H2,(H4,4,5,6)(H,7,8,9)	-0.632
InChI=1S/C10H11NO2/c1-2-3-10(13)11-8-4-6-9(12)7-5-8/h2-7,12H,1H3,(H,11,13)/b3-2+	-2.646
InChI=1S/C8H9Br/c1-2-7-5-3-4-6-8(7)9/h3-6H,2H2,1H3	-3.67
InChI=1S/C13H19ClNO3PS2/c1-4-7-13(16)15(10-21-19(20,17-2)18-3)12-9-6-5-8-11(12)14/h5-6,8-9H,4,7,10H2,1-3H3	-5.204
InChI=1S/C7H6N2/c1-2-6-7(8-4-1)3-5-9-6/h1-5,9H	-1.618
InChI=1S/C12H15NO2/c1-4-9-15-11-8-6-5-7-10(11)12(14)13(2)3/h4-8H,1,9H2,2-3H3	-2.111
InChI=1S/C10H21N/c1-8-6-9(2,3)11-10(4,5)7-8/h8,11H,6-7H2,1-5H3	-1.802
InChI=1S/C2H2ClF3/c3-1-2(4,5)6/h1H2	-1.11

"InChi"	"logS(M)"
InChI=1S/C9H5Cl4NO2/c10-4-1-2-5(6(11)3-4)8(7(14)15)9(12,13)16-8/h1-3H,(H2,14,15)	-3.73
InChI=1S/C5H8O2/c1-3-5(7)4(2)6/h3H2,1-2H3	-0.176
InChI=1S/C22H24N2O6S2/c25-19(11-15-7-3-1-4-8-15)23-17(21(27)28)13-31-32-14-18(22(29)30)h1-10,17-18H,11-14H2,(H,23,25)(H,24,26)(H,27,28)(H,29,30)	-1.833
InChI=1S/C20H23NO4S/c1-23-16-9-11-5-7-14(21)13-10-15(22)17(26-4)8-6-12(13)18(11)20(25h6,8-10,14H,5,7,21H2,1-4H3	-3.11
InChI=1S/C18H19N/c1-2-17-18(13-14-19-17,15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3-12H,2,13-14H2,1H3	-6.571
InChI=1S/C12H10O4/c1-12(8-5-3-2-4-6-8)10(13)7-9(16-12)11(14)15/h2-7H,1H3,(H,14,15)	-2.541
InChI=1S/C16H12BrN5/c1-22-15-7-14-13(5-10(15)8-20-22)16(19-9-18-14)21-12-4-2-3-11(17)h2-9H,1H3,(H,18,19,21)	-3.48
InChI=1S/C12H5Cl5/c13-7-2-1-3-8(14)10(7)6-4-5-9(15)12(17)11(6)16/h1-5H	-6.78
InChI=1S/C11H12N2O2S/c1-7(13(15)11(12)14)10-6-8-4-2-3-5-9(8)16-10/h2-7,15H,1H3,(H2,12,14)	-3.37
InChI=1S/C14H17N5O7S2/c1-4-27(21,22)9-6-5-7-15-12(9)28(23,24)19-14(20)18-13-16-10(25-2)8h5-8H,4H2,1-3H3,(H2,16,17,18,19,20)	-4.635
InChI=1S/C15H21NOS/c1-15(2,13-9-5-3-6-10-13)18-14(17)16-11-7-4-8-12-16/h3,5-6,9-10H,4,7-8,11-12H2,1-2H3	-4.12
InChI=1S/C15H15ClN2O3/c16-10-6-4-5-9-11(10)13(20)18(12(9)19)15(14(17)21)7-2-1-3-8-15/h4-6H,1-3,7-8H2,(H2,17,21)	-4.01
InChI=1S/C12H17NO3/c1-3-16-11-6-4-10(5-7-11)13-12(15)8-9(2)14/h4-7,9,14H,3,8H2,1-2H3,(H,13,15)	-2.321
InChI=1S/C14H8Br6O2/c15-7-3-9(17)13(10(18)4-7)21-1-2-22-14-11(19)5-8(16)6-12(14)20/h3-6H,1-2H2	-6.536
InChI=1S/C11H18ClN5S/c1-13-11-14-9(12)8(18-3)10(15-11)17-6-4-16(2)5-7-17/h4-7H2,1-3H3,(H,13,14,15)	-2.844
InChI=1S/C15H24O/c1-6-15(5,16)11-9-13-12(2)8-7-10-14(13,3)4/h6,9,11,16H,1,7-8,10H2,2-5H3/b11-9+	-3.164
InChI=1S/C10H22/c1-3-5-7-9-10-8-6-4-2/h3-10H2,1-2H3	-6.437
InChI=1S/C7H8FN3O3/c1-10(2)7(14)11-3-4(8)5(12)9-6(11)13/h3H,1-2H3,(H,9,12,13)	-1.53
InChI=1S/C7H7FN2O3/c1-2-5(11)10-6(12)4(8)3-9-7(10)13/h3H,2H2,1H3,(H,9,13)	-0.7
InChI=1S/C23H28O6/c1-17(24)26-13-15-28-21-9-5-19(6-10-21)23(3,4)20-7-11-22(12-8-20)h5-12H,13-16H2,1-4H3	-8.059
InChI=1S/C4H6FNS/c5-2-1-3-7-4-6/h1-3H2	-1.48
InChI=1S/C10H16O4/c1-3-9(11)14-7-10(4-2)5-12-8-13-6-10/h3H,1,4-8H2,2H3	-1.333

"InChi"	"logS(M)"
InChI=1S/C11H20O4/c1-5-11(6-2,7-14-9(3)12)8-15-10(4)13/h5-8H2,1-4H3	-3.125
InChI=1S/C15H24O/c1-10-8-11(14(2,3)4)13(16)12(9-10)15(5,6)7/h8-9,16H,1-7H3	-5.462
InChI=1S/C14H28O4/c1-6-9-10-12(7-2)11-16-13(15)17-18-14(4,5)8-3/h12H,6-11H2,1-5H3	-6.088
InChI=1S/C11H25NO2/c1-2-3-4-5-6-7-8-12-9-11(14)10-13/h11-14H,2-10H2,1H3	-2.22
InChI=1S/C20H30N2O4/c1-3-26-20(25)17(12-11-16-8-5-4-6-9-16)21-15(2)14-22-13-7-10-18(24-6,8-9,15,17-18,21H,3,7,10-14H2,1-2H3,(H,23,24)	-1.24
InChI=1S/C7H5NO5/c9-6-4(7(10)11)2-1-3-5(6)8(12)13/h1-3,9H,(H,10,11)	-2.149
InChI=1S/C29H33ClN2O2/c1-31(2)27(33)29(24-9-5-3-6-10-24,25-11-7-4-8-12-25)19-22-32-20-13-16,34H,17-22H2,1-2H3	-7.071
InChI=1S/C12H4Cl6O/c13-5-3-4-8(11(18)9(5)16)19-12-7(15)2-1-6(14)10(12)17/h1-4H	-7.96
InChI=1S/C13H14N2O2/c1-2-3-6-14-10-8-11(16)12-9(13(10)17)5-4-7-15-12/h4-5,7-8,14H,2-3,6H2,1H3	-1.374
InChI=1S/C5H7NS/c1-2-3-4-6-5-7/h2H,1,3-4H2	-2.391
InChI=1S/C16H24N2O2/c1-14-8-5-6-11-18(14)12-7-13-20-16(19)17-15-9-3-2-4-10-15/h2-4,9-10,14H,5-8,11-13H2,1H3,(H,17,19)	-3.385
InChI=1S/C22H28N2O3/c1-17-6-8-20(9-7-17)24-12-10-23(11-13-24)15-21(26)16-27-22-5-3-4-h3-9,14,21,26H,10-13,15-16H2,1-2H3	-3.158
InChI=1S/C9H10N2O/c12-9(11-6-7-11)10-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,12)	-1.47
InChI=1S/C7H6FNO/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H2,9,10)	-0.721
InChI=1S/C2H3Br2NO/c3-1(4)2(5)6/h1H,(H2,5,6)	-1.057
InChI=1S/C19H18N2O5/c1-11(22)25-17-13-7-3-5-9-15(13)21(19(20)24)16-10-6-4-8-14(16)18(h3-10,17-18H,1-2H3,(H2,20,24)	-3.55
InChI=1S/C5H9N3O/c1-2-8-3-4(9)7-5(8)6/h2-3H2,1H3,(H2,6,7,9)	-0.165
InChI=1S/C12H13N3/c1-9-8-10(2)14-12(13-9)15-11-6-4-3-5-7-11/h3-8H,1-2H3,(H,13,14,15)	-3.217
InChI=1S/C12H24N2O3/c1-7(2)5-9(13)11(15)14-10(12(16)17)6-8(3)4/h7-10H,5-6,13H2,1-4H3,(H,14,15)(H,16,17)	-0.69
InChI=1S/C7H10N2O/c1-3-8-5-6-9(4-2)7(8)10/h3-4H,1-2,5-6H2	-1.156
InChI=1S/C6H6O2S/c7-6(8)3-5-1-2-9-4-5/h1-2,4H,3H2,(H,7,8)	-0.91
InChI=1S/C14H18O6/c15-13(19-7-9-5-17-9)11-3-1-2-4-12(11)14(16)20-8-10-6-18-10/h1-2,9-12H,3-8H2	-1.34
InChI=1S/C16H32O2/c1-3-5-7-9-10-12-14-15(16(17)18)13-11-8-6-4-2/h15H,3-14H2,1-2H3,(H,17,18)	-6.075
InChI=1S/C5H11NO4/c1-2-5(3-7,4-8)6(9)10/h7-8H,2-4H2,1H3	0.826

"InChi"	"logS(M)"
InChI=1S/C9H10O4/c10-5-6-13-9(12)7-3-1-2-4-8(7)11/h1-4,10-11H,5-6H2	-1.157
InChI=1S/C14H13NO/c1-12(16)15(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-11H,1H3	-2.467
InChI=1S/C7H7N/c1-2-7-5-3-4-6-8-7/h2-6H,1H2	-0.582
InChI=1S/C9H14N2O4/c1-3-9(4-2)6(13)10-8(15)11(5-12)7(9)14/h12H,3-5H2,1-2H3,(H,10,13,15)	-3.93
InChI=1S/C16H19N3O2/c1-12-14(18-10-6-7-11-18)15(20)17(2)16(21)19(12)13-8-4-3-5-9-13/h3-5,8-9H,6-7,10-11H2,1-2H3	-2.809
InChI=1S/C15H21NO4/c16-12(8-10-6-7-13(17)14(18)9-10)15(19)20-11-4-2-1-3-5-11/h6-7,9,11-12,17-18H,1-5,8,16H2	-1.27
InChI=1S/C15H20O4/c1-2-3-9-13(12-7-5-4-6-8-12)19-15(18)11-10-14(16)17/h4-8,13H,2-3,9-11H2,1H3,(H,16,17)	-3.908
InChI=1S/C19H17NOS/c21-17-11-12-19(18(22)20-17)15-7-3-1-5-13(15)9-10-14-6-2-4-8-16(14)h1-8H,9-12H2,(H,20,21,22)	-5.339
InChI=1S/C12H18O/c1-8(2)10-6-5-7-11(9(3)4)12(10)13/h5-9,13H,1-4H3	-3.158
InChI=1S/C3H8N2O/c1-5(2)3(4)6/h1-2H3,(H2,4,6)	0.212
InChI=1S/C11H20O/c1-5-10(3)8-7-9-11(4,12)6-2/h6,8,12H,2,5,7,9H2,1,3-4H3/b10-8-	-2.409
InChI=1S/C6H9N3O2/c1-8-6(11)9(2)5(10)3-4-7/h3H2,1-2H3,(H,8,11)	0.171
InChI=1S/C7H7NO2S/c9-11(10)7-4-2-1-3-6(7)5-8-11/h1-4,8H,5H2	-1.521
InChI=1S/C10H18O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h9H,2-8H2,1H3	-1.629
InChI=1S/C13H28O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h14H,2-13H2,1H3	-3.302
InChI=1S/C8H13N3O4/c1-2-15-6-7(12)5-10-4-3-9-8(10)11(13)14/h3-4,7,12H,2,5-6H2,1H3	-1.195
InChI=1S/C17H17ClFN3O3/c1-17(20)6-21(7-17)14-11(19)4-9-13(12(14)18)22(8-2-3-8)5-10(15(9)h4-5,8H,2-3,6-7,20H2,1H3,(H,24,25)	-5.33
InChI=1S/C16H14N2O6S/c1-10(19)18-25(23,24)12-8-6-11(7-9-12)17-15(20)13-4-2-3-5-14(13)1h2-9H,1H3,(H,17,20)(H,18,19)(H,21,22)	-2.52
InChI=1S/C8H10NO6P/c1-5-8(11)7(3-10)6(2-9-5)4-15-16(12,13)14/h2-3,11H,4H2,1H3,(H2,12,13,14)	-1.316
InChI=1S/C8H15NO3/c1-4-5(2)7(8(11)12)9-6(3)10/h5,7H,4H2,1-3H3,(H,9,10)(H,11,12)	-0.591
InChI=1S/C12H3Cl7O/c13-4-1-6(15)8(2-5(4)14)20-9-3-7(16)10(17)12(19)11(9)18/h1-3H	-9.5
InChI=1S/C9H18/c1-8-5-4-6-9(2,3)7-8/h8H,4-7H2,1-3H3	-4.853
InChI=1S/C9H16N4OS/c1-5-15-8-12-11-6(9(2,3)4)7(14)13(8)10/h5,10H2,1-4H3	-2.735
InChI=1S/C9H12N2O3S2/c1-2-11-5-7-3-6-4-8(16(10,12)13)14-9(6)15-7/h3-4,11H,2,5H2,1H3,(H2,10,12,13)	-1.04

"InChi"	"logS(M)"
InChI=1S/C9H10N4O2/c1-2-3-7(14)13-8-6(4-12-13)9(15)11-5-10-8/h4-5H,2-3H2,1H3,(H,10,11,15)	-3.27
InChI=1S/C3H2Cl2F4/c4-3(5,1(6)7)2(8)9/h1-2H	-3.455
InChI=1S/C7H7NO/c8-7-3-1-6(5-9)2-4-7/h1-5H,8H2	-0.872
InChI=1S/C20H31NO3/c1-16(2)15-24-19-10-8-18(9-11-19)20(22)23-14-6-13-21-12-5-4-7-17(h8-11,16-17H,4-7,12-15H2,1-3H3	-5.129
InChI=1S/C5H10O/c1-5(2)3-4-6-5/h3-4H2,1-2H3	-0.956
InChI=1S/C12H12O2/c13-11-6-10(7-12(14)8-11)9-4-2-1-3-5-9/h1-5,10H,6-8H2	-2.51
InChI=1S/C8H16O3/c1-3-4-5-10-6-7-11-8(2)9/h3-7H2,1-2H3	-1.25
InChI=1S/C10H14N2O3/c1-4-10(5-6(2)3)7(13)11-9(15)12-8(10)14/h4,6H,1,5H2,2-3H3,(H2,11,12,13,14,15)	-2.12
InChI=1S/C19H29NO/c21-19(17-9-3-1-4-10-17,18-11-5-2-6-12-18)13-16-20-14-7-8-15-20/h1,3-4,9-10,18,21H,2,5-8,11-16H2	-4.7
InChI=1S/C10H12O2/c11-10(12)8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H,11,12)	-1.78
InChI=1S/C9H6ClNOS2/c10-6-1-3-7(4-2-6)11-8(12)5-14-9(11)13/h1-4H,5H2	-2.056
InChI=1S/C2H4N4O2/c3-1(7)5-6-2(4)8/h(H2,3,7)(H2,4,8)/b6-5+	-3.546
InChI=1S/C19H29NO2/c1-3-18(17-11-5-4-6-12-17)19(21)22-15-9-14-20-13-8-7-10-16(20)2/h4-6,11-12,16,18H,3,7-10,13-15H2,1-2H3	-4.638
InChI=1S/C7H8N2O2/c8-6-4-2-1-3-5(6)7(10)9-11/h1-4,11H,8H2,(H,9,10)	-0.748
InChI=1S/C2H5NO2/c1-2-3(4)5/h2H2,1H3	-0.22
InChI=1S/C4H6O4S/c5-3(6)1-9-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)	0.425
InChI=1S/C12H17NO3/c14-7-10(15)8-16-11-5-1-3-9-4-2-6-13-12(9)11/h1,3,5,10,13-15H,2,4,6-8H2	-2.039
InChI=1S/C10H19N3O2S/c1-3-11-9(16)12-5-7-13(8-6-12)10(14)15-4-2/h3-8H2,1-2H3,(H,11,16)	-1.79
InChI=1S/C9H18O3/c1-3-4-5-9(2)11-7-8(6-10)12-9/h8,10H,3-7H2,1-2H3	-2.134
InChI=1S/C12H12N2OS/c1-8-11(16-9(2)13-8)12(15)14-10-6-4-3-5-7-10/h3-7H,1-2H3,(H,14,15)	-1.73
InChI=1S/C26H6Cl8N2O4/c27-14-10-11(15(28)19(32)18(14)31)24(38)9(23(10)37)7-5-4-6-2-1-3-h1-5,9H	-7.727
InChI=1S/C14H22O/c1-5-10(3)12-7-8-14(15)13(9-12)11(4)6-2/h7-11,15H,5-6H2,1-4H3	-4.744
InChI=1S/C4H11NO/c1-5(2)3-4-6/h6H,3-4H2,1-2H3	1.05
InChI=1S/C10H12O4/c11-5-8-1-3-10(4-2-8)14-7-9(13)6-12/h1-5,9,12-13H,6-7H2	-0.784
InChI=1S/C13H19NO3/c1-4-14(5-2)13(16)10-7-8-11(15)12(9-10)17-6-3/h7-9,15H,4-6H2,1-3H3	-2.251

"InChi"	"logS(M)"
InChI=1S/C11H22N2O4/ c1-8(2)4-5-11(3,6-16-9(12)14)7-17-10(13)15/h8H,4-7H2,1-3H3, (H2,12,14)(H2,13,15)	-2.613
InChI=1S/C18H10N2O/ c21-18-13-8-4-6-11-5-3-7-12(16(11)13)17-19-14-9-1-2-10-15(14)20(1 h1-10H	-5.59
InChI=1S/C10H12ClNO2/c11-7-9(14-10(12)13)6-8-4-2-1-3-5-8/ h1-5,9H,6-7H2,(H2,12,13)	-2.775
InChI=1S/C18H23NO/ c1-15-9-7-8-12-17(15)18(20-14-13-19(2)3)16-10-5-4-6-11-16/ h4-12,18H,13-14H2,1-3H3	-3.377
InChI=1S/C10H6Cl2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H	-5.358
InChI=1S/C8H18/c1-5-6-7-8(2,3)4/h5-7H2,1-4H3	-5.757
InChI=1S/C15H19N3O2/ c1-2-18-9-3-4-14(11-18)20-15(19)17-13-7-5-12(10-16)6-8-13/ h5-8,14H,2-4,9,11H2,1H3,(H,17,19)	-3.326
InChI=1S/C14H30O2S2/ c15-9-13-17-11-7-5-3-1-2-4-6-8-12-18-14-10-16/h15-16H,1-14H2	-4.37
InChI=1S/C4H7N3S/c1-2-5-4-7-6-3-8-4/h3H,2H2,1H3,(H,5,7)	-1.001
InChI=1S/C8H8ClNO/c9-8-2-1-6-5-11-10-4-7(6)3-8/h1-3,10H,4-5H2	-2.453
InChI=1S/C6H10N3O6P/c1-5-7-4-6(9(10)11)8(5)2-3-15-16(12,13)14/ h4H,2-3H2,1H3,(H2,12,13,14)	-1.38
InChI=1S/C7H14N4O3/c1-8-7(10-11(12)13)9-4-6-2-3-14-5-6/h6H, 2-5H2,1H3,(H2,8,9,10)	-0.569
InChI=1S/C6H6O4/c7-2-4-1-5(8)6(9)3-10-4/h1,3,7,9H,2H2	0.818
InChI=1S/C15H24O3/ c1-4-6-7-8-12-10-13(16)9-11(3)14(12)15(17)18-5-2/h9,12,14H, 4-8,10H2,1-3H3	-3.187
InChI=1S/C10H11NO3/c1-7(10(13)14)11-9(12)8-5-3-2-4-6-8/h2-7H, 1H3,(H,11,12)(H,13,14)	-1.684
InChI=1S/C12H8Cl2/c13-11-8-4-7-10(12(11)14)9-5-2-1-3-6-9/h1-8H	-5.35
InChI=1S/C8H15NO3/c1-3-4-5-7(8(11)12)9-6(2)10/h7H, 3-5H2,1-2H3,(H,9,10)(H,11,12)	-0.682
InChI=1S/C30H44N2O10/ c1-31(11-9-15-41-29(33)21-17-23(35-3)27(39-7)24(18-21)36-4)13-14- h17-20H,9-16H2,1-8H3	-3.404
InChI=1S/C22H22FN3O3/ c23-17-7-5-15(6-8-17)20(27)16-9-11-25(12-10-16)13-14-26-21(28)18- h1-8,16H,9-14H2,(H,24,29)	-4.597
InChI=1S/C7H12N2O2/c1-4(2)6-7(11)8-3-5(10)9-6/h4,6H, 3H2,1-2H3,(H,8,11)(H,9,10)	-0.893
InChI=1S/C8H8N2O2/c1-10-4-3-7(12-2)6(5-9)8(10)11/h3-4H,1-2H3	-1.784
InChI=1S/C20H17F2N3O3/ c21-12-1-3-13(4-2-12)25-11-15(20(27)28)19(26)14-9-16(22)18(10-17(h1-4,9-11,23H,5-8H2,(H,27,28)	-3.13
InChI=1S/C18H33ClN2O5S/ c1-5-6-10-7-11(21(3)8-10)17(25)20-12(9(2)19)16-14(23)13(22)15(24) h9-16,18,22-24H,5-8H2,1-4H3,(H,20,25)	-4.143
InChI=1S/C12H16O6/ c13-6-8-9(14)10(15)11(16)12(18-8)17-7-4-2-1-3-5-7/h1-5,8-16H,6H2	-1.46

"InChi"	"logS(M)"
InChI=1S/C16H14O2/c17-16(12-11-14-7-3-1-4-8-14)18-13-15-9-5-2-6-10-15/h1-12H,13H2/b12-11+	-4.821
InChI=1S/C12H16O/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h6-10,13H,1-5H2	-3.468
InChI=1S/C3H9O3P/c1-5-7(3,4)6-2/h1-3H3	-0.094
InChI=1S/C8H5NO2S/c10-8(11)7-5-3-1-2-4-6(5)12-9-7/h1-4H,(H,10,11)	-2.259
InChI=1S/C14H18ClNO3/c1-10(2)7-8-19-13-5-3-11(9-12(13)15)4-6-14(17)16-18/h3-6,9-10,18H,7-8H2,1-2H3,(H,16,17)/b6-4+	-4.555
InChI=1S/C7H3BrClNO2/c8-3-1-6-5(2-4(3)9)10-7(11)12-6/h1-2H,(H,10,11)	-3.13
InChI=1S/C18H30O/c1-16(2,3)12-10-13(17(4,5)6)15(19)14(11-12)18(7,8)9/h10-11,19H,1-9H3	-3.875
InChI=1S/C12H4Cl6O/c13-5-1-3-7(11(17)9(5)15)19-8-4-2-6(14)10(16)12(8)18/h1-4H	-8.14
InChI=1S/C18H14NO6P/c20-19(21)15-11-13-18(14-12-15)25-26(22,23-16-7-3-1-4-8-16)24-17-h1-14H	-4.96
InChI=1S/C32H32N2O/c33-30(21-26-13-5-1-6-14-26)23-32(35)31(22-27-15-7-2-8-16-27)34(2h1-20,23,31H,21-22,24-25,33H2/b30-23-	-7.663
InChI=1S/C6H11N7O3S2/c1-13(4(7)8)2-3(14)10-5-11-12-6(17-5)18(9,15)16/h2H2,1H3,(H3,7,8)(H2,9,15,16)(H,10,11,14)	-1.14
InChI=1S/C14H29NO2/c1-10(2)7-14(8-11(3)4,9-12(5)6)13(16)15-17/h10-12,17H,7-9H2,1-6H3,(H,15,16)	-4
InChI=1S/C15H21NO4/c1-10-7-6-8-11(2)14(10)16(13(17)9-19-4)12(3)15(18)20-5/h6-8,12H,9H2,1-5H3	-1.6
InChI=1S/C10H12N2O3/c11-9(7-4-2-1-3-5-7)10(15)12-6-8(13)14/h1-5,9H,6,11H2,(H,12,15)(H,13,14)	-1.41
InChI=1S/C24H46O4/c1-3-5-7-9-11-13-15-17-19-21-23(25)27-28-24(26)22-20-18-16-14-12-h3-22H2,1-2H3	-6.601
InChI=1S/C5H7ClO3/c1-4(7)9-3-5(8)2-6/h2-3H2,1H3	-0.351
InChI=1S/C7H7NO3/c8-7(11)5-3-4(9)1-2-6(5)10/h1-3,9-10H,(H2,8,11)	-1.683
InChI=1S/C9H16O/c1-4-8(2)6-5-7-9(3)10/h6H,4-5,7H2,1-3H3/b8-6+	-2.193
InChI=1S/C6H15N/c1-5(7)6(2,3)4/h5H,7H2,1-4H3/p+1	0.986
InChI=1S/C6H14FN/c7-5-3-1-2-4-6-8/h1-6,8H2	-0.564
InChI=1S/C26H50N4O2/c1-23(2)15-21(16-24(3,4)27-23)29(19-31)13-11-9-10-12-14-30(20-32)h19-22,27-28H,9-18H2,1-8H3	-1.54
InChI=1S/C11H16O4/c1-11(13,7-12)8-15-10-5-3-4-9(6-10)14-2/h3-6,12-13H,7-8H2,1-2H3	-1.598
InChI=1S/C10H10O2/c1-8(12-9(2)11)10-6-4-3-5-7-10/h3-7H,1H2,2H3	-2.114
InChI=1S/C9H19NOS/c1-4-7-10(8-5-2)9(11)12-6-3/h4-8H2,1-3H3	-2.703

"InChi"	"logS(M)"
InChI=1S/C18H17NO5/c1-23-15-9-7-12(11-16(15)24-2)8-10-17(20)19-14-6-4-3-5-13(14)18(2h3-11H,1-2H3,(H,19,20)(H,21,22)/b10-8+	-5.532
InChI=1S/C15H12ClN5O4/c1-3-20-14(22)10(7-17)8(2)13(15(20)23)19-18-11-5-4-9(16)6-12(11)2h4-6,23H,3H2,1-2H3/b19-18+	-6.69
InChI=1S/C14H15N5O6S/c1-8-15-12(18-14(16-8)25-3)17-13(21)19-26(22,23)10-7-5-4-6-9(10)1h4-7H,1-3H3,(H2,15,16,17,18,19,21)	-1.604
InChI=1S/C14H29NO2/c1-4-7-8-9-10-11-12-14(5-2,6-3)13(16)15-17/h17H,4-12H2,1-3H3,(H,15,16)	-5.22
InChI=1S/C13H26N2O4/c1-4-7-8-15-12(17)19-10-13(5-2,6-3)9-18-11(14)16/h4-10H2,1-3H3,(H2,14,16)(H,15,17)	-3.696
InChI=1S/C9H18N6O6/c16-1-13(2-17)7-10-8(14(3-18)4-19)12-9(11-7)15(5-20)6-21/h16-21H,1-6H2	0.514
InChI=1S/C11H11NO6/c1-6(2)18-11(15)7-4-3-5-8(12(16)17)9(7)10(13)14/h3-6H,1-2H3,(H,13,14)/p-1	-2.347
InChI=1S/C13H22N2O/c1-15(2)13(16)14-12-7-8-6-11(12)10-5-3-4-9(8)10/h8-12H,3-7H2,1-2H3,(H,14,16)	-3.01
InChI=1S/C21H27NO3/c1-2-14-22-15-18(23)16-25-21-11-7-6-10-19(21)20(24)13-12-17-8-4-3h3-11,18,22-23H,2,12-16H2,1H3	-3.564
InChI=1S/C9H10N4O4S3/c1-6-2-4-7(5-3-6)20(16,17)13-8-11-12-9(18-8)19(10,14)15/h2-5H,1H3,(H,11,13)(H2,10,14,15)	-1.22
InChI=1S/C8H17NO2/c1-4-11-8(10)6-5-7-9(2)3/h4-7H2,1-3H3	-0.254
InChI=1S/C12H4Cl6/c13-6-3-4-7(14)11(17)9(6)5-1-2-8(15)12(18)10(5)16/h1-4H	-7.65
InChI=1S/C9H11NO/c1-8(11)10-7-9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,10,11)	-1.101
InChI=1S/C21H24N4O2/c1-23-12-14-24(15-13-23)16-25-19(26)21(22-20(25)27,17-8-4-2-5-9-1h2-11H,12-16H2,1H3,(H,22,27)	-2.851
InChI=1S/C8H10O3/c1-10-6-4-3-5-7(11-2)8(6)9/h3-5,9H,1-2H3	-0.953
InChI=1S/C14H10Cl2O4/c15-9-5-1-3-7-11(9)19-14(13(17)18)20-12-8-4-2-6-10(12)16/h1-8,14H,(H,17,18)	-2.83
InChI=1S/C11H18N2O3S2/c14-18(15,16)17-10-9-12-7-4-8-13-11-5-2-1-3-6-11/h1-3,5-6,12-13H,4,7-10H2,(H,14,15,16)	-2.547
InChI=1S/C44H52N4O6S2/c1-25-23-27(3)43(55(51,52)47-31-15-9-7-10-16-31)29(5)39(25)45-35-h13-14,19-24,31-32,45-48H,7-12,15-18H2,1-6H3	-4.819
InChI=1S/C21H25NO3/c1-2-22-15-9-14-19(16-22)25-20(23)21(24,17-10-5-3-6-11-17)18-12-7h3-8,10-13,19,24H,2,9,14-16H2,1H3	-3.397
InChI=1S/C9H14O2/c1-3-4-5-6-7-8-9(10)11-2/h3-6H2,1-2H3	-3.009

"InChi"	"logS(M)"
InChI=1S/C13H21NO2/c1-10-4-6-13(7-5-10)14(8-11(2)15)9-12(3)16/h4-7,11-12,15-16H,8-9H2,1-3H3	-1.504
InChI=1S/C12H16O4S/c1-4-17(13,14)16-9-5-6-11-10(7-9)12(2,3)8-15-11/h5-7H,4,8H2,1-3H3	-2.992
InChI=1S/C10H11NO4/c1-2-15-10(13)9(11-7-12)5-8-3-4-14-6-8/h3-7H,2H2,1H3,(H,11,12)/b9-5-	-2.748
InChI=1S/C10H20O2S/c1-9(2)6-4-3-5-7-12-10(11)8-13/h9,13H,3-8H2,1-2H3	-4.285
InChI=1S/C12H25NO/c1-4-5-6-7-8-9-10-11-12(14)13(2)3/h4-11H2,1-3H3	-2.768
InChI=1S/C16H16N2O2/c1-18(2)17-12-16(19)13-8-10-15(11-9-13)20-14-6-4-3-5-7-14/h3-12H,1-2H3/b17-12+	-3.553
InChI=1S/C13H10N2O/c14-12-8-4-1-2-6-10(8)15-13-9(12)5-3-7-11(13)16/h1-7,16H,(H2,14,15)	-2.906
InChI=1S/C7H11N3/c1-10(6-2-4-8)7-3-5-9/h2-3,6-7H2,1H3	0.863
InChI=1S/C2H4O3S/c3-6-4-1-2-5-6/h1-2H2/p+1	0.221
InChI=1S/C7H5NS/c1-3-8-5-7-6(1)2-4-9-7/h1-5H	-1.675
InChI=1S/C5HCl4N/c6-2-1-3(7)5(9)10-4(2)8/h1H	-3.861
InChI=1S/C14H13N3/c1-2-10-7-8-13(15-9-10)14-16-11-5-3-4-6-12(11)17-14/h3-9H,2H2,1H3,(H,16,17)	-3.262
InChI=1S/C8HCl3N2O/c9-5-3(1-12)6(10)7(11)8(14)4(5)2-13/h14H	-3.329
InChI=1S/C21H16N2O5S/c1-28-16-11-15(23-29(26,27)12-7-3-2-4-8-12)17-18(19(16)22)21(25)1h2-11,23H,22H2,1H3	-2.356
InChI=1S/C19H20N2O2/c1-2-21(13-14-22)19-20-17(15-9-5-3-6-10-15)18(23-19)16-11-7-4-8-1h3-12,22H,2,13-14H2,1H3	-4.912
InChI=1S/C12H22N2O/c1-3-4-5-12(15)14-10-6-7-11(14)9-13(2)8-10/h10-11H,3-9H2,1-2H3	-1.841
InChI=1S/C12H6Cl4O/c13-9-3-1-7(5-11(9)15)17-8-2-4-10(14)12(16)6-8/h1-6H	-6.98
InChI=1S/C13H22O2/c1-6-12(14)15-13(5,7-2)10-8-9-11(3)4/h7,9H,2,6,8,10H2,1,3-5H3	-4.382
InChI=1S/C13H16N2O2/c1-9(16)14-6-5-10-8-15-13-4-3-11(17-2)7-12(10)13/h3-4,7-8,15H,5-6H2,1-2H3,(H,14,16)	-5.09
InChI=1S/C16H9F3O2/c17-16(18,19)10-7-5-9(6-8-10)13-14(20)11-3-1-2-4-12(11)15(13)21/h1-8,13H	-4.545
InChI=1S/C10H14N2O4/c1-10(12-11,9(15)16)5-6-2-3-7(13)8(14)4-6/h2-4,12-14H,5,11H2,1H3,(H,15,16)	0.034
InChI=1S/C8H6O2/c9-6-8(10)7-4-2-1-3-5-7/h1-6H	-0.74
InChI=1S/C9H12BrNO2S/c1-2-7-11-14(12,13)9-5-3-8(10)4-6-9/h3-6,11H,2,7H2,1H3	-3.542
InChI=1S/C15H15NO3/c1-2-19-14-11-7-6-10-13(14)15(17)16(18)12-8-4-3-5-9-12/h3-11,18H,2H2,1H3	-3.37

"InChi"	"logS(M)"
InChI=1S/C22H42O6/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20(25)27-17-19(24)22-21(26)1h18-19,21-24,26H,2-17H2,1H3	-6.906
InChI=1S/C10H17NO2/c1-2-13-10(12)9-7-8-3-5-11(9)6-4-8/h8-9H,2-7H2,1H3	-0.949
InChI=1S/C9H18Cl3N2O2P/c10-2-6-13-5-1-9-16-17(13,15)14(7-3-11)8-4-12/h1-9H2	-2.733
InChI=1S/C12H4Cl6/c13-6-2-1-3-7(14)9(6)5-4-8(15)11(17)12(18)10(5)16/h1-4H	-8.13
InChI=1S/C13H13NO3/c1-2-17-13(16)12(15)14-9-5-7-10-6-3-4-8-11(10)14/h3-8H,2,9H2,1H3	-2.303
InChI=1S/C4H8S2/c1-2-5-4-6-3-1/h1-4H2	-2.042
InChI=1S/C9H12O/c1-8-4-2-3-5-9(8)6-7-10/h2-5,10H,6-7H2,1H3	-1.043
InChI=1S/C6H14N2/c1-5-3-8-6(2)4-7-5/h5-8H,3-4H2,1-2H3/p+2	0.486
InChI=1S/C14H15N/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1,3-4,7-8H,2,5-6,9-10H2	-4.42
InChI=1S/C7H5ClN2O2/c8-3-1-4-6(2-5(3)11)12-7(9)10-4/h1-2,11H,(H2,9,10)	-1.32
InChI=1S/C7H11NO5/c1-4(9)8-5(7(12)13)2-3-6(10)11/h5H,2-3H2,1H3,(H,8,9)(H,10,11)(H,12,13)	-0.71
InChI=1S/C9H20O3/c1-2-3-4-5-6-12-8-9(11)7-10/h9-11H,2-8H2,1H3	-2.171
InChI=1S/C7H10O5S2/c1-2-14-7(13)12-4(6(10)11)3-5(8)9/h4H,2-3H2,1H3,(H,8,9)(H,10,11)	-1.29
InChI=1S/C10H11NO4/c1-11(2)8-4-3-6(9(12)13)5-7(8)10(14)15/h3-5H,1-2H3,(H,12,13)(H,14,15)	-2.02
InChI=1S/C10H10N4O/c11-8-3-1-7(2-4-8)9(15)14-10-12-5-6-13-10/h1-6H,11H2,(H2,12,13,14,15)	-1.025
InChI=1S/C9H10O2/c1-7(10)9(11)8-5-3-2-4-6-8/h2-6,9,11H,1H3	-1.177
InChI=1S/C16H18ClN/c1-13(11-14-7-3-2-4-8-14)18-12-15-9-5-6-10-16(15)17/h2-10,13,18H,11-12H2,1H3	-3.993
InChI=1S/C9H12N2O/c1-7-3-2-4-8-10-6-5-9(12)11(7)8/h5-7H,2-4H2,1H3	-1.966
InChI=1S/C4H8O2/c1-4(6)2-3-5/h3-4,6H,2H2,1H3	1.055
InChI=1S/C10H12O2/c1-8(11)2-3-9-4-6-10(12)7-5-9/h4-7,12H,2-3H2,1H3	-1.552
InChI=1S/C7H17O3PS3/c1-4-9-11(12,10-5-2)13-7-14(8)6-3/h4-7H2,1-3H3/p+1	-1.538
InChI=1S/C7H14N2O/c1-3-4-5-6-8-9(2)7-10/h6-7H,3-5H2,1-2H3/b8-6+	-1.444
InChI=1S/C9H16ClN5/c1-5-11-7-12-6(10)13-8(14-7)15-9(2,3)4/h5H2,1-4H3,(H2,11,12,13,14,15)	-4.43
InChI=1S/C15H21N/c1-2-16-15-13-9-8-12(10-13)14(15)11-6-4-3-5-7-11/h3-7,12-16H,2,8-10H2,1H3	-2.496
InChI=1S/C18H20N2O/c1-3-20(4-2)19-14-18(21)17-12-10-16(11-13-17)15-8-6-5-7-9-15/h5-14H,3-4H2,1-2H3/b19-14+	-4.23

"InChi"	"logS(M)"
InChI=1S/C18H34O6/c1-3-5-11-21-13-15-23-17(19)9-7-8-10-18(20)24-16-14-22-12-6-4-2/h3-16H2,1-2H3	-4.959
InChI=1S/C17H22O5/c1-8-7-12-14(9(2)16(20)22-12)15(21-10(3)18)17(4)11(8)5-6-13(17)19h5-6,8-9,11-12,14-15H,7H2,1-4H3	-2.19
InChI=1S/C7H15Cl2N/c1-2-5-10(6-3-8)7-4-9/h2-7H2,1H3	-1.681
InChI=1S/C12H24N2O4/c1-8(2)12(5,6-17-10(13)15)7-18-11(16)14-9(3)4/h8-9H,6-7H2,1-5H3,(H2,13,15)(H,14,16)	-3.05
InChI=1S/C14H17Cl2N3O/c1-2-3-6-14(20,8-19-10-17-9-18-19)12-5-4-11(15)7-13(12)16/h4-5,7,9-10,20H,2-3,6,8H2,1H3	-4.267
InChI=1S/C29H31N5/c30-27-16-17-28(32-31-27)34-22-20-33(21-23-34)19-18-29(24-10-4-1h1-17H,18-23H2,(H2,30,31)	-6.574
InChI=1S/C12H10N2O/c15-12(10-4-2-1-3-5-10)14-11-6-8-13-9-7-11/h1-9H,(H,13,14,15)	-2.417
InChI=1S/C12H19NO/c1-8(14)13-12-5-9-2-10(6-12)4-11(3-9)7-12/h9-11H,2-7H2,1H3,(H,13,14)	-2.636
InChI=1S/C14H13N3O2S/c1-19-13-7-9(20(2)18)3-4-10(13)14-16-11-5-6-15-8-12(11)17-14/h3-8H,1-2H3,(H,16,17)/p+1	-2.363
InChI=1S/C10H16N2O4/c1-7(13)11(8(2)14)5-6-12(9(3)15)10(4)16/h5-6H2,1-4H3	-2.279
InChI=1S/C10H19N5O/c1-5-11-8-12-9(15(6-2)7-3)14-10(13-8)16-4/h5-7H2,1-4H3,(H,11,12,13,14)	-2.999
InChI=1S/C21H39N7O12/c1-5-21(36,4-30)16(40-17-9(26-2)13(34)10(31)6(3-29)38-17)18(37-5)h4-18,26,29,31-36H,3H2,1-2H3,(H4,22,23,27)(H4,24,25,28)	0.235
InChI=1S/C18H16F3N3O/c1-23(2)16-11-17(25)24(13-6-4-3-5-7-13)15-10-12(18(19,20)21)8-9-1h3-10H,11H2,1-2H3	-3.524
InChI=1S/C20H44N2/c1-17(15-19(3,4)5)9-11-21-13-14-22-12-10-18(2)16-20(6,7)8/h17-18,21-22H,9-16H2,1-8H3	-2.24
InChI=1S/C6H6FN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2	-0.527
InChI=1S/C23H34O2/c1-7-22(24)25-17-15-19(3)11-8-10-18(2)13-14-21-20(4)12-9-16-23(21h8,10-11,13-15H,7,9,12,16-17H2,1-6H3/b11-8+,14-13+,18-10+,19-15+	-7.535
InChI=1S/C9H7NO/c11-9-5-6-10-8-4-2-1-3-7(8)9/h1-6H,(H,10,11)	-1.481
InChI=1S/C9H9NO2/c1-2-9(11)7-3-5-8(10-12)6-4-7/h3-6H,2H2,1H3	-2.13
InChI=1S/C12H15ClN2O/c1-3-15(4-2)14-9-12(16)10-5-7-11(13)8-6-10/h5-9H,3-4H2,1-2H3/b14-9+	-2.971
InChI=1S/C9H9NO2/c1-2-9(12)10-7-3-5-8(11)6-4-7/h2-6,11H,1H2,(H,10,12)	-0.925
InChI=1S/C6H10O3S2/c1-3-9-6(10)11-4(2)5(7)8/h4H,3H2,1-2H3,(H,7,8)	-1.449

"InChi"	"logS(M)"
InChI=1S/C16H22INO2/ c1-13-5-2-3-10-18(13)11-4-12-20-16(19)14-6-8-15(17)9-7-14/ h6-9,13H,2-5,10-12H2,1H3	-5.254
InChI=1S/C31H36N2O6S2/ c1-5-32(6-2)25-15-9-23(10-16-25)30(24-11-17-26(18-12-24)33(7-3)8- h9-21,30H,5-8H2,1-4H3,(H,34,35,36)(H,37,38,39)	-0.698
InChI=1S/C11H16O/c1-8-7-9(11(2,3)4)5-6-10(8)12/h5-7,12H,1-4H3	-3.21
InChI=1S/C11H22N2O4/ c1-4-6-13-10(15)17-8-11(3,5-2)7-16-9(12)14/h4-8H2,1-3H3, (H2,12,14)(H,13,15)	-2.653
InChI=1S/C9H8O3/c1-12-9(11)8(10)7-5-3-2-4-6-7/h2-6H,1H3	-1.914
InChI=1S/C30H62/ c1-25(2)15-11-19-29(7)23-13-21-27(5)17-9-10-18-28(6)22-14-24-30(8 h25-30H,9-24H2,1-8H3	-5.149
InChI=1S/C6H14N4O2/c1-3(2)4(9-5(7)11)10-6(8)12/h3-4H,1-2H3, (H3,7,9,11)(H3,8,10,12)	-1.81
InChI=1S/C14H22N2O5/ c1-14(12(18)21-9-20-3,10-7-5-4-6-8-10)11(17)16-13(19)15-2/h7H, 4-6,8-9H2,1-3H3,(H2,15,16,17,19)	-2.42
InChI=1S/C21H32O3/ c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-10- h12-13,16-18,22,24H,4-11H2,1-3H3	-4.16
InChI=1S/C10H22O4/c1-8(5-11)14-10(3)7-13-9(2)6-12-4/h8-11H, 5-7H2,1-4H3	0.685
InChI=1S/C15H14F3N5O7S/ c1-28-9-6-10(29-2)21-13(20-9)22-14(25)23-31(26,27)11-7(12(24)30-3 h4-6H,1-3H3,(H2,20,21,22,23,25)	-3.89
InChI=1S/C9H12N4O/c1-13(2)12-11-8-5-3-7(4-6-8)9(10)14/h3-6H, 1-2H3,(H2,10,14)/b12-11+	-1.628
InChI=1S/C7H11N3O4/c1-14-5-6(11)4-9-3-2-8-7(9)10(12)13/ h2-3,6,11H,4-5H2,1H3	-0.743
InChI=1S/C8H6/c1-2-8-6-4-3-5-7-8/h1,3-7H	-2.35
InChI=1S/C12H22N2O4/ c1-5-6-14-11(16)18-8-12(4,9(2)3)7-17-10(13)15/h5,9H, 1,6-8H2,2-4H3,(H2,13,15)(H,14,16)	-2.981
InChI=1S/C12H15NOS/ c15-12(13-6-8-14-9-7-13)10-11-4-2-1-3-5-11/h1-5H,6-10H2	-1.814
InChI=1S/C15H22O4/ c1-9-3-4-14(7-16)11(5-9)19-12-6-10(17)13(14,2)15(12)8-18-15/ h5,10-12,16-17H,3-4,6-8H2,1-2H3	-2.61
InChI=1S/C10H11N3O3S/ c1-7-5-10(11)13(12-7)8-3-2-4-9(6-8)17(14,15)16/h2-4,6,11H, 5H2,1H3,(H,14,15,16)/b11-10-	-1.139
InChI=1S/C14H19O6P/ c1-11(20-21(16,17-3)18-4)10-14(15)19-12(2)13-8-6-5-7-9-13/ h5-10,12H,1-4H3/b11-10-	-2.497
InChI=1S/C12H24N2O2/c1-3-5-7-11(15)13-9-10-14-12(16)8-6-4-2/ h3-10H2,1-2H3,(H,13,15)(H,14,16)	-1.815
InChI=1S/C17H17ClO6/ c1-8-5-9(21-2)6-12(19)17(8)16(20)13-10(22-3)7-11(23-4)14(18)15(13 h6-8H,5H2,1-4H3	-4.4

"InChi"	"logS(M)"
InChI=1S/C23H36N2O/c1-7-8-12-20-15-22(2,3)25(23(4,5)16-20)21(26)18-24(6)17-19-13-10-9-11,13-15H,7-8,12,16-18H2,1-6H3	-6.7
InChI=1S/C11H15ClO2/c1-10(2,13)11(3,14)8-4-6-9(12)7-5-8/h4-7,13-14H,1-3H3	-2.82
InChI=1S/C11H12Cl2O3/c1-2-5-15-11(14)7-16-10-4-3-8(12)6-9(10)13/h3-4,6H,2,5,7H2,1H3	-4.25
InChI=1S/C24H30N2O2S/c1-18(28)20-7-8-24-22(17-20)26(21-5-2-3-6-23(21)29-24)13-4-12-25-h2-3,5-8,17,19,27H,4,9-16H2,1H3	-6.604
InChI=1S/C12H3Cl7/c13-5-2-7(15)6(14)1-4(5)10-11(18)8(16)3-9(17)12(10)19/h1-3H	-8.94
InChI=1S/C10H20N2O4/c1-4-10(3,6-15-8(11)13)7-16-9(14)12-5-2/h4-7H2,1-3H3,(H2,11,13)(H,12,14)	-2.133
InChI=1S/C10H8ClNO2/c1-2-5-12-8-6-7(11)3-4-9(8)14-10(12)13/h2-4,6H,1,5H2	-3.448
InChI=1S/C13H26N2O4/c1-4-6-7-13(3,9-18-11(14)16)10-19-12(17)15-8-5-2/h4-10H2,1-3H3,(H2,14,16)(H,15,17)	-3.696
InChI=1S/C16H13NO3/c1-10(16(18)19)12-7-8-14-13(9-12)17-15(20-14)11-5-3-2-4-6-11/h2-10H,1H3,(H,18,19)	-3.603
InChI=1S/C14H21NO2/c1-3-10-14(11-4-2,13(16)15-17)12-8-6-5-7-9-12/h5-9,17H,3-4,10-11H2,1-2H3,(H,15,16)	-2.89
InChI=1S/C12H13NO3/c14-11(13-7-4-8-13)9-16-12(15)10-5-2-1-3-6-10/h1-3,5-6H,4,7-9H2	-1.609
InChI=1S/C12H14N4O2/c1-8-10(14-12(13)18)11(17)16(15(8)2)9-6-4-3-5-7-9/h3-7H,1-2H3,(H3,13,14,18)	-1.52
InChI=1S/C14H20N4O/c15-14-16-10-13(19-14)11-17-6-8-18(9-7-17)12-4-2-1-3-5-12/h1-5,13H,6-11H2,(H2,15,16)	-1.825
InChI=1S/C22H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24/h2-21H2,1H3,(H,23,24)	-7.328
InChI=1S/C8H15N3O7/c1-11(10-17)8(16)9-4-6(14)5(13)3(2-12)18-7(4)15/h3-7,12-15H,2H2,1H3,(H,9,16)	-1.719
InChI=1S/C14H11NO/c1-10-6-8-11(9-7-10)14-15-12-4-2-3-5-13(12)16-14/h2-9H,1H3	-4.168
InChI=1S/C11H12N2O2/c1-2-12-11-13-10(14)9(15-11)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H,12,13,14)	-1.131
InChI=1S/C11H15NO2/c1-8(2)9-5-4-6-10(7-9)14-11(13)12-3/h4-8H,1-3H3,(H,12,13)	-3.357
InChI=1S/C23H28N2O2/c1-24-20-12-13-21(24)17-25(16-20)14-15-27-23(26)22(18-8-4-2-5-9-1h2-11,20-22H,12-17H2,1H3	-4.026
InChI=1S/C18H30O4/c1-15(2)17(19)21-13-11-9-7-5-6-8-10-12-14-22-18(20)16(3)4/h1,3,5-14H2,2,4H3	-6.35

"InChi"	"logS(M)"
InChI=1S/C22H32N2O2/c1-23-14-19-12-13-20(15-23)24(19)21(26)22(16-25,17-8-4-2-5-9-17)1h2,4-5,8-9,18-20,25H,3,6-7,10-16H2,1H3	-4.122
InChI=1S/C14H23NO4S2/c1-12(11-20-21(16,17)18)15-10-4-3-5-13-6-8-14(19-2)9-7-13/h6-9,12,15H,3-5,10-11H2,1-2H3,(H,16,17,18)	-2.49
InChI=1S/C15H20O4S/c1-11(2)19-14(16)15(9-4-10-15)20(17,18)13-7-5-12(3)6-8-13/h5-8,11H,4,9-10H2,1-3H3	-3.34
InChI=1S/C8H15N5O/c1-4-9-6-11-7(10-5(2)3)13-8(14)12-6/h5H,4H2,1-3H3,(H3,9,10,11,12,13,14)	-4.524
InChI=1S/C8H7N3/c9-6-2-1-3-7-8(6)11-5-4-10-7/h1-5H,9H2	-1.362
InChI=1S/C10H8O2/c11-8-5-7-3-1-2-4-9(7)10(12)6-8/h1-6,11-12H	-1.949
InChI=1S/C7H5Cl2NO/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H2,10,11)	-1.843
InChI=1S/C32H35N5/c1-2-19-33-30-25-34-31(35-26-30)37-23-21-36(22-24-37)20-18-32(27h2-17,25-26,33H,1,18-24H2	-7.324
InChI=1S/C3H6N2O2/c1-3(6)5(2)4-7/h1-2H3	-0.768
InChI=1S/C52H76O24/c1-18-29(72-34-14-30(43(58)21(4)68-34)73-33-13-28(54)42(57)20(3)h10,12,19-24,27-28,30-37,41-45,49-51,53-61,64-65H,11,13-17H2,1-9H3	-0.863
InChI=1S/C10H11N3O5/c14-9(15)5-6-11-10(16)12-7-1-3-8(4-2-7)13(17)18/h1-4H,5-6H2,(H,14,15)(H2,11,12,16)	-2.7
InChI=1S/C20H20O6/c21-20-12-23-19(14-9-5-2-6-10-14)25-17(20)16-15(26-20)11-22-18(2h1-10,15-19,21H,11-12H2	-4.438
InChI=1S/C22H27NO6/c1-16(17-3-4-19-14-20(26-2)6-5-18(19)13-17)22(25)29-12-11-28-21(2h3-6,13-14,16H,7-12,15H2,1-2H3	-4.3
InChI=1S/C23H25BrN6O10/c1-13(31)25-18-11-20(28(5-7-39-14(2)32)6-8-40-15(3)33)22(38-4)12-h9-12H,5-8H2,1-4H3,(H,25,31)/b27-26+	-5.495
InChI=1S/C19H26O3/c1-7-8-13-12(4)16(10-15(13)20)22-18(21)17-14(9-11(2)3)19(17,5)6/h7,9,14,16-17H,1,8,10H2,2-6H3	-4.818
InChI=1S/C7H6N2O2S2/c1-3(10)8-5-6-4(2-12-13-6)9-7(5)11/h2H,1H3,(H,8,10)(H,9,11)	-1.475
InChI=1S/C10H13NO/c1-3-9-4-6-10(7-5-9)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)	-2.145
InChI=1S/C14H19Cl2NO2/c1-9-4-5-12(14(18)19)6-13(9)17(7-10(2)15)8-11(3)16/h4-6,10-11H,7-8H2,1-3H3,(H,18,19)	-5.625
InChI=1S/C17H19ClN2OS/c1-19(2)8-3-9-20-14-6-5-13(21)11-17(14)22-16-7-4-12(18)10-15(16)2h4-7,10-11,21H,3,8-9H2,1-2H3	-5.48
InChI=1S/C10H12N4O4S2/c1-7(15)18-4-2-13-3-5-19-10(13)12-9-11-6-8(20-9)14(16)17/h6H,2-5H2,1H3/b12-10+	-2.495
InChI=1S/C9H16Cl3NO2/c1-4-6(5(2)3)7(14)13-8(15)9(10,11)12/h5-6,8,15H,4H2,1-3H3,(H,13,14)	-2.857

"InChi"	"logS(M)"
InChI=1S/C25H36O4/c1-22-10-11-25(28-14-15-29-25)16-17(22)4-5-18-19-6-7-21(24(3)26-1h4-5,19-21H,6-16H2,1-3H3	-6.7
InChI=1S/C17H26O3/c1-3-4-5-6-7-8-15(18)11-9-14-10-12-16(19)17(13-14)20-2/h10,12-13,19H,3-9,11H2,1-2H3	-4.865
InChI=1S/C12H6Cl4S/c13-7-1-3-8(4-2-7)17-12-6-10(15)9(14)5-11(12)16/h1-6H	-7.034
InChI=1S/C4H11N3O3S2/c5-4(6)7-2-1-3-11-12(8,9)10/h1-3H2,(H4,5,6,7)(H,8,9,10)	0.671
InChI=1S/C42H70O35/c43-1-8-29-15(50)22(57)36(64-8)72-30-9(2-44)66-38(24(59)17(30)52h8-63H,1-7H2	-1.84
InChI=1S/C12H3Cl7O/c13-4-1-2-6(10(17)8(4)15)20-7-3-5(14)9(16)12(19)11(7)18/h1-3H	-9.12
InChI=1S/C19H16O5/c1-2-22-19(21)12-23-14-8-9-15-16(20)11-17(24-18(15)10-14)13-6-4-3h3-11H,2,12H2,1H3	-4.709
InChI=1S/C15H21N3O2/c1-15-7-8-17(3)13(15)18(4)12-6-5-10(9-11(12)15)20-14(19)16-2/h5-6,9,13H,7-8H2,1-4H3,(H,16,19)	-1.55
InChI=1S/C14H19Cl2NO2/c15-8-10-17(11-9-16)13-6-4-12(5-7-13)2-1-3-14(18)19/h4-7H,1-3,8-11H2,(H,18,19)	-3.4
InChI=1S/C11H22N2O3S2/c12-11(9-17-18(14,15)16)13-8-4-7-10-5-2-1-3-6-10/h10H,1-9H2,(H2,12,13)(H,14,15,16)	-3.746
InChI=1S/C6H6N4O2/c1-10-4-3(2-7-6(10)12)8-5(11)9-4/h2H,1H3,(H2,8,9,11)	-0.794
InChI=1S/C4H10O2S/c5-1-3-7-4-2-6/h5-6H,1-4H2	0.913
InChI=1S/C10H13N/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-4,10H,5-7,11H2	-1.044
InChI=1S/C11H13NO4/c1-3-15-10(13)12-8-6-4-5-7-9(8)16-11(12)14-2/h4-7,11H,3H2,1-2H3	-3.022
InChI=1S/C15H14O/c1-12(16)15(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-11,15H,1H3	-3.143
InChI=1S/C22H42N2O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-23-18-19-24(22)20-2h9-10,25H,2-8,11-21H2,1H3/b10-9+	-3.846
InChI=1S/C14H10Cl4/c1-8-4-9(14(18)7-13(8)17)5-10-6-11(15)2-3-12(10)16/h2-4,6-7H,5H2,1H3	-8.06
InChI=1S/C17H16N2O2/c20-12-11-18-17-19-15(13-7-3-1-4-8-13)16(21-17)14-9-5-2-6-10-14/h1-10,20H,11-12H2,(H,18,19)	-3.82
InChI=1S/C11H15Cl2O2PS2/c1-3-7-18-16(17,14-4-2)15-11-6-5-9(12)8-10(11)13/h5-6,8H,3-4,7H2,1-2H3	-6.693
InChI=1S/C7H14O2/c1-3-5-6-9-7(8)4-2/h3-6H2,1-2H3	-1.938
InChI=1S/C13H18O2/c1-13(2,3)10-4-6-11(7-5-10)14-8-12-9-15-12/h4-7,12H,8-9H2,1-3H3	-3.43

"InChi"	"logS(M)"
InChI=1S/C12H10BrN3O4S/c13-11-7-9(16(17)18)3-6-12(11)15-21(19,20)10-4-1-8(14)2-5-10/h1-7,15H,14H2	-4.78
InChI=1S/C12H14N8/c13-11(14)19-17-9-5-6-10(18-20-12(15)16)8-4-2-1-3-7(8)9/h1-6H,(H4,13,14,19)(H4,15,16,20)/b17-9+,18-10+	-3.29
InChI=1S/C44H34Cl2N6O4/c1-23-13-15-29(45)21-37(23)49-51-39-31-11-7-5-9-27(31)19-33(41(3 h5-22,49-50H,1-4H3,(H,47,55)(H,48,56)/b51-39-,52-40-	-7.678
InChI=1S/C6H15N5/c1-2-3-4-10-6(9)11-5(7)8/h2-4H2,1H3,(H6,7,8,9,10,11)	0.676
InChI=1S/C17H23NO5/c1-11(2)18(12(3)4)16(20)10-22-17(21)14-8-6-7-9-15(14)23-13(5)19/h6-9,11-12H,10H2,1-5H3	-3.25
InChI=1S/C12H7Cl3O/c13-8-1-3-11(4-2-8)16-12-6-9(14)5-10(15)7-12/h1-7H	-5.52
InChI=1S/C11H22N2O4/c1-3-4-5-6-11(2,7-16-9(12)14)8-17-10(13)15/h3-8H2,1-2H3,(H2,12,14)(H2,13,15)	-2.675
InChI=1S/C21H30O2/c1-5-6-7-8-15-12-16(22)13-19-20(15)17-11-14(2)9-10-18(17)21(3,4)2 h11-13,17-18,22H,5-10H2,1-4H3	-7.401
InChI=1S/C21H22ClNS/c22-16-10-11-21-19(15-16)17(18-7-2-3-9-20(18)24-21)8-6-14-23-12-4 h2-3,7-11,15H,1,4-6,12-14H2/b17-8+	-8.133
InChI=1S/C5H8O/c1-2-6-5-3-4-5/h2,5H,1,3-4H2	-1.1
InChI=1S/C10H18O2/c1-4-5-6-7-8-12-10(11)9(2)3/h5-6,9H,4,7-8H2,1-3H3/b6-5+	-3.174
InChI=1S/C20H23NS/c1-21-12-6-7-15(14-21)13-18-16-8-2-4-10-19(16)22-20-11-5-3-9-17(1 h2-5,8-11,15,18H,6-7,12-14H2,1H3	-4.882
InChI=1S/C8H20NO6P/c1-9(2,3)4-5-14-16(12,13)15-7-8(11)6-10/h8,10-11H,4-7H2,1-3H3	0.59
InChI=1S/C10H12ClNO2/c1-14-10(13)9(12)6-7-2-4-8(11)5-3-7/h2-5,9H,6,12H2,1H3	-1.181
InChI=1S/C16H22N2O4S2/c19-24(20,21)23-13-11-17-10-4-1-5-12-22-16-9-8-14-6-2-3-7-15(14)1 h2-3,6-9,17H,1,4-5,10-13H2,(H,19,20,21)	-2.87
InChI=1S/C9H7BrO2/c10-8-3-1-2-7(6-8)4-5-9(11)12/h1-6H,(H,11,12)/b5-4+	-2.636
InChI=1S/C9H7NO3/c1-12-9(11)7(6-10)5-8-3-2-4-13-8/h2-5H,1H3/b7-5-	-2.168
InChI=1S/C3H6O2/c1-2-5-3-4-1/h1-3H2	1.13
InChI=1S/C7H6ClNO/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H2,9,10)	-0.883
InChI=1S/C20H22N4O10S/c1-9(25)33-10(2)34-19(28)15-11(7-32-20(21)29)8-35-18-14(17(27)24 h4-6,10,14,18H,7-8H2,1-3H3,(H2,21,29)(H,22,26)/b23-13+	-3.68
InChI=1S/C6H11NO2/c1-5(8)4-6(9)7(2)3/h4H2,1-3H3	0.889
InChI=1S/C27H43NO/c1-16-5-8-23-17(2)25-24(28(23)15-16)14-22-20-7-6-18-13-19(29)9-11 h6,16-17,19-25,29H,5,7-15H2,1-4H3	-8.482

"InChi"	"logS(M)"
InChI=1S/C18H17NO/c20-17-11-18(12-19-17)15-7-3-1-5-13(15)9-10-14-6-2-4-8-16(14)18/h1-8H,9-12H2,(H,19,20)	-5.18
InChI=1S/C7H5Cl4NO/c1-13-6-3-4(7(9,10)11)2-5(8)12-6/h2-3H,1H3	-4.364
InChI=1S/C13H18N2O/c16-13(11-15-9-5-2-6-10-15)14-12-7-3-1-4-8-12/h1,3-4,7-8H,2,5-6,9-11H2,(H,14,16)	-3.108
InChI=1S/C10H15NO3/c1-14-10-4-2-8(3-5-10)11-6-9(13)7-12/h2-5,9,11-13H,6-7H2,1H3	-0.295
InChI=1S/C16H24N2O2/c1-4-9-18-10-8-14(11-18)20-16(19)17-15-12(2)6-5-7-13(15)3/h5-7,14H,4,8-11H2,1-3H3,(H,17,19)	-3.936
InChI=1S/C11H17N/c1-9(11(2,3)12)10-7-5-4-6-8-10/h4-9H,12H2,1-3H3	-1.627
InChI=1S/C12H15NO3/c1-4-16-12-7-5-11(6-8-12)13(9(2)14)10(3)15/h5-8H,4H2,1-3H3	-1.947
InChI=1S/C11H15NO2/c1-2-3-4-8-14-11(13)10-6-5-7-12-9-10/h5-7,9H,2-4,8H2,1H3	-2.378
InChI=1S/C8H12N2/c9-10-7-6-8-4-2-1-3-5-8/h1-5,10H,6-7,9H2	-0.67
InChI=1S/C8H16/c1-7(2)6-8(3,4)5/h1,6H2,2-5H3	-4.688
InChI=1S/C14H21NOS/c1-3-10-15(11-4-2)14(16)17-12-13-8-6-5-7-9-13/h5-9H,3-4,10-12H2,1-2H3	-4.28
InChI=1S/C8H9BrO/c1-5-3-7(9)4-6(2)8(5)10/h3-4,10H,1-2H3	-3.075
InChI=1S/C9H16O2/c1-7-5-3-4-6-9(7)11-8(2)10/h7,9H,3-6H2,1-2H3	-2.55
InChI=1S/C7H14N2O3S2/c8-7(5-13-14(10,11)12)9-6-3-1-2-4-6/h6H,1-5H2,(H2,8,9)(H,10,11,12)	-1.66
InChI=1S/C2H3F3/c1-2(3,4)5/h1H3	-2.043
InChI=1S/C14H22N2O3/c1-16(2)8-11-18-9-3-10-19-14(17)12-4-6-13(15)7-5-12/h4-7H,3,8-11,15H2,1-2H3	-1.177
InChI=1S/C34H32N6O6/c1-21(41)31(33(43)35-25-11-7-5-8-12-25)39-37-27-17-15-23(19-29(2' h5-20,31-32H,1-4H3,(H,35,43)(H,36,44)/b39-37+,40-38+	-8.617
InChI=1S/C10H23NO3S2/c1-3-5-6-7-10(4-2)11-8-9-15-16(12,13)14/h10-11H,3-9H2,1-2H3,(H,12,13,14)	-1.753
InChI=1S/C17H20ClNO/c1-19(2)13-12-17(20,14-8-4-3-5-9-14)15-10-6-7-11-16(15)18/h3-11,20H,12-13H2,1-2H3	-3.618
InChI=1S/C9H13O2P/c1-6-4-7(2)9(12(10)11)8(3)5-6/h4-5,12H,1-3H3,(H,10,11)	-2.79
InChI=1S/C16H12ClFN2O/c1-20-14-7-6-10(17)8-12(14)16(19-9-15(20)21)11-4-2-3-5-13(11)18/h2-8H,9H2,1H3	-3.756
InChI=1S/C7H4Cl4O/c1-2-3(8)5(10)6(11)7(12)4(2)9/h12H,1H3	-4.602
InChI=1S/C10H13N5O3/c1-7(16)18-3-2-17-6-15-5-13-8-4-12-10(11)14-9(8)15/h4-5H,2-3,6H2,1H3,(H2,11,12,14)	-0.97
InChI=1S/C19H21NO2/c1-20(2)14-8-13-19(15-9-4-3-5-10-15)17-12-7-6-11-16(17)18(21)22-1h3-7,9-12H,8,13-14H2,1-2H3	-2.9

"InChi"	"logS(M)"
InChI=1S/C5H12N2O/c1-4(2)3-5(8)7-6/h4H,3,6H2,1-2H3,(H,7,8)	-1.095
InChI=1S/C6H16O7P2/c1-5-11-15(8,12-6-2)13-14(7,9-3)10-4/h5-6H2,1-4H3	-0.658
InChI=1S/C11H16NO5PS/c1-8(2)10-7-9(5-6-11(10)12(13)14)17-18(19,15-3)16-4/h5-8H,1-4H3	-5.275
InChI=1S/C7H14N2O/c10-6-7-5-8-1-3-9(7)4-2-8/h7,10H,1-6H2	0.847
InChI=1S/C20H27O4P/c1-3-5-12-18(4-2)17-22-25(21,23-19-13-8-6-9-14-19)24-20-15-10-7-11-16-20/h6-11,13-16,18H,3-5,12,17H2,1-2H3	-5.28
InChI=1S/C14H23N3O4S/c1-10-9-17(4-5-21-10)22(19,20)16-14(18)15-8-13-7-11-2-3-12(13)6-12-3,10-13H,4-9H2,1H3,(H2,15,16,18)	-2.26
InChI=1S/C7H6Cl2O/c1-10-7-5(8)3-2-4-6(7)9/h2-4H,1H3	-3.102
InChI=1S/C17H21NO4/c1-11-12(2)22-17-13(16(11)19)4-5-15(20-3)14(17)10-18-6-8-21-9-7-1h4-5H,6-10H2,1-3H3	-2.358
InChI=1S/C8H7N3O/c9-8-11-10-7(12-8)6-4-2-1-3-5-6/h1-5H,(H2,9,11)	-0.716
InChI=1S/C12H19NO3S2/c1-2-11(12-6-4-3-5-7-12)10-13-8-9-17-18(14,15)16/h3-7,11,13H,2,8-10H2,1H3,(H,14,15,16)	-1.489
InChI=1S/C3H8O2/c1-5-3-2-4/h4H,2-3H2,1H3	1.119
InChI=1S/C7H6Cl2O/c1-4-2-5(8)7(10)6(9)3-4/h2-3,10H,1H3	-1.42
InChI=1S/C9H12ClO4P/c1-12-15(11,13-2)14-9-7-4-3-6(7)5-8(9)10/h3-4,6-7H,5H2,1-2H3	-2.057
InChI=1S/C11H14N2O2/c1-11(2,10(12)15)13-9(14)8-6-4-3-5-7-8/h3-7H,1-2H3,(H2,12,15)(H,13,14)	-1.615
InChI=1S/C9H8N2O/c1-11-6-10-9(12)7-4-2-3-5-8(7)11/h2-6H,1H3	-1.434
InChI=1S/C19H23N3O/c1-3-21(4-2)13-14-22-18-12-8-7-11-17(18)20-16-10-6-5-9-15(16)19(2h5-12,20H,3-4,13-14H2,1-2H3	-5.162
InChI=1S/C8H10N2O/c9-8-2-1-6-4-10-11-5-7(6)3-8/h1-3,10H,4-5,9H2	-1.256
InChI=1S/C21H23NO5/c1-4-16(24)27-21-8-7-13(23)19-20(21)9-10-22(2)15(21)11-12-5-6-14(h5-8,15,19H,4,9-11H2,1-3H3	-2.792
InChI=1S/C16H13N/c1-2-9-14(10-3-1)17-16-12-6-8-13-7-4-5-11-15(13)16/h1-12,17H	-4.864
InChI=1S/C2H5FO/c3-1-2-4/h4H,1-2H2	1.193
InChI=1S/C10H11ClN2OS/c11-7-1-3-9(4-2-7)15-6-8-5-13-10(12)14-8/h1-4,8H,5-6H2,(H2,12,13)	-3.356
InChI=1S/C2H4ClNO2/c1-2(3)4(5)6/h2H,1H3	-1.437
InChI=1S/C10H12O3/c1-2-9(10(11)12)13-8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H,11,12)	-2.042
InChI=1S/C6H15NO/c1-3-7(4-2)5-6-8/h8H,3-6H2,1-2H3	0.931
InChI=1S/C13H11N3O2S/c1-2-18-13(17)16-11-6-4-3-5-9(11)15-12(16)10-7-19-8-14-10/h3-8H,2H2,1H3	-2.92
InChI=1S/C6H8NO3P/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,7H2,(H2,8,9,10)	-0.124

"InChi"	"logS(M)"
InChI=1S/C13H10N2S/c14-13-15-12(8-16-13)11-6-5-9-3-1-2-4-10(9)7-11/h1-8H,(H2,14,15)	-4.85
InChI=1S/C18H14ClNO/c19-17-8-6-15(7-9-17)18(21,14-4-2-1-3-5-14)16-10-12-20-13-11-16/h1-13,21H	-4.123
InChI=1S/C19H17ClN4/c20-18-8-6-16(7-9-18)10-11-19(12-21,13-24-15-22-14-23-24)17-4-2-1h1-9,14-15H,10-11,13H2	-6.226
InChI=1S/C9H13NO3/c1-6(2)4-8(11)7(5-10)9(12)13-3/h6-7H,4H2,1-3H3	-2.73
InChI=1S/C15H29NO3/c1-3-4-5-6-7-8-9-10-11-12-14(17)16(2)13-15(18)19/h3-13H2,1-2H3,(H,18,19)	-2.735
InChI=1S/C8H10N4O2/c1-2-3-12-6-5(9-4-10-6)7(13)11-8(12)14/h4H,2-3H2,1H3,(H,9,10)(H,11,13,14)	-2.209
InChI=1S/C7H12N2O2/c1-5-2-3-6(8-10)7(4-5)9-11/h5,9,11H,2-4H2,1H3	-1.662
InChI=1S/C12H7ClF3NO2S/c13-11-17-9(12(14,15)16)8(20-11)10(18)19-6-7-4-2-1-3-5-7/h1-5H,6H2	-5.809
InChI=1S/C7H5NO4/c9-6(10)4-1-2-8-5(3-4)7(11)12/h1-3H,(H,9,10)(H,11,12)	-1.827
InChI=1S/C22H12/c1-2-7-17-16(6-1)18-11-10-14-9-8-13-4-3-5-15-12-19(17)22(18)21(14h1-12H	-9.163
InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4)h9,18-19,21-25,28H,6-8,10-17H2,1-5H3	-7.1
InChI=1S/C16H24N6O5/c1-3-20(4-2)16(24)21-9-7-19(8-10-21)12-14(23)18-17-11-13-5-6-15(2h5-6,11H,3-4,7-10,12H2,1-2H3,(H,18,23)/b17-11+	-3.675
InChI=1S/C16H22ClNO2/c1-13-5-2-3-10-18(13)11-4-12-20-16(19)14-6-8-15(17)9-7-14/h6-9,13H,2-5,10-12H2,1H3	-4.141
InChI=1S/C6H7N3O2/c1-3-5-4-7-6(8(5)2)9(10)11/h3-4H,1H2,2H3	-1.255
InChI=1S/C18H18ClNO4/c1-24-16-10-8-15(9-11-16)20(12-2-3-17(21)22)18(23)13-4-6-14(19)7-h4-11H,2-3,12H2,1H3,(H,21,22)	-4.042
InChI=1S/C9H13NO3S2/c11-15(12,13)14-7-6-10-8-9-4-2-1-3-5-9/h1-5,10H,6-8H2,(H,11,12,13)	-0.178
InChI=1S/C35H42N2O9/c1-40-21-8-9-22-23-11-12-37-18-20-15-29(46-30(38)10-7-19-13-27(4h7-10,13-14,16,20,24,26,29,31,34,36H,11-12,15,17-18H2,1-6H3/b10-7+	-6.124
InChI=1S/C8H17NO2/c1-4-9(5-2)7-8(10)11-6-3/h4-7H2,1-3H3	-0.254
InChI=1S/C23H20N2O3S/c26-22-21(16-17-29(28)20-14-8-3-9-15-20)23(27)25(19-12-6-2-7-13-1h1-15,21H,16-17H2/p+1	-4.113
InChI=1S/C16H13NO/c1-12(11-17)14-8-5-9-15(10-14)16(18)13-6-3-2-4-7-13/h2-10,12H,1H3	-3.858
InChI=1S/C9H16NO2/c1-8(2)5-7(11)6-9(3,4)10(8)12/h5-6H2,1-4H3	0.103

"InChi"	"logS(M)"
InChI=1S/C3H5ClO/c4-1-3-2-5-3/h3H,1-2H2	-0.147
InChI=1S/C20H20N2O2/c1-15(2)13-14-18-19(23)21(16-9-5-3-6-10-16)22(20(18)24)17-11-7-4-h3-13,18H,14H2,1-2H3	-5.224
InChI=1S/C8H15NO3/c1-5(2)4-7(8(11)12)9-6(3)10/h5,7H,4H2,1-3H3,(H,9,10)(H,11,12)	-1.33
InChI=1S/C5H5N5/c6-5-9-3-1-7-2-8-4(3)10-5/h1-2H,(H3,6,7,8,9,10)	-2.43
InChI=1S/C9H10ClNO/c1-6-5-8(10)3-4-9(6)11-7(2)12/h3-5H,1-2H3,(H,11,12)	-2.31
InChI=1S/C15H12N2O/c1-10(18)16-13-7-6-12-8-11-4-2-3-5-14(11)17-15(12)9-13/h2-9H,1H3,(H,16,18)	-4.106
InChI=1S/C4H8N2O3/c1-3-9-4(7)6(2)5-8/h3H2,1-2H3	-0.553
InChI=1S/C7H13N3O4/c8-3-6(12)10-4(7(13)14)1-2-5(9)11/h4H,1-3,8H2,(H2,9,11)(H,10,12)(H,13,14)	-0.194
InChI=1S/C18H20O4/c1-2-18-20-13-17(22-18)12-19-14-8-10-16(11-9-14)21-15-6-4-3-5-7-1h3-11,17-18H,2,12-13H2,1H3	-4.787
InChI=1S/C7H16FN/c8-6-4-2-1-3-5-7-9/h1-7,9H2	-1.087
InChI=1S/C12H16N3O3PS/c1-3-16-19(20,17-4-2)18-12-13-10-15(14-12)11-8-6-5-7-9-11/h5-10H,3-4H2,1-2H3	-3.905
InChI=1S/C7H12O3/c8-6(9)7(10)4-2-1-3-5-7/h10H,1-5H2,(H,8,9)	-0.333
InChI=1S/C14H12O2/c15-13-8-6-12(7-9-13)14(16)10-11-4-2-1-3-5-11/h1-9,15H,10H2	-1.501
InChI=1S/C8H9FN2O4/c1-2-6(12)15-4-11-3-5(9)7(13)10-8(11)14/h3H,2,4H2,1H3,(H,10,13,14)	-0.81
InChI=1S/C9H5ClO2/c10-7-2-3-8-6(5-7)1-4-9(11)12-8/h1-5H	-2.359
InChI=1S/C13H15N/c1-3-10-14(2)13-9-8-11-6-4-5-7-12(11)13/h1,4-7,13H,8-10H2,2H3	-1.944
InChI=1S/C18H38/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3-18H2,1-2H3	-7.628
InChI=1S/C18H17N5O4/c1-10(24)16(23-22-13-5-3-4-6-15(13)27-2)17(25)19-11-7-8-12-14(9-1h3-9,16H,1-2H3,(H,19,25)(H2,20,21,26)/b23-22+	-7.631
InChI=1S/C27H40O2/c1-16(2)18-11-20(24(28)22(14-18)26(5,6)7)13-21-12-19(17(3)4)15-23h11-12,14-17,28-29H,13H2,1-10H3	-9.868
InChI=1S/C13H11N3O4S2/c1-16-10(12(18)15-13-14-6-7-21-13)11(17)8-4-2-3-5-9(8)22(16,19)20h2-7,17H,1H3,(H,14,15,18)	-3.061
InChI=1S/C12H8Cl3NO/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6H,16H2	-5.045
InChI=1S/C22H27N5O2/c1-3-17(2)27-22(29)26(16-23-27)20-6-4-18(5-7-20)24-12-14-25(15-13h4-11,16-17,28H,3,12-15H2,1-2H3	-4.829
InChI=1S/C12H5Cl5O/c13-6-2-1-3-7(14)12(6)18-11-5-9(16)8(15)4-10(11)17/h1-5H	-7.12
InChI=1S/C11H14N2/c1-13(2)8-9-7-12-11-6-4-3-5-10(9)11/h3-7,12H,8H2,1-2H3	-1.454

"InChi"	"logS(M)"
InChI=1S/C10H13NO/c1-3-9-6-4-5-7-10(9)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)	-1.591
InChI=1S/C8H8O3/c1-11-8-3-2-6(5-9)4-7(8)10/h2-5,10H,1H3	-1.826
InChI=1S/C40H50N8O6/c1-4-26(2)34-40(54)48-32(19-12-22-42-48)39(53)47-31(18-11-21-41-4h5-10,14-17,21-22,26,29-34H,4,11-13,18-20,23-25H2,1-3H3,(H,43,50)(H,44,49)	-4.04
InChI=1S/C15H14O3/c16-14-9-5-4-8-13(14)15(17)18-11-10-12-6-2-1-3-7-12/h1-9,16H,10-11H2	-4.489
InChI=1S/C9H8N2O2/c1-5-2-3-6-7(4-5)11-9(13)8(12)10-6/h2-4H,1H3,(H,10,12)(H,11,13)	-3.042
InChI=1S/C9H7BrO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6H,(H,11,12)/b6-3+	-2.991
InChI=1S/C18H15N5O5/c1-9(24)15(23-22-12-5-3-2-4-11(12)17(26)27)16(25)19-10-6-7-13-14(h2-8,15H,1H3,(H,19,25)(H,26,27)(H2,20,21,28)/b23-22+	-7.331
InChI=1S/C19H28O/c1-18-9-3-4-16(18)15-6-5-13-12-14(20)7-11-19(13,2)17(15)8-10-18/h3,9,13,15-17H,4-8,10-12H2,1-2H3	-6.07
InChI=1S/C14H22N2O3/c1-4-15-9-11(14(18)19-5-2)13(17)16-10(3)7-6-8-12(15)16/h9-10,12H,4-8H2,1-3H3	-1.721
InChI=1S/C3H4O2/c4-1-3-2-5-3/h1,3H,2H2	1.142
InChI=1S/C9H12O2/c1-8(10)7-11-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3	-1.003
InChI=1S/C10H10N2O2/c1-10(7-5-3-2-4-6-7)8(13)11-9(14)12-10/h2-6H,1H3,(H2,11,12,13,14)	-1.46
InChI=1S/C9H7F3O/c1-6(13)7-3-2-4-8(5-7)9(10,11)12/h2-5H,1H3	-2.482
InChI=1S/C17H16Br2N2O4/c18-9-11-20(12-10-19)14-5-7-16(8-6-14)25-17(22)13-1-3-15(4-2-13)2h1-8H,9-12H2	-7.053
InChI=1S/C17H20N4/c18-15-11-19-8-7-17(15)20-9-10-21-14(12-20)6-5-13-3-1-2-4-16(13)2h1-4,7-8,11,14H,5-6,9-10,12,18H2	-3.495
InChI=1S/C16H33NO2/c1-2-3-4-5-6-7-8-9-10-11-12-17(18)13-15-19-16-14-17/h2-16H2,1H3	-4.84
InChI=1S/C28H32O15/c1-10-21(32)23(34)25(36)27(40-10)39-9-19-22(33)24(35)26(37)28(43h3-8,10,19,21-30,32-37H,9H2,1-2H3	-7.506
InChI=1S/C8H15NO/c1-2-3-6-9-7-4-5-8(9)10/h2-7H2,1H3	-1.399
InChI=1S/C11H16O2/c1-3-11(2,13)10(12)9-7-5-4-6-8-9/h4-8,10,12-13H,3H2,1-2H3	-1.724
InChI=1S/C7H12O4S2/c1-4(6(8)9)12-3-13-5(2)7(10)11/h4-5H,3H2,1-2H3,(H,8,9)(H,10,11)	-1.82
InChI=1S/C12H14N2O6S/c1-8(15)14-21(19,20)10-4-2-9(3-5-10)13-11(16)6-7-12(17)18/h2-5H,6-7H2,1H3,(H,13,16)(H,14,15)(H,17,18)	-2.686
InChI=1S/C7H5Cl3O/c8-5-1-4(3-11)2-6(9)7(5)10/h1-2,11H,3H2	-3.095
InChI=1S/C7H7NO4/c1-12-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3	-2.841
InChI=1S/C7H6BrNO/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H2,9,10)	-2.163

"InChi"	"logS(M)"
InChI=1S/C27H33N3O8/c1-26(37)13-7-6-8-16(31)17(13)21(32)18-14(26)11-15-20(29(2)3)22(3h6-8,14-15,20,31,33-34,37-38H,4-5,9-12H2,1-3H3,(H,28,36)	-1.42
InChI=1S/C12H17NO2/c1-9(13-3)12(15-10(2)14)11-7-5-4-6-8-11/h4-9,12-13H,1-3H3	-1.337
InChI=1S/C11H6O3/c12-10-4-2-7-1-3-9-8(5-6-13-9)11(7)14-10/h1-6H	-2.336
InChI=1S/C15H10Cl2N2O2/c16-10-6-5-9(12(17)7-10)8-19-13-4-2-1-3-11(13)14(18-19)15(20)21/h1-7H,8H2,(H,20,21)	-5.566
InChI=1S/C10H14N2O/c1-2-11-8-12-10(13)9-6-4-3-5-7-9/h3-7,11H,2,8H2,1H3,(H,12,13)	-0.075
InChI=1S/C35H33NO2/c37-34(24-28-14-5-1-6-15-28,25-29-16-7-2-8-17-29)32-22-13-23-33(3h1-23,37-38H,24-27H2	-9.63
InChI=1S/C4H7NO2/c1-2-4(7)5-3-6/h2,6H,1,3H2,(H,5,7)	0.81
InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h5,10-11H,4,6-8H2,1-3H3	-2.707
InChI=1S/C16H15NO2S2/c18-15(19)11-17(14-9-5-2-6-10-14)16(20)21-12-13-7-3-1-4-8-13/h1-10H,11-12H2,(H,18,19)	-3.92
InChI=1S/C14H18N2O/c1-16-7-3-4-14(16)12-9-15-13-6-5-10(17-2)8-11(12)13/h5-6,8-9,14-15H,3-4,7H2,1-2H3	-1.861
InChI=1S/C13H20O3/c1-2-3-4-11-5-7-13(8-6-11)16-10-12(15)9-14/h5-8,12,14-15H,2-4,9-10H2,1H3	-3.298
InChI=1S/C6H8O4/c7-5(8)3-1-2-4-6(9)10/h1,3H,2,4H2,(H,7,8)(H,9,10)/b3-1+	-1.204
InChI=1S/C19H23N3O4/c1-25-16-7-6-13(10-17(16)26-2)8-9-21-18(23)12-22-15-5-3-4-14(11-1h3-7,10-11,22H,8-9,12H2,1-2H3,(H2,20,24)(H,21,23)	-2.69
InChI=1S/C7H6F3NO2S/c8-7(9,10)5-1-3-6(4-2-5)14(11,12)13/h1-4H,(H2,11,12,13)	-1.981
InChI=1S/C15H15F3N2O2/c1-10(2)14(21,12-7-19-9-20-8-12)11-3-5-13(6-4-11)22-15(16,17)18/h3-10,21H,1-2H3	-3.438
InChI=1S/C9H8ClNO2/c1-5-9(12)11-7-4-6(10)2-3-8(7)13-5/h2-5H,1H3,(H,11,12)	-2.459
InChI=1S/C9H8N6O8S3/c1-13-8(24-9(11-13)25(10,20)21)12-26(22,23)7-3-2-5(14(16)17)4-6(7h2-4H,1H3,(H2,10,20,21)/b12-8-	-2.74
InChI=1S/C4H8N4O8/c9-6(10)5(1-3-15-7(11)12)2-4-16-8(13)14/h1-4H2	-1.219
InChI=1S/C16H22N4O3/c1-3-6-13-14(9-8-12(11(2)21)16(13)22)23-10-5-4-7-15-17-19-20-18-1h8-9,22H,3-7,10H2,1-2H3,(H,17,18,19,20)	-4.204
InChI=1S/C9H20O2/c1-3-5-6-9(4-2,7-10)8-11/h10-11H,3-8H2,1-2H3	-1.26
InChI=1S/C11H17NO3/c1-7(2)12-6-11(15)8-3-9(13)5-10(14)4-8/h3-5,7,11-15H,6H2,1-2H3	0.675
InChI=1S/C12H7Cl3/c13-10-7-12(15)11(14)6-9(10)8-4-2-1-3-5-8/h1-7H	-6.27

"InChi"	"logS(M)"
InChI=1S/C15H8Cl2FNO/c16-9-7-12(17)15-13(8-9)19-6-5-14(15)20-11-3-1-10(18)2-4-11/h1-8H	-6.424
InChI=1S/C22H23NO2/c1-2-22(18-12-6-3-7-13-18,19-14-8-4-9-15-19)25-21(24)23-20-16-10-h1,3-4,6-9,12-15,20H,5,10-11,16-17H2,(H,23,24)	-7.088
InChI=1S/C10H12O3/c1-3-13-9-5-4-8(7-11)6-10(9)12-2/h4-7H,3H2,1-2H3	-2.191
InChI=1S/C13H11ClFNO/c14-12-7-11(16)4-5-13(12)17-8-9-2-1-3-10(15)6-9/h1-7H,8,16H2	-4.693
InChI=1S/C9H11NO3S/c1-7(9(10)11)14(12,13)8-5-3-2-4-6-8/h2-7H,1H3,(H2,10,11)	-1.64
InChI=1S/C11H13N3O6S/c1-21-5-4-9(11(15)16)12-8-3-2-7(13(17)18)6-10(8)14(19)20/h2-3,6,9,12H,4-5H2,1H3,(H,15,16)	-2.886
InChI=1S/C12H16N2O/c15-12(10-5-4-8-13-9-10)14-11-6-2-1-3-7-11/h4-5,8-9,11H,1-3,6-7H2,(H,14,15)	-2.319
InChI=1S/C8H6N4O8/c13-7(14)3-9-8-5(11(17)18)1-4(10(15)16)2-6(8)12(19)20/h1-2,9H,3H2,(H,13,14)	-2.392
InChI=1S/C42H30N6O12/c49-37(25-7-1-13-43-19-25)55-31-32(56-38(50)26-8-2-14-44-20-26)3 h1-24,31-36H	-5.48
InChI=1S/C12H7Cl3O/c13-9-6-7-10(14)12(11(9)15)16-8-4-2-1-3-5-8/h1-7H	-5.95
InChI=1S/C10H10N2O/c1-8(13)9-4-2-3-5-10(9)12-7-6-11/h2-5,12H,7H2,1H3	-2.087
InChI=1S/C24H46O6/c1-9-13-15-19(11-3)21(25)27-29-23(5,6)17-18-24(7,8)30-28-22(26)20h19-20H,9-18H2,1-8H3	-7.188
InChI=1S/C3H6O3/c1-4-2-6-3-5-1/h1-3H2	0.372
InChI=1S/C5H6N2/c6-4-2-1-3-5-7/h1-3H2	1.026
InChI=1S/C36H60O30/c37-1-7-25-13(43)19(49)31(55-7)62-26-8(2-38)57-33(21(51)15(26)45) h7-54H,1-6H2	-0.91
InChI=1S/C20H16N2O2/c1-11-6-9-17(12(2)10-11)22-19(23)14-5-3-4-13-16(21)8-7-15(18(13)1 h3-10H,21H2,1-2H3	-4.892
InChI=1S/C12H20N2O4/c1-5-6-14-11(16)18-8-12(4,9(2)3)7-17-10(13)15/h1,9H,6-8H2,2-4H3,(H2,13,15)(H,14,16)	-1.125
InChI=1S/C6H10N2O2/c1-2-8-4-3-7-5(9)6(8)10/h2-4H2,1H3,(H,7,9)	-0.758
InChI=1S/C9H9NO2/c1-11-8-3-7(6-10)4-9(5-8)12-2/h3-5H,1-2H3	-2.109
InChI=1S/C13H10O2/c14-10-11-6-8-13(9-7-11)15-12-4-2-1-3-5-12/h1-10H	-3.864
InChI=1S/C2H3Cl2NO2/c1-2(3,4)5(6)7/h1H3	-1.76
InChI=1S/C11H6ClN3O3/c12-6-1-2-7-8(5-6)14-11(13-7)9-3-4-10(18-9)15(16)17/h1-5H,(H, 13,14)	-4.82

"InChi"	"logS(M)"
InChI=1S/C19H20N2O3/c1-3-4-5-10-17-18(12(2)21-24-17)20-15-11-16(22)19(23)14-9-7-6-8-1h6-9,11,22H,3-5,10H2,1-2H3/b20-15+	-3.18
InChI=1S/C13H24Cl6O8P2/c14-1-5-22-28(20,23-6-2-15)26-11-13(9-18,10-19)12-27-29(21,24-7-3h1-12H2	-3.4
InChI=1S/C12H11ClN6O2S2/c13-9-5-10(15-6-7-2-1-3-22-7)8(12-16-18-19-17-12)4-11(9)23(14,20)2h1-5,15H,6H2,(H2,14,20,21)(H,16,17,18,19)	-2.321
InChI=1S/C17H27NO2/c1-11-9-12(16(2,3)4)14(20-15(19)18-8)13(10-11)17(5,6)7/h9-10H,1-8H3,(H,18,19)	-4.598
InChI=1S/C17H23N5O14/c18-5(7(24)4(23)2-35-16(19)33)12(28)20-6(15(31)32)10-8(25)9(26)13h1,4-10,13,23-26H,2,18H2,(H2,19,33)(H,20,28)(H,29,30)(H,31,32)(H,21,27,34)	0.283
InChI=1S/C6H12/c1-3-5-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+	-3.226
InChI=1S/C9H15F/c1-2-3-4-5-6-7-8-9-10/h1H,3-9H2	-3.595
InChI=1S/C8H7ClO2/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4H,1H3,(H,10,11)	-3.065
InChI=1S/C39H72O4/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-38(40)42-36-37(3)h18-21,37H,4-17,22-36H2,1-3H3/b20-18+,21-19+	-4.782
InChI=1S/C8H8N4/c1-5-6(2)12-8-7(11-5)3-9-4-10-8/h3-4H,1-2H3	-0.46
InChI=1S/C19H15ClF3NO7/c1-3-29-17(25)10(2)30-18(26)13-9-12(5-6-15(13)24(27)28)31-16-7-4-h4-10H,3H2,1-2H3	-6.623
InChI=1S/C15H23NO/c1-14-8-5-6-11-16(14)12-7-13-17-15-9-3-2-4-10-15/h2-4,9-10,14H,5-8,11-13H2,1H3	-3.347
InChI=1S/C53H58O6P2/c1-49(2,39-21-13-9-14-22-39)43-29-31-47(45(33-43)51(5,6)41-25-17-h9-34H,35-38H2,1-8H3	-7.232
InChI=1S/C13H10N2O3/c16-12-6-4-10(5-7-12)14-15-11-3-1-2-9(8-11)13(17)18/h1-8,16H,(H,17,18)/b15-14+	-3.85
InChI=1S/C20H8I4O5/c21-11-5-9-17(13(23)15(11)25)28-18-10(6-12(22)16(26)14(18)24)20(5h1-6,25-26H	-3.077
InChI=1S/C9H8O3/c10-8-3-1-2-7(6-8)4-5-9(11)12/h1-6,10H,(H,11,12)/b5-4+	-2.099
InChI=1S/C8H14O4/c1-3-8(4-2,7(11)12)5-6(9)10/h3-5H2,1-2H3,(H,9,10)(H,11,12)	-0.796
InChI=1S/C16H12ClNO5/c1-9(15(19)20)21-11-3-5-12(6-4-11)22-16-18-13-7-2-10(17)8-14(13)2h2-9H,1H3,(H,19,20)	-3.092
InChI=1S/C7H14O/c8-7-5-3-1-2-4-6-7/h7-8H,1-6H2	-0.88
InChI=1S/C13H12FN3O2S2/c14-9-1-3-10(4-2-9)16-13(20)17-11-5-7-12(8-6-11)21(15,18)19/h1-8H,(H2,15,18,19)(H2,16,17,20)	-2.99
InChI=1S/C5H6N2O2/c1-3-2-4(8)5(9)7-6-3/h2H,1H3,(H,6,8)(H,7,9)	0.134

"InChi"	"logS(M)"
InChI=1S/C8H15NO2/c9-8(7(10)11)5-3-1-2-4-6-8/h1-6,9H2,(H,10,11)	-1.833
InChI=1S/C10H12O4/c1-5-4-7(11)6(2)9(12)8(5)10(13)14-3/h4,11-12H,1-3H3	-4.037
InChI=1S/C21H28N2S2/c1-5-6-14-24-20(23-19-8-7-13-22-15-19)25-16-17-9-11-18(12-10-17)2h7-13,15H,5-6,14,16H2,1-4H3/b23-20+	-5.571
InChI=1S/C9H18N2O2/c1-4-13-9(12)11-6-7(2)10-5-8(11)3/h7-8,10H,4-6H2,1-3H3	0.65
InChI=1S/C10H15NO/c1-2-3-8-12-10-6-4-9(11)5-7-10/h4-7H,2-3,8,11H2,1H3	-2.653
InChI=1S/C10H14O2/c1-10(2)7-4-3-6(5-7)8(11)9(10)12/h6-7H,3-5H2,1-2H3	-1.52
InChI=1S/C13H10ClN3O4S2/c14-9-6-10-12(7-11(9)22(15,18)19)23(20,21)17-13(16-10)8-4-2-1-3-5-h1-7H,(H,16,17)(H2,15,18,19)	-4.157
InChI=1S/C25H31NO6/c1-13-26-25(20(30)12-31-14(2)27)21(32-13)10-18-17-6-5-15-9-16(28)h7-9,17-19,21-22,29H,5-6,10-12H2,1-4H3	-4.074
InChI=1S/C7H5Cl3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H	-3.567
InChI=1S/C4H3BrN2O/c5-3-1-6-2-7-4(3)8/h1-2H,(H,6,7,8)	-0.447
InChI=1S/C12H3Cl5O2/c13-4-1-2-5-6(3-4)19-12-10(17)8(15)7(14)9(16)11(12)18-5/h1-3H	-9.473
InChI=1S/C9H8N2/c10-8-5-1-3-7-4-2-6-11-9(7)8/h1-6H,10H2	-1.244
InChI=1S/C6H8O6/c7-4(8)1-3(6(11)12)2-5(9)10/h3H,1-2H2,(H,7,8)(H,9,10)(H,11,12)	0.275
InChI=1S/C14H21NO3/c1-10-9-13(11(2)18-10)14(16)15(17-3)12-7-5-4-6-8-12/h9,12H,4-8H2,1-3H3	-2.92
InChI=1S/C8H18O4/c1-9-3-5-11-7-8-12-6-4-10-2/h3-8H2,1-2H3	0.749
InChI=1S/C8H10BrNO2S/c1-2-10-13(11,12)8-5-3-7(9)4-6-8/h3-6,10H,2H2,1H3	-3.02
InChI=1S/C28H37N3O5S/c1-27(2,3)30-25(34)24-28(4,5)37-18-31(24)26(35)23(33)21(16-19-12-h6-15,21,23-24,33H,16-18H2,1-5H3,(H,29,32)(H,30,34)	-3.83
InChI=1S/C27H50O6/c1-5-9-12-15-18-24(28)31-21-27(8-4,22-32-25(29)19-16-13-10-6-2)23h5-23H2,1-4H3	-6.974
InChI=1S/C10H14O/c1-8-5-4-6-10(2,3)9(8)7-11/h4-5,7H,6H2,1-3H3	-2.465
InChI=1S/C17H34O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-17(20)21-15-16(19)14-18/h16,18-19H,2-15H2,1H3	-7.398
InChI=1S/C10H10O4/c1-7(11)13-9-5-3-4-6-10(9)14-8(2)12/h3-6H,1-2H3	-2.072
InChI=1S/C18H18N4O6/c1-11(23)17(18(24)19-14-6-4-5-7-16(14)28-3)21-20-13-9-8-12(27-2)1h4-10,17H,1-3H3,(H,19,24)/b21-20+	-8.308
InChI=1S/C22H28N2O3/c1-2-22(26)18-8-10-21(11-9-18)27-17-20(25)16-23-12-14-24(15-13-2h3-11,20,25H,2,12-17H2,1H3	-3.11
InChI=1S/C2HF6NO4S2/c3-1(4,5)14(10,11)9-15(12,13)2(6,7)8/h9H	0.454

"InChi"	"logS(M)"
InChI=1S/C8H16O3/c1-7(9)11-6-5-8(2,3)10-4/h5-6H2,1-4H3	-0.439
InChI=1S/C11H12N4O3S/c1-18-11-10(13-6-7-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H,12H2,1H3,(H,13,15)	-1.842
InChI=1S/C16H26/c1-2-3-4-5-6-7-8-10-13-16-14-11-9-12-15-16/h9,11-12,14-15H,2-8,10,13H2,1H3	-7.959
InChI=1S/C11H16N2O4/c1-4-6-11(7-5-2,9(15)17-3)8(14)13-10(12)16/h4-5H,1-2,6-7H2,3H3,(H3,12,13,14,16)	-2.17
InChI=1S/C18H27NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19)24-1h4,11,13-15,22H,5-10H2,1-3H3/b12-4+	-1.576
InChI=1S/C18H39O7P/c1-4-7-10-20-13-16-23-26(19,24-17-14-21-11-8-5-2)25-18-15-22-12-9h4-18H2,1-3H3	-2.779
InChI=1S/C9H11FN2O4/c1-2-3-7(13)16-5-12-4-6(10)8(14)11-9(12)15/h4H,2-3,5H2,1H3,(H,11,14,15)	-1.31
InChI=1S/C8H6O4/c9-4-5-1-2-7(10)6(3-5)8(11)12/h1-4,10H,(H,11,12)	-2.635
InChI=1S/C8H10N4O4S/c13-3-1-11-2-4-16-8(11)10-7-9-5-6(17-7)12(14)15/h5,13H,1-4H2/b10-8-	-0.833
InChI=1S/C13H26N2O4/c1-5-7-15-12(17)19-9-13(4,10(3)6-2)8-18-11(14)16/h10H,5-9H2,1-4H3,(H2,14,16)(H,15,17)	-3.634
InChI=1S/C10H20N2O3S2/c11-10(8-16-17(13,14)15)12-7-6-9-4-2-1-3-5-9/h9H,1-8H2,(H2,11,12)(H,13,14,15)	-3.225
InChI=1S/C11H18N2O3/c1-5-11(6-2)8(14)12-10(13-9(11)15)16-7(3)4/h7H,5-6H2,1-4H3,(H,12,13,14,15)	-2.081
InChI=1S/C15H11N3O3/c19-14-9-16-15(10-4-2-1-3-5-10)12-8-11(18(20)21)6-7-13(12)17-14/h1-8H,9H2,(H,17,19)	-3.8
InChI=1S/C11H16N2O/c1-2-3-8-13-10-7-5-4-6-9(10)11(12)14/h4-7,13H,2-3,8H2,1H3,(H2,12,14)	-2.594
InChI=1S/C15H15N3/c1-8-12(16)5-3-10-7-11-4-6-13(17)9(2)15(11)18-14(8)10/h3-7H,16-17H2,1-2H3	-4.245
InChI=1S/C15H16N2O3S/c1-10-3-4-12(9-11(10)2)15(18)17-21(19,20)14-7-5-13(16)6-8-14/h3-9H,16H2,1-2H3,(H,17,18)	-4.374
InChI=1S/C14H18O7/c1-7(16)8-2-4-9(5-3-8)20-14-13(19)12(18)11(17)10(6-15)21-14/h2-5,10-15,17-19H,6H2,1H3	-1.17
InChI=1S/C17H19NO3/c1-20-13-5-2-9-8-11-10-3-4-12(19)16-17(10,6-7-18-11)14(9)15(13)21h2-5,10-12,16,18-19H,6-8H2,1H3	-0.863
InChI=1S/C14H21N3O2S/c1-15-20(18,19)10-11-4-5-14-13(8-11)12(9-16-14)6-7-17(2)3/h4-5,8-9,15-16H,6-7,10H2,1-3H3	-1.141

"InChi"	"logS(M)"
InChI=1S/C6H6O4/c7-5(8)3-1-2-4-6(9)10/h1-4H,(H,7,8)(H,9,10)/b3-1+,4-2+	-2.852
InChI=1S/C20H31NO2/c1-2-3-5-13-19-14-8-9-15-21(19)16-10-17-23-20(22)18-11-6-4-7-12-1h4,6-7,11-12,19H,2-3,5,8-10,13-17H2,1H3	-5.426
InChI=1S/C12H16O4/c1-2-11(15)10-5-3-4-6-12(10)16-8-9(14)7-13/h3-6,9,13-14H,2,7-8H2,1H3	-1.717
InChI=1S/C9H9N5O6S3/c1-13-8(21-9(11-13)22(10,17)18)12-23(19,20)7-4-2-6(3-5-7)14(15)16/h2-5H,1H3,(H2,10,17,18)/b12-8+	-2.7
InChI=1S/C12H18O3/c1-3-4-7-15-9-10-5-6-11(13)12(8-10)14-2/h5-6,8,13H,3-4,7,9H2,1-2H3	-2.095
InChI=1S/C29H39NO9/c1-27(2,33)8-5-10-29(34,16-23(31)36-4)26(32)39-25-22(35-3)15-28-9h13-15,24-25,33-34H,5-12,16-17H2,1-4H3	-4.339
InChI=1S/C11H21N5S/c1-6-12-9-14-10(13-8(4)7(2)3)16-11(15-9)17-5/h7-8H,6H2,1-5H3,(H2,12,13,14,15,16)	-3.708
InChI=1S/C11H14N2O2S/c1-14-8-2-4-10(5-3-8)16-7-9-6-13-11(12)15-9/h2-5,9H,6-7H2,1H3,(H2,12,13)	-2.451
InChI=1S/C9H17NOS/c1-2-12-9(11)10-7-5-3-4-6-8-10/h2-8H2,1H3	-2.286
InChI=1S/C12H22O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3	-3.975
InChI=1S/C9H12O4/c10-5-8(12)6-13-9-3-1-7(11)2-4-9/h1-4,8,10-12H,5-6H2	0.053
InChI=1S/C9H10N4/c1-5-6(2)12-9-8(11-5)4-10-7(3)13-9/h4H,1-3H3	-1.144
InChI=1S/C12H22O4/c1-3-15-11(13)9-7-5-6-8-10-12(14)16-4-2/h3-10H2,1-2H3	-2.53
InChI=1S/C20H29NO2/c1-2-3-5-13-19-14-8-9-15-21(19)16-10-17-23-20(22)18-11-6-4-7-12-1h2-4,6-7,11-12,19H,5,8-10,13-17H2,1H3/b3-2+	-5.227
InChI=1S/C8H10FN3/c1-12(2)11-10-8-5-3-7(9)4-6-8/h3-6H,1-2H3/b11-10+	-2.643
InChI=1S/C41H63NO15/c1-10-19(3)34(47)56-33-28(46)27-23(17-42-16-18(2)11-12-25(42)38(h18-20,23-33,43,46,49-52H,10-17H2,1-9H3	-5.939
InChI=1S/C7H5NO4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H,(H,9,10)	-1.35
InChI=1S/C9H10N2O3/c10-5-8(12)11-7-3-1-6(2-4-7)9(13)14/h1-4H,5,10H2,(H,11,12)(H,13,14)	-1.851
InChI=1S/C11H15N3O4/c1-12-10(15)17-6-8-4-3-5-9(14-8)7-18-11(16)13-2/h3-5H,6-7H2,1-2H3,(H,12,15)(H,13,16)	-1.263
InChI=1S/C9H10N2O2S/c12-11(13)8-3-1-7(2-4-8)9-10-5-6-14-9/h1-4,9-10H,5-6H2	-1.551
InChI=1S/C22H26N2O2/c1-3-5-13-23-17-11-12-18(24-14-6-4-2)20-19(17)21(25)15-9-7-8-10-1h7-12,23-24H,3-6,13-14H2,1-2H3	-7.932
InChI=1S/C9H7Cl2N5/c10-4-1-2-6(11)5(3-4)7-14-8(12)16-9(13)15-7/h1-3H,(H4,12,13,14,15,16)	-2.751

"InChi"	"logS(M)"
InChI=1S/C29H30N2O6/c1-5-6-17-23-27(32)30(21-13-9-7-10-14-21)31(22-15-11-8-12-16-22)2h7-16,18-19H,5-6,17H2,1-4H3	-6.928
InChI=1S/C18H21N3O/c1-20(2)12-7-13-21-16-10-5-3-8-14(16)18(22)19-15-9-4-6-11-17(15)2h3-6,8-11H,7,12-13H2,1-2H3,(H,19,22)	-5.256
InChI=1S/C8H7IO3/c1-12-8(11)5-2-3-7(10)6(9)4-5/h2-4,10H,1H3	-3.314
InChI=1S/C29H50O2/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-29(8)19-17-26-25(7)27h20-22,30H,9-19H2,1-8H3	-8.52
InChI=1S/C18H20N2O3/c21-17(13-5-7-19-15-4-2-1-3-12(13)15)16-9-11-6-8-20(16)10-14(11)1h1-5,7,11,14,16-17,21H,6,8-10H2,(H,22,23)	-1.94
InChI=1S/C13H9FN2/c14-8-5-6-12-10(7-8)13(15)9-3-1-2-4-11(9)16-12/h1-7H,(H2,15,16)	-2.4
InChI=1S/C13H20O/c1-8(2)12-6-10-5-11(7-14)13(12)4-9(10)3/h7-8,11-13H,4-6H2,1-3H3	-3.851
InChI=1S/C15H18ClN3O/c16-13-7-5-12(6-8-13)15(20)9-3-1-2-4-14(15)19-11-17-10-18-19/h5-8,10-11,14,20H,1-4,9H2	-3.368
InChI=1S/C19H19N5O4S/c1-3-23(11-10-18(25)28-2)14-6-4-13(5-7-14)20-21-19-16-12-15(24(26h4-9,12H,3,10-11H2,1-2H3/b21-20+	-7.315
InChI=1S/C18H26N2O5S/c1-6-7-11-23-16(21)19(4)26-20(5)17(22)24-14-10-8-9-13-12-18(2,3)2h8-10H,6-7,11-12H2,1-5H3	-4.541
InChI=1S/C7H10O3/c1-6(5-8)3-4-10-7(2)9/h3,5H,4H2,1-2H3/b6-3-	-0.461
InChI=1S/C10H10O5/c1-4(11)8-6(13)3-7(14)9(5(2)12)10(8)15/h3,13-15H,1-2H3	-2.735
InChI=1S/C42H72O14/c1-20(2)10-9-13-42(8,56-37-34(52)32(50)30(48)25(19-44)55-37)21-1h10,21-37,43-52H,9,11-19H2,1-8H3	-6.145
InChI=1S/C7H6O2/c8-5-6-2-1-3-7(9)4-6/h1-5,9H	-1.23
InChI=1S/C4H11N/c1-4(2)3-5/h4H,3,5H2,1-2H3	1.136
InChI=1S/C11H10N2O3S/c14-9(15)6-8-10(16)13(11(17)12-8)7-4-2-1-3-5-7/h1-5,8H,6H2,(H,12,17)(H,14,15)	-1.764
InChI=1S/C18H30O/c1-7-12(4)15-10-16(13(5)8-2)18(19)17(11-15)14(6)9-3/h10-14,19H,7-9H2,1-6H3	-5.55
InChI=1S/C14H17N3O9/c1-6(18)23-5-9-11(24-7(2)19)12(25-8(3)20)13(26-9)17-14(22)16-10(2h4,9,11-13H,5H2,1-3H3,(H,16,21,22)	-3.046
InChI=1S/C9H14N2/c10-7-4-8-11-9-5-2-1-3-6-9/h1-3,5-6,11H,4,7-8,10H2	-1.654
InChI=1S/C4H11NO/c1-3-5(6)4-2/h6H,3-4H2,1-2H3	0.704
InChI=1S/C14H12O2/c1-14(2)12-8-10-6-4-3-5-9(10)7-11(12)13(15)16-14/h3-8H,1-2H3	-2.984
InChI=1S/C20H23N3O3/c1-20(2,3)14-11-13(9-10-18(24)26-4)12-17(19(14)25)23-21-15-7-5-6-h5-8,11-12,25H,9-10H2,1-4H3	-6.849

"InChi"	"logS(M)"
InChI=1S/C3H8O/c1-3-4-2/h3H2,1-2H3	-0.08
InChI=1S/C16H13FO4/c1-9-6-11(8-13(15(9)19)16(20)21)14(18)7-10-2-4-12(17)5-3-10/h2-6,8,19H,7H2,1H3,(H,20,21)	-4.464
InChI=1S/C8H9N3O2/c1-6(12)10-11-8(13)7-4-2-3-5-9-7/h2-5H,1H3,(H,10,12)(H,11,13)	-1.332
InChI=1S/C12H2Cl8O/c13-3-1-5(9(17)11(19)7(3)15)21-6-2-4(14)8(16)12(20)10(6)18/h1-2H	-10.1
InChI=1S/C4H4N2O2/c7-3-1-2-4(8)6-5-3/h1-2H,(H,5,7)(H,6,8)	-1.271
InChI=1S/C20H15NO4/c22-15-9-5-13(6-10-15)20(14-7-11-16(23)12-8-14)19(24)21-17-3-1-2-h1-12,22-23H,(H,21,24)	-3.962
InChI=1S/C3H9N/c1-3(2)4/h3H,4H2,1-2H3	1.228
InChI=1S/C14H14O2/c15-10-13-8-4-5-9-14(13)16-11-12-6-2-1-3-7-12/h1-9,15H,10-11H2	-2.7
InChI=1S/C21H21NO4/c1-15-19(25-14-16-5-3-2-4-6-16)8-7-17-18(23)13-20(26-21(15)17)22-h2-8,13H,9-12,14H2,1H3	-5.16
InChI=1S/C8H8N2S/c1-5-3-2-4-6-7(5)10-8(11)9-6/h2-4H,1H3,(H2,9,10,11)	-3.136
InChI=1S/C12H6Cl4O/c13-7-1-3-9(4-2-7)17-11-6-8(14)5-10(15)12(11)16/h1-6H	-7.14
InChI=1S/C10H8O2/c11-9-5-7-3-1-2-4-8(7)6-10(9)12/h1-6,11-12H	-2.738
InChI=1S/C7H5NO2/c8-4-5-1-2-6(9)7(10)3-5/h1-3,9-10H	-1.024
InChI=1S/C11H17N/c1-11(2,12-3)9-10-7-5-4-6-8-10/h4-8,12H,9H2,1-3H3	-1.549
InChI=1S/C16H17NO4/c1-11-6-4-5-7-15(11)17(19)16(18)12-8-13(20-2)10-14(9-12)21-3/h4-10,19H,1-3H3	-3.65
InChI=1S/C13H10N2O3/c16-10-7-5-9(6-8-10)14-15-12-4-2-1-3-11(12)13(17)18/h1-8,16H,(H,17,18)/b15-14+	-3.33
InChI=1S/C13H16ClNO/c1-15-13(9-5-4-8-12(13)16)10-6-2-3-7-11(10)14/h2-3,6-7,15H,4-5,8-9H2,1H3	-1.929
InChI=1S/C15H19ClO4S/c1-11(2)20-14(17)15(9-3-4-10-15)21(18,19)13-7-5-12(16)6-8-13/h5-8,11H,3-4,9-10H2,1-2H3	-4.65
InChI=1S/C22H25N3O/c1-24-14-12-19(13-15-24)25-22(26)20(16-17-8-4-2-5-9-17)21(23-25)1h2-11,19,23H,12-16H2,1H3	-4.66
InChI=1S/C17H12F3NO3/c1-9(16(22)23)11-4-7-14-13(8-11)21-15(24-14)10-2-5-12(6-3-10)17(1h2-9H,1H3,(H,22,23)	-4.921
InChI=1S/C3H5ClO2/c1-2(4)3(5)6/h2H,1H3,(H,5,6)	0.965
InChI=1S/C9H8O2/c1-10-8-2-3-9-7(6-8)4-5-11-9/h2-6H,1H3	-2.519
InChI=1S/C13H26N2O4/c1-5-7-13(6-2,8-18-11(14)16)9-19-12(17)15-10(3)4/h10H,5-9H2,1-4H3,(H2,14,16)(H,15,17)	-3.634
InChI=1S/C13H26N2/c14-12-5-1-10(2-6-12)9-11-3-7-13(15)8-4-11/h10-13H,1-9,14-15H2	-1.624

"InChi"	"logS(M)"
InChI=1S/C11H12O4S/c12-10(13)6-9(7-16-11(14)15)8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,12,13)(H,14,15)	-1.24
InChI=1S/C8H8N4O/c1-4-5(2)12-7-6(11-4)8(13)10-3-9-7/h3H,1-2H3,(H,9,10,12,13)	-2.29
InChI=1S/C15H21NO2/c1-11-7-13(9-15(2,3)8-11)18-14(17)12-5-4-6-16-10-12/h4-6,10-11,13H,7-9H2,1-3H3	-4.114
InChI=1S/C8H10N2O/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4H,9H2,1H3,(H2,10,11)	-0.577
InChI=1S/C4H8O3/c1-3-7-4(5)6-2/h3H2,1-2H3	-0.344
InChI=1S/C7H16O3/c1-3-9-6-7-10-5-4-8-2/h3-7H2,1-2H3	0.829
InChI=1S/C11H14O2/c1-11(2,3)9-6-4-8(5-7-9)10(12)13/h4-7H,1-3H3,(H,12,13)	-3.578
InChI=1S/C6H4FNO3/c7-4-1-2-5(8(10)11)6(9)3-4/h1-3,9H	-2.05
InChI=1S/C10H20O/c1-8(2)10(11)6-4-5-9(3)7-10/h8-9,11H,4-7H2,1-3H3	-0.24
InChI=1S/C6H4F3N5/c7-6(8,9)3-2-4(12-1-11-2)14-5(10)13-3/h1H,(H3,10,11,12,13,14)	-3.135
InChI=1S/C7H5Cl3O/c1-3-4(8)2-5(9)7(11)6(3)10/h2,11H,1H3	-3.276
InChI=1S/C25H18Cl2N2/c26-21-13-15(9-11-23(21)28)25(16-10-12-24(29)22(27)14-16)19-7-3-1-14H,28-29H2	-6.904
InChI=1S/C12H10O4S/c13-9-3-1-5-11(7-9)17(15,16)12-6-2-4-10(14)8-12/h1-8,13-14H	-2.33
InChI=1S/C4H4OS/c5-4-2-1-3-6-4/h1,3H,2H2	-0.223
InChI=1S/C6H7NS/c1-8-6-4-2-3-5-7-6/h2-5H,1H3	-1.576
InChI=1S/C7H15NO2/c1-4-8(5-2)7(9)10-6-3/h4-6H2,1-3H3	-1.065
InChI=1S/C7H9NO2/c8-4-5-1-2-6(9)7(10)3-5/h1-3,9-10H,4,8H2	0.857
InChI=1S/C7H11NO4S2/c1-2-14-7(13)8-4(6(11)12)3-5(9)10/h4H,2-3H2,1H3,(H,8,13)(H,9,10)(H,11,12)	-1.386
InChI=1S/C11H12N2S/c1-2-4-9(5-3-1)10-8-13-6-7-14-11(13)12-10/h1-5,10H,6-8H2	-2.263
InChI=1S/C18H30N2O3/c1-4-18(22)15-7-9-17(10-8-15)23-14-16(21)13-19-11-12-20(5-2)6-3/h7-10,16,19,21H,4-6,11-14H2,1-3H3	-1.708
InChI=1S/C7H13N3/c1-10(2)4-3-7-5-8-6-9-7/h5-6H,3-4H2,1-2H3,(H,8,9)	0.836
InChI=1S/C8H7ClN2O2/c1-12-6-3-7-5(2-4(6)9)11-8(10)13-7/h2-3H,1H3,(H2,10,11)	-2.481
InChI=1S/C11H7ClF3N5O3/c12-7-2-1-6(11(13,14)15)3-8(7)17-9(21)4-19-5-16-10(18-19)20(22)23/h1-3,5H,4H2,(H,17,21)	-5.968
InChI=1S/C15H17NO3/c1-3-10-16(11-4-2)14(17)12-19-15(18)13-8-6-5-7-9-13/h3-9H,1-2,10-12H2	-2.563
InChI=1S/C12H24N2O3S2/c13-12(10-18-19(15,16)17)14-9-5-4-8-11-6-2-1-3-7-11/h11H,1-10H2,(H2,13,14)(H,15,16,17)	-4.266

"InChi"	"logS(M)"
InChI=1S/C14H20Br2N2/c1-18(12-5-3-2-4-6-12)9-10-7-11(15)8-13(16)14(10)17/h7-8,12H,2-6,9,17H2,1H3	-1.973
InChI=1S/C12H10N2O5/c1-2-14-7-4-9-8(18-5-19-9)3-6(7)11(15)10(13-14)12(16)17/h3-4H,2,5H2,1H3,(H,16,17)	-3.179
InChI=1S/C17H35NO/c1-5-7-12-16(6-2)14-18-17(19)13-10-8-9-11-15(3)4/h15-16H,5-14H2,1-4H3,(H,18,19)	-5.732
InChI=1S/C15H11NO3/c17-14(18)9-10-6-7-13-12(8-10)16-15(19-13)11-4-2-1-3-5-11/h1-8H,9H2,(H,17,18)	-3.143
InChI=1S/C20H40N2O8/c1-10(2)21(11(3)4)18(22(12(5)6)13(7)8)20(29)30-9-14(23)15(24)16(2h10-18,23-26H,9H2,1-8H3,(H,27,28)	0.36
InChI=1S/C33H35NO2/c35-32(28-18-9-3-10-19-28,24-26-14-5-1-6-15-26)30-22-13-23-31(34-h1-12,14-21,30-31,34-36H,13,22-25H2	-7.729
InChI=1S/C19H26I3N3O9/c1-8(30)24(3-11(32)6-28)17-14(20)13(19(34)23-10(4-26)5-27)15(21)1h10-12,26-29,32-33H,3-7H2,1-2H3,(H,23,34)	-4.101
InChI=1S/C10H16N2O3/c1-4-10(5-6(2)3)7(13)11-9(15)12-8(10)14/h6H,4-5H2,1-3H3,(H2,11,12,13,14,15)	-5.142
InChI=1S/C5H3ClN4/c6-4-3-5(9-1-7-3)10-2-8-4/h1-2H,(H,7,8,9,10)	-1.49
InChI=1S/C5H10O/c1-2-6-5-3-4-5/h5H,2-4H2,1H3	-0.641
InChI=1S/C21H25ClN2O3/c1-16(25)18-6-2-5-9-21(18)27-15-17(26)14-23-10-12-24(13-11-23)20h2-9,17,26H,10-15H2,1H3	-3.388
InChI=1S/C14H10ClNO/c15-10-5-3-9-4-6-13-11(2-1-7-16-13)14(17)12(9)8-10/h1-3,5,7-8H,4,6H2	-5.495
InChI=1S/C10H8ClN3O2/c11-7-3-1-2-4-8(7)13-9(15)14-10-12-5-6-16-10/h1-6H,(H2,12,13,14,15)	-3.028
InChI=1S/C12H15NO3/c1-13(2)11(14)8-9-16-12(15)10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3	-1.099
InChI=1S/C2H6N4O2/c3-5-1(7)2(8)6-4/h3-4H2,(H,5,7)(H,6,8)	0.928
InChI=1S/C23H30N2O2/c1-18(2)10-11-23(22(24)26,12-13-25-14-16-27-17-15-25)21-9-5-7-19-h3-10H,11-17H2,1-2H3,(H2,24,26)	-5.039
InChI=1S/C11H23NO2/c1-10(2)7-9(14)8-11(3,4)12(10)5-6-13/h9,13-14H,5-8H2,1-4H3	-0.86
InChI=1S/C19H39NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-19(22)18(2)21/h18,21H,3-17H2,1-2H3,(H,20,22)	-3.651
InChI=1S/C13H9ClN2/c14-10-3-1-8-5-9-2-4-11(15)7-13(9)16-12(8)6-10/h1-7H,15H2	-4.58
InChI=1S/C9H18N2O4/c1-3-6(2)7(4-14-8(10)12)5-15-9(11)13/h6-7H,3-5H2,1-2H3,(H2,10,12)(H2,11,13)	-1.601
InChI=1S/C9H9N3O5/c13-9-11(4-1-5-16-9)10-6-7-2-3-8(17-7)12(14)15/h2-3,6H,1,4-5H2/b10-6+	-3.476

"InChi"	"logS(M)"
InChI=1S/C23H25NO3/c1-2-23(26)18-8-10-21(11-9-18)27-16-20(25)14-19-15-24-13-12-22(1 h3-13,19-20,25H,2,14-16H2,1H3	-4.085
InChI=1S/C9H7Cl2NO2/c10-6-4-2-1-3-5(6)9(8(12)13)7(11)14-9/ h1-4,7H,(H2,12,13)	-2.489
InChI=1S/C12H15NO3/c1-3-4-12(15)16-11-7-5-10(6-8-11)13-9(2)14/ h5-8H,3-4H2,1-2H3,(H,13,14)	-2.83
InChI=1S/C8H14FN3O2S/c9-3-4-12(11-14)8(13)10-7-1-5-15-6-2-7/ h7H,1-6H2,(H,10,13)	-2.138
InChI=1S/C20H23ClO3/ c1-4-20(3,19(22)23-5-2)24-18-12-8-16(9-13-18)14-15-6-10-17(21)11- h6-13H,4-5,14H2,1-3H3	-6.968
InChI=1S/C21H20Br8O2/ c1-21(2,11-3-15(26)19(16(27)4-11)30-9-13(24)7-22)12-5-17(28)20(18 h3-6,13-14H,7-10H2,1-2H3	-9.816
InChI=1S/C17H22N2O4S2/ c1-11(2)8-19(3)9-13-6-12(4-5-15(13)20)17(21)14-7-16(24-10-14)25(1 h4-7,10-11,20H,8-9H2,1-3H3,(H2,18,22,23)	-1.42
InChI=1S/C43H64O10/ c1-27-17-29(19-31(35(27)46)39(3,4)5)13-15-33(44)48-21-41(9,10)37- h17-20,37-38,46-47H,13-16,21-26H2,1-12H3	-8.268
InChI=1S/C7H13NO/c1-6(2)8-5-3-4-7(8)9/h6H,3-5H2,1-2H3	-0.814
InChI=1S/C7H5BrO2/c8-6-1-5(4-9)2-7(10)3-6/h1-4,10H	-3.25
InChI=1S/C3H4Cl2/c1-3(5)2-4/h2H,1H3/b3-2-	-1.614
InChI=1S/C14H13NO/ c15-13-8-6-11(7-9-13)10-14(16)12-4-2-1-3-5-12/h1-9H,10,15H2	-1.805
InChI=1S/C18H28N2O/ c1-17(2)11-8-12-18(3,4)20(17)16(21)14-19-13-15-9-6-5-7-10-15/ h5-7,9-10,19H,8,11-14H2,1-4H3	-4.481
InChI=1S/C23H23N3OS/ c1-24(2)17-10-12-19-21(14-17)28-22-15-18(25(3)4)11-13-20(22)26(1 h5-15H,1-4H3	-6.876
InChI=1S/C11H20N2O5/ c1-4-5-11(3,6-17-9(12)15)7-18-10(16)13-8(2)14/h4-7H2,1-3H3, (H2,12,15)(H,13,14,16)	-1.889
InChI=1S/C33H40N2O9/ c1-38-19-7-8-20-21-9-10-35-16-18-13-27(44-32(36)17-11-25(39-2)30(h7-8,11-12,14,18,22,24,27-28,31,34H,9-10,13,15-16H2,1-6H3	-3.921
InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h4,6-8H, 1,5H2,2-3H3	-2.552
InChI=1S/C7H6N2O5/c1-14-7-3-5(8(10)11)2-6(4-7)9(12)13/h2-4H, 1H3	-2.814
InChI=1S/C7H12FN/c8-6-4-2-1-3-5-7-9/h1-6H2	-2.332
InChI=1S/C7H6N4O2/c1-3-6(12)11-5-4(10-3)7(13)9-2-8-5/h2H,1H3, (H2,8,9,11,12,13)	-2.15
InChI=1S/C11H12O4/c1-14-9-5-3-8(4-6-11(12)13)10(7-9)15-2/ h3-7H,1-2H3,(H,12,13)/b6-4+	-2.232
InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/ h6,13-14H,2,5,7-10H2,1,3-4H3/b11-6-	-6.337
InChI=1S/C11H12O2/c1-10(12)13-9-5-8-11-6-3-2-4-7-11/h2-8H, 9H2,1H3/b8-5+	-2.793

"InChi"	"logS(M)"
InChI=1S/C19H24N2O2/c1-19(18(20)22,9-10-21-11-13-23-14-12-21)17-8-4-6-15-5-2-3-7-16(1h2-8H,9-14H2,1H3,(H2,20,22)	-3.104
InChI=1S/C7H12O3/c1-2-7(9)10-6-4-3-5-8/h2,8H,1,3-6H2	0.841
InChI=1S/C14H9NO2S/c16-14(11-5-2-1-3-6-11)17-13-8-4-7-12(9-13)15-10-18/h1-9H	-4.85
InChI=1S/C9H21O4PS3/c1-6-12-14(15,13-7-2)16-8-17(10,11)9(3,4)5/h6-8H2,1-5H3	-2.895
InChI=1S/C9H18O/c1-7(2)8-3-5-9(10)6-4-8/h7-10H,3-6H2,1-2H3	-2.068
InChI=1S/C6H7NO4S2/c1-11-6(8)5-4(2-3-12-5)13(7,9)10/h2-3H,1H3,(H2,7,9,10)	-0.837
InChI=1S/C12H20O2/c1-5-11(13)14-10-6-9(2)7-12(3,4)8-10/h5,9-10H,1,6-8H2,2-4H3	-4.03
InChI=1S/C4H8O/c1-4(2)5-3/h1H2,2-3H3	1.142
InChI=1S/C15H14BrNO2/c1-17-15(18)13-9-11(16)8-12(14(13)19-2)10-6-4-3-5-7-10/h3-9H,1-2H3,(H,17,18)	-4.899
InChI=1S/C18H20/c1-15(16-10-6-4-7-11-16)14-18(2,3)17-12-8-5-9-13-17/h4-13H,1,14H2,2-3H3	-6.012
InChI=1S/C15H21NO5/c1-18-12-9-11(10-13(19-2)14(12)20-3)15(17)16-7-5-4-6-8-21-16/h9-10H,4-8H2,1-3H3	-3.508
InChI=1S/C6H12N2O8/c9-7(10)15-5-3-13-1-2-14-4-6-16-8(11)12/h1-6H2	-1.561
InChI=1S/C10H8N2O3/c1-6-2-3-7-8(12(14)15)4-5-9(13)10(7)11-6/h2-5,13H,1H3	-3.96
InChI=1S/C6H11NO2S2/c1-3-11-6(10)7-4(2)5(8)9/h4H,3H2,1-2H3,(H,7,10)(H,8,9)	-0.961
InChI=1S/C23H38N2O5/c1-16(2)20-7-6-18(5)21(23(28)30-17(3)4)22(20)29-15-19(27)14-25-1(h6-7,16-17,19,26-27H,8-15H2,1-5H3	-4.264
InChI=1S/C20H23NO4/c22-13-4-3-12-9-15-20(24)6-5-14(23)18-19(20,16(12)17(13)25-18)7-8h3-4,11,15,18,22,24H,1-2,5-10H2	-2.321
InChI=1S/C6H14O2/c1-6(2,8-3)4-5-7/h7H,4-5H2,1-3H3	-0.073
InChI=1S/C10H13NO/c1-2-4-9(5-3-1)10-8-11-6-7-12-10/h1-5,10-11H,6-8H2	-0.332
InChI=1S/C6H7NS/c8-5-6-3-1-2-4-7-6/h1-4,8H,5H2	0.079
InChI=1S/C7H8ClNO2S/c1-6-2-4-7(5-3-6)12(10,11)9-8/h2-5,9H,1H3	-0.36
InChI=1S/C14H16N2O2/c1-17-13-7-9(3-5-11(13)15)10-4-6-12(16)14(8-10)18-2/h3-8H,15-16H2,1-2H3	-3.61
InChI=1S/C5H5NOS/c6-5(7)4-2-1-3-8-4/h1-3H,(H2,6,7)	-0.574
InChI=1S/C12H30O13P4/c1-7-17-26(13,18-8-2)23-28(15,21-11-5)25-29(16,22-12-6)24-27(14,1h7-12H2,1-6H3	0.296
InChI=1S/C23H34N3O10P/c1-11(2)8-16(26-37(33,34)36-23-20(29)19(28)18(27)12(3)35-23)21(3h4-7,10-12,16-20,23-24,27-29H,8-9H2,1-3H3,(H,25,30)(H,31,32)(H2,26,33,34)	-3.102

"InChi"	"logS(M)"
InChI=1S/C6H7N5/c1-11-3-10-5(7)4-6(11)9-2-8-4/h2-3H,7H2,1H3	-0.481
InChI=1S/C8H6N2O/c9-7-5-3-1-2-4-6(5)8(11)10-7/h1-4H,(H2,9,10,11)	-1.688
InChI=1S/C4H5Cl3/c1-3(6)4(7)2-5/h4H,1-2H2	-2.424
InChI=1S/C9H14N2O3S/c1-2-3-9(4-5-12)6(13)10-8(15)11-7(9)14/h12H,2-5H2,1H3,(H2,10,11,13,14,15)	-1.61
InChI=1S/C10H12O3/c1-13-9-5-2-8(3-6-9)4-7-10(11)12/h2-3,5-6H,4,7H2,1H3,(H,11,12)	-2.214
InChI=1S/C12H27NO2/c1-2-3-4-5-6-7-8-13(9-11-14)10-12-15/h14-15H,2-12H2,1H3	-2.191
InChI=1S/C6H4I2/c7-5-2-1-3-6(8)4-5/h1-4H	-4.518
InChI=1S/C12H16O2/c1-4-14-11(13)12(2,3)10-8-6-5-7-9-10/h5-9H,4H2,1-3H3	-3.046
InChI=1S/C18H22/c1-3-7-15(8-4-1)17-11-13-18(14-12-17)16-9-5-2-6-10-16/h1,3,5,9,11-16H,2,4,6-8,10H2	-6.592
InChI=1S/C37H45NO12/c1-16-11-10-12-17(2)36(46)38-23-15-24(40)26-27(32(23)44)31(43)21h10-16,18-20,25,29-30,33,41-43H,1-9H3,(H,38,46)/b11-10-,14-13-,17-12-	-8.374
InChI=1S/C22H18N2O5S/c1-12-7-9-13(10-8-12)30(27,28)24-16-11-17(29-2)20(23)19-18(16)21(h3-11,24H,23H2,1-2H3	-5.113
InChI=1S/C33H54O7/c1-20(2)8-7-9-21(3)25-10-11-26-24-18-28(39-22(4)34)33(38)19-23(4(h20-21,23-28,38H,7-19H2,1-6H3,(H,35,36)	-8.181
InChI=1S/C12H10N4S/c1-2-4-9(5-3-1)6-17-12-10-11(14-7-13-10)15-8-16-12/h1-5,7-8H,6H2,(H,13,14,15,16)	-4.026
InChI=1S/C16H32N2O6/c19-11-5-7-13-23-15(21)17-9-3-1-2-4-10-18-16(22)24-14-8-6-12-20/h19-20H,1-14H2,(H,17,21)(H,18,22)	-1.93
InChI=1S/C6H14N2O4S2/c1-12-4-2-3-8-6(7)5-13-14(9,10)11/h2-5H2,1H3,(H2,7,8)(H,9,10,11)	-0.355
InChI=1S/C13H21N3O5S3/c1-4-16(11(17)7-15-3)10-5-8(2)23(18,19)13-9(10)6-12(22-13)24(14,2(h6,8,10,15H,4-5,7H2,1-3H3,(H2,14,20,21)	-1.21
InChI=1S/C5H7Cl2NO4/c6-3(7)4(10)8-2(1-9)5(11)12/h2-3,9H,1H2,(H,8,10)(H,11,12)	-0.03
InChI=1S/C8H10O3/c1-5(2)7(9)11-8(10)6(3)4/h1,3H2,2,4H3	-0.197
InChI=1S/C12H10N2O4S/c15-14(16)12-9-5-4-8-11(12)13-19(17,18)10-6-2-1-3-7-10/h1-9,13H	-4.01
InChI=1S/C32H22O4/c33-31(25-15-19-29(20-16-25)35-27-7-3-1-4-8-27)23-11-13-24(14-12-h1-22H	-7.974
InChI=1S/C25H43N13O10/c26-3-1-2-10(27)4-16(41)32-12-6-30-23(47)18(11-5-17(42)37-24(28)3h7,10-12,14-15,17-18,39-40,42H,1-6,8-9,26-27H2,(H,30,47)(H,32,41)(H,33,45)(H,34,43)(H,35,46)(H,38,44)(H3,28,36,37)(H3,29,31,48)/b13-7+	0.164

"InChi"	"logS(M)"
InChI=1S/C11H22N2O4S/c1-11(2,7-14)9(16)10(17)13-4-3-8(15)12-5-6-18/h9,14,16,18H,3-7H2,1-2H3,(H,12,15)(H,13,17)	-0.796
InChI=1S/C8H18NO/c1-7(2,3)9(10)8(4,5)6/h1-6H3	-2.114
InChI=1S/C8H11N/c1-6-4-7(2)9-8(3)5-6/h4-5H,1-3H3	-0.539
InChI=1S/C8H18OS2/c1-3-5-7-10-11(9)8-6-4-2/h3-8H2,1-2H3/p+1	-2.289
InChI=1S/C3H8O2/c4-2-1-3-5/h4-5H,1-3H2	1.119
InChI=1S/C15H14BrF2N3O3/c1-3-24-20-14(22)9-7-21(2)15(23)12(18)13(9)19-11-5-4-8(16)6-10(11h4-7,19H,3H2,1-2H3,(H,20,22)	-4.19
InChI=1S/C16H17Cl6N5/c1-27(2)8-4-7-23-14-25-12(24-13(26-14)16(20,21)22)10-5-3-6-11(9-1h3,5-6,9H,4,7-8H2,1-2H3,(H,23,24,25,26)	-6.94
InChI=1S/C9H20N2O/c1-5-10(6-2)9(12)11(7-3)8-4/h5-8H2,1-4H3	-0.634
InChI=1S/C22H28N2O4/c1-17(25)19-7-3-5-9-21(19)28-16-18(26)15-23-11-13-24(14-12-23)20h3-10,18,26H,11-16H2,1-2H3	-2.876
InChI=1S/C15H24N4O4/c1-11(2)8-18(9-12(3)4)10-14(20)17-16-7-13-5-6-15(23-13)19(21)22/h5-7,11-12H,8-10H2,1-4H3,(H,17,20)/b16-7+	-4.069
InChI=1S/C6H5N3S/c7-4-1-2-6-5(3-4)8-9-10-6/h1-3H,7H2	-1.304
InChI=1S/C20H29N3O2/c1-3-5-12-23(13-6-4-2)14-8-11-21-17-15-18(24)19-16(20(17)25)9-7-1h7,9-10,15,21H,3-6,8,11-14H2,1-2H3	-3.617
InChI=1S/C7H15NO2/c1-2-3-4-5-6-10-7(8)9/h2-6H2,1H3,(H2,8,9)	-1.92
InChI=1S/C6H9N3/c1-5(3-7)9-6(2)4-8/h5-6,9H,1-2H3	0.89
InChI=1S/C23H29NO2/c1-19-11-8-9-16-24(19)17-10-18-26-23(25)22(20-12-4-2-5-13-20)21-1h2-7,12-15,19,22H,8-11,16-18H2,1H3	-5.783
InChI=1S/C19H26N2O/c1-2-19(22)21-17-11-6-12-18(21)15-20(14-17)13-7-10-16-8-4-3-5-9-1h3-5,7-10,17-18H,2,6,11-15H2,1H3/b10-7+	-4.178
InChI=1S/C5H6O3/c1-4(6)2-3-5(7)8/h2-3H,1H3,(H,7,8)/b3-2+	-0.233
InChI=1S/C20H16N4O5S/c1-13-17(12-21)19(25)24(2)20(26)18(13)23-22-14-7-6-8-15(11-14)29h3-11,22H,1-2H3/b23-18-	-8.783
InChI=1S/C11H9ClN4S/c12-9-3-1-2-8-7(4-5-14-10(8)9)6-15-16-11(13)17/h1-6H,(H3,13,16,17)/b15-6+	-3.503
InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-4H,1-2,5-8H2	-4.023
InChI=1S/C17H16N2O2S/c1-12-6-7-13-4-2-3-5-16(13)17(12)19-22(20,21)15-10-8-14(18)9-11-1h2-11,19H,18H2,1H3	-4.5
InChI=1S/C17H18FN3O3/c1-17(19)7-20(8-17)14-5-13-10(4-12(14)18)15(22)11(16(23)24)6-21(1h4-6,9H,2-3,7-8,19H2,1H3,(H,23,24)	-5.62
InChI=1S/C7H14NO4PS2/c1-8(7(10)11-2)6(9)5-15-13(4,14)12-3/h5H2,1-4H3	-1.956
InChI=1S/C8H14O/c1-3-5-6-7-8(9)4-2/h2,8-9H,3,5-7H2,1H3	-1.287

"InChi"	"logS(M)"
InChI=1S/C16H25NO/c1-15-8-5-6-11-17(15)12-7-13-18-14-16-9-3-2-4-10-16/h2-4,9-10,15H,5-8,11-14H2,1H3	-3.69
InChI=1S/C37H67NO12/c1-14-26-20(4)29(40)21(5)28(39)18(2)16-36(9,44)33(50-35-30(41)25(h18-27,29-33,35,40-42,44H,14-17H2,1-13H3	-6.087
InChI=1S/C14H18N4O2/c1-4-15-14(20)16-12-10(2)17(3)18(13(12)19)11-8-6-5-7-9-11/h5-9H,4H2,1-3H3,(H2,15,16,20)	-1.83
InChI=1S/C15H13NO3S/c17-15-10-13-8-4-5-9-14(13)20(18,19)16(15)11-12-6-2-1-3-7-12/h1-9H,10-11H2	-3.153
InChI=1S/C20H25NO/c22-20(18-10-4-1-5-11-18,19-12-6-2-7-13-19)14-17-21-15-8-3-9-16-2h1-2,4-7,10-13,22H,3,8-9,14-17H2	-3.952
InChI=1S/C20H22O3/c1-4-5-6-7-12-23-20(21)15(2)16-8-9-18-14-19(22-3)11-10-17(18)13-1h8-11,13-15H,4,7,12H2,1-3H3	-7.33
InChI=1S/C3H4N4/c4-3-5-1-2-6-7-3/h1-2H,(H2,4,5,7)	1.017
InChI=1S/C18H26O2/c1-8-10-13(5)15(9-2)20-17(19)16-14(11-12(3)4)18(16,6)7/h2,10-11,14-16H,8H2,1,3-7H3/b13-10+	-6.393
InChI=1S/C11H18O3/c1-6-8(12)3-2-7-9(13)4-5-10(14)11(6)7/h6-7,9-11,13-14H,2-5H2,1H3	-0.3
InChI=1S/C12H2Cl6O2/c13-3-1-5-6(2-4(3)14)20-12-10(18)8(16)7(15)9(17)11(12)19-5/h1-2H	-10.949
InChI=1S/C10H18O6/c1-9(11)15-7-5-13-3-4-14-6-8-16-10(2)12/h3-8H2,1-2H3	0.63
InChI=1S/C12H16N2O3/c1-3-5-7-12(8-6-4-2)9(15)13-11(17)14-10(12)16/h3-6H,7-8H2,1-2H3,(H2,13,14,15,16,17)/b5-3+,6-4+	-2.197
InChI=1S/C9H10BrNO3/c10-6-1-2-8(14-4-3-12)7(5-6)9(11)13/h1-2,5,12H,3-4H2,(H2,11,13)	-1.269
InChI=1S/C3H7O4P/c1-2-3(7-2)8(4,5)6/h2-3H,1H3,(H2,4,5,6)	0.807
InChI=1S/C7H6Cl2/c8-7(9)6-4-2-1-3-5-6/h1-5,7H	-2.809
InChI=1S/C14H23NO/c1-11(2)13-7-6-12(3)10-14(13)16-9-8-15(4)5/h6-7,10-11H,8-9H2,1-5H3	-3.044
InChI=1S/C13H9ClN2O3/c14-8-1-6-12(11(7-8)13(18)19)16-15-9-2-4-10(17)5-3-9/h1-7,17H,(H,18,19)/b16-15+	-3.86
InChI=1S/C29H36O15/c1-13-22(36)23(37)24(38)29(41-13)44-27-25(39)28(40-9-8-15-3-6-17(h2-7,10-11,13,20,22-34,36-39H,8-9,12H2,1H3/b7-4+	-3.877
InChI=1S/C11H20O2/c1-4-11(12)13-9-7-5-6-8-10(2)3/h4,10H,1,5-9H2,2-3H3	-4.171
InChI=1S/C38H76N2O4/c1-3-5-7-21-27-35(41)29-23-17-13-9-11-15-19-25-31-37(43)39-33-34h35-36,41-42H,3-34H2,1-2H3,(H,39,43)(H,40,44)	-6.735
InChI=1S/C18H26N2O/c1-2-18(21)20-16-10-11-17(20)14-19(13-16)12-6-9-15-7-4-3-5-8-15/h3-5,7-8,16-17H,2,6,9-14H2,1H3	-3.854

"InChi"	"logS(M)"
InChI=1S/C9H10N4O3/ c1-5(14)13-4-10-7-6(13)8(15)12(3)9(16)11(7)2/h4H,1-3H3	-1.4
InChI=1S/C15H10BrCl2NO2/ c16-8-14(20)19-13-6-5-9(17)7-11(13)15(21)10-3-1-2-4-12(10)18/ h1-7H,8H2,(H,19,20)	-6.889
InChI=1S/C15H22N2O2/ c1-3-17-10-6-8-13(11-17)19-15(18)16-14-9-5-4-7-12(14)2/ h4-5,7,9,13H,3,6,8,10-11H2,1-2H3,(H,16,18)	-3.366
InChI=1S/C14H24ClN5S/ c1-14(2,3)18-13-16-11(15)10(21-5)12(17-13)20-8-6-19(4)7-9-20/ h6-9H2,1-5H3,(H,16,17,18)	-2.986
InChI=1S/C2H7NO4S/c3-1-2-7-8(4,5)6/h1-3H2,(H,4,5,6)	0.85
InChI=1S/C14H12O4/ c15-11-7-13(14(16)17)18-12-6-9-4-2-1-3-8(9)5-10(11)12/h5-7H, 1-4H2,(H,16,17)	-1.05
InChI=1S/C16H12N2O2/ c1-11-7-13(3-5-15(11)17-9-19)14-4-6-16(18-10-20)12(2)8-14/h3-8H, 1-2H3	-2.308
InChI=1S/C6H10O4S2/c1-5-6(2)12(9,10)4-3-11(5,7)8/h3-4H2,1-2H3	-1.66
InChI=1S/C18H29NO2/ c1-18(2,3)19-12-15(20)13-21-17-11-7-6-10-16(17)14-8-4-5-9-14/ h6-7,10-11,14-15,19-20H,4-5,8-9,12-13H2,1-3H3	-1.619
InChI=1S/C19H25NO4/ c1-11(2)9-14-15(19(14,3)4)18(23)24-10-20-16(21)12-7-5-6-8-13(12)1 h9,14-15H,5-8,10H2,1-4H3	-5.26
InChI=1S/C15H15ClN4O6S/ c1-3-26-13(21)9-6-4-5-7-10(9)27(23,24)20-15(22)19-14-17-11(16)8-1 h4-8H,3H2,1-2H3,(H2,17,18,19,20,22)	-4.58
InChI=1S/C9H14N2/c1-8(11-10)7-9-5-3-2-4-6-9/h2-6,8,11H, 7,10H2,1H3	-1.115
InChI=1S/C5H11NO3/c1-3-5(4-2)9-6(7)8/h5H,3-4H2,1-2H3	-2.452
InChI=1S/C10H10N4O5/ c1-11-10(15)6-4-8(12-2-3-12)9(14(18)19)5-7(6)13(16)17/h4-5H, 2-3H2,1H3,(H,11,15)	-2.85
InChI=1S/C21H23NO6/ c1-11(23)22-15-7-5-12-9-18(27-3)20(25)21(28-4)19(12)13-6-8-17(26- h6,8-10,15,25H,5,7H2,1-4H3,(H,22,23)	-2.42
InChI=1S/C9H19NO3/c1-3-4-5-9(2,6-11)7-13-8(10)12/h11H, 3-7H2,1-2H3,(H2,10,12)	-1.735
InChI=1S/C10H18O/c1-9(2)5-4-6-10(3)7-8-11/h5,8,10H, 4,6-7H2,1-3H3	-3.244
InChI=1S/C12H6Cl2O2/ c13-7-1-3-9-11(5-7)16-12-6-8(14)2-4-10(12)15-9/h1-6H	-7.181
InChI=1S/C22H28N2O2/ c1-7-17-8-10-18(11-9-17)20(25)23-24(22(4,5)6)21(26)19-13-15(2)12- h8-14H,7H2,1-6H3,(H,23,25)	-5.628
InChI=1S/C5H10O/c1-5(2)3-4-6/h6H,1,3-4H2,2H3	0.019
InChI=1S/C21H34N2O/ c1-7-22(8-2)16-19(24)23-20(3,4)14-18(15-21(23,5)6)17-12-10-9-11-1 h9-13,18H,7-8,14-16H2,1-6H3	-5.361
InChI=1S/C6H13NO6/c7-3(6(12)13)5(11)4(10)2(9)1-8/h2-5,8-11H, 1,7H2,(H,12,13)	-0.859

"InChi"	"logS(M)"
InChI=1S/C6H8N2/c1-6(5-8)3-2-4-7/h6H,2-3H2,1H3	-0.316
InChI=1S/C25H50O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25(28)29-2h24,26-27H,2-23H2,1H3	-6.919
InChI=1S/C13H12O3/c1-8-7-12(9(2)16-8)13(15)10-3-5-11(14)6-4-10/h3-7,14H,1-2H3	-2.873
InChI=1S/C4H12NO3P/c1-5(2)9(6,7-3)8-4/h1-4H3	0.087
InChI=1S/C14H13N/c1-3-7-13-11(5-1)9-15-10-12-6-2-4-8-14(12)13/h1-8,15H,9-10H2	-3.497
InChI=1S/C2H2FN/c3-1-2-4/h1H2	0.278
InChI=1S/C21H13N/c1-3-7-17-14(5-1)11-12-20-19(17)13-16-10-9-15-6-2-4-8-18(15)21(16h1-13H	-6.245
InChI=1S/C40H58N8O8/c1-25(2)17-30(34(49)21-35(50)44-31(18-26(3)4)36(51)42-22-28-13-1h8-16,23-26,30-34,49H,17-22H2,1-7H3,(H,41,43)(H,42,51)(H,44,50)(H,45,53)(H,46,52)(H,47,54)	-2.38
InChI=1S/C16H20N2/c1-18(2)13-11-15(14-8-4-3-5-9-14)16-10-6-7-12-17-16/h3-10,12,15H,11,13H2,1-2H3	-1.028
InChI=1S/C13H11NO2/c14-13(16)11-8-4-7-10(12(11)15)9-5-2-1-3-6-9/h1-8,15H,(H2,14,16)	-2.567
InChI=1S/C10H12O2/c1-2-10(11)12-8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3	-2.345
InChI=1S/C19H20N2O/c1-21(2)13-17(14-8-4-3-5-9-14)19(22)16-12-20-18-11-7-6-10-15(16)1h3-12,17,20H,13H2,1-2H3	-2.944
InChI=1S/C12H22O4/c1-15-11(13)9-7-5-3-4-6-8-10-12(14)16-2/h3-10H2,1-2H3	-3.283
InChI=1S/C12H13NO2S/c1-9-11(16-8-7-15-9)12(14)13-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3,(H,13,14)	-3.14
InChI=1S/C18H18O4S2/c19-17(20)15(13-7-3-1-4-8-13)23-11-12-24-16(18(21)22)14-9-5-2-6-1h1-10,15-16H,11-12H2,(H,19,20)(H,21,22)	-3.41
InChI=1S/C20H24N2O6/c1-11(2)10-28-20(24)17-13(4)21-12(3)16(19(23)27-5)18(17)14-8-6-7-h6-9,11,18,21H,10H2,1-5H3	-4.198
InChI=1S/C22H14O4/c23-21(24)17-11-3-7-13-5-1-9-15(19(13)17)16-10-2-6-14-8-4-12-18(2h1-12H,(H,23,24)(H,25,26)	-2.233
InChI=1S/C9H18N2O4/c1-3-9(4-2,5-14-7(10)12)6-15-8(11)13/h3-6H2,1-2H3,(H2,10,12)(H2,11,13)	-1.632
InChI=1S/C10H14O/c1-7-4-8(2)10(6-11)9(3)5-7/h4-5,11H,6H2,1-3H3	-2.109
InChI=1S/C10H21NO/c1-7(2)10(5,8(3)4)9(12)11-6/h7-8H,1-6H3,(H,11,12)	-1.395
InChI=1S/C7H6N2O2S2/c8-13(10,11)7-9-5-3-1-2-4-6(5)12-7/h1-4H,(H2,8,10,11)	-2.63
InChI=1S/C7H10N4O3/c1-10-5(8)4(9-3-12)6(13)11(2)7(10)14/h3H,8H2,1-2H3,(H,9,12)	-1.183

"InChi"	"logS(M)"
InChI=1S/C17H19N3O6/c1-10(20-25-5)11-7-6-8-12(15(11)16(21)24-4)26-17-18-13(22-2)9-14(h6-9H,1-5H3/b20-10+	-3.604
InChI=1S/C17H25N3O4S2/c1-5-23-16(21)11-12-20(13-15-9-7-6-8-10-15)26-19(3)17(22)24-18-14-h6-10H,5,11-13H2,1-4H3/b18-14-	-4.301
InChI=1S/C9H6ClNO/c10-7-3-4-8(12)9-6(7)2-1-5-11-9/h1-5,12H	-3.976
InChI=1S/C11H12O3/c1-2-14-10-6-4-3-5-9(10)7-8-11(12)13/h3-8H,2H2,1H3,(H,12,13)/p-1/b8-7+	-3.325
InChI=1S/C10H9ClO4/c1-6(12)9(10(13)14)15-8-5-3-2-4-7(8)11/h2-5,9H,1H3,(H,13,14)	-2.1
InChI=1S/C18H20N2O3/c1-3-13-9-5-6-10-14(13)19-17(21)18(22)20-15-11-7-8-12-16(15)23-4-h5-12H,3-4H2,1-2H3,(H,19,21)(H,20,22)	-6.018
InChI=1S/C15H19N3O8/c1-7(19)23-6-10-12(24-8(2)20)13(25-9(3)21)14(26-10)18-5-4-11(16)1h4-5,10,12-14H,6H2,1-3H3,(H2,16,17,22)	-2.519
InChI=1S/C11H15N3O5/c15-10-12(1-7-4-17-7)11(16)14(3-9-6-19-9)13(10)2-8-5-18-8/h7-9H,1-6H2	-1.127
InChI=1S/C9H13NOS/c1-9(11,7-10)12-8-5-3-2-4-6-8/h2-6,11H,7,10H2,1H3	-0.015
InChI=1S/C3H8N4O2/c4-2(8)6-1-7-3(5)9/h1H2,(H3,4,6,8)(H3,5,7,9)	-0.652
InChI=1S/C13H22O2/c1-9(2)12(14)15-11-6-10(3)7-13(4,5)8-11/h10-11H,1,6-8H2,2-5H3	-4.599
InChI=1S/C21H30N2/c1-5-16-10-14(11-17(6-2)20(16)22)9-15-12-18(7-3)21(23)19(8-4)13-1h10-13H,5-9,22-23H2,1-4H3	-5.849
InChI=1S/C17H32O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-17(18)4-2/h4H,2-3,5-16H2,1H3	-4.429
InChI=1S/C9H16N4O/c1-4-7-11-8(10-5-2)13-9(12-7)14-6-3/h4-6H2,1-3H3,(H,10,11,12,13)	-3.437
InChI=1S/C8H17NO/c1-2-8(10)7-5-3-4-6-9-7/h7-10H,2-6H2,1H3	-0.81
InChI=1S/C11H15N3O2/c1-2-3-4-10(15)13-14-11(16)9-5-7-12-8-6-9/h5-8H,2-4H2,1H3,(H,13,15)(H,14,16)	-1.01
InChI=1S/C12H9N3O2S/c1-17-12(16)15-10-5-3-2-4-8(10)14-11(15)9-6-18-7-13-9/h2-7H,1H3	-3.11
InChI=1S/C6H16N2/c7-5-3-1-2-4-6-8/h1-8H2	0.739
InChI=1S/C14H22O2/c1-10(2)14-7-5-13(3,6-8-14)11(9-14)12(15)16-4/h5,7,10-11H,6,8-9H2,1-4H3	-4.201
InChI=1S/C19H31N7O4/c27-10-6-25(7-11-28)18-20-14-15-16(22-18)17(24-4-2-1-3-5-24)23-19h14,27-30H,1-13H2	-2.033
InChI=1S/C9H6BrCl2NO2/c10-7-9(15-7,8(13)14)5-2-1-4(11)3-6(5)12/h1-3,7H,(H2,13,14)	-3.691
InChI=1S/C12H13N5/c13-11(14)17-12(15)16-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H6,13,14,15,16,17)	-2.55

"InChi"	"logS(M)"
InChI=1S/C23H34O5/c1-13(24)28-12-20(27)18-7-6-17-16-5-4-14-10-15(25)8-9-22(14,2)21(h14-18,21,25H,4-12H2,1-3H3	-4.062
InChI=1S/C7H14O2/c1-4-9-7(8)5-6(2)3/h6H,4-5H2,1-3H3	-1.813
InChI=1S/C45H86O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-43(46)49-40-42(51-45(48)39-h42H,4-41H2,1-3H3	-8.647
InChI=1S/C6H10O3/c1-3-5(7)6(8)9-4-2/h3,5,7H,1,4H2,2H3	0.363
InChI=1S/C15H19ClN2O4S2/c1-11-10-14(18-15-12(11)4-2-5-13(15)16)22-8-3-6-17-7-9-23-24(19,2h2,4-5,10,17H,3,6-9H2,1H3,(H,19,20,21)	-3.198
InChI=1S/C15H21NO3/c1-3-10-16(11-4-2)14(17)12-19-15(18)13-8-6-5-7-9-13/h5-9H,3-4,10-12H2,1-2H3	-2.379
InChI=1S/C13H16O4S/c1-3-17-12(14)13(8-9-13)18(15,16)11-6-4-10(2)5-7-11/h4-7H,3,8-9H2,1-2H3	-3.01
InChI=1S/C9H12/c1-2-8-5-7-3-4-9(8)6-7/h2-4,7,9H,5-6H2,1H3/b8-2+	-3.177
InChI=1S/C12H22O4/c1-9(2)15-11(13)7-5-6-8-12(14)16-10(3)4/h9-10H,5-8H2,1-4H3	-3.107
InChI=1S/C7H7N5/c1-8-7-11-4-5-6(12-7)10-3-2-9-5/h2-4H,1H3,(H,8,10,11,12)	-1.712
InChI=1S/C18H30N2O3/c1-3-10-20(11-4-2)12-15-22-13-5-14-23-18(21)16-6-8-17(19)9-7-16/h6-9H,3-5,10-15,19H2,1-2H3	-3.263
InChI=1S/C3H6N2O3/c1-5(4-8)2-3(6)7/h2H2,1H3,(H,6,7)	0.928
InChI=1S/C7H16N2O3S2/c1-6(2)3-4-9-7(8)5-13-14(10,11)12/h6H,3-5H2,1-2H3,(H2,8,9)(H,10,11,12)	-1.771
InChI=1S/C6H8O4/c1-9-5(7)3-4-6(8)10-2/h3-4H,1-2H3/b4-3+	-0.267
InChI=1S/C9H21NO3S2/c1-3-4-5-6-9(2)10-7-8-14-15(11,12)13/h9-10H,3-8H2,1-2H3,(H,11,12,13)	-1.231
InChI=1S/C44H59N7O5/c1-8-12-14-30(10-3)28-55-39(53)33-18-24-36(25-19-33)46-42-48-41(h16-27,30-31H,8-15,28-29H2,1-7H3,(H,51,52)(H3,45,46,47,48,49,50)	-8.185
InChI=1S/C8H7N/c1-7-3-2-4-8(5-7)6-9/h2-5H,1H3	-2.041
InChI=1S/C23H36O3/c1-5-21(25)26-20-9-8-17-16-7-6-15-12-19(24)14(2)13-23(15,4)18(16)h14-18,20H,5-13H2,1-4H3	-6.167
InChI=1S/C6H13NO2S/c7-10(8,9)6-4-2-1-3-5-6/h6H,1-5H2,(H2,7,8,9)	-1.413
InChI=1S/C9H8N2O/c1-7(12)11-9-4-2-8(6-10)3-5-9/h2-5H,1H3,(H,11,12)	-1.805
InChI=1S/C12H24O6/c1-2-14-5-6-16-9-10-18-12-11-17-8-7-15-4-3-13-1/h1-12H2	-0.548
InChI=1S/C10H13NO4S/c1-3-15-10(12)11-16(13,14)9-6-4-8(2)5-7-9/h4-7H,3H2,1-2H3,(H,11,12)	-2.243
InChI=1S/C13H13N/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H,14H2	-1.723
InChI=1S/C3H9NO2/c4-1-3(6)2-5/h3,5-6H,1-2,4H2	1.04

"InChi"	"logS(M)"
InChI=1S/C17H27NO3/c1-6-18(7-2)10-11-21-16-14(12(3)4)9-8-13(5)15(16)17(19)20/h8-9,12H,6-7,10-11H2,1-5H3,(H,19,20)	-4.36
InChI=1S/C15H21NO4/c1-3-4-5-6-11-19-15(18)20-14-9-7-13(8-10-14)16-12(2)17/h7-10H,3-6,11H2,1-2H3,(H,16,17)	-4.32
InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h4-8H,1-3H3/b5-4+	-2.778
InChI=1S/C16H25NO3/c1-11(2)13-8-7-12(3)14(16(18)19-6)15(13)20-10-9-17(4)5/h7-8,11H,9-10H2,1-6H3	-3.313
InChI=1S/C13H12/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h1-10H,11H2	-4.17
InChI=1S/C10H16O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h7-9,11H,1,4-5H2,2-3H3	-2.096
InChI=1S/C6H6N4/c7-5-4-1-2-8-6(4)10-3-9-5/h1-3H,(H3,7,8,9,10)	-0.261
InChI=1S/C12H19N6OP/c1-16(2)20(19,17(3)4)18-12(13)14-11(15-18)10-8-6-5-7-9-10/h5-9H,1-4H3,(H2,13,14,15)	-3.071
InChI=1S/C16H12Cl2N4O4/c1-9(23)15(16(24)19-12-5-3-2-4-11(12)18)21-20-13-7-6-10(17)8-14(1h2-8,15H,1H3,(H,19,24)/b21-20+	-7.722
InChI=1S/C18H38NO3P/c1-4-7-15-19-18(13-11-10-12-14-18)23(20,21-16-8-5-2)22-17-9-6-3/h19H,4-17H2,1-3H3	-3.311
InChI=1S/C11H12ClNO3/c1-2-16-10-5-3-8(7-9(10)12)4-6-11(14)13-15/h3-7,15H,2H2,1H3,(H,13,14)/b6-4+	-3.053
InChI=1S/C5H8O4/c1-5(2,3(6)7)4(8)9/h1-2H3,(H,6,7)(H,8,9)	-0.167
InChI=1S/C10H10O2/c1-10(2)8-6-4-3-5-7(8)9(11)12-10/h3-6H,1-2H3	-1.868
InChI=1S/C15H12ClN5O4/c1-3-20-14(22)10(7-17)8(2)13(15(20)23)19-18-11-5-4-9(16)6-12(11)2h4-6,18H,3H2,1-2H3/b19-13-	-4.967
InChI=1S/C11H14Br2N2O2/c1-3-15(4-2)10(16)7-14-5-8(12)11(17)9(13)6-14/h5-6H,3-4,7H2,1-2H3	-2.31
InChI=1S/C6H17N2O4PS/c7-2-1-3-8-4-6(9)5-14-13(10,11)12/h6,8-9H,1-5,7H2,(H2,10,11,12)	0.612
InChI=1S/C9H10O3/c1-6-7(5-10)3-4-8(11)9(6)12-2/h3-5,11H,1-2H3	-1.375
InChI=1S/C12H20ClN5OS/c1-14-12-15-10(13)9(20-2)11(16-12)18-5-3-17(4-6-18)7-8-19/h19H,3-8H2,1-2H3,(H,14,15,16)	-0.903
InChI=1S/C5H7N3O3/c9-4-3-7-2-1-6-5(7)8(10)11/h1-2,9H,3-4H2	-0.337
InChI=1S/C10H10N2O4S/c1-7-6-10(13)12(11-7)8-2-4-9(5-3-8)17(14,15)16/h2-5H,6H2,1H3,(H,14,15,16)	-1.693
InChI=1S/C6H12O/c1-3-6(4-2)5-7/h5-6H,3-4H2,1-2H3	-1.52
InChI=1S/C21H32O3/c1-19-11-13(12-22)18(23)10-14(19)4-5-15-16(19)6-8-20(2)17(15)7-9-h12,14-17,22,24H,4-11H2,1-3H3/b13-12+	-4.805

"InChi"	"logS(M)"
InChI=1S/C13H10N2O4/c16-13(17)11-6-1-2-7-12(11)14-9-4-3-5-10(8-9)15(18)19/h1-8,14H,(H,16,17)	-6.43
InChI=1S/C13H18O3/c1-2-3-9-15-10-11-16-13(14)12-7-5-4-6-8-12/h4-8H,2-3,9-11H2,1H3	-3.322
InChI=1S/C5H3BrN4/c6-4-3-5(9-1-7-3)10-2-8-4/h1-2H,(H,7,8,9,10)	-2.025
InChI=1S/C11H15N3O2/c1-7-4-3-5-9-13(2)6-8(10(12)15)11(16)14(7)9/h5-7H,3-4H2,1-2H3,(H2,12,15)	-2.227
InChI=1S/C5H9NO4/c1-6-3(5(9)10)2-4(7)8/h3,6H,2H2,1H3,(H,7,8)(H,9,10)	-0.754
InChI=1S/C7H8O3/c1-5-3-6(9-2)4-7(8)10-5/h3-4H,1-2H3	0.123
InChI=1S/C12H20O/c1-11(2)7-6-9-12(3)8-4-5-10-13/h7-8,10H,4-6,9H2,1-3H3/b12-8+	-3.538
InChI=1S/C12H10ClNO2S/c13-10-6-8-11(9-7-10)14-17(15,16)12-4-2-1-3-5-12/h1-9,14H	-4.03
InChI=1S/C24H30N2O/c25-19-7-4-17(5-8-19)10-13-26-14-12-24-11-2-1-3-21(24)23(26)15-18h4-9,16,21,23,27H,1-3,10-15,25H2	-4.069
InChI=1S/C12H8Cl2/c13-11-6-4-9(5-7-11)10-2-1-3-12(14)8-10/h1-8H	-6.4
InChI=1S/C11H12N2O2/c1-2-11(8-6-4-3-5-7-8)9(14)12-10(15)13-11/h3-7H,2H2,1H3,(H2,12,13,14,15)	-2.64
InChI=1S/C11H18ClN3O4/c12-6-7-15(14-19)11(18)13-9(10(16)17)8-4-2-1-3-5-8/h8-9H,1-7H2,(H,13,18)(H,16,17)	-3.937
InChI=1S/C9H20O2/c1-3-4-5-6-9(2,7-10)8-11/h10-11H,3-8H2,1-2H3	-2.188
InChI=1S/C17H18FN3O3/c1-19-9-6-20(7-9)15-5-14-11(4-13(15)18)16(22)12(17(23)24)8-21(14)h4-5,8-10,19H,2-3,6-7H2,1H3,(H,23,24)	-5.41
InChI=1S/C14H24N2O3/c1-3-5-6-7-8-9-10-14(4-2)11(17)15-13(19)16-12(14)18/h3-10H2,1-2H3,(H2,15,16,17,18,19)	-3.94
InChI=1S/C19H23N7O3/c1-28-10-8-21-17-14(19(27)22-9-11-29-2)23-13-15(20)24-16(25-18(1h3-7H,8-11H2,1-2H3,(H,22,27)(H3,20,21,24,25,26)	-3.356
InChI=1S/C4H9NO2/c1-3-7-4(6)5-2/h3H2,1-2H3,(H,5,6)	0.826
InChI=1S/C16H24N2O2/c1-3-13-11(2)17-14-5-4-12(16(19)15(13)14)10-18-6-8-20-9-7-18/h12,17H,3-10H2,1-2H3	-2.983
InChI=1S/C9H10O2/c1-2-4-8(5-3-1)10-6-9-7-11-9/h1-5,9H,6-7H2	-1.796
InChI=1S/C10H14N2O2/c11-10(14)8-4-1-2-5-9(8)12-6-3-7-13/h1-2,4-5,12-13H,3,6-7H2,(H2,11,14)	-1.216
InChI=1S/C14H11N/c1-10-5-4-7-12-9-11-6-2-3-8-13(11)15-14(10)12/h2-9H,1H3	-5.021
InChI=1S/C11H18O/c1-11(2)9-4-3-8(5-6-12)10(11)7-9/h3,9-10,12H,4-7H2,1-2H3	-2.696
InChI=1S/C7H17O2PS3/c1-7(2)12-5-6-13-10(11,8-3)9-4/h7H,5-6H2,1-4H3	-3.429
InChI=1S/C12H6Cl4O/c13-7-3-8(14)5-10(4-7)17-9-1-2-11(15)12(16)6-9/h1-6H	-7.32

"InChi"	"logS(M)"
InChI=1S/C6H14N2/c7-5-3-1-2-4-6(5)8/h5-6H,1-4,7-8H2/p+2	0.889
InChI=1S/C11H14O2/c1-8(9(2)11(12)13)10-6-4-3-5-7-10/h3-9H, 1-2H3,(H,12,13)	-2.772
InChI=1S/C8H6O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)(H, 11,12)	-3.22
InChI=1S/C8H16O/c1-2-8(9)6-4-3-5-7-8/h9H,2-7H2,1H3	-1.832
InChI=1S/C11H22O/c1-8(2)10-6-5-9(3)7-11(10)12-4/h8-11H, 5-7H2,1-4H3	-3.93
InChI=1S/C6H10N2O2/c1-3-6(2)4(9)7-5(10)8-6/h3H2,1-2H3, (H2,7,8,9,10)	-1.736
InChI=1S/C37H68O8/ c1-9-17-21-29(13-5)33(38)42-25-37(26-43-34(39)30(14-6)22-18-10-2, h29-32H,9-28H2,1-8H3	-9.205
InChI=1S/C18H26N2O/ c1-4-18(21)20-15(2)13-19(14-16(20)3)12-8-11-17-9-6-5-7-10-17/ h5-11,15-16H,4,12-14H2,1-3H3/b11-8+	-3.767
InChI=1S/C9H9NO3S/c1-10-9(11)6-7-4-2-3-5-8(7)14(10,12)13/ h2-5H,6H2,1H3	-1.14
InChI=1S/C10H14Cl2N2O2/ c1-3-5-13-8(15)7-14(6-4-2)10(16)9(11)12/h3-4,9H,1-2,5-7H2,(H, 13,15)	-1.04
InChI=1S/C17H26N2O/ c1-3-17(20)19(16-10-6-4-7-11-16)15(2)14-18-12-8-5-9-13-18/ h4,6-7,10-11,15H,3,5,8-9,12-14H2,1-2H3	-2.946
InChI=1S/C8H7NO5/c10-3-5-1-7-8(14-4-13-7)2-6(5)9(11)12/ h1-2,10H,3-4H2	-3.06
InChI=1S/C13H18O3/c1-3-4-7-16-12-6-5-11(8-10(12)2)9-13(14)15/ h5-6,8H,3-4,7,9H2,1-2H3,(H,14,15)	-3.442
InChI=1S/C8H8O2/c1-6-2-3-7-8(4-6)10-5-9-7/h2-4H,5H2,1H3	-2.417
InChI=1S/C31H38N2O3/ c1-8-32(9-2)26-18-28-24(16-20(26)5)30(22-14-12-13-15-23(22)31(34) h12-19,28H,8-11H2,1-7H3	-7.687
InChI=1S/C21H28N2O/ c1-4-21(24)23(20-13-9-6-10-14-20)17-18(2)22(3)16-15-19-11-7-5-8-1 h5-14,18H,4,15-17H2,1-3H3	-3.694
InChI=1S/C16H15FO2/ c17-10-11-19-16(18)12-13-6-8-15(9-7-13)14-4-2-1-3-5-14/h1-9H, 10-12H2	-5.01
InChI=1S/C55H86O24/ c1-10-23(2)46(71)79-43-44(72-24(3)60)55(22-59)26(17-50(43,4)5)25- h10-11,26-44,47-49,56-59,61-68H,12-22H2,1-9H3,(H,69,70)/b23-10+	-1.103
InChI=1S/C10H13N5O4S/ c11-10-13-7-4(8(20)14-10)12-2-15(7)9-6(18)5(17)3(1-16)19-9/ h2-3,5-6,9,16-18H,1H2,(H3,11,13,14,20)	-1.976
InChI=1S/C13H14O6/ c1-3-17-12(15)8-18-13(16)10-6-4-5-7-11(10)19-9(2)14/h4-7H, 3,8H2,1-2H3	-2.58
InChI=1S/C11H12O3/c1-2-8-13-11(12)9-14-10-6-4-3-5-7-10/h2-7H, 1,8-9H2	-2.536
InChI=1S/C11H13NO2/c1-8(7-9(2)13)12-10-5-3-4-6-11(10)14/ h3-6,14H,7H2,1-2H3/b12-8-	-3.55

"InChi"	"logS(M)"
InChI=1S/C9H18O/c1-8(5-6-10)7-9(2,3)4/h6,8H,5,7H2,1-4H3	-2.676
InChI=1S/C17H24ClNO2/c1-4-7-11-21-13-19(16(20)12-18)17-14(5-2)9-8-10-15(17)6-3/h4,7-10H,5-6,11-13H2,1-3H3/b7-4+	-4.029
InChI=1S/C7H7Cl2NO2S/c1-6-2-4-7(5-3-6)13(11,12)10(8)9/h2-5H,1H3	-3.51
InChI=1S/C15H13ClN2/c16-12-6-7-14-13(10-12)15(18-9-8-17-14)11-4-2-1-3-5-11/h1-7,10,17H,8-9H2	-4.392
InChI=1S/C11H13Cl2NO3/c1-11(2)14(10(15)9(12)13)6-8(17-11)7-4-3-5-16-7/h3-5,8-9H,6H2,1-2H3	-3.15
InChI=1S/C33H29NO2/c35-32(28-18-9-3-10-19-28,24-26-14-5-1-6-15-26)30-22-13-23-31(34-h1-23,35-36H,24-25H2	-8.587
InChI=1S/C15H26O/c1-7-15(6)9-8-12(14(4,5)16)10-13(15)11(2)3/h7,12-13,16H,1-2,8-10H2,3-6H3	-3.059
InChI=1S/C11H15NO4S/c1-3-12(4-2)17(15,16)10-7-5-9(6-8-10)11(13)14/h5-8H,3-4H2,1-2H3,(H,13,14)	-2.597
InChI=1S/C10H12N4O5S3/c1-14-9(20-10(12-14)21(11,15)16)13-22(17,18)8-5-3-7(19-2)4-6-8/h3-6H,1-2H3,(H2,11,15,16)/b13-9+	-2.76
InChI=1S/C18H25NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19)24-1h4-5,11,14-15,22H,6-10H2,1-3H3/b12-4+	-0.595
InChI=1S/C14H20N2O/c1-2-14(17)16(12-6-4-3-5-7-12)13-8-10-15-11-9-13/h3-7,13,15H,2,8-11H2,1H3/p+1	-0.835
InChI=1S/C8H13N3O2/c1-3-8(4-2,5-9)6(12)11-7(10)13/h3-4H2,1-2H3,(H3,10,11,12,13)	-1.564
InChI=1S/C19H17NO2/c1-20-17(21)12-19(18(20)22)15-8-4-2-6-13(15)10-11-14-7-3-5-9-16(1h2-9H,10-12H2,1H3	-5.55
InChI=1S/C9H18N2O4/c1-3-4-7(15-9(11)13)5-6(2)14-8(10)12/h6-7H,3-5H2,1-2H3,(H2,10,12)(H2,11,13)	-1.601
InChI=1S/C15H19F3N4O/c16-15(17,18)11-2-1-3-12(8-11)22-6-4-21(5-7-22)10-13-9-20-14(19)2h1-3,8,13H,4-7,9-10H2,(H2,19,20)	-3.482
InChI=1S/C4H12O4P2S4/c1-5-9(11,6-2)13-14-10(12,7-3)8-4/h1-4H3	-4.398
InChI=1S/C16H24N2/c1-2-9-16-15(7-1)8-3-4-12-18(16)14-13-17-10-5-6-11-17/h1-2,7,9H,3-6,8,10-14H2	-3.523
InChI=1S/C2H6N4O4/c7-5(8)3-1-2-4-6(9)10/h3-4H,1-2H2	-1.815
InChI=1S/C3H3Br/c1-2-3-4/h1H,3H2	-0.902
InChI=1S/C11H16N2O3S/c1-2-3-9-12-11(14)13-17(15,16)10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3,(H2,12,13,14)	-3.05
InChI=1S/C6H14O2/c1-3-7-5-6-8-4-2/h3-6H2,1-2H3	-0.77
InChI=1S/C13H24N2O4/c1-5-7-15-12(17)19-9-13(4,10(3)6-2)8-18-11(14)16/h5,10H,1,6-9H2,2-4H3,(H2,14,16)(H,15,17)	-3.503

"InChi"	"logS(M)"
InChI=1S/C5H11ClO/c1-4(6)5(2)7-3/h4-5H,1-3H3	-1.999
InChI=1S/C10H17NO2/c12-10(8-6-7-8)11(13)9-4-2-1-3-5-9/h8-9,13H,1-7H2	-2.04
InChI=1S/C16H19N3O2/c1-12-14(18-10-6-7-11-18)15(20)19(16(21)17(12)2)13-8-4-3-5-9-13/h3-5,8-9H,6-7,10-11H2,1-2H3	-3.211
InChI=1S/C17H20N2O3/c1-3-21-15-11-14(16(22-4-2)10-13(15)18)19-17(20)12-8-6-5-7-9-12/h5-11H,3-4,18H2,1-2H3,(H,19,20)	-2.406
InChI=1S/C20H20Cl2N8O4/c1-9(31)17(19(33)25-23)29-27-12-4-5-13(14(21)8-12)11-3-6-16(15(22h3-8,17-18H,23-24H2,1-2H3,(H,25,33)(H,26,34)/b29-27+,30-28+	-8.705
InChI=1S/C20H22N4O6S/c1-28-12-17(25)21-16-11-14(31-13-7-5-4-6-8-13)9-10-15(16)22-18(23h4-11H,12H2,1-3H3,(H,21,25)(H2,22,23,24,26,27)	-3.142
InChI=1S/C6H10O4/c7-5(3-1-9-3)6(8)4-2-10-4/h3-8H,1-2H2	0.834
InChI=1S/C29H25N5O5/c1-2-3-14-39-28(37)20-10-6-7-11-22(20)33-34-25-19-9-5-4-8-17(19)1h4-13,15-16,33H,2-3,14H2,1H3,(H,30,36)(H2,31,32,38)/b34-25-	-8.214
InChI=1S/C6H8N2OS/c1-2-3-8-5(9)4-7-6(8)10/h2H,1,3-4H2,(H,7,10)	-0.876
InChI=1S/C4H7ClO3S/c5-3-1-9(7,8)2-4(3)6/h3-4,6H,1-2H2	0.768
InChI=1S/C14H12N2O4/c1-15-11(17)7-6-10(14(15)20)16-12(18)8-4-2-3-5-9(8)13(16)19/h2-5,10H,6-7H2,1H3	-2.99
InChI=1S/C15H10Cl2O3/c16-12-6-5-10(7-13(12)17)14(18)8-9-3-1-2-4-11(9)15(19)20/h1-7H,8H2,(H,19,20)	-5.049
InChI=1S/C23H26N4/c1-3-8-20(9-4-1)22(21-10-5-2-6-11-21)13-15-26-16-18-27(19-17-26)2h1-12,14,22H,13,15-19H2	-4.537
InChI=1S/C17H18F2N4O3/c1-17(21)5-22(6-17)14-10(18)12(20)9-13(11(14)19)23(7-2-3-7)4-8(15h4,7H,2-3,5-6,20-21H2,1H3,(H,25,26)	-4.38
InChI=1S/C10H18N8/c11-7-17-9(13)15-5-3-1-2-4-6-16-10(14)18-8-12/h1-6H2,(H3,13,15,17)(H3,14,16,18)	-4.435
InChI=1S/C7H15N3O6/c8-7(16)10-9-1-3(12)5(14)6(15)4(13)2-11/h1,3-6,11-15H,2H2,(H3,8,10,16)/b9-1+	-0.426
InChI=1S/C12H24O3/c1-4-7-10-13-11(8-5-2)15-12(14-10)9-6-3/h10-12H,4-9H2,1-3H3	-3.889
InChI=1S/C12H3Cl7/c13-5-2-1-4(9(16)12(5)19)8-10(17)6(14)3-7(15)11(8)18/h1-3H	-8.42
InChI=1S/C14H4Br10/c15-5-3(6(16)10(20)13(23)9(5)19)1-2-4-7(17)11(21)14(24)12(22)8(4)h1-2H2	-9.13
InChI=1S/C14H28N2O4/c1-4-6-8-14(3,10-19-12(15)17)11-20-13(18)16-9-7-5-2/h4-11H2,1-3H3,(H2,15,17)(H,16,18)	-4.217
InChI=1S/C14H18O3/c15-13(16)14(17,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8,12,17H,2,5-6,9-10H2,(H,15,16)	-2.601

"InChi"	"logS(M)"
InChI=1S/C9H20N2S/c1-2-3-4-5-6-7-8-12-9(10)11/h2-8H2,1H3,(H3,10,11)	0.16
InChI=1S/C8H7ClO2/c1-5-6(8(10)11)3-2-4-7(5)9/h2-4H,1H3,(H,10,11)	-2.773
InChI=1S/C3H5NO4/c1-8-3(5)2-4(6)7/h2H2,1H3	-0.891
InChI=1S/C12H6O3/c13-11-8-5-1-3-7-4-2-6-9(10(7)8)12(14)15-11/h1-6H	-6.297
InChI=1S/C11H15NO/c1-9(12(2)3)11(13)10-7-5-4-6-8-10/h4-9H,1-3H3	-1.245
InChI=1S/C8H8N2O2S/c1-4-5(3-9)7(10)13-6(4)8(11)12-2/h10H2,1-2H3	-4.992
InChI=1S/C17H24O/c1-11(18)14-9-12(16(2,3)4)10-15-13(14)7-8-17(15,5)6/h9-10H,7-8H2,1-6H3	-4.871
InChI=1S/C12H3Cl7/c13-5-3-8(16)11(18)12(19)9(5)4-1-6(14)10(17)7(15)2-4/h1-3H	-9.1
InChI=1S/C12H5Cl5O/c13-6-1-2-11(8(14)3-6)18-7-4-9(15)12(17)10(16)5-7/h1-5H	-7.89
InChI=1S/C10H18N2O5/c1-4-10(5-2,7(13)12-9(11)15)8(14)17-6-16-3/h4-6H2,1-3H3,(H3,11,12,13,15)	-2.17
InChI=1S/C22H31N3O5/c1-28-18-14-17(15-19(29-2)22(18)30-3)6-7-20(26)25-12-10-23(11-13-h6-7,14-15H,4-5,8-13,16H2,1-3H3/b7-6+	-2.711
InChI=1S/C9H9NO2/c1-10-7-4-2-3-5-8(7)12-6-9(10)11/h2-5H,6H2,1H3	-2.144
InChI=1S/C20H23N3O/c1-23(2)15-9-14-21-20-22-18(16-10-5-3-6-11-16)19(24-20)17-12-7-4-h3-8,10-13H,9,14-15H2,1-2H3,(H,21,22)	-4.104
InChI=1S/C13H22O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h7,9H,5-6,8,10H2,1-4H3/b12-9-	-3.697
InChI=1S/C5H3BrO3/c6-3-1-2-9-4(3)5(7)8/h1-2H,(H,7,8)	-1.17
InChI=1S/C6H4Cl2N2O2/c7-4-1-3(10(11)12)2-5(8)6(4)9/h1-2H,9H2	-4.471
InChI=1S/C14H16ClN3O2/c1-9-12(16(2)3)13(19)17(4)14(20)18(9)11-7-5-10(15)6-8-11/h5-8H,1-4H3	-2.678
InChI=1S/C7H14N2O3S/c1-7(2,13(4)11)5-9-12-6(10)8-3/h5H,1-4H3,(H,8,10)/p+1/b9-5+	-0.867
InChI=1S/C12H17NO/c1-2-3-4-5-12(14)10-6-8-11(13)9-7-10/h6-9H,2-5,13H2,1H3	-2.92
InChI=1S/C17H20N2O3/c1-12(2)22-17(20)19-18-15-11-14(9-10-16(15)21-3)13-7-5-4-6-8-13/h4-12,18H,1-3H3,(H,19,20)	-4.902
InChI=1S/C20H18O3/c1-20(14-2-8-17(21)9-3-14,15-4-10-18(22)11-5-15)16-6-12-19(23)13-h2-13,21-23H,1H3	-4.087
InChI=1S/C11H10N2O2/c14-9-5-6-13-10(9)12-8-4-2-1-3-7(8)11(13)15/h1-4,9,14H,5-6H2	-2.106
InChI=1S/C19H21NS/c1-20-11-8-15(9-12-20)19-16-5-3-2-4-14(16)6-7-18-17(19)10-13-21-1h2-5,10,13H,6-9,11-12H2,1H3	-5.901

"InChi"	"logS(M)"
InChI=1S/C10H18N2O/c1-3-10(13)12-8-4-5-9(12)7-11(2)6-8/h8-9H,3-7H2,1-2H3	-2.108
InChI=1S/C6H4ClF/c7-5-3-1-2-4-6(5)8/h1-4H	-2.416
InChI=1S/C11H25NO/c1-3-5-8-12(9-6-4-2)10-7-11-13/h13H,3-11H2,1-2H3	-1.697
InChI=1S/C7H6Cl2/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2	-3.207
InChI=1S/C12H10N6O4/c1-4-2-6-7(14-11(21)13-6)3-5(4)17-18-8-9(19)15-12(22)16-10(8)20/h2-3,8,17-18H,1H3,(H2,15,16,19,20,22)	-6.489
InChI=1S/C12H27NO3S2/c1-2-3-4-5-6-7-8-9-10-13-11-12-17-18(14,15)16/h13H,2-12H2,1H3,(H,14,15,16)	-2.859
InChI=1S/C9H6Cl2N2O2/c10-4-8(14)13-9-12-6-3-5(11)1-2-7(6)15-9/h1-3H,4H2,(H,12,13,14)	-3.265
InChI=1S/C7H11NO3/c1-8-4-5(3-6(8)9)7(10)11-2/h5H,3-4H2,1-2H3	0.804
InChI=1S/C34H30Cl2N6O4/c1-19-5-11-25(12-6-19)37-33(45)31(21(3)43)41-39-29-15-9-23(17-27(h5-18,31-32H,1-4H3,(H,37,45)(H,38,46)/b41-39+,42-40+	-8.102
InChI=1S/C20H25NO4/c1-2-19(23)16-8-10-18(11-9-16)25-14-17(22)12-21-13-20(24)15-6-4-3h3-11,17,20-22,24H,2,12-14H2,1H3	-2.002
InChI=1S/C12H3Cl7/c13-4-1-2-5(14)10(17)8(4)9-11(18)6(15)3-7(16)12(9)19/h1-3H	-7.94
InChI=1S/C10H12N4O6/c1-2-19-9(15)6-13(10(11)16)12-5-7-3-4-8(20-7)14(17)18/h3-5H,2,6H2,1H3,(H2,11,16)/b12-5+	-2.441
InChI=1S/C16H28O2/c17-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-18-16/h1,3H,2,4-15H2/b3-1-	-5.629
InChI=1S/C7H15NO4S2/c1-13(9,10)8-14(11,12)7-5-3-2-4-6-7/h7-8H,2-6H2,1H3	-0.33
InChI=1S/C6H10O4/c7-5(8)3-1-2-4-6(9)10/h1-4H2,(H,7,8)(H,9,10)	-0.82
InChI=1S/C9H11Cl2NOS/c10-8-2-1-7(3-9(8)11)14-5-6(13)4-12/h1-3,6,13H,4-5,12H2	-1.616
InChI=1S/C20H23Cl2NO2/c1-23-10-9-14-11-18(24-2)19(25-3)12-15(14)17(23)8-7-13-5-4-6-16(2h4-6,11-12,17H,7-10H2,1-3H3	-5.67
InChI=1S/C12H16/c1-5-10-6-8-11(9-7-10)12(2,3)4/h5-9H,1H2,2-4H3	-4.563
InChI=1S/C11H22N2O4/c1-4-5-8(2)11(3,6-16-9(12)14)7-17-10(13)15/h8H,4-7H2,1-3H3,(H2,12,14)(H2,13,15)	-2.613
InChI=1S/C10H10Cl2N2O2/c11-8-5-7(6-9(12)13-8)10(15)14-1-3-16-4-2-14/h5-6H,1-4H2	-1.482
InChI=1S/C16H22ClNO3/c1-4-12-8-7-9-13(5-2)16(12)18(14(19)10-17)11-15(20)21-6-3/h7-9H,4-6,10-11H2,1-3H3	-3.473
InChI=1S/C12H18/c1-7-8(2)10(4)12(6)11(5)9(7)3/h1-6H3	-5.23
InChI=1S/C20H25NO/c1-4-19(22)20(15-16-21(2)3,17-11-7-5-8-12-17)18-13-9-6-10-14-18/h5-14H,4,15-16H2,1-3H3	-2.996

"InChi"	"logS(M)"
InChI=1S/C10H15BrN2O4S2/c11-9-2-3-10(13-8-9)17-6-1-4-12-5-7-18-19(14,15)16/h2-3,8,12H,1,4-7H2,(H,14,15,16)	-1.654
InChI=1S/C15H24N2O2/c1-5-17(6-2)11(3)12(4)19-15(18)13-7-9-14(16)10-8-13/h7-12H,5-6,16H2,1-4H3	-3.42
InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h8-11H,1,4-6H2,2-3H3	-1.711
InChI=1S/C9H10O4/c1-2-13-9(12)6-3-4-7(10)8(11)5-6/h3-5,10-11H,2H2,1H3	-1.856
InChI=1S/C8H14O2S2/c9-8(10)4-2-1-3-7-5-6-11-12-7/h7H,1-6H2,(H,9,10)	-2.375
InChI=1S/C13H21O3PS/c1-11(2)15-17(14,16-12(3)4)18-10-13-8-6-5-7-9-13/h5-9,11-12H,10H2,1-4H3	-2.858
InChI=1S/C30H41N3O5S/c1-19-12-11-13-20(2)25(19)38-17-23(34)31-22(16-21-14-9-8-10-15-2 h8-15,22,24,26,35H,16-18H2,1-7H3,(H,31,34)(H,32,36)	-5.01
InChI=1S/C19H30N2O2/c1-14(2)20(15(3)4)11-12-21-18-10-9-17(23-5)13-16(18)7-6-8-19(21)2 h9-10,13-15H,6-8,11-12H2,1-5H3	-4.466
InChI=1S/C8H5N3O3S2/c12-7(5-2-1-3-15-5)10-8-9-4-6(16-8)11(13)14/h1-4H,(H,9,10,12)	-4.738
InChI=1S/C8H7NO2/c9-6-2-1-5-4-11-8(10)7(5)3-6/h1-3H,4,9H2	-2.041
InChI=1S/C11H21BrO2/c12-10-8-6-4-2-1-3-5-7-9-11(13)14/h1-10H2,(H,13,14)	-3.699
InChI=1S/C5H6N2O2S/c6-5-7-3(2-10-5)1-4(8)9/h2H,1H2,(H2,6,7)(H,8,9)	-1.982
InChI=1S/C15H24O/c1-2-3-4-5-6-7-8-9-14-10-12-15(16)13-11-14/h10-13,16H,2-9H2,1H3	-4.498
InChI=1S/C11H15NO4/c1-8-4-2-3-5-10(8)15-6-9(13)7-16-11(12)14/h2-5,9,13H,6-7H2,1H3,(H2,12,14)	-1.461
InChI=1S/C6H5Cl2NO3S/c7-3-1-5(9)6(2-4(3)8)13(10,11)12/h1-2H,9H2,(H,10,11,12)	-2.105
InChI=1S/C6H10O5/c1-4(5(7)9-2)11-6(8)10-3/h4H,1-3H3	-0.6
InChI=1S/C22H30Cl2N10/c23-15-5-9-17(10-6-15)31-21(27)33-19(25)29-13-3-1-2-4-14-30-20(26 h5-12H,1-4,13-14H2,(H5,25,27,29,31,33)(H5,26,28,30,32,34)	-2.801
InChI=1S/C5H7F6NO2/c6-4(7,8)3(14,5(9,10)11)12-1-2-13/h12-14H,1-2H2	-0.022
InChI=1S/C19H23N3O6/c1-20(19(23)17-6-7-18(28-17)22(24)25)14-15-2-4-16(5-3-15)27-13-1(h2-7H,8-14H2,1H3	-2.29
InChI=1S/C24H29NO/c26-20-10-9-19-16-23-21-8-4-5-12-24(21,22(19)17-20)13-15-25(23)14 h1-3,6-7,9-10,17,21,23,26H,4-5,8,11-16H2	-5.782
InChI=1S/C13H10Cl2O4S/c14-11-7(13(18)9-2-1-5-20-9)3-4-8(12(11)15)19-6-10(16)17/h1-5,13,18H,6H2,(H,16,17)	-3.928
InChI=1S/C11H18O2/c1-5-11(4,13-9-12)8-6-7-10(2)3/h5,7,9H,1,6,8H2,2-4H3	-4.041

"InChi"	"logS(M)"
InChI=1S/C28H37N3O4S/c1-18-12-14-20(15-13-18)24(33)29-21(16-19-10-8-7-9-11-19)22(32)2(h7-15,21-23,32H,16-17H2,1-6H3,(H,29,33)(H,30,34)	-4.11
InChI=1S/C12H13ClN2O2/c13-11-3-1-10(2-4-11)12(16)9-14-15-5-7-17-8-6-15/h1-4,9H,5-8H2/b14-9+	-1.903
InChI=1S/C17H24N2O/c1-4-5-9-15-13-14-8-6-7-10-16(14)17(18-15)20-12-11-19(2)3/h6-8,10,13H,4-5,9,11-12H2,1-3H3	-4.658
InChI=1S/C14H12N2O/c17-13(10-6-2-1-3-7-10)14-15-11-8-4-5-9-12(11)16-14/h1-9,13,17H,(H,15,16)	-2.503
InChI=1S/C12H19N/c1-7-10-8-11(2,3)13(6)12(4,5)9-10/h1,8H,9H2,2-6H3	-1.829
InChI=1S/C12H21BrN2O4/c1-6(2)5-9(13)11(17)14-7(3)10(16)15-8(4)12(18)19/h6-9H,5H2,1-4H3,(H,14,17)(H,15,16)(H,18,19)	-1.43
InChI=1S/C10H12N2OS/c11-10-12-6-8(13-10)7-14-9-4-2-1-3-5-9/h1-5,8H,6-7H2,(H2,11,12)	-2.163
InChI=1S/C14H11Cl2NO3/c15-6-1-2-8(7(16)5-6)17-13(18)11-9-3-4-10(20-9)12(11)14(17)19/h1-2,5,9-12H,3-4H2	-2.01
InChI=1S/C14H20N2O2/c1-18-13-7-5-6-12(10-13)15-14(17)11-16-8-3-2-4-9-16/h5-7,10H,2-4,8-9,11H2,1H3,(H,15,17)	-3.326
InChI=1S/C12H12N2O3/c15-7-5-10-11(16)13-9-4-2-1-3-8(9)12(17)14(10)6-7/h1-4,7,10,15H,5-6H2,(H,13,16)	-2.37
InChI=1S/C6H13NO2/c1-5(2)3-4-9-6(7)8/h5H,3-4H2,1-2H3,(H2,7,8)	-1.44
InChI=1S/C12H13I3N2O2/c1-17(2)6-16-12-9(14)5-8(13)7(11(12)15)3-4-10(18)19/h5-6H,3-4H2,1-2H3,(H,18,19)/b16-6+	-7.129
InChI=1S/C16H14N4O/c1-12-15(18-17-13-8-4-2-5-9-13)16(21)20(19-12)14-10-6-3-7-11-14/h2-11,15H,1H3/b18-17+	-7.541
InChI=1S/C10H14O2S/c1-8-2-4-10(5-3-8)13-7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3	-1.951
InChI=1S/C5H10O4/c1-4(6)3-5(2,7)9-8-4/h6-7H,3H2,1-2H3	0.571
InChI=1S/C6H12N5O2PS2/c1-12-14(15,13-2)16-3-4-9-5(7)11-6(8)10-4/h3H2,1-2H3,(H4,7,8,9,10,11)	-3.069
InChI=1S/C5H10O3/c1-3-8-5(7)4(2)6/h4,6H,3H2,1-2H3	0.928
InChI=1S/C17H17NO2/c1-2-20-16(19)13-18-17(14-9-5-3-6-10-14)15-11-7-4-8-12-15/h3-12H,2,13H2,1H3	-3.427
InChI=1S/C10H6ClNO3/c11-8(13)5-12-9(14)6-3-1-2-4-7(6)10(12)15/h1-4H,5H2	-1.007
InChI=1S/C10H18O/c1-8-4-6-9(7-5-8)10(2,3)11/h4,9,11H,5-7H2,1-3H3	-2.337
InChI=1S/C5H9NS/c1-2-5-6-3-4-7-5/h2-4H2,1H3	-2.707

"InChi"	"logS(M)"
InChI=1S/C23H27N3O2/c1-17-21(23(27)26(24(17)3)20-12-8-5-9-13-20)16-25-14-15-28-22(18(h4-13,18,22H,14-16H2,1-3H3	-3.568
InChI=1S/C15H15NO3/c1-8-4-2-3-5-9(8)16-14(17)12-10-6-7-11(19-10)13(12)15(16)18/h2-5,10-13H,6-7H2,1H3	-0.977
InChI=1S/C10H13NO4S/c1-8(13)11-9-2-4-10(5-3-9)16(14,15)7-6-12/h2-5,12H,6-7H2,1H3,(H,11,13)	-2.307
InChI=1S/C8H18O4S2/c1-5-8(4,13(9,10)6-2)14(11,12)7-3/h5-7H2,1-4H3	-1.91
InChI=1S/C12H22O4/c13-11(14)9-7-5-3-1-2-4-6-8-10-12(15)16/h1-10H2,(H,13,14)(H,15,16)	-3.76
InChI=1S/C7H9N3O/c1-4-3-5(2)10-7(9-4)6(8)11/h3H,1-2H3,(H2,8,11)	0.122
InChI=1S/C14H21N3O4/c1-6-9(2)15-13-11(16(18)19)7-10(14(3,4)5)8-12(13)17(20)21/h7-9,15H,6H2,1-5H3	-5.47
InChI=1S/C57H110O9/c1-4-7-10-31-40-51(58)43-34-25-19-13-16-22-28-37-46-55(61)64-49-5h51-54,58-60H,4-50H2,1-3H3	-7.274
InChI=1S/C15H12N2S2/c18-13-15(17-14(19)16-13,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H,(H2,16,17,18,19)	-2.711
InChI=1S/C31H51NO10/c1-8-25-22(16-34)13-17(2)9-10-23(35)18(3)14-21(11-12-33)30(19(4)2h9-10,12-13,18-22,24-25,27-31,34,36,38-39H,8,11,14-16H2,1-7H3/b10-9-,17-13-	-3.393
InChI=1S/C14H12O3/c15-13-9-5-4-8-12(13)14(16)17-10-11-6-2-1-3-7-11/h1-9,15H,10H2	-4.414
InChI=1S/C13H26O3/c1-6-9-10-11(7-2)12(14)15-16-13(4,5)8-3/h11H,6-10H2,1-5H3	-4.117
InChI=1S/C6H2Cl3NO2/c7-3-1-4(8)6(10(11)12)5(9)2-3/h1-2H	-4.559
InChI=1S/C12H18O4/c1-9(2)11(13)15-7-5-6-8-16-12(14)10(3)4/h1,3,5-8H2,2,4H3	-2.969
InChI=1S/C14H17NO5/c1-3-19-13(17)9-15(2)12(16)10-20-14(18)11-7-5-4-6-8-11/h4-8H,3,9-10H2,1-2H3	-1.67
InChI=1S/C15H10O2/c16-14-11-8-4-5-9-12(11)15(17)13(14)10-6-2-1-3-7-10/h1-9,13H	-3.298
InChI=1S/C9H12N2O2/c10-9(13)7-3-1-2-4-8(7)11-5-6-12/h1-4,11-12H,5-6H2,(H2,10,13)	-1.783
InChI=1S/C10H6Cl2N2/c11-8-6-9(12)14-10(13-8)7-4-2-1-3-5-7/h1-6H	-4.954
InChI=1S/C6H6N4S/c1-11-6-4-5(8-2-7-4)9-3-10-6/h2-3H,1H3,(H,7,8,9,10)	-2.335
InChI=1S/C10H19ClNO5P/c1-6-12(7-2)10(13)9(11)8(3)17-18(14,15-4)16-5/h6-7H2,1-5H3/b9-8+	0.523
InChI=1S/C12H12N2O3/c1-3-17-12(16)9-7-13-10-6-4-5-8(2)14(10)11(9)15/h4-7H,3H2,1-2H3	-1.715
InChI=1S/C8H18O2/c1-7(2,3)9-10-8(4,5)6/h1-6H3	-2.932
InChI=1S/C8H16O/c1-3-5-6-7-8(9)4-2/h3-7H2,1-2H3	-1.693

"InChi"	"logS(M)"
InChI=1S/C15H21NO3/c1-10(2)8-13-14(17)16-12(15(18)19-13)9-11-6-4-3-5-7-11/h3-7,10,12-13,15,18H,8-9H2,1-2H3,(H,16,17)	-2.12
InChI=1S/C19H22N2O/c1-20(13-12-16-8-4-2-5-9-16)18-14-19(22)21(15-18)17-10-6-3-7-11-17/h2-11,18H,12-15H2,1H3	-3.408
InChI=1S/C7H5NO4/c9-6(10)4-1-5(7(11)12)3-8-2-4/h1-3H,(H,9,10)(H,11,12)	-2.223
InChI=1S/C9H20S/c1-4-5-6-7-8-9(2,3)10/h10H,4-8H2,1-3H3	-3.99
InChI=1S/C11H9NO4/c1-16-6-2-3-9-7(4-6)8(11(14)15)5-10(13)12-9/h2-5H,1H3,(H,12,13)(H,14,15)/p-1	-3.11
InChI=1S/C12H15N7O6S3/c13-5-9(20)15-6-10(21)16-7-1-3-8(4-2-7)28(24,25)19-11-17-18-12(26)h1-4H,5-6,13H2,(H,15,20)(H,16,21)(H,17,19)(H2,14,22,23)	-1.29
InChI=1S/C24H36O3/c1-4-5-6-22(26)27-17-11-13-23(2)16(15-17)7-8-18-19-9-10-21(25)24(h7,17-20H,4-6,8-15H2,1-3H3	-4.76
InChI=1S/C13H19N3O4S2/c14-10-12-4-5-13(16-11-12)20-8-3-1-2-6-15-7-9-21-22(17,18)19/h4-5,11,15H,1-3,6-9H2,(H,17,18,19)	-1.421
InChI=1S/C26H32O4/c1-23(2)15-26(7,18-11-8-16(9-12-18)21(27)24(3,4)29)20-14-17(10-13h8-14,29-30H,15H2,1-7H3	-5.964
InChI=1S/C10H13N5O5/c16-1-4-6(17)7(18)10(20-4)15-3-13-5-8(14-19)11-2-12-9(5)15/h2-4,6-7,10,16-19H,1H2,(H,11,12,14)	-0.359
InChI=1S/C6H14O4/c7-1-3-9-5-6-10-4-2-8/h7-8H,1-6H2	0.823
InChI=1S/C18H32O2/c19-18(20)16-10-8-6-4-2-1-3-5-7-9-13-17-14-11-12-15-17/h11,14,17H,1-10,12-13,15-16H2,(H,19,20)	-7.18
InChI=1S/CHCl3/c2-1(3)4/h1H/i1D	-1.418
InChI=1S/C12H8O2/c13-12-11-9(7-14-12)6-5-8-3-1-2-4-10(8)11/h1-6H,7H2	-3.306
InChI=1S/C15H24N2O3/c1-4-17(5-2)11-10-16-15(18)12-20-14-8-6-13(19-3)7-9-14/h6-9H,4-5,10-12H2,1-3H3,(H,16,18)	-2.776
InChI=1S/C8H13N3O3/c1-2-3-7-6-9-8(11(13)14)10(7)4-5-12/h6,12H,2-5H2,1H3	-1.881
InChI=1S/C12H6F2N2O2/c13-12(14)17-10-3-1-2-8(11(10)18-12)9-6-16-5-7(9)4-15/h1-3,5-6,16H	-5.139
InChI=1S/C5H13NO/c1-6(2)4-3-5-7/h7H,3-5H2,1-2H3	0.986
InChI=1S/C23H30N2O/c1-18(2)12-13-23(22(24)26,14-17-25-15-5-6-16-25)21-11-7-9-19-8-3-h3-4,7-12H,5-6,13-17H2,1-2H3,(H2,24,26)	-5.996
InChI=1S/C3H2ClF5/c4-3(8,9)2(6,7)1-5/h1H2	-3.7
InChI=1S/C5H10N2O/c1-6-3-4-7(2)5(6)8/h3-4H2,1-2H3	0.636
InChI=1S/C12H18O3/c1-2-5-10-6-3-4-7-12(10)15-9-11(14)8-13/h3-4,6-7,11,13-14H,2,5,8-9H2,1H3	-2.775

"InChi"	"logS(M)"
InChI=1S/C17H20N2O6S/c1-17(2)12(16(22)23)19-14(21)11(15(19)26-17)18-13(20)10-8(24-3)6-h5-7,11-12,15H,1-4H3,(H,18,20)(H,22,23)	-3.015
InChI=1S/C12H5Cl5/c13-7-1-6(2-8(14)3-7)12-10(16)4-9(15)5-11(12)17/h1-5H	-7.92
InChI=1S/C9H9NO5/c1-6(11)15-9-5-7(10(12)13)3-4-8(9)14-2/h3-5H,1-2H3	-2.947
InChI=1S/C9H6O6/c10-7(11)4-1-2-5(8(12)13)6(3-4)9(14)15/h1-3H,(H,10,11)(H,12,13)(H,14,15)	-1
InChI=1S/C6H2Cl3NO2/c7-3-1-2-4(10(11)12)6(9)5(3)8/h1-2H	-3.94
InChI=1S/C17H25NO2/c1-5-16(19)20-17(15-9-7-6-8-10-15)11-14(3)18(4)12-13(17)2/h6-10,13-14H,5,11-12H2,1-4H3	-2.874
InChI=1S/C7H7ClN6O2/c8-1-2-14-7(16)13-3-10-4(5(9)15)6(13)11-12-14/h3H,1-2H2,(H2,9,15)	-2.311
InChI=1S/C34H15NO4/c36-33-21-7-3-1-5-16(21)18-9-12-23-28-19(10-13-24(33)29(18)28)20-h1-15H	-4.399
InChI=1S/C12H10Cl2N6O2S/c1-20-10-8(9(13)17-11(14)18-10)16-12(20)19-23(21,22)7-4-2-6(15)3-h2-5H,15H2,1H3,(H,16,19)	-2.555
InChI=1S/C8H4Cl4O3/c9-3-1-4(10)8(7(12)6(3)11)15-2-5(13)14/h1H,2H2,(H,13,14)	-3.41
InChI=1S/C12H14ClNO4/c1-7(15)4-12(16)14-9-6-10(17-2)8(13)5-11(9)18-3/h5-6H,4H2,1-3H3,(H,14,16)	-2.979
InChI=1S/C16H13ClFNO3/c1-10(16(21)22)19(12-7-8-14(18)13(17)9-12)15(20)11-5-3-2-4-6-11/h2-10H,1H3,(H,21,22)	-4.247
InChI=1S/C16H28O4/c1-11(2)9-19-15(17)13-7-5-6-8-14(13)16(18)20-10-12(3)4/h11-14H,5-10H2,1-4H3	-4.191
InChI=1S/C15H10ClI2NO3/c1-8(20)22-14-12(6-10(17)7-13(14)18)15(21)19-11-4-2-9(16)3-5-11/h2-7H,1H3,(H,19,21)	-7.825
InChI=1S/C24H27NO2/c1-3-5-12-19(4-2)18-27-24(26)22(17-25)23(20-13-8-6-9-14-20)21-15-h6-11,13-16,19H,3-5,12,18H2,1-2H3	-6.558
InChI=1S/C18H6Cl4N2O/c19-13-11-12(14(20)16(22)15(13)21)18(25)24-9-6-2-4-7-3-1-5-8(10(7h1-6H	-7.134
InChI=1S/C17H25N3O3S/c1-11(2)10-14(15(21)19-13-8-9-23-16(13)22)20-17(24)18-12-6-4-3-5-h3-7,11,13-14,16,22H,8-10H2,1-2H3,(H,19,21)(H2,18,20,24)	-2.37
InChI=1S/C11H21N/c1-7-8(6-12)4-9-5-10(7)11(9,2)3/h7-10H,4-6,12H2,1-3H3	-2.516
InChI=1S/C3H5NO2/c1-3(5)2-4-6/h2,6H,1H3/b4-2+	-0.128
InChI=1S/C9H15N3O2/c1-3-5-12-7(10)6-8(13)11(4-2)9(12)14/h6H,3-5,10H2,1-2H3	-2.134
InChI=1S/C10H7N3O/c11-6-7-14-13-10(8-12)9-4-2-1-3-5-9/h1-5H,7H2/b13-10+	-3.29

"InChi"	"logS(M)"
InChI=1S/C12H16N2/c1-14(2)8-7-10-9-13-12-6-4-3-5-11(10)12/h3-6,9,13H,7-8H2,1-2H3	-1.226
InChI=1S/C18H23N3O3/c1-2-18(22)20-16-9-10-17(20)13-19(12-16)11-3-4-14-5-7-15(8-6-14)2h3-8,16-17H,2,9-13H2,1H3/b4-3+	-4.219
InChI=1S/C13H17NO5/c1-9(8-17-3)18-13(16)19-12-6-4-11(5-7-12)14-10(2)15/h4-7,9H,8H2,1-3H3,(H,14,15)	-2.48
InChI=1S/C10H20O/c1-8(2)10(3)6-4-5-9(11)7-10/h8-9,11H,4-7H2,1-3H3	-0.6
InChI=1S/C3H6Cl2O2S/c4-1-2-8(6,7)3-5/h1-3H2	-1.5
InChI=1S/C11H13NO3S/c1-8(2)12-11(13)7-9-5-3-4-6-10(9)16(12,14)15/h3-6,8H,7H2,1-2H3	-2.121
InChI=1S/C20H17NO/c1-21-18-13-7-5-11-16(18)20(22,15-9-3-2-4-10-15)17-12-6-8-14-19(1h2-14,22H,1H3	-3.903
InChI=1S/C26H21F6NO5/c1-24(2)18(11-12-20(34)38-23(25(27,28)29)26(30,31)32)21(24)22(35h3-13,18-19,21,23H,1-2H3/b12-11+	-7.433
InChI=1S/C12H12N2O3S/c15-10(16)7-6-9-11(17)14(12(18)13-9)8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,13,18)(H,15,16)	-2.285
InChI=1S/C5H5N5S/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)	-3.31
InChI=1S/C19H39N3O/c1-4-21(5-2)11-6-7-16(3)20-15-19-18(10-14-23)17-8-12-22(19)13-9-1h16-20,23H,4-15H2,1-3H3	-2.821
InChI=1S/C10H21NO/c1-4-5-6-7-8-9-10(12)11(2)3/h4-9H2,1-3H3	-1.6
InChI=1S/C19H19ClF3NO5/c1-3-26-8-9-27-18(25)12(2)28-14-4-6-15(7-5-14)29-17-16(20)10-13(1h4-7,10-12H,3,8-9H2,1-2H3	-5.874
InChI=1S/C9H13ClN2/c1-7(12-11)5-8-3-2-4-9(10)6-8/h2-4,6-7,12H,5,11H2,1H3	-2.288
InChI=1S/C35H54O10/c1-18-31(39)26(36)15-30(42-18)45-32-19(2)43-29(16-27(32)37)44-22h13,18-19,21-27,29-32,36-37,39-40H,5-12,14-17H2,1-4H3	-5.662
InChI=1S/C7H6O4/c1-2-3(8)5(10)7-6(11-7)4(2)9/h6-8H,1H3	-2.545
InChI=1S/C7H6N2O2S/c8-5-6-1-3-7(4-2-6)12(9,10)11/h1-4H,(H2,9,10,11)	-0.992
InChI=1S/C18H30O6/c1-4-7-10-22-16(19)13-15(18(21)24-12-9-6-3)14-17(20)23-11-8-5-2/h13H,4-12,14H2,1-3H3/b15-13-	-6.583
InChI=1S/C6H14O6S2/c1-13(7,8)11-5-3-4-6-12-14(2,9)10/h3-6H2,1-2H3	-2.27
InChI=1S/C13H18N4O4/c1-4-5-6-9(18)21-8-17-7-14-11-10(17)12(19)16(3)13(20)15(11)2/h7H,4-6,8H2,1-3H3	-2.37
InChI=1S/C8H10O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h5-6H,1-4H2	-1.565
InChI=1S/C30H29Cl2N5/c1-3-36(4-2)18-17-33-26-20-30-28(19-27(26)34-23-13-9-21(31)10-14h5-16,19-20,34H,3-4,17-18H2,1-2H3/b33-26+	-6.713

"InChi"	"logS(M)"
InChI=1S/C20H13N/c1-3-7-15-13(5-1)9-11-17-19(15)20-16-8-4-2-6-14(16)10-12-18(20)21h1-12,21H	-6.628
InChI=1S/C7H7NO5S/c8-4-1-2-5(7(9)10)6(3-4)14(11,12)13/h1-3H,8H2,(H,9,10)(H,11,12,13)	-1.86
InChI=1S/C13H10ClNOS/c1-16-9-3-4-10-13(7-9)17-12-5-2-8(14)6-11(12)15-10/h2-7,15H,1H3	-4.979
InChI=1S/C19H33NO3S2/c21-25(22,23)24-18-17-20-16-12-7-5-3-1-2-4-6-9-13-19-14-10-8-11-1h8,10-11,14-15,20H,1-7,9,12-13,16-18H2,(H,21,22,23)	-5.392
InChI=1S/C2H3Cl2NO/c3-1(4)2(5)6/h1H,(H2,5,6)	-0.256
InChI=1S/C14H11Cl3O2/c15-14(16,17)13(9-1-5-11(18)6-2-9)10-3-7-12(19)8-4-10/h1-8,13,18-19H	-4.818
InChI=1S/C6H5N3S3/c7-3-10-1-6(12-5-9)2-11-4-8/h6H,1-2H2	-1.935
InChI=1S/C12H14N4O4S2/c1-19-11(17)15-9(21)13-7-5-3-4-6-8(7)14-10(22)16-12(18)20-2/h3-6H,1-2H3,(H2,13,15,17,21)(H2,14,16,18,22)	-4.11
InChI=1S/C11H16O/c1-11(2,9-12)8-10-6-4-3-5-7-10/h3-7,12H,8-9H2,1-2H3	-2.042
InChI=1S/C10H20O3/c1-3-5-6-8-13-10(11)7-9-12-4-2/h3-9H2,1-2H3	-2.196
InChI=1S/C11H13N3O5/c15-3-6-7(16)8(17)11(19-6)14-2-1-5-9(14)12-4-13-10(5)18/h1-2,4,6-8,11,15-17H,3H2,(H,12,13,18)	-0.22
InChI=1S/C25H31N3O/c1-26(2)22-13-7-19(8-14-22)25(29,20-9-15-23(16-10-20)27(3)4)21-11h7-18,29H,1-6H3	-6.235
InChI=1S/C9H10O4S/c1-7(9(10)11)14(12,13)8-5-3-2-4-6-8/h2-7H,1H3,(H,10,11)	-0.89
InChI=1S/C13H22N2O4/c1-4-6-7-13(3,9-18-11(14)16)10-19-12(17)15-8-5-2/h2H,4,6-10H2,1,3H3,(H2,14,16)(H,15,17)	-3.009
InChI=1S/C7H10N2O3/c1-3(2)4-5(10)8-7(12)9-6(4)11/h3-4H,1-2H3,(H2,8,9,10,11,12)	-1.456
InChI=1S/C14H21N3O2/c1-3-4-5-6-11-17(2)16-15-13-9-7-12(8-10-13)14(18)19/h7-10H,3-6,11H2,1-2H3,(H,18,19)/b16-15+	-2.52
InChI=1S/C16H26O3/c1-2-3-4-5-6-7-8-9-10-11-12-14-13-15(17)19-16(14)18/h10-11,14H,2-9,12-13H2,1H3/b11-10+	-4.426
InChI=1S/C3H8N2O/c1-3-5(2)4-6/h3H2,1-2H3	0.532
InChI=1S/C23H27FN4O2/c1-15-18(23(29)28-10-3-2-4-21(28)25-15)9-13-27-11-7-16(8-12-27)22h5-6,14,16H,2-4,7-13H2,1H3	-5.279
InChI=1S/C13H11N3O/c1-9-6-7-13(17)12(8-9)16-14-10-4-2-3-5-11(10)15-16/h2-8,17H,1H3	-5.353
InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h12H,2-11H2,1H3	-5.061
InChI=1S/C6H10O3/c1-6(2)3-9-5(8)4(6)7/h4,7H,3H2,1-2H3	0.652

"InChi"	"logS(M)"
InChI=1S/C18H14F3N5O3/c1-9(27)15(26-25-12-5-3-2-4-11(12)18(19,20)21)16(28)22-10-6-7-13-h2-8,15H,1H3,(H,22,28)(H2,23,24,29)/b26-25+	-7.456
InChI=1S/C19H15NO8/c21-13(22)7-20(8-14(23)24)6-9-5-12-15(19(28)16(9)25)18(27)11-4-2-h1-5,25,28H,6-8H2,(H,21,22)(H,23,24)	-1.808
InChI=1S/C23H22O8/c1-3-27-21(25)13-29-16-10-19(30-14-22(26)28-4-2)23-17(24)12-18(3h5-12H,3-4,13-14H2,1-2H3	-5.496
InChI=1S/C6H14O2/c7-5-3-1-2-4-6-8/h7-8H,1-6H2	1.626
InChI=1S/C16H21ClN2O4S2/c17-14-12-16(19-15-7-3-2-6-13(14)15)23-10-5-1-4-8-18-9-11-24-25(2h2-3,6-7,12,18H,1,4-5,8-11H2,(H,20,21,22)	-3.671
InChI=1S/C10H8O4/c11-7-1-3-9(13-7)5-6-10(9)4-2-8(12)14-10/h1-4H,5-6H2	-0.428
InChI=1S/C16H20N4O2/c1-5-6-11-14(21)19-13-9-10(2)7-8-12(13)17-16(18(3)4)20(19)15(11)2h7-9,22H,5-6H2,1-4H3	-3.63
InChI=1S/C8H7NO5/c1-14-7-3-2-5(8(10)11)4-6(7)9(12)13/h2-4H,1H3,(H,10,11)	-2.661
InChI=1S/C14H16N4O3/c1-2-17-8-10(13(20)21)11(19)9-7-15-14(16-12(9)17)18-5-3-4-6-18/h7-8H,2-6H2,1H3,(H,20,21)	-3.664
InChI=1S/C9H8INO4/c10-4-8(13)11-5-1-2-6(9(14)15)7(12)3-5/h1-3,12H,4H2,(H,11,13)(H,14,15)	-3.322
InChI=1S/C7H14O2/c1-4-6(3)7(8)9-5-2/h6H,4-5H2,1-3H3	-2.336
InChI=1S/C10H21NO3/c1-5-10(6-2,7-12)8-14-9(13)11(3)4/h12H,5-8H2,1-4H3	-2.165
InChI=1S/C13H13NO4/c1-3-13(2,12(17)18)14-10(15)8-6-4-5-7-9(8)11(14)16/h4-7H,3H2,1-2H3,(H,17,18)	-1.91
InChI=1S/C18H28O2/c1-4-7-9-14-17(18(19-5-2)20-6-3)15-16-12-10-8-11-13-16/h8,10-13,15,18H,4-7,9,14H2,1-3H3/b17-15-	-5.172
InChI=1S/C10H18/c1-5-10(4)8-6-7-9(2)3/h5,7,10H,1,6,8H2,2-4H3	-5.965
InChI=1S/C17H16N2O/c20-16-17(19-11-18-16)14-7-3-1-5-12(14)9-10-13-6-2-4-8-15(13)17/h1-8,19H,9-11H2,(H,18,20)	-4.273
InChI=1S/C9H12O/c1-7-3-5-9(6-4-7)8(2)10/h3-6,8,10H,1-2H3	-1.428
InChI=1S/C15H13N3O3/c19-13(11-7-3-1-4-8-11)16-15(21)18-17-14(20)12-9-5-2-6-10-12/h1-10H,(H,17,20)(H2,16,18,19,21)	-3.294
InChI=1S/C10H16O2/c1-9(2)7-4-5-10(3,12-9)8(11)6-7/h7H,4-6H2,1-3H3	-0.925
InChI=1S/C14H16ClN3O4S2/c15-10-5-11-13(6-12(10)23(16,19)20)24(21,22)18-14(17-11)9-4-7-1-2h1-2,5-9,14,17-18H,3-4H2,(H2,16,19,20)	-5.191
InChI=1S/C10H11N/c1-8(2)10-5-3-9(7-11)4-6-10/h3-6,8H,1-2H3	-2.989
InChI=1S/C24H32O4/c1-14-12-18-19(22(4)9-6-17(27)13-21(14)22)7-10-23(5)20(18)8-11-24h13,18-20H,1,6-12H2,2-5H3	-6.108

"InChi"	"logS(M)"
InChI=1S/C13H26N2O4/c1-5-6-7-13(4,8-18-11(14)16)9-19-12(17)15-10(2)3/h10H,5-9H2,1-4H3,(H2,14,16)(H,15,17)	-3.634
InChI=1S/C12H18O3/c1-2-3-10-4-6-12(7-5-10)15-9-11(14)8-13/h4-7,11,13-14H,2-3,8-9H2,1H3	-2.775
InChI=1S/C13H11NO/c15-14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,15H	-3.373
InChI=1S/C16H35N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h2-17H2,1H3	-3.584
InChI=1S/C13H22N2O4S2/c1-12-5-7-15-13(11-12)19-9-4-2-3-6-14-8-10-20-21(16,17)18/h5,7,11,14H,2-4,6,8-10H2,1H3,(H,16,17,18)	-1.932
InChI=1S/C13H15NO4/c15-12(14-6-8-17-9-7-14)10-18-13(16)11-4-2-1-3-5-11/h1-5H,6-10H2	-1.773
InChI=1S/C15H13NO3/c1-10-5-4-6-11(9-10)16-14(17)12-7-2-3-8-13(12)15(18)19/h2-9H,1H3,(H,16,17)(H,18,19)	-2.407
InChI=1S/C14H9NO3/c15-9-5-6-10(16)12-11(9)13(17)7-3-1-2-4-8(7)14(12)18/h1-6,16H,15H2	-3.824
InChI=1S/C17H23ClO4S/c1-13(2)22-16(19)17(11-5-3-4-6-12-17)23(20,21)15-9-7-14(18)8-10-15h7-10,13H,3-6,11-12H2,1-2H3	-5.52
InChI=1S/C13H28O3/c1-11(2)5-7-15-9-13(14)10-16-8-6-12(3)4/h11-14H,5-10H2,1-4H3	-1.366
InChI=1S/C5H3ClO3/c6-4-2-1-3(9-4)5(7)8/h1-2H,(H,7,8)	-1.69
InChI=1S/C16H18N2O5/c1-4-13(19)22-9-23-16(21)12-8-18(5-2)15-11(14(12)20)7-6-10(3)17-15h6-8H,4-5,9H2,1-3H3	-2.83
InChI=1S/C9H8N2O/c12-9-6-10-11(7-9)8-4-2-1-3-5-8/h1-7,12H	-1.962
InChI=1S/C15H15N3O2/c1-10-3-8-15(20)14(9-10)18-17-13-6-4-12(5-7-13)16-11(2)19/h3-9,17H,1-2H3,(H,16,19)/b18-14+	-5.358
InChI=1S/C43H22N6O13S3/c44-47-31-19-15-24-27(39(31)51)9-4-12-35(24)63(54,55)60-34-22-18-22H	-6.821
InChI=1S/C13H18O2/c1-2-3-4-5-6-11-7-9-12(10-8-11)13(14)15/h7-10H,2-6H2,1H3,(H,14,15)	-3.65
InChI=1S/C19H17N3O3S/c23-19(20-15-9-3-1-4-10-15)21-17-13-7-8-14-18(17)22-26(24,25)16-14,22H,(H2,20,21,23)	-4.578
InChI=1S/C6H8O2/c1-2-3-4-5-6(7)8/h2-5H,1H3,(H,7,8)/b3-2+,5-4+	-1.77
InChI=1S/C15H20N2O4S3/c1-15(2,3)17-9-11-4-6-12(7-5-11)23(18,19)13-8-14(22-10-13)24(16,2h4-8,10,17H,9H2,1-3H3,(H2,16,20,21)	-1.98
InChI=1S/C4H4N2O/c7-4-5-2-1-3-6-4/h1-3H,(H,5,6,7)	0.675
InChI=1S/C8H8N2OS/c1-11-5-2-3-6-7(4-5)10-8(12)9-6/h2-4H,1H3,(H2,9,10,12)	-2.751
InChI=1S/C12H9Cl2NO2S/c13-10-7-4-8-11(12(10)14)15-18(16,17)9-5-2-1-3-6-9/h1-8,15H	-4.73

"InChi"	"logS(M)"
InChI=1S/C12H4Cl6O/c13-5-1-2-6(14)12(11(5)18)19-10-4-8(16)7(15)3-9(10)17/h1-4H	-7.88
InChI=1S/C8H14O2/c1-4-5-8(6(2)9)7(3)10/h8H,4-5H2,1-3H3	-0.88
InChI=1S/C4H8N2O/c7-4-5-2-1-3-6-4/h1-3H2,(H2,5,6,7)	-1.034
InChI=1S/C8H13N3O2/c1-3-4-11-6(9)5-7(12)10(2)8(11)13/h5H,3-4,9H2,1-2H3	-1.611
InChI=1S/C5H7NO2/c1-4(3-6)8-5(2)7/h4H,1-2H3	0.247
InChI=1S/C12H6Cl4/c13-9-3-1-7(2-4-9)8-5-10(14)12(16)11(15)6-8/h1-6H	-7.96
InChI=1S/C7H8ClNO3S/c1-4-2-7(13(10,11)12)6(9)3-5(4)8/h2-3H,9H2,1H3,(H,10,11,12)	-2.406
InChI=1S/C15H12N2O3/c1-20-10-6-9(16)11-12(13(10)17)15(19)8-5-3-2-4-7(8)14(11)18/h2-6H,16-17H2,1H3	-5.746
InChI=1S/C26H32O3/c1-25-14-12-19(27)16-18(25)8-9-20-21-10-11-23(26(21,2)15-13-22(2(h3-7,16,20-23H,8-15H2,1-2H3	-4.48
InChI=1S/C11H12N4O5/c1-7(16)19-5-14-4-12-10-9(11(14)18)3-15(13-10)6-20-8(2)17/h3-4H,5-6H2,1-2H3	-1.99
InChI=1S/C13H8N2O2S/c16-13(10-3-2-6-14-8-10)17-12-5-1-4-11(7-12)15-9-18/h1-8H	-4.3
InChI=1S/C25H21N7O5/c1-13(33)21(24(36)28-18-10-11-19-20(12-18)30-25(37)29-19)32-31-1 h2-12,21H,1H3,(H2,26,34)(H,27,35)(H,28,36)(H2,29,30,37)/b32-31+	-6.673
InChI=1S/C25H28O6/c1-5-23(26)30-17-15-28-21-11-7-19(8-12-21)25(3,4)20-9-13-22(14-10 h5-14H,1-2,15-18H2,3-4H3	-5.999
InChI=1S/C8H16N2O4/c1-3-6(4-13-7(9)11)5-14-8(12)10-2/h6H,3-5H2,1-2H3,(H2,9,11)(H,10,12)	-1.12
InChI=1S/C11H13NO3/c1-12(2)10(13)8-15-11(14)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3	-1.372
InChI=1S/C12H20N2S8/c15-11(13-7-3-1-4-8-13)17-19-21-22-20-18-12(16)14-9-5-2-6-10-14/h1-10H2	-7.632
InChI=1S/C19H21FN2O4/c1-10-2-3-12-16-13(18(24)14(19(25)26)9-22(10)16)8-15(20)17(12)21 h8-11,23H,2-7H2,1H3,(H,25,26)	-3.78
InChI=1S/C18H25NO3/c1-19-9-8-18-7-3-4-13(20)16(18)12(19)10-11-5-6-14(22-2)17(21)15(1 h5-6,12-13,16,20-21H,3-4,7-10H2,1-2H3	-1.851
InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h8-9H,5-7,10H2,1-4H3/b9-8+	-4.187
InChI=1S/C4H4O4/c5-3(6)1-2-4(7)8/h1-2H,(H,5,6)(H,7,8)/b2-1+	-1.22
InChI=1S/C8H20O7P2/c1-7(2)13-17(10,14-8(3)4)15-16(9,11-5)12-6/h7-8H,1-6H3	-1.575
InChI=1S/C20H34O4/c1-17(2)19(21)23-15-13-11-9-7-5-6-8-10-12-14-16-24-20(22)18(3)4/h1,3,5-16H2,2,4H3	-7.484
InChI=1S/C10H7NO2/c12-9-6-7-10(13)11(9)8-4-2-1-3-5-8/h1-7H	-2.327

"InChi"	"logS(M)"
InChI=1S/C60H114O8/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-56(62)65-53-55((h54-55,59-61H,4-53H2,1-3H3	-7.285
InChI=1S/C17H16ClNO/c1-19-9-14-12-4-2-3-5-16(12)20-17-7-6-11(18)8-13(17)15(14)10-19/ h2-8,14-15H,9-10H2,1H3	-2.13
InChI=1S/C17H31N3O4/c1-5-10(3)13(18)16(22)20-9-7-8-12(20)15(21)19-14(17(23)24)11(4)6- h10-14H,5-9,18H2,1-4H3,(H,19,21)(H,23,24)	-2.561
InChI=1S/C14H10N2O/c17-14-13(15-10-6-2-1-3-7-10)11-8-4-5-9-12(11)16-14/h1-9H,(H, 15,16,17)	-2.847
InChI=1S/C6H5NO3/c8-6(9)5-2-1-3-7(10)4-5/h1-4H,(H,8,9)	-1.298
InChI=1S/C13H17N5O5/c1-10(19)17-6-4-16(5-7-17)9-12(20)15-14-8-11-2-3-13(23-11)18(21)2 h2-3,8H,4-7,9H2,1H3,(H,15,20)/b14-8+	-2.177
InChI=1S/C16H12N2O5/c1-9(16(19)20)11-4-7-14-13(8-11)17-15(23-14)10-2-5-12(6-3-10)18(2 h2-9H,1H3,(H,19,20)	-4.166
InChI=1S/C6H4N2O5/c9-6-2-4(7(10)11)1-5(3-6)8(12)13/h1-3,9H	-1.663
InChI=1S/C10H10N2OS/c1-7-9(13)12(10(14)11-7)8-5-3-2-4-6-8/ h2-7H,1H3,(H,11,14)	-2.081
InChI=1S/C11H22O/c1-3-4-5-6-7-8-9-10-11(2)12/h3-10H2,1-2H3	-4.202
InChI=1S/C12H14O4/c1-8(13)9-4-6-10(7-5-9)16-12(2,3)11(14)15/ h4-7H,1-3H3,(H,14,15)	-2.033
InChI=1S/C12H19N3O5/c16-6-3-13-11-2-1-10(9-12(11)15(19)20)14(4-7-17)5-8-18/ h1-2,9,13,16-18H,3-8H2	-1.795
InChI=1S/C11H9NO2/c1-2-10-8-4-3-7(6-12)5-9(8)11(13)14-10/ h3-5,10H,2H2,1H3	-2.31
InChI=1S/C4H8N2O3S/c5-2(3(7)8)1-10-4(6)9/h2H,1,5H2,(H2,6,9) (H,7,8)	-0.417
InChI=1S/C18H19Cl2NO2/c1-14-4-2-3-5-17(14)18(22)23-16-8-6-15(7-9-16)21(12-10-19)13-11-2 h2-9H,10-13H2,1H3	-6.261
InChI=1S/C7H4I2O3/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,10H,(H, 11,12)	-4.202
InChI=1S/C13H24O4/c1-9(2)11-14-5-13(6-15-11)7-16-12(10(3)4)17-8-13/h9-12H, 5-8H2,1-4H3	-3.11
InChI=1S/C12H9NO3/c14-12-8-10(6-7-11(12)13(15)16)9-4-2-1-3-5-9/h1-8,14H	-3.856
InChI=1S/C21H23NO4/c1-13(2)11-19(20(23)24)22-21(25)26-12-18-16-9-5-3-7-14(16)15-8-4- h3-10,13,18-19H,11-12H2,1-2H3,(H,22,25)(H,23,24)	-3.74
InChI=1S/C10H12O3/c1-13-9(7-10(11)12)8-5-3-2-4-6-8/h2-6,9H, 7H2,1H3,(H,11,12)	-1.695
InChI=1S/C4H6NO6P/c6-5(7)4-1-9-12(8,10-2-4)11-3-4/h1-3H2	-0.81
InChI=1S/C5H11NO3/c1-2-9-3-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)	0.524
InChI=1S/C14H22O4/c1-11(2)13(15)17-9-7-5-6-8-10-18-14(16)12(3)4/h1,3,5-10H2,2,4H3	-4.044

"InChi"	"logS(M)"
InChI=1S/C9H9NO2/c1-5-7-3-2-6(10)4-8(7)9(11)12-5/h2-5H,10H2,1H3	-1.789
InChI=1S/C21H22N2O5/c1-14(21(27)28-13-19(25)23(2)12-18(22)24)16-9-6-10-17(11-16)20(2(h3-11,14H,12-13H2,1-2H3,(H2,22,24)	-2.42
InChI=1S/C4H10N2O6/c1-3(11-5(7)8)4(2)12-6(9)10/h3-4H,1-2H3,(H,7,8)(H,9,10)/q+2	-1.89
InChI=1S/C8H8O3/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3,(H,9,10)	-1.93
InChI=1S/C10H13ClN2S/c1-7-6-8(11)4-5-9(7)13(3)10(14)12-2/h4-6H,1-3H3,(H,12,14)	-3.66
InChI=1S/C15H19N5S/c1-3-20(4-2)9-10-21-15-17-13-11-7-5-6-8-12(11)16-14(13)18-19-15/h5-8H,3-4,9-10H2,1-2H3,(H,16,18)	-3.09
InChI=1S/C2H6ClO3P/c3-1-2-7(4,5)6/h1-2H2,(H2,4,5,6)	0.84
InChI=1S/C20H33NO/c1-15(12-21-13-16(2)22-17(3)14-21)11-18-7-9-19(10-8-18)20(4,5)6/h7-10,15-17H,11-14H2,1-6H3	-2.482
InChI=1S/C18H19N3O2/c1-12-7-5-6-8-17(12)20-19-16-9-10-18(13(2)11-16)21(14(3)22)15(4)2h5-11H,1-4H3/b20-19+	-3.647
InChI=1S/C3H7NO2/c1-4-2-3(5)6/h4H,2H2,1H3,(H,5,6)	0.527
InChI=1S/C11H15N3O6/c1-2-8-7-12-11(14(18)19)13(8)5-6-20-10(17)4-3-9(15)16/h7H,2-6H2,1H3,(H,15,16)	-2.335
InChI=1S/C8H14ClN3O2/c9-5-6-12(11-14)8(13)10-7-3-1-2-4-7/h7H,1-6H2,(H,10,13)	-2.682
InChI=1S/C10H16O2/c1-8(7-10(11)12)9-5-3-2-4-6-9/h7,9H,2-6H2,1H3,(H,11,12)/b8-7+	-3.266
InChI=1S/C25H24N2O7S/c1-2-33-13-5-12-27-35(31,32)16-10-8-15(9-11-16)34-20-14-19(28)21-h3-4,6-11,14,27-28H,2,5,12-13,26H2,1H3	-4.787
InChI=1S/C15H19N/c1-2-6-13(7-3-1)14-9-10-15-8-4-5-11-16(15)12-14/h1-3,6-7,12,15H,4-5,8-11H2	-3.367
InChI=1S/C8H9NO/c9-8(10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,9,10)	-0.572
InChI=1S/C36H28Cl2N8O6/c1-3-51-35(49)31-29(33(47)45(43-31)23-11-7-5-8-12-23)41-39-27-17-h5-20,29-30H,3-4H2,1-2H3/b41-39+,42-40+	-8.527
InChI=1S/C12H12N2O2/c15-11-10-6-3-7-14(10)12(16)8-4-1-2-5-9(8)13-11/h1-2,4-5,10H,3,6-7H2,(H,13,15)	-3.75
InChI=1S/C14H21NO3/c1-3-5-8-18-13-7-6-11(9-12(13)4-2)10-14(16)15-17/h6-7,9,17H,3-5,8,10H2,1-2H3,(H,15,16)	-3.608
InChI=1S/C9H8N4O5/c10-9(14)5-3-7(11-1-2-11)8(13(17)18)4-6(5)12(15)16/h3-4H,1-2H2,(H2,10,14)	-2.3
InChI=1S/C17H15NO2S/c1-2-20-16(19)11-12-7-9-13(10-8-12)17-18-14-5-3-4-6-15(14)21-17/h3-10H,2,11H2,1H3	-4.36
InChI=1S/C7H5ClO/c8-7-3-1-6(5-9)2-4-7/h1-5H	-2.177

"InChi"	"logS(M)"
InChI=1S/C13H18O7/c14-6-8(15)12-10(17)9(16)11(18)13(20-12)19-7-4-2-1-3-5-7/h1-5,8-18H,6H2	-1.554
InChI=1S/C10H14N4O2/c1-3-4-5-14-8-7(11-6-12-8)9(15)13(2)10(14)16/h6H,3-5H2,1-2H3,(H,11,12)	-1.924
InChI=1S/C19H31NO3/c1-3-5-6-7-8-9-10-11-14-23-16-12-13-17(19(21)15-16)18(4-2)20-22/h12-13,15,21-22H,3-11,14H2,1-2H3/b20-18+	-4.06
InChI=1S/C21H29NO/c1-15(2)8-11-22-12-10-21-9-4-3-5-18(21)20(22)13-16-6-7-17(23)14-1h6-8,14,18,20,23H,3-5,9-13H2,1-2H3	-4.335
InChI=1S/C7H16O4/c1-9-4-5-11-7-6-10-3-2-8/h8H,2-7H2,1H3	0.785
InChI=1S/C6H4N2O/c1-2-4-6-5(3-1)7-9-8-6/h1-4H	-1.522
InChI=1S/C21H36N6O6/c28-16(29)10-4-1-7-13-22-19-25-20(23-14-8-2-5-11-17(30)31)27-21(2h1-15H2,(H,28,29)(H,30,31)(H,32,33)(H3,22,23,24,25,26,27)	-2.542
InChI=1S/C18H30N2O2/c1-3-5-12-20(13-6-4-2)14-7-15-22-18(21)16-8-10-17(19)11-9-16/h8-11H,3-7,12-15,19H2,1-2H3	-3.695
InChI=1S/C13H8O/c14-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)13/h1-8H	-3.852
InChI=1S/C12H16O2/c1-9(2)7-10-3-5-11(6-4-10)8-12(13)14/h3-6,9H,7-8H2,1-2H3,(H,13,14)	-3.07
InChI=1S/C12H19ClNO3P/c1-12(2,3)9-6-7-11(10(13)8-9)17-18(15,14-4)16-5/h6-8H,1-5H3,(H,14,15)	-3.164
InChI=1S/C10H8O4/c1-13-9-4-6-2-3-10(12)14-8(6)5-7(9)11/h2-5,11H,1H3	-2.38
InChI=1S/C13H16O6/c1-5-17-12(15)9-7(3)19-8(4)10(11(9)14)13(16)18-6-2/h5-6H2,1-4H3	-1.526
InChI=1S/C15H24N2O3/c1-4-5-8-16-12-6-7-13(14(18)11-12)15(19)20-10-9-17(2)3/h6-7,11,16,18H,4-5,8-10H2,1-3H3	-3.183
InChI=1S/C27H34ClN3O4S/c1-26(2,3)30-24(34)22-27(4,5)36-16-31(22)25(35)21(32)20(15-17-9-7h6-14,20-22,32H,15-16H2,1-5H3,(H,29,33)(H,30,34)	-4.28
InChI=1S/C8H7ClO3/c9-6-2-1-3-7(4-6)12-5-8(10)11/h1-4H,5H2,(H,10,11)	-2.195
InChI=1S/C7H7N/c1-2-7-3-5-8-6-4-7/h2-6H,1H2	-0.558
InChI=1S/C7H3N3O8/c11-7(12)6-4(9(15)16)1-3(8(13)14)2-5(6)10(17)18/h1-2H,(H,11,12)	-1.098
InChI=1S/C20H23NO3/c1-14-9-8-10-15(2)19(14)21(16(3)20(23)24-4)18(22)13-17-11-6-5-7-1h5-12,16H,13H2,1-4H3	-3.944
InChI=1S/C8H19O4P/c1-3-5-7-11-13(9,10)12-8-6-4-2/h3-8H2,1-2H3,(H,9,10)	-1.087
InChI=1S/C9H12ClN3O4S2/c1-2-9-12-6-3-5(10)7(18(11,14)15)4-8(6)19(16,17)13-9/h3-4,9,12-13H,2H2,1H3,(H2,11,14,15)	-2.883
InChI=1S/C8H10O/c1-9-7-8-5-3-2-4-6-8/h2-6H,7H2,1H3	-1.61

"InChi"	"logS(M)"
InChI=1S/C18H18N6O5S2/c19-12(8-1-3-10(25)4-2-8)15(26)21-13-16(27)24-14(18(28)29)9(7-31-h1-5,12-13,17,25H,6-7,19H2,(H,21,26)(H,28,29)(H,20,22,23)	-2.266
InChI=1S/C7H5NO4/c9-6(10)4-1-2-8-3-5(4)7(11)12/h1-3H,(H,9,10)(H,11,12)	-1.854
InChI=1S/C12H4Cl6/c13-6-1-5(2-7(14)3-6)10-11(17)8(15)4-9(16)12(10)18/h1-4H	-8.27
InChI=1S/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5,7-8,12H,6,9H2,1-4H3/b7-5+	-3.138
InChI=1S/C10H19NO3/c1-2-3-4-5-6-7-9(12)11-8-10(13)14/h2-8H2,1H3,(H,11,12)(H,13,14)	-2.112
InChI=1S/C9H6ClN/c10-9-5-3-8(4-6-9)2-1-7-11/h1-6H/b2-1+	-2.781
InChI=1S/C9H17NO/c11-9-7-5-3-1-2-4-6-8-10-9/h1-8H2,(H,10,11)	-1.074
InChI=1S/C16H20N4O2/c1-5-6-11-14(21)19-13-9-10(2)7-8-12(13)17-16(18(3)4)20(19)15(11)2h7-9,11H,5-6H2,1-4H3	-3.538
InChI=1S/C11H13NO3/c1-8(13)7-11(14)12-9-5-3-4-6-10(9)15-2/h3-6H,7H2,1-2H3,(H,12,14)	-1.806
InChI=1S/C9H18O2/c1-4-5-9(10)11-7-6-8(2)3/h8H,4-7H2,1-3H3	-2.933
InChI=1S/C21H21O3P/c1-16-10-4-7-13-19(16)22-25(23-20-14-8-5-11-17(20)2)24-21-15-9-6-h4-15H,1-3H3	-7.78
InChI=1S/C12H6Cl4O/c13-7-1-3-8(4-2-7)17-9-5-10(14)12(16)11(15)6-9/h1-6H	-7.35
InChI=1S/C22H30O3/c1-20-10-6-16(24)14-15(20)4-5-17-18(20)7-11-21(2)19(17)8-12-22(21h14,17-19,23,25H,4-8,10-13H2,1-2H3	-3.526
InChI=1S/C6H15NO3S2/c1-2-3-4-7-5-6-11-12(8,9)10/h7H,2-6H2,1H3,(H,8,9,10)	0.27
InChI=1S/C12H11N3O/c13-10-6-4-9(5-7-10)12(16)15-11-3-1-2-8-14-11/h1-8H,13H2,(H,14,15,16)	-1.743
InChI=1S/C10H16N2O/c1-8(12-11)7-9-3-5-10(13-2)6-4-9/h3-6,8,12H,7,11H2,1-2H3	-1.774
InChI=1S/C8H10N4O4/c1-2-11(8(9)13)10-5-6-3-4-7(16-6)12(14)15/h3-5H,2H2,1H3,(H2,9,13)/b10-5+	-2.939
InChI=1S/C15H13N/c16-12-15(14-9-5-2-6-10-14)11-13-7-3-1-4-8-13/h1-10,15H,11H2	-4.126
InChI=1S/C6H8N2O3/c1-6(2)3(9)7-5(11)8-4(6)10/h1-2H3,(H2,7,8,9,10,11)	-1.74
InChI=1S/C7H4Cl2F3N/c8-4-1-3(7(10,11)12)2-5(9)6(4)13/h1-2H,13H2	-3.592
InChI=1S/C10H16O5/c1-4-13-7-8(9(11)14-5-2)10(12)15-6-3/h7H,4-6H2,1-3H3	-1.593
InChI=1S/C6H14O/c1-5-7-6(2,3)4/h5H2,1-4H3	-0.93
InChI=1S/C13H11NO2/c15-12-7-3-1-5-10(12)9-14-11-6-2-4-8-13(11)16/h1-9,14,16H/b10-9+	-2.091
InChI=1S/C14H17N3O/c1-3-8-16-9-17-13(10(16)2)15-12-7-5-4-6-11(12)14(17)18/h4-7,10H,3,8-9H2,1-2H3	-2.67

"InChi"	"logS(M)"
InChI=1S/C10H9NO3/c1-6(12)14-8-2-3-9-7(4-8)5-10(13)11-9/h2-4H,5H2,1H3,(H,11,13)	-1.54
InChI=1S/C6H12O2/c1-2-5-3-4-6(7)8-5/h5-7H,2-4H2,1H3	-0.065
InChI=1S/C12H2Cl6O/c13-4-1-3-7-6(2-5(14)8(15)10(7)17)19-12(3)11(18)9(4)16/h1-2H	-10.3
InChI=1S/C12H8BrNS/c13-8-5-6-10-12(7-8)15-11-4-2-1-3-9(11)14-10/h1-7,14H	-6.112
InChI=1S/C8H11N5O2S/c1-11-3-4-12(2)8(11)10-7-9-5-6(16-7)13(14)15/h5H,3-4H2,1-2H3	-1.154
InChI=1S/C21H34O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)8-9-20(13,2)19(15)18(24)11-h13-19,23-24H,4-11H2,1-3H3	-4.067
InChI=1S/C6H5ClO2/c7-5-2-1-4(8)3-6(5)9/h1-3,8-9H	-1.071
InChI=1S/C22H16N4O/c27-18-12-10-17(11-13-18)24-26-22-15-14-21(19-8-4-5-9-20(19)22)25h1-15,26H/b25-23+	-6.009
InChI=1S/C10H12BrNO3/c1-12-10(14)8-6-7(11)2-3-9(8)15-5-4-13/h2-3,6,13H,4-5H2,1H3,(H,12,14)	-2.226
InChI=1S/C19H25NO5S/c1-20(14-15-8-6-5-7-9-15)10-11-26(21,22)16-12-17(23-2)19(25-4)18(h5-9,12-13H,10-11,14H2,1-4H3	-2.82
InChI=1S/C17H34N4O10/c18-2-6-10(24)12(26)8(21)16(28-6)30-14-5(20)1-4(19)9(23)15(14)31-h4-17,22-27H,1-3,18-21H2	0.342
InChI=1S/C8H14O2/c1-6(2)4-8(10)5-7(3)9/h6H,4-5H2,1-3H3	-1.6
InChI=1S/C14H14O/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10H,11-12H2	-3.695
InChI=1S/C9H14O2/c10-9-6-5-7-3-1-2-4-8(7)11-9/h7-8H,1-6H2	-0.587
InChI=1S/C24H16N2/c25-17-23-14-11-21(12-15-23)9-6-19-4-7-20(8-5-19)10-13-22-2-1-3-2h1-16H/b9-6+,13-10+	-8.124
InChI=1S/C17H34O6/c1-9-10-13-19-14(18)11-12-17(8,22-20-15(2,3)4)23-21-16(5,6)7/h9-13H2,1-8H3	-5.19
InChI=1S/C13H12N2O/c14-12-9-5-4-8-11(12)13(16)15-10-6-2-1-3-7-10/h1-9H,14H2,(H,15,16)	-3.057
InChI=1S/C17H14N2O2/c1-17(2,13-3-7-15(8-4-13)20-11-18)14-5-9-16(10-6-14)21-12-19/h3-10H,1-2H3	-5.47
InChI=1S/C16H21NO3/c1-2-14-10-6-7-11-17(14)15(18)12-20-16(19)13-8-4-3-5-9-13/h3-5,8-9,14H,2,6-7,10-12H2,1H3	-2.72
InChI=1S/C9H9NO/c1-11-8-2-3-9-7(6-8)4-5-10-9/h2-6,10H,1H3	-2.035
InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2	0.56
InChI=1S/C12H17NO2/c1-2-3-6-9-15-11-8-5-4-7-10(11)12(13)14/h4-5,7-8H,2-3,6,9H2,1H3,(H2,13,14)	-2.633
InChI=1S/C14H12N2O3/c1-10-4-2-3-5-13(10)15-14(17)11-6-8-12(9-7-11)16(18)19/h2-9H,1H3,(H,15,17)	-3.596
InChI=1S/C4H10O3/c1-7-3-4(6)2-5/h4-6H,2-3H2,1H3	0.974

"InChi"	"logS(M)"
InChI=1S/C12H9NO6/c1-2-18-12(15)11-6-9(14)8-5-7(13(16)17)3-4-10(8)19-11/h3-6H,2H2,1H3	-2.919
InChI=1S/C10H15NO3/c1-11(2)6-10(14)7-3-4-8(12)9(13)5-7/h3-5,10,12-14H,6H2,1-2H3	0.705
InChI=1S/C5H10O3/c1-7-4-3-5(6)8-2/h3-4H2,1-2H3	0.803
InChI=1S/C15H20N2O/c1-18-13-4-5-15-14(10-13)12(11-16-15)6-9-17-7-2-3-8-17/h4-5,10-11,16H,2-3,6-9H2,1H3	-2.384
InChI=1S/C6H12N2O2S3/c7-5(9)1-3-11-13-12-4-2-6(8)10/h1-4H2,(H2,7,9)(H2,8,10)	-1.294
InChI=1S/C24H34O4/c1-14-12-18-19(22(4)9-6-17(27)13-21(14)22)7-10-23(5)20(18)8-11-24h13-14,18-20H,6-12H2,1-5H3	-5.508
InChI=1S/C16H21NO8S/c1-10(2)24-15(18)9-14(16(19)25-11(3)4)26(22,23)13-7-5-12(6-8-13)1h5-8,10-11,14H,9H2,1-4H3	-4.29
InChI=1S/C7H7BrN2O/c8-5-1-3-6(4-2-5)10-7(9)11/h1-4H,(H3,9,10,11)	-1.634
InChI=1S/C10H14O2/c1-9-5-2-3-6-10(9)12-8-4-7-11/h2-3,5-6,11H,4,7-8H2,1H3	-1.731
InChI=1S/C17H17F2N3O3/c1-20-8-5-21(6-8)15-12(18)4-10-14(13(15)19)22(9-2-3-9)7-11(16(10)h4,7-9,20H,2-3,5-6H2,1H3,(H,24,25)	-5.31
InChI=1S/C2H3ClF2/c3-1-2(4)5/h2H,1H2	-0.923
InChI=1S/C12H4Cl4O2/c13-5-1-2-7-8(3-5)17-9-4-6(14)10(15)11(16)12(9)18-7/h1-4H	-8.874
InChI=1S/C20H26O2/c1-11(2)18(16-9-12(3)7-14(5)19(16)21)17-10-13(4)8-15(6)20(17)22/h7-11,18,21-22H,1-6H3	-6.167
InChI=1S/C10H15N5/c11-9(12)15-10(13)14-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H6,11,12,13,14,15)	0.011
InChI=1S/C10H14O2/c1-3-10(12-9(2)11)7-5-4-6-8-10/h1H,4-8H2,2H3	-2.352
InChI=1S/C6H9N3O2/c1-3-5-4-7-6(8(5)2)9(10)11/h4H,3H2,1-2H3	-1.971
InChI=1S/C8H17Cl2N/c1-2-3-6-11(7-4-9)8-5-10/h2-8H2,1H3	-2.204
InChI=1S/C18H24I3N3O7/c1-8(27)22-16-14(20)11(17(30)23(2)4-9(28)6-25)13(19)12(15(16)21)1h9-10,25-26,28-29H,4-7H2,1-3H3,(H,22,27)	-3.842
InChI=1S/C17H19ClN2O2S/c1-19(2)6-3-7-20-13-5-4-11(21)8-16(13)23-17-10-15(22)12(18)9-14(1h4-5,8-10,21-22H,3,6-7H2,1-2H3	-5.895
InChI=1S/C5H12S/c1-2-3-4-5-6/h6H,2-5H2,1H3	-2.825
InChI=1S/C11H13ClO3/c1-2-3-6-15-11(14)8-4-5-10(13)9(12)7-8/h4-5,7,13H,2-3,6H2,1H3	-3.51
InChI=1S/C6HBr5O3S/c7-1-2(8)4(10)6(15(12,13)14)5(11)3(1)9/h(H,12,13,14)	-2.006
InChI=1S/C13H12O3/c1-16-12-5-4-10-6-9(7-13(14)15)2-3-11(10)8-12/h2-6,8H,7H2,1H3,(H,14,15)	-2.791

"InChi"	"logS(M)"
InChI=1S/C13H14N2O5/ c1-14-12(19)10(15(13(14)20)7-11(17)18)6-8-2-4-9(16)5-3-8/ h2-5,10,16H,6-7H2,1H3,(H,17,18)	-0.05
InChI=1S/C10H14N4O2/ c1-4-5-6-11-7-8(12-6)13(2)10(16)14(3)9(7)15/h4-5H2,1-3H3,(H, 11,12)	-1.794
InChI=1S/C10H11N5O/ c1-8-7-15(10(16)14-13-8)12-6-9-3-2-4-11-5-9/h2-6H,7H2,1H3,(H, 14,16)/b12-6+	-2.874
InChI=1S/C6H14S/c1-5(2)7-6(3)4/h5-6H,1-4H3	-2.24
InChI=1S/C11H6ClN3O3/ c12-7-2-1-3-8(6-7)15-9(16)13-10-14(11(15)17)4-5-18-10/h1-6H	-2.404
InChI=1S/C27H24N6O6S/ c1-14-10-21(22(39-3)13-23(14)40(37,38)28-2)32-33-24-17-7-5-4-6-15 h4-13,28,32H,1-3H3,(H,29,35)(H2,30,31,36)/b33-24-	-8.217
InChI=1S/C9H15N3O3/c1-4-13-7-10-8(14-5-2)12-9(11-7)15-6-3/ h4-6H2,1-3H3	-1.484
InChI=1S/C11H11NO4/c1-2-16-11(13)8-5-9-3-6-10(7-4-9)12(14)15/ h3-8H,2H2,1H3/b8-5+	-3.481
InChI=1S/C4H12NO3PS/c1-4(2,5)3-10-9(6,7)8/h3,5H2,1-2H3, (H2,6,7,8)	0.609
InChI=1S/C6H12O2/c1-8-6-4-2-3-5-7/h5H,2-4,6H2,1H3	0.457
InChI=1S/C24H31FO6/ c1-13-9-18-17-6-5-15-10-16(28)7-8-21(15,3)23(17,25)19(29)11-22(18 h7-8,10,13,17-19,26,29H,5-6,9,11-12H2,1-4H3	-4.9
InChI=1S/C7H8N4S/c1-2-11-4-10-5-6(11)8-3-9-7(5)12/h3-4H, 2H2,1H3,(H,8,9,12)	-1.295
InChI=1S/C26H38O2/ c1-10-11-18(19-14-21(25(4,5)6)23(27)12-16(19)2)20-15-22(26(7,8)9) h12-15,18,27-28H,10-11H2,1-9H3	-7.981
InChI=1S/C11H14N4O2/ c1-7-5-9(16-3)13-11(12-7)15-10(17-4)6-8(2)14-15/h5-6H,1-4H3	-1.986
InChI=1S/C2H7N3S/c1-4-2(6)5-3/h3H2,1H3,(H2,4,5,6)	-0.466
InChI=1S/C7H15NO/c1-4-5-7(2,3)6(8)9/h4-5H2,1-3H3,(H2,8,9)	-1.154
InChI=1S/C19H21ClO6/ c1-5-24-13-9-12(23-4)15-17(16(13)20)26-19(18(15)22)10(3)7-11(21)8 h8-10H,5-7H2,1-4H3	-4.7
InChI=1S/C10H6N2O4/ c13-10(14)7-3-4-8(12(15)16)6-2-1-5-11-9(6)7/h1-5H,(H,13,14)	-3.166
InChI=1S/C15H30O/c1-3-5-7-9-11-13-15(16)14-12-10-8-6-4-2/ h3-14H2,1-2H3	-5.684
InChI=1S/C13H24O2/c1-10(2)11-12(3,4)9-14-13(15-11)7-5-6-8-13/ h10-11H,5-9H2,1-4H3	-3.524
InChI=1S/C7H6INO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H, 10,11)	-2.878
InChI=1S/C12H16N2O3/ c1-3-17-12(16)9-7-13-10-6-4-5-8(2)14(10)11(9)15/h7-8H, 3-6H2,1-2H3	-1.454
InChI=1S/C27H31N3O/ c1-3-30(26-12-9-25(21(2)17-26)18-22(19-28)20-29)15-16-31-27-13-1 h9-14,17-18,23H,3-8,15-16H2,1-2H3	-8.386

"InChi"	"logS(M)"
InChI=1S/C8H7NS2/c1-10-8-9-6-4-2-3-5-7(6)11-8/h2-5H,1H3	-3.161
InChI=1S/C11H14BrNO2/c1-6(2)13-11(15)9-5-8(12)4-7(3)10(9)14/h4-6,14H,1-3H3,(H,13,15)	-4.183
InChI=1S/C21H21BrN6O6/c1-5-7-26(8-6-2)18-11-16(23-13(3)29)17(12-20(18)34-4)24-25-21-15(h5-6,9-12H,1-2,7-8H2,3-4H3,(H,23,29)/b25-24+	-7.009
InChI=1S/C11H13ClN2O3/c12-10-2-1-8-6-14(3-4-16-11(13)15)17-7-9(8)5-10/h1-2,5H,3-4,6-7H2,(H2,13,15)	-2.54
InChI=1S/C8H22N2O5P2/c1-7-13-16(11,9(3)4)15-17(12,10(5)6)14-8-2/h7-8H2,1-6H3	-1.064
InChI=1S/C8H10O2/c1-10-8-4-2-7(6-9)3-5-8/h2-5,9H,6H2,1H3	-0.745
InChI=1S/C6H6N4O/c1-11-6-4-5(8-2-7-4)9-3-10-6/h2-3H,1H3,(H,7,8,9,10)	-1.53
InChI=1S/C18H24I3N3O8/c1-24(4-9(28)6-26)18(31)12-13(19)11(17(30)22-3-8(27)5-25)14(20)16h8-9,25-28H,3-7H2,1-2H3,(H,22,30)(H,23,29)	-4.523
InChI=1S/C7H8N4O3/c12-3-10-2-8-6-5(7(10)14)1-9-11(6)4-13/h1-2,12-13H,3-4H2	-1.72
InChI=1S/C17H24N4O4S/c1-3-5-7-13(22)24-11-21-10-20-15-16(21)18-9-19-17(15)26-12-25-14h9-10H,3-8,11-12H2,1-2H3	-4.33
InChI=1S/C10H14/c1-3-9-6-5-7-10(4-2)8-9/h5-8H,3-4H2,1-2H3	-3.748
InChI=1S/C9H14O2/c10-8-4-7-9(11-8)5-2-1-3-6-9/h1-7H2	-1.971
InChI=1S/C12H3Cl7/c13-4-1-6(14)9(7(15)2-4)5-3-8(16)11(18)12(19)10(5)17/h1-3H	-8.68
InChI=1S/C12H5Cl5/c13-7-1-2-8(9(14)5-7)6-3-10(15)12(17)11(16)4-6/h1-5H	-8.55
InChI=1S/C8H17NO/c1-4-6(3)7(5-2)8(9)10/h6-7H,4-5H2,1-3H3,(H2,9,10)	-2.145
InChI=1S/C22H25NO2/c1-25-21-11-9-20(10-12-21)22(24)8-5-15-23-16-13-19(14-17-23)18-6h2-4,6-7,9-13H,5,8,14-17H2,1H3	-4.782
InChI=1S/C18H19F2N3O3/c1-8-18(2,21)7-23(8)15-12(19)5-10-14(13(15)20)22(9-3-4-9)6-11(16(h5-6,8-9H,3-4,7,21H2,1-2H3,(H,25,26)	-5.04
InChI=1S/C20H14O3/c21-19(17-8-4-5-9-18(17)20(22)23)16-12-10-15(11-13-16)14-6-2-1-3-h1-13H,(H,22,23)	-4.828
InChI=1S/C6H4Br2O/c7-4-1-2-6(9)5(8)3-4/h1-3,9H	-2.123
InChI=1S/C11H22N2O/c1-3-5-7-12-9-10-13(11(12)14)8-6-4-2/h3-10H2,1-2H3	-2.896
InChI=1S/C17H17N3O3/c1-9(2)17(3)16(23)19-14(20-17)13-11(15(21)22)8-10-6-4-5-7-12(10)1h4-9H,1-3H3,(H,21,22)(H,19,20,23)	-3.72
InChI=1S/C6H6BrNO2S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H2,8,9,10)	-2.084
InChI=1S/C14H12O3/c15-13(7-8-14(16)17)12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9H,7-8H2,(H,16,17)	-3.853
InChI=1S/C6H12O/c1-5-3-4-6(2)7-5/h5-6H,3-4H2,1-2H3	0.072

"InChi"	"logS(M)"
InChI=1S/C18H26O/c1-11-9-19-10-13-7-15-16(8-14(11)13)18(5,6)12(2)17(15,3)4/h7-8,11-12H,9-10H2,1-6H3	-5.169
InChI=1S/C11H14N4O2/c1-7(2)5-15-10(16)8-9(12-6-13(8)3)14(4)11(15)17/h6H,1,5H2,2-4H3	-2.166
InChI=1S/C3H4Cl2/c4-2-1-3-5/h1-2H,3H2/b2-1+	-1.707
InChI=1S/C33H35N5O5/c1-32(35-29(39)21-15-23-22-10-6-11-24-28(22)20(17-34-24)16-25(23h3-6,8-11,15,17,21,25-27,34,42H,7,12-14,16,18H2,1-2H3,(H,35,39)	-5.301
InChI=1S/C11H17NO3/c1-7(12)11(13)9-6-8(14-2)4-5-10(9)15-3/h4-7,11,13H,12H2,1-3H3	-0.058
InChI=1S/C9H4Cl6O4/c10-3-4(11)8(13)2(6(18)19)1(5(16)17)7(3,12)9(8,14)15/h1-2H,(H,16,17)(H,18,19)	-2.046
InChI=1S/C8H9NOS/c10-6-9-8(11)7-4-2-1-3-5-7/h1-5,10H,6H2,(H,9,11)	-1.14
InChI=1S/C17H20N2O5/c1-4-6-14(20)23-10-24-17(22)13-9-19(5-2)16-12(15(13)21)8-7-11(3)1h7-9H,4-6,10H2,1-3H3	-2.95
InChI=1S/C12H27NO3S2/c1-3-4-5-6-7-8-9-12(2)13-10-11-17-18(14,15)16/h12-13H,3-11H2,1-2H3,(H,14,15,16)	-2.796
InChI=1S/C14H11N3O3S/c1-20-14(19)17-13-15-9-5-4-8(7-10(9)16-13)12(18)11-3-2-6-21-11/h2-7H,1H3,(H2,15,16,17,19)	-3.556
InChI=1S/C8H17NO/c1-3-5-7(6-4-2)8(9)10/h7H,3-6H2,1-2H3,(H2,9,10)	-2.319
InChI=1S/C19H17NO2/c1-14(19(21)20-17-9-3-2-4-10-17)22-18-12-11-15-7-5-6-8-16(15)13-1h2-14H,1H3,(H,20,21)	-5.589
InChI=1S/C12H25NO3/c1-4-6-8-13-11(15)16-10-12(3,9-14)7-5-2/h14H,4-10H2,1-3H3,(H,13,15)	-3.278
InChI=1S/C19H22FN3O/c20-17-8-6-16(7-9-17)18(24)4-3-11-22-12-14-23(15-13-22)19-5-1-2-1h1-2,5-10H,3-4,11-15H2	-3.398
InChI=1S/C10H12N2O2/c1-14-9-5-4-8(6-11-9)12-10(13)7-2-3-7/h4-7H,2-3H2,1H3,(H,12,13)	-2.14
InChI=1S/C21H15NO3/c1-12-6-8-13(9-7-12)22-16-10-11-17(23)19-18(16)20(24)14-4-2-3-5-1h2-11,22-23H,1H3	-7.549
InChI=1S/C15H11NO2S/c17-14(18)9-10-6-7-12-13(8-10)19-15(16-12)11-4-2-1-3-5-11/h1-8H,9H2,(H,17,18)	-3.646
InChI=1S/C9H20O3/c1-4-5-11-7-9(3)12-6-8(2)10/h8-10H,4-7H2,1-3H3	-0.07
InChI=1S/C8H6Br2/c1-2-6-5-7(9)3-4-8(6)10/h2-5H,1H2	-4.579
InChI=1S/C14H12Cl2/c15-9-11-1-5-13(6-2-11)14-7-3-12(10-16)4-8-14/h1-8H,9-10H2	-10.099
InChI=1S/C10H11NO4/c1-2-9(10(12)13)7-3-5-8(6-4-7)11(14)15/h3-6,9H,2H2,1H3,(H,12,13)	-2.562
InChI=1S/C15H16O/c1-15(2,12-6-4-3-5-7-12)13-8-10-14(16)11-9-13/h3-11,16H,1-2H3	-4.096

"InChi"	"logS(M)"
InChI=1S/C12H16F3NO/c1-9(16-5-6-17)7-10-3-2-4-11(8-10)12(13,14)15/h2-4,8-9,16-17H,5-7H2,1H3	-1.884
InChI=1S/C22H27NO/c1-16-21-14-18-8-9-19(24)15-20(18)22(16,2)11-13-23(21)12-10-17-6-h3-9,15-16,21,24H,10-14H2,1-2H3	-4.942
InChI=1S/C7H17NO3S2/c1-2-3-4-5-8-6-7-12-13(9,10)11/h8H,2-7H2,1H3,(H,9,10,11)	-0.249
InChI=1S/C9H7NO6/c1-16-9(13)6-3-2-5(8(11)12)4-7(6)10(14)15/h2-4H,1H3,(H,11,12)	-2.657
InChI=1S/C22H17NOS/c1-23(20-12-10-16-6-2-4-8-18(16)14-20)22(25)24-21-13-11-17-7-3-5-h2-15H,1H3	-8.313
InChI=1S/C8H16O3/c1-6(2)5-11-7(9)8(3,4)10/h6,10H,5H2,1-4H3	-0.728
InChI=1S/C7H7ClN2O/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3H,9H2,(H2,10,11)	-1.977
InChI=1S/C13H19NO3/c1-16-11-6-8-4-3-5-9(14)7-10(8)12(15)13(11)17-2/h6,9,15H,3-5,7,14H2,1-2H3	-1.927
InChI=1S/C28H34O15/c1-10-21(32)23(34)25(36)27(40-10)39-9-19-22(33)24(35)26(37)28(43h3-7,10,17,19,21-30,32-37H,8-9H2,1-2H3	-5.01
InChI=1S/C12H16BrNO2/c1-3-4-5-14-12(16)10-7-9(13)6-8(2)11(10)15/h6-7,15H,3-5H2,1-2H3,(H,14,16)	-4.303
InChI=1S/C5H10O2S2/c1-4(6)7-2-5(9)3-8/h5,8-9H,2-3H2,1H3	-1.221
InChI=1S/C12H19NO3/c1-12(2,3)13-7-11(16)8-4-9(14)6-10(15)5-8/h4-6,11,13-16H,7H2,1-3H3	-0.025
InChI=1S/C12H17N3O2/c1-3-4-9-15(2)14-13-11-7-5-10(6-8-11)12(16)17/h5-8H,3-4,9H2,1-2H3,(H,16,17)/b14-13+	-1.81
InChI=1S/C10H12N4O2/c1-4-5-14-9(15)7-8(11-6-12(7)2)13(3)10(14)16/h4,6H,1,5H2,2-3H3	-1.596
InChI=1S/C8H15N7O2S3/c9-6(15-20(12,16)17)1-2-18-3-5-4-19-8(13-5)14-7(10)11/h4H,1-3H2,(H2,9,15)(H2,12,16,17)(H4,10,11,13,14)	-2.65
InChI=1S/C10H2O6/c11-7-3-1-4-6(10(14)16-8(4)12)2-5(3)9(13)15-7/h1-2H	-1.406
InChI=1S/C12H11Cl2NO4/c1-12(6-18-2)10(16)15(11(17)19-12)9-4-7(13)3-8(14)5-9/h3-5H,6H2,1-2H3	-4.66
InChI=1S/C10H20N2O/c1-3-12(4-2)10(13)9-6-5-7-11-8-9/h9,11H,3-8H2,1-2H3	-1.212
InChI=1S/C5H10N6O2/c1-3(9-11-5(7)13)2-8-10-4(6)12/h2H,1H3,(H3,6,10,12)(H3,7,11,13)/b8-2+,9-3-	-1.95
InChI=1S/C12H17N3O2/c1-2-3-4-5-11(16)14-15-12(17)10-6-8-13-9-7-10/h6-9H,2-5H2,1H3,(H,14,16)(H,15,17)	-1.24
InChI=1S/C12H24N2O4/c1-9(15)11(17)13-7-5-3-4-6-8-14-12(18)10(2)16/h9-10,15-16H,3-8H2,1-2H3,(H,13,17)(H,14,18)	-0.7

"InChi"	"logS(M)"
InChI=1S/C12H14O4S/c1-16-11(13)12(8-5-9-12)17(14,15)10-6-3-2-4-7-10/h2-4,6-7H,5,8-9H2,1H3	-3.001
InChI=1S/C8H13N2O5P/c1-5-8(11)7(2-9)6(3-10-5)4-15-16(12,13)14/h3,11H,2,4,9H2,1H3,(H2,12,13,14)	0.605
InChI=1S/C10H18O4/c1-3-13-9(11)7-5-6-8-10(12)14-4-2/h3-8H2,1-2H3	-1.679
InChI=1S/C13H17NO3/c1-3-4-9-17-13(16)11-5-7-12(8-6-11)14-10(2)15/h5-8H,3-4,9H2,1-2H3,(H,14,15)	-3.46
InChI=1S/C17H20O2/c1-12(2)11-17(13-3-7-15(18)8-4-13)14-5-9-16(19)10-6-14/h3-10,12,17-19H,11H2,1-2H3	-3.367
InChI=1S/C11H14N2O4/c12-6-10(15)13-9(11(16)17)5-7-1-3-8(14)4-2-7/h1-4,9,14H,5-6,12H2,(H,13,15)(H,16,17)	-0.73
InChI=1S/C8H12Cl4O2/c1-3-7(9,4-2)6(13)14-5-8(10,11)12/h3-5H2,1-2H3	-4.32
InChI=1S/C22H32O3/c1-3-4-21(24)25-20-10-9-19-18-7-5-14-13-15(23)6-8-16(14)17(18)11-h13,16-20H,3-12H2,1-2H3	-5.91
InChI=1S/C9H16O2/c1-2-3-4-5-8-6-7-9(10)11-8/h8H,2-7H2,1H3	-1.855
InChI=1S/C9H14N2/c1-5-4-6(2)9(11)7(3)8(5)10/h4H,10-11H2,1-3H3	-0.821
InChI=1S/C10H10O/c1-3-10(2,11)9-7-5-4-6-8-9/h1,4-8,11H,2H3	-1.193
InChI=1S/C8H9NO4/c10-4-3-6-1-2-8(11)7(5-6)9(12)13/h1-2,5,10-11H,3-4H2	-1.156
InChI=1S/C13H13NO2/c14-12(8-13(15)16)11-7-3-5-9-4-1-2-6-10(9)11/h1-7,12H,8,14H2,(H,15,16)	-1.59
InChI=1S/C49H76O20/c1-21-43(67-38-17-32(53)44(22(2)62-38)68-39-18-33(64-24(4)51)45(h13,21-23,26-35,37-46,50,52-54,56-59H,7-12,14-20H2,1-6H3	-6.436
InChI=1S/C19H16Cl2N2O4S/c1-11-4-7-14(8-5-11)28(25,26)27-19-17(12(2)22-23(19)3)18(24)15-9-h4-10H,1-3H3	-6.895
InChI=1S/C21H27NO/c23-21(19-11-4-1-5-12-19,20-13-6-2-7-14-20)15-10-18-22-16-8-3-9-1h1-2,4-7,11-14,23H,3,8-10,15-18H2	-4.696
InChI=1S/C6HCl4NO2/c7-2-1-3(8)5(10)6(4(2)9)11(12)13/h1H	-5.096
InChI=1S/C12H12N2O3/c1-13-10(15)9(8-6-4-3-5-7-8)11(16)14(2)12(13)17/h3-7,9H,1-2H3	-1.585
InChI=1S/C13H24N2O5/c1-3-4-13(2,9-19-11(14)16)10-20-12(17)15-5-7-18-8-6-15/h3-10H2,1-2H3,(H2,14,16)	-2.56
InChI=1S/C13H11N3/c14-10-1-3-12-8(6-10)5-9-7-11(15)2-4-13(9)16-12/h1-7H,14-15H2	-3.106
InChI=1S/C8H8ClNO3S/c1-6(11)10-7-2-4-8(5-3-7)14(9,12)13/h2-5H,1H3,(H,10,11)	-2.877
InChI=1S/C6H12N2/c1-2-8-5-3-7(1)4-6-8/h1-6H2	0.603
InChI=1S/C13H14/c1-10(2)12-9-5-7-11-6-3-4-8-13(11)12/h3-10H,1-2H3	-4.782

"InChi"	"logS(M)"
InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h4,9-11H,1,5-6H2,2-3H3	-1.72
InChI=1S/C11H12N4O4S/c1-7(16)18-5-15-4-14-9-10(15)12-3-13-11(9)20-6-19-8(2)17/h3-4H,5-6H2,1-2H3	-2.54
InChI=1S/C2H4ClF/c3-1-2-4/h1-2H2	-0.529
InChI=1S/C14H14O/c1-11-7-3-5-9-13(11)15-14-10-6-4-8-12(14)2/h3-10H,1-2H3	-4.844
InChI=1S/C5H11NO2/c1-3-6-4(2)5(7)8/h4,6H,3H2,1-2H3,(H,7,8)	0.652
InChI=1S/C22H13N3O3/c26-13-23-19-7-1-16(2-8-19)22(17-3-9-20(10-4-17)24-14-27)18-5-11-h1-12,22H	-6.565
InChI=1S/C19H24O3/c1-4-5-6-11-22-19(20)14(2)15-7-8-17-13-18(21-3)10-9-16(17)12-15/h7-10,12-14H,4-6,11H2,1-3H3	-6.97
InChI=1S/C18H36O3/c1-2-3-4-11-14-17(19)15-12-9-7-5-6-8-10-13-16-18(20)21/h17,19H,2-16H2,1H3,(H,20,21)	-5.488
InChI=1S/C12H18Cl2N2O/c1-12(2,3)16-6-10(17)7-4-8(13)11(15)9(14)5-7/h4-5,10,16-17H,6,15H2,1-3H3	-1.922
InChI=1S/C7H17O4P/c1-4-6-10-12(8,9-3)11-7-5-2/h4-7H2,1-3H3	-0.659
InChI=1S/C12H7Cl3O/c13-8-6-10(14)12(11(15)7-8)16-9-4-2-1-3-5-9/h1-7H	-6.11
InChI=1S/C10H15NO3S/c11-15(13,14)10-6-4-9(5-7-10)3-1-2-8-12/h4-7,12H,1-3,8H2,(H2,11,13,14)	-1.193
InChI=1S/C10H10Cl2O3/c1-2-14-10(13)6-15-9-4-3-7(11)5-8(9)12/h3-5H,2,6H2,1H3	-3.35
InChI=1S/C7H11NO2/c1-3-7(2)4-5(9)8-6(7)10/h3-4H2,1-2H3,(H,8,9,10)	-0.556
InChI=1S/C6H13NO/c1-5-3-7-4-6(2)8-5/h5-7H,3-4H2,1-2H3	0.939
InChI=1S/C11H20N2O2/c1-4-11(2,3)8-5-6-9(12-14)10(7-8)13-15/h8,14-15H,4-7H2,1-3H3/b12-9+,13-10+	-3.965
InChI=1S/C13H20Cl6N2O6/c1-3-4-11(2,5-26-9(24)20-7(22)12(14,15)16)6-27-10(25)21-8(23)13(1' h7-8,22-23H,3-6H2,1-2H3,(H,20,24)(H,21,25)	-7.155
InChI=1S/C6H7NO6S2/c7-5-2-1-4(14(8,9)10)3-6(5)15(11,12)13/h1-3H,7H2,(H,8,9,10)(H,11,12,13)	-1.77
InChI=1S/C3H7BrO/c4-2-1-3-5/h5H,1-3H2	0.009
InChI=1S/C11H19ClN2O/c1-2-11(15)14-9-3-4-10(14)8-13(7-9)6-5-12/h9-10H,2-8H2,1H3	-1.788
InChI=1S/C40H26N2O4/c1-19-13-20(2)16-23(15-19)41-37(43)29-9-5-25-27-7-11-31-36-32(40(h5-18H,1-4H3	-7.476
InChI=1S/C10H20O3/c1-3-4-5-6-10(2)12-8-9(7-11)13-10/h9,11H,3-8H2,1-2H3	-2.657
InChI=1S/C7H8N2O3S/c8-7(10)5-1-3-6(4-2-5)13(9,11)12/h1-4H,(H2,8,10)(H2,9,11,12)	-2.301
InChI=1S/C6H7NO/c7-4-5-2-1-3-6(5)8/h5H,1-3H2	-0.357
InChI=1S/C7H13NO3/c1-5(2)3-6(7(10)11)8-4-9/h4-6H,3H2,1-2H3,(H,8,9)(H,10,11)	-0.733

"InChi"	"logS(M)"
InChI=1S/C14H21NO/c1-3-7-14(8-9-15(2)11-14)12-5-4-6-13(16)10-12/h4-6,10,16H,3,7-9,11H2,1-2H3	-2.011
InChI=1S/C13H26N2O4/c1-4-7-8-13(5-2,9-18-11(14)16)10-19-12(17)15-6-3/h4-10H2,1-3H3,(H2,14,16)(H,15,17)	-3.696
InChI=1S/C8H19N/c1-5-7(3)9-8(4)6-2/h7-9H,5-6H2,1-4H3/p+1	-1.769
InChI=1S/C9H9NO/c1-2-9-10-7-5-3-4-6-8(7)11-9/h3-6H,2H2,1H3	-2.63
InChI=1S/C12H5Cl5/c13-7-3-1-6(2-4-7)8-5-9(14)11(16)12(17)10(8)15/h1-5H	-7.31
InChI=1S/C8H7NO3S/c10-8-5-6-3-1-2-4-7(6)13(11,12)9-8/h1-4H,5H2,(H,9,10)	-0.859
InChI=1S/C13H17IN2O6/c1-2-3-11(18)21-6-9-8(17)4-10(22-9)16-5-7(14)12(19)15-13(16)20/h5,8-10,17H,2-4,6H2,1H3,(H,15,19,20)	-2.84
InChI=1S/C14H19NO4/c1-3-4-9-19-12-7-5-11(10-13(12)18-2)6-8-14(16)15-17/h5-8,10,17H,3-4,9H2,1-2H3,(H,15,16)/b8-6+	-3.14
InChI=1S/C11H12N2O/c14-11(8-13-7-6-12-9-13)10-4-2-1-3-5-10/h1-7,9,11,14H,8H2	-1.656
InChI=1S/C4H6O2/c1-3(5-1)4-2-6-4/h3-4H,1-2H2	1.065
InChI=1S/C9H20O6/c10-1-4-13-7-9(15-6-3-12)8-14-5-2-11/h9-12H,1-8H2	0.649
InChI=1S/C21H30O2/c1-5-6-7-8-15-12-18(22)20-16-11-14(2)9-10-17(16)21(3,4)23-19(20)1h11-13,16-17,22H,5-10H2,1-4H3	-6.866
InChI=1S/C6H9Cl2NO4/c1-13-6(12)3(2-10)9-5(11)4(7)8/h3-4,10H,2H2,1H3,(H,9,11)	-0.06
InChI=1S/C12H25NO3S2/c1-2-11(12-6-3-4-7-12)10-13-8-5-9-17-18(14,15)16/h11-13H,2-10H2,1H3,(H,14,15,16)	-2.623
InChI=1S/C22H28O3/c1-20-9-5-15(23)13-14(20)3-4-16-17(20)6-10-21(2)18(16)7-11-22(21)h3-4,13,16-18H,5-12H2,1-2H3	-4.101
InChI=1S/C13H15NO5/c1-3-14-12(16)8-18-13(17)10-6-4-5-7-11(10)19-9(2)15/h4-7H,3,8H2,1-2H3,(H,14,16)	-1.68
InChI=1S/C11H12N2OS2/c1-2-4-10-9(3-1)12-11(15-10)16-13-5-7-14-8-6-13/h1-4H,5-8H2	-3.811
InChI=1S/C9H11NO2/c1-10-9(11)7-5-3-4-6-8(7)12-2/h3-6H,1-2H3,(H,10,11)	-1.504
InChI=1S/C29H38N2O4/c1-6-18-17-31-10-8-20-14-27(33-3)29(35-5)16-23(20)25(31)12-21(18h13-16,24-25,30H,6-12,17H2,1-5H3	-5.646
InChI=1S/C20H31NO5/c1-7-24-20(23)18-15(4)9-10-16(14(2)3)19(18)26-13-17(22)25-12-8-11h9-10,14H,7-8,11-13H2,1-6H3	-4.387
InChI=1S/C21H24F3N3OS2/c1-13(2)26(14(3)4)11-12-29-20(28)27-16-8-5-7-15(21(22,23)24)18(16h5-10,13-14H,11-12H2,1-4H3	-6.674
InChI=1S/C10H16N2O3/c1-11-5-7-3-4-8(6-11)12(7)9(13)10(14)15-2/h7-8H,3-6H2,1-2H3	-1.096

"InChi"	"logS(M)"
InChI=1S/C32H62N4O6/c1-5-9-15-27(7-3)29-17-23-41-35(29)21-25-39-31(37)33-19-13-11-12-h27-30H,5-26H2,1-4H3,(H,33,37)(H,34,38)	-5.791
InChI=1S/C9H20O2/c1-4-8(3)9(5-2,6-10)7-11/h8,10-11H,4-7H2,1-3H3	-2.126
InChI=1S/CH2ClF/c2-1-3/h1H2	-0.82
InChI=1S/C18H15O3PS/c23-22(19-16-10-4-1-5-11-16,20-17-12-6-2-7-13-17)21-18-14-8-3-9-1h1-15H	-6.955
InChI=1S/C16H23ClN2O2/c1-4-11-21-15-12-13(17)7-8-14(15)16(20)18-9-10-19(5-2)6-3/h4,7-8,12H,1,5-6,9-11H2,2-3H3,(H,18,20)	-4.417
InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)8(12)10-9-7/h1-4H,(H,9,11)(H,10,12)	-1.788
InChI=1S/C9H20O2/c1-4-5-8(2)9(3,6-10)7-11/h8,10-11H,4-7H2,1-3H3	-2.126
InChI=1S/C14H14N2O5S/c1-2-21-13-7-3-11(4-8-13)15-22(19,20)14-9-5-12(6-10-14)16(17)18/h3-10,15H,2H2,1H3	-4.72
InChI=1S/C42H67NO16/c1-21(2)16-32(47)57-40-25(6)53-34(20-42(40,8)50)58-37-24(5)54-41(h12-13,15,21-25,27,29-31,34-41,49-50H,14,16-20H2,1-11H3/b13-12-	-6.922
InChI=1S/C10H9NO2/c1-11-8-5-3-2-4-7(8)6-9(11)10(12)13/h2-6H,1H3,(H,12,13)	-2.6
InChI=1S/C11H6O3/c12-11-2-1-7-5-8-3-4-13-9(8)6-10(7)14-11/h1-6H	-3.74
InChI=1S/C9H16ClN3O3/c10-5-6-13(12-16)9(15)11-7-1-3-8(14)4-2-7/h7-8,14H,1-6H2,(H,11,15)	-1.876
InChI=1S/C15H29NO3/c1-2-3-4-5-6-7-8-9-10-15(19)16(11-13-17)12-14-18/h2,17-18H,1,3-14H2	-2.762
InChI=1S/C7H5BrN2O/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3H,(H2,9,10)	-2.726
InChI=1S/C9H7ClOS/c1-5-2-6(10)3-8-9(5)7(11)4-12-8/h2-3H,4H2,1H3	-3.094
InChI=1S/C8H2F12O/c9-2-3(21-1-4(10,11)12)6(15,16)8(19,20)7(17,18)5(2,13)14/h1H2	-4.521
InChI=1S/C17H23N3O/c1-19(2)12-13-20(17-6-4-5-11-18-17)14-15-7-9-16(21-3)10-8-15/h4-11H,12-14H2,1-3H3	-3.066
InChI=1S/C17H18Cl2N4O4/c1-11-8-12(22(4-6-24)5-7-25)2-3-16(11)20-21-17-14(18)9-13(23(26)2h2-3,8-10,24-25H,4-7H2,1H3/b21-20+	-5.959
InChI=1S/C9H10O2/c1-6-3-4-8(9(10)11)7(2)5-6/h3-5H,1-2H3,(H,10,11)	-2.97
InChI=1S/C10H22O4/c1-8(11)5-13-10(3)7-14-9(2)6-12-4/h8-11H,5-7H2,1-4H3	0.685
InChI=1S/C10H9NO6S2/c11-9-3-4-10(19(15,16)17)7-2-1-6(5-8(7)9)18(12,13)14/h1-5H,11H2,(H,12,13,14)(H,15,16,17)	-1.643
InChI=1S/C7H12/c1-4-5-6-7(2)3/h7H,4H2,1-3H3	-2.745

"InChi"	"logS(M)"
InChI=1S/C10H15NO/c1-11(2)8-9-12-10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3	-0.911
InChI=1S/C5H9NO2S2/c1-2-10-5(9)6-3-4(7)8/h2-3H2,1H3,(H,6,9)(H,7,8)	-1.088
InChI=1S/C15H12N2O/c1-10(18)16-13-6-7-15-12(9-13)8-11-4-2-3-5-14(11)17-15/h2-9H,1H3,(H,16,18)	-4.106
InChI=1S/C14H16N4/c1-18(2)14-9-7-13(8-10-14)17-16-12-5-3-11(15)4-6-12/h3-10H,15H2,1-2H3/b17-16+	-4.594
InChI=1S/C14H13N3O2S/c1-2-7-19-14(18)17-12-6-4-3-5-10(12)16-13(17)11-8-20-9-15-11/h3-6,8-9H,2,7H2,1H3	-3.52
InChI=1S/C11H18N2O3S/c1-2-3-4-5-11(6-7-14)8(15)12-10(17)13-9(11)16/h14H,2-7H2,1H3,(H2,12,13,15,16,17)	-2.38
InChI=1S/C17H25NO2/c1-14-7-9-16(10-8-14)17(19)20-13-5-12-18-11-4-3-6-15(18)2/h7-10,15H,3-6,11-13H2,1-2H3	-4.273
InChI=1S/C4H6O2/c1-3-6-4(2)5/h3H,1H2,2H3	-0.634
InChI=1S/C50H66O8/c1-45(2,3)35-25-31(15-19-39(35)51)49(13,32-16-20-40(52)36(26-32)4 h15-22,25-28,51-54H,23-24,29-30H2,1-14H3	-6.201
InChI=1S/C12H10Cl2N2O2S/c13-11-6-3-9(7-12(11)14)16-19(17,18)10-4-1-8(15)2-5-10/h1-7,16H,15H2	-4.94
InChI=1S/C10H14N2O5/c1-5-3-12(10(16)11-9(5)15)8-2-6(14)7(4-13)17-8/h3,6-8,13-14H,2,4H2,1H3,(H,11,15,16)	-0.742
InChI=1S/C11H22N2O4/c1-4-11(5-8(2)3,6-16-9(12)14)7-17-10(13)15/h8H,4-7H2,1-3H3,(H2,12,14)(H2,13,15)	-2.613
InChI=1S/C10H12O2/c1-8-11-7-10(12-8)9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3	-1.805
InChI=1S/C7H5ClN2O4S/c8-3-1-4-6(14-7(9)10-4)5(2-3)15(11,12)13/h1-2H,(H2,9,10)(H,11,12,13)	-2.08
InChI=1S/C12H13N3O/c1-8-11-13-10-6-4-3-5-9(10)12(16)15(11)7-14(8)2/h3-6,8H,7H2,1-2H3	0.03
InChI=1S/C7H3F9/c1-2-3(8)5(11,12)7(15,16)6(13,14)4(2,9)10/h1H3	-4.21
InChI=1S/C9H7N3O3/c1-5-10-8-3-2-6(12(14)15)4-7(8)9(13)11-5/h2-4H,1H3,(H,10,11,13)	-2.22
InChI=1S/C13H16N2O2/c1-2-13(8-7-11(16)15-12(13)17)9-3-5-10(14)6-4-9/h3-6H,2,7-8,14H2,1H3,(H,15,16,17)	-1.97
InChI=1S/C13H20Br2N2O4S2/c14-11-9-12(15)13(17-10-11)21-7-4-2-1-3-5-16-6-8-22-23(18,19)20/h9-10,16H,1-8H2,(H,18,19,20)	-4.552
InChI=1S/C14H20N4O2S/c1-2-3-4-5-6-7-11(19)20-10-21-14-12-13(16-8-15-12)17-9-18-14/h8-9H,2-7,10H2,1H3,(H,15,16,17,18)	-4.62

"InChi"	"logS(M)"
InChI=1S/C13H16O2/c1-2-3-4-8-11-15-13(14)12-9-6-5-7-10-12/h3-7,9-10H,2,8,11H2,1H3/b4-3+	-3.705
InChI=1S/C12H16N2O2/c1-10(15)13-6-8-14(9-7-13)11-2-4-12(16)5-3-11/h2-5,16H,6-9H2,1H3	-1.818
InChI=1S/C5H5N3O2/c9-8(10)7-5-3-1-2-4-6-5/h1-4H,(H,6,7)	-0.66
InChI=1S/C8H18O/c1-4-7(3)6-8(9)5-2/h7-9H,4-6H2,1-3H3	-1.86
InChI=1S/C15H20O6/c1-5-12(16)19-9-15(8-4,10-20-13(17)6-2)11-21-14(18)7-3/h5-7H,1-3,8-11H2,4H3	-2.773
InChI=1S/C8H12N2O2/c9-6-1-2-8(7(10)5-6)12-4-3-11/h1-2,5,11H,3-4,9-10H2	-0.234
InChI=1S/C10H17NO4/c11-9(12)13-6-8-7-14-10(15-8)4-2-1-3-5-10/h8H,1-7H2,(H2,11,12)	-1.89
InChI=1S/C13H22N4O3S/c1-7-20-9(18)8-21-11-14-10(13(2,3)4)15-17(11)12(19)16(5)6/h7-8H2,1-6H3	-2.861
InChI=1S/C6H6INO2S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H2,8,9,10)	-2.623
InChI=1S/C8H16O4/c1-5-9-6(2)11-8(4)12-7(3)10-5/h5-8H,1-4H3	-2.9
InChI=1S/C15H18N4/c1-10-7-5-6-8-14(10)13(4)18-19-15-16-11(2)9-12(3)17-15/h5-9H,1-4H3,(H,16,17,19)/b18-13-	-3.196
InChI=1S/C8H13N3O2/c1-3-4-5-7-6-9-8(10(7)2)11(12)13/h6H,3-5H2,1-2H3	-3.015
InChI=1S/C7H3Cl2F3/c8-5-2-1-4(3-6(5)9)7(10,11)12/h1-3H	-3.268
InChI=1S/C9H6Cl2O2/c10-7-3-1-6(5-8(7)11)2-4-9(12)13/h1-5H,(H,12,13)/b4-2+	-3.257
InChI=1S/C6H10N2O4/c9-3-7-1-5(11)8(4-10)2-6(7)12/h9-10H,1-4H2	-0.417
InChI=1S/C15H17N5O6S/c1-9-16-13(18-14(17-9)26-4)20(2)15(22)19-27(23,24)11-8-6-5-7-10(11)5-8H,1-4H3,(H,19,22)	-3.898
InChI=1S/C15H24O/c1-13(2)7-6-11(16)12-14(3,4)10-5-8-15(12,13)9-10/h10,12H,5-9H2,1-4H3	-4.098
InChI=1S/C16H20N4O6/c1-3-25-15(23)17-9-11(19-5-6-19)14(22)10(18-16(24)26-4-2)12(13(9)3-8H2,1-2H3,(H,17,23)(H,18,24)	-2.141
InChI=1S/C13H18ClN3O4S2/c14-9-6-10-12(7-11(9)22(15,18)19)23(20,21)17-13(16-10)5-8-3-1-2-4-8H6-8,13,16-17H,1-5H2,(H2,15,18,19)	-4.105
InChI=1S/C10H15NO/c1-2-3-8-11-9-4-6-10(12)7-5-9/h4-7,11-12H,2-3,8H2,1H3	-2.342
InChI=1S/C16H14O4/c17-14(18)11-16(15(19)20,12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10H,11H2,(H,17,18)(H,19,20)	-2.432
InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h2-4,8H,1,5-7H2	-3.335
InChI=1S/C7H16S/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3	-4.155
InChI=1S/C17H18O2/c1-3-7-14-10-11-16(17(12-14)18-2)19-13-15-8-5-4-6-9-15/h3-6,8-12H,1,7,13H2,2H3	-5.102

"InChi"	"logS(M)"
InChI=1S/C29H14N2O5/c30-24-18(10-9-17-23(24)28(35)16-8-4-3-7-15(16)25(17)32)29-31-21-h1-12H,30H2	-5.496
InChI=1S/C10H7NO3/c12-9-5-7(10(13)14)6-3-1-2-4-8(6)11-9/h1-5H,(H,11,12)(H,13,14)	-1.994
InChI=1S/C13H15ClN2/c1-16-7-3-6-12(16)9-8-15-11-5-2-4-10(14)13(9)11/h2,4-5,8,12,15H,3,6-7H2,1H3	-2.375
InChI=1S/C6H9NS/c1-2-3-4-5-7-6-8/h2H,1,3-5H2	-2.9
InChI=1S/C12H4Cl6/c13-5-1-7(12(18)10(17)4-5)11-8(15)2-6(14)3-9(11)16/h1-4H	-8.71
InChI=1S/C24H30ClNO2/c1-17(2)11-13-26-14-12-19-15-23(27-3)24(28-4)16-21(19)22(26)10-7-h5-6,8-9,11,15-16,22H,7,10,12-14H2,1-4H3	-6.804
InChI=1S/C7H10N2O2S/c1-5-2-3-6(4-7(5)8)12(9,10)11/h2-4H,8H2,1H3,(H2,9,10,11)	-1.917
InChI=1S/C5H11NO3/c1-2-3-4-5-9-6(7)8/h2-5H2,1H3	-2.568
InChI=1S/C18H15ClN6O2/c19-17-13-16(25(26)27)7-8-18(17)23-22-14-3-5-15(6-4-14)24(11-1-9-h3-8,13H,1-2,11-12H2/b23-22+	-4.282
InChI=1S/C10H10O2/c1-2-3-8-4-5-9-10(6-8)12-7-11-9/h2-6H,7H2,1H3/b3-2+	-3.262
InChI=1S/C5H12O4S2/c1-5(2,10(3,6)7)11(4,8)9/h1-4H3	-1.45
InChI=1S/C5H10N2O3/c1-5(2,3(8)9)7-4(6)10/h1-2H3,(H,8,9)(H3,6,7,10)	-1.165
InChI=1S/C14H18O5/c1-11(15)18-10-14(19-12(2)16)9-17-8-13-6-4-3-5-7-13/h3-7,14H,8-10H2,1-2H3	-2.649
InChI=1S/C3H7N/c4-3-1-2-3/h3H,1-2,4H2	1.243
InChI=1S/C9H10FNO/c1-6-3-4-9(8(10)5-6)11-7(2)12/h3-5H,1-2H3,(H,11,12)	-1.74
InChI=1S/C6H12O/c1-2-3-4-5-6-7/h3-4,7H,2,5-6H2,1H3/b4-3+	-0.786
InChI=1S/C7H5ClN2O/c8-4-1-2-5-6(3-4)11-7(9)10-5/h1-3H,(H2,9,10)	-2.532
InChI=1S/C20H30O/c1-16(8-6-9-17(2)13-15-21)11-12-19-18(3)10-7-14-20(19,4)5/h6,8-9,11-13,21H,7,10,14-15H2,1-5H3/b9-6+,12-11+,16-8+,17-13+	-3.81
InChI=1S/C3H5NO/c1-3(5)2-4/h3,5H,1H3	1.148
InChI=1S/C10H14O2/c1-8-5-3-4-6-10(8)12-7-9(2)11/h3-6,9,11H,7H2,1-2H3	-1.668
InChI=1S/C5H12N2S/c1-6(2)5(8)7(3)4/h1-4H3	-1.389
InChI=1S/C12H16FNO3/c1-2-3-6-17-11-5-4-9(7-10(11)13)8-12(15)14-16/h4-5,7,16H,2-3,6,8H2,1H3,(H,14,15)	-2.819
InChI=1S/C13H20N2O5/c1-3-6-13(2,8-19-11(14)16)9-20-12(17)15-10-5-4-7-18-10/h4-5,7H,3,6,8-9H2,1-2H3,(H2,14,16)(H,15,17)	-3.506
InChI=1S/C12H9Br2NO2S/c13-9-6-7-12(11(14)8-9)15-18(16,17)10-4-2-1-3-5-10/h1-8,15H	-5.01

"InChi"	"logS(M)"
InChI=1S/C32H66O/c1-3-5-7-9-11-13-15-17-18-20-22-24-26-28-30-32(31-33)29-27-25-23-h32-33H,3-31H2,1-2H3	-5.669
InChI=1S/C14H26O2/c1-5-7-14(15)16-11-10-13(4)9-6-8-12(2)3/h8,13H,5-7,9-11H2,1-4H3	-5.143
InChI=1S/C3H8N2O/c1-4-3(6)5-2/h1-2H3,(H2,4,5,6)	0.939
InChI=1S/C13H17NO4/c1-2-14(8-9-15)12(16)10-18-13(17)11-6-4-3-5-7-11/h3-7,15H,2,8-10H2,1H3	-1.37
InChI=1S/C11H22O2/c1-5-6-7-10-12-9(2)8-11(3,4)13-10/h9-10H,5-8H2,1-4H3	-2.453
InChI=1S/C11H16N2O2/c1-3-13(11(12)14)9-5-7-10(8-6-9)15-4-2/h5-8H,3-4H2,1-2H3,(H2,12,14)	-1.85
InChI=1S/C9H9ClO2S/c1-6-4-7(10)2-3-8(6)12-5-9(11)13/h2-4H,5H2,1H3,(H,11,13)	-3.16
InChI=1S/C15H15NO4/c1-19-13-8-11(9-14(10-13)20-2)15(17)16(18)12-6-4-3-5-7-12/h3-10,18H,1-2H3	-3.1
InChI=1S/C10H14O4/c11-4-6-13-9-2-1-3-10(8-9)14-7-5-12/h1-3,8,11-12H,4-7H2	-1.02
InChI=1S/C11H14O3/c1-4-9(12)8-5-6-10(13-2)11(7-8)14-3/h5-7H,4H2,1-3H3	-2.164
InChI=1S/C9H8O4/c1-7(10)12-13-9(11)8-5-3-2-4-6-8/h2-6H,1H3	-2.45
InChI=1S/C12H6Cl4/c13-9-4-2-1-3-7(9)8-5-6-10(14)12(16)11(8)15/h1-6H	-6.83
InChI=1S/C11H15FN2O4/c1-2-3-4-5-6-18-11(17)14-7-8(12)9(15)13-10(14)16/h7H,2-6H2,1H3,(H,13,15,16)	-2.24
InChI=1S/C12H16N4O2S/c1-2-3-4-5-9(17)18-8-19-12-10-11(14-6-13-10)15-7-16-12/h6-7H,2-5,8H2,1H3,(H,13,14,15,16)	-3.63
InChI=1S/C12H18O4/c1-10-2-4-11(5-3-10)16-9-12(6-13,7-14)8-15/h2-5,13-15H,6-9H2,1H3	-2.122
InChI=1S/C8H9N3S2/c9-7(12)11-8(13)10-6-4-2-1-3-5-6/h1-5H,(H4,9,10,11,12,13)	-0.371
InChI=1S/C10H14O/c11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-9H,1-5H2	-2.511
InChI=1S/C22H26FNO2/c1-17-4-8-19(9-5-17)22(26)12-15-24(16-13-22)14-2-3-21(25)18-6-10-h4-11,26H,2-3,12-16H2,1H3	-4.35
InChI=1S/C10H13NO4/c11-10(14)8-3-1-2-4-9(8)15-6-7(13)5-12/h1-4,7,12-13H,5-6H2,(H2,11,14)	0.054
InChI=1S/C18H21ClN2O2S/c1-20(2)9-4-10-21-13-11-12(19)5-7-15(13)24-16-8-6-14(22)18(23-3)1h5-8,11,22H,4,9-10H2,1-3H3	-5.549
InChI=1S/C12H23NO3/c1-5-6-12(4,8-14)9-16-11(15)13-7-10(2)3/h14H,2,5-9H2,1,3-4H3,(H,13,15)	-3.196
InChI=1S/C20H28O3S/c1-8-23-24(21,22)18-13-16(20(5,6)7)12-14-11-15(19(2,3)4)9-10-17(1h9-13H,8H2,1-7H3	-7.594
InChI=1S/C5H5NO2/c7-4-1-2-6-5(8)3-4/h1-3H,(H2,6,7,8)	-1.25

"InChi"	"logS(M)"
InChI=1S/C8H12O6/c1-2-13-7-5(11)8(12)14-6(7)4(10)3-9/h4,6,9-11H,2-3H2,1H3	0.581
InChI=1S/CH5N3O/c2-1(5)4-3/h3H2,(H3,2,4,5)	1.125
InChI=1S/C18H25N5O4/c1-11(25-2)17(24)22-5-7-23(8-6-22)18-20-13-10-15(27-4)14(26-3)9-12(13)19-18/h9-11H,5-8H2,1-4H3,(H2,19,20,21)	-2.911
InChI=1S/C5H5N3O2/c6-4-3(5(9)10)7-1-2-8-4/h1-2H,(H2,6,8)(H,9,10)	-1.763
InChI=1S/C12H15NO2/c1-3-9-15-11-8-6-5-7-10(11)12(14)13-4-2/h3,5-8H,1,4,9H2,2H3,(H,13,14)	-2.938
InChI=1S/C9H20/c1-4-6-8-9(3)7-5-2/h9H,4-8H2,1-3H3	-6.047
InChI=1S/C11H13NO4/c1-15-9-5-3-8(7-10(9)16-2)4-6-11(13)12-14/h3-7,14H,1-2H3,(H,12,13)/b6-4+	-1.576
InChI=1S/C28H28ClF2N3O/c29-21-7-12-27-26(18-21)32-28(35)34(27)24-13-16-33(17-14-24)15-1h3-12,18,24-25H,1-2,13-17H2,(H,32,35)	-8.878
InChI=1S/C4H8OS/c1-3(5)4(2)6/h4,6H,1-2H3	-0.07
InChI=1S/C12H5Cl5/c13-6-1-2-9(15)8(3-6)12-10(16)4-7(14)5-11(12)17/h1-5H	-7.47
InChI=1S/C14H17ClN2O/c1-16-8-12-6-7-13(9-16)17(12)14(18)10-2-4-11(15)5-3-10/h2-5,12-13H,6-9H2,1H3	-2.567
InChI=1S/C16H26N2O3/c1-21-14(19)3-2-4-17-15(20)18-16-8-11-5-12(9-16)7-13(6-11)10-16/h11-13H,2-10H2,1H3,(H2,17,18,20)	-2.25
InChI=1S/C8H16N2O4/c1-2-3-6(4-13-7(9)11)5-14-8(10)12/h6H,2-5H2,1H3,(H2,9,11)(H2,10,12)	-1.143
InChI=1S/C19H22N2OS/c1-13(20(3)4)12-21-16-7-5-6-8-18(16)23-19-10-9-15(14(2)22)11-17(1h5-11,13H,12H2,1-4H3	-5.242
InChI=1S/C5H9NO4/c6-3(5(9)10)1-2-4(7)8/h3H,1-2,6H2,(H,7,8)(H,9,10)	-0.992
InChI=1S/C12H24N2O4/c1-4-6-12(3,8-17-10(13)15)9-18-11(16)14-7-5-2/h4-9H2,1-3H3,(H2,13,15)(H,14,16)	-3.175
InChI=1S/C7H10N2/c1-5-4-6(8)2-3-7(5)9/h2-4H,8-9H2,1H3	-0.507
InChI=1S/C13H13ClN2O2S/c1-9-8-11(15)4-7-13(9)19(17,18)16-12-5-2-10(14)3-6-12/h2-8,16H,15H2,1H3	-4.42
InChI=1S/C14H9BrN2O/c15-10-6-7-12-11(8-10)13(17-14(18)16-12)9-4-2-1-3-5-9/h1-8H,(H,16,17,18)	-3.711
InChI=1S/C15H22N2O4/c1-9(2)7-12(16)14(19)17-13(15(20)21)8-10-3-5-11(18)6-4-10/h3-6,9,12-13,18H,7-8,16H2,1-2H3,(H,17,19)(H,20,21)	-1.58
InChI=1S/C11H20O2/c1-9(2)5-7-11(12-9)8-6-10(3,4)13-11/h5-8H2,1-4H3	-1.964
InChI=1S/C37H62O12/c1-10-28(40)45-30(24(7)33(41)42)23(6)31-22(5)25(39)17-36(47-31)1h19-27,29-32,38-39,43H,10-18H2,1-9H3,(H,41,42)	-7.529

"InChi"	"logS(M)"
InChI=1S/C24H50N4/c1-21(2)15-19(16-22(3,4)27-21)25-13-11-9-10-12-14-26-20-17-23(5,6h19-20,25-28H,9-18H2,1-8H3	-2.351
InChI=1S/C15H15NO4/c1-19-9-5-3-2-4-8(9)16-14(17)12-10-6-7-11(20-10)13(12)15(16)18/h2-5,10-13H,6-7H2,1H3	-0.695
InChI=1S/C18H19Br2NO2/c1-14-2-4-15(5-3-14)18(22)23-17-8-6-16(7-9-17)21(12-10-19)13-11-2h2-9H,10-13H2,1H3	-7.06
InChI=1S/C6H5FO/c7-5-1-3-6(8)4-2-5/h1-4,8H	-0.21
InChI=1S/C10H18O6/c1-6(2)10(16,8(13)14)5-4-9(3,15)7(11)12/h6,15-16H,4-5H2,1-3H3,(H,11,12)(H,13,14)	-1.69
InChI=1S/C19H23N4O6PS/c1-13(23(12-24)11-16-10-21-14(2)22-18(16)20)17(8-9-29-30(26,27)28h3-7,10,12H,8-9,11H2,1-2H3,(H2,20,21,22)(H2,26,27,28)/b17-13-	-3.539
InChI=1S/C22H25NO5S/c1-12(24)23-16-8-6-13-10-18(26-2)21(27-3)22(28-4)20(13)14-7-9-19(h7,9-11,16H,6,8H2,1-5H3,(H,23,24)	-4.436
InChI=1S/C8H12N4/c1-2-10-8(11-3-1)12-6-4-9-5-7-12/h1-3,9H,4-7H2	0.19
InChI=1S/C24H32O6/c1-21-8-5-14(25)11-23(21,28)10-7-16-15(21)6-9-22(2)18(13-3-4-17(2h3-4,12,14-16,18-20,25,27-28H,5-11H2,1-2H3	-3.302
InChI=1S/C16H17NO2/c1-13-7-5-6-10-15(13)17(19)16(18)12-11-14-8-3-2-4-9-14/h2-10,19H,11-12H2,1H3	-2.79
InChI=1S/C19H16ClNO4/c1-24-17-10-18(25-2)15(9-14(17)20)21-19(23)13-7-11-5-3-4-6-12(11)h3-10,22H,1-2H3,(H,21,23)	-5.378
InChI=1S/C13H11NO2/c15-13(16)11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/h1-9,14H,(H,15,16)	-4.96
InChI=1S/C19H25N3/c1-3-21(4-2)13-14-22-18-11-7-5-9-16(18)15-20-17-10-6-8-12-19(17)2h5-12,20H,3-4,13-15H2,1-2H3	-4.829
InChI=1S/C2HF5/c3-1(4)2(5,6)7/h1H	-1.416
InChI=1S/C5H12FO2P/c1-4-9(6,7)8-5(2)3/h5H,4H2,1-3H3	-0.95
InChI=1S/C20H22O3/c1-20(2,3)16-9-5-14(6-10-16)18(21)13-19(22)15-7-11-17(23-4)12-8-1h5-12H,13H2,1-4H3	-7.061
InChI=1S/C13H18O5/c1-3-11(16)9-4-5-12(13(6-9)17-2)18-8-10(15)7-14/h4-6,10,14-15H,3,7-8H2,1-2H3	-1.563
InChI=1S/C19H22N2O3/c1-2-3-14-17(19(23)24)18(22)21(16-12-8-5-9-13-16)20-15-10-6-4-7-1h4-13,17,20H,2-3,14H2,1H3,(H,23,24)	-4.147
InChI=1S/C13H17NO4/c1-3-8-18-11-6-4-10(9-12(11)17-2)5-7-13(15)14-16/h4-7,9,16H,3,8H2,1-2H3,(H,14,15)/b7-5+	-2.62
InChI=1S/C10H16/c1-3-5-7-9-10-8-6-4-2/h3,5-8H,1,4,9-10H2,2H3/b7-5+,8-6+	-3.342
InChI=1S/C9H17N/c1-8-6-5-7-9(2,3)10(8)4/h6H,5,7H2,1-4H3	-0.937

"InChi"	"logS(M)"
InChI=1S/C20H28Cl4N2O4/c1-3-29-11-9-25(19(27)17(21)22)13-15-5-7-16(8-6-15)14-26(10-12-3(h5-8,17-18H,3-4,9-14H2,1-2H3	-4.849
InChI=1S/C11H9NO2/c1-11(2)9-4-3-7(6-12)5-8(9)10(13)14-11/h3-5H,1-2H3	-2.91
InChI=1S/C7H6O4/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3,8-9H,(H,10,11)	-0.771
InChI=1S/C11H13N5O3/c12-10-13-3-8-9(15-10)16(6-14-8)2-1-7-4-18-11(17)19-5-7/h3,6-7H,1-2,4-5H2,(H2,12,13,15)	-1.43
InChI=1S/C12H13N/c1-2-13-12-9-5-7-10-6-3-4-8-11(10)12/h3-9,13H,2H2,1H3	-3.192
InChI=1S/C34H50O8/c1-23-19-25(21-27(31(23)37)33(3,4)5)9-11-29(35)41-17-15-39-13-14-h19-22,37-38H,9-18H2,1-8H3	-5.768
InChI=1S/C8H10OS/c1-5-4-8(6(2)9)7(3)10-5/h4H,1-3H3	-2.537
InChI=1S/C11H14N2O3/c1-7-4-3-5-9-12-6-8(11(15)16-2)10(14)13(7)9/h6-7H,3-5H2,1-2H3	-2.269
InChI=1S/C7H13NO/c9-7-5-3-1-2-4-6-8-7/h1-6H2,(H,8,9)	-0.335
InChI=1S/C12H22O/c1-2-3-4-5-6-8-11-9-7-10-12(11)13/h11H,2-10H2,1H3	-3.769
InChI=1S/C8H12N4O3/c1-6-4-9-8(12(14)15)11(6)5-7(13)10(2)3/h4H,5H2,1-3H3	-2.682
InChI=1S/C13H12N2O/c1-10-6-5-9-14-12(10)15-13(16)11-7-3-2-4-8-11/h2-9H,1H3,(H,14,15,16)	-2.505
InChI=1S/C7H6F3N/c8-7(9,10)5-3-1-2-4-6(5)11/h1-4H,11H2	-1.676
InChI=1S/C12H21NO2/c14-12(10-6-4-5-7-10)13(15)11-8-2-1-3-9-11/h10-11,15H,1-9H2	-3.16
InChI=1S/C31H38N2O11/c1-14(2)7-8-16-13-17(9-11-19(16)34)27(37)33-21-22(35)18-10-12-20(h9-14,23,25-26,29,34-36H,7-8H2,1-6H3,(H2,32,39)(H,33,37)	-5.713
InChI=1S/C7H14N2O/c8-7(10)9-6-4-2-1-3-5-6/h6H,1-5H2,(H3,8,9,10)	-1.247
InChI=1S/C24H48O2/c1-3-5-7-9-11-13-14-16-18-20-22-23(24(25)26)21-19-17-15-12-10-8-6h23H,3-22H2,1-2H3,(H,25,26)	-5.868
InChI=1S/C9H11NO2/c1-7(11)10-8-3-5-9(12-2)6-4-8/h3-6H,1-2H3,(H,10,11)	-1.3
InChI=1S/C9H9NOS/c1-2-11-9-5-3-8(4-6-9)10-7-12/h3-6H,2H2,1H3	-4.26
InChI=1S/C2H6N4O2/c3-1(5-7)2(4)6-8/h5,7H,3-4H2/b2-1+	-0.777
InChI=1S/C7H10O/c8-6-7-4-2-1-3-5-7/h1-2,6-7H,3-5H2	-0.978
InChI=1S/C10H13NO3/c1-10(11,9(13)14)6-7-2-4-8(12)5-3-7/h2-5,12H,6,11H2,1H3,(H,13,14)	-0.501
InChI=1S/C11H15NO3/c1-12(2)11(14)9-5-3-4-6-10(9)15-8-7-13/h3-6,13H,7-8H2,1-2H3	-0.587
InChI=1S/C12H14O4/c1-3-15-11(13)9-5-7-10(8-6-9)12(14)16-4-2/h5-8H,3-4H2,1-2H3	-2.719
InChI=1S/C10H19N3O3/c1-4-16-10(15)13-6-7(2)12(9(11)14)5-8(13)3/h7-8H,4-6H2,1-3H3,(H2,11,14)	-0.55

"InChi"	"logS(M)"
InChI=1S/C9H18N2O3S2/c10-9(7-15-16(12,13)14)11-8-5-3-1-2-4-6-8/h8H,1-7H2,(H2,10,11)(H,12,13,14)	-3.703
InChI=1S/C26H34O6/c1-14(27)31-22-21(15-4-7-20(29)30-13-15)25(3)11-9-18-19(26(25)23(h4,7,13,16-19,21-23,28H,5-6,8-12H2,1-3H3	-4.05
InChI=1S/C27H50O6/c1-7-13-16-21(10-4)25(28)31-19-24(33-27(30)23(12-6)18-15-9-3)20-3h21-24H,7-20H2,1-6H3	-6.974
InChI=1S/C11H20O2/c1-10(2)5-4-6-11(3)7-8-13-9-12/h5,9,11H,4,6-8H2,1-3H3	-4.056
InChI=1S/C27H44O3/c1-18(8-6-14-26(3,4)30)23-12-13-24-20(9-7-15-27(23,24)5)10-11-21-h10-11,18,22-25,28-30H,2,6-9,12-17H2,1,3-5H3/b20-10+,21-11-	-8.725
InChI=1S/C11H15ClO4/c12-9-3-1-2-4-10(9)16-8-11(5-13,6-14)7-15/h1-4,13-15H,5-8H2	-2.351
InChI=1S/C16H15F2N3O3/c17-11-3-9-13(12(18)14(11)20-4-7(19)5-20)21(8-1-2-8)6-10(15(9)22)h3,6-8H,1-2,4-5,19H2,(H,23,24)	-5.27
InChI=1S/C12H13N2O3P/c13-14-18(15,16-11-7-3-1-4-8-11)17-12-9-5-2-6-10-12/h1-10H,13H2,(H,14,15)	-2.237
InChI=1S/C12H16N4O4/c1-11(7-13,5-3-9(17)18)15-16-12(2,8-14)6-4-10(19)20/h3-6H2,1-2H3,(H,17,18)(H,19,20)/p-2/b16-15+	-2.008
InChI=1S/C14H22N2O/c1-2-3-4-5-6-7-11-16-14(17)13-9-8-10-15-12-13/h8-10,12H,2-7,11H2,1H3,(H,16,17)	-3.008
InChI=1S/C19H26N2/c1-15(2)9-10-16(3)20-18-11-13-19(14-12-18)21-17-7-5-4-6-8-17/h4-8,11-16,20-21H,9-10H2,1-3H3	-5.625
InChI=1S/C13H20O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h6-7,9-10H,5,8H2,1-4H3/b10-6+,12-9-	-3.297
InChI=1S/C5H14N2O/c1-5(8)4-7-3-2-6/h5,7-8H,2-4,6H2,1H3	0.927
InChI=1S/C16H19ClO3/c17-14-10-12(15(18)8-9-16(19)20)6-7-13(14)11-4-2-1-3-5-11/h6-7,10-11H,1-5,8-9H2,(H,19,20)	-5.537
InChI=1S/C13H17NO3/c1-2-3-9-14-12(15)10-17-13(16)11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3,(H,14,15)	-2.759
InChI=1S/C6H14N2O6/c1-6(14-8(11)12)4-2-3-5-13-7(9)10/h6H,2-5H2,1H3,(H,9,10)(H,11,12)/q+2	-2.84
InChI=1S/C13H18O/c1-10(2)12-5-4-6-13(9-12)11(3)7-8-14/h4-6,8-11H,7H2,1-3H3	-3.677
InChI=1S/C10H14O8/c1-5(11)15-9(16-6(2)12)10(17-7(3)13)18-8(4)14/h9-10H,1-4H3	-2.1
InChI=1S/C39H66O6/c1-31(2)22-16-10-7-13-19-27-43-37(40)34-25-26-35(38(41)44-28-20-h25-26,30-33H,7-24,27-29H2,1-6H3	-5.707
InChI=1S/C6H5Cl2N/c7-4-1-5(8)3-6(9)2-4/h1-3H,9H2	-2.315
InChI=1S/C9H7NO/c11-8-5-7-3-1-2-4-9(7)10-6-8/h1-6,11H	-2.393

"InChi"	"logS(M)"
InChI=1S/C18H36O2/ c1-3-5-7-9-10-11-12-13-14-16-18(19)20-17-15-8-6-4-2/ h3-17H2,1-2H3	-6.755
InChI=1S/C10H9ClN2O2/ c11-5-6-13-9(14)7-3-1-2-4-8(7)12-10(13)15/h1-4H,5-6H2,(H,12,15)	-3.575
InChI=1S/C2H8N2O/c3-4-1-2-5/h4-5H,1-3H2	1.119
InChI=1S/C15H11ClO/ c16-14-9-6-12(7-10-14)8-11-15(17)13-4-2-1-3-5-13/h1-11H/b11-8+	-4.645
InChI=1S/C6H11N/c1-3-5-7-6-4-2/h3-4,7H,1-2,5-6H2	-0.079
InChI=1S/C11H8O3/c12-9-6-5-7-3-1-2-4-8(7)10(9)11(13)14/ h1-6,12H,(H,13,14)	-3.128
InChI=1S/C18H10Cl2O2S2/ c1-7-3-9(19)5-11-13(7)15(21)17(23-11)18-16(22)14-8(2)4-10(20)6-12 h3-6H,1-2H3/b18-17-	-7.932
InChI=1S/C3H8N2O/c1-2-3(6)5-4/h2,4H2,1H3,(H,5,6)	-0.302
InChI=1S/C8H19O3PS3/c1-4-10-12(13,11-5-2)14-7-8-15(9)6-3/ h4-8H2,1-3H3/p+1	-1.861
InChI=1S/C15H21NO2/ c1-4-14(17)18-15(10-11-16(3)12(15)2)13-8-6-5-7-9-13/h5-9,12H, 4,10-11H2,1-3H3	-2.519
InChI=1S/C12H3Cl7O/ c13-4-1-6(15)9(3-5(4)14)20-12-10(18)7(16)2-8(17)11(12)19/h1-3H	-9.05
InChI=1S/C21H26O2/ c1-5-6-7-8-15-12-18(22)20-16-11-14(2)9-10-17(16)21(3,4)23-19(20)1 h9-13,22H,5-8H2,1-4H3	-6.742
InChI=1S/C8H12O4/c1-4-8(12-7(3)10)5-11-6(2)9/h4,8H, 1,5H2,2-3H3	-0.818
InChI=1S/C12H4Cl6/ c13-7-4-9(15)8(14)3-6(7)5-1-10(16)12(18)11(17)2-5/h1-4H	-8.21
InChI=1S/C21H28N2O3/ c1-17(24)20-9-5-6-10-21(20)26-16-19(25)15-22-11-13-23(14-12-22)18 h2-10,17,19,24-25H,11-16H2,1H3	-2.795
InChI=1S/C36H28O8P2/ c37-45(39-31-13-5-1-6-14-31,40-32-15-7-2-8-16-32)43-35-25-21-29(2 h1-28H	-7.813
InChI=1S/C12H24N2O4/ c1-5-6-7-12(2,8-17-10(13)15)9-18-11(16)14(3)4/h5-9H2,1-4H3, (H2,13,15)	-3.106
InChI=1S/C11H13ClO2/c1-7(2)10(11(13)14)8-3-5-9(12)6-4-8/ h3-7,10H,1-2H3,(H,13,14)	-3.26
InChI=1S/C13H11NO4/ c1-16-13-11-8(4-5-17-11)9(6-14)7-2-3-10(15)18-12(7)13/h2-5H, 6,14H2,1H3	-0.9
InChI=1S/C15H20N2/ c1-4-9-17(10-5-1)11-8-13-12-16-15-7-3-2-6-14(13)15/ h2-3,6-7,12,16H,1,4-5,8-11H2	-2.68
InChI=1S/C16H23NO4/ c1-2-16(19)13-3-5-15(6-4-13)21-12-14(18)11-17-7-9-20-10-8-17/ h3-6,14,18H,2,7-12H2,1H3	-0.766
InChI=1S/C17H17N3O6S2/ c1-9(21)26-6-10-7-28-16-13(15(23)20(16)14(10)17(24)25)19-12(22)8 h2-5,13,16H,6-8H2,1H3,(H,19,22)(H,24,25)	-2.615

"InChi"	"logS(M)"
InChI=1S/C18H35NO/c1-2-3-4-5-6-7-8-9-10-13-16-19-17-14-11-12-15-18(19)20/h2-17H2,1H3	-6.218
InChI=1S/C9H14O2/c1-6-7(8(10)11)4-5-9(6,2)3/h4-5H2,1-3H3,(H,10,11)	-2.887
InChI=1S/C8H13N3O3/c1-8(2,14-4)6-5-9-7(10(6)3)11(12)13/h5H,1-4H3	-1.963
InChI=1S/C7H12N4O5/c8-7(16)11-2-5(13)9-1-4(12)10-3-6(14)15/h1-3H2,(H,9,13)(H,10,12)(H,14,15)(H3,8,11,16)	-1.351
InChI=1S/C16H24N4O2/c1-2-21-15-6-4-3-5-14(15)20-9-7-19(8-10-20)12-13-11-18-16(17)22-1h3-6,13H,2,7-12H2,1H3,(H2,17,18)	-2.453
InChI=1S/C20H16N2O4/c1-2-20(25)14-8-16-17-12(7-11-5-3-4-6-15(11)21-17)9-22(16)18(23)1h3-8,25H,2,9-10H2,1H3	-3.226
InChI=1S/C13H13ClN2O2S/c1-9-2-7-13(12(14)8-9)16-19(17,18)11-5-3-10(15)4-6-11/h2-8,16H,15H2,1H3	-4.32
InChI=1S/C13H24N2O4/c1-4-6-7-13(3,9-18-11(14)16)10-19-12(17)15-8-5-2/h5H,2,4,6-10H2,1,3H3,(H2,14,16)(H,15,17)	-3.565
InChI=1S/C16H32O2/c1-3-5-7-9-11-13-15-18-16(17)14-12-10-8-6-4-2/h3-15H2,1-2H3	-6.71
InChI=1S/C14H15Cl2N3O2/c1-2-11-6-20-14(21-11,7-19-9-17-8-18-19)12-4-3-10(15)5-13(12)16/h3-5,8-9,11H,2,6-7H2,1H3	-3.613
InChI=1S/C15H24O2/c1-12(2)6-4-7-14-8-5-9-15(10-14)11-17-13(3)16/h6,8,15H,4-5,7,9-11H2,1-3H3	-4.976
InChI=1S/C17H16O3/c1-11-7-8-14(9-12(11)2)16(18)10-13-5-3-4-6-15(13)17(19)20/h3-9H,10H2,1-2H3,(H,19,20)	-4.586
InChI=1S/C17H19N3/c1-19(2)14-7-5-12-9-13-6-8-15(20(3)4)11-17(13)18-16(12)10-14/h5-11H,1-4H3	-2.579
InChI=1S/C8H7BrN4O4S3/c9-5-1-3-6(4-2-5)20(16,17)13-7-11-12-8(18-7)19(10,14)15/h1-4H,(H,11,13)(H2,10,14,15)	-2.13
InChI=1S/C9H5ClINO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H	-1.822
InChI=1S/C12H7Cl3O/c13-8-5-6-12(10(15)7-8)16-11-4-2-1-3-9(11)14/h1-7H	-4.95
InChI=1S/C11H13BrN2/c1-14(2)7-8-6-13-11-4-3-9(12)5-10(8)11/h3-6,13H,7H2,1-2H3	-4.06
InChI=1S/C10H14N4O3/c1-12-6-11-8-7(12)9(15)14(4-5-17-3)10(16)13(8)2/h6H,4-5H2,1-3H3	-2.147
InChI=1S/C45H32N6O6/c52-39-37(40(53)47(32-21-9-2-10-22-32)46(39)31-19-7-1-8-20-31)45(h1-30,37-38H	-8.063
InChI=1S/C5H12O2/c1-5(2)7-4-3-6/h5-6H,3-4H2,1-2H3	-0.018
InChI=1S/C6H13O9P/c7-1-2(8)4(10)6(5(11)3(1)9)15-16(12,13)14/h1-11H,(H2,12,13,14)	0.108

"InChi"	"logS(M)"
InChI=1S/C15H14O3/c1-9(2)7-8-12-13(16)10-5-3-4-6-11(10)14(17)15(12)18/h3-7,16H,8H2,1-2H3	-4.124
InChI=1S/C18H26O2/c1-13(2)18-10-9-17(4,20-18)16(11-18)19-12-15-8-6-5-7-14(15)3/h5-8,13,16H,9-12H2,1-4H3	-3.639
InChI=1S/C7H6O6S/c8-6-2-1-4(14(11,12)13)3-5(6)7(9)10/h1-3,8H,(H,9,10)(H,11,12,13)	0.655
InChI=1S/C10H22O/c1-9(2)5-7-11-8-6-10(3)4/h9-10H,5-8H2,1-4H3	-3.76
InChI=1S/C5H9N3O4/c6-3(9)1-2(4(10)11)8-5(7)12/h2H,1H2,(H2,6,9)(H,10,11)(H3,7,8,12)	-0.511
InChI=1S/C6H11NO2/c8-6(9)5-1-3-7-4-2-5/h5,7H,1-4H2,(H,8,9)	0.39
InChI=1S/C8H18O5/c9-1-3-11-5-7-13-8-6-12-4-2-10/h9-10H,1-8H2	0.712
InChI=1S/C9H5ClN4/c10-7-2-1-3-8(4-7)13-14-9(5-11)6-12/h1-4,13H	-3.58
InChI=1S/C11H24N2S/c1-2-3-4-5-6-7-8-9-10-14-11(12)13/h2-10H2,1H3,(H3,12,13)	-2.71
InChI=1S/C14H14O4/c1-4-14(3,5-2)18-13(17)11-9-7-6-8-10(11)12(15)16/h1,6-9H,5H2,2-3H3,(H,15,16)	-2.667
InChI=1S/C9H9ClO3/c1-2-13-9(12)6-3-4-8(11)7(10)5-6/h3-5,11H,2H2,1H3	-3.223
InChI=1S/C12H13NO3/c14-7-10(15)8-16-11-5-1-3-9-4-2-6-13-12(9)11/h1-6,10,14-15H,7-8H2	-1.661
InChI=1S/C19H18O6/c20-17(21)16-15(24-19(25-16)13-9-5-2-6-10-13)14-11-22-18(23-14)1 h1-10,14-16,18-19H,11H2,(H,20,21)	-2.45
InChI=1S/C14H20N4O4/c1-4-5-6-7-10(19)22-9-18-8-15-12-11(18)13(20)17(3)14(21)16(12)2/h8H,4-7,9H2,1-3H3	-2.64
InChI=1S/C5H6O2/c1-3-4-7-5(2)6/h1H,4H2,2H3	-0.416
InChI=1S/C20H42/c1-4-6-8-10-12-13-15-17-19-20(3)18-16-14-11-9-7-5-2/h20H,4-19H2,1-3H3	-6.451
InChI=1S/C6H13NO3S2/c8-12(9,10)11-4-3-7-5-6-1-2-6/h6-7H,1-5H2,(H,8,9,10)	0.444
InChI=1S/C19H28N2/c1-20(2)14-9-15-21-18-12-6-4-3-5-10-16(18)17-11-7-8-13-19(17)21/h7-8,11,13H,3-6,9-10,12,14-15H2,1-2H3	-5.166
InChI=1S/C6H10N4/c1-2-4-6-7-8-9-10(6)5-3-1/h1-5H2	-1.64
InChI=1S/C8H4N2S2/c11-5-9-7-1-2-8(4-3-7)10-6-12/h1-4H	-5.375
InChI=1S/C15H20N2O/c18-15-11-14(16-9-5-2-6-10-16)12-17(15)13-7-3-1-4-8-13/h1,3-4,7-8,14H,2,5-6,9-12H2	-2.519
InChI=1S/C5H10O/c1-2-3-5-4-6-5/h5H,2-4H2,1H3	-0.573
InChI=1S/C19H34O6/c1-4-5-6-7-8-9-10-11-12-13-19(22)24-15-18(25-17(3)21)14-23-16(2)2 h18H,4-15H2,1-3H3	-6.378
InChI=1S/C7H17N/c1-2-3-4-5-6-7-8/h2-8H2,1H3	-1.85

"InChi"	"logS(M)"
InChI=1S/C23H26FN3O2/c24-19-10-8-18(9-11-19)21(28)7-4-14-26-15-12-23(13-16-26)22(29)2 h1-3,5-6,8-11H,4,7,12-17H2,(H,25,29)	-4.671
InChI=1S/C2H2Cl3NO/c3-2(4,5)1(6)7/h(H2,6,7)	-1.097
InChI=1S/C16H16ClNO3/c1-16(2,21-14-7-5-13(17)6-8-14)15(19)20-11-12-4-3-9-18-10-12/h3-10H,11H2,1-2H3	-2.744
InChI=1S/C7H6OS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)	-1.606
InChI=1S/C8H9ClO3/c1-11-6-4-3-5(9)8(12-2)7(6)10/h3-4,10H,1-2H3	-1.56
InChI=1S/C5H6N2O/c1-4-2-5(8)7-3-6-4/h2-3H,1H3,(H,6,7,8)	-0.653
InChI=1S/C7H12FNS/c8-5-3-1-2-4-6-10-7-9/h1-6H2	-3.043
InChI=1S/C17H19ClN4O4/c1-12-10-13(21(6-8-23)7-9-24)2-4-16(12)19-20-17-5-3-14(22(25)26)1 h2-5,10-11,23-24H,6-9H2,1H3/b20-19+	-6.57
InChI=1S/C7H8O7/c8-4(9)1-7(2-5(10)11)6(12)13-3-14-7/h1-3H2,(H, 8,9)(H,10,11)	-0.611
InChI=1S/C4H9Cl/c1-4(2)3-5/h4H,3H2,1-2H3	-2
InChI=1S/C17H28O2/c1-11-6-8-14(17(4,5)19-13(3)18)10-16-12(2)7-9-15(11)16/h11-12,14H,6-10H2,1-5H3	-5.023
InChI=1S/C7H4ClNO4/c8-5-2-1-4(7(10)11)3-6(5)9(12)13/h1-3H,(H, 10,11)	-2.76
InChI=1S/C9H10N2O3/c1-2-5-14-9-4-3-7(11(12)13)6-8(9)10/h2-4,6H,1,5,10H2	-2.8
InChI=1S/C6H14N2O2/c7-4-2-1-3-5(8)6(9)10/h5H,1-4,7-8H2,(H, 9,10)	0.835
InChI=1S/C12H15N5O4/c1-8(18)15-12-13-5-10-11(16-12)17(6-14-10)7-20-3-4-21-9(2)19/h5-6H,3-4,7H2,1-2H3,(H,13,15,16,18)	-0.73
InChI=1S/C7H6F3NO2S/c8-7(9,10)14(12,13)11-6-4-2-1-3-5-6/h1-5,11H	-3.448
InChI=1S/C15H14N2/c1-9-5-3-7-11-13(16)12-8-4-6-10(2)15(12)17-14(9)11/h3-8H,1-2H3,(H2,16,17)	-4.917
InChI=1S/C6H13NO4/c8-2-3-5(10)6(11)4(9)1-7-3/h3-11H,1-2H2	0.404
InChI=1S/C11H14N2S/c1-13-8-3-7-12-11(13)6-5-10-4-2-9-14-10/h2,4-6,9H,3,7-8H2,1H3/b6-5+	-4.381
InChI=1S/C12H5Cl5/c13-7-3-6(4-8(14)5-7)11-9(15)1-2-10(16)12(11)17/h1-5H	-7.95
InChI=1S/C7H7N3/c8-6-1-2-7-5(3-6)4-9-10-7/h1-4H,8H2,(H,9,10)	-0.729
InChI=1S/C7H13NO/c1-5(2)7(9)8-6(3)4/h6H,1H2,2-4H3,(H,8,9)	-0.62
InChI=1S/C12H14O4/c1-8(2)12(14)16-10-5-4-9(7-13)6-11(10)15-3/h4-8H,1-3H3	-2.589
InChI=1S/C27H30O3/c1-3-27(30-25(29)18-7-5-4-6-8-18)16-14-24-23-11-9-19-17-20(28)10-h1,4-8,17,21-24H,9-16H2,2H3	-7.75
InChI=1S/C9H11FO/c1-2-3-7-6-8(10)4-5-9(7)11/h4-6,11H, 2-3H2,1H3	-1.887
InChI=1S/C10H14O4S/c1-8-2-4-10(5-3-8)15(13,14)7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3	-0.449

"InChi"	"logS(M)"
InChI=1S/C4H6O2/c1-3(5)4(2)6/h1-2H3	0.366
InChI=1S/C8H14O4/c9-7(10)5-3-1-2-4-6-8(11)12/h1-6H2,(H,9,10)(H,11,12)	-1.167
InChI=1S/C18H22N4O2S/c1-17(2)14-8-9-18(17,3)15-13(14)10-20-16(21-15)22-25(23,24)12-6-4-7,10,14H,8-9,19H2,1-3H3,(H,20,21,22)	-4.08
InChI=1S/C27H44O3/c1-18-8-12-22(28)17-21(18)11-10-20-7-6-16-27(5)23(13-14-24(20)27)10-11,19,22-25,28-30H,1,6-9,12-17H2,2-5H3/b20-10+,21-11+	-8.731
InChI=1S/C9H21O4P/c1-4-7-11-14(10,12-8-5-2)13-9-6-3/h4-9H2,1-3H3	-1.541
InChI=1S/C15H24O2/c1-14(2,3)11-7-10(9-16)8-12(13(11)17)15(4,5)6/h7-8,16-17H,9H2,1-6H3	-4.013
InChI=1S/C10H15NO2/c1-2-11-7-10(13)8-4-3-5-9(12)6-8/h3-6,10-13H,2,7H2,1H3	-3.454
InChI=1S/C11H7FN2O4/c12-8-6-14(10(16)13-9(8)15)11(17)18-7-4-2-1-3-5-7/h1-6H,(H,13,15,16)	-2.44
InChI=1S/C12H11IN2O2/c1-8-10(13)11(16)15(12(17)14(8)2)9-6-4-3-5-7-9/h3-7H,1-2H3	-2.641
InChI=1S/C14H21NO2/c1-9-6-10(2)12(11(3)7-9)8-14(4,5)13(16)15-17/h6-7,17H,8H2,1-5H3,(H,15,16)	-3.52
InChI=1S/C10H10ClFO/c11-7-1-2-10(13)8-3-5-9(12)6-4-8/h3-6H,1-2,7H2	-2.723
InChI=1S/C25H31N3/c1-26(2)22-13-7-19(8-14-22)25(20-9-15-23(16-10-20)27(3)4)21-11-17-7-18,25H,1-6H3	-5.458
InChI=1S/C12H13N3O2/c16-9-7-8(13-1-2-13)12(17)11(15-5-6-15)10(9)14-3-4-14/h7H,1-6H2	-0.335
InChI=1S/C10H14O3/c1-8-2-4-10(5-3-8)13-7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3	-1.732
InChI=1S/C12H22O2/c1-5-14-11(13)9-7-6-8-10-12(2,3)4/h5H,1,6-10H2,2-4H3	-4.581
InChI=1S/C18H22N2O2S/c1-14(12-19(2)3)13-20-15-8-4-6-10-17(15)23(21,22)18-11-7-5-9-16(1h4-11,14H,12-13H2,1-3H3	-3.855
InChI=1S/C23H18N4O2/c1-3-26(4-2)15-10-9-14-11-16-21(29-20(14)12-15)17(13-24)23(28)27-h5-12H,3-4H2,1-2H3	-7.202
InChI=1S/C23H29N3O2/c1-18-11-13-19(14-12-18)24(2)23(28)20-9-5-6-10-21(20)25(3)22(27)1h5-6,9-14H,4,7-8,15-17H2,1-3H3	-5.455
InChI=1S/C16H21NO4/c1-10(2)17-8-13(19)9-20-14-6-4-5-12-7-15(11(3)18)21-16(12)14/h4-7,10,13,17,19H,8-9H2,1-3H3	-2.042
InChI=1S/C7H7NO3/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4,9H,5H2	-1.884
InChI=1S/C12H16N2O2/c1-2-11-12(16-9-15-11)7-10(1)8-14-5-3-13-4-6-14/h1-2,7,13H,3-6,8-9H2	-0.809

"InChi"	"logS(M)"
InChI=1S/C12H14O3/c1-4-5-10-6-7-11(15-9(2)13)12(8-10)14-3/h4,6-8H,1,5H2,2-3H3	-2.702
InChI=1S/C13H22N2O6/c1-8(2)13(5,6-20-11(18)14-9(3)16)7-21-12(19)15-10(4)17/h8H,6-7H2,1-5H3,(H,14,16,18)(H,15,17,19)	-2.083
InChI=1S/C11H18O2/c1-10(2)5-4-6-11(3)7-8-13-9-12/h5,7,9H,4,6,8H2,1-3H3/b11-7+	-3.746
InChI=1S/C13H12N2O5S/c1-20-12-6-2-10(3-7-12)14-21(18,19)13-8-4-11(5-9-13)15(16)17/h2-9,14H,1H3	-4.64
InChI=1S/C12H4Br6O/c13-5-2-8(16)12(9(17)3-5)19-10-4-6(14)1-7(15)11(10)18/h1-4H	-8.198
InChI=1S/C9H4Cl2N4/c10-8-2-1-6(3-9(8)11)14-15-7(4-12)5-13/h1-3,14H	-4.185
InChI=1S/C22H27N3O3S2/c1-30(27,28)17-7-8-21-19(15-17)25(18-5-2-3-6-20(18)29-21)12-4-11-h2-3,5-8,15-16H,4,9-14H2,1H3,(H2,23,26)	-4.371
InChI=1S/C8H18O/c1-3-4-5-6-8(2)7-9/h8-9H,3-7H2,1-2H3	-2.528
InChI=1S/C13H25NO/c15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-13/h1-12H2,(H,14,15)	-2.626
InChI=1S/C9H6N2O2/c12-8-4-3-7(11-13)6-2-1-5-10-9(6)8/h1-5,12H	-1.2
InChI=1S/C5H12O2/c1-2-3-5(7)4-6/h5-7H,2-4H2,1H3	0.982
InChI=1S/C22H25N3O4S/c1-2-29-22(27)23-16-7-8-20-18(15-16)25(17-5-3-4-6-19(17)30-20)21(h3-8,15H,2,9-14H2,1H3,(H,23,27)	-3.9
InChI=1S/C6H12O3/c1-3-8-4-5-9-6(2)7/h3-5H2,1-2H3	0.272
InChI=1S/C17H19NO4/c1-18-7-6-16-13-9-2-3-10(19)14(13)22-15(16)11(20)4-5-17(16,21)12(h2-3,12,15,19,21H,4-8H2,1H3	-1.099
InChI=1S/C20H24N2O2S/c1-3-22(4-2)12-11-21-16-10-9-14(13-23)20-18(16)19(24)15-7-5-6-8-1h5-10,21,23H,3-4,11-13H2,1-2H3	-4.689
InChI=1S/C21H27ClN2O2/c22-20-8-6-19(7-9-20)21(18-4-2-1-3-5-18)24-12-10-23(11-13-24)14-1h1-9,21,25H,10-17H2	-2.942
InChI=1S/C10H14O5/c1-7(2)10(13)15-5-4-14-9(12)6-8(3)11/h1,4-6H2,2-3H3	-1.064
InChI=1S/C6H13NO2/c1-3-5(6(8)9)7-4-2/h5,7H,3-4H2,1-2H3,(H,8,9)	-0.419
InChI=1S/C15H11N3O/c19-15-16-13(11-7-3-1-4-8-11)14(17-18-15)12-9-5-2-6-10-12/h1-10H,(H,16,18,19)	-4.161
InChI=1S/C11H18N2O2S/c1-3-5-6-7-11(4-2)8(14)12-10(16)13-9(11)15/h3-7H2,1-2H3,(H2,12,13,14,15,16)	-3.71
InChI=1S/C18H24N4O2S/c1-11(2)15-9-4-12(3)16-10-20-18(21-17(15)16)22-25(23,24)14-7-5-13h5-8,10-12,15H,4,9,19H2,1-3H3,(H,20,21,22)	-4.18
InChI=1S/C21H28O3/c1-7-8-9-10-15-14(4)18(12-17(15)22)24-20(23)19-16(11-13(2)3)21(19h7-9,11,16,18-19H,1,10,12H2,2-6H3/b9-8+	-6.215

"InChi"	"logS(M)"
InChI=1S/C24H8O6/c25-21-13-5-1-9-10-2-6-15-20-16(24(28)30-23(15)27)8-4-12(18(10)20)3-7-14(22(13)26)19(9)11(17(21)20)h1-8H	-5.594
InChI=1S/C6H7N/c1-6-4-2-3-5-7-6/h2-5H,1H3	1.031
InChI=1S/C11H25NO3S2/c1-3-5-6-8-11(7-4-2)12-9-10-16-17(13,14)15/h11-12H,3-10H2,1-2H3,(H,13,14,15)	-2.273
InChI=1S/C8H16N2O2S/c11-13(12,9-5-1-2-6-9)10-7-3-4-8-10/h1-8H2	-0.44
InChI=1S/C7H17NO5/c1-8-2-4(10)6(12)7(13)5(11)3-9/h4-13H,2-3H2,1H3	0.408
InChI=1S/C20H24N2O2/c1-3-13-11-22-9-7-15(13)18(12-22)20(23)16-6-8-21-19-5-4-14(24-2)10-17(16)19/h3-6,8,10,13,15,18,20,23H,1,7,9,11-12H2,2H3	-3.36
InChI=1S/C17H18N2O6S/c1-17(2)11(16(24)25)19-13(21)10(14(19)26-17)18-12(20)9(15(22)23)8-7-5-3-4-6-7/h3-7,9-11,14H,1-2H3,(H,18,20)(H,22,23)(H,24,25)	-2.924
InChI=1S/C9H11NO3/c1-13-8-4-2-3-7(5-8)9(12)10-6-11/h2-5,11H,6H2,1H3,(H,10,12)	-1.29
InChI=1S/C11H17NO3S/c12-16(14,15)11-7-5-10(6-8-11)4-2-1-3-9-13/h5-8,13H,1-4,9H2,(H2,12,14,15)	-1.971
InChI=1S/C15H19N3O/c1-3-8-17-9-10-18-14(11(17)2)16-13-7-5-4-6-12(13)15(18)19/h4-7,11H,3,8-10H2,1-2H3	-2.31
InChI=1S/C10H9Cl2NO/c1-6(2)10(14)13-7-3-4-8(11)9(12)5-7/h3-5H,1H2,2H3,(H,13,14)	-4.433
InChI=1S/C12H3Cl7/c13-6-2-1-4(8(15)10(6)17)5-3-7(14)11(18)12(19)9(5)16/h1-3H	-8.057
InChI=1S/C12H22O2S/c13-15(14,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h11-12H,1-10H2	-2.06
InChI=1S/C7H6ClNO2/c1-5-2-3-6(9(10)11)4-7(5)8/h2-4H,1H3	-3.544
InChI=1S/C5H6N6/c6-3-2-4(9-1-8-2)11-5(7)10-3/h1H,(H5,6,7,8,9,10,11)	-1.8
InChI=1S/C4H5Br3FNO2/c5-4(6,7)3(11)9-2(10)1-8/h3,11H,1H2,(H,9,10)	-1.935
InChI=1S/C7H10N2/c1-5-2-3-6(8)4-7(5)9/h2-4H,8-9H2,1H3	-0.507
InChI=1S/C8H16ClF/c9-7-5-3-1-2-4-6-8-10/h1-8H2	-4.23
InChI=1S/C7H15NS/c1-3-7(4-2)8-5-6-9-7/h8H,3-6H2,1-2H3	-1.268
InChI=1S/C7H12N2O2/c1-3-5(4-2)6(10)9-7(8)11/h3H,4H2,1-2H3,(H3,8,9,10,11)/b5-3-	-2.157
InChI=1S/C21H34N2O5/c1-15(2)18-6-5-16(3)19(21(26)27-4)20(18)28-14-17(25)13-23-9-7-22(8-10-23)h5-6,15,17,24-25H,7-14H2,1-4H3	-3.284
InChI=1S/C7H14N2O3/c1-2-3-4-5(6(10)11)9-7(8)12/h5H,2-4H2,1H3,(H,10,11)(H3,8,9,12)	-2.16
InChI=1S/C10H11ClO3/c1-10(2,9(12)13)14-8-5-3-7(11)4-6-8/h3-6H,1-2H3,(H,12,13)	-2.566
InChI=1S/C12H11NO/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9H,13H2	-3.08

"InChi"	"logS(M)"
InChI=1S/C10H23O4P/c1-4-7-9-13-15(11,12-6-3)14-10-8-5-2/h4-10H2,1-3H3	-1.846
InChI=1S/C10H6Cl2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1-6H	-5.7
InChI=1S/C11H12O4S/c12-10(13)6-9(16-7-11(14)15)8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,12,13)(H,14,15)	-1.55
InChI=1S/C17H16O4/c1-13(21-17(19)15-10-6-3-7-11-15)12-20-16(18)14-8-4-2-5-9-14/h2-11,13H,12H2,1H3	-4.567
InChI=1S/C21H26N2O/c1-2-21(24)23(19-11-7-4-8-12-19)20-13-15-22(16-14-20)17-18-9-5-3-h3-12,20H,2,13-17H2,1H3	-3.415
InChI=1S/C5H10O/c1-4-5(2,3)6/h4,6H,1H2,2-3H3	0.351
InChI=1S/C11H25NO3S2/c1-3-5-6-7-8-11(4-2)12-9-10-16-17(13,14)15/h11-12H,3-10H2,1-2H3,(H,13,14,15)	-2.273
InChI=1S/C12H10Cl2N2O2S/c13-10-2-1-3-11(12(10)14)16-19(17,18)9-6-4-8(15)5-7-9/h1-7,16H,15H2	-4.73
InChI=1S/C12H6Cl4O/c13-7-2-4-11(10(16)5-7)17-12-6-8(14)1-3-9(12)15/h1-6H	-6.77
InChI=1S/C4H11N/c1-4(2,3)5/h5H2,1-3H3	1.136
InChI=1S/C13H21ClN2O4S2/c14-12-5-6-13(16-11-12)20-9-4-2-1-3-7-15-8-10-21-22(17,18)19/h5-6,11,15H,1-4,7-10H2,(H,17,18,19)	-2.686
InChI=1S/C7H13NO2/c1-4-7(9)10-6-5-8(2)3/h4H,1,5-6H2,2-3H3	0.224
InChI=1S/C14H16Cl2O2/c15-12-8-10(13(16)14(17)18)6-7-11(12)9-4-2-1-3-5-9/h6-9,13H,1-5H2,(H,17,18)	-5.542
InChI=1S/C9H9Cl2NO2/c1-12-9(13)14-5-6-3-2-4-7(10)8(6)11/h2-4H,5H2,1H3,(H,12,13)	-3.139
InChI=1S/C6H7NO4/c1-10-4-5-2-3-6(11-5)7(8)9/h2-3H,4H2,1H3	-1.155
InChI=1S/C6H10O4/c7-3-1-9-6-4(8)2-10-5(3)6/h3-8H,1-2H2	1.177
InChI=1S/C24H26N2O4/c1-28-21-10-4-5-11-22(21)29-14-13-25-15-17(27)16-30-23-12-6-9-20-h2-12,17,25-27H,13-16H2,1H3	-4.26
InChI=1S/C8H8O4/c1-12-7-3-5(4-9)2-6(10)8(7)11/h2-4,10-11H,1H3	-0.918
InChI=1S/C24H32O5/c1-21-8-5-15(25)12-23(21,27)10-7-17-16(21)6-9-22(2)18(11-19-24(17h3-4,13,15-19,25,27H,5-12H2,1-2H3	-3.773
InChI=1S/C15H21N3O3S/c1-11-5-7-14(8-6-11)22(20,21)17-15(19)16-18-9-12-3-2-4-13(12)10-1h5-8,12-13H,2-4,9-10H2,1H3,(H2,16,17,19)	-4.29
InChI=1S/C11H16O/c1-8-5-6-9(10(12)7-8)11(2,3)4/h5-7,12H,1-4H3	-2.673
InChI=1S/C8H9NO4S/c1-6-3-4-7(14(2,12)13)5-8(6)9(10)11/h3-5H,1-2H3	-2.765
InChI=1S/C12H18Br6/c13-7-1-2-8(14)10(16)5-6-12(18)11(17)4-3-9(7)15/h7-12H,1-6H2	-7.873
InChI=1S/C30H58O2/c1-3-5-7-9-11-13-15-16-17-18-19-20-22-24-26-28-30(31)32-29-27-25-h16-17H,3-15,18-29H2,1-2H3/b17-16+	-6.955
InChI=1S/C8H6N2O/c11-7-3-1-2-6-4-9-5-10-8(6)7/h1-5,11H	-2.036

"InChi"	"logS(M)"
InChI=1S/C16H15F3O/ c1-2-15(20,12-7-4-3-5-8-12)13-9-6-10-14(11-13)16(17,18)19/ h3-11,20H,2H2,1H3	-4.196
InChI=1S/C12H10N2O2/ c15-10-6-7-11(12(16)8-10)14-13-9-4-2-1-3-5-9/h1-8,13,16H/b14-11+	-3.03
InChI=1S/C24H28N2/ c1(9-19-25-21-11-17-23-13-5-3-6-14-23)2-10-20-26-22-12-18-24-15-7 h3-8,11-18,21-22H,1-2,9-10,19-20H2/b17-11+,18-12+,25-21+,26-22+	-3.894
InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-6H2,1-3H3	-4.773
InChI=1S/C12H5Cl5/ c13-6-1-2-8(10(15)4-6)9-3-7(14)5-11(16)12(9)17/h1-5H	-7.82
InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4H,5-7H2,1-3H3	-4.287
InChI=1S/C9H7NO4/c11-9(12)6-3-7-1-4-8(5-2-7)10(13)14/h1-6H,(H, 11,12)/b6-3+	-2.416
InChI=1S/C22H42O8/ c1-3-5-11-25-13-15-27-17-19-29-21(23)9-7-8-10-22(24)30-20-18-28-1 h3-20H2,1-2H3	-2.882
InChI=1S/C12H16N4O4/ c1-4-5-8(17)20-7-16-6-13-10-9(16)11(18)15(3)12(19)14(10)2/h6H, 4-5,7H2,1-3H3	-1.86
InChI=1S/C14H11Cl2NO2/ c1-9-3-2-4-11(7-9)17(19)14(18)12-6-5-10(15)8-13(12)16/h2-8,19H, 1H3	-4.47
InChI=1S/C3H9NO/c1-4-2-3-5/h4-5H,2-3H2,1H3	1.124
InChI=1S/C18H22O3/ c1-12(17(19)21-18(2,3)4)13-6-7-15-11-16(20-5)9-8-14(15)10-13/ h6-12H,1-5H3	-6.5
InChI=1S/C14H12O2/ c15-14(16)10-11-5-4-8-13(9-11)12-6-2-1-3-7-12/h1-9H,10H2,(H, 15,16)	-3.081
InChI=1S/C7H5NO3/c9-5-6-1-3-7(4-2-6)8(10)11/h1-5H	-1.81
InChI=1S/C16H23NO/ c1-18-16-8-3-2-7-15(16)13-9-10-14-6-4-5-11-17(14)12-13/ h2-3,7-8,13-14H,4-6,9-12H2,1H3	-3.552
InChI=1S/C3H6O3/c1-5-3(4)6-2/h1-2H3	0.185
InChI=1S/C22H30O4/ c1-21(2,3)17-11-13(25-7)9-15(19(17)23)16-10-14(26-8)12-18(20(16)2 h9-12,23-24H,1-8H3	-6.776
InChI=1S/C15H16N2O3/ c1-2-13(18)17-11-8-9-12(17)15(20)16(14(11)19)10-6-4-3-5-7-10/ h3-7,11-12H,2,8-9H2,1H3	-1.712
InChI=1S/C50H42Cl2N6O8/ c1-25(2)65-49(63)31-17-15-27(5)39(21-31)55-57-43-33-13-9-7-11-29(h7-26,59-60H,1-6H3,(H,53,61)(H,54,62)/b57-55+,58-56+	-7.007
InChI=1S/C17H8Br2O/ c18-9-4-5-10-11-6-7-15(19)12-2-1-3-13(16(11)12)17(20)14(10)8-9/ h1-8H	-8.696
InChI=1S/C12H22O4/c1-2-3-4-5-6-7-8-9-10(11(13)14)12(15)16/ h10H,2-9H2,1H3,(H,13,14)(H,15,16)	-3.302
InChI=1S/C12H13N3O3/ c16-12(9-13-14-7-1-2-8-14)10-3-5-11(6-4-10)15(17)18/h3-6,9H, 1-2,7-8H2/b13-9+	-2.621

"InChi"	"logS(M)"
InChI=1S/C4H8N2/c1-4-5-2-3-6-4/h2-3H2,1H3,(H,5,6)	-0.26
InChI=1S/C16H33N3O/c1-3-18(4-2)11-8-17-13-16-15(7-12-20)14-5-9-19(16)10-6-14/h14-17,20H,3-13H2,1-2H3	-1.319
InChI=1S/C9H16N2O2/c1-3-7(2)8(9(12)13)11-6-4-5-10/h7-8,11H,3-4,6H2,1-2H3,(H,12,13)	-0.982
InChI=1S/C12H8O4/c1-14-12-7-2-3-11(13)16-10(7)6-9-8(12)4-5-15-9/h2-6H,1H3	-3.6
InChI=1S/C20H25N3O/c24-19(10-9-18-6-2-1-3-7-18)11-13-22-14-16-23(17-15-22)20-8-4-5-1h1-10,12,19,24H,11,13-17H2/b10-9+	-3.222
InChI=1S/C9H8O5/c1-14-7-5(8(10)11)3-2-4-6(7)9(12)13/h2-4H,1H3,(H,10,11)(H,12,13)	-2.293
InChI=1S/C11H8N2O/c1-2-5-9-8(4-1)12-11(13-9)10-6-3-7-14-10/h1-7H,(H,12,13)	-3.414
InChI=1S/C12H8Cl2O/c13-9-6-7-11(14)12(8-9)15-10-4-2-1-3-5-10/h1-8H	-4.97
InChI=1S/C31H48O6/c1-17(2)9-8-10-20(28(35)36)26-22-15-24(34)27-29(5)13-12-23(33)18(h9,18,21-25,27,33-34H,8,10-16H2,1-7H3,(H,35,36)/b26-20+	-8.303
InChI=1S/C12H17NO2/c1-2-3-4-5-9-15-12(14)11-7-6-8-13-10-11/h6-8,10H,2-5,9H2,1H3	-2.654
InChI=1S/C13H18N2O3/c14-9-5-4-8-11(13(17)18)15-12(16)10-6-2-1-3-7-10/h1-3,6-7,11H,4-5,8-9,14H2,(H,15,16)(H,17,18)	-2.284
InChI=1S/C8H12O3/c1-2-8(9)11-6-7-4-3-5-10-7/h2,7H,1,3-6H2	-0.295
InChI=1S/C12H22O3/c1-9-5-3-7-11(13-9)15-12-8-4-6-10(2)14-12/h9-12H,3-8H2,1-2H3	-1.108
InChI=1S/C4H7ClO/c1-2-6-4-3-5/h2H,1,3-4H2	-2.395
InChI=1S/C12H7Br4O5P/c13-5-1-7(15)11(9(17)3-5)12-8(16)2-6(14)4-10(12)21-22(18,19)20/h1-4,17H,(H2,18,19,20)	-7.896
InChI=1S/C4H10N2O/c1-5-4(7)6(2)3/h1-3H3,(H,5,7)	0.303
InChI=1S/C11H20N3O3PS/c1-6-14(7-2)11-12-9(3)8-10(13-11)17-18(19,15-4)16-5/h8H,6-7H2,1-5H3	-4.133
InChI=1S/C20H27ClN2O3/c1-2-16-14-22-19(25)26-20(16)9-12-23(13-10-20)11-3-4-18(24)15-5-7h5-8,16H,2-4,9-14H2,1H3,(H,22,25)	-4.514
InChI=1S/C16H20N2O2/c1-11(9-13(3)19)17-15-5-7-16(8-6-15)18-12(2)10-14(4)20/h5-8H,9-10H2,1-4H3/b17-11-,18-12-	-1.89
InChI=1S/C8H8N4O3/c1-5(13)15-4-12-7-6(2-11-12)8(14)10-3-9-7/h2-3H,4H2,1H3,(H,9,10,14)	-2.56
InChI=1S/C10H10N2O4/c1-7(13)11-5-9-4-10(12(14)15)3-2-8(9)6-16-11/h2-4H,5-6H2,1H3	-2.253
InChI=1S/C14H8N2S4/c1-3-7-11-9(5-1)15-13(17-11)19-20-14-16-10-6-2-4-8-12(10)18-14/h1-8H	-4.522

"InChi"	"logS(M)"
InChI=1S/C35H53N3O9/c1-22(2)30(33(41)36-15-16-43-6)38-32(40)25(17-24-19-28(44-7)31(4(h10-14,19-20,22,25-27,30,39H,15-18,21H2,1-9H3,(H,36,41)(H,37,42)(H,38,40)	-4
InChI=1S/C19H20O7/c1-11(20)18-14(23)5-3-7-16(18)25-9-13(22)10-26-17-8-4-6-15(24)19(h3-8,13,22-24H,9-10H2,1-2H3	-2.173
InChI=1S/C9H10O2/c1-7-5-3-4-6-8(7)9(10)11-2/h3-6H,1-2H3	-1.757
InChI=1S/C15H24N2O/c1-6-17(7-2)10-14(18)16-15-12(4)8-11(3)9-13(15)5/h8-9H,6-7,10H2,1-5H3,(H,16,18)	-3.07
InChI=1S/C23H29NO4/c1-2-22(26)18-8-10-21(11-9-18)28-17-20(25)16-24-14-12-23(27,13-15h3-11,20,25,27H,2,12-17H2,1H3	-3.374
InChI=1S/C21H30O2/c1-5-6-7-8-16-12-19(22)21(20(23)13-16)18-11-15(4)9-10-17(18)14(2)h11-13,17-18,22-23H,2,5-10H2,1,3-4H3	-7.412
InChI=1S/C9H18NO2/c1-8(2)5-7(11)6-9(3,4)10(8)12/h7,11H,5-6H2,1-4H3	0.563
InChI=1S/C3H3N3O2/c7-6(8)3-4-1-2-5-3/h1-2H,(H,4,5)	-0.545
InChI=1S/C7H7N3/c8-6-2-1-5-4-9-10-7(5)3-6/h1-4H,8H2,(H,9,10)	-0.728
InChI=1S/C7H11N3O/c1-5-4-6(11)7(9-8-5)10(2)3/h4H,1-3H3,(H,8,11)	-0.524
InChI=1S/C10H20O2/c1-4-7-8-9(5-2)10(11)12-6-3/h9H,4-8H2,1-3H3	-3.423
InChI=1S/C9H9NO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H,(H2,10,11)/b7-6+	-1.497
InChI=1S/C22H27NO4/c1-17(24)18-6-5-9-21(14-18)27-16-20(25)15-23-12-10-22(26,11-13-2h2-9,14,20,25-26H,10-13,15-16H2,1H3	-2.853
InChI=1S/C10H14O2S/c1-8-4-2-3-5-10(8)13-7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3	-1.951
InChI=1S/C9H10FNO/c1-6-5-8(10)3-4-9(6)11-7(2)12/h3-5H,1-2H3,(H,11,12)	-1.359
InChI=1S/C6H3F3O/c7-4-1-3(10)2-5(8)6(4)9/h1-2,10H	-0.154
InChI=1S/C4H2O3/c5-3-1-2-4(6)7-3/h1-2H	0.618
InChI=1S/C41H68N8O9/c1-27(2)20-31(35(52)24-36(53)45-32(21-28(3)4)37(54)43-14-11-15-45h8-10,12-13,25-28,31-35,50-52H,11,14-24H2,1-7H3,(H,42,44)(H,43,54)(H,45,53)(H,46,56)(H,47,55)(H,48,57)	-2.37
InChI=1S/C8H18O/c1-7(2)6-9-8(3,4)5/h7H,6H2,1-5H3	0.885
InChI=1S/C12H9N3O5S/c1-7(16)20-9-5-3-2-4-8(9)11(17)14-12-13-6-10(21-12)15(18)19/h2-6H,1H3,(H,13,14,17)	-3.423
InChI=1S/C9H6Cl2O2/c10-7-2-1-3-8(11)6(7)4-5-9(12)13/h1-5H,(H,12,13)/b5-4+	-3.257
InChI=1S/C12H25N3O4/c1-4-12(8-18-10(13)16,9-19-11(14)17)7-15(5-2)6-3/h4-9H2,1-3H3,(H2,13,16)(H2,14,17)	-0.781
InChI=1S/C13H24O2/c1-5-13(3,4)11-8-6-7-9-12(11)15-10(2)14/h11-12H,5-9H2,1-4H3	-4.446
InChI=1S/C4H11N5/c1-9(2)4(7)8-3(5)6/h1-2H3,(H5,5,6,7,8)	0.889

"InChi"	"logS(M)"
InChI=1S/C13H6Cl5NO3/c14-4-1-6(16)11(20)8(2-4)19-13(22)9-10(18)5(15)3-7(17)12(9)21/h1-3,20-21H,(H,19,22)	-7.106
InChI=1S/C14H26O2/c1-11(2)9-13(5,15)7-8-14(6,16)10-12(3)4/h11-12,15-16H,9-10H2,1-6H3	-2.124
InChI=1S/C12H19N3O/c1-3-6-10(7-4-2)11(16)15-12-13-8-5-9-14-12/h5,8-10H,3-4,6-7H2,1-2H3,(H,13,14,15,16)	-3.13
InChI=1S/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h2,5,7-10H,1H2	0.28
InChI=1S/C13H11N3O2/c17-12-3-1-2-10(8-12)9-15-16-13(18)11-4-6-14-7-5-11/h1-9,17H,(H,16,18)/b15-9+	-1.329
InChI=1S/C21H27NO2/c1-2-11-21(18-4-3-5-20(24)15-18)12-14-22(16-21)13-10-17-6-8-19(23h3-9,15,23-24H,2,10-14,16H2,1H3	-4.061
InChI=1S/C12H18N2O5S2/c1-18-10-4-3-9(7-11(10)19-2)5-6-14-12(13)8-20-21(15,16)17/h3-4,7H,5-6,8H2,1-2H3,(H2,13,14)(H,15,16,17)	-2.414
InChI=1S/C8H12N2O3/c1-5(10-6(2)11)7(12)3-4-8(9)13/h1,3-4H2,2H3,(H2,9,13)(H,10,11)	0.735
InChI=1S/C12H22O/c13-12-10-8-6-4-2-1-3-5-7-9-11-12/h1-11H2	-3.846
InChI=1S/C10H6Cl6O/c11-6-7(12)9(14)5-3(1-2-4(5)17)8(6,13)10(9,15)16/h1-5,17H	-5.46
InChI=1S/C16H24N2O/c1-10-8-13(16(3,4)5)15(19)11(2)12(10)9-14-17-6-7-18-14/h8,19H,6-7,9H2,1-5H3,(H,17,18)	-5.279
InChI=1S/C10H11ClN2O/c1-13(2)12-7-10(14)8-3-5-9(11)6-4-8/h3-7H,1-2H3/b12-7+	-1.927
InChI=1S/C2H7NO4S2/c1-8(4,5)3-9(2,6)7/h3H,1-2H3	0.04
InChI=1S/C10H15NO2S/c1-2-3-9-11-14(12,13)10-7-5-4-6-8-10/h4-8,11H,2-3,9H2,1H3	-2.676
InChI=1S/C13H20N2O3/c1-3-15(4-2)7-8-18-13(17)11-6-5-10(14)9-12(11)16/h5-6,9,16H,3-4,7-8,14H2,1-2H3	-2.09
InChI=1S/C11H21N/c1-10(2)8-5-6-9(7-8)11(10,3)12-4/h8-9,12H,5-7H2,1-4H3	-2.173
InChI=1S/C8H10N2O3/c1-2-13-8-4-3-6(10(11)12)5-7(8)9/h3-5H,2,9H2,1H3	-3.211
InChI=1S/C10H12O3/c1-7-3-8(2)5-9(4-7)13-6-10(11)12/h3-5H,6H2,1-2H3,(H,11,12)	-2.353
InChI=1S/C4H10N2O6/c1-2-4(12-6(9)10)3-11-5(7)8/h4H,2-3H2,1H3,(H,7,8)(H,9,10)/q+2	-1.89
InChI=1S/C20H24N2O4/c1-21-11-10-15-12-19(25-2)20(26-3)13-16(15)18(21)9-8-14-6-4-5-7-17h4-7,12-13,18H,8-11H2,1-3H3	-4.629
InChI=1S/C12H12N2O2/c1-14(2)12(16)11(15)9-7-13-10-6-4-3-5-8(9)10/h3-7,13H,1-2H3	-1.371
InChI=1S/C8H10ClNO2/c1-11-7-4-6(10)8(12-2)3-5(7)9/h3-4H,10H2,1-2H3	-3.006
InChI=1S/C8H5Cl3O3/c9-4-1-5(10)8(11)6(2-4)14-3-7(12)13/h1-2H,3H2,(H,12,13)	-3

"InChi"	"logS(M)"
InChI=1S/C13H19ClN2O2/c1-2-3-7-18-8-6-16-12-5-4-10(14)9-11(12)13(15)17/h4-5,9,16H,2-3,6-8H2,1H3,(H2,15,17)	-3.729
InChI=1S/C8H6O2/c9-8-7-4-2-1-3-6(7)5-10-8/h1-4H,5H2	-0.863
InChI=1S/C13H16N2O4/c1-13(2,12(19)14-8-10(16)17)15-11(18)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H,14,19)(H,15,18)(H,16,17)	-0.56
InChI=1S/C9H6O5/c10-8(9(11)12)5-1-2-6-7(3-5)14-4-13-6/h1-3H,4H2,(H,11,12)	-1.191
InChI=1S/C19H26O3/c1-17-9-10-19(22)15(14(17)5-6-16(17)21)4-3-12-11-13(20)7-8-18(12,h11,14-15,22H,3-10H2,1-2H3	-2.68
InChI=1S/C14H20Cl2N2O/c1-3-17-14(19)12-5-4-11(2)13(10-12)18(8-6-15)9-7-16/h4-5,10H,3,6-9H2,1-2H3,(H,17,19)	-4.751
InChI=1S/C16H22N4O/c1-4-11-19(12-5-2)16(21)15-13(3)20(18-17-15)14-9-7-6-8-10-14/h6-10H,4-5,11-12H2,1-3H3	-2.269
InChI=1S/C7H13N3O/c8-7(11)10-9-6-4-2-1-3-5-6/h1-5H2,(H3,8,10,11)	-1.413
InChI=1S/C28H36O15/c1-11-21(34)23(36)25(38)27(40-11)43-26-24(37)22(35)19(10-29)42-28h4,6-9,11,19,21-29,31-38H,3,5,10H2,1-2H3	-3.185
InChI=1S/C13H14/c1-9-7-8-11(3)13-10(2)5-4-6-12(9)13/h4-8H,1-3H3	-4.92
InChI=1S/C11H14N2O/c1-14-9-2-3-11-10(6-9)8(4-5-12)7-13-11/h2-3,6-7,13H,4-5,12H2,1H3	-1.247
InChI=1S/C18H23N3O3/c1-2-18(22)20-15-9-10-16(20)13-19(12-15)11-5-7-14-6-3-4-8-17(14)2h3-8,15-16H,2,9-13H2,1H3/b7-5+	-4.219
InChI=1S/C10H13N3O2/c1-3-13(2)12-11-9-6-4-8(5-7-9)10(14)15/h4-7H,3H2,1-2H3,(H,14,15)/b12-11+	-0.42
InChI=1S/C12H22O2/c1-9(13)14-11-8-6-5-7-10(11)12(2,3)4/h10-11H,5-8H2,1-4H3	-4.297
InChI=1S/CH4N2O2S/c2-1(3)6(4)5/h(H3,2,3)(H,4,5)/p+1	-0.557
InChI=1S/C6H14O2/c1-5(7)4-6(2,3)8/h5,7-8H,4H2,1-3H3	0.927
InChI=1S/C24H32ClFO5/c1-20(2)30-19-10-16-15-6-5-13-9-14(27)7-8-21(13,3)23(15,26)17(28)h9,15-17,19,28H,5-8,10-12H2,1-4H3	-5.328
InChI=1S/C19H21NO3/c1-20-9-8-19-12-5-7-15(22-3)18(19)23-17-14(21-2)6-4-11(16(17)19)1h4-7,13,18H,8-10H2,1-3H3	-2.66
InChI=1S/C17H22O2/c1-19-17(18)16-10-8-14-11-13(7-9-15(14)16)12-5-3-2-4-6-12/h7,9,11-12,16H,2-6,8,10H2,1H3	-5.996
InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3	1.119
InChI=1S/C10H11NO3/c1-11-9(12)7-14-10(13)8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,11,12)	-1.718
InChI=1S/C13H22O2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(14)15/h6,9-11H,4-5,7-8H2,1-3H3,(H,14,15)	-4.608

"InChi"	"logS(M)"
InChI=1S/C20H41NO/c1-4-7-10-11-12-13-14-15-16-17-20(22)21(18-8-5-2)19-9-6-3/h4-19H2,1-3H3	-7.016
InChI=1S/C25H38O2/c1-7-8-9-10-17(3)18(4)19-14-22(26)24-20-13-16(2)11-12-21(20)25(5,h14-18,26H,7-13H2,1-6H3	-9.472
InChI=1S/C10H9NO4S/c11-8-5-4-6-7(2-1-3-9(6)12)10(8)16(13,14)15/h1-5,12H,11H2,(H,13,14,15)	-2.06
InChI=1S/C18H25NO4/c1-6-9-19-10-14(20)11-23-17-15(12(2)3)8-7-13(4)16(17)18(21)22-5/h1,7-8,12,14,19-20H,9-11H2,2-5H3	-2.709
InChI=1S/C12H13NO2/c1-15-9-12(14)13-8-4-6-10-5-2-3-7-11(10)13/h2-7H,8-9H2,1H3	-1.844
InChI=1S/C30H47N/c1-3-5-7-9-11-13-15-19-27-21-17-23-29(25-27)31-30-24-18-22-28(26-h17-18,21-26,31H,3-16,19-20H2,1-2H3	-7.926
InChI=1S/C18H34O4/c1-3-5-7-11-15-21-17(19)13-9-10-14-18(20)22-16-12-8-6-4-2/h3-16H2,1-2H3	-5.083
InChI=1S/C10H9Cl2NO2/c1-5-2-3-6(7(11)4-5)10(9(13)14)8(12)15-10/h2-4,8H,1H3,(H2,13,14)	-3.059
InChI=1S/C7H5NO5/c9-6-2-1-4(8(12)13)3-5(6)7(10)11/h1-3,9H,(H,10,11)	-2.263
InChI=1S/C10H10N2O4S/c11-17(15,16)8-3-1-7(2-4-8)12-9(13)5-6-10(12)14/h1-4H,5-6H2,(H2,11,15,16)	-1.285
InChI=1S/C17H18N2O4/c1-11-3-7-13(8-4-11)18-15(20)17(22,23)16(21)19-14-9-5-12(2)6-10-1h3-10,22-23H,1-2H3,(H,18,20)(H,19,21)	-3.1
InChI=1S/C10H12N4O3/c1-4-6(15)14-5-11-8-7(14)9(16)13(3)10(17)12(8)2/h5H,4H2,1-3H3	-1.1
InChI=1S/C8H18O3/c1-2-3-4-5-11-7-8(10)6-9/h8-10H,2-7H2,1H3	-1.083
InChI=1S/C12H18N2O/c1-4-13-8-11(15)14-12-9(2)6-5-7-10(12)3/h5-7,13H,4,8H2,1-3H3,(H,14,15)	-1.833
InChI=1S/C15H16N2S/c1-11-7-3-5-9-13(11)16-15(18)17-14-10-6-4-8-12(14)2/h3-10H,1-2H3,(H2,16,17,18)	-4.75
InChI=1S/C13H7Br2N3O6/c14-9-3-7(4-10(15)13(9)19)6-16-24-12-2-1-8(17(20)21)5-11(12)18(22h1-6,16H	-6.664
InChI=1S/C17H14O3/c1-2-14-16(13-5-3-4-6-15(13)20-14)17(19)11-7-9-12(18)10-8-11/h3-10,18H,2H2,1H3	-4.177
InChI=1S/C18H26N4O2/c1-3-9-21-16-14(17(23)22(10-4-2)18(21)24)19-15(20-16)13(11-5-6-11h11-13H,3-10H2,1-2H3,(H,19,20)	-4.59
InChI=1S/C7H7BrO/c8-7-4-2-1-3-6(7)5-9/h1-4,9H,5H2	-2.158
InChI=1S/C20H20FNO4/c1-3-4-11-24-20(23)14(2)25-16-6-8-17(9-7-16)26-19-10-5-15(13-22)1h5-10,12,14H,3-4,11H2,1-2H3	-5.708
InChI=1S/C3H6F2O/c1-6-2-3(4)5/h3H,2H2,1H3	-0.284

"InChi"	"logS(M)"
InChI=1S/C18H36O2/c1-4-6-13-17(5-2)14-9-7-8-11-16(3)12-10-15-18(19)20/h16-17H,4-15H2,1-3H3,(H,19,20)	-5.056
InChI=1S/C18H18ClN3S/c1-21-8-10-22(11-9-21)18-14-12-13(19)6-7-16(14)23-17-5-3-2-4-15(1h2-7,12H,8-11H2,1H3	-4.098
InChI=1S/C5H11NO/c1-4(2)3-5(6)7/h4H,3H2,1-2H3,(H2,6,7)	-0.883
InChI=1S/C10H13NO/c1-9(12)11-8-7-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3,(H,11,12)	-1.408
InChI=1S/C14H21NO2/c1-2-3-4-5-6-7-11-17-14(16)13-9-8-10-15-12-13/h8-10,12H,2-7,11H2,1H3	-3.093
InChI=1S/C10H14O3/c1-9(2)6-4-5-10(9,3)8(12)13-7(6)11/h6H,4-5H2,1-3H3	-3.099
InChI=1S/C13H15Cl2N3O6/c14-12(15)13(21)17-9(6-24-10(19)5-16)11(20)7-1-3-8(4-2-7)18(22)23h1-4,9,11-12,20H,5-6,16H2,(H,17,21)	-1.72
InChI=1S/C17H24O4/c1-2-3-4-5-6-7-8-9-16(18)21-15-12-10-14(11-13-15)17(19)20/h10-13H,2-9H2,1H3,(H,19,20)	-5.425
InChI=1S/C10H13Cl2FN2O2S2/c1-8-4-6-9(7-5-8)15(18-10(11,12)13)19(16,17)14(2)3/h4-7H,1-3H3	-5.586
InChI=1S/C36H72O2/c1-34(2)30-26-22-18-14-10-6-5-9-13-17-21-25-29-33-38-36(37)32-28-h34-35H,5-33H2,1-4H3	-7.086
InChI=1S/C7H16O/c1-4-7(8,5-2)6-3/h8H,4-6H2,1-3H3	-0.85
InChI=1S/C13H4Cl4N2O7/c14-5-1-7(16)11(3-9(5)18(21)22)25-13(20)26-12-4-10(19(23)24)6(15)h1-4H	-6.813
InChI=1S/C11H8N2/c1-2-4-10-8(3-1)9-5-6-12-7-11(9)13-10/h1-7,13H	-3.73
InChI=1S/C17H20O3/c1-4-9-20-17(18)12(2)13-5-6-15-11-16(19-3)8-7-14(15)10-13/h5-8,10-12H,4,9H2,1-3H3	-5.82
InChI=1S/C7H11N3O2/c1-5(2)7-8-4-6(9(7)3)10(11)12/h4-5H,1-3H3	-1.26
InChI=1S/C5H12O2/c1-4-5(2,3)7-6/h6H,4H2,1-3H3	-0.217
InChI=1S/C19H23NO3/c1-11(2)14-6-5-12(3)19-15(10-14)13(4)9-16(19)20-17(21)7-8-18(22)2h5-6,9-11H,7-8H2,1-4H3,(H,20,21)(H,22,23)	-5.389
InChI=1S/C10H14N4O4/c1-3-4-5-8(13(15)16)6-9-7-11-10(12(9)2)14(17)18/h6-7H,3-5H2,1-2H3/b8-6-	-3.493
InChI=1S/C7H4INS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H	-4.05
InChI=1S/C4H11O4P/c1-4-8-9(5,6-2)7-3/h4H2,1-3H3	0.511
InChI=1S/C6H14N2O/c1-8(2)5-3-4-7-6-9/h6H,3-5H2,1-2H3,(H,7,9)	0.885
InChI=1S/C13H13ClN2O3S/c1-19-13-11(14)3-2-4-12(13)16-20(17,18)10-7-5-9(15)6-8-10/h2-8,16H,15H2,1H3	-4.15
InChI=1S/C17H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-2/h3-16H2,1-2H3	-7.83

"InChi"	"logS(M)"
InChI=1S/C34H35N3O10/c1-15-28(38)20(35)12-23(46-15)47-22-14-34(44,16(2)36-37-33(43)17-11,15,20,22-23,28,38,40,42,44H,12-14,35H2,1-3H3,(H,37,43)/b36-16+	-8.043
InChI=1S/C19H18N4O3/c1-3-26-19(25)14-9-11-15(12-10-14)20-21-17-13(2)22-23(18(17)24)16-4-12,17H,3H2,1-2H3/b21-20+	-6.351
InChI=1S/C19H22N2OS/c1-14(22)15-9-10-19-17(13-15)21(12-6-11-20(2)3)16-7-4-5-8-18(16)24-5,7-10,13H,6,11-12H2,1-3H3	-3.565
InChI=1S/C15H15ClN2OS/c16-10-2-5-14-13(8-10)18(7-1-6-17)12-4-3-11(19)9-15(12)20-14/h2-5,8-9,19H,1,6-7,17H2	-5.659
InChI=1S/C15H20N2O4/c1-3-15(4-2,12(18)17-14(16)20)13(19)21-10-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-2H3,(H3,16,17,18,20)	-3.66
InChI=1S/C12H10Cl2N2O2S/c13-8-1-6-11(14)12(7-8)16-19(17,18)10-4-2-9(15)3-5-10/h1-7,16H,15H2	-4.4
InChI=1S/C7H15NO2/c1-5(2)4-6(8-3)7(9)10/h5-6,8H,4H2,1-3H3,(H,9,10)	-0.515
InChI=1S/C6H14NO5P/c1-11-13(10,12-2)4-3-6(9)7-5-8/h8H,3-5H2,1-2H3,(H,7,9)	1.578
InChI=1S/C4HCl5/c5-2(4(8)9)1-3(6)7/h1H	-4.23
InChI=1S/C18H22N2O/c1-4-8-17(18(21)20-19-13(2)3)16-12-7-10-14-9-5-6-11-15(14)16/h4-7,9-13,17,19H,1,8H2,2-3H3,(H,20,21)	-4.673
InChI=1S/C18H19NO4/c1-19-8-7-17-14-10-3-4-12(22-2)15(14)23-16(17)11(20)5-6-18(17,21)h3-6,13,16,21H,7-9H2,1-2H3	-2.459
InChI=1S/C16H12O5/c1-20-11-6-13(18)15-14(7-11)21-8-12(16(15)19)9-2-4-10(17)5-3-9/h2-8,17-18H,1H3	-4.481
InChI=1S/C14H26O2/c1-6-15-14(16-7-2)11-13(5)10-8-9-12(3)4/h9,11,14H,6-8,10H2,1-5H3/b13-11-	-2.355
InChI=1S/C24H31FO5S/c1-13-10-18-17-7-6-15-11-16(27)8-9-21(15,3)23(17,25)19(28)12-22(1h8-9,11,13,17-19,28H,6-7,10,12H2,1-5H3	-6.22
InChI=1S/C21H26N2O3/c1-17(24)18-6-5-9-21(14-18)26-16-20(25)15-22-10-12-23(13-11-22)1h2-9,14,20,25H,10-13,15-16H2,1H3	-2.588
InChI=1S/C24H32O6/c1-13-9-16-17-6-8-24(29,20(28)12-30-14(2)25)23(17,4)11-19(27)21(1h5,7,10,13,16-17,19,21,27,29H,6,8-9,11-12H2,1-4H3	-4.421
InChI=1S/C6H4Cl2N2O2/c7-4-1-3(6(11)10-12)2-5(8)9-4/h1-2,12H,(H,10,11)	-1.321
InChI=1S/C7H4Cl2O2/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3H,(H,10,11)	-2.332
InChI=1S/C7H13NO3/c1-4(2)6(7(10)11)8-5(3)9/h4,6H,1-3H3,(H,8,9)(H,10,11)	-0.36
InChI=1S/C9H14N2O2S/c1-10-8-4-6-9(7-5-8)14(12,13)11(2)3/h4-7,10H,1-3H3	-3.08

"InChi"	"logS(M)"
InChI=1S/C24H10N2O4/c27-21-13-5-1-9-10-2-6-15-20-16(24(30)26-23(15)29)8-4-12(18(10)20h1-8H,(H,25,27,28)(H,26,29,30)	-7.591
InChI=1S/C15H30O8/c1-2-3-4-13(21)23-12-15(8-19,9-20)11-22-10-14(5-16,6-17)7-18/h16-20H,2-12H2,1H3	-6.83
InChI=1S/C21H23ClFN3O/c1-3-25(4-2)11-12-26-19-10-9-15(22)13-17(19)21(24-14-20(26)27)16h5-10,13H,3-4,11-12,14H2,1-2H3	-3.926
InChI=1S/C17H16Cl2FNO2/c18-8-10-21(11-9-19)15-4-6-16(7-5-15)23-17(22)13-2-1-3-14(20)12-1h1-7,12H,8-11H2	-5.993
InChI=1S/C16H22O3/c1-11-8-12(10-16(2,3)9-11)19-15(18)13-6-4-5-7-14(13)17/h4-7,11-12,17H,8-10H2,1-3H3	-5.817
InChI=1S/C13H9NO/c15-14-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)13/h1-8,15H	-4.84
InChI=1S/C9H12OS/c1-6-4-8(10)5-7(2)9(6)11-3/h4-5,10H,1-3H3	-2.588
InChI=1S/C14H10Cl4/c1-8-4-10(14(18)7-12(8)16)5-9-2-3-11(15)6-13(9)17/h2-4,6-7H,5H2,1H3	-7.49
InChI=1S/C4H4BrN3O2/c1-2-3(8(9)10)7-4(5)6-2/h1H3,(H,6,7)	-1.791
InChI=1S/C6H11NS/c1-5-4-8-6(2,3)7-5/h4H2,1-3H3	-3.476
InChI=1S/C10H9NO3S/c11-9-6-5-7-3-1-2-4-8(7)10(9)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-1.7
InChI=1S/C8H8N4O6/c9-8(15)11(4-7(13)14)10-3-5-1-2-6(18-5)12(16)17/h1-3H,4H2,(H2,9,15)(H,13,14)/b10-3+	-0.752
InChI=1S/C20H19O4P/c1-16-12-14-19(15-13-16)23-25(21,22-18-9-4-3-5-10-18)24-20-11-7-6h3-15H,1-2H3	-6.373
InChI=1S/C6H4N4S/c11-5-2-8-4-1-7-3-9-6(4)10-5/h1-3H,(H,7,9,10,11)	-2.71
InChI=1S/C10H13NO2/c1-8(2)13-10(12)11-9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)	-3.001
InChI=1S/C17H21N3O2/c1-3-21-15-9-5-13(6-10-15)19-17(18)20-14-7-11-16(12-8-14)22-4-2/h5-12H,3-4H2,1-2H3,(H3,18,19,20)	-2.476
InChI=1S/C4H6O5/c5-3(6)1-9-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)	0.493
InChI=1S/C20H29N5O3/c1-22-18(15-19(26)23(2)20(22)27)21-9-6-10-24-11-13-25(14-12-24)16h4-5,7-8,15,21H,6,9-14H2,1-3H3	-3.391
InChI=1S/C17H17F2N3O3/c1-17(20)6-21(7-17)14-11(18)4-9-13(12(14)19)22(8-2-3-8)5-10(15(9)h4-5,8H,2-3,6-7,20H2,1H3,(H,24,25)	-5.64
InChI=1S/C3H6Br2O/c4-1-3(5)2-6/h3,6H,1-2H2	-0.622
InChI=1S/C11H20O4/c1-3-14-10(12)8-6-5-7-9-11(13)15-4-2/h3-9H2,1-2H3	-2.041
InChI=1S/C7H13NOS/c1-4-5-10-7(2,3)6(8)9/h4H,1,5H2,2-3H3,(H2,8,9)	-1.466

"InChi"	"logS(M)"
InChI=1S/C12H6Cl4/c13-8-3-1-7(2-4-8)10-5-9(14)6-11(15)12(10)16/h1-6H	-6.77
InChI=1S/C10H14N2O2/c1-3-12(10(11)13)8-4-6-9(14-2)7-5-8/h4-7H,3H2,1-2H3,(H2,11,13)	-1.27
InChI=1S/C7H6N2/c1-3-8-5-7-6(1)2-4-9-7/h1-5,9H	-0.942
InChI=1S/C9H16N8/c1-3-5-6-17(4-2)9-13-7(10)12-8(14-9)15-16-11/h3-6H2,1-2H3,(H2,10,12,13,14)	-3.52
InChI=1S/C2H4N4/c3-6-1-4-5-2-6/h1-2H,3H2	1.075
InChI=1S/C12H24O11/c13-1-4(16)7(18)11(5(17)2-14)23-12-10(21)9(20)8(19)6(3-15)22-12/h4-21H,1-3H2	0.287
InChI=1S/C13H10N2O/c16-13-14-11-8-4-5-9-12(11)15(13)10-6-2-1-3-7-10/h1-9H,(H,14,16)	-2.425
InChI=1S/C8H13NO2/c10-5-6-1-3-9-4-2-7(11)8(6)9/h1,7-8,10-11H,2-5H2	0.712
InChI=1S/C16H22O6/c1-4-20-13-10-15(22-6-3)14(21-5-2)9-11(13)12(17)7-8-16(18)19/h9-10H,4-8H2,1-3H3,(H,18,19)	-3.3
InChI=1S/C12H6Cl4O/c13-7-4-5-10(9(15)6-7)17-11-3-1-2-8(14)12(11)16/h1-6H	-6.65
InChI=1S/C19H24N2S/c1-4-20(5-2)15(3)14-21-16-10-6-8-12-18(16)22-19-13-9-7-11-17(19)2h6-13,15H,4-5,14H2,1-3H3	-2.15
InChI=1S/C8H16N2O/c1-3-9-6-5-7-10(4-2)8(9)11/h3-7H2,1-2H3	-1.332
InChI=1S/C15H11ClF3NO4/c1-2-23-14-8-10(4-5-12(14)20(21)22)24-13-6-3-9(7-11(13)16)15(17,1h3-8H,2H2,1H3	-6.494
InChI=1S/C9H18O2/c1-3-5-6-8-11-9(10)7-4-2/h3-8H2,1-2H3	-2.467
InChI=1S/C20H25N3O4/c1-21-20(25)15-5-4-6-16(12-15)23-13-19(24)22-10-9-14-7-8-17(26-2)h4-8,11-12,23H,9-10,13H2,1-3H3,(H,21,25)(H,22,24)	-1.85
InChI=1S/C14H20O/c1-11(10-15)9-12-5-7-13(8-6-12)14(2,3)4/h5-8,10-11H,9H2,1-4H3	-3.792
InChI=1S/C10H16O/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9,11H,1-6H2	-1.63
InChI=1S/C21H33NO3/c1-3-4-7-16-24-20-12-10-19(11-13-20)21(23)25-17-8-15-22-14-6-5-9-h10-13,18H,3-9,14-17H2,1-2H3	-6.016
InChI=1S/C5H11NO2/c1-5(2,3)8-4(6)7/h1-3H3,(H2,6,7)	0.1
InChI=1S/C5H10S2/c1-5-6-3-2-4-7-5/h5H,2-4H2,1H3	-2.397
InChI=1S/C16H19FN4O3/c1-18-21-9-11(16(23)24)15(22)10-7-12(17)14(8-13(10)21)20-5-3-19(2h7-9,18H,3-6H2,1-2H3,(H,23,24)	-3.73
InChI=1S/C11H14OS2/c1-12-10-5-3-9(4-6-10)11-13-7-2-8-14-11/h3-6,11H,2,7-8H2,1H3	-4.176
InChI=1S/C7H17O4P/c1-4-7-11-12(8,9-5-2)10-6-3/h4-7H2,1-3H3	0.406
InChI=1S/C11H14OS2/c1-12-10-6-3-2-5-9(10)11-13-7-4-8-14-11/h2-3,5-6,11H,4,7-8H2,1H3	-4.176
InChI=1S/C21H32O9/c1-4-19(22)28-13-7-10-25-16-18(27-12-9-15-30-21(24)6-3)17-26-11-8h4-6,18H,1-3,7-17H2	-2.553

"InChi"	"logS(M)"
InChI=1S/C9H13N3O6/c10-9(17)4-6(15)3(11-12-4)8-7(16)5(14)2(1-13)18-8/h2,5,7-8,13-16H,1H2,(H2,10,17)(H,11,12)	0.254
InChI=1S/C15H23N3O2/c1-3-4-5-6-7-12-18(2)17-16-14-10-8-13(9-11-14)15(19)20/h8-11H,3-7,12H2,1-2H3,(H,19,20)/b17-16+	-3.39
InChI=1S/C7H7ClO2/c1-10-7-4-5(8)2-3-6(7)9/h2-4,9H,1H3	-1.501
InChI=1S/C4H12N3O4P/c1-7(4(5)6)2-3-11-12(8,9)10/h2-3H2,1H3,(H3,5,6)(H2,8,9,10)	0.705
InChI=1S/C10H19N/c1-7-10(2,3)8-4-5-9(6-8)11-7/h7-9,11H,4-6H2,1-3H3	-1.752
InChI=1S/C7H17NO/c1-3-8(4-2)6-5-7-9/h9H,3-7H2,1-2H3	0.389
InChI=1S/C3H7N/c1-3-2-4-3/h3-4H,2H2,1H3	1.243
InChI=1S/C10H14O3/c1-8-3-2-4-10(5-8)13-7-9(12)6-11/h2-5,9,11-12H,6-7H2,1H3	-1.732
InChI=1S/C9H10N4O4S3/c10-20(16,17)9-12-11-8(18-9)13-19(14,15)6-7-4-2-1-3-5-7/h1-5H,6H2,(H,11,13)(H2,10,16,17)	-2.7
InChI=1S/C16H21N3O2/c1-5-18(6-2)14-12(3)17(4)16(21)19(15(14)20)13-10-8-7-9-11-13/h7-11H,5-6H2,1-4H3	-3.098
InChI=1S/C12H11N3/c1-3-7-11(8-4-1)13-15-14-12-9-5-2-6-10-12/h1-10H,(H,13,14)	-2.596
InChI=1S/C6H12N2O5/c7-5(9)12-3-1-11-2-4-13-6(8)10/h1-4H2,(H2,7,9)(H2,8,10)	-0.516
InChI=1S/C18H19ClO6/c1-5-24-10-6-9(2)18(13(20)7-10)17(21)14-11(22-3)8-12(23-4)15(19)16h7-9H,5-6H2,1-4H3	-4.6
InChI=1S/C8H17NO/c1-8(2)7-9-3-5-10-6-4-9/h8H,3-7H2,1-2H3	-0.709
InChI=1S/C15H21NO4/c1-3-5-10-20-13-8-6-12(7-9-15(17)16-18)11-14(13)19-4-2/h6-9,11,18H,3-5,10H2,1-2H3,(H,16,17)/b9-7+	-3.662
InChI=1S/C10H20N2O4/c1-2-3-4-5-8(6-15-9(11)13)7-16-10(12)14/h8H,2-7H2,1H3,(H2,11,13)(H2,12,14)	-2.184
InChI=1S/C18H19Br2NO2/c1-14-3-2-4-15(13-14)18(22)23-17-7-5-16(6-8-17)21(11-9-19)12-10-2h2-8,13H,9-12H2,1H3	-7.06
InChI=1S/C8H7NO3/c1-11-5-2-3-7-6(4-5)9-8(10)12-7/h2-4H,1H3,(H,9,10)	-1.283
InChI=1S/C6H13NO2/c1-2-3-4-5-6(8)7-9/h9H,2-5H2,1H3,(H,7,8)	-0.738
InChI=1S/C10H13NO2/c1-7(2)11-10(13)8-5-3-4-6-9(8)12/h3-7,12H,1-2H3,(H,11,13)	-1.986
InChI=1S/C12H6Cl4O/c13-7-1-3-9(4-2-7)17-12-10(15)5-8(14)6-11(12)16/h1-6H	-6.83
InChI=1S/C14H11N/c1-10-11-6-2-4-8-13(11)15-14-9-5-3-7-12(10)14/h2-9H,1H3	-5.021
InChI=1S/C17H17Br2NO2/c18-10-12-20(13-11-19)15-6-8-16(9-7-15)22-17(21)14-4-2-1-3-5-14/h1-9H,10-13H2	-6.491

"InChi"	"logS(M)"
InChI=1S/C11H13N5O5S3/c1-7(17)13-8-3-5-9(6-4-8)24(20,21)15-10-16(2)14-11(22-10)23(12,18)h3-6H,1-2H3,(H,13,17)(H2,12,18,19)/b15-10+	-1.69
InChI=1S/C9H18N2O4/c1-4-9(2,5-14-7(10)12)6-15-8(13)11-3/h4-6H2,1-3H3,(H2,10,12)(H,11,13)	-1.611
InChI=1S/C13H29NO2/c1-2-3-4-5-6-7-8-9-10-14-11-13(16)12-15/h13-16H,2-12H2,1H3	-3.11
InChI=1S/C8H16O4/c1-2-10-5-6-12-8-7-11-4-3-9-1/h1-8H2	-0.453
InChI=1S/C21H32O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)8-9-20(13,2)19(15)18(24)11-h13-17,19,23H,4-11H2,1-3H3	-3.915
InChI=1S/C12H10O2/c13-11-7-6-10(8-12(11)14)9-4-2-1-3-5-9/h1-8,13-14H	-2.066
InChI=1S/C26H20N2O2S2/c29-25(19-11-3-1-4-12-19)27-21-15-7-9-17-23(21)31-32-24-18-10-8-1h1-18H,(H,27,29)(H,28,30)	-6.978
InChI=1S/C15H11NO2/c1-16-12-8-4-7-11-13(12)15(18)10-6-3-2-5-9(10)14(11)17/h2-8,16H,1H3	-6.3
InChI=1S/C6H4N4O4/c11-3-1-2(9-6(14)10-3)8-5(13)4(12)7-1/h(H,7,12)(H3,8,9,10,11,13,14)	-4.06
InChI=1S/C4H9NO3/c5-3(1-2-6)4(7)8/h3,6H,1-2,5H2,(H,7,8)	0.924
InChI=1S/C16H19NO6/c1-11(18)23-16-13(20-2)9-12(10-14(16)21-3)5-6-15(19)17-7-4-8-22-1h5-6,9-10H,4,7-8H2,1-3H3/b6-5+	-1.945
InChI=1S/C8H10N4O3S2/c13-3-1-11-2-4-16-8(11)10-7-9-5-6(17-7)12(14)15/h5,13H,1-4H2/b10-8-	-1.676
InChI=1S/C16H20N2O3S2/c1-11(2)8-18-9-12-4-3-5-13(6-12)16(19)14-7-15(22-10-14)23(17,20)2h3-7,10-11,18H,8-9H2,1-2H3,(H2,17,20,21)	-2.05
InChI=1S/C14H18N2/c1-10-7-8-14(16(10)2)12-9-15-13-6-4-3-5-11(12)13/h3-6,9-10,14-15H,7-8H2,1-2H3	-2.032
InChI=1S/C23H32O5/c1-22-11-9-15(24)13-14(22)3-4-16-17-5-6-19(23(17,2)12-10-18(16)22h13,16-19H,3-12H2,1-2H3,(H,25,26)	-5.08
InChI=1S/C5H6N2S/c1-8-5-6-3-2-4-7-5/h2-4H,1H3	-0.402
InChI=1S/C16H25NO3/c1-11(2)14-10-15(20-13(4)18)12(3)9-16(14)19-8-7-17(5)6/h9-11H,7-8H2,1-6H3	-2.937
InChI=1S/C6H4I2/c7-5-1-2-6(8)4-3-5/h1-4H	-5.372
InChI=1S/C10H13ClO3/c1-7-4-9(2-3-10(7)11)14-6-8(13)5-12/h2-4,8,12-13H,5-6H2,1H3	-2.533
InChI=1S/C18H20N2S/c1-19-11-10-14(12-19)13-20-15-6-2-4-8-17(15)21-18-9-5-3-7-16(18)2h2-9,14H,10-13H2,1H3	-5.93
InChI=1S/C6H8N2O3/c9-6-4(7-10)2-1-3-5(6)8-11/h10-11H,1-3H2/b7-4-,8-5+	-1.023
InChI=1S/C5H8O3/c1-2-5(7)8-4-3-6/h2,6H,1,3-4H2	0.935

"InChi"	"logS(M)"
InChI=1S/C15H12O7/c16-7-4-10(19)12-11(5-7)22-15(14(21)13(12)20)6-1-2-8(17)9(18)3-6/h1-5,14-19,21H	-1.14
InChI=1S/C11H20O4/c1-4-7-8-9(10(12)14-5-2)11(13)15-6-3/h9H,4-8H2,1-3H3	-2.816
InChI=1S/C9H13NO2/c1-12-9-5-3-2-4-8(9)10-6-7-11/h2-5,10-11H,6-7H2,1H3	-1.702
InChI=1S/C9H12O/c1-6-4-5-7(2)9(10)8(6)3/h4-5,10H,1-3H3	-1.936
InChI=1S/C9H7NO2/c1-5-3-2-4-6-7(5)8(11)9(12)10-6/h2-4H,1H3,(H,10,11,12)	-1.231
InChI=1S/C11H14O2/c1-2-6-11(12)13-9-10-7-4-3-5-8-10/h3-5,7-8H,2,6,9H2,1H3	-3.117
InChI=1S/C8H18O2/c1-2-3-4-5-7-10-8-6-9/h9H,2-8H2,1H3	-1.169
InChI=1S/C11H12O3/c1-2-11(12)14-9-8-13-10-6-4-3-5-7-10/h2-7H,1,8-9H2	-2.564
InChI=1S/C11H14N2O4/c12-9(11(17)13-6-10(15)16)5-7-1-3-8(14)4-2-7/h1-4,9,14H,5-6,12H2,(H,13,17)(H,15,16)	-1.1
InChI=1S/C10H9NO3S/c11-8-5-4-7-2-1-3-10(9(7)6-8)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-2.54
InChI=1S/C15H10ClNO2S/c16-11-4-2-10(3-5-11)15-17-12-7-9(8-14(18)19)1-6-13(12)20-15/h1-7H,8H2,(H,18,19)	-4.449
InChI=1S/C13H10O2S/c14-13(15)11-8-4-5-9-12(11)16-10-6-2-1-3-7-10/h1-9H,(H,14,15)	-4.15
InChI=1S/C4H5BrO2/c1-3(5)2-4(6)7/h2H,1H3,(H,6,7)/b3-2-	-0.6
InChI=1S/C15H30O2/c1-2-16-14-17-15-12-10-8-6-4-3-5-7-9-11-13-15/h15H,2-14H2,1H3	-5.335
InChI=1S/C11H11ClO4S/c1-16-10(13)11(6-7-11)17(14,15)9-4-2-8(12)3-5-9/h2-5H,6-7H2,1H3	-3.309
InChI=1S/C13H17N/c1-4-11-5-7-12(8-6-11)9-13(2,3)10-14/h5-8H,4,9H2,1-3H3	-3.351
InChI=1S/C17H27NO3S/c1-3-6-14(18-21-4-2)17-15(19)9-13(10-16(17)20)12-7-5-8-22-11-12/h12-13,19H,3-11H2,1-2H3/b18-14+	-3.58
InChI=1S/C20H28O/c1-3-20(21)13-11-18-17-9-8-14-6-4-5-7-15(14)16(17)10-12-19(18,20)h1,6,15-18,21H,4-5,7-13H2,2H3	-5.569
InChI=1S/C19H23I2NO2/c1-12(8-9-14-6-4-3-5-7-14)22-13(2)18(23)15-10-16(20)19(24)17(21)1h3-7,10-13,18,22-24H,8-9H2,1-2H3	-6.378
InChI=1S/C11H21N5S/c1-6-17-11-15-9(12-7(2)3)14-10(16-11)13-8(4)5/h7-8H,6H2,1-5H3,(H2,12,13,14,15,16)	-4.203
InChI=1S/C5H4ClN/c6-5-3-1-2-4-7-5/h1-4H	-0.754
InChI=1S/C11H10O/c1-12-11-8-4-6-9-5-2-3-7-10(9)11/h2-8H,1H3	-4.199
InChI=1S/C9H8O4/c10-8(11)5-6-3-1-2-4-7(6)9(12)13/h1-4H,5H2,(H,10,11)(H,12,13)	-1.052
InChI=1S/C25H36O10/c1-6-22(4,31)21(30)35-16-15-11(3)17(27)25(32)20-23(5)12(10(2)7-13h7,11-18,20,26-28,31-32H,6,8-9H2,1-5H3	-2.441

"InChi"	"logS(M)"
InChI=1S/C16H21ClN2/c1-18-14-8-9-15(18)12-19(11-14)10-4-6-13-5-2-3-7-16(13)17/h2-7,14-15H,8-12H2,1H3/b6-4+	-3.17
InChI=1S/C13H16O2/c1-2-3-11-15-13(14)10-9-12-7-5-4-6-8-12/h4-10H,2-3,11H2,1H3/b10-9+	-1.611
InChI=1S/C18H22N6O4/c1-23(2)9-12-3-5-13(6-4-12)17(26)28-8-7-27-11-24-10-20-14-15(24)2h3-6,10H,7-9,11H2,1-2H3,(H3,19,21,22,25)	-2.47
InChI=1S/C16H20O/c1-2-3-4-5-6-13-7-8-15-12-16(17)10-9-14(15)11-13/h7-12,17H,2-6H2,1H3	-5.146
InChI=1S/C6H7NO3S2/c8-4-3-12-6(11)7(4)2-1-5(9)10/h1-3H2,(H,9,10)	0.197
InChI=1S/C7H11F/c1-2-3-4-5-6-7-8/h1H,3-7H2	-2.552
InChI=1S/C11H24O3/c1-3-5-7-13-9-11(12)10-14-8-6-4-2/h11-12H,3-10H2,1-2H3	-1.626
InChI=1S/C12H20O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h6,8H,5,7,9H2,1-4H3/b11-8-	-3.755
InChI=1S/C9H10ClN2O5PS/c1-15-18(14,16-2)19-5-12-8-7(17-9(12)13)3-6(10)4-11-8/h3-4H,5H2,1-2H3	-2.47
InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4H,1-2,5-7H2	-3.34
InChI=1S/C12H5Cl5/c13-8-3-1-2-6(12(8)17)7-4-10(15)11(16)5-9(7)14/h1-5H	-7.21
InChI=1S/C13H9ClN2/c14-10-2-1-8-5-9-6-11(15)3-4-12(9)16-13(8)7-10/h1-7H,15H2	-4.58
InChI=1S/C12H10N2O4/c15-8-10-3-1-2-9(13-10)4-5-11-6-7-12(18-11)14(16)17/h1-7,15H,8H2/b5-4+	-2.556
InChI=1S/C7H7NO3S3/c8-14(10,11)6-3-5-7(13-6)4(9)1-2-12-5/h3H,1-2H2,(H2,8,10,11)	-3.49
InChI=1S/C12H5Cl5/c13-7-3-1-2-6(4-7)10-11(16)8(14)5-9(15)12(10)17/h1-5H	-7.76
InChI=1S/C10H16O/c1-7-4-8(2)10(6-11)9(3)5-7/h4,6,8-10H,5H2,1-3H3	-1.844
InChI=1S/C8H8O2/c9-7-10-6-8-4-2-1-3-5-8/h1-5,7H,6H2	-1.673
InChI=1S/C7H5NO4/c9-7(10)5-1-3-6(4-2-5)8(11)12/h1-4H,(H,9,10)	-2.8
InChI=1S/C7H17O3P/c1-6(2)9-11(5,8)10-7(3)4/h6-7H,1-5H3	-0.052
InChI=1S/C5H9N3/c1-3-5(6)4(2)8-7-3/h6H2,1-2H3,(H,7,8)	-0.215
InChI=1S/C5H8N2O5/c6-5(12)7-2(4(10)11)1-3(8)9/h2H,1H2,(H,8,9)(H,10,11)(H3,6,7,12)	0.194
InChI=1S/C28H27ClF5NO/c29-26-12-7-21(18-25(26)28(32,33)34)27(36)13-16-35(17-14-27)15-1h3-12,18,24,36H,1-2,13-17H2	-8.385
InChI=1S/C6H8O4/c1-3-2-6(3,4(7)8)5(9)10/h3H,2H2,1H3,(H,7,8)(H,9,10)	0.841
InChI=1S/C5H6N2S/c8-4-5-3-6-1-2-7-5/h1-3,8H,4H2	-0.49
InChI=1S/C16H12O2/c1-11-15(17)13-9-5-6-10-14(13)18-16(11)12-7-3-2-4-8-12/h2-10H,1H3	-4.272

"InChi"	"logS(M)"
InChI=1S/C11H7F13O2/c1-2-5(25)26-4-3-6(12,13)7(14,15)8(16,17)9(18,19)10(20,21)11(22,23)h2H,1,3-4H2	-6.354
InChI=1S/C33H60O8/c1-5-9-13-17-21-29(34)38-25-33(26-39-30(35)22-18-14-10-6-2,27-40-h5-28H2,1-4H3	-7.068
InChI=1S/C10H7NO2/c12-10(13)8-5-1-3-7-4-2-6-11-9(7)8/h1-6H,(H,12,13)	-1.745
InChI=1S/C12H15N5O5/c1-7(18)14-12-15-10-9(11(20)16-12)13-5-17(10)6-21-3-4-22-8(2)19/h5H,3-4,6H2,1-2H3,(H2,14,15,16,18,20)	-2.14
InChI=1S/C6H13NO/c7-6(5-8)3-1-2-4-6/h8H,1-5,7H2	0.856
InChI=1S/C9H10O/c1-7-3-4-9(6-10)5-8(7)2/h3-6H,1-2H3	-2.277
InChI=1S/C2H4BrNO/c3-1-2(4)5/h1H2,(H2,4,5)	0.064
InChI=1S/C10H20O4/c1-9(2,5-11)7-14-8(13)10(3,4)6-12/h11-12H,5-7H2,1-4H3	0.068
InChI=1S/C12H4Cl6O/c13-5-1-2-8(6(14)3-5)19-9-4-7(15)10(16)12(18)11(9)17/h1-4H	-8.44
InChI=1S/C33H33N3O/c1-35(2)27-18-14-24(15-19-27)33(37,25-16-20-28(21-17-25)36(3)4)3h5-23,34,37H,1-4H3	-6.989
InChI=1S/C45H66N8O7/c1-29(2)19-36(41(56)48-26-33-18-12-17-32(20-33)25-46)50-40(55)24h7,10-12,15-18,20,27-30,35-39,54H,6,8-9,13-14,19,21-26,46H2,1-5H3,(H,47,49)(H,48,56)(H,50,55)(H,51,58)(H,52,57)(H,53,59)	-4.7
InChI=1S/C7H7NO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,8H2,(H,9,10)	-1.366
InChI=1S/C5H12N2O6/c1-4(12-6(8)9)3-5(2)13-7(10)11/h4-5H,3H2,1-2H3,(H,8,9)(H,10,11)/q+2	-2.22
InChI=1S/C6H5N3/c1-2-5-6(7-3-1)9-4-8-5/h1-4H,(H,7,8,9)	-0.327
InChI=1S/C6H9N11/c7-1-11-2(8)14-5(13-1)17-6-15-3(9)12-4(10)16-6/h(H9,7,8,9,10,11,12,13,14,15,16,17)	-4.225
InChI=1S/C19H13F/c1-12-15-8-4-2-6-13(15)10-17-16-9-5-3-7-14(16)11-18(20)19(12)17/h2-11H,1H3	-7.31
InChI=1S/C9H20O/c1-3-5-6-7-8-9(10)4-2/h9-10H,3-8H2,1-2H3	-2.661
InChI=1S/C7H14O2/c1-6-4-3-5-7(8-2)9-6/h6-7H,3-5H2,1-2H3	-0.592
InChI=1S/C7H4ClNS/c8-6-1-3-7(4-2-6)10-5-9/h1-4H	-3.039
InChI=1S/C10H18O/c1-2-3-4-5-6-7-8-9-10-11/h6-7,10H,2-5,8-9H2,1H3/b7-6+	-3.302
InChI=1S/C8H18O4/c1-2-10-5-6-12-8-7-11-4-3-9/h9H,2-8H2,1H3	0.749
InChI=1S/C9H21O3PS3/c1-6-11-13(14,12-7-2)15-8-16(10)9(3,4)5/h6-8H2,1-5H3/p+1	-2.442
InChI=1S/C14H24O4/c15-13-9-7-5-3-1-2-4-6-8-10-14(16)18-12-11-17-13/h1-12H2	-3.534
InChI=1S/C16H15ClN2OS/c1-3-10-8-12-15(11-6-4-5-7-13(11)17)18-9-14(20)19(2)16(12)21-10/h4-8H,3,9H2,1-2H3	-4.241
InChI=1S/C12H8Cl2O/c13-9-6-7-12(11(14)8-9)15-10-4-2-1-3-5-10/h1-8H	-4.63

"InChi"	"logS(M)"
InChI=1S/C15H21BrO3/c1-2-3-4-5-6-7-10-19-15(18)12-8-9-14(17)13(16)11-12/h8-9,11,17H,2-7,10H2,1H3	-4.52
InChI=1S/C11H13NO3/c1-8-3-2-4-9(5-8)12-6-10(7-13)15-11(12)14/h2-5,10,13H,6-7H2,1H3	-2.237
InChI=1S/C6H12BrF/c7-5-3-1-2-4-6-8/h1-6H2	-3.588
InChI=1S/C17H20O4/c1-11(18)10-21-17(19)12(2)13-4-5-15-9-16(20-3)7-6-14(15)8-13/h4-9,11-12,18H,10H2,1-3H3	-3.31
InChI=1S/C13H29N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h2-14H2,1H3	-4.162
InChI=1S/C7H6N2/c1-2-6-3-5-9-7(6)8-4-1/h1-5H,(H,8,9)	-1.618
InChI=1S/C14H10O3/c15-13(11-7-3-1-4-8-11)17-14(16)12-9-5-2-6-10-12/h1-10H	-4.355
InChI=1S/C22H26N2O/c25-22(19-9-5-2-6-10-19)20(17-7-3-1-4-8-17)15-23-21-16-24-13-11-1h1-10,18,20-21,23H,11-16H2	-3.699
InChI=1S/C20H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22/h6-7,9-10,12-13,15-16H,2-5,8,11,14,17-19H2,1H3,(H,21,22)/b7-6+,10-9+,13-12+,16-15+	-6.986
InChI=1S/C18H35NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17(20)19-16-18(21)22/h2-16H2,1H3,(H,19,20)(H,21,22)	-5.593
InChI=1S/C8H6Cl5NO2/c1-15-5-3(9)6(8(11,12)13)14-7(16-2)4(5)10/h1-2H3	-5.512
InChI=1S/C9H15Cl3O2/c1-4-7(5-2)8(13)14-6(3)9(10,11)12/h6-7H,4-5H2,1-3H3	-5.037
InChI=1S/C6H14N2O5S2/c7-6(5-14-15(10,11)12)8-1-3-13-4-2-9/h9H,1-5H2,(H2,7,8)(H,10,11,12)	0.588
InChI=1S/C8H7N3O5/c1-4-6(8(9)12)2-5(10(13)14)3-7(4)11(15)16/h2-3H,1H3,(H2,9,12)	-2.353
InChI=1S/C15H22N4O2/c1-20-13-4-2-12(3-5-13)19-8-6-18(7-9-19)11-14-10-17-15(16)21-14/h2-5,14H,6-11H2,1H3,(H2,16,17)	-1.899
InChI=1S/C8H10N2O3S/c1-3-2-14-7-4(9)6(11)10(7)5(3)8(12)13/h4,7H,2,9H2,1H3,(H,12,13)	-3.045
InChI=1S/C12H8O3S/c13-16(14)11-7-3-1-5-9(11)15-10-6-2-4-8-12(10)16/h1-8H	-4.481
InChI=1S/C8H12N2O3S/c1-8(2)4(7(12)13)10-5(11)3(9)6(10)14-8/h3-4,6H,9H2,1-2H3,(H,12,13)	-1.944
InChI=1S/C33H45NO11/c1-16(35)45-33-21-18(13-31(39,28(43-6)26(33)37)27(21)44-29(38)17h7-11,18-28,36-37,39H,12-15H2,1-6H3	-2.014
InChI=1S/C10H10ClNO2/c11-6-5-9-12-10(13)7-3-1-2-4-8(7)14-9/h1-4,9H,5-6H2,(H,12,13)	-3.387
InChI=1S/C52H99N5O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-47-45-49(58)56(h47-48,53-55H,3-46H2,1-2H3	-10.235
InChI=1S/C13H20O4/c1-2-3-8-16-12-6-4-5-7-13(12)17-10-11(15)9-14/h4-7,11,14-15H,2-3,8-10H2,1H3	-2.573

"InChi"	"logS(M)"
InChI=1S/C12H4Cl6/c13-7-1-5(2-8(14)11(7)17)6-3-9(15)12(18)10(16)4-6/h1-4H	-8.85
InChI=1S/C8H14O/c1-2-9-8-6-4-3-5-7-8/h2,8H,1,3-7H2	-2.583
InChI=1S/C18H22N4O5/c1-14-19-12-17(22(24)25)21(14)8-11-27-18(23)16-4-2-15(3-5-16)13-2h2-5,12H,6-11,13H2,1H3	-2.89
InChI=1S/C12H10Cl2N2O2S/c13-9-3-1-2-4-11(9)16-19(17,18)12-6-5-8(15)7-10(12)14/h1-7,16H,15H2	-5.11
InChI=1S/C7H6ClNO/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H2,9,10)	-1.66
InChI=1S/C9H12ClO2PS3/c1-11-13(14,12-2)16-7-15-9-5-3-8(10)4-6-9/h3-6H,7H2,1-2H3	-5.294
InChI=1S/C17H26O10/c1-6-9(19)3-7-8(15(23)24-2)5-25-16(11(6)7)27-17-14(22)13(21)12(20h5-7,9-14,16-22H,3-4H2,1-2H3	-0.591
InChI=1S/C4H6O4S2/c5-3(6)1(9)2(10)4(7)8/h1-2,9-10H,(H,5,6)(H,7,8)	0.199
InChI=1S/C25H32O2/c1-3-25(26)15-13-23-22-10-8-17-16-19(27-18-6-4-5-7-18)9-11-20(17)h1,9,11,16,18,21-23,26H,4-8,10,12-15H2,2H3	-6.984
InChI=1S/C9H14N2S2/c1-5-8(10)6(12-2)4-7(13-3)9(5)11/h4H,10-11H2,1-3H3	-2.857
InChI=1S/C8H10ClN3/c1-12(2)11-10-8-5-3-4-7(9)6-8/h3-6H,1-2H3/b11-10+	-3.129
InChI=1S/C15H24N2O3/c18-13(19)2-1-3-16-14(20)17-15-7-10-4-11(8-15)6-12(5-10)9-15/h10-12H,1-9H2,(H,18,19)(H2,16,17,20)	-1.6
InChI=1S/C10H9NO6/c1-15-7-3-6(11(13)14)5-4-17-10(12)8(5)9(7)16-2/h3H,4H2,1-2H3	-3.21
InChI=1S/C15H17N/c1-3-7-14(8-4-1)11-12-16-13-15-9-5-2-6-10-15/h1-10,16H,11-13H2	-2.723
InChI=1S/C8H19O3P/c1-2-3-4-5-6-7-8-12(9,10)11/h2-8H2,1H3,(H2,9,10,11)	-3.015
InChI=1S/C9H13N/c1-6-4-8(3)9(10)5-7(6)2/h4-5H,10H2,1-3H3	-1.955
InChI=1S/C14H28O2/c1-15-14(16-2)12-10-8-6-4-3-5-7-9-11-13-14/h3-13H2,1-2H3	-4.126
InChI=1S/C9H18/c1-8(2)9-6-4-3-5-7-9/h8-9H,3-7H2,1-2H3	-5.312
InChI=1S/C10H16O2/c1-8(2)10(11)12-9-6-4-3-5-7-9/h9H,1,3-7H2,2H3	-3.089
InChI=1S/C21H28O4/c1-15(22)13-24-19-9-5-17(6-10-19)21(3,4)18-7-11-20(12-8-18)25-14-h5-12,15-16,22-23H,13-14H2,1-4H3	-3.5
InChI=1S/C8H9N5/c1-13(2)7-4-10-6-3-9-5-11-8(6)12-7/h3-5H,1-2H3	-0.09
InChI=1S/C6H4Br2/c7-5-3-1-2-4-6(5)8/h1-4H	-3.5
InChI=1S/C11H18N2O3/c1-5-11(6-2)8(14)12-10(16)13(7(3)4)9(11)15/h7H,5-6H2,1-4H3,(H,12,14,16)	-2.867
InChI=1S/C9H11NO2/c1-2-10-9(12)7-5-3-4-6-8(7)11/h3-6,11H,2H2,1H3,(H,10,12)	-1.528
InChI=1S/C9H15Cl6O4P/c10-4-1-7(13)17-20(16,18-8(14)2-5-11)19-9(15)3-6-12/h7-9H,1-6H2	-3.634

"InChi"	"logS(M)"
InChI=1S/C17H19NO2/c1-18-9-8-17-7-3-2-4-12(17)13(18)10-11-5-6-14(19)16(20)15(11)17/h2-7,12-13,19-20H,8-10H2,1H3	-1.72
InChI=1S/C20H42O/c1-3-5-7-9-11-12-14-16-18-20(19-21)17-15-13-10-8-6-4-2/h20-21H,3-19H2,1-2H3	-6.475
InChI=1S/C6H6FN3O3/c1-8-5(12)10-2-3(7)4(11)9-6(10)13/h2H,1H3,(H,8,12)(H,9,11,13)	-2.28
InChI=1S/C8H11NO6S2/c9-7-2-1-3-8(6-7)16(10,11)5-4-15-17(12,13)14/h1-3,6H,4-5,9H2,(H,12,13,14)	-1.424
InChI=1S/C8H16O3/c1-3-4-5-6-11-8(10)7(2)9/h7,9H,3-6H2,1-2H3	-1.205
InChI=1S/C15H17NO6/c1-11(17)22-13-5-3-2-4-12(13)15(19)21-10-14(18)16-6-8-20-9-7-16/h2-5H,6-10H2,1H3	-1.8
InChI=1S/C8H14O3/c1-3-7(6(2)9)4-5-8(10)11/h7H,3-5H2,1-2H3,(H,10,11)	-0.451
InChI=1S/C7H14O2/c1-4-7(8)9-5-6(2)3/h6H,4-5H2,1-3H3	-1.884
InChI=1S/C5H10O/c1-5(2)3-4-6/h4-5H,3H2,1-2H3	-0.759
InChI=1S/C5H7NO3/c1-5(2)3(7)6-4(8)9-5/h1-2H3,(H,6,7,8)	-0.36
InChI=1S/C19H41N/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-2/h20H,3-19H2,1-2H3	-7.243
InChI=1S/C10H16O2/c1-3-4-5-6-7-8-9-10(11)12-2/h3-7H2,1-2H3	-3.652
InChI=1S/C18H12N3O9PS/c22-19(23)13-1-7-16(8-2-13)28-31(32,29-17-9-3-14(4-10-17)20(24)25h1-12H	-5.679
InChI=1S/C15H23NO2/c1-2-3-4-5-6-7-8-12-18-15(17)14-10-9-11-16-13-14/h9-11,13H,2-8,12H2,1H3	-3.096
InChI=1S/C13H16O4/c1-3-9(4-2)13(16)17-11-8-6-5-7-10(11)12(14)15/h5-9H,3-4H2,1-2H3,(H,14,15)	-1.84
InChI=1S/C8H8N2O/c1-5-2-3-7-6(4-5)10-8(9)11-7/h2-4H,1H3,(H2,9,10)	-1.961
InChI=1S/C12H16O2/c1-10(2)12(13)14-9-8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3	-3.08
InChI=1S/C13H11ClO/c14-12-6-7-13(15)11(9-12)8-10-4-2-1-3-5-10/h1-7,9,15H,8H2	-3.167
InChI=1S/C13H10N4O3/c18-12-10-6-16-17(11(10)14-7-15-12)8-20-13(19)9-4-2-1-3-5-9/h1-7H,8H2,(H,14,15,18)	-4.05
InChI=1S/C16H26N2O/c1-2-3-4-5-6-7-8-9-13-18-16(19)15-11-10-12-17-14-15/h10-12,14H,2-9,13H2,1H3,(H,18,19)	-3.076
InChI=1S/C12H20ClN5OS/c1-17-4-6-18(7-5-17)11-9(20-2)10(13)15-12(16-11)14-3-8-19/h19H,3-8H2,1-2H3,(H,14,15,16)	-0.903
InChI=1S/C10H9NO4S/c11-7-2-1-6-3-8(16(13,14)15)5-10(12)9(6)4-7/h1-5,12H,11H2,(H,13,14,15)	-2.883

"InChi"	"logS(M)"
InChI=1S/C10H10N4O2S/c11-8-1-3-9(4-2-8)17(15,16)14-10-7-12-5-6-13-10/h1-7H,11H2,(H,13,14)	-3.7
InChI=1S/C4H10S/c1-4(2,3)5/h5H,1-3H3	-1.788
InChI=1S/C10H7ClO/c11-10-8-4-2-1-3-7(8)5-6-9(10)12/h1-6,12H	-2.77
InChI=1S/C8H11N/c1-6-4-3-5-7(2)8(6)9/h3-5H,9H2,1-2H3	-1.168
InChI=1S/C36H45NO2S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-26-37-35(38)29-23-22-2h17-18,20-25H,2-16,19,26H2,1H3	-7.967
InChI=1S/C12H14N2O3/c1-14-11(15)10(13-12(14)16)7-8-3-5-9(17-2)6-4-8/h3-6,10H,7H2,1-2H3,(H,13,16)	-0.89
InChI=1S/C32H46N8O6S2/c1-19(2)31(43)45-11-9-27(21(5)39(17-41)15-25-13-35-23(7)37-29(25)h13-14,17-20H,9-12,15-16H2,1-8H3,(H2,33,35,37)(H2,34,36,38)/b27-21-,28-22+	-7.467
InChI=1S/C17H19N5O/c18-13-15-12-16(14-4-2-1-3-5-14)20-21-17(15)19-6-7-22-8-10-23-11-h1-5,12H,6-11H2,(H,19,21)	-2.327
InChI=1S/C9H10BrNO/c1-6-5-8(10)3-4-9(6)11-7(2)12/h3-5H,1-2H3,(H,11,12)	-1.756
InChI=1S/C19H22N2O4/c1-25-12-2-3-16-14(9-12)13(4-6-20-16)18(22)17-8-11-5-7-21(17)10-1h2-4,6,9,11,15,17-18,22H,5,7-8,10H2,1H3,(H,23,24)	-2.03
InChI=1S/C7H8N2O/c1-6(10)9-7-4-2-3-5-8-7/h2-5H,1H3,(H,8,9,10)	-0.716
InChI=1S/C2H3Br3O2/c3-2(4,5)1(6)7/h1,6-7H	-1.708
InChI=1S/C15H16ClN3O4S2/c1-9(10-5-3-2-4-6-10)15-18-12-7-11(16)13(24(17,20)21)8-14(12)25(2h2-9,15,18-19H,1H3,(H2,17,20,21)	-4.822
InChI=1S/C14H22O/c1-2-3-5-10-14(12-15)11-13-8-6-4-7-9-13/h4,6-9,14-15H,2-3,5,10-12H2,1H3	-3.843
InChI=1S/C10H13Cl2NO/c11-5-7-13(8-6-12)9-1-3-10(14)4-2-9/h1-4,14H,5-8H2	-3.324
InChI=1S/C20H16O4/c21-15-9-5-13(6-10-15)19(14-7-11-16(22)12-8-14)17-3-1-2-4-18(17)2h1-12,19,21-22H,(H,23,24)	-3.263
InChI=1S/C36H16Cl2N4O4/c37-23-14-22(36-40-26-12-10-20-28(30(26)42-36)34(46)18-8-4-2-6-1h1-14H,(H,39,41)(H,40,42)	-4.525
InChI=1S/C44H64N8O9/c1-26(2)16-32(37(53)22-38(54)48-33(17-27(3)4)39(55)51-36(42(58)5h8-15,18,24-27,32-37,53H,16-17,19-23,45H2,1-7H3,(H,46,47)(H,48,54)(H,49,57)(H,50,56)(H,51,55)(H,52,60)(H,58,59)	-2.82
InChI=1S/C5H5N3O3/c1-7-4(3-9)2-6-5(7)8(10)11/h2-3H,1H3	-0.638
InChI=1S/C5H8O4/c1-8-4(6)3-5(7)9-2/h3H2,1-2H3	0.027
InChI=1S/C26H47O3P/c1-24(2)18-12-7-5-9-16-22-27-30(29-26-20-14-11-15-21-26)28-23-17h11,14-15,20-21,24-25H,5-10,12-13,16-19,22-23H2,1-4H3	-6.382
InChI=1S/C6H12Cl2O/c1-5(3-7)9-6(2)4-8/h5-6H,3-4H2,1-2H3	-2.003
InChI=1S/C5H4Cl6O3/c6-4(7,8)1-13-3(12)14-2-5(9,10)11/h1-2H2	-4.922

"InChi"	"logS(M)"
InChI=1S/C11H22N2O4/c1-3-5-6-11(4-2,7-16-9(12)14)8-17-10(13)15/h3-8H2,1-2H3,(H2,12,14)(H2,13,15)	-2.675
InChI=1S/C13H20N2O/c1-3-15(4-2)11-13(16)14-10-12-8-6-5-7-9-12/h5-9H,3-4,10-11H2,1-2H3,(H,14,16)	-2.635
InChI=1S/C11H11NO2/c1-12-10(13)7-9(11(12)14)8-5-3-2-4-6-8/h2-6,9H,7H2,1H3	-1.431
InChI=1S/C9H5BrO6/c10-3-1-4(7(11)12)6(9(15)16)5(2-3)8(13)14/h1-2H,(H,11,12)(H,13,14)(H,15,16)	-1.448
InChI=1S/C11H9NO4/c1-14-8-3-6(4-12)7-5-16-11(13)9(7)10(8)15-2/h3H,5H2,1-2H3	-3.48
InChI=1S/C11H17NO2/c13-8-6-12(7-9-14)10-11-4-2-1-3-5-11/h1-5,13-14H,6-10H2	0.208
InChI=1S/C9H15N3/c1-12(2)8-7-11-9-5-3-4-6-10-9/h3-6H,7-8H2,1-2H3,(H,10,11)	-0.06
InChI=1S/C9H22N2O2/c1-10(2)5-8-13-9-6-11(3)4-7-12/h12H,4-9H2,1-3H3	0.476
InChI=1S/C12H16ClNOS/c1-3-14(4-2)12(15)16-9-10-7-5-6-8-11(10)13/h5-8H,3-4,9H2,1-2H3	-4.031
InChI=1S/C17H16Br2N2O4/c18-8-10-20(11-9-19)14-4-6-16(7-5-14)25-17(22)13-2-1-3-15(12-13)2h1-7,12H,8-11H2	-7.053
InChI=1S/C19H23N3O/c1-21(2)13-8-14-23-19-17-11-6-7-12-18(17)22(20-19)15-16-9-4-3-5-1h3-7,9-12H,8,13-15H2,1-2H3	-4.047
InChI=1S/C3H8O2/c1-3(5)2-4/h3-5H,2H2,1H3	1.119
InChI=1S/C18H19ClN6O5/c1-4-23(5-2)12-6-7-15(16(9-12)20-11(3)26)21-22-18-14(19)8-13(24(2h6-10H,4-5H2,1-3H3,(H,20,26)/b22-21+	-7.116
InChI=1S/C12H15NO3/c1-2-8-13-11(14)9-16-12(15)10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,13,14)	-2.539
InChI=1S/C16H12O4/c1-2-19-15(17)13-9-12-11-6-4-3-5-10(11)7-8-14(12)20-16(13)18/h3-9H,2H2,1H3	-3.528
InChI=1S/C12H11IN2O2S/c13-9-1-5-11(6-2-9)15-18(16,17)12-7-3-10(14)4-8-12/h1-8,15H,14H2	-4.52
InChI=1S/C3H3N3O3/c7-1-4-2(8)6-3(9)5-1/h(H3,4,5,6,7,8,9)	-1.808
InChI=1S/C18H19F2N3O3/c1-2-13-12(21)7-23(13)16-11(19)5-9-15(14(16)20)22(8-3-4-8)6-10(17h5-6,8,12-13H,2-4,7,21H2,1H3,(H,25,26)	-3.81
InChI=1S/C4H7NO/c1-3(2)4(5)6/h1H2,2H3,(H2,5,6)	0.375
InChI=1S/C12H5Cl5O/c13-6-1-2-10(8(15)3-6)18-11-5-7(14)4-9(16)12(11)17/h1-5H	-7.64
InChI=1S/C21H27NO2/c1-4-10-20(21(23)24-16-15-22(5-2)6-3)19-14-9-12-17-11-7-8-13-18(1h4,7-9,11-14,20H,1,5-6,10,15-16H2,2-3H3	-5.006
InChI=1S/C8H12N2O3/c1-4-5-6(11)9(2)8(13)10(3)7(5)12/h5H,4H2,1-3H3	-0.615
InChI=1S/C14H30O2/c1-2-3-4-5-6-7-8-9-10-11-13-16-14-12-15/h15H,2-14H2,1H3	-1.459

"InChi"	"logS(M)"
InChI=1S/C10H11N5/c1-7-12-9(11)15-10(13-7)14-8-5-3-2-4-6-8/h2-6H,1H3,(H3,11,12,13,14,15)	-2.753
InChI=1S/C2H7NO3S2/c3-1-2-7-8(4,5)6/h1-3H2,(H,4,5,6)	0.804
InChI=1S/C18H26O4/c1-3-5-9-13-21-17(19)15-11-7-8-12-16(15)18(20)22-14-10-6-4-2/h7-8,11-12H,3-6,9-10,13-14H2,1-2H3	-3.49
InChI=1S/C9H12N2O3/c1-6(2)14-9-4-3-7(11(12)13)5-8(9)10/h3-6H,10H2,1-2H3	-2.66
InChI=1S/C33H62O6/c1-5-9-12-15-18-21-24-30(34)37-27-33(8-4,28-38-31(35)25-22-19-16-h5-29H2,1-4H3	-6.841
InChI=1S/C9H11N/c1-7-6-8-4-2-3-5-9(8)10-7/h2-5,7,10H,6H2,1H3	-2.288
InChI=1S/C10H11NO3S/c1-2-11-10(12)9-6-4-3-5-8(9)7-15(11,13)14/h3-6H,2,7H2,1H3	-2.052
InChI=1S/C7H4ClNO4/c8-4-1-2-6(9(12)13)5(3-4)7(10)11/h1-3H,(H,10,11)	-1.319
InChI=1S/C20H24O3/c1-3-20(18(21)9-10-19(20)22)12-11-14-5-4-6-15-13-16(23-2)7-8-17(1h7-8,11,13H,3-6,9-10,12H2,1-2H3/b14-11+	-4.173
InChI=1S/C12H14N2O4/c1-14(7-10(13)15)11(16)8-18-12(17)9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H2,13,15)	-0.92
InChI=1S/C6H12O/c1-3-5-6-7-4-2/h4H,2-3,5-6H2,1H3	-2.338
InChI=1S/C8H10N2O/c1-7(11)9-10-8-5-3-2-4-6-8/h2-6,10H,1H3,(H,9,11)	-0.926
InChI=1S/C22H28N2O2/c1-24-16-6-5-8-19(24)13-10-17-7-3-4-9-21(17)23-22(25)18-11-14-20(h3-4,7,9,11-12,14-15,19H,5-6,8,10,13,16H2,1-2H3,(H,23,25)	-5.391
InChI=1S/C5H10O3/c1-3-7-5(6)8-4-2/h3-4H2,1-2H3	-0.798
InChI=1S/C8H6N2/c1-2-4-8-6-10-9-5-7(8)3-1/h1-6H	-0.415
InChI=1S/C19H19ClFNO3/c1-12(2)25-19(24)13(3)22(15-9-10-17(21)16(20)11-15)18(23)14-7-5-4h4-13H,1-3H3	-4.306
InChI=1S/C9H11NO2/c1-2-9(11)7-3-5-8(10-12)6-4-7/h3-6,10,12H,2H2,1H3	-1.436
InChI=1S/C9H9N3O2/c1-11-8(13)10-12(9(11)14)7-5-3-2-4-6-7/h2-6H,1H3,(H,10,13)	-2.98
InChI=1S/C12H28N2S/c1-5-13(6-2)9-11-15-12-10-14(7-3)8-4/h5-12H2,1-4H3	-2.366
InChI=1S/C8H8Cl2O/c1-4-3-6(11)8(10)5(2)7(4)9/h3,11H,1-2H3	-2.98
InChI=1S/C9H7NO2/c1-10-7-5-3-2-4-6(7)8(11)9(10)12/h2-5H,1H3	-0.873
InChI=1S/C16H17NO3/c18-11-3-1-8-7-10-9-2-4-12(19)15-16(9,5-6-17-10)13(8)14(11)20-15/h1-4,9-10,12,15,17-19H,5-7H2	-0.026
InChI=1S/C16H23NO3/c1-13-5-2-3-10-17(13)11-4-12-20-16(19)14-6-8-15(18)9-7-14/h6-9,13,18H,2-5,10-12H2,1H3	-3.02
InChI=1S/C16H22ClN3O/c1-15(2,3)16(21,10-20-12-18-11-19-20)9-8-13-4-6-14(17)7-5-13/h4-7,11-12,21H,8-10H2,1-3H3	-3.932

"InChi"	"logS(M)"
InChI=1S/C14H24O4/c1-3-9-17-13(15)11-7-5-6-8-12(11)14(16)18-10-4-2/h11-12H,3-10H2,1-2H3	-3.263
InChI=1S/C12H14ClN2O3PS/c1-3-16-19(20,17-4-2)18-15-12(9-14)10-7-5-6-8-11(10)13/h5-8H,3-4H2,1-2H3/b15-12+	-5.292
InChI=1S/C11H21N/c1-3-4-5-6-7-8-9-11(2)10-12/h11H,3-9H2,1-2H3	-4.632
InChI=1S/C19H36O4/c1-3-5-7-9-11-14-18(20)22-16-13-17-23-19(21)15-12-10-8-6-4-2/h3-17H2,1-2H3	-7.517
InChI=1S/C36H74S2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-38-36-34-32-h3-36H2,1-2H3	-6.058
InChI=1S/C10H9NO2/c1-7(12)13-10-6-11-9-5-3-2-4-8(9)10/h2-6,11H,1H3	-2.196
InChI=1S/CH4O3S/c1-5(2,3)4/h1H3,(H,2,3,4)	1.017
InChI=1S/C12H15NO3/c1-3-8-16-12(15)10-4-6-11(7-5-10)13-9(2)14/h4-7H,3,8H2,1-2H3,(H,13,14)	-3.29
InChI=1S/C14H24N2O4/c1-4-7-8-14(6-3,10-19-12(15)17)11-20-13(18)16-9-5-2/h2H,4,6-11H2,1,3H3,(H2,15,17)(H,16,18)	-3.53
InChI=1S/C19H14N2/c1-2-8-14(9-3-1)20-19-15-10-4-6-12-17(15)21-18-13-7-5-11-16(18)19/h1-13H,(H,20,21)	-6.225
InChI=1S/C14H18N2/c1-10-5-6-13-11(8-10)12(9-15-13)14-4-3-7-16(14)2/h5-6,8-9,14-15H,3-4,7H2,1-2H3	-2.144
InChI=1S/C17H17NO3/c1-2-21-17(20)13-10-11-18-14(13)8-9-15(18)16(19)12-6-4-3-5-7-12/h3-9,13H,2,10-11H2,1H3	-4.2
InChI=1S/C8H7N/c9-7-6-8-4-2-1-3-5-8/h1-5H,6H2	-3.069
InChI=1S/C12H17ClO2/c1-11(2,14)8-12(3,15)9-4-6-10(13)7-5-9/h4-7,14-15H,8H2,1-3H3	-3.278
InChI=1S/C26H32F2O7/c1-13(29)33-12-20(32)26-21(34-22(2,3)35-26)10-15-16-9-18(27)17-8-h6-8,15-16,18-19,21,31H,9-12H2,1-5H3	-5.019
InChI=1S/C3H6O3/c4-1-3(6)2-5/h1,3,5-6H,2H2	-0.489
InChI=1S/C11H8F3NO/c12-11(13,14)10(16)15-7-3-5-8-4-1-2-6-9(8)15/h1-6H,7H2	-3.155
InChI=1S/C4H7NO4/c1-2-9-4(6)3-5(7)8/h2-3H2,1H3	-1.412
InChI=1S/C26H34N2O/c1-27(2)21-9-6-19(7-10-21)12-15-28-16-14-26-13-4-3-5-23(26)25(28)h6-11,18,23,25,29H,3-5,12-17H2,1-2H3	-5.208
InChI=1S/C19H21NO3/c1-2-8-20-9-7-19-12-4-6-15(22)18(19)23-17-14(21)5-3-11(16(17)19)1h2-6,12-13,15,18,21-22H,1,7-10H2	-2.051
InChI=1S/C8H17NO/c1-4-7(3)6-8(5-2)9-10/h7,10H,4-6H2,1-3H3/b9-8-	-2.131
InChI=1S/C8H14N2O2/c1-6(2)7(8(11)12)10-5-3-4-9/h6-7,10H,3,5H2,1-2H3,(H,11,12)	-1.12

"InChi"	"logS(M)"
InChI=1S/C10H8N4O3/c15-9(13-10-11-5-6-12-10)7-1-3-8(4-2-7)14(16)17/h1-6H,(H2,11,12,13,15)	-2.259
InChI=1S/C21H29N3O/c1-16(2)24(17(3)4)15-13-21(20(22)25,18-10-6-5-7-11-18)19-12-8-9-1 h5-12,14,16-17H,13,15H2,1-4H3,(H2,22,25)	-1.7
InChI=1S/C20H24N6O5/c21-20-23-17-16(18(27)24-20)22-12-26(17)13-30-9-10-31-19(28)15-3 h1-4,12H,5-11,13H2,(H3,21,23,24,27)	-2.75
InChI=1S/C12H18N2O/c1-12(2,3)11(15)14-13-9-10-7-5-4-6-8-10/h4-8,13H,9H2,1-3H3,(H,14,15)	-2.285
InChI=1S/C3H9NO3S2/c1-4-2-3-8-9(5,6)7/h4H,2-3H2,1H3,(H,5,6,7)	0.766
InChI=1S/C5H10O/c1-2-3-4-5-6/h5H,2-4H2,1H3	-0.85
InChI=1S/C7H14O/c1-3-5-6-7(8)4-2/h3-6H2,1-2H3	-1.424
InChI=1S/C9H4O5/c10-7(11)4-1-2-5-6(3-4)9(13)14-8(5)12/h1-3H,(H,10,11)	-0.896
InChI=1S/C15H20O4S/c1-12-6-8-13(9-7-12)20(17,18)15(14(16)19-2)10-4-3-5-11-15/h6-9H,3-5,10-11H2,1-2H3	-4.61
InChI=1S/C6H6O3/c1-4-6(8)5(7)2-3-9-4/h2-3,8H,1H3	-1.063
InChI=1S/C10H11NO3/c1-10(2)6-7-4-3-5-8(11(12)13)9(7)14-10/h3-5H,6H2,1-2H3	-3.207
InChI=1S/C11H12Cl2O3/c1-7(2)16-11(14)6-15-10-4-3-8(12)5-9(10)13/h3-5,7H,6H2,1-2H3	-3.848
InChI=1S/C10H18O4/c1-2-3-4-8(7-10(13)14)5-6-9(11)12/h8H,2-7H2,1H3,(H,11,12)(H,13,14)	-1.397
InChI=1S/C4H7NO/c1-4(2,6)3-5/h6H,1-2H3	1.07
InChI=1S/C23H14Cl2N6O8S2/c24-21-29-22(25)31-23(30-21)28-12-7-9(5-6-14(12)40(34,35)36)27-1 h1-8,27H,26H2,(H,34,35,36)(H,37,38,39)(H,28,29,30,31)	0.196
InChI=1S/C8H11N3O4/c1-3-15-8(12)5-10-4-7(11(13)14)9-6(10)2/h4H,3,5H2,1-2H3	-2.002
InChI=1S/C12H12N2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H,13-14H2	-2.7
InChI=1S/C19H29NO4/c1-5-23-19(21)17-15(4)6-7-16(14(2)3)18(17)24-13-10-20-8-11-22-12-h6-7,14H,5,8-13H2,1-4H3	-3.81
InChI=1S/C3H3Cl3O3/c4-3(5,6)1(7)2(8)9/h1,7H,(H,8,9)	0.36
InChI=1S/C30H41FO7/c1-25(2,3)15-24(35)36-16-22(34)30-23(37-26(4,5)38-30)13-20-19-9-8 h10-12,19-21,23,33H,8-9,13-16H2,1-7H3	-5.124
InChI=1S/C12H22O2/c1-5-7-8-11(6-2)9-14-12(13)10(3)4/h11H,3,5-9H2,1-2,4H3	-4.806
InChI=1S/C6H12ClO4P/c1-3-9-12(8,10-4-2)11-6-5-7/h5-6H,3-4H2,1-2H3/b6-5+	-1.332
InChI=1S/C6H6N4O/c1-4-2-5(11)6-8-7-3-10(6)9-4/h2-3,9H,1H3	-0.281
InChI=1S/C11H15NO/c1-11(2,3)12(13)9-10-7-5-4-6-8-10/h4-9H,1-3H3/b12-9-	-1.57
InChI=1S/C12H24N2O4/c1-4-6-7-14-11(16)18-9-12(3,5-2)8-17-10(13)15/h4-9H2,1-3H3,(H2,13,15)(H,14,16)	-3.175

"InChi"	"logS(M)"
InChI=1S/C9H10N4O4/c1-11-6-5(7(14)12(2)8(11)15)13(4-10-6)9(16)17-3/h4H,1-3H3	-1.24
InChI=1S/C19H24O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h7,9,11,14-16H,3-6,8,10H2,1-2H3	-2.82
InChI=1S/C12H18N6O/c13-11-16-8-10(19-11)9-17-4-6-18(7-5-17)12-14-2-1-3-15-12/h1-3,10H,4-9H2,(H2,13,16)	-1.293
InChI=1S/C11H16N2O2S/c1-4-6-11(7(3)5-2)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3H3,(H2,12,13,14,15,16)	-3.291
InChI=1S/C15H16O3/c1-18-13-9-7-12(8-10-13)15(17)14(16)11-5-3-2-4-6-11/h2-10,14-17H,1H3	-1.39
InChI=1S/C26H22N4O4/c1-2-34-22-10-6-5-9-21(22)28-26(33)20-15-17-7-3-4-8-19(17)23(24(2h3-15,29H,2H2,1H3,(H2,27,32)(H,28,33)/b30-23-	-7.582
InChI=1S/C9H20O/c1-3-5-7-9(10)8-6-4-2/h9-10H,3-8H2,1-2H3	-2.49
InChI=1S/C22H23F4NO2/c23-19-8-6-16(7-9-19)20(28)5-2-12-27-13-10-21(29,11-14-27)17-3-1-h1,3-4,6-9,15,29H,2,5,10-14H2	-5.035
InChI=1S/C16H15NO2/c17-15-11-5-4-10-14(15)16(18)19-12-6-9-13-7-2-1-3-8-13/h1-11H,12,17H2/b9-6+	-6.04
InChI=1S/C9H3N3/c10-4-7-1-8(5-11)3-9(2-7)6-12/h1-3H	-1.124
InChI=1S/C12H6Cl4/c13-8-3-1-2-7(4-8)12-10(15)5-9(14)6-11(12)16/h1-6H	-7.155
InChI=1S/C10H6ClN5O/c11-7-1-2-8-9(5-7)16(17)14-10(13-8)15-4-3-12-6-15/h1-6H	-3.63
InChI=1S/C6H10N2O6/c9-7(10)13-5-2-1-3-6(4-5)14-8(11)12/h5-6H,1-4H2	-2.33
InChI=1S/C12H4Br6/c13-7-3-1-5(9(15)11(7)17)6-2-4-8(14)12(18)10(6)16/h1-4H	-7.756
InChI=1S/C14H17N3O/c1-9-8-16(3)10(2)13-15-12-7-5-4-6-11(12)14(18)17(9)13/h4-7,9-10H,8H2,1-3H3	-2.09
InChI=1S/C9H10O2/c1-7(10)8-4-3-5-9(6-8)11-2/h3-6H,1-2H3	-1.869
InChI=1S/C5H10O3/c1-5(2-6,3-7)4-8/h2,7-8H,3-4H2,1H3	0.929
InChI=1S/C10H6Cl2/c11-9-5-7-3-1-2-4-8(7)6-10(9)12/h1-6H	-5.36
InChI=1S/C7H9NO3S3/c8-14(10,11)6-3-5-7(13-6)4(9)1-2-12-5/h3-4,9H,1-2H2,(H2,8,10,11)	-2.25
InChI=1S/C10H15BrO/c1-9(2)6-4-5-10(9,3)8(12)7(6)11/h6-7H,4-5H2,1-3H3	-3.693
InChI=1S/C7H9N/c1-2-7-4-3-5-8-6-7/h3-6H,2H2,1H3	0.538
InChI=1S/C4H8O2S2/c5-3-1-7-8-2-4(3)6/h3-6H,1-2H2	0.672
InChI=1S/C4H5NOS/c1-4(6)2-7-3-5/h2H2,1H3	-0.216
InChI=1S/C10H14O2S/c1-2-3-4-13-10-6-8(11)5-9(12)7-10/h5-7,11-12H,2-4H2,1H3	-2.519
InChI=1S/C7H10BrCl3O2/c1-4(2)5(8)6(12)13-3-7(9,10)11/h4-5H,3H2,1-2H3	-4.8

"InChi"	"logS(M)"
InChI=1S/C20H28O2/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(16,3)10-5-11-20(17,4)18(21)22/h6,8,12-13,17H,5,7,9-11H2,1-4H3,(H,21,22)	-4.658
InChI=1S/C4H8Br2/c5-3-1-2-4-6/h1-4H2	-2.79
InChI=1S/C12H10ClN/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H,14H2	-4.638
InChI=1S/C8H23N5/c9-1-3-11-5-7-13-8-6-12-4-2-10/h11-13H,1-10H2	0.723
InChI=1S/C14H10O3/c15-13(16)14(17)11-7-3-1-5-9(11)10-6-2-4-8-12(10)14/h1-8,17H,(H,15,16)	-1.966
InChI=1S/C14H17N3O3/c1-15-10-6-7-11(15)9-16(8-10)14(18)12-4-2-3-5-13(12)17(19)20/h2-5,10-11H,6-9H2,1H3	-2.326
InChI=1S/C12H6Cl4O/c13-7-1-3-10(15)12(5-7)17-8-2-4-9(14)11(16)6-8/h1-6H	-7.07
InChI=1S/C12H18N4O5/c1-2-3-4-9(17)8-15(12(13)18)14-7-10-5-6-11(21-10)16(19)20/h5-7,9,17H,2-4,8H2,1H3,(H2,13,18)/b14-7+	-3.572
InChI=1S/C54H90N6O18/c1-22(2)34-49(67)73-31(19)43(61)55-38(26(9)10)53(71)77-41(29(15)16)51(69)74-32(20)44(62)56-39(27(11)12)54(72)78-42(30(17)18)50(68)75-33(21)45(63)57-40(28(13)14)52(70)76-35(23(3)4)47(65)59-36(24(5)6)48(66)58-37(25(7)8)46(64)60-34/h22-42H,1-21H3,(H,55,61)(H,56,62)(H,57,63)(H,58,64)(H,59,65)(H,60,66)	-8.625
InChI=1S/C15H11ClN2/c16-12-6-7-14-13(10-12)15(18-9-8-17-14)11-4-2-1-3-5-11/h1-8,10H,9H2	-4.194
InChI=1S/C7H7NO2/c8-7(10)5-3-1-2-4-6(5)9/h1-4,9H,(H2,8,10)	-1.76
InChI=1S/C15H30O2/c1-4-5-6-7-8-9-10-11-12-13-15(16)17-14(2)3/h14H,4-13H2,1-3H3	-5.385
InChI=1S/C20H38O4S/c1-5-9-11-17(7-3)13-23-19(21)15-25-16-20(22)24-14-18(8-4)12-10-6-h17-18H,5-16H2,1-4H3	-6.655
InChI=1S/C23H27NO2/c25-22(26-17-16-24-14-8-3-9-15-24)21-18-23(21,19-10-4-1-5-11-19)2h1-2,4-7,10-13,21H,3,8-9,14-18H2	-5.024
InChI=1S/C21H24N6O3/c1-12-5-7-14(8-6-12)24-26-18-16(9-21(3,4)10-17(18)28)25-27-20(30)h5-8,11,24H,9-10H2,1-4H3,(H,27,30)(H,22,23,29)/b25-16+,26-18-	-6.536
InChI=1S/C12H13NO4/c1-9(14)13(2)11(15)8-17-12(16)10-6-4-3-5-7-10/h3-7H,8H2,1-2H3	-2.866
InChI=1S/C10H10N4OS/c1-14-7-5-3-2-4-6(7)8(9(14)15)12-13-10(11)16/h2-5H,1H3,(H3,11,13,16)/b12-8-	-3.008
InChI=1S/C18H38O/c1-18(2)16-14-12-10-8-6-4-3-5-7-9-11-13-15-17-19/h18-19H,3-17H2,1-2H3	-6.256
InChI=1S/C10H12N4O4/c1-6(15)18-5-14-4-11-8-7(14)9(16)13(3)10(17)12(8)2/h4H,5H2,1-3H3	-1.83
InChI=1S/C22H28N2O3/c1-17-14-19(18(2)25)8-9-22(17)27-16-21(26)15-23-10-12-24(13-11-2h3-9,14,21,26H,10-13,15-16H2,1-2H3	-3.158

"InChi"	"logS(M)"
InChI=1S/C7H7Cl2N3O2S/c1-2-3-15-7-10-5(8)4(12(13)14)6(9)11-7/h2-3H2,1H3	-4.387
InChI=1S/C19H14/c1-13-5-4-8-14-9-10-17-11-15-6-2-3-7-16(15)12-18(17)19(13)14/h2-12H,1H3	-6.644
InChI=1S/C10H20O2/c1-8(2)5-6-12-10(11)7-9(3)4/h8-9H,5-7H2,1-4H3	-3.554
InChI=1S/C10H9N/c1-8-6-9-4-2-3-5-10(9)7-11-8/h2-7H,1H3	-2.19
InChI=1S/C17H18Cl2N2OS/c1-21(2)10-9-17(22)20-15-8-5-13(19)11-16(15)23-14-6-3-12(18)4-7-1h3-8,11H,9-10H2,1-2H3,(H,20,22)	-6.102
InChI=1S/C9H17N3O2/c10-9(13)12-11-6-7-14-8-4-2-1-3-5-8/h6,8H,1-5,7H2,(H3,10,12,13)/b11-6+	-1.74
InChI=1S/C24H19NO6/c1-15(26)29-19-11-7-17(8-12-19)24(18-9-13-20(14-10-18)30-16(2)27)h3-14H,1-2H3,(H,25,28)	-5.556
InChI=1S/C12HCl9O/c13-2-1-3(5(15)6(16)4(2)14)22-12-10(20)8(18)7(17)9(19)11(12)21/h1H	-10.55
InChI=1S/C12H10N2O/c15-12(10-5-4-8-13-9-10)14-11-6-2-1-3-7-11/h1-9H,(H,14,15)	-3.093
InChI=1S/C13H7Br2N3O6/c14-9-3-7(4-10(15)13(9)19)6-16-24-12-2-1-8(17(20)21)5-11(12)18(22h1-6,19H/b16-6+	-5.19
InChI=1S/C10H13NO3/c1-11-9(10(13)14)6-7-2-4-8(12)5-3-7/h2-5,9,11-12H,6H2,1H3,(H,13,14)	-2.132
InChI=1S/C6H14OS2/c1-5(2)8-9(7)6(3)4/h5-6H,1-4H3/p+1	-0.823
InChI=1S/C4H6N2O/c7-2-4-1-5-3-6-4/h1,3,7H,2H2,(H,5,6)	0.815
InChI=1S/C21H26Cl2O/c1-20(2,3)13-21(4,5)16-7-9-19(24)15(11-16)10-14-6-8-17(22)12-18(1h6-9,11-12,24H,10,13H2,1-5H3	-8.224
InChI=1S/C4H11NO2/c1-4(5,2-6)3-7/h6-7H,2-3,5H2,1H3	0.978
InChI=1S/C7H4Cl2N2O/c8-3-1-5-6(2-4(3)9)12-7(10)11-5/h1-2H,(H2,10,11)	-2.994
InChI=1S/C17H28N2O2/c1-5-19(6-2)16(11-13(3)4)12-21-17(20)14-7-9-15(18)10-8-14/h7-10,13,16H,5-6,11-12,18H2,1-4H3	-3.573
InChI=1S/C6H3FN2O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H	-2.668
InChI=1S/C13H13BrN2O2/c1-9-11(14)12(17)16(13(18)15(9)2)8-10-6-4-3-5-7-10/h3-7H,8H2,1-2H3	-3.338
InChI=1S/C5H8O2/c1-4(6)5(2)3-7-5/h3H2,1-2H3	0.38
InChI=1S/C7H16N2O2/c8-5-3-1-2-4-6-9-7(10)11/h9H,1-6,8H2,(H,10,11)	-0.095
InChI=1S/C18H28O2/c1-6-13-20-18(19)14-17(5)12-8-11-16(4)10-7-9-15(2)3/h1,8,12,14-16H,7,9-11,13H2,2-5H3/b12-8+,17-14-	-4.724
InChI=1S/C12H18O4/c1-10-4-2-3-5-11(10)16-9-12(6-13,7-14)8-15/h2-5,13-15H,6-9H2,1H3	-2.122

"InChi"	"logS(M)"
InChI=1S/C24H21N5O4/c25-15-4-16-28(17-18-33-24(30)19-5-2-1-3-6-19)22-11-7-20(8-12-22)h1-3,5-14H,4,16-18H2/b27-26+	-7.17
InChI=1S/C6H6N2O6S/c7-4-1-3(8(10)11)2-5(6(4)9)15(12,13)14/h1-2,9H,7H2,(H,12,13,14)	-1.766
InChI=1S/C20H16/c1-2-16-18-10-6-4-8-15(18)13-20-17-9-5-3-7-14(17)11-12-19(16)20/h3-13H,2H2,1H3	-6.796
InChI=1S/C9H10O2/c1-2-5-9-8(4-1)10-6-3-7-11-9/h1-2,4-5H,3,6-7H2	-2.461
InChI=1S/C7H6O2/c8-5-6-3-1-2-4-7(6)9/h1-5,9H	-0.86
InChI=1S/C35H54O6P2/c1-23-15-25(31(3,4)5)29(26(16-23)32(6,7)8)40-42-36-19-35(20-37-42h15-18H,19-22H2,1-14H3	-7.801
InChI=1S/C4H9NO5/c6-1-4(2-7,3-8)5(9)10/h6-8H,1-3H2	0.821
InChI=1S/C4H9N/c1-2-4-5-3-1/h5H,1-4H2	1.15
InChI=1S/C13H15NO4/c1-3-8-18-11-6-4-10(9-12(11)17-2)5-7-13(15)14-16/h3-7,9,16H,1,8H2,2H3,(H,14,15)/b7-5+	-2.488
InChI=1S/C16H13N3O2/c1-21-13-8-11-4-3-7-18-15(11)14(9-13)19-16(20)12-5-2-6-17-10-12/h2-10H,1H3,(H,19,20)	-4.446
InChI=1S/C18H21NO5/c1-11(18(21)24-12(2)23-17(20)10-19)13-4-5-15-9-16(22-3)7-6-14(15)h4-9,11-12H,10,19H2,1-3H3	-2.44
InChI=1S/C8H10O3S2/c1-7(13(9,10)11)12-8-5-3-2-4-6-8/h2-7H,1H3,(H,9,10,11)	-0.49
InChI=1S/C4H4N2/c5-3-1-2-4-6/h1-2H2	0.175
InChI=1S/C18H21NO3/c1-2-19-17(21)22-14-18(13-20,15-9-5-3-6-10-15)16-11-7-4-8-12-16/h3-12,20H,2,13-14H2,1H3,(H,19,21)	-3.734
InChI=1S/C10H21N/c1-9(11-2)8-10-6-4-3-5-7-10/h9-11H,3-8H2,1-2H3	-2.313
InChI=1S/C9H18N2O4S2/c10-6(8(12)13)4-16-2-1-3-17-5-7(11)9(14)15/h6-7H,1-5,10-11H2,(H,12,13)(H,14,15)	-2.49
InChI=1S/C19H28N2O4S2/c1-2-8-16-15-19(21-18-10-5-4-9-17(16)18)25-13-7-3-6-11-20-12-14-2h4-5,9-10,15,20H,2-3,6-8,11-14H2,1H3,(H,22,23,24)	-4.482
InChI=1S/C12H13NO3/c14-7-10(15)8-16-12-6-5-9-3-1-2-4-11(9)13-12/h1-6,10,14-15H,7-8H2	-2.051
InChI=1S/C14H31N3/c1-13(2)10-12(11-14(3,4)16-13)15-8-7-9-17(5)6/h12,15-16H,7-11H2,1-6H3	0.316
InChI=1S/C6H4N2O3S/c7-8-5-1-3-6(4-2-5)12(9,10)11/h1-4H/p+1	-2.42
InChI=1S/C13H27NO/c1-3-4-11-15-12-7-10-14-9-6-5-8-13(14)2/h13H,3-12H2,1-2H3	-2.745
InChI=1S/C6H6ClNO/c7-4-1-2-5(8)6(9)3-4/h1-3,9H,8H2	-2.391

"InChi"	"logS(M)"
InChI=1S/C12H15NO4/c1-13(7-8-14)11(15)9-17-12(16)10-5-3-2-4-6-10/h2-6,14H,7-9H2,1H3	-1.09
InChI=1S/C6H7F3O3/c1-2-12-5(11)3-4(10)6(7,8)9/h2-3H2,1H3	-1.663
InChI=1S/C12H9NO/c14-8-5-6-10-9-3-1-2-4-11(9)13-12(10)7-8/h1-7,13-14H	-3.748
InChI=1S/C12H4Cl6O/c13-5-1-2-9(6(14)3-5)19-12-8(16)4-7(15)10(17)11(12)18/h1-4H	-8.47
InChI=1S/C15H19NO4/c1-2-11(4-12(3-1)17-9-15-10-20-15)16(5-13-7-18-13)6-14-8-19-14/h1-4,13-15H,5-10H2	-2.193
InChI=1S/C7H8O3S/c1-6-2-4-7(5-3-6)11(8,9)10/h2-5H,1H3,(H,8,9,10)	0.556
InChI=1S/C4H9NO3/c1-2-4(3-6)5(7)8/h4,6H,2-3H2,1H3	-0.344
InChI=1S/C6H8N2O4S2/c7-13(9,10)5-2-1-3-6(4-5)14(8,11)12/h1-4H,(H2,7,9,10)(H2,8,11,12)	-2.169
InChI=1S/C14H14O2/c1-3-7-13(8-4-1)15-11-12-16-14-9-5-2-6-10-14/h1-10H,11-12H2	-3.989
InChI=1S/C11H13NO3/c1-8-7-9(3-5-10(8)15-2)4-6-11(13)12-14/h3-7,14H,1-2H3,(H,12,13)/b6-4+	-2.299
InChI=1S/C3H5N3S/c1-2-5-6-3(4)7-2/h1H3,(H2,4,6)	0.151
InChI=1S/C10H9N3O2/c14-9(13-10-11-6-7-15-10)12-8-4-2-1-3-5-8/h1-7H,(H2,11,12,13,14)	-2.225
InChI=1S/C17H22N4O/c1-14-13-16(15-5-3-2-4-6-15)19-20-17(14)18-7-8-21-9-11-22-12-10-2h2-6,13H,7-12H2,1H3,(H,18,20)	-2.102
InChI=1S/C8H14O2S/c9-8(10)6-11-7-4-2-1-3-5-7/h7H,1-6H2,(H,9,10)	-1.338
InChI=1S/C5H10O2/c1-5(2,3-6)4-7/h3,7H,4H2,1-2H3	-0.328
InChI=1S/C12H16N2O/c1-13(2)11-8-12(15)14(9-11)10-6-4-3-5-7-10/h3-7,11H,8-9H2,1-2H3	-1.065
InChI=1S/C8H9NO2/c1-6-3-4-8(9(10)11)5-7(6)2/h3-5H,1-2H3	-3.179
InChI=1S/C47H73NO17/c1-27-17-15-13-11-9-7-5-6-8-10-12-14-16-18-34(64-46-44(58)41(48)4h5-18,27-38,40-44,46,49-54,56-58,61H,19-26,48H2,1-4H3,(H,59,60)/b6-5-,9-7-,10-8-,13-11-,14-12-,17-15-,18-16-	-3.091
InChI=1S/C15H16F5NO2S2/c1-6(2)5-7-8(13(22)24-3)10(12(16)17)21-11(15(18,19)20)9(7)14(23)2h6,12H,5H2,1-4H3	-5.457
InChI=1S/C7H11NO2/c1-4-7(3,5-2)10-6(8)9/h1H,5H2,2-3H3,(H2,8,9)	-0.946
InChI=1S/C27H56N2O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-27(30)28h4-26H2,1-3H3,(H,28,30)	-6.628
InChI=1S/C9H9NO2/c1-7(11)9(12)10-8-5-3-2-4-6-8/h2-6H,1H3,(H,10,12)	-1.368
InChI=1S/C5H10N2S2/c8-5(9)7-3-1-6-2-4-7/h6H,1-4H2,(H,8,9)	-0.908
InChI=1S/C11H22N2O4/c1-5-6-11(2,7-16-9(14)12-3)8-17-10(15)13-4/h5-8H2,1-4H3,(H,12,14)(H,13,15)	-2.632

"InChi"	"logS(M)"
InChI=1S/C20H26O4/c21-19(23-15-9-3-1-4-10-15)17-13-7-8-14-18(17)20(22)24-16-11-5-2-h7-8,13-16H,1-6,9-12H2	-5.513
InChI=1S/C9H18O3/c1-8(2,3)7(10)11-12-9(4,5)6/h1-6H3	-2.068
InChI=1S/C20H10Cl2N2O2/c21-9-1-3-15-11(5-9)19(25)13-8-18-14(7-17(13)23-15)20(26)12-6-10(h1-8H,(H,23,25)(H,24,26)	-7.42
InChI=1S/C14H18N2O2/c1-4-14(5-2)12(17)15(3)16(13(14)18)11-9-7-6-8-10-11/h6-10H,4-5H2,1-3H3	-2.69
InChI=1S/C4H9NO2S/c5-3(1-2-8)4(6)7/h3,8H,1-2,5H2,(H,6,7)	0.813
InChI=1S/C10H13FN2O4/c1-2-3-4-8(14)17-6-13-9(15)7(11)5-12-10(13)16/h5H,2-4,6H2,1H3,(H,12,16)	-1.66
InChI=1S/C12H5Cl5O/c13-6-3-10(16)12(17)11(4-6)18-7-1-2-8(14)9(15)5-7/h1-5H	-7.83
InChI=1S/C7H6N4/c1-5-2-9-7-6(11-5)3-8-4-10-7/h2-4H,1H3	0.06
InChI=1S/C18H15NO3/c1-22-15-8-6-14(7-9-15)19-18(21)16-10-12-4-2-3-5-13(12)11-17(16)2h2-11,20H,1H3,(H,19,21)	-5.263
InChI=1S/C23H25F3N2OS/c24-23(25,26)17-7-8-22-20(16-17)18(19-4-1-2-6-21(19)30-22)5-3-9-2h1-2,4-8,16,29H,3,9-15H2/b18-5-	-6.099
InChI=1S/C15H18O7/c1-5(2)14(18)6-11(17)22-8(14)7(16)12(3)13(4-20-13)9-10(21-9)15(6,h6-10,16,18-19H,1,4H2,2-3H3	-1.42
InChI=1S/C11H14I2N2O2/c1-3-15(4-2)10(16)7-14-5-8(12)11(17)9(13)6-14/h5-6H,3-4,7H2,1-2H3	-3.18
InChI=1S/C22H23O4P/c1-22(2,3)18-14-16-21(17-15-18)26-27(23,24-19-10-6-4-7-11-19)25-2h4-17H,1-3H3	-5.077
InChI=1S/C18H26O4/c1-13(2)9-11-21-17(19)15-7-5-6-8-16(15)18(20)22-12-10-14(3)4/h5-8,13-14H,9-12H2,1-4H3	-5.445
InChI=1S/C16H35O4P/c1-5-9-11-15(7-3)13-19-21(17,18)20-14-16(8-4)12-10-6-2/h15-16H,5-14H2,1-4H3,(H,17,18)	-3.362
InChI=1S/C23H16N4O8S/c24-26-27-25-17-10-8-14-15(21(17)30)2-1-3-19(14)36(33,34)35-13-6-h1-7,9-11,24,28,31-32H,8H2/b26-24+,27-25+	-5.105
InChI=1S/C18H13NO3/c20-17(14-9-3-4-10-15(14)18(21)22)19-16-11-5-7-12-6-1-2-8-13(12)1h1-11H,(H,19,20)(H,21,22)	-3.163
InChI=1S/C9H15NO3S/c11-7-6-14-8(10-7)4-2-1-3-5-9(12)13/h8H,1-6H2,(H,10,11)(H,12,13)	-2.073
InChI=1S/C11H23NO/c1-4-5-6-7-8-9-10-11(13)12(2)3/h4-10H2,1-3H3	-2.144
InChI=1S/C15H18N4/c1-18(2)17-15(16)19-9-12-7-3-5-11-6-4-8-13(10-19)14(11)12/h3-8H,9-10H2,1-2H3,(H2,16,17)	-1.07

"InChi"	"logS(M)"
InChI=1S/C12H9F2N5O2S/c1-7-5-6-19-11(15-7)16-12(17-19)22(20,21)18-10-8(13)3-2-4-9(10)14h2-6,18H,1H3	-3.825
InChI=1S/C6H6N2O3/c7-5-2-1-4(9)3-6(5)8(10)11/h1-3,9H,7H2	-1.834
InChI=1S/C11H22O4/c1-2-3-4-5-6-7-11(14)15-9-10(13)8-12/h10,12-13H,2-9H2,1H3	0.179
InChI=1S/C7H7NO5S3/c8-16(12,13)6-3-5-7(14-6)4(9)1-2-15(5,10)11/h3H,1-2H2,(H2,8,12,13)	-3.67
InChI=1S/C4H6N2O/c1-3-2-4(7)6-5-3/h2H2,1H3,(H,6,7)	-1.415
InChI=1S/C11H15NO2S/c1-7-5-9(14-11(13)12-3)6-8(2)10(7)15-4/h5-6H,1-4H3,(H,12,13)	-3.921
InChI=1S/C7H12O2/c1-5(2)7(8)9-6(3)4/h6H,1H2,2-4H3	-2.059
InChI=1S/C12H15NO/c1-2-9-4-3-5-11-10(6-7-14)8-13-12(9)11/h3-5,8,13-14H,2,6-7H2,1H3	-1.915
InChI=1S/C3H5Cl2NO2/c1-2-3(4,5)6(7)8/h2H2,1H3	-1.5
InChI=1S/C19H19N7O5/c1-4-24(5-2)14-6-7-16(17(9-14)21-12(3)27)22-23-19-13(11-20)8-15(2h6-10H,4-5H2,1-3H3,(H,21,27)/b23-22+	-6.328
InChI=1S/C6H3ClN2O2/c7-5-1-4(10)3(2-8)6(11)9-5/h1H,(H2,9,10,11)	-1.232
InChI=1S/C14H16O6/c1-14(2)19-8-9(20-14)7-18-13(17)11-6-4-3-5-10(11)12(15)16/h3-6,9H,7-8H2,1-2H3,(H,15,16)	-1.23
InChI=1S/C9H10O3/c1-2-12-9-4-3-7(6-10)5-8(9)11/h3-6,11H,2H2,1H3	-1.733
InChI=1S/C8H15NO/c1-3-5-6-7(4-2)8(9)10/h4H,3,5-6H2,1-2H3,(H2,9,10)/b7-4-	-1.372
InChI=1S/C11H15ClN2O2/c1-8(2)13-14-11(15)7-16-10-5-3-9(12)4-6-10/h3-6,8,13H,7H2,1-2H3,(H,14,15)	-2.696
InChI=1S/C8H12O5/c1-5(9)6(8(11)13-3)4-7(10)12-2/h6H,4H2,1-3H3	-0.525
InChI=1S/C4H7ClO2/c1-2-7-4(6)3-5/h2-3H2,1H3	-0.8
InChI=1S/C19H14/c1-13-17-8-4-3-7-15(17)12-16-11-10-14-6-2-5-9-18(14)19(13)16/h2-12H,1H3	-6.565
InChI=1S/C25H21N/c26-24-18-16-23(17-19-24)25(20-10-4-1-5-11-20,21-12-6-2-7-13-21)22h1-19H,26H2	-6.872
InChI=1S/C10H14O7/c1-4-5(10(15)16)2-7(17-4)9(14)8(13)6(12)3-11/h2,6,8-9,11-14H,3H2,1H3,(H,15,16)/p-1	-1.277
InChI=1S/C16H20N8O2S/c1-16(2)11(12-20-22-23-21-12)24-14(26)10(15(24)27-16)19-13(25)9(h3-6,9-11,15H,17-18H2,1-2H3,(H,19,25)(H,20,21,22,23)	-1.57
InChI=1S/C11H15ClO3/c1-7-3-10(4-8(2)11(7)12)15-6-9(14)5-13/h3-4,9,13-14H,5-6H2,1-2H3	-3.103
InChI=1S/C8H7ClN4/c9-6-1-3-7(4-2-6)13-8(11)12-5-10/h1-4H,(H3,11,12,13)	-1.961
InChI=1S/C6H11ClO/c1-6(8)4-2-3-5-7/h2-5H2,1H3	-1.416

"InChi"	"logS(M)"
InChI=1S/C14H13N5O/c1-2-8-19-9-15-11-12(19)17-14(18-13(11)20)16-10-6-4-3-5-7-10/h2-7,9H,1,8H2,(H2,16,17,18,20)	-5.09
InChI=1S/C5H12O2/c1-3-6-5-7-4-2/h3-5H2,1-2H3	-0.173
InChI=1S/C8H17N/c1-9(2)8-6-4-3-5-7-8/h8H,3-7H2,1-2H3	-0.977
InChI=1S/C6H14O2/c1-3-4-8-5-6(2)7/h6-7H,3-5H2,1-2H3	0.927
InChI=1S/C6H10O4/c1-6(2,5(9)10)3-4(7)8/h3H2,1-2H3,(H,7,8)(H,9,10)	-0.32
InChI=1S/C11H13N3O5/c12-11(15)18-4-3-13-6-8-1-2-10(14(16)17)5-9(8)7-19-13/h1-2,5H,3-4,6-7H2,(H2,12,15)	-2.3
InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1-2H3	-0.08
InChI=1S/C11H11Br2NO4/c1-5(15)14-9(11(17)18)4-6-2-7(12)10(16)8(13)3-6/h2-3,9,16H,4H2,1H3,(H,14,15)(H,17,18)	-2.183
InChI=1S/C9H11NO2/c1-10(2)9(12)7-5-3-4-6-8(7)11/h3-6,11H,1-2H3	-0.201
InChI=1S/C9H15NO2/c1-3-9(4-2)6-5-7(11)10-8(9)12/h3-6H2,1-2H3,(H,10,11,12)	-4.53
InChI=1S/C20H20ClNO3/c1-12-18(23)15-9-10-17(24-4)16(11-22(2)3)20(15)25-19(12)13-5-7-14h5-10H,11H2,1-4H3	-4.673
InChI=1S/C10H9Cl3O3/c1-2-15-10(14)5-16-9-4-7(12)6(11)3-8(9)13/h3-4H,2,5H2,1H3	-4.849
InChI=1S/C7H5N3O/c11-7-5-3-1-2-4-6(5)8-10-9-7/h1-4H,(H,8,9,11)	-2.332
InChI=1S/C4H8N4O4S3/c1-8-3(7-14(2,9)10)13-4(6-8)15(5,11)12/h1-2H3,(H2,5,11,12)/b7-3+	-2.05
InChI=1S/C9H10O3/c1-7(9(10)11)12-8-5-3-2-4-6-8/h2-7H,1H3,(H,10,11)	-1.51
InChI=1S/C9H11N3O3S/c1-6(2-3-7(13)14)11-12-8(15)9-10-4-5-16-9/h4-5H,2-3H2,1H3,(H,12,15)(H,13,14)/b11-6-	-1.73
InChI=1S/C17H16ClN3O/c18-12-5-6-15-13(11-12)17(21-9-7-19-8-10-21)20-14-3-1-2-4-16(14)2h1-6,11,19H,7-10H2	-4.089
InChI=1S/C18H25NO/c1-4-9-19-10-8-18(5-2)13(3)17(19)11-14-6-7-15(20)12-16(14)18/h4,6-7,12-13,17,20H,1,5,8-11H2,2-3H3	-3.485
InChI=1S/C12H3Cl7/c13-5-1-2-6(14)10(17)8(5)4-3-7(15)11(18)12(19)9(4)16/h1-3H	-8.59
InChI=1S/C18H26N2O/c1-4-18(21)19-13-15(2)20(16(3)14-19)12-8-11-17-9-6-5-7-10-17/h5-11,15-16H,4,12-14H2,1-3H3/b11-8+	-3.767
InChI=1S/C12H5Cl5O/c13-6-1-3-7(4-2-6)18-9-5-8(14)10(15)12(17)11(9)16/h1-5H	-8.06
InChI=1S/C7H8N2O3/c1-12-7-4-5(9(10)11)2-3-6(7)8/h2-4H,8H2,1H3	-3.205
InChI=1S/C16H32N2O/c1-2-3-4-5-6-7-8-9-10-11-16-17-12-13-18(16)14-15-19/h19H,2-15H2,1H3	-3.899

"InChi"	"logS(M)"
InChI=1S/C16H21NO6S/c1-12(2)23-15(18)16(10-4-3-5-11-16)24(21,22)14-8-6-13(7-9-14)17(1h6-9,12H,3-5,10-11H2,1-2H3	-4.88
InChI=1S/C7H13NO2/c8-7(6(9)10)4-2-1-3-5-7/h1-5,8H2,(H,9,10)	-0.719
InChI=1S/C5H12N2O2/c6-5(9)1-2-7-3-4-8/h7-8H,1-4H2,(H2,6,9)	-0.121
InChI=1S/C8H6O5/c9-6-2-4(7(10)11)1-5(3-6)8(12)13/h1-3,9H,(H,10,11)(H,12,13)	-2.005
InChI=1S/C16H16O4/c1-2-11-6-12(17-7-13-8-18-13)4-5-15(11)16(3-1)20-10-14-9-19-14/h1-6,13-14H,7-10H2	-3.919
InChI=1S/C14H13NO3/c1-18-11-6-4-5-10(9-11)15-13-8-3-2-7-12(13)14(16)17/h2-9,15H,1H3,(H,16,17)	-4.8
InChI=1S/C10H11ClO3/c1-2-13-10(12)7-14-9-5-3-8(11)4-6-9/h3-6H,2,7H2,1H3	-2.421
InChI=1S/C20H21N3O/c1-22-12-14-23(15-13-22)20-21-18(16-8-4-2-5-9-16)19(24-20)17-10-6h2-11H,12-15H2,1H3	-4.042
InChI=1S/C7H15NO3S2/c9-13(10,11)12-5-4-8-6-7-2-1-3-7/h7-8H,1-6H2,(H,9,10,11)	-0.079
InChI=1S/C15H24O4/c1-4-5-6-7-13-12(10-15(17)18-3)8-9-14(13)19-11(2)16/h12H,4-10H2,1-3H3	-3.722
InChI=1S/C16H18ClN/c17-11-12-18(13-15-7-3-1-4-8-15)14-16-9-5-2-6-10-16/h1-10H,11-14H2	-3.673
InChI=1S/C9H22N2/c1-8(4-5-10)6-9(2,3)7-11/h8H,4-7,10-11H2,1-3H3	0.478
InChI=1S/C12H3Cl7O/c13-4-1-2-5(14)12(9(4)17)20-7-3-6(15)8(16)11(19)10(7)18/h1-3H	-8.89
InChI=1S/C6H13NO2/c1-2-3-4-5(7)6(8)9/h5H,2-4,7H2,1H3,(H,8,9)	-1.039
InChI=1S/C9H9ClO4/c10-7-1-2-8(6(3-7)4-11)14-5-9(12)13/h1-3,11H,4-5H2,(H,12,13)	-2.035
InChI=1S/C11H17NO/c1-3-4-9-12-10-7-5-6-8-11(10)13-2/h5-8,12H,3-4,9H2,1-2H3	-2.943
InChI=1S/C61H112O13/c1-13-19-34-51(16-4)57(65)72-45-60(42-69-54(62)37-28-22-25-31-48h48-53H,13-47H2,1-12H3	-7.324
InChI=1S/C18H36O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h15-17H,6-14H2,1-5H3	-5.475
InChI=1S/C10H14N2O2/c1-3-14-9-6-4-8(5-7-9)12(2)10(11)13/h4-7H,3H2,1-2H3,(H2,11,13)	-1.66
InChI=1S/C16H25N3O3/c1-12-14(18-8-10-22-11-9-18)15(20)17(2)16(21)19(12)13-6-4-3-5-7-1h13H,3-11H2,1-2H3	-3.147
InChI=1S/C13H17N/c1-11(9-13(2,3)10-14)12-7-5-4-6-8-12/h4-8,11H,9H2,1-3H3	-3.235
InChI=1S/C36H32Cl4N6O4/c1-17-7-9-29(19(3)11-17)41-35(49)33(21(5)47)45-43-31-15-25(37)23(h7-16,33-34H,1-6H3,(H,41,49)(H,42,50)/b45-43+,46-44+	-8.463

"InChi"	"logS(M)"
InChI=1S/C7H15NO/c1-4-6(5(2)3)7(8)9/h5-6H,4H2,1-3H3,(H2,8,9)	-1.124
InChI=1S/C10H11Cl3O2/c1-6(14)4-15-5-7-8(11)2-3-9(12)10(7)13/h2-3,6,14H,4-5H2,1H3	-3.567
InChI=1S/C34H64O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-31-37-33(35)29-30-34(36)38-h29-30H,3-28,31-32H2,1-2H3/b30-29+	-6.554
InChI=1S/C11H24O/c1-2-3-4-5-6-7-8-9-10-11-12/h12H,2-11H2,1H3	-4.48
InChI=1S/C12H9NOS/c14-8-5-6-10-12(7-8)15-11-4-2-1-3-9(11)13-10/h1-7,13-14H	-2.575
InChI=1S/C11H6O4/c12-8-2-1-6-5-7-3-4-14-10(7)9(13)11(6)15-8/h1-5,13H	-3.22
InChI=1S/C23H49NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-23-20-21-24(2)h4-23H2,1-3H3	-6.852
InChI=1S/C16H26N2O/c1-5-13(2)16(15(17)19,11-12-18(3)4)14-9-7-6-8-10-14/h6-10,13H,5,11-12H2,1-4H3,(H2,17,19)	-3.261
InChI=1S/C3H6ClNO2/c1-2-3(4)5(6)7/h3H,2H2,1H3	-1.189
InChI=1S/C7H10N2O2S/c1-3-11-7(10)9-5-4-8(2)6(9)12/h4-5H,3H2,1-2H3	-0.473
InChI=1S/C10H14O3/c11-6-7-12-8-9-13-10-4-2-1-3-5-10/h1-5,11H,6-9H2	-0.717
InChI=1S/C13H10O4S/c1-7-9(12(15)16)11(14)10(13(17)18-7)8-5-3-2-4-6-8/h2-6,17H,1H3,(H,15,16)	-2.254
InChI=1S/C4H5NO2/c1-7-4(6)2-3-5/h2H2,1H3	-0.264
InChI=1S/C8H10O8/c9-5(10)1-3(7(13)14)4(8(15)16)2-6(11)12/h3-4H,1-2H2,(H,9,10)(H,11,12)(H,13,14)(H,15,16)	-0.18
InChI=1S/C9H18N3OP/c1-7-4-10(7)14(13,11-5-8(11)2)12-6-9(12)3/h7-9H,4-6H2,1-3H3	-0.65
InChI=1S/C42H78O5/c1-4-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-40(44)46-38-42(6-h19-22,43H,4-18,23-39H2,1-3H3/b21-19+,22-20+	-8.721
InChI=1S/C16H13ClF3NO4/c1-9(15(22)23-2)24-11-3-5-12(6-4-11)25-14-13(17)7-10(8-21-14)16(1h3-9H,1-2H3	-4.606
InChI=1S/C6H6N2O3/c9-3-6(1-2-6)4(10)8-5(11)7-3/h1-2H2,(H2,7,8,9,10,11)	-1.89
InChI=1S/C22H27NO2/c1-18-9-11-20(12-10-18)22(25)13-16-23(17-14-22)15-5-8-21(24)19-6-h2-4,6-7,9-12,25H,5,8,13-17H2,1H3	-1.62
InChI=1S/C9H14N2O2S/c1-3-5-9(4-2)6(12)10-8(14)11-7(9)13/h3-5H2,1-2H3,(H2,10,11,12,13,14)	-2.8
InChI=1S/C19H20N8O5/c20-15-14-16(27-19(21)26-15)23-8-11(24-14)7-22-10-3-1-9(2-4-10)17h1-4,8,12,22H,5-7H2,(H,25,30)(H,28,29)(H,31,32)(H4,20,21,23,26,27)	-2.162
InChI=1S/C21H28N2O3/c1-16(21(24)26-13-12-23-10-8-22(2)9-11-23)17-4-5-19-15-20(25-3)7-h4-7,14-16H,8-13H2,1-3H3	-1.49

"InChi"	"logS(M)"
InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8H,5-6,9H2,1-4H3/b8-7+	-3.08
InChI=1S/C26H25N3O3S/c30-26(29-20-5-1-3-7-24(20)33-25-8-4-2-6-21(25)29)17-28-13-11-27(h1-10,15H,11-14,16-18H2	-5.056
InChI=1S/C12HCl9/c13-2-1-3(14)6(15)7(16)4(2)5-8(17)10(19)12(21)11(20)9(5)18/h1H	-10.104
InChI=1S/C5H2Br2O3/c6-2-1-10-4(3(2)7)5(8)9/h1H,(H,8,9)	-2.089
InChI=1S/C10H20O/c1-9(11)7-8-10-5-3-2-4-6-10/h9-11H,2-8H2,1H3	-2.767
InChI=1S/C6HCl3N2S/c7-2-1-3(8)5-6(4(2)9)11-12-10-5/h1H	-4.98
InChI=1S/C13H13N3O3S/c1-10(17)15-11-5-7-12(8-6-11)20(18,19)16-13-4-2-3-9-14-13/h2-9H,1H3,(H,14,16)(H,15,17)	-3.716
InChI=1S/C11H6BrNS/c12-11-9-4-2-1-3-8(9)5-6-10(11)13-7-14/h1-6H	-4.32
InChI=1S/C42H69NO15/c1-23(2)19-32(47)56-40-27(6)53-34(22-42(40,8)50)57-37-26(5)54-41(h12-14,16,18,23-27,29-31,34-41,46,49-50H,15,17,19-22H2,1-11H3/b13-12-,16-14-	-4.343
InChI=1S/C26H40O3/c1-4-5-6-7-8-24(28)29-23-12-11-21-20-10-9-18-17-19(27)13-15-25(18h17,20-23H,4-16H2,1-3H3	-7.868
InChI=1S/C7H10N2O3/c1-3-7(2)4(10)8-6(12)9-5(7)11/h3H2,1-2H3,(H2,8,9,10,11,12)	-1.23
InChI=1S/C12H9ClO/c13-11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/h1-9H	-4.78
InChI=1S/C17H18N2O4/c18-15(20)22-11-17(12-23-16(19)21,13-7-3-1-4-8-13)14-9-5-2-6-10-1h1-10H,11-12H2,(H2,18,20)(H2,19,21)	-3.13
InChI=1S/C9H18N2O2/c1-7(2)9(13)10-11(4,5)6-8(3)12/h8,12H,1,6H2,2-5H3	0.73
InChI=1S/C9H13NO4S/c11-9(7-15(12,13)14)6-10-8-4-2-1-3-5-8/h1-5,9-11H,6-7H2,(H,12,13,14)/p-1	0.119
InChI=1S/C10HCl7/c11-2-1-3(12)6(13)5-4(2)7(14)9(16)10(17)8(5)15/h1H	-8.775
InChI=1S/C6H13NO2/c7-5-3-1-2-4-6(8)9/h1-5,7H2,(H,8,9)	0.585
InChI=1S/C17H16Br2ClNO2/c18-8-10-21(11-9-19)15-4-6-16(7-5-15)23-17(22)13-2-1-3-14(20)12-1h1-7,12H,8-11H2	-7.291
InChI=1S/C15H14ClNO3/c16-9-3-1-8(2-4-9)7-17-14(18)12-10-5-6-11(20-10)13(12)15(17)19/h1-4,10-13H,5-7H2	-2.368
InChI=1S/C10H9ClN4O2S/c11-7-5-13-10(14-6-7)15-18(16,17)9-3-1-2-8(12)4-9/h1-6H,12H2,(H,13,14,15)	-1.538
InChI=1S/C43H75NO16/c1-15-29-43(11,52)36(48)24(5)33(47)22(3)20-41(9,51)38(25(6)34(26(h22-29,32,34-38,40,48-49,51-52H,15-21H2,1-14H3	-6.271
InChI=1S/C15H23NO5/c1-8-6-15(2,21)7-10(14(8)20)11(17)3-9-4-12(18)16-13(19)5-9/h8-11,17,21H,3-7H2,1-2H3,(H,16,18,19)	-0.497

"InChi"	"logS(M)"
InChI=1S/C11H15Cl2NO3S/c1-9-2-3-10(18(15,16)17)8-11(9)14(6-4-12)7-5-13/h2-3,8H,4-7H2,1H3,(H,15,16,17)	-4.374
InChI=1S/C20H25NO2/c1-3-21(4-2)15-16-23-20(22)19(17-11-7-5-8-12-17)18-13-9-6-10-14-1h5-14,19H,3-4,15-16H2,1-2H3	-4.217
InChI=1S/C8H18O/c1-4-5-8(9)6-7(2)3/h7-9H,4-6H2,1-3H3	-1.908
InChI=1S/C18H18N4O2/c1-13-16(20-18(24)19-14-9-5-3-6-10-14)17(23)22(21(13)2)15-11-7-4-h3-12H,1-2H3,(H2,19,20,24)	-2.3
InChI=1S/C26H28N2O3/c1-30-24-12-11-20(17-25(24)31-2)26(29)27-23-10-6-9-21-18-28(16-1h3-12,17H,13-16,18H2,1-2H3,(H,27,29)	-5.416
InChI=1S/C6H2Cl4O2/c7-1-2(8)4(10)6(12)5(11)3(1)9/h11-12H	-3.55
InChI=1S/C8H17Cl2N2O2P/c9-3-6-12(7-4-10)15(13)11-5-1-2-8-14-15/h1-8H2,(H,11,13)	-0.962
InChI=1S/C11H20N2O4/c1-5-11(6-2,8(14)13-10(12)16)9(15)17-7(3)4/h7H,5-6H2,1-4H3,(H3,12,13,14,16)	-2.77
InChI=1S/C4H4N2O2S/c1-2-3(4(7)8)5-6-9-2/h1H3,(H,7,8)	-0.46
InChI=1S/C13H20O2/c1-2-3-4-5-6-7-11-8-9-12(14)10-13(11)15/h8-10,14-15H,2-7H2,1H3	-4.007
InChI=1S/C9H10N2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-5H,6-7H2,(H,10,11)/p+1	-1.127
InChI=1S/C7H5BrO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)	-2.05
InChI=1S/C13H19NO3/c1-3-14(4-2)13(16)11-7-5-6-8-12(11)17-10-9-15/h5-8,15H,3-4,9-10H2,1-2H3	-1.63
InChI=1S/C11H15N3O2/c1-3-8-14(2)13-12-10-6-4-9(5-7-10)11(15)16/h4-7H,3,8H2,1-2H3,(H,15,16)/b13-12+	-1.43
InChI=1S/C6H15O3PS3/c1-4-13(7)6-5-12-10(11,8-2)9-3/h4-6H2,1-3H3/p+1	-0.914
InChI=1S/C17H20O2/c1-10-5-14(6-11(2)16(10)18)9-15-7-12(3)17(19)13(4)8-15/h5-8,18-19H,9H2,1-4H3	-3.409
InChI=1S/C10H6Cl2N2O/c11-8-6-13-14(10(15)9(8)12)7-4-2-1-3-5-7/h1-6H	-3.382
InChI=1S/C18H16N2O2/c21-16-18(20-17(22)19-16)14-10-3-1-6-12(14)8-5-9-13-7-2-4-11-15(1h1-4,6-7,10-11H,5,8-9H2,(H2,19,20,21,22)	-5.546
InChI=1S/C14H16N2/c15-13-7-3-11(4-8-13)1-2-12-5-9-14(16)10-6-12/h3-10H,1-2,15-16H2	-3.646
InChI=1S/C16H28O/c1-2-3-4-13-5-7-14(8-6-13)15-9-11-16(17)12-10-15/h13-15H,2-12H2,1H3	-6.374
InChI=1S/C9H12/c1-3-5-7-9-8-6-4-2/h1-2H,5-9H2	-2.983
InChI=1S/C8H13NO3/c1-2-12-8(11)9-5-3-7(10)4-6-9/h2-6H2,1H3	0.767
InChI=1S/C11H11NO3S/c1-2-7-12-11(13)10-6-4-3-5-9(10)8-16(12,14)15/h2-6H,1,7-8H2	-2.443
InChI=1S/C7H10N2/c8-9-6-7-4-2-1-3-5-7/h1-5,9H,6,8H2	0.913

"InChi"	"logS(M)"
InChI=1S/C8H9N5/c1-13(2)8-6-7(11-5-12-8)10-4-3-9-6/h3-5H,1-2H3	-1.022
InChI=1S/C8H19O2PS2/c1-4-7-12-11(9,10-6-3)13-8-5-2/h4-8H2,1-3H3	-2.509
InChI=1S/C6H12ClNO/c1-3-6(7,4-2)5(8)9/h3-4H2,1-2H3,(H2,8,9)	-1.029
InChI=1S/C11H16N4O4/c16-3-8-6(17)1-9(19-8)15-5-14-10-7(18)2-12-4-13-11(10)15/h4-9,16-18H,1-3H2,(H,12,13)	0.571
InChI=1S/C22H38O5/c1-4-5-14-22(2,26)15-10-12-18-17(19(23)16-20(18)24)11-8-6-7-9-13-h10,12,17-18,20,24,26H,4-9,11,13-16H2,1-3H3/b12-10+	-6.314
InChI=1S/C11H24O3/c1-5-11(6-2,9-12)10(13-7-3)14-8-4/h10,12H,5-9H2,1-4H3	-1.962
InChI=1S/C12H3Cl7/c13-6-1-4(2-7(14)10(6)17)5-3-8(15)11(18)12(19)9(5)16/h1-3H	-8.72
InChI=1S/C19H14O/c20-19(17-9-5-2-6-10-17)18-13-11-16(12-14-18)15-7-3-1-4-8-15/h1-14H	-5.279
InChI=1S/C7H8N2O/c10-6-8-9-7-4-2-1-3-5-7/h1-6,9H,(H,8,10)	-0.441
InChI=1S/C11H16O3/c1-2-9-3-5-11(6-4-9)14-8-10(13)7-12/h3-6,10,12-13H,2,7-8H2,1H3	-2.251
InChI=1S/C20H13NO4/c21-18-15(25-11-6-2-1-3-7-11)10-14(22)16-17(18)20(24)13-9-5-4-8-1h1-10,22H,21H2	-4.219
InChI=1S/C13H17NO2/c1-13(2,10-15)14-12(16)9-8-11-6-4-3-5-7-11/h3-9,15H,10H2,1-2H3,(H,14,16)/b9-8+	-1.812
InChI=1S/C14H19N5O4/c1-3-18(4-2)11(20)5-6-12(21)23-9-19-13-10(7-17-19)14(22)16-8-15-1h7-8H,3-6,9H2,1-2H3,(H,15,16,22)	-0.99
InChI=1S/C9H8N2OS/c1-7(12)11-9-4-2-3-8(5-9)10-6-13/h2-5H,1H3,(H,11,12)	-3.53
InChI=1S/C24H40N2/c1-16-20-8-9-22-19-7-6-17-14-18(25(3)4)10-12-23(17,2)21(19)11-13-h6,16,18-22H,7-15H2,1-5H3	-5.447
InChI=1S/C6H8O4S2/c7-5(8)3-1-2-4(6(9)10)12-11-3/h3-4H,1-2H2,(H,7,8)(H,9,10)	-1.171
InChI=1S/C2HClF2/c3-2(5)1-4/h1H/b2-1+	-1.285
InChI=1S/C7H4N4O5/c12-6-5(9-10-7(13)8-6)3-1-2-4(16-3)11(14)15/h1-2H,(H2,8,10,12,13)	-2.782
InChI=1S/C12H15NO5/c1-9(14)13-10-3-5-11(6-4-10)18-12(15)17-8-7-16-2/h3-6H,7-8H2,1-2H3,(H,13,14)	-1.69
InChI=1S/C13H17ClO3/c1-2-3-4-5-8-17-13(16)10-6-7-12(15)11(14)9-10/h6-7,9,15H,2-5,8H2,1H3	-4.09
InChI=1S/C12H8O2/c13-12-7-10-9-4-2-1-3-8(9)5-6-11(10)14-12/h1-6H,7H2	-2.708
InChI=1S/C14H21N3O/c1-11-4-3-5-12(2)14(11)16-13(18)10-17-8-6-15-7-9-17/h3-5,15H,6-10H2,1-2H3,(H,16,18)/p+2	0.443

"InChi"	"logS(M)"
InChI=1S/C15H23NOS/c1-5-16(13(4)12(2)3)15(17)18-11-14-9-7-6-8-10-14/h6-10,12-13H,5,11H2,1-4H3	-4.734
InChI=1S/C13H18N2O2/c1-10-5-3-4-6-12(10)14-13(16)17-11-7-8-15(2)9-11/h3-6,11H,7-9H2,1-2H3,(H,14,16)	-2.324
InChI=1S/C10H7BrN2O/c11-8-6-12-9(13-10(8)14)7-4-2-1-3-5-7/h1-6H,(H,12,13,14)	-3.479
InChI=1S/C11H13NO3/c13-10(14)7-4-8-12-11(15)9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H,12,15)(H,13,14)	-1.202
InChI=1S/C16H19NO2/c1-18-14-7-3-12(4-8-14)11-16(17)13-5-9-15(19-2)10-6-13/h3-10,16H,11,17H2,1-2H3	-2.936
InChI=1S/C6H10O4S2/c7-5(8)3(11)1-2-4(12)6(9)10/h3-4,11-12H,1-2H2,(H,7,8)(H,9,10)	-2.476
InChI=1S/C27H25O4P/c1-21(2)23-18-24(22-12-6-3-7-13-22)20-27(19-23)31-32(28,29-25-14-h3-21H,1-2H3	-6.848
InChI=1S/C22H32O3/c1-12-9-15-17-6-5-16(13(2)23)22(17,4)11-19(25)20(15)21(3)8-7-14(2h10,12,15-17,19-20,25H,5-9,11H2,1-4H3	-3.618
InChI=1S/C9H6N4O/c10-5-8(6-11)13-12-7-2-1-3-9(14)4-7/h1-4,12,14H	-2.95
InChI=1S/C16H35NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-15-16-21-22(18,19)20/h17H,2-16H2,1H3,(H,18,19,20)	-4.945
InChI=1S/C8H9N3O/c1-4-2-6-7(3-5(4)9)11-8(12)10-6/h2-3H,9H2,1H3,(H2,10,11,12)	-1.977
InChI=1S/C20H24N2OS/c1-4-18(23)15-10-11-20-17(14-15)22(13-7-12-21(2)3)16-8-5-6-9-19(1h5-6,8-11,14H,4,7,12-13H2,1-3H3	-4.49
InChI=1S/C15H24O6/c1-6-14(16)20-12(4)9-18-8-11(3)19-10-13(5)21-15(17)7-2/h6-7,11-13H,1-2,8-10H2,3-5H3	-1.876
InChI=1S/C10H9NO3S/c11-10-8-4-2-1-3-7(8)5-6-9(10)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-2.96
InChI=1S/C11H13NO4/c1-3-15-11(14)16-10-6-4-9(5-7-10)12-8(2)13/h4-7H,3H2,1-2H3,(H,12,13)	-2.67
InChI=1S/C8H10O8S/c9-5(10)1-3(7(13)14)17-4(8(15)16)2-6(11)12/h3-4H,1-2H2,(H,9,10)(H,11,12)(H,13,14)(H,15,16)	-0.491
InChI=1S/C7H7ClO/c1-5-3-2-4-6(8)7(5)9/h2-4,9H,1H3	-0.774
InChI=1S/C15H22N2O4/c1-9(2)7-13(15(20)21)17-14(19)12(16)8-10-3-5-11(18)6-4-10/h3-6,9,12-13,18H,7-8,16H2,1-2H3,(H,17,19)(H,20,21)	-2.07
InChI=1S/C11H17NO2/c1-8(2)12-7-11(14)9-3-5-10(13)6-4-9/h3-6,8,11-14H,7H2,1-2H3	-0.312
InChI=1S/C13H19N3O6S/c1-4-6-14(7-5-2)13-11(15(17)18)8-10(23(3,21)22)9-12(13)16(19)20/h8-9H,4-7H2,1-3H3	-5.76
InChI=1S/C12H24N3O4P/c16-20(13,14-3-9-18-10-4-14)15-5-11-19-12-6-15/h1-12H2	0.298

"InChi"	"logS(M)"
InChI=1S/C22H45NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23(19-21-24)20-22-2h9-10,24-25H,2-8,11-22H2,1H3/b10-9+	-4.78
InChI=1S/C7H9NO4S3/c8-15(11,12)6-3-4-5(9)1-2-14(10)7(4)13-6/h3,5,9H,1-2H2,(H2,8,11,12)/p+1	-1.35
InChI=1S/C6H10N4/c1-4-9-3-5(2-7)6(8)10-4/h3H,2,7H2,1H3,(H2,8,9,10)	0.49
InChI=1S/C19H21NO4/c1-20-5-4-10-7-15(22)19(24-3)18-12-9-16(23-2)14(21)8-11(12)6-13(2h7-9,13,21-22H,4-6H2,1-3H3	-3.101
InChI=1S/C9H12FN3O3/c1-2-3-4-11-8(15)13-5-6(10)7(14)12-9(13)16/h5H,2-4H2,1H3,(H,11,15)(H,12,14,16)	-2.446
InChI=1S/C25H41NO9/c1-6-26-9-22(10-32-2)12(27)7-13(33-3)24-11-8-23(30)19(28)14(11)25h11-21,27-31H,6-10H2,1-5H3	0.301
InChI=1S/C5H12N2O/c1-3-7(4-2)5(6)8/h3-4H2,1-2H3,(H2,6,8)	-0.232
InChI=1S/C10H13NO2/c1-11(2)9-6-4-8(5-7-9)10(12)13-3/h4-7H,1-3H3	-3.05
InChI=1S/C11H13NO3/c1-8(13)12-10(11(14)15)7-9-5-3-2-4-6-9/h2-6,10H,7H2,1H3,(H,12,13)(H,14,15)	-1.41
InChI=1S/C13H24O3/c1-5-13(4,7-6-10(2)3)12(14)16-9-11-8-15-11/h10-11H,5-9H2,1-4H3	-3.513
InChI=1S/C15H20N2O4S2/c1-12-11-15(17-14-6-3-2-5-13(12)14)21-9-4-7-16-8-10-22-23(18,19)2h2-3,5-6,11,16H,4,7-10H2,1H3,(H,18,19,20)	-2.397
InChI=1S/C16H16N2O4S/c1-11(19)17-13-3-7-15(8-4-13)23(21,22)16-9-5-14(6-10-16)18-12(2)2h3-10H,1-2H3,(H,17,19)(H,18,20)	-3.576
InChI=1S/C14H22N2O4/c1-3-5-7-19-12-9-11(14(17)16-18)10-13(15-12)20-8-6-4-2/h9-10,18H,3-8H2,1-2H3,(H,16,17)	-4.2
InChI=1S/C16H21NO3/c1-12-7-6-8-13(2)17(12)15(18)11-20-16(19)14-9-4-3-5-10-14/h3-5,9-10,12-13H,6-8,11H2,1-2H3	-3.26
InChI=1S/C13H9ClN2/c14-10-6-3-5-9-12(15)8-4-1-2-7-11(8)16-13(9)10/h1-7H,(H2,15,16)	-4.58
InChI=1S/C27H24N6O7S/c1-28-41(37,38)23-13-21(39-2)20(12-22(23)40-3)32-33-24-16-7-5-4-6h4-13,28,32H,1-3H3,(H,29,35)(H2,30,31,36)/b33-24-	-7.892
InChI=1S/C17H20N4O6/c1-4-19-17(24)27-14-9-11(8-13(15(14)22)21(25)26)7-12(10-18)16(23)h7-9,22H,4-6H2,1-3H3,(H,19,24)/b12-7-	-3.18
InChI=1S/C12H15N3O/c1-9-11(13-2)12(16)15(14(9)3)10-7-5-4-6-8-10/h4-8,13H,1-3H3	-1.122
InChI=1S/C14H12O3/c15-14(16)13(11-7-3-1-4-8-11)17-12-9-5-2-6-10-12/h1-10,13H,(H,15,16)	-3
InChI=1S/C13H15NO3/c1-3-17-13(15)14-11-7-5-4-6-10(11)8-9-12(14)16-2/h4-9,12H,3H2,1-2H3	-3.814

"InChi"	"logS(M)"
InChI=1S/C30H35F2N3O/c1-22-5-3-6-23(2)30(22)33-29(36)21-35-19-17-34(18-20-35)16-4-7-28h3,5-6,8-15,28H,4,7,16-21H2,1-2H3,(H,33,36)	-3.692
InChI=1S/C18H20FN3O3/c1-2-14-13(20)8-22(14)16-6-15-10(5-12(16)19)17(23)11(18(24)25)7-2h5-7,9,13-14H,2-4,8,20H2,1H3,(H,24,25)	-3.91
InChI=1S/C8H8N2O4/c11-7(9-13)5-1-2-6(4-3-5)8(12)10-14/h1-4,13-14H,(H,9,11)(H,10,12)	-1.288
InChI=1S/C19H18N2O3/c22-15-6-5-10-11-9-14-19(7-8-20(14)18(24)16(11)23)12-3-1-2-4-13(1h1-6,10-11,14,16-17,23H,7-9H2	-2.11
InChI=1S/C9H8Cl2N2O2/c10-7-3-6(4-8(11)12-7)9(14)13-1-2-15-5-13/h3-4H,1-2,5H2	-1.43
InChI=1S/C17H25NO2/c1-19-16-9-7-13(11-17(16)20-2)14-6-8-15-5-3-4-10-18(15)12-14/h7,9,11,14-15H,3-6,8,10,12H2,1-2H3	-3.399
InChI=1S/C32H22N4O2/c1-3-35-29-19-9-5-7-11-21(19)31(37)23-13-17(15-25(33-35)27(23)29h5-16H,3-4H2,1-2H3	-4.393
InChI=1S/C8H12Cl2N6O/c9-1-3-16(4-2-10)15-14-8-6(7(11)17)12-5-13-8/h5,15H,1-4H2,(H2,11,17)/b14-8-	-2.385
InChI=1S/C13H17NO/c1-4-14-13(15)11(3)10(2)12-8-6-5-7-9-12/h5-9H,4H2,1-3H3,(H,14,15)/b11-10-	-3.138
InChI=1S/C15H14N2O3/c1-11(18)20-14-9-7-13(8-10-14)17-15(19)16-12-5-3-2-4-6-12/h2-10H,1H3,(H2,16,17,19)	-4.44
InChI=1S/C17H24N2O/c1-2-17(20)19-15-8-9-16(19)13-18(12-15)11-10-14-6-4-3-5-7-14/h3-7,15-16H,2,8-13H2,1H3	-3.143
InChI=1S/C15H13NO/c1-17-15-10-11-6-2-4-8-13(11)16-14-9-5-3-7-12(14)15/h2-10,16H,1H3	-4.514
InChI=1S/C18H21NO/c20-18(15-7-3-1-4-8-15,16-9-5-2-6-10-16)17-11-13-19-14-12-17/h1-10,17,19-20H,11-14H2	-1.39
InChI=1S/C10H7BrO/c11-9-3-1-8-6-10(12)4-2-7(8)5-9/h1-6,12H	-3.303
InChI=1S/C10H18N2O4/c1-4-10(5-2,8(14)16-6-3)7(13)12-9(11)15/h4-6H2,1-3H3,(H3,11,12,13,15)	-2.08
InChI=1S/C9H8N2O/c1-6-7-3-2-4-8(12)9(7)11-5-10-6/h2-5,12H,1H3	-2.603
InChI=1S/C15H28N2O/c1-7-16(8-2)12-13(18)17-14(3,4)10-9-11-15(17,5)6/h9-10H,7-8,11-12H2,1-6H3	-3.596
InChI=1S/C6H5IO/c7-5-2-1-3-6(8)4-5/h1-4,8H	-2.728
InChI=1S/C20H40O/c1-17(2)9-6-10-18(3)11-7-12-19(4)13-8-14-20(5)15-16-21/h15,17-19,21H,6-14,16H2,1-5H3/b20-15-	-4.862
InChI=1S/C6H7F3N4OS/c1-10-4(14)13(2)5-12-11-3(15-5)6(7,8)9/h1-2H3,(H,10,14)	-2.058
InChI=1S/C6H6Cl2N2O4S2/c7-4-1-3(15(9,11)12)2-5(6(4)8)16(10,13)14/h1-2H,(H2,9,11,12)(H2,10,13,14)	-4.017

"InChi"	"logS(M)"
InChI=1S/C17H11NO7/c1-23-12-4-2-3-8-9(12)5-11(18(21)22)14-10(17(19)20)6-13-16(15(8)14)2-6H,7H2,1H3,(H,19,20)	-6.764
InChI=1S/C21H25ClN2O3/c22-19-8-6-18(7-9-19)21(17-4-2-1-3-5-17)24-12-10-23(11-13-24)14-15-9,21H,10-16H2,(H,25,26)	-0.747
InChI=1S/C13H12N2O/c14-11-6-4-5-10(9-11)13(16)15-12-7-2-1-3-8-12/h1-9H,14H2,(H,15,16)	-2.27
InChI=1S/C16H30O2/c1-4-5-6-7-8-9-10-11-12-13-14-18-16(17)15(2)3/h2,4-14H2,1,3H3	-8.406
InChI=1S/C18H26O/c1-11-8-14(16(19)9-12(11)2)15-10-13-6-7-18(15,5)17(13,3)4/h8-9,13,15,19H,6-7,10H2,1-5H3	-6.174
InChI=1S/C13H21NO4S2/c1-18-13-7-5-12(6-8-13)4-2-3-9-14-10-11-19-20(15,16)17/h5-8,14H,2-4,9-11H2,1H3,(H,15,16,17)	-2.03
InChI=1S/C11H10O2/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-2,4,6-7H,3,5H2,(H,12,13)	-2.794
InChI=1S/C29H50N2O8/c1-5-36-26(32)18-24(28(34)38-7-3)30-22-13-9-20(10-14-22)17-21-11-15-20-25,30-31H,5-19H2,1-4H3	-3.744
InChI=1S/C6H5N5O2/c7-6-10-4-3(5(13)11-6)8-1-2(12)9-4/h1H,(H4,7,9,10,11,12,13)	-4.55
InChI=1S/C8H16O3/c1-3-4-8(2)10-6-7(5-9)11-8/h7,9H,3-6H2,1-2H3	-1.614
InChI=1S/C18H16ClNO3/c1-3-22-18(21)11(2)13-6-9-16-15(10-13)20-17(23-16)12-4-7-14(19)8-4-11H,3H2,1-2H3	-5.98
InChI=1S/C7H16NO4PS2/c1-10-5-4-8-7(9)6-15-13(14,11-2)12-3/h4-6H2,1-3H3,(H,8,9)	-1.136
InChI=1S/C14H8N2O8/c17-11-3-1-7(15(21)22)5-9(11)13(19)14(20)10-6-8(16(23)24)2-4-12(1h1-6,17-18H	-3.521
InChI=1S/C12H7Cl3O/c13-8-2-1-3-9(6-8)16-10-4-5-11(14)12(15)7-10/h1-7H	-5.437
InChI=1S/C13H14N2O6/c1-8(16)21-10-5-3-2-4-9(10)13(19)20-7-12(18)15-6-11(14)17/h2-5H,6-7H2,1H3,(H2,14,17)(H,15,18)	-2.52
InChI=1S/C17H21NO2/c1-12(13-6-4-3-5-7-13)17(19)20-16-10-14-8-9-15(11-16)18(14)2/h3-7,14-16H,1,8-11H2,2H3	-2.893
InChI=1S/C13H10N2O3/c16-12-7-6-10(8-11(12)13(17)18)15-14-9-4-2-1-3-5-9/h1-8,16H,(H,17,18)/b15-14+	-3.05
InChI=1S/C12H11O2P/c13-15(14,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H,(H,13,14)	-2.335
InChI=1S/C13H10ClNO2/c14-9-4-3-5-10(8-9)15-12-7-2-1-6-11(12)13(16)17/h1-8,15H,(H,16,17)	-5.3
InChI=1S/C24H51N3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26-23-19-24-27-22-1h9-10,26-27H,2-8,11-25H2,1H3/b10-9+	-3.718

"InChi"	"logS(M)"
InChI=1S/C4H7Br/c1-2-3-4-5/h2H,1,3-4H2	-2.247
InChI=1S/C8H10FN3O3/c1-2-3-10-7(14)12-4-5(9)6(13)11-8(12)15/h4H,2-3H2,1H3,(H,10,14)(H,11,13,15)	-1.83
InChI=1S/C6H6N2O/c9-8-5-6-1-3-7-4-2-6/h1-5,7H	0.549
InChI=1S/C12H2Cl6O/c13-4-1-3-6(2-5(4)14)19-12-7(3)8(15)9(16)10(17)11(12)18/h1-2H	-10.66
InChI=1S/C15H21NO3/c1-11(2)16(12(3)4)14(17)10-19-15(18)13-8-6-5-7-9-13/h5-9,11-12H,10H2,1-4H3	-3.34
InChI=1S/C16H22N2O4S2/c1-12-4-5-15-14(10-12)13(2)11-16(18-15)22-8-3-6-17-7-9-23-24(19,2h4-5,10-11,17H,3,6-9H2,1-2H3,(H,19,20,21)	-2.966
InChI=1S/C15H14INO3/c16-11-8-12(10-4-2-1-3-5-10)14(19)13(9-11)15(20)17-6-7-18/h1-5,8-9,18-19H,6-7H2,(H,17,20)	-4.366
InChI=1S/C15H14NO2PS/c1-2-17-19(20,15-6-4-3-5-7-15)18-14-10-8-13(12-16)9-11-14/h3-11H,2H2,1H3	-5.704
InChI=1S/C20H30O4/c1-4-7-11-16(6-3)15-24-20(22)18-13-10-9-12-17(18)19(21)23-14-8-5-h9-10,12-13,16H,4-8,11,14-15H2,1-3H3	-7.22
InChI=1S/C7H2Cl3NO2/c8-2-1-3(9)6-5(4(2)10)11-7(12)13-6/h1H,(H,11,12)	-3.399
InChI=1S/C11H22O2/c1-3-4-5-6-7-8-9-10-13-11(2)12/h3-10H2,1-2H3	-4.471
InChI=1S/C16H19N3O2/c1-5-11-18-15(20)14(17(3)4)12(2)19(16(18)21)13-9-7-6-8-10-13/h5-10H,1,11H2,2-4H3	-2.972
InChI=1S/C40H44N12O10S2/c53-21-17-51(18-22-54)39-47-35(41-29-7-3-1-4-8-29)45-37(49-39)43-h1-16,25-26,53-56H,17-24H2,(H,57,58,59)(H,60,61,62)(H2,41,43,45,47,49)(H2,42,44,46,48,50)/b12-11+	-1.059
InChI=1S/C9H11N5O4S3/c1-14-8(19-9(12-14)20(11,15)16)13-21(17,18)7-4-2-6(10)3-5-7/h2-5H,10H2,1H3,(H2,11,15,16)/b13-8+	-2.5
InChI=1S/C18H24N2O/c1-2-18(21)20-16-10-11-17(20)14-19(13-16)12-6-9-15-7-4-3-5-8-15/h3-9,16-17H,2,10-14H2,1H3/b9-6+	-3.656
InChI=1S/C14H17NO6S/c1-10(2)21-13(16)14(8-3-9-14)22(19,20)12-6-4-11(5-7-12)15(17)18/h4-7,10H,3,8-9H2,1-2H3	-3.76
InChI=1S/C11H21N/c1-8-9-5-6-10(7-9)11(2,3)12(8)4/h8-10H,5-7H2,1-4H3	-1.651
InChI=1S/C13H9NO2/c15-13-14-12(8-16-13)11-6-5-9-3-1-2-4-10(9)7-11/h1-8H,(H,14,15)	-2.936
InChI=1S/C7H14NO3PS2/c1-3-10-12(9,11-4-2)8-7-13-5-6-14-7/h3-6H2,1-2H3	-2.594
InChI=1S/C15H19Cl2N3O/c1-15(2,3)14(21)13(20-9-18-8-19-20)6-10-4-5-11(16)7-12(10)17/h4-5,7-9,13-14,21H,6H2,1-3H3	-4.562

"InChi"	"logS(M)"
InChI=1S/C8H7N5O6S3/c9-21(16,17)8-11-10-7(20-8)12-22(18,19)6-3-1-5(2-4-6)13(14)15/h1-4H,(H,10,12)(H2,9,16,17)	-1.33
InChI=1S/C14H12FNO2/c1-10-5-2-3-8-13(10)16(18)14(17)11-6-4-7-12(15)9-11/h2-9,18H,1H3	-2.53
InChI=1S/C12H6Cl4O/c13-7-1-4-12(11(16)5-7)17-8-2-3-9(14)10(15)6-8/h1-6H	-7
InChI=1S/C6H7NO2/c1-3-6(4-7)9-5(2)8/h3,6H,1H2,2H3	-0.899
InChI=1S/C8H18O/c1-8(2)6-4-3-5-7-9/h8-9H,3-7H2,1-2H3	-2.304
InChI=1S/C12H7BrClNO2/c1-2-10(16)17-12-8(13)6-9(14)7-4-3-5-15-11(7)12/h2-6H,1H2	-4.717
InChI=1S/C14H10BrN/c15-9-11-5-7-12(8-6-11)14-4-2-1-3-13(14)10-16/h1-8H,9H2	-6.657
InChI=1S/C27H42O4/c1-16(15-28)5-8-23(30)17(2)25-24(31)14-22-20-7-6-18-13-19(29)9-11h6,16-17,19-22,25,28-29H,5,7-15H2,1-4H3	-5.396
InChI=1S/C11H14O2/c1-2-3-4-9-5-7-10(8-6-9)11(12)13/h5-8H,2-4H2,1H3,(H,12,13)	-3.08
InChI=1S/C11H16O/c1-8-5-6-10(12)9(7-8)11(2,3)4/h5-7,12H,1-4H3	-2.692
InChI=1S/C18H34O5/c1-4-7-9-10-12-17(21)23-15-18(6-3,13-19)14-22-16(20)11-8-5-2/h19H,4-15H2,1-3H3	-5.983
InChI=1S/C8H7ClO3/c9-6-1-3-7(4-2-6)12-5-8(10)11/h1-4H,5H2,(H,10,11)	-2.29
InChI=1S/C10H21NO4/c1-5-10(6-2,7-12)8-15-9(13)11(3)14-4/h12H,5-8H2,1-4H3	-2.484
InChI=1S/C24H27NO6/c1-25(2)13-15-31-23-20(19(26)11-8-16-6-9-17(27-3)10-7-16)21(28-4)h6-12,14H,13,15H2,1-5H3/b11-8+	-4.459
InChI=1S/C6H5Cl2N/c7-4-2-1-3-5(9)6(4)8/h1-3H,9H2	-2.13
InChI=1S/C23H30N2O3/c1-17-7-8-21(13-18(17)2)25-11-9-24(10-12-25)15-22(27)16-28-23-6-4h4-8,13-14,22,27H,9-12,15-16H2,1-3H3	-3.727
InChI=1S/C10H6N2OS2/c1-5-2-3-6-7(4-5)12-9-8(11-6)14-10(13)15-9/h2-4H,1H3	-5.37
InChI=1S/C6H14N2O6/c1-5(13-7(9)10)3-4-6(2)14-8(11)12/h5-6H,3-4H2,1-2H3,(H,9,10)(H,11,12)/q+2	-2.68
InChI=1S/C10H14O3/c1-10(12,7-11)8-13-9-5-3-2-4-6-9/h2-6,11-12H,7-8H2,1H3	-1.31
InChI=1S/C12H10N2O/c15-12-8-6-11(7-9-12)14-13-10-4-2-1-3-5-10/h1-9,15H/b14-13+	-3.95
InChI=1S/C6H11BrN2O2/c1-3(2)4(7)5(10)9-6(8)11/h3-4H,1-2H3,(H3,8,9,10,11)	-1.802
InChI=1S/C15H19NO5/c1-18-12-8-11(9-13(19-2)15(12)20-3)4-5-14(17)16-6-7-21-10-16/h4-5,8-9H,6-7,10H2,1-3H3/b5-4+	-1.921
InChI=1S/C18H28N2O2/c1-13-8-6-9-14(2)16(13)19-17(21)22-15-10-7-11-20(12-15)18(3,4)5/h6,8-9,15H,7,10-12H2,1-5H3,(H,19,21)	-4.884
InChI=1S/C6H8O4/c1-6(4(7)8)2-3-10-5(6)9/h2-3H2,1H3,(H,7,8)	0.841

"InChi"	"logS(M)"
InChI=1S/C14H10N2S/c1-3-7-11(8-4-1)13-15-16-14(17-13)12-9-5-2-6-10-12/h1-10H	-3.263
InChI=1S/C7H3ClF3NO2/c8-5-2-1-4(7(9,10)11)3-6(5)12(13)14/h1-3H	-2.534
InChI=1S/C8H10Cl2N2O2S/c1-12(15(11,13)14)5-6-2-3-7(9)4-8(6)10/h2-4H,5H2,1H3,(H2,11,13,14)	-2.772
InChI=1S/C13H11N3O2S/c14-10-2-1-8-5-9-6-11(19(15,17)18)3-4-12(9)16-13(8)7-10/h1-7H,14H2,(H2,15,17,18)	-2.968
InChI=1S/C24H51N/c1-22(2)16-10-7-13-19-25(20-14-8-11-17-23(3)4)21-15-9-12-18-24(5)h22-24H,7-21H2,1-6H3	-4.057
InChI=1S/C27H34O3/c1-26-14-12-20(28)17-19(26)8-9-21-22-10-11-24(27(22,2)15-13-23(2 h3-7,17,21-24H,8-16H2,1-2H3	-4.66
InChI=1S/C11H18N2O3/c14-9(15)6-2-4-7-3-1-5-8-10(7)13-11(16)12-8/h7-8,10H,1-6H2,(H,14,15)(H2,12,13,16)	-0.96
InChI=1S/C10H8O4/c1-5-2-10(13)14-9-4-8(12)7(11)3-6(5)9/h2-4,11-12H,1H3	-3.284
InChI=1S/C6H9N3O3/c10-7-4-2-1-3-5(8-11)6(4)9-12/h7,10-11H,1-3H2/b8-5+	0.767
InChI=1S/C13H18O3/c14-8-11(15)9-16-13-7-3-5-10-4-1-2-6-12(10)13/h3,5,7,11,14-15H,1-2,4,6,8-9H2	-3.233
InChI=1S/C27H32ClNO2/c1-4-29(5-2)18-19-31-26-16-12-24(13-17-26)27(30,23-10-6-21(3)7-11 h6-17,30H,4-5,18-20H2,1-3H3	-7.112
InChI=1S/C7H14N2S/c1-3-8-5-6-9(4-2)7(8)10/h3-6H2,1-2H3	-0.313
InChI=1S/C4H8O2/c1-4-5-2-3-6-4/h4H,2-3H2,1H3	0.879
InChI=1S/C13H20N2O/c1-2-3-4-5-6-10-15-13(16)12-8-7-9-14-11-12/h7-9,11H,2-6,10H2,1H3,(H,15,16)	-3.2
InChI=1S/C27H36N4O2/c32-26(28-22-7-3-1-4-8-22)30-24-15-11-20(12-16-24)19-21-13-17-25(h11-18,22-23H,1-10,19H2,(H2,28,30,32)(H2,29,31,33)	-5.143
InChI=1S/C8H9NO2/c10-6-9-8(11)7-4-2-1-3-5-7/h1-5,10H,6H2,(H,9,11)	-0.52
InChI=1S/C40H64N2O4/c1-37(2,3)29-23-27(24-30(35(29)45)38(4,5)6)17-19-33(43)41-21-15-1 h23-26,45-46H,13-22H2,1-12H3,(H,41,43)(H,42,44)	-7.804
InChI=1S/C8H5NO2S/c10-8(11)6-1-3-7(4-2-6)9-5-12/h1-4H,(H,10,11)	-3.98
InChI=1S/C4H6O3S/c5-8(6)1-3-4(2-8)7-3/h3-4H,1-2H2	0.872
InChI=1S/C44H26Cl4N6O4/c45-31-15-7-19-35(37(31)47)51-53-39-25-11-3-1-9-23(25)21-29(41(3 h1-22,51-52H,(H,49,57)(H,50,58)/b53-39-,54-40+	-9.228
InChI=1S/C14H15OP/c1-2-16(15,13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12H,2H2,1H3	-2.906
InChI=1S/C37H46O5/c1-34(2,3)22-13-15-28(24(19-22)30-25-20-23(35(4,5)6)14-16-29(25)4 h13-20,30,38H,1-12H3	-8.849

"InChi"	"logS(M)"
InChI=1S/C17H22N4O4/c1-9(2)25-16(22)14-12(23-3)6-10(7-13(14)24-4)5-11-8-20-17(19)21-11-6-9H,5H2,1-4H3,(H4,18,19,20,21)	-3.195
InChI=1S/C17H19ClO6/c1-8-5-9(19)6-12(23-4)17(8)16(20)13-10(21-2)7-11(22-3)14(18)15(13)h7-8,12H,5-6H2,1-4H3	-4.611
InChI=1S/C10H14O4/c11-5-7-13-9-1-2-10(4-3-9)14-8-6-12/h1-4,11-12H,5-8H2	-1.23
InChI=1S/C10H9NO/c1-11-9-5-3-2-4-8(9)6-7-10(11)12/h2-7H,1H3	-1.047
InChI=1S/C24H31N3OS/c1-3-7-22(28)19-10-11-24-21(18-19)27(20-8-4-5-9-23(20)29-24)13-6-h4-5,8-11,18H,3,6-7,12-17H2,1-2H3	-6.395
InChI=1S/C13H15ClN6O7S/c1-20-10(8(9(14)18-20)11(21)27-4)28(23,24)19-13(22)17-12-15-6(25-h5H,1-4H3,(H2,15,16,17,19,22)	-4.464
InChI=1S/C12H5Cl5/c13-6-4-8(12(17)10(15)5-6)7-2-1-3-9(14)11(7)16/h1-5H	-6.96
InChI=1S/C6H6BrO3P/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H2,8,9,10)	-2.132
InChI=1S/C15H14N2O/c16-15(18)14-11-5-2-1-4-10(11)7-8-13-12(14)6-3-9-17-13/h1-6,9,14H,7-8H2,(H2,16,18)	-2.434
InChI=1S/C20H20N2O4/c1-14-18(25-13-15-4-2-3-7-21-15)6-5-16-17(23)12-19(26-20(14)16)22h2-7,12H,8-11,13H2,1H3	-4.45
InChI=1S/C12H19NO4S2/c1-17-12-6-2-4-11(10-12)5-3-7-13-8-9-18-19(14,15)16/h2,4,6,10,13H,3,5,7-9H2,1H3,(H,14,15,16)	-1.509
InChI=1S/C30H28O8/c1-15-24(33)19(27(36)22(16(2)31)25(15)34)14-20-26(35)18-12-13-30h5-13,33-37H,14H2,1-4H3/b11-10+	-8.889
InChI=1S/C11H18N2/c1-10(12-13(2)3)9-11-7-5-4-6-8-11/h4-8,10,12H,9H2,1-3H3	-1.925
InChI=1S/C8H8N2O3S/c9-14(11,12)5-7-6-3-1-2-4-8(6)13-10-7/h1-4H,5H2,(H2,9,11,12)	-2.424
InChI=1S/C12H17NO2S/c1-2-3-8-16-11-6-4-10(5-7-11)9-12(14)13-15/h4-7,15H,2-3,8-9H2,1H3,(H,13,14)	-3.078
InChI=1S/C13H17NO3/c1-2-3-10-17-12-7-4-11(5-8-12)6-9-13(15)14-16/h4-9,16H,2-3,10H2,1H3,(H,14,15)/b9-6+	-3.296
InChI=1S/C6H8NO3P/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H,7H2,(H2,8,9,10)	-1.605
InChI=1S/C10H12BrNO3/c1-6(13)5-15-9-3-2-7(11)4-8(9)10(12)14/h2-4,6,13H,5H2,1H3,(H2,12,14)	-1.727
InChI=1S/C32H30N2O2/c1-17-13-19(3)29(20(4)14-17)33-25-11-12-26(34-30-21(5)15-18(2)16h7-16,33-34H,1-6H3	-7.825
InChI=1S/C12H15NO4/c1-3-17-10-6-4-9(8-11(10)16-2)5-7-12(14)13-15/h4-8,15H,3H2,1-2H3,(H,13,14)/b7-5+	-2.099
InChI=1S/C11H20O2/c1-4-7-8-10(5-2)9-13-11(12)6-3/h6,10H,3-5,7-9H2,1-2H3	-4.283

"InChi"	"logS(M)"
InChI=1S/C14H10O4/c15-12-8-4-3-7-11(12)13(16)9-5-1-2-6-10(9)14(17)18/h1-8,15H,(H,17,18)	-2.343
InChI=1S/C9H12N2O4/c12-5-1-4-10-8-3-2-7(13)6-9(8)11(14)15/h2-3,6,10,12-13H,1,4-5H2	-2.111
InChI=1S/C13H17IN2O6/c1-6(2)12(19)21-5-9-8(17)3-10(22-9)16-4-7(14)11(18)15-13(16)20/h4,6,8-10,17H,3,5H2,1-2H3,(H,15,18,20)	-2.76
InChI=1S/C20H41N5O7/c1-20(28)8-29-19(14(27)17(20)25-3)31-15-11(23)6-12(24-2)16(13(15)h9-19,24-28H,4-8,21-23H2,1-3H3	0.054
InChI=1S/C11H10N2O/c1-2-3-8-4-5-9-6-12-7-13-10(9)11(8)14/h2,4-7,14H,1,3H2	-3.62
InChI=1S/C20H22N2O/c1-22-11-5-8-20(22)18-13-21-19-10-9-16(12-17(18)19)23-14-15-6-3-2h2-4,6-7,9-10,12-13,20-21H,5,8,11,14H2,1H3	-3.875
InChI=1S/C11H14O2/c1-2-9(8-11(12)13)10-6-4-3-5-7-10/h3-7,9H,2,8H2,1H3,(H,12,13)	-2.834
InChI=1S/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3-7,11H,1-2H3/b4-3+	-2.365
InChI=1S/C4H8N2O3/c5-4(7)2-1-3-6(8)9/h1-3H2,(H2,5,7)	-0.969
InChI=1S/C15H18N2O3/c1-4-15(5-2)13(20-11(3)18)16-17(14(15)19)12-9-7-6-8-10-12/h6-10H,4-5H2,1-3H3	-3.54
InChI=1S/C5H10O3/c1-5(6)8-4-3-7-2/h3-4H2,1-2H3	0.928
InChI=1S/C12H11N3O5S/c13-8-1-3-9(4-2-8)14-11-6-5-10(15(16)17)7-12(11)21(18,19)20/h1-7,14H,13H2,(H,18,19,20)	-1.598
InChI=1S/C14H22ClN5OS/c1-18-3-5-19(6-4-18)13-11(22-2)12(15)16-14(17-13)20-7-9-21-10-8-2h3-10H2,1-2H3	-2.062
InChI=1S/C8H6S/c1-2-4-8-7(3-1)5-6-9-8/h1-6H	-3.014
InChI=1S/C15H11NO2/c1-8-6-7-11-12(13(8)16)15(18)10-5-3-2-4-9(10)14(11)17/h2-7H,16H2,1H3	-5.854
InChI=1S/C7H5BrO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)	-3.525
InChI=1S/C7H6Cl2/c1-5-6(8)3-2-4-7(5)9/h2-4H,1H3	-3.792
InChI=1S/C6H7N3O/c7-9-6(10)5-2-1-3-8-4-5/h1-4H,7H2,(H,9,10)	-0.137
InChI=1S/C22H31N3O2/c1-5-25(15-16-26-19(4)27-17-18(2)3)22-13-11-21(12-14-22)24-23-20h6-14,18-19H,5,15-17H2,1-4H3/b24-23+	-7.091
InChI=1S/C21H40O4/c1-5-7-9-11-13-15-19(22)24-17-21(3,4)18-25-20(23)16-14-12-10-8-6-h5-18H2,1-4H3	-6.853
InChI=1S/C34H28ClN5O7/c1-45-27-13-10-20(33(43)37-21-11-8-18(9-12-21)32(36)42)15-26(27)h4-17,39H,1-3H3,(H2,36,42)(H,37,43)(H,38,44)/b40-30-	-7.866
InChI=1S/C13H16N4O4S/c1-3-9(18)20-7-17-6-16-11-12(17)14-5-15-13(11)22-8-21-10(19)4-2/h5-6H,3-4,7-8H2,1-2H3	-2.78

"InChi"	"logS(M)"
InChI=1S/C7H13O4P/c1-6(2)7-3-9-12(8,10-4-7)11-5-7/h6H,3-5H2,1-2H3	-1.125
InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3	-0.466
InChI=1S/C11H10O3/c12-10-6-8(11(13)14)5-7-3-1-2-4-9(7)10/h1-4,8H,5-6H2,(H,13,14)	-2.103
InChI=1S/C14H18N4O2S/c1-19-10-5-8(6-11(20-2)12(10)21-3)4-9-7-17-14(16)18-13(9)15/h5-7H,4H2,1-3H3,(H4,15,16,17,18)	-2.75
InChI=1S/C7H6Cl2/c1-5-2-3-6(8)4-7(5)9/h2-4H,1H3	-3.809
InChI=1S/C12H10N2O4S/c15-14(16)11-8-6-10(7-9-11)13-19(17,18)12-4-2-1-3-5-12/h1-9,13H	-3.93
InChI=1S/C7H2Cl4O2/c8-3-1-2(7(12)13)4(9)6(11)5(3)10/h1H,(H,12,13)	-4.606
InChI=1S/C11H14O2/c1-9(8-11(12)13)7-10-5-3-2-4-6-10/h2-6,9H,7-8H2,1H3,(H,12,13)	-2.834
InChI=1S/C10H14NO5PS/c1-4-8-7-9(5-6-10(8)11(12)13)16-17(18,14-2)15-3/h5-7H,4H2,1-3H3	-4.908
InChI=1S/C17H28N2O2/c1-5-18(6-2)16(20)14-12-9-10-13(11-12)15(14)17(21)19(7-3)8-4/h9-10,12-15H,5-8,11H2,1-4H3	-3.068
InChI=1S/C38H60N8O9/c1-22(2)15-27(31(47)19-32(48)43-28(16-23(3)4)33(49)41-14-13-26(3	-2.22
InChI=1S/C20H25N3/c1-2-7-19(8-3-1)23-14-12-22(13-15-23)16-18-11-10-17-6-4-5-9-20(17	-3.756
InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)9-8(12)10-7/h1-4H,(H2,9,10,11,12)	-3.099
InChI=1S/C9H12N4O3S/c1-5-9(2,3)16-7(11-5)12-8-10-4-6(17-8)13(14)15/h4-5H,1-3H3,(H,10,11,12)	-2.057
InChI=1S/C7H7Cl2N3O/c1-12(10)7(13)4-2-5(8)11-6(9)3-4/h2-3H,10H2,1H3	-2.359
InChI=1S/C10H14O2/c1-10(2,3)8-6-7(11)4-5-9(8)12/h4-6,11-12H,1-3H3	-1.221
InChI=1S/C9H7NO6/c1-16-9(13)6-2-5(8(11)12)3-7(4-6)10(14)15/h2-4H,1H3,(H,11,12)	-2.074
InChI=1S/C5H10Cl2O2/c6-1-3-8-5-9-4-2-7/h1-5H2	-1.346
InChI=1S/C17H14N2/c1-10-14-9-18-8-7-12(14)11(2)17-16(10)13-5-3-4-6-15(13)19-17/h3-9,19H,1-2H3	-6.206
InChI=1S/C15H19NO/c1-11(2)16-10-15(17)14-8-7-12-5-3-4-6-13(12)9-14/h3-9,11,15-17H,10H2,1-2H3	-2.427
InChI=1S/C8H6ClNO2/c1-10-6-4-5(9)2-3-7(6)12-8(10)11/h2-4H,1H3	-2.535
InChI=1S/C9H8Cl2N2O2/c10-7(11)9(15)13-6-4-2-1-3-5(6)8(12)14/h1-4,7H,(H2,12,14)(H,13,15)	-2.437
InChI=1S/C4H6Cl2/c5-3-1-2-4-6/h1-2H,3-4H2/b2-1+	-2.167

"InChi"	"logS(M)"
InChI=1S/C8H7IN4O4S3/c9-5-1-3-6(4-2-5)20(16,17)13-7-11-12-8(18-7)19(10,14)15/h1-4H,(H,11,13)(H2,10,14,15)	-2.2
InChI=1S/C7H11N3O3/c1-7(2,11)5-4-8-6(9(5)3)10(12)13/h4,11H,1-3H3	-1.309
InChI=1S/C17H15NO2/c19-17(20-13-14-7-2-1-3-8-14)18-12-6-10-15-9-4-5-11-16(15)18/h1-11H,12-13H2	-5.334
InChI=1S/C12H16N3O4PS/c1-3-18-20(17,19-4-2)21-9-15-12(16)10-7-5-6-8-11(10)13-14-15/h5-8H,3-4,9H2,1-2H3	-1.993
InChI=1S/C10H6O7/c11-7(10(16)17)6-4(8(12)13)2-1-3-5(6)9(14)15/h1-3H,(H,12,13)(H,14,15)(H,16,17)	-0.454
InChI=1S/C3H5NO3/c5-2-4-1-3(6)7/h2H,1H2,(H,4,5)(H,6,7)	0.267
InChI=1S/C18H26ClN3O/c1-3-22(11-12-23)10-4-5-14(2)21-17-8-9-20-18-13-15(19)6-7-16(17)1h6-9,13-14,23H,3-5,10-12H2,1-2H3,(H,20,21)	-3.032
InChI=1S/C20H30O2/c1-12-10-14(21)11-13-4-5-15-16-6-7-18(22)19(16,2)9-8-17(15)20(12,h11-12,15-18,22H,4-10H2,1-3H3	-3.526
InChI=1S/C13H29N/c1-3-10-13(4-2)11-8-6-5-7-9-12-14/h13H,3-12,14H2,1-2H3	-3.698
InChI=1S/C10H9N3S2/c14-9(13-10-11-6-7-15-10)12-8-4-2-1-3-5-8/h1-7H,(H2,11,12,13,14)	-2.807
InChI=1S/C5H10O2/c1-2-5-6-3-4-7-5/h5H,2-4H2,1H3	0.292
InChI=1S/C6H5F3N2O2/c1-3(12)10-5-11-4(2-13-5)6(7,8)9/h2H,1H3,(H,10,11,12)	-1.387
InChI=1S/C12H27NO3S2/c1-3-5-6-7-8-9-12(4-2)13-10-11-17-18(14,15)16/h12-13H,3-11H2,1-2H3,(H,14,15,16)	-2.796
InChI=1S/C14H30O/c1-3-5-6-7-8-9-10-11-13-14(15)12-4-2/h14-15H,3-13H2,1-2H3	-5.837
InChI=1S/C12H8N6O16/c19-9(33-5-11(13(21)22,14(23)24)15(25)26)7-3-1-2-4-8(7)10(20)34-6h1-4H,5-6H2	-3.578
InChI=1S/C15H7Cl2F3N2O2/c16-9-6-11-12(7-10(9)17)22(13(21-11)15(18,19)20)14(23)24-8-4-2-1-h1-7H	-4.46
InChI=1S/C11H12N2O/c1-9-7-11(14)13(12-9)8-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3	-2.4
InChI=1S/C12H5Cl5O/c13-6-4-5-9(11(17)10(6)16)18-12-7(14)2-1-3-8(12)15/h1-5H	-7.23
InChI=1S/C15H18N4O7S/c1-4-25-10-7-5-6-8-11(10)26-27(21,22)19-15(20)18-14-16-12(23-2)9-h5-9H,4H2,1-3H3,(H2,16,17,18,19,20)	-4.185
InChI=1S/C15H19N3O2/c1-10(2)16-13-11(3)17(4)15(20)18(14(13)19)12-8-6-5-7-9-12/h5-10,16H,1-4H3	-2.051
InChI=1S/C8H10N2O/c1-10(8(9)11)7-5-3-2-4-6-7/h2-6H,1H3,(H2,9,11)	-0.656
InChI=1S/C11H14O4/c1-8(13)9-2-4-11(5-3-9)15-7-10(14)6-12/h2-5,10,12,14H,6-7H2,1H3	-1.196

"InChi"	"logS(M)"
InChI=1S/C15H17Br2NO2/c1-2-3-4-5-6-7-14(19)20-15-12(16)8-11(10-18)9-13(15)17/h8-9H,2-7H2,1H3	-6.702
InChI=1S/C8H9O3PS/c1-9-12(13)10-6-7-4-2-3-5-8(7)11-12/h2-5H,6H2,1H3	-3.571
InChI=1S/C9H15N3O2S/c1-12(2,3)7(8(13)14)4-6-5-10-9(15)11-6/h5,7H,4H2,1-3H3,(H2-,10,11,13,14,15)	-0.46
InChI=1S/C16H24O4/c1-11-5-3-2-4-6-12-9-13(17)10-14(12)15(18)7-8-16(19)20-11/h4,6-8,11-15,17-18H,2-3,5,9-10H2,1H3/b6-4-,8-7-	-5.67
InChI=1S/C32H44O4/c1-20(33)35-25-14-12-21(31(8,9)18-29(2,3)4)16-23(25)27-24-17-22(1h12-17,27H,18-19H2,1-11H3	-6.693
InChI=1S/C15H24N2O3/c18-12-15(13(19)17-14(20)16-12)10-8-6-4-2-1-3-5-7-9-11-15/h1-11H2,(H2,16,17,18,19,20)	-5.8
InChI=1S/C22H29N3O/c1-7-21(3,4)15-13-16(22(5,6)8-2)20(26)19(14-15)25-23-17-11-9-10-1h9-14,26H,7-8H2,1-6H3	-8.546
InChI=1S/C21H30N2O2/c1-20(2)14-18(17-8-6-5-7-9-17)15-21(3,4)23(20)19(24)16-22-10-12-2h5-9,14H,10-13,15-16H2,1-4H3	-4.589
InChI=1S/C6H6N2S/c7-6(9)5-3-1-2-4-8-5/h1-4H,(H2,7,9)	-0.261
InChI=1S/C11H13NO/c1-9-7-8-11(13)12(9)10-5-3-2-4-6-10/h2-6,9H,7-8H2,1H3	-0.846
InChI=1S/C7H11N3O2/c1-5(2)6-4-8-7(9(6)3)10(11)12/h4-5H,1-3H3	-1.756
InChI=1S/C7H6N2/c1-4-9-7-2-3-8-5-6(1)7/h1-5,9H	-0.942
InChI=1S/C8H12INO2/c1-2-3-6-10-8(11)12-7-4-5-9/h2-3,6-7H2,1H3,(H,10,11)	-3.203
InChI=1S/C15H21ClO3/c1-2-3-4-5-6-7-10-19-15(18)12-8-9-14(17)13(16)11-12/h8-9,11,17H,2-7,10H2,1H3	-4.38
InChI=1S/C12H16O2/c1-10(13)14-12(2,3)9-11-7-5-4-6-8-11/h4-8H,9H2,1-3H3	-2.395
InChI=1S/C14H19ClN4O/c15-12-3-1-2-4-13(12)19-7-5-18(6-8-19)10-11-9-17-14(16)20-11/h1-4,11H,5-10H2,(H2,16,17)	-2.947
InChI=1S/C11H12O3/c1-2-14-10-6-4-3-5-9(10)7-8-11(12)13/h3-8H,2H2,1H3,(H,12,13)/b8-7+	-2.523
InChI=1S/C21H18ClNO6/c1-12-16(10-20(26)29-11-19(24)25)17-9-15(28-2)7-8-18(17)23(12)21(h3-9H,10-11H2,1-2H3,(H,24,25)	-5.095
InChI=1S/C20H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-20-18-21/h9-10,21H,2-8,11-20H2,1H3/b10-9+	-2.495
InChI=1S/C7H12O2/c1-3-5-6-9-7(8)4-2/h4H,2-3,5-6H2,1H3	-1.877
InChI=1S/C10H12N2O2/c1-7(13)12-5-8-2-3-10(11)4-9(8)6-14-12/h2-4H,5-6,11H2,1H3	-1.017
InChI=1S/C23H29NO/c1-3-22(25)23(20-12-6-4-7-13-20,21-14-8-5-9-15-21)19(2)18-24-16-1h4-9,12-15,19H,3,10-11,16-18H2,1-2H3	-4.939

"InChi"	"logS(M)"
InChI=1S/C4H7FOS/c1-4(6)7-3-2-5/h2-3H2,1H3	-0.652
InChI=1S/C10H20N2O4/c1-4-5-10(2,6-15-8(11)13)7-16-9(14)12-3/h4-7H2,1-3H3,(H2,11,13)(H,12,14)	-2.133
InChI=1S/C17H20O5/c1-11(17(20)22-10-15(19)9-18)12-3-4-14-8-16(21-2)6-5-13(14)7-12/h3-8,11,15,18-19H,9-10H2,1-2H3	-2.62
InChI=1S/C13H11N/c14-11-5-6-13-10(8-11)7-9-3-1-2-4-12(9)13/h1-6,8H,7,14H2	-4.315
InChI=1S/C4H8N4O3/c1-7-3-11-2-5-4(7)6-8(9)10/h2-3H2,1H3,(H,5,6)	-1.002
InChI=1S/C6H12N4/c1-7-2-9-4-8(1)5-10(3-7)6-9/h1-6H2	0.792
InChI=1S/C10H12OS2/c1-11-9-5-3-2-4-8(9)10-12-6-7-13-10/h2-5,10H,6-7H2,1H3	-3.655
InChI=1S/C18H27NO3/c1-3-4-5-6-7-8-9-10-18(21)22-17-13-11-16(12-14-17)19-15(2)20/h11-14H,3-10H2,1-2H3,(H,19,20)	-4.53
InChI=1S/C3HBr2ClO2/c4-2(5)1(6)3(7)8/h(H,7,8)	-0.687
InChI=1S/C4H5N3O2/c5-2-1-6-4(9)7-3(2)8/h1H,5H2,(H2,6,7,8,9)	-2.41
InChI=1S/C26H16O2S2/c27-25-19-13-7-15-21(29-17-9-3-1-4-10-17)23(19)26(28)24-20(25)14-h1-16H	-5.517
InChI=1S/C18H28N2O4/c1-3-5-9-23-16-13-15(14-17(19-16)24-10-6-4-2)18(21)20-7-11-22-12-h13-14H,3-12H2,1-2H3	-4.363
InChI=1S/C10H12O3/c11-10(12)7-4-8-13-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H,11,12)	-2.094
InChI=1S/C6H7NO/c1-6-2-4-7(8)5-3-6/h2-5H,1H3	0.962
InChI=1S/C23H28O11/c1-20-9-22(29)13-7-23(20,32-18-16(27)15(26)14(25)12(8-24)31-18)2h2-6,12-16,18-19,24-27,29H,7-10H2,1H3	-1.32
InChI=1S/C11H17NO/c1-8-5-10(7-12(3)4)6-9(2)11(8)13/h5-6,13H,7H2,1-4H3	-0.938
InChI=1S/C30H50O/c1-19(2)20-11-14-27(5)17-18-29(7)21(25(20)27)9-10-23-28(6)15-13-2h20-25,31H,1,9-18H2,2-8H3	-10.845
InChI=1S/C20H14O4/c21-19(23-15-9-3-1-4-10-15)17-13-7-8-14-18(17)20(22)24-16-11-5-2-h1-14H	-6.589
InChI=1S/C12H22O6/c1-15-7-9-17-11(13)5-3-4-6-12(14)18-10-8-16-2/h3-10H2,1-2H3	-1.266
InChI=1S/C22H30N2O/c1-17(2)24(18(3)4)16-15-22(21(23)25,19-11-7-5-8-12-19)20-13-9-6-1h5-14,17-18H,15-16H2,1-4H3,(H2,23,25)	-5.211
InChI=1S/C14H18N2O/c17-14-13(15-9-4-5-10-15)8-11-16(14)12-6-2-1-3-7-12/h1-3,6-7,13H,4-5,8-11H2	-2.337
InChI=1S/C12H16N2O3/c1-5-7-12(8-6-2)9(15)13(3)11(17)14(4)10(12)16/h5-6H,1-2,7-8H2,3-4H3	-2.407

"InChi"	"logS(M)"
InChI=1S/C22H33NO5/c1-5-26-22(25)20-17(4)9-10-18(16(2)3)21(20)28-15-19(24)27-14-13-2h9-10,16H,5-8,11-15H2,1-4H3	-5.319
InChI=1S/C21H27NO/c1-5-20(23)21(16-17(2)22(3)4,18-12-8-6-9-13-18)19-14-10-7-11-15-1h6-15,17H,5,16H2,1-4H3	-3.805
InChI=1S/C12H14N4O5/c1-7(2)13-12(17)8-5-10(14-3-4-14)11(16(20)21)6-9(8)15(18)19/h5-7H,3-4H2,1-2H3,(H,13,17)	-3.5
InChI=1S/C15H24N4O2S2/c1-4-7-22-23-14(5-6-20)11(2)19(10-21)9-13-8-17-12(3)18-15(13)16/h8,10,20H,4-7,9H2,1-3H3,(H2,16,17,18)/b14-11-	-3.151
InChI=1S/C15H22BrNO/c1-14(2,3)12(16)13(18)17-15(4,5)11-9-7-6-8-10-11/h6-10,12H,1-5H3,(H,17,18)	-4.946
InChI=1S/C13H12N2O4S/c14-8-5-6-10(15)12(7-8)20(18,19)11-4-2-1-3-9(11)13(16)17/h1-7H,14-15H2,(H,16,17)	-1.839
InChI=1S/C8H9NO3/c10-7-3-1-2-5-9(7)6-4-8(11)12/h1-3,5H,4,6H2,(H,11,12)	-0.6
InChI=1S/C17H23N7O5/c1-23-6-4-9(20-16(23)19)8-12(25)21-10-2-3-13(29-14(10)15(26)27)24h2-3,5,7,9-10,13-14H,4,6,8H2,1H3,(H2,19,20)(H,21,25)(H,26,27)(H2,18,22,28)	0.149
InChI=1S/C11H22N2O4/c1-4-5-6-11(2,7-16-9(12)14)8-17-10(15)13-3/h4-8H2,1-3H3,(H2,12,14)(H,13,15)	-2.653
InChI=1S/C18H22N2O2/c1-2-17(21)20-15-10-11-16(20)18(22)19(13-15)12-6-9-14-7-4-3-5-8-1h3-9,15-16H,2,10-13H2,1H3/b9-6+	-2.892
InChI=1S/C14H31N/c1-4-5-6-7-8-9-10-11-12-13-14-15(2)3/h4-14H2,1-3H3	-4.426
InChI=1S/C20H25N3O2/c1-3-14(11-24)22-20(25)13-7-16-15-5-4-6-17-19(15)12(9-21-17)8-18(h4-7,9,13-14,18,21,24H,3,8,10-11H2,1-2H3,(H,22,25)	-2.691
InChI=1S/C6H8N4O3S/c1-7-6(14)8-2-3(11)9-5(13)10-4(2)12/h2H,1H3,(H2,7,8,14)(H2,9,10,11,12,13)	-0.46
InChI=1S/C9H13ClN4O5S2/c1-13-4-9(15)14-6-2-5(10)7(20(11,16)17)3-8(6)21(12,18)19/h2-3,13H,4H2,1H3,(H,14,15)(H2,11,16,17)(H2,12,18,19)	-1.27
InChI=1S/C21H30O6/c1-4-7-12-25-19(22)16-10-11-17(20(23)26-13-8-5-2)18(15-16)21(24)2h10-11,15H,4-9,12-14H2,1-3H3	-4.807
InChI=1S/C11H16O/c1-9(10(2)12)8-11-6-4-3-5-7-11/h3-7,9-10,12H,8H2,1-2H3	-1.697
InChI=1S/C12H5Cl5O/c13-6-1-2-7(14)11(3-6)18-12-5-9(16)8(15)4-10(12)17/h1-5H	-7.56
InChI=1S/C7H8F9NO3S/c1-17(2-3-18)21(19,20)7(15,16)5(10,11)4(8,9)6(12,13)14/h18H,2-3H2,1H3	-3.404
InChI=1S/C10H11NO4/c12-6-8(10(14)15)11-9(13)7-4-2-1-3-5-7/h1-5,8,12H,6H2,(H,11,13)(H,14,15)	-0.91

"InChi"	"logS(M)"
InChI=1S/C12H8N2/c1-2-6-10-9(5-1)13-11-7-3-4-8-12(11)14-10/h1-8H	-3.7
InChI=1S/C9H6OS/c11-9-6-5-7-3-1-2-4-8(7)10-9/h1-6H	-1.802
InChI=1S/C19H17NO3/c1-2-23-16-9-7-15(8-10-16)20-19(22)17-11-13-5-3-4-6-14(13)12-18(1h3-12,21H,2H2,1H3,(H,20,22)	-5.312
InChI=1S/C6H9NO3/c1-3-6(2)4(8)7-5(9)10-6/h3H2,1-2H3,(H,7,8,9)	0.02
InChI=1S/C20H22Cl2N2OS/c21-15-4-7-17(8-5-15)26-19-9-6-16(22)14-18(19)23-20(25)10-13-24-1h4-9,14H,1-3,10-13H2,(H,23,25)	-6.785
InChI=1S/C19H26N2O/c1-2-19(22)21-17-11-12-18(21)15-20(14-17)13-7-6-10-16-8-4-3-5-9-1h3-6,8-10,17-18H,2,7,11-15H2,1H3/b10-6+	-4.178
InChI=1S/C28H32Cl2N6/c1-19(33-25-7-9-31-27-15-21(29)3-5-23(25)27)17-35-11-13-36(14-12-h3-10,15-16,19-20H,11-14,17-18H2,1-2H3,(H,31,33)(H,32,34)	-8.194
InChI=1S/C12H9ClN2O3/c13-11-10(18-8-4-2-1-3-5-8)7-6-9(12(11)14)15(16)17/h1-7H,14H2	-5.025
InChI=1S/C16H18N2O2/c1-12-6-2-5-9-15(12)20-11-10-18-14-8-4-3-7-13(14)16(17)19/h2-9,18H,10-11H2,1H3,(H2,17,19)	-3.683
InChI=1S/C9H9BrO3/c1-2-13-9(12)6-3-4-8(11)7(10)5-6/h3-5,11H,2H2,1H3	-3.39
InChI=1S/C7H8N2O3S/c8-7(10)5-2-1-3-6(4-5)13(9,11)12/h1-4H,(H2,8,10)(H2,9,11,12)	-2.155
InChI=1S/C22H29NO5/c1-14(2)11-20(23)22(25)28-10-9-27-21(24)15(3)16-5-6-18-13-19(26-4h5-8,12-15,20H,9-11,23H2,1-4H3	-3.82
InChI=1S/C18H27NO2/c1-16-10-6-8-14-19(16)13-7-3-9-15-21-18(20)17-11-4-2-5-12-17/h2,4-5,11-12,16H,3,6-10,13-15H2,1H3	-4.382
InChI=1S/C7H11NOS2/c1-2-3-4-8-6(9)5-11-7(8)10/h2-5H2,1H3	-1.163
InChI=1S/C10H21NOS/c1-4-7-11(8-5-2)10(12)13-9-6-3/h4-9H2,1-3H3	-3.3
InChI=1S/C3H9NO3S/c1-3(4)2-8(5,6)7/h3H,2,4H2,1H3,(H,5,6,7)	0.856
InChI=1S/C28H38O19/c1-12(29)37-9-20-22(40-15(4)32)24(42-17(6)34)25(43-18(7)35)27(45-h20-27H,9-11H2,1-8H3	-2.873
InChI=1S/C7H16N2O4S/c1-3-6(4-2)5-13-7(10)9-14(8,11)12/h6H,3-5H2,1-2H3,(H,9,10)(H2,8,11,12)	-1.749
InChI=1S/C9H11Cl2O3PS/c1-6-4-7(10)9(8(11)5-6)14-15(16,12-2)13-3/h4-5H,1-3H3	-5.437
InChI=1S/C8H7NO2/c10-8-5-11-7-4-2-1-3-6(7)9-8/h1-4H,5H2,(H,9,10)	-2.572
InChI=1S/C18H20N2O4/c1-2-3-6-11-19-15(21)10-9-14(18(19)24)20-16(22)12-7-4-5-8-13(12)1h4-5,7-8,14H,2-3,6,9-11H2,1H3	-4.7
InChI=1S/C6H9NO5/c1-3(8)7-4(6(11)12)2-5(9)10/h4H,2H2,1H3,(H,7,8)(H,9,10)(H,11,12)	0.757

"InChi"	"logS(M)"
InChI=1S/C20H19NO/c21-19(16-10-4-1-5-11-16)20(22,17-12-6-2-7-13-17)18-14-8-3-9-15-1h1-15,19,22H,21H2	-3.143
InChI=1S/C12H26O/c1-3-5-7-8-10-12(11-13)9-6-4-2/h12-13H,3-11H2,1-2H3	-5.27
InChI=1S/C19H31NO3/c1-13(2)12-23-19(21)17-15(5)8-9-16(14(3)4)18(17)22-11-10-20(6)7/h8-9,13-14H,10-12H2,1-7H3	-4.814
InChI=1S/C6H10O4S2/c7-5(8)1-3-11-12-4-2-6(9)10/h1-4H2,(H,7,8)(H,9,10)	-0.93
InChI=1S/C25H22ClNO3/c1-17(2)24(18-11-13-20(26)14-12-18)25(28)30-23(16-27)19-7-6-10-2h3-15,17,23-24H,1-2H3	-8.322
InChI=1S/C6H6ClO3P/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H,(H2,8,9,10)	-1.6
InChI=1S/C11H16O3/c1-8-5-3-4-6-11(8)14-7-10(13)9(2)12/h3-6,9-10,12-13H,7H2,1-2H3	-1.849
InChI=1S/C5H9NO3S/c1-3(10)5(9)6-2-4(7)8/h3,10H,2H2,1H3,(H,6,9)(H,7,8)	0.162
InChI=1S/C23H16O6/c24-20-16(14-7-3-1-5-12(14)9-18(20)22(26)27)11-17-15-8-4-2-6-13(1h1-10,24-25H,11H2,(H,26,27)(H,28,29)	-0.553
InChI=1S/C15H21NO5/c1-19-10-8-16(9-11-20-2)14(17)12-21-15(18)13-6-4-3-5-7-13/h3-7H,8-12H2,1-2H3	-1.57
InChI=1S/C14H20N2O2/c1-11-6-3-4-8-13(11)15-14(17)18-12-7-5-9-16(2)10-12/h3-4,6,8,12H,5,7,9-10H2,1-2H3,(H,15,17)	-2.845
InChI=1S/C10H15NO3S2/c11-16(13,14)10-5-3-9(4-6-10)15-8-2-1-7-12/h3-6,12H,1-2,7-8H2,(H2,11,13,14)	-2.514
InChI=1S/C12H17ClO3/c1-2-3-9-6-10(13)4-5-12(9)16-8-11(15)7-14/h4-6,11,14-15H,2-3,7-8H2,1H3	-3.576
InChI=1S/C17H20N2O5/c1-5-19-8-13(17(22)24-9-23-16(21)10(2)3)14(20)12-7-6-11(4)18-15(1h6-8,10H,5,9H2,1-4H3	-3.02
InChI=1S/C17H12I2O3/c1-2-13-15(10-5-3-4-6-14(10)22-13)16(20)9-7-11(18)17(21)12(19)8-9h3-8,21H,2H2,1H3	-8.02
InChI=1S/C10H15NO3/c1-7-4-8(11)2-3-10(7)14-6-9(13)5-12/h2-4,9,12-13H,5-6,11H2,1H3	-1.057
InChI=1S/C7H6Cl2O/c1-10-6-4-2-3-5(8)7(6)9/h2-4H,1H3	-3.309
InChI=1S/C4H8O2/c1-2-6-4-3-5-1/h1-4H2	1.055
InChI=1S/C9H10O3/c1-12-8-4-2-7(3-5-8)6-9(10)11/h2-5H,6H2,1H3,(H,10,11)	-1.231
InChI=1S/C19H16O3/c20-18-15-9-3-4-11-16(15)22-19(21)17(18)14-10-5-7-12-6-1-2-8-13(1h1-4,6,8-9,11,14,20H,5,7,10H2	-4.86
InChI=1S/C14H22N4O6S2/c1-5-7-16(8-6-2)14-12(17(19)20)9-11(10-13(14)18(21)22)26(23,24)15h9-10H,5-8H2,1-4H3/p+1	-4.86
InChI=1S/C7H16O/c1-5-7(3,4)8-6-2/h5-6H2,1-4H3	-1.472

"InChi"	"logS(M)"
InChI=1S/C14H12N2O2/c17-13(11-7-3-1-4-8-11)15-16-14(18)12-9-5-2-6-10-12/h1-10H,(H,15,17)(H,16,18)	-1.588
InChI=1S/C16H12FNO3/c1-9(16(19)20)11-4-7-14-13(8-11)18-15(21-14)10-2-5-12(17)6-3-10/h2-9H,1H3,(H,19,20)	-3.905
InChI=1S/C3H9N/c1-2-3-4/h2-4H2,1H3	1.228
InChI=1S/C15H15NO3/c17-14(11-19-13-9-5-2-6-10-13)15(18)16-12-7-3-1-4-8-12/h1-10,14,17H,11H2,(H,16,18)	-2.41
InChI=1S/C8H9NO4/c1-4-5(2-3-6(10)11)8(13)9-7(4)12/h2-3H2,1H3,(H,10,11)(H,9,12,13)	-0.661
InChI=1S/C11H22O/c1-4-6-7-9-11(12)10(3)8-5-2/h8,11-12H,4-7,9H2,1-3H3/b10-8-	-3.432
InChI=1S/C6H15O4PS2/c1-4-13(8)6-5-12-11(7,9-2)10-3/h4-6H2,1-3H3/p+1	0.609
InChI=1S/C7H11N7S/c1-4(2)9-5-10-6(13-14-8)12-7(11-5)15-3/h4H,1-3H3,(H,9,10,11,12)	-3.48
InChI=1S/C15H15NO2/c1-16(2)15(18)13-10-6-9-12(14(13)17)11-7-4-3-5-8-11/h3-10,17H,1-2H3	-2.762
InChI=1S/C17H13N3O/c1-20-15-8-7-12(10-18)9-14(15)17(19-11-16(20)21)13-5-3-2-4-6-13/h2-9H,11H2,1H3	-3.01
InChI=1S/C10H19N3O4/c1-6(2)3-7(11)10(17)13-4-8(14)12-5-9(15)16/h6-7H,3-5,11H2,1-2H3,(H,12,14)(H,13,17)(H,15,16)	0.212
InChI=1S/C8H18O/c1-4-6-8(9)7(3)5-2/h7-9H,4-6H2,1-3H3	-1.841
InChI=1S/C57H110O6/c1-51(2)43-37-31-25-19-13-7-10-16-22-28-34-40-46-55(58)61-49-54((h51-54H,7-50H2,1-6H3	-8.459
InChI=1S/C13H17ClO3/c1-3-16-13(15)5-4-8-17-12-7-6-11(14)9-10(12)2/h6-7,9H,3-5,8H2,1-2H3	-4.41
InChI=1S/C10H14O/c1-7(2)9-6-4-5-8(3)10(9)11/h4-7,11H,1-3H3	-1.274
InChI=1S/C12H18O7/c1-3-5-16-11(13)18-9-7-15-8-10-19-12(14)17-6-4-2/h3-4H,1-2,5-10H2	-2.065
InChI=1S/C22H30N6O4/c1-3-8-27(9-4-2)13-16-6-5-7-17(12-16)21(30)32-11-10-31-15-28-14-2h5-7,12,14H,3-4,8-11,13,15H2,1-2H3,(H3,23,25,26,29)	-0.35
InChI=1S/C20H25NO3/c1-2-20(23)17-8-10-19(11-9-17)24-15-18(22)14-21-13-12-16-6-4-3-5-h3-11,18,21-22H,2,12-15H2,1H3	-2.851
InChI=1S/C9H12N2O/c10-9(12)11-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H3,10,11,12)	-1.347
InChI=1S/C12H11NO4/c14-10(15)6-3-7-13-11(16)8-4-1-2-5-9(8)12(13)17/h1-2,4-5H,3,6-7H2,(H,14,15)	-2.392
InChI=1S/C5H5N3O4/c1-7-2-3(8(11)12)4(9)6-5(7)10/h2H,1H3,(H,6,9,10)	-1.998
InChI=1S/C9H12O/c1-2-3-8-4-6-9(10)7-5-8/h4-7,10H,2-3H2,1H3	-2.028

"InChi"	"logS(M)"
InChI=1S/C16H30O4/c1-3-5-7-9-11-13-15(17)19-20-16(18)14-12-10-8-6-4-2/h3-14H2,1-2H3	-7.612
InChI=1S/C7H12N2O2/c1-5-3-2-4-6(8-10)7(5)9-11/h5,10-11H,2-4H2,1H3/b8-6+,9-7-	-1.592
InChI=1S/C24H32O4/c1-4-22(25)27-16-7-9-17-15(14-16)6-8-19-18(17)12-13-24(3)20(19)10h7,9,14,18-21H,4-6,8,10-13H2,1-3H3	-7.133
InChI=1S/C15H22Cl2N2O3S/c1-13-2-4-14(5-3-13)23(20,21)19-10-11-22-15(12-19)18(8-6-16)9-7-17h2-5,15H,6-12H2,1H3	-3.005
InChI=1S/C9H12ClNOS/c1-9(12,6-11)13-8-4-2-7(10)3-5-8/h2-5,12H,6,11H2,1H3	-0.815
InChI=1S/C15H19NO/c1-13(11-14-7-4-3-5-8-14)16(2)12-15-9-6-10-17-15/h3-10,13H,11-12H2,1-2H3	-2.864
InChI=1S/C21H25Cl2NO3/c1-24-8-7-13-10-19(25-2)20(26-3)12-16(13)18(24)6-5-14-9-15(22)11-h9-12,18H,5-8H2,1-4H3	-6.398
InChI=1S/C21H25FN2O2/c1-26-21-7-3-2-5-19(21)24-15-13-23(14-16-24)12-4-6-20(25)17-8-10-h2-3,5,7-11H,4,6,12-16H2,1H3	-3.44
InChI=1S/C12H5Cl5/c13-6-4-9(15)11(10(16)5-6)7-2-1-3-8(14)12(7)17/h1-5H	-7.4
InChI=1S/C33H44N4O10/c1-7-11-25(38)44-18-24(46-27(40)13-9-3)30(47-28(41)14-10-4)23(45h15-16,23-24,30H,7-14,17-18H2,1-6H3,(H,36,42,43)	-8.512
InChI=1S/C10H19NO/c12-10-8-6-4-2-1-3-5-7-9-11-10/h1-9H2,(H,11,12)	-1.886
InChI=1S/C19H25N3O2S2/c1-14(20(2)3)13-22-16-8-6-7-9-18(16)25-19-11-10-15(12-17(19)22)26h6-12,14H,13H2,1-5H3	-5.181
InChI=1S/C7H6O4/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3,8-9H,(H,10,11)	-1.41
InChI=1S/C11H8N4/c1-2-4-8(5-3-1)10-14-9-6-12-7-13-11(9)15-10/h1-7H,(H,12,13,14,15)	-3.06
InChI=1S/C6H4N2O5/c9-6-4(7(10)11)2-1-3-5(6)8(12)13/h1-3,9H	-2.767
InChI=1S/C21H30O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)11-19(24)21(13,3)18(15)8-9-h10,15-19,24H,4-9,11H2,1-3H3	-3.82
InChI=1S/C12H4Cl6/c13-6-2-1-5(3-7(6)14)10-11(17)8(15)4-9(16)12(10)18/h1-4H	-8.48
InChI=1S/C15H29NO7/c1-2-3-4-5-6-7-8-16-15(21)22-9-10-11(17)12(18)13(19)14(20)23-10/h10-14,17-20H,2-9H2,1H3,(H,16,21)	-2.35
InChI=1S/C13H17ClN2O3S/c14-10-6-8-12(9-7-10)20(18,19)16-13(17)15-11-4-2-1-3-5-11/h6-9,11H,1-5H2,(H2,15,16,17)	-4.397
InChI=1S/C12H12N4O/c13-12(14)16-15-7-10-9-4-2-1-3-8(9)5-6-11(10)17/h1-7,17H,(H4,13,14,16)/b15-7+	-2.46
InChI=1S/C12H23N/c1-7-10-8-11(2,3)13(6)12(4,5)9-10/h8H,7,9H2,1-6H3	-2.518

"InChi"	"logS(M)"
InChI=1S/C13H9Cl2NO2/ c14-9-6-7-11(12(15)8-9)13(17)16(18)10-4-2-1-3-5-10/h1-8,18H	-3.672
InChI=1S/C16H22N2/ c1-4-18-15(9-10-16(18,2)3)13-11-17-14-8-6-5-7-12(13)14/ h5-8,11,15,17H,4,9-10H2,1-3H3	-2.659
InChI=1S/C16H15NO2/ c1-2-11-19-15-13(12-7-4-3-5-8-12)9-6-10-14(15)16(17)18/h2-10H, 1,11H2,(H2,17,18)	-3.519
InChI=1S/C8H14O4/c1-11-7(9)5-3-4-6-8(10)12-2/h3-6H2,1-2H3	-1.463
InChI=1S/C12H6Cl2N2O6/ c13-5-1-7(11(17)9(3-5)15(19)20)8-2-6(14)4-10(12(8)18)16(21)22/ h1-4,17-18H	-5.881
InChI=1S/C40H54N8O6/ c1-4-26(2)34-40(54)48-32(19-12-22-42-48)37(51)43-29(18-11-21-41) h5-10,14-17,22,26,29-34H,4,11-13,18-21,23-25,41H2,1-3H3,(H, 43,51)(H,44,50)(H,45,49)	-2.7
InChI=1S/C5H11NO/c1-3-6(4-2)5-7/h5H,3-4H2,1-2H3	0.995
InChI=1S/C13H16N2O/ c1-8-13-10(5-6-14-8)11-7-9(16-2)3-4-12(11)15-13/h3-4,7-8,14-15H, 5-6H2,1-2H3	-2.048
InChI=1S/C4H5Cl2NO2/c5-1-3(8)7-4(9)2-6/h1-2H2,(H,7,8,9)	-2.23
InChI=1S/C5H10O2/c1-4(3-6)5(2)7/h3-5,7H,1-2H3	-0.491
InChI=1S/C9H14O3/c1-7(2)9(10)12-6-8-4-3-5-11-8/h8H, 1,3-6H2,2H3	-0.952
InChI=1S/C52H102O4/ c1-5-7-9-11-12-13-14-15-16-17-20-23-30-35-41-47-52(54)56-50(44-3 h49-50H,5-48H2,1-4H3	-8.755
InChI=1S/C26H35N3O3/ c1-6-18(2)10-9-15-32-24(30)14-13-19-16-20(26(3,4)5)25(31)23(17-19 h7-8,11-12,16-18,31H,6,9-10,13-15H2,1-5H3	-6.164
InChI=1S/C14H13NO2/ c15-13(16)14(17,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,17H, (H2,15,16)	-1.437
InChI=1S/C24H28N2O/ c1-2-24(27)26-22-13-14-23(26)18-25(17-22)16-21(20-11-7-4-8-12-20 h3-12,15,22-23H,2,13-14,16-18H2,1H3/b21-15-	-5.716
InChI=1S/C6H16FN2OP/c1-5(2)8-11(7,10)9-6(3)4/h5-6H,1-4H3, (H2,8,9,10)	-0.357
InChI=1S/C12H9N3O5/ c16-9-3-1-8(2-4-9)12(17)14-13-7-10-5-6-11(20-10)15(18)19/ h1-7,16H,(H,14,17)/b13-7+	-3.656
InChI=1S/C5H7N3O2/c1-4-3-7(2)5(6-4)8(9)10/h3H,1-2H3	-1.451
InChI=1S/C16H18N2O4S/ c1-11(2)22-14-7-3-12(4-8-14)16(19)18-23(20,21)15-9-5-13(17)6-10-1 h3-11H,17H2,1-2H3,(H,18,19)	-4.3
InChI=1S/C12H18N2O7S/ c13-22(19,20)7-3-1-6(2-4-7)14-12-11(18)10(17)9(16)8(5-15)21-12/ h1-4,8-12,14-18H,5H2,(H2,13,19,20)	-0.98
InChI=1S/C9H7NO/c11-9-8-4-2-1-3-7(8)5-6-10-9/h1-6H,(H,10,11)	-2.484
InChI=1S/C15H13Cl2N3O2/ c1-2-7-22-13-9-12(10(16)8-11(13)17)20-15(21)19-6-4-3-5-14(19)18-2 h1,8-9H,3-7H2	-4.325

"InChi"	"logS(M)"
InChI=1S/C16H16N2O5S/c17-11-1-5-13(6-2-11)24(22,23)14-7-3-12(4-8-14)18-15(19)9-10-16(2h1-8H,9-10,17H2,(H,18,19)(H,20,21)	-2.136
InChI=1S/C18H24ClN3O/c1-6-14-15(19)16(22(5)21-14)17(23)20-11-12-7-9-13(10-8-12)18(2,3)h7-10H,6,11H2,1-5H3,(H,20,23)	-5.109
InChI=1S/C12H22O2/c1-9(13)14-11-7-5-10(6-8-11)12(2,3)4/h10-11H,5-8H2,1-4H3	-3.7
InChI=1S/C18H23NO/c1-18(20-15-14-19(2)3,16-10-6-4-7-11-16)17-12-8-5-9-13-17/h4-13H,14-15H2,1-3H3	-3.197
InChI=1S/C24H44Cl6/c1-3-7-19(25)9-5-11-21(27)13-15-23(29)17-18-24(30)16-14-22(28)12-h19-24H,3-18H2,1-2H3	-7.966
InChI=1S/C11H6Cl2N2/c12-10-3-1-2-8(11(10)13)9-6-15-5-7(9)4-14/h1-3,5-6,15H	-4.694
InChI=1S/C14H12O3/c1-7-4-12(15)17-14-9(3)13-10(6-11(7)14)5-8(2)16-13/h4-6H,1-3H3	-5.28
InChI=1S/C15H17ClN4/c1-2-3-8-15(9-17,10-20-12-18-11-19-20)13-4-6-14(16)7-5-13/h4-7,11-12H,2-3,8,10H2,1H3	-3.31
InChI=1S/C12H4Cl6O/c13-6-2-1-5(3-7(6)14)19-12-10(17)8(15)4-9(16)11(12)18/h1-4H	-8.3
InChI=1S/C14H21N5O4/c1-2-5-17-6-8-18(9-7-17)11-13(20)16-15-10-12-3-4-14(23-12)19(21)2h3-4,10H,2,5-9,11H2,1H3,(H,16,20)/b15-10+	-3.464
InChI=1S/C20H34N2O3/c1-3-5-12-22(13-6-4-2)14-17-24-15-7-16-25-20(23)18-8-10-19(21)11-h8-11H,3-7,12-17,21H2,1-2H3	-4.307
InChI=1S/C15H21NO3/c1-3-19-14(18)15(7-9-16(2)10-8-15)12-5-4-6-13(17)11-12/h4-6,11,17H,3,7-10H2,1-2H3	-1.563
InChI=1S/C6H12O/c1-4-6(7)5(2)3/h5H,4H2,1-3H3	-0.811
InChI=1S/C4H11NO8P2/c6-4(7)1-5(2-14(8,9)10)3-15(11,12)13/h1-3H2,(H,6,7)(H2,8,9,10)(H2,11,12,13)	-0.026
InChI=1S/C7H7NO5S/c1-5-2-3-6(8(9)10)4-7(5)14(11,12)13/h2-4H,1H3,(H,11,12,13)	0.492
InChI=1S/C8H14O2/c1-7(9)10-8-5-3-2-4-6-8/h8H,2-6H2,1H3	-1.67
InChI=1S/C6H12N6/c1-7-4-10-5(8-2)12-6(9-3)11-4/h1-3H3,(H3,7,8,9,10,11,12)	-1.505
InChI=1S/C22H32N2O5/c1-6-23(7-2)22(26)17-13-24-9-8-15-10-20(27-4)21(28-5)11-16(15)18(h10-11,17-19H,6-9,12-13H2,1-5H3	-3.814
InChI=1S/C9H14O/c1-6-4-5-7(2)9(10)8(6)3/h5-6,8H,4H2,1-3H3	-1.885
InChI=1S/C6H5N5O/c7-6-10-4-3(5(12)11-6)8-1-2-9-4/h1-2H,(H3,7,9,10,11,12)	-3.97
InChI=1S/C4H6O3/c5-3-1-2-4(6)7/h3H,1-2H2,(H,6,7)	0.807
InChI=1S/C13H22N2O4/c1-5-7-15-12(17)19-9-13(4,10(3)6-2)8-18-11(14)16/h1,10H,6-9H2,2-4H3,(H2,14,16)(H,15,17)	-2.945

"InChi"	"logS(M)"
InChI=1S/C9H11NO/c1-10-6-8-4-2-3-5-9(8)7-11-10/h2-5H,6-7H2,1H3	-1.933
InChI=1S/C2H2F2O2/c3-1(4)2(5)6/h1H,(H,5,6)	1.018
InChI=1S/C9H16O4/c1-6(4-7(10)11)5-9(2,3)8(12)13/h6H,4-5H2,1-3H3,(H,10,11)(H,12,13)	-0.279
InChI=1S/C11H12N2S/c1-9-8-11(14)12(2)13(9)10-6-4-3-5-7-10/h3-8H,1-2H3	-1.667
InChI=1S/C18H14/c1-3-8-15(9-4-1)17-12-7-13-18(14-17)16-10-5-2-6-11-16/h1-14H	-5.183
InChI=1S/C6H7F3O2/c1-4(2)5(10)11-3-6(7,8)9/h1,3H2,2H3	-2.268
InChI=1S/C7H8O3/c1-2-6-7(9)5(8)3-4-10-6/h3-4,9H,2H2,1H3	-1.176
InChI=1S/C9H10O2/c1-2-9(11)7-3-5-8(10)6-4-7/h3-6,10H,2H2,1H3	-2.639
InChI=1S/C3H9O6P/c4-1-3(5)2-9-10(6,7)8/h3-5H,1-2H2,(H2,6,7,8)	0.764
InChI=1S/C14H20O/c1-3-7-13(8-4-1)11-12-15-14-9-5-2-6-10-14/h1,3-4,7-8,14H,2,5-6,9-12H2	-2.418
InChI=1S/C55H37Cl5F6N8O8/c1-26-20-41(68-53(80)49(28(3)76)74-72-43-22-30(5-17-38(43)59)51(7h4-25,48-49H,1-3H3,(H,67,79)(H,68,80)(H,69,77)(H,70,78)/b73-71+,74-72+	-7.692
InChI=1S/C14H19N3/c1-2-7-13-12(5-1)6-3-4-10-17(13)11-14-15-8-9-16-14/h1-2,5,7H,3-4,6,8-11H2,(H,15,16)	-3.477
InChI=1S/C10H19N/c1-7-9-4-5-10(6-9)8(2)11(7)3/h7-10H,4-6H2,1-3H3	-1.545
InChI=1S/C12H12O2/c13-11-6-10(7-12(14)8-11)9-4-2-1-3-5-9/h1-5,8,10,13H,6-7H2	-2.511
InChI=1S/C8H19N/c1-3-4-5-6-7-8(2)9/h8H,3-7,9H2,1-2H3	-1.465
InChI=1S/C5H12N2O/c1-3-4-5-7(2)6-8/h3-5H2,1-2H3	-0.7
InChI=1S/C14H19ClN2O2/c1-2-17-8-4-7-13(10-17)19-14(18)16-12-6-3-5-11(15)9-12/h3,5-6,9,13H,2,4,7-8,10H2,1H3,(H,16,18)	-3.598
InChI=1S/C23H29N5O3/c1-5-7-8-16(6-2)14-25-21(29)17-9-11-18(12-10-17)26-27-20-15(3)19(h9-12,16,26H,5-8,14H2,1-4H3,(H,25,29)/b27-20-	-7.025
InChI=1S/C11H9FN2O2/c12-9-7-14(11(16)13-10(9)15)6-8-4-2-1-3-5-8/h1-5,7H,6H2,(H,13,15,16)	-2.65
InChI=1S/C8H16O/c1-4-7(3)6-8(9)5-2/h7H,4-6H2,1-3H3	-1.631
InChI=1S/C19H19N5O4/c1-15(25)28-14-13-23(12-2-11-20)18-7-3-16(4-8-18)21-22-17-5-9-19(h3-10H,2,12-14H2,1H3/b22-21+	-4.28
InChI=1S/C9H13N3O2/c1-3-5-12-7(10)6-8(13)11(4-2)9(12)14/h3,6H,1,4-5,10H2,2H3	-1.08
InChI=1S/C13H10N2/c14-11-5-6-13-10(8-11)7-9-3-1-2-4-12(9)15-13/h1-8H,14H2	-4.094
InChI=1S/C15H20O2/c1-11(15(16)17)12-7-9-14(10-8-12)13-5-3-2-4-6-13/h7-11,13H,2-6H2,1H3,(H,16,17)	-4.482
InChI=1S/C12H4Cl6/c13-5-1-2-7(14)6(3-5)10-8(15)4-9(16)11(17)12(10)18/h1-4H	-8.01

"InChi"	"logS(M)"
InChI=1S/C16H23NO2/c1-13-8-6-7-11-17(13)12-14(2)19-16(18)15-9-4-3-5-10-15/h3-5,9-10,13-14H,6-8,11-12H2,1-2H3	-3.277
InChI=1S/C10H20O2/c1-9(6-8-11)5-4-7-10(2,3)12/h8-9,12H,4-7H2,1-3H3	-0.692
InChI=1S/C9H6Cl2FNO2/c10-6-3-4(12)1-2-5(6)9(8(13)14)7(11)15-9/h1-3,7H,(H2,13,14)	-2.792
InChI=1S/C17H18FN3O3/c1-8-13(19)7-20(8)15-5-14-10(4-12(15)18)16(22)11(17(23)24)6-21(14h4-6,8-9,13H,2-3,7,19H2,1H3,(H,23,24)	-4.63
InChI=1S/C10H6Cl4O4/c1-17-9(15)3-5(11)7(13)4(10(16)18-2)8(14)6(3)12/h1-2H3	-5.822
InChI=1S/C7H14N4S2/c1-4-5(2)9-7(13)11-10-6(12)8-3/h4-5H,1H2,2-3H3,(H2,8,10,12)(H2,9,11,13)	-1.366
InChI=1S/C8H9NO/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3,(H2,9,10)	-1.196
InChI=1S/C43H35Cl5N8O6/c1-20-16-35(52-43(62)39(24(5)58)56-54-37-18-26(13-15-30(37)47)41h6-19,38-39H,1-5H3,(H,49,59)(H,50,60)(H,51,61)(H,52,62)/b55-53+,56-54+	-7.972
InChI=1S/C24H48O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-22-26-24(25)23(6-3)21-8h23H,4-22H2,1-3H3	-6.868
InChI=1S/C8H15N5S/c1-4-9-6-11-7(10-5-2)13-8(12-6)14-3/h4-5H2,1-3H3,(H2,9,10,11,12,13)	-2.73
InChI=1S/C8H11NO3S/c1-9(2)7-4-3-5-8(6-7)13(10,11)12/h3-6H,1-2H3,(H,10,11,12)	0.298
InChI=1S/C2H3F3O2/c3-2(4,5)1(6)7/h1,6-7H	-0.085
InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,7-8H,1,6H2,2-4H3/b10-8+	-3.973
InChI=1S/C7H8O2/c8-5-6-1-3-7(9)4-2-6/h1-4,8-9H,5H2	-1.268
InChI=1S/C16H28O4/c1-5-9-15(10-6-2,13(17)18)16(11-7-3,12-8-4)14(19)20/h5,9H,6-8,10-12H2,1-4H3,(H,17,18)(H,19,20)/b9-5+	-3.495
InChI=1S/C7H15NOS/c1-5(2)10-7(3,4)6(8)9/h5H,1-4H3,(H2,8,9)	-1.535
InChI=1S/C8H10O/c1-7-3-5-8(9-2)6-4-7/h3-6H,1-2H3	-2.34
InChI=1S/C15H17NO7/c1-3-21-14(19)8-16-13(18)9-22-15(20)11-6-4-5-7-12(11)23-10(2)17/h4-7H,3,8-9H2,1-2H3,(H,16,18)	-1.87
InChI=1S/C8H9N3O2S/c1-6-10-14(12,13)7-4-3-5-9-8(7)11(6)2/h3-5H,1-2H3	-0.699
InChI=1S/C17H23NO6S/c1-18-13-7-8-14(18)10-15(9-13)24-17(19)16(11-23-25(20,21)22)12-5-h2-6,13-16H,7-11H2,1H3,(H,20,21,22)	-1.567
InChI=1S/C14H16N4O4S/c1-3-18-9-8-13(16-14(18)20)17-23(21,22)12-6-4-11(5-7-12)15-10(2)1h4-9H,3H2,1-2H3,(H,15,19)(H,16,17,20)	-2.71
InChI=1S/C7H6N4O5/c8-6(12)7(13)10-9-3-4-1-2-5(16-4)11(14)15/h1-3H,(H2,8,12)(H,10,13)/b9-3+	-1.607
InChI=1S/C12H4Cl4O2/c13-5-1-9-10(2-6(5)14)18-12-4-8(16)7(15)3-11(12)17-9/h1-4H	-9.207

"InChi"	"logS(M)"
InChI=1S/C10H16O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h2-3,9H,4-8H2,1H3/b3-2+	-1.489
InChI=1S/C9H12N2O3/c1-7-2-3-8(10-4-5-12)9(6-7)11(13)14/h2-3,6,10,12H,4-5H2,1H3	-2.747
InChI=1S/C12H9Br/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H	-5.553
InChI=1S/C21H32N6O3/c1-4-19(28)27(18-9-7-6-8-10-18)21(17-30-3)11-13-24(14-12-21)15-16h6-10H,4-5,11-17H2,1-3H3	-4.081
InChI=1S/C15H21ClN2O2/c1-3-18-9-5-7-12(10-18)20-15(19)17-14-11(2)6-4-8-13(14)16/h4,6,8,12H,3,5,7,9-10H2,1-2H3,(H,17,19)	-4.167
InChI=1S/C25H43NO18/c1-6-11(26-8-2-7(3-27)12(30)15(33)13(8)31)14(32)19(37)24(40-6)43-h2,6,8-39H,3-5H2,1H3	0.19
InChI=1S/C5H8N2O2/c1-3-5(9)6-2-4(8)7-3/h3H,2H2,1H3,(H,6,9)(H,7,8)	0.29
InChI=1S/C5H6O4/c1-3(5(8)9)2-4(6)7/h2H,1H3,(H,6,7)(H,8,9)/b3-2-	0.779
InChI=1S/C16H17NO4/c1-11-5-4-6-13(7-11)17(19)16(18)12-8-14(20-2)10-15(9-12)21-3/h4-10,19H,1-3H3	-3.61
InChI=1S/C9H13NO2/c1-4-12-9(11)8-6(2)5-7(3)10-8/h5,10H,4H2,1-3H3	-2.621
InChI=1S/C7H9NO2/c9-6-3-1-5-2-4-7(10)8(5)6/h5H,1-4H2	0.731
InChI=1S/C10H13NO2/c1-8(12)7-11-9-5-3-4-6-10(9)13-2/h3-6,11H,7H2,1-2H3	-1.781
InChI=1S/C14H11NS/c1-10-6-8-11(9-7-10)14-15-12-4-2-3-5-13(12)16-14/h2-9H,1H3	-4.35
InChI=1S/C15H22N2O2/c1-4-17-9-8-13(10-17)19-15(18)16-14-11(2)6-5-7-12(14)3/h5-7,13H,4,8-10H2,1-3H3,(H,16,18)	-3.415
InChI=1S/C8H9N5/c1-13(2)8-11-5-6-7(12-8)10-4-3-9-6/h3-5H,1-2H3	0.359
InChI=1S/C16H17NO2/c1-13-6-5-9-15(12-13)17(19)16(18)11-10-14-7-3-2-4-8-14/h2-9,12,19H,10-11H2,1H3	-3.41
InChI=1S/C17H23N3O2/c1-5-18(6-2)15-13(4)20(14-11-9-8-10-12-14)17(22)19(7-3)16(15)21/h8-12H,5-7H2,1-4H3	-3.442
InChI=1S/C12H13N5O6S2/c1-6-13-10(16-12(14-6)23-3)15-11(19)17-25(20,21)7-4-5-24-8(7)9(18h4-5H,1-3H3,(H2,13,14,15,16,17,19)	-2.238
InChI=1S/C7H5NOS/c9-7-3-1-6(2-4-7)8-5-10/h1-4,9H	-2.67
InChI=1S/C8H6Cl3NO/c1-4(13)12-8-3-6(10)5(9)2-7(8)11/h2-3H,1H3,(H,12,13)	-3.049
InChI=1S/C12H15NO5/c1-3-16-12(15)18-8-17-11-6-4-10(5-7-11)13-9(2)14/h4-7H,3,8H2,1-2H3,(H,13,14)	-2.43
InChI=1S/C12H12ClNO/c1-3-10(2)14(12(15)9-13)11-7-5-4-6-8-11/h1,4-8,10H,9H2,2H3	-2.647
InChI=1S/C12H18O4/c1-4-11(13)15-8-6-10(3)7-9-16-12(14)5-2/h4-5,10H,1-2,6-9H2,3H3	-2.621

"InChi"	"logS(M)"
InChI=1S/C19H15ClN2O2/c20-15-6-7-17(22-19(24)14-8-10-21-11-9-14)16(12-15)18(23)13-4-2-1-3-5-12,18,23H,(H,22,24)	-5.53
InChI=1S/C12H13N3O2S/c1-14-12(13)15-18(16,17)11-7-6-9-4-2-3-5-10(9)8-11/h2-8H,1H3,(H3,13,14,15)	-3.1
InChI=1S/C8H13NO/c1-2-9-7-5-3-4-6-8(9)10/h2H,1,3-7H2	-0.451
InChI=1S/C17H18BrNO4/c18-13-10-14(12-4-2-1-3-5-12)16(23-9-8-21)15(11-13)17(22)19-6-7-20-5,10-11,20-21H,6-9H2,(H,19,22)	-4.02
InChI=1S/C9H11ClN2O3S/c1-11-9(13)6-3-4-7(10)8(5-6)16(14,15)12-2/h3-5,12H,1-2H3,(H,11,13)	-1.707
InChI=1S/C10H20N2S2/c1-3-7-11(8-4-1)13-14-12-9-5-2-6-10-12/h1-10H2	-2.341
InChI=1S/C13H11N3O2/c17-12(10-4-2-1-3-5-10)15-16-13(18)11-6-8-14-9-7-11/h1-9H,(H,15,17)(H,16,18)	-2.54
InChI=1S/C9H18O3/c1-3-5-7-12-9(10)6-8-11-4-2/h3-8H2,1-2H3	-1.639
InChI=1S/C16H33NO2/c1-3-6-15(7-4-2)8-5-9-16-14-19-13-11-17(16)10-12-18/h15-16,18H,3-14H2,1-2H3	0.964
InChI=1S/C11H13NO3/c1-2-7-15-10-5-3-9(4-6-10)8-11(13)12-14/h2-6,14H,1,7-8H2,(H,12,13)	-1.865
InChI=1S/C6H15NO2/c1-7(2)3-5-9-6-4-8/h8H,3-6H2,1-2H3	-0.124
InChI=1S/C17H16N2O2S/c1-19(2)13-6-4-12(5-7-13)17-18-14-9-11(10-16(20)21)3-8-15(14)22-17h3-9H,10H2,1-2H3,(H,20,21)	-4.111
InChI=1S/C15H30O4/c1-2-3-4-5-6-7-8-9-10-11-15(18)19-13-14(17)12-16/h14,16-17H,2-13H2,1H3	-4.66
InChI=1S/C10H14N2O3/c11-10(15)8-3-1-2-4-9(8)12-5-7(14)6-13/h1-4,7,12-14H,5-6H2,(H2,11,15)	-1.361
InChI=1S/C20H28O3/c1-19-9-7-14(22)11-13(19)3-4-15-16-5-6-18(23-12-21)20(16,2)10-8-17h11-12,15-18H,3-10H2,1-2H3	-4.93
InChI=1S/C15H17N3/c1-11-7-3-5-9-13(11)17-15(16)18-14-10-6-4-8-12(14)2/h3-10H,1-2H3,(H3,16,17,18)	-3.534
InChI=1S/C10H11NO4/c1-2-3-10(12)15-9-6-4-8(5-7-9)11(13)14/h4-7H,2-3H2,1H3	-3.94
InChI=1S/C9H10ClN5O2/c10-8-2-1-7(5-12-8)6-14-4-3-11-9(14)13-15(16)17/h1-2,5H,3-4,6H2,(H,11,13)	-2.622
InChI=1S/C17H18N2O6/c20-8-12-13(21)14(22)15(23)17(25-12)19-10-5-2-1-4-9(10)18-16(19)1h1-7,12-15,17,20-23H,8H2	-2.33
InChI=1S/C11H14N2/c1-12-7-6-9-8-13-11-5-3-2-4-10(9)11/h2-5,8,12-13H,6-7H2,1H3	-0.945
InChI=1S/C16H28O2/c1-6-16(5,18)15(17)12-8-11-14(4)10-7-9-13(2)3/h8-9,11-12,15,17-18H,6-7,10H2,1-5H3/b12-8+,14-11-	-5.275

"InChi"	"logS(M)"
InChI=1S/C4H6Cl2FNO2/c5-3(6)4(10)8-2(9)1-7/h3-4,10H,1H2,(H,8,9)	0.302
InChI=1S/C13H18O3/c1-3-5-11-7-4-6-10(2)13(11)16-9-12(15)8-14/h3-4,6-7,12,14-15H,1,5,8-9H2,2H3	-3.213
InChI=1S/C7H5N5O8/c1-8(12(19)20)7-5(10(15)16)2-4(9(13)14)3-6(7)11(17)18/h2-3H,1H3	-3.589
InChI=1S/C9H7NO2/c1-5-3-2-4-6-7(5)10-9(12)8(6)11/h2-4H,1H3,(H,10,11,12)	-1.231
InChI=1S/C20H14NO4/c1-21-8-15-12(4-5-16-20(15)25-10-22-16)13-3-2-11-6-17-18(24-9-23-h2-8H,9-10H2,1H3/q+1	-5.112
InChI=1S/C18H16N2O/c1-12-7-9-16(13(2)11-12)19-20-18-15-6-4-3-5-14(15)8-10-17(18)21/h3-11,19H,1-2H3/b20-18-	-6.705
InChI=1S/C8H10O3/c1-2-5-11-8(9)7-4-3-6-10-7/h3-4,6H,2,5H2,1H3	-1.976
InChI=1S/C7H14O2/c1-6(8)5-7(2,3)9-4/h5H2,1-4H3	0.333
InChI=1S/C9H10O3/c1-9(12,8(10)11)7-5-3-2-4-6-7/h2-6,12H,1H3,(H,10,11)	-0.895
InChI=1S/C10H20O/c1-5-9(2)7-6-8-10(3,4)11/h5,9,11H,1,6-8H2,2-4H3	-2.221
InChI=1S/C7H3Cl3O2/c8-4-2-6(10)5(9)1-3(4)7(11)12/h1-2H,(H,11,12)	-2.445
InChI=1S/C12H19N3O6S2/c16-15(17)11-4-5-12(14-10-11)21-8-3-1-2-6-13-7-9-22-23(18,19)20/h4-5,10,13H,1-3,6-9H2,(H,18,19,20)	-1.924
InChI=1S/C14H28O4/c1-12(2,3)15-17-14(10-8-7-9-11-14)18-16-13(4,5)6/h7-11H2,1-6H3	-5.386
InChI=1S/C12H5Cl5/c13-7-1-2-9(14)8(5-7)6-3-10(15)12(17)11(16)4-6/h1-5H	-7.315
InChI=1S/C17H16N2O/c1-11(2)16-15(13-7-3-4-8-14(13)19-16)17(20)12-6-5-9-18-10-12/h3-11,19H,1-2H3	-4.098
InChI=1S/C9H17NO7/c1-2-17-9(16)10-5(3-11)7(14)8(15)6(13)4-12/h3,5-8,12-15H,2,4H2,1H3,(H,10,16)	0.114
InChI=1S/C29H40O9/c1-15-9-23(31)29(34)25(36-15)37-21-11-17-3-4-20-19(27(17,14-30)12h10,14-15,17-23,25,31,33-34H,3-9,11-13H2,1-2H3	-4.671
InChI=1S/C30H12Br2O2/c31-22-10-9-16-21-12-14-5-7-18-25-20(15-3-1-2-4-17(15)29(18)33)11h1-12H	-4.45
InChI=1S/C15H16O3/c1-10(15(16)18-3)11-4-5-13-9-14(17-2)7-6-12(13)8-11/h4-10H,1-3H3	-4.78
InChI=1S/C7H5BrO2/c8-6-3-5(4-9)1-2-7(6)10/h1-4,10H	-2.179
InChI=1S/C12H13NO5/c1-8(14)13-10(11(15)16)7-18-12(17)9-5-3-2-4-6-9/h2-6,10H,7H2,1H3,(H,13,14)(H,15,16)	-3.22
InChI=1S/C11H14N4O2S2/c1-2-3-10-13-14-11(18-10)15-19(16,17)9-6-4-8(12)5-7-9/h4-7H,2-3,12H2,1H3,(H,14,15)	-3.308

"InChi"	"logS(M)"
InChI=1S/C11H10ClNO3S/c1-2-16-9(14)6-13-10-7(12)4-3-5-8(10)17-11(13)15/h3-5H,2,6H2,1H3	-3.762
InChI=1S/C7H5ClO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)	-1.89
InChI=1S/C11H16N2O/c1-8-4-3-5-9(2)10(8)6-7-13-11(12)14/h3-5H,6-7H2,1-2H3,(H3,12,13,14)	-2.486
InChI=1S/C7H15NO2/c1-4-10-7(9)8-5-6(2)3/h6H,4-5H2,1-3H3,(H,8,9)	-0.768
InChI=1S/C15H21N3O/c1-11(5-3-7-16)18-14-10-13(19-2)9-12-6-4-8-17-15(12)14/h4,6,8-11,18H,3,5,7,16H2,1-2H3	-2.305
InChI=1S/C15H14Cl2F3N3O3/c1-3-26-13(24)10(17)4-8-5-12(11(18)6-9(8)16)23-15(25)22(14(19)20)h5-6,10,14H,3-4H2,1-2H3	-4.273
InChI=1S/C15H17ClN2O2/c1-15(2,3)13(19)14(18-9-8-17-10-18)20-12-6-4-11(16)5-7-12/h4-10,14H,1-3H3	-3.703
InChI=1S/C6H14O5/c7-1-5(9)3-11-4-6(10)2-8/h5-10H,1-4H2	0.779
InChI=1S/C7H12F6N2O/c1-15(2)4-3-14-5(16,6(8,9)10)7(11,12)13/h14,16H,3-4H2,1-2H3	-0.445
InChI=1S/C4H7NS/c1-4-5-2-3-6-4/h2-3H2,1H3	-2.149
InChI=1S/C7H13NO3S/c1-5(9)8-6(7(10)11)3-4-12-2/h6H,3-4H2,1-2H3,(H,8,9)(H,10,11)/p-1	-0.322
InChI=1S/C13H19N3O2/c1-3-4-5-10-16(2)15-14-12-8-6-11(7-9-12)13(17)18/h6-9H,3-5,10H2,1-2H3,(H,17,18)/b15-14+	-2.37
InChI=1S/C6H12O2/c1-4-6(7)8-5(2)3/h5H,4H2,1-3H3	-1.291
InChI=1S/C19H13Cl/c1-12-16-9-7-13-4-2-3-5-17(13)19(16)10-14-6-8-15(20)11-18(12)14/h2-11H,1H3	-7.44
InChI=1S/C6H14N2/c1-7-3-5-8(2)6-4-7/h3-6H2,1-2H3	0.942
InChI=1S/C9H11N5O4S3/c1-14-8(19-9(12-14)20(11,15)16)13-21(17,18)7-4-2-3-6(10)5-7/h2-5H,10H2,1H3,(H2,11,15,16)/b13-8+	-2.45
InChI=1S/C11H13BrO3/c1-2-3-6-15-11(14)8-4-5-10(13)9(12)7-8/h4-5,7,13H,2-3,6H2,1H3	-3.67
InChI=1S/C10H14N2O/c1-7(2)12-9-6-4-3-5-8(9)10(11)13/h3-7,12H,1-2H3,(H2,11,13)	-2.269
InChI=1S/C20H36O4/c1-3-5-7-9-11-13-17-23-19(21)15-16-20(22)24-18-14-12-10-8-6-4-2/h15-16H,3-14,17-18H2,1-2H3/b16-15+	-6.356
InChI=1S/C15H12O3/c1-8-5-10-7-9-3-2-4-11(16)13(9)15(18)14(10)12(17)6-8/h2-7,16-18H,1H3	-3.058
InChI=1S/C17H27NO4/c1-10(2)18-8-15(20)9-21-16-7-11(3)17(22-14(6)19)13(5)12(16)4/h7,10,15,18,20H,8-9H2,1-6H3	-2.72
InChI=1S/C12H13N5O4/c13-1-5-2-17(11-7(5)10(14)15-4-16-11)12-9(20)8(19)6(3-18)21-12/h2,4,6,8-9,12,18-20H,3H2,(H2,14,15,16)	-2.191

"InChi"	"logS(M)"
InChI=1S/C11H20O4/c12-10(13)8-6-4-2-1-3-5-7-9-11(14)15/h1-9H2,(H,12,13)(H,14,15)	-1.627
InChI=1S/C19H15ClN2O5/c20-12-6-7-14-13(10-12)17(11-4-2-1-3-5-11)22-19(18(26)21-14)27-16h1-7,10,19H,8-9H2,(H,21,26)(H,23,24)	-4.228
InChI=1S/C10H8O2/c1-7-6-8-4-2-3-5-9(8)12-10(7)11/h2-6H,1H3	-2.395
InChI=1S/C26H29Cl2N5O3/c1-32-6-8-33(9-7-32)5-4-10-36-25-13-21-18(11-24(25)35-3)26(17(15-h11-14,16H,4-10H2,1-3H3,(H,30,31)	-4.88
InChI=1S/C17H12N2O4/c20-16-9-12-5-2-1-4-11(12)8-15(16)17(21)18-13-6-3-7-14(10-13)19(2h1-10,20H,(H,18,21)	-6.644
InChI=1S/C20H27NO2/c1-15(13-17-9-5-7-11-19(17)22-3)21-16(2)14-18-10-6-8-12-20(18)23-h5-12,15-16,21H,13-14H2,1-4H3	-2
InChI=1S/C16H26N2O3S/c1-5-6-7-8-9-16(19)18(4)14-10-12-15(13-11-14)22(20,21)17(2)3/h10-13H,5-9H2,1-4H3	-3.68
InChI=1S/C18H25NO2/c1-19-10-9-18-8-4-3-5-13(18)14(19)11-12-6-7-15(21-2)17(20)16(12)1h6-7,13-14,20H,3-5,8-11H2,1-2H3	-3.049
InChI=1S/C12H16O/c1-10-8-12(2,9-13-10)11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3	-2.433
InChI=1S/C3H2ClF5O/c4-1(5)3(8,9)10-2(6)7/h1-2H	-1.516
InChI=1S/C4H8N2S/c1-6-2-3-7-4(6)5/h5H,2-3H2,1H3/b5-4-	-0.731
InChI=1S/C18H20FN3O3/c1-9-14(20-2)8-21(9)16-6-15-11(5-13(16)19)17(23)12(18(24)25)7-22(h5-7,9-10,14,20H,3-4,8H2,1-2H3,(H,24,25)	-4.57
InChI=1S/C19H14O3/c20-16-7-1-13(2-8-16)19(14-3-9-17(21)10-4-14)15-5-11-18(22)12-6-1h1-12,20-21H	-2.384
InChI=1S/C14H5Cl6NO3/c15-4-2-1-3-5(8(4)16)21-13(22)6-7(14(23)24)10(18)12(20)11(19)9(6)h1-3H,(H,21,22)(H,23,24)	-4.505
InChI=1S/C19H23ClN2/c1-21(2)12-5-13-22-18-7-4-3-6-15(18)8-9-16-10-11-17(20)14-19(16)2h3-4,6-7,10-11,14H,5,8-9,12-13H2,1-2H3	-6.031
InChI=1S/C12H15N3O/c1-10-2-3-12(16)15(14-10)9-6-11-4-7-13-8-5-11/h4-5,7-8H,2-3,6,9H2,1H3	-1.136
InChI=1S/C21H18O/c22-21(19-14-8-3-9-15-19)16-20(17-10-4-1-5-11-17)18-12-6-2-7-13-1h1-15,20H,16H2	-5.551
InChI=1S/C16H26N2O3/c1-3-18(4-2)10-13-20-11-5-12-21-16(19)14-6-8-15(17)9-7-14/h6-9H,3-5,10-13,17H2,1-2H3	-2.221
InChI=1S/C21H19N3/c1-24(2)16-13-11-15(12-14-16)22-21-17-7-3-5-9-19(17)23-20-10-6-4-h3-14H,1-2H3,(H,22,23)	-6.69
InChI=1S/C13H21N3O2/c1-9-11(14(2)3)12(17)16(13(18)15(9)4)10-7-5-6-8-10/h10H,5-8H2,1-4H3	-2.651

"InChi"	"logS(M)"
InChI=1S/C10H13NO3/c1-13-8-4-3-7(6-10(11)12)5-9(8)14-2/h3-5H,6H2,1-2H3,(H2,11,12)	-0.788
InChI=1S/C21H23F2NO2/c22-18-7-3-16(4-8-18)20(25)2-1-13-24-14-11-21(26,12-15-24)17-5-9-h3-10,26H,1-2,11-15H2	-2.83
InChI=1S/C20H23NO5/c1-11(22)21-16-8-5-12-9-17(24-2)19(25-3)20(26-4)18(12)14-7-6-13(2h6-7,9-10,16,23H,5,8H2,1-4H3,(H,21,22)	-3.553
InChI=1S/C11H14O4/c1-9(12)14-7-10(13)8-15-11-5-3-2-4-6-11/h2-6,10,13H,7-8H2,1H3	-1.13
InChI=1S/C13H18N2O4/c1-7(2)11(13(18)19)15-5-10-9(6-16)4-14-8(3)12(10)17/h4-5,7,11,16-17H,6H2,1-3H3,(H,18,19)/b15-5+	-1.6
InChI=1S/C16H14O/c1-13-7-9-14(10-8-13)11-12-16(17)15-5-3-2-4-6-15/h2-12H,1H3/b12-11+	-4.413
InChI=1S/C5H15N2O3PS/c6-2-1-3-7-4-5-12-11(8,9)10/h7H,1-6H2,(H2,8,9,10)	0.669
InChI=1S/C7H10O6S3/c8-4(9)1-14-7(15-2-5(10)11)16-3-6(12)13/h7H,1-3H2,(H,8,9)(H,10,11)(H,12,13)	-1.424
InChI=1S/C15H16O5/c1-17-12-7-11(20-15(16)8-12)4-2-10-3-5-13-14(6-10)19-9-18-13/h3,5-6,8,11H,2,4,7,9H2,1H3	-2.676
InChI=1S/C11H15NO/c1-4-11(13)9-5-7-10(8-6-9)12(2)3/h5-8H,4H2,1-3H3	-2.495
InChI=1S/C10H11BrN2O6/c11-10(12(16)17,13(18)19)6-8(14)9(15)7-4-2-1-3-5-7/h1-5,8-9,14-15H,6H2	-1.707
InChI=1S/C12H8Cl2/c13-10-7-4-8-11(14)12(10)9-5-2-1-3-6-9/h1-8H	-5.21
InChI=1S/C14H15N/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10,14H,11,15H2	-2.36
InChI=1S/C21H38N2O/c1-2-3-4-5-6-7-8-9-10-22-20(24)23-21-14-17-11-18(15-21)13-19(12-17h17-19H,2-16H2,1H3,(H2,22,23,24)	-5.83
InChI=1S/C15H25NO4S2/c1-20-15-10-5-4-9-14(15)8-3-2-6-11-16-12-7-13-21-22(17,18)19/h4-5,9-10,16H,2-3,6-8,11-13H2,1H3,(H,17,18,19)	-3.073
InChI=1S/C11H24N2O3/c1-5-6-11(4,7-14)8-16-10(15)13-12-9(2)3/h9,12,14H,5-8H2,1-4H3,(H,13,15)	-2.494
InChI=1S/C21H28N2O2/c1-23(13-12-16-8-11-20(24-2)21(14-16)25-3)15-18-10-9-17-6-4-5-7-1h4-8,11,14,18,22H,9-10,12-13,15H2,1-3H3	-3.915
InChI=1S/C33H41N5O6S2/c1-33(2,3)37-31(42)26-19-46-20-38(26)32(43)29(40)24(15-21-9-6-5-7h5-14,16,24-26,29,40H,15,17-20H2,1-4H3,(H,35,39)(H,36,41)(H,37,42)	-3.95
InChI=1S/C13H13N3O/c1-9-5-4-8-15-12(9)16-13(17)10-6-2-3-7-11(10)14/h2-8H,14H2,1H3,(H,15,16,17)	-2.616
InChI=1S/C2H2Br4/c3-1(4)2(5)6/h1-2H	-2.72
InChI=1S/C6H4ClNO3/c7-4-1-2-5(8(10)11)6(9)3-4/h1-3,9H	-2.637

"InChi"	"logS(M)"
InChI=1S/C10H11NO3S/c1-2-11-10(12)7-8-5-3-4-6-9(8)15(11,13)14/h3-6H,2,7H2,1H3	-1.662
InChI=1S/C11H13NO4/c1-7(13)9(11(15)16)12-10(14)8-5-3-2-4-6-8/h2-7,9,13H,1H3,(H,12,14)(H,15,16)	-1.23
InChI=1S/C11H12BrNO2/c1-6-4-7(12)5-9(10(6)14)11(15)13-8-2-3-8/h4-5,8,14H,2-3H2,1H3,(H,13,15)	-3.836
InChI=1S/C14H16N2O5/c1-8(13(18)19)16-12(17)11(15-14(16)20)7-9-3-5-10(21-2)6-4-9/h3-6,8,11H,7H2,1-2H3,(H,15,20)(H,18,19)	-0.86
InChI=1S/C16H12ClN5O/c1-9(15-19-21-22-20-15)11-4-7-14-13(8-11)18-16(23-14)10-2-5-12(17h2-9H,1H3,(H,19,20,21,22)	-8.144
InChI=1S/C12H16O3/c1-2-3-8-15-11-6-4-10(5-7-11)9-12(13)14/h4-7H,2-3,8-9H2,1H3,(H,13,14)	-2.871
InChI=1S/C8H19NO2/c1-3-7(10)5-9-6-8(11)4-2/h7-11H,3-6H2,1-2H3	0.792
InChI=1S/C12H18N2O/c15-12-6-5-11-14(12)10-4-3-9-13-7-1-2-8-13/h1-2,5-11H2	-0.653
InChI=1S/C13H15FN2/c1-16-6-2-3-13(16)11-8-15-12-5-4-9(14)7-10(11)12/h4-5,7-8,13,15H,2-3,6H2,1H3	-1.877
InChI=1S/C10H15NO2/c1-9(2)6-4-5-10(9,3)8(13)11-7(6)12/h6H,4-5H2,1-3H3,(H,11,12,13)	-1.434
InChI=1S/C16H23N3O2/c1-18-14-6-7-15(18)11-19(10-14)8-9-21-16(20)12-2-4-13(17)5-3-12/h2-5,14-15H,6-11,17H2,1H3	-1.424
InChI=1S/C10H12O3/c1-7(2)13-10(12)8-3-5-9(11)6-4-8/h3-7,11H,1-2H3	-2.417
InChI=1S/C4H6N2/c1-6-3-2-5-4-6/h2-4H,1H3	1.086
InChI=1S/C14H17N3O3S/c1-15-9-10-6-7-16(12(15)8-10)13(18)4-2-11-3-5-14(21-11)17(19)20/h2-5,10,12H,6-9H2,1H3/b4-2+	-3.064
InChI=1S/C18H16N2O4/c21-16(22)12-19-15(11-13-7-3-1-4-8-13)17(23)20(18(19)24)14-9-5-2-h1-10,15H,11-12H2,(H,21,22)	-2.91
InChI=1S/C6H11N2O4PS3/c1-10-5-7-8(6(9)16-5)4-15-13(14,11-2)12-3/h4H2,1-3H3	-3.1
InChI=1S/C20H32/c1-3-5-6-8-18-11-15-20(16-12-18)19-13-9-17(7-4-2)10-14-19/h9-10,13-14,18,20H,3-8,11-12,15-16H2,1-2H3	-6.773
InChI=1S/C9H10NO3PS/c1-11-14(15,12-2)13-9-5-3-8(7-10)4-6-9/h3-6H,1-2H3	-3.723
InChI=1S/C19H21N3/c1-21-10-12-22(13-11-21)19-17-8-4-2-6-15(17)14-16-7-3-5-9-18(16)2h2-9H,10-14H2,1H3	-3.216
InChI=1S/C6H8N2/c7-5-6-1-3-8-4-2-6/h1-4H,5,7H2	0.966
InChI=1S/C16H22N2O/c1-2-16(19)18-13-11-17(12-14-18)10-6-9-15-7-4-3-5-8-15/h3-9H,2,10-14H2,1H3/b9-6+	-2.849
InChI=1S/C13H26N2O4/c1-5-8-13(4,9-18-11(14)16)10-19-12(17)15(6-2)7-3/h5-10H2,1-4H3,(H2,14,16)	-3.627

"InChi"	"logS(M)"
InChI=1S/C8H17NO2/c1-2-3-4-5-6-7(9)8(10)11/h7H,2-6,9H2,1H3,(H,10,11)	-1.547
InChI=1S/C14H18O4/c1-3-17-10-11-18-14(15)9-6-12-4-7-13(16-2)8-5-12/h4-9H,3,10-11H2,1-2H3/b9-6+	-2.7
InChI=1S/C16H23N3OS/c1-12(2)19-14(17-16(3,4)5)21-11-18(15(19)20)13-9-7-6-8-10-13/h6-10,12H,11H2,1-5H3/b17-14-	-5.531
InChI=1S/C32H26Cl2N6O4/c1-19(41)29(31(43)35-23-9-5-3-6-10-23)39-37-27-15-13-21(17-25(27)h3-18,29-30H,1-2H3,(H,35,43)(H,36,44)/b39-37+,40-38+	-9.197
InChI=1S/C20H22O3/c1-20(2,19(21)22)23-16-12-10-15(11-13-16)18-9-5-7-14-6-3-4-8-17(1h3-4,6,8,10-13,18H,5,7,9H2,1-2H3,(H,21,22)	-5.58
InChI=1S/C12H2Cl8O/c13-3-1-4(14)9(18)12(8(3)17)21-6-2-5(15)7(16)11(20)10(6)19/h1-2H	-10.1
InChI=1S/C14H18N4O3S/c1-3-10(2)18-9-8-13(16-14(18)19)17-22(20,21)12-6-4-11(15)5-7-12/h4-10H,3,15H2,1-2H3,(H,16,17,19)	-2.76
InChI=1S/C8H11N/c1-6-3-4-8(9)5-7(6)2/h3-5H,9H2,1-2H3	-1.504
InChI=1S/C11H16O3/c1-2-9-4-3-5-11(6-9)14-8-10(13)7-12/h3-6,10,12-13H,2,7-8H2,1H3	-2.251
InChI=1S/C22H33Cl2N3O4/c1-5-31-22(30)20(15(2)3)26-21(29)19(25-16(4)28)14-17-6-8-18(9-7-1h6-9,15,19-20H,5,10-14H2,1-4H3,(H,25,28)(H,26,29)	-5.847
InChI=1S/C13H18O4/c1-2-5-12(16)11-6-3-4-7-13(11)17-9-10(15)8-14/h3-4,6-7,10,14-15H,2,5,8-9H2,1H3	-2.237
InChI=1S/C18H18N6O5S2/c1-12-2-6-15(7-3-12)31(28,29)24-18(25)23-17-20-11-10-16(22-17)21-h2-11H,1H3,(H2,19,26,27)(H3,20,21,22,23,24,25)	-4.3
InChI=1S/C10H11NO2S/c1-2-13-10(12)11-7-14-9-6-4-3-5-8(9)11/h3-6H,2,7H2,1H3	-3.275
InChI=1S/C5H8FN/c6-4-2-1-3-5-7/h1-4H2	-1.289
InChI=1S/C22H21O2P/c1-16-14-17(2)21(18(3)15-16)22(23)25(24,19-10-6-4-7-11-19)20-12-8h4-15H,1-3H3	-5.011
InChI=1S/C15H13NO3/c1-11(17)19-14-9-7-13(8-10-14)16-15(18)12-5-3-2-4-6-12/h2-10H,1H3,(H,16,18)	-4.14
InChI=1S/C20H24N4O2S/c1-22-11-13-23(14-12-22)10-5-15-26-20(25)24-16-6-2-3-7-17(16)27-1h2-4,6-9H,5,10-15H2,1H3	-5.458
InChI=1S/C7H11N3O3/c1-2-6-5-8-7(10(12)13)9(6)3-4-11/h5,11H,2-4H2,1H3	-1.359
InChI=1S/C20H21NOS/c1-13-4-3-5-16(10-13)21(2)20(23)22-17-8-9-18-14-6-7-15(11-14)19(1h3-5,8-10,12,14-15H,6-7,11H2,1-2H3	-7.177
InChI=1S/C6HF5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H	-0.52
InChI=1S/C19H25NO4/c1-20-8-7-19-12-4-5-14(21)18(19)24-17-15(23-10-22-2)6-3-11(16(17)h3,6,12-14,18,21H,4-5,7-10H2,1-2H3	-1.96

"InChi"	"logS(M)"
InChI=1S/C17H15O6P/c18-16(19)9-11(17(20)21)10-24(22)15-8-4-2-6-13(15)12-5-1-3-7-14(1h1-8,11H,9-10H2,(H,18,19)(H,20,21)	-2.814
InChI=1S/C6H3N3O8/c10-5-2(7(12)13)1-3(8(14)15)6(11)4(5)9(16)17/h1,10-11H	-3.51
InChI=1S/C11H22O3/c1-4-6-7-10(5-2)8-14-11(13)9(3)12/h9-10,12H,4-8H2,1-3H3	-2.674
InChI=1S/C15H18N2O3/c1-4-15(11-8-6-5-7-9-11)12(18)16-14(17-13(15)19)20-10(2)3/h5-10H,4H2,1-3H3,(H,16,17,18,19)	-2.73
InChI=1S/C14H14N2O3S/c1-10(17)16-12-4-8-14(9-5-12)20(18,19)13-6-2-11(15)3-7-13/h2-9H,15H2,1H3,(H,16,17)	-3.612
InChI=1S/C14H18N2O5/c1-9-4-3-5-10(2)14(9)15-11(17)6-16(7-12(18)19)8-13(20)21/h3-5H,6-8H2,1-2H3,(H,15,17)(H,18,19)(H,20,21)	0.469
InChI=1S/C11H14ClNO3/c1-2-5-16-10-4-3-8(6-9(10)12)7-11(14)13-15/h3-4,6,15H,2,5,7H2,1H3,(H,13,14)	-2.797
InChI=1S/C16H13N3O/c1-20-16-17-14(12-8-4-2-5-9-12)15(18-19-16)13-10-6-3-7-11-13/h2-11H,1H3	-4.04
InChI=1S/C16H19N3/c1-3-19(4-2)16-12-10-15(11-13-16)18-17-14-8-6-5-7-9-14/h5-13H,3-4H2,1-2H3/b18-17+	-5.982
InChI=1S/C8H12N2O2S/c1-3-8(4-2)5(11)9-7(12)10-6(8)13/h3-4H2,1-2H3,(H2,9,10,11,12,13)	-1.106
InChI=1S/C20H25N3O/c1-4-23(5-2)20(24)14-9-16-15-7-6-8-17-19(15)13(11-21-17)10-18(16)h6-9,11,14,18,21H,4-5,10,12H2,1-3H3	-5.188
InChI=1S/C4H4O3/c5-3-1-2-4(6)7-3/h1-2H2	-0.202
InChI=1S/C9H8Cl2FNO2/c10-7(11)9(15)13-8(14)5-1-3-6(12)4-2-5/h1-4,7,9,15H,(H,13,14)	-1.715
InChI=1S/C18H29NO3/c1-7-19(8-2)11-12-22-17-15(13(3)4)10-9-14(5)16(17)18(20)21-6/h9-10,13H,7-8,11-12H2,1-6H3	-4.354
InChI=1S/C19H12O6S/c20-11-5-7-16-14(9-11)19(15-10-12(21)6-8-17(15)24-16)13-3-1-2-4-1h1-10,20-21H	-3.5
InChI=1S/C12H14N2O2/c13-7-4-8-14-11(12(15)16)9-10-5-2-1-3-6-10/h1-3,5-6,11,14H,4,8-9H2,(H,15,16)	-1.494
InChI=1S/C11H7FN2O3/c12-8-6-13-11(17)14(10(8)16)9(15)7-4-2-1-3-5-7/h1-6H,(H,13,17)	-2.26
InChI=1S/C22H27N3O2/c1-17-10-12-18(13-11-17)23-22(27)19-8-4-5-9-20(19)24(2)21(26)16-2h4-5,8-13H,3,6-7,14-16H2,1-2H3,(H,23,27)	-5.114
InChI=1S/C12H14N4O3S2/c1-3-11-14-15-12(20-11)16-21(18,19)10-6-4-9(5-7-10)13-8(2)17/h4-7H,3H2,1-2H3,(H,13,17)(H,15,16)	-3.4
InChI=1S/C9H18N2O4/c1-9(2,5-14-7(10)12)6-15-8(13)11(3)4/h5-6H2,1-4H3,(H2,10,12)	-1.541

"InChi"	"logS(M)"
InChI=1S/C15H12N2O2/c1-19-15(18)9-6-7-13-11(8-9)14(16)10-4-2-3-5-12(10)17-13/h2-8H,1H3,(H2,16,17)	-4.061
InChI=1S/C17H10F6N4S/c18-16(19,20)25-13-14(26-17(21,22)23)28-15(24-11-7-3-1-4-8-11)27(h1-10H/b24-15-,25-13+,26-14-	-5.42
InChI=1S/C15H12Br4O2/c1-15(2,7-3-9(16)13(20)10(17)4-7)8-5-11(18)14(21)12(19)6-8/h3-6,20-21H,1-2H3	-5.694
InChI=1S/C6H4Cl3N/c7-3-1-5(9)6(10)2-4(3)8/h1-2H,10H2	-3.436
InChI=1S/C10H15N3/c1-11-10(12-2)13-8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H2,11,12,13)	-2.932
InChI=1S/C10H11N3O2/c11-7(10(14)15)5-9-6-3-1-2-4-8(6)12-13-9/h1-4,7H,5,11H2,(H,12,13)(H,14,15)	-1.409
InChI=1S/C16H22BrNO2/c1-13-5-2-3-10-18(13)11-4-12-20-16(19)14-6-8-15(17)9-7-14/h6-9,13H,2-5,10-12H2,1H3	-4.674
InChI=1S/C6H4N4O2/c11-3-1-7-4-5(10-3)8-2-9-6(4)12/h1-2H,(H2,8,9,10,11,12)	-2.82
InChI=1S/C27H26N2O2/c1-27(2,19-3-11-23(12-4-19)30-25-15-7-21(28)8-16-25)20-5-13-24(14h3-18H,28-29H2,1-2H3	-7.192
InChI=1S/C21H33NO5/c1-14(2)17-10-9-16(5)19(21(24)27-15(3)4)20(17)26-13-18(23)25-12-8h9-10,14-15H,8,11-13H2,1-7H3	-4.844
InChI=1S/C9H12O2S/c10-6-8(11)7-12-9-4-2-1-3-5-9/h1-5,8,10-11H,6-7H2	-1.382
InChI=1S/C6H6O3/c1-4-2-5(7)3-6(8)9-4/h2-3,7H,1H3	0.376
InChI=1S/C3H4Cl2O2/c1-3(4,5)2(6)7/h1H3,(H,6,7)	0.545
InChI=1S/C11H12N4O5/c1-2-12-11(16)7-5-9(13-3-4-13)10(15(19)20)6-8(7)14(17)18/h5-6H,2-4H2,1H3,(H,12,16)	-3.13
InChI=1S/C10H10O2/c1-8(2)10(11)12-9-6-4-3-5-7-9/h3-7H,1H2,2H3	-2.495
InChI=1S/C6H14/c1-4-5-6(2)3/h6H,4-5H2,1-3H3	-3.74
InChI=1S/C12H16Cl2N2O/c1-9-2-3-10(12(15)17)8-11(9)16(6-4-13)7-5-14/h2-3,8H,4-7H2,1H3,(H2,15,17)	-3.729
InChI=1S/C17H21NO4/c1-11(6-12-2-4-14(19)5-3-12)18-10-17(22)13-7-15(20)9-16(21)8-13/h2-5,7-9,11,17-22H,6,10H2,1H3	-0.865
InChI=1S/C8H20N2OS/c1-5-9(6-2)12(11)10(7-3)8-4/h5-8H2,1-4H3/p+1	-1.28
InChI=1S/C8H6ClNO/c1-5-10-7-4-6(9)2-3-8(7)11-5/h2-4H,1H3	-2.91
InChI=1S/C18H28N2O2/c1-3-15(2)18(17(19)21,16-7-5-4-6-8-16)9-10-20-11-13-22-14-12-20/h4-8,15H,3,9-14H2,1-2H3,(H2,19,21)	-3.236
InChI=1S/C12H15N3O6/c16-10-13(1-7-4-19-7)11(17)15(3-9-6-21-9)12(18)14(10)2-8-5-20-8/h7-9H,1-6H2	-2.469
InChI=1S/C9H8INO3/c10-7-3-1-2-6(4-7)9(14)11-5-8(12)13/h1-4H,5H2,(H,11,14)(H,12,13)	-3.03

"InChi"	"logS(M)"
InChI=1S/C26H12N4O2/c31-25-15-11-12-16-22-14(24-28-18-6-2-4-8-20(18)30(24)26(16)32)1(h1-12H	-5.633
InChI=1S/C14H13N3O2/c15-11-5-1-10(2-6-11)14(19)17-12-7-3-9(4-8-12)13(16)18/h1-8H,15H2,(H2,16,18)(H,17,19)	-4.916
InChI=1S/C32H24N6O5/c1-43-27-14-11-19(30(40)33-20-8-3-2-4-9-20)16-26(27)37-38-28-22-1h2-17,37H,1H3,(H,33,40)(H,34,41)(H2,35,36,42)/b38-28-	-8.479
InChI=1S/C10H12N4O4/c1-4-18-10(17)14-5-11-7-6(14)8(15)13(3)9(16)12(7)2/h5H,4H2,1-3H3	-1.65
InChI=1S/C13H14ClNO2/c1-9(13(16)17)10-4-5-12(11(14)8-10)15-6-2-3-7-15/h2-5,8-9H,6-7H2,1H3,(H,16,17)	-3.318
InChI=1S/C8H8N4O2S/c1-5(13)14-4-15-8-6-7(10-2-9-6)11-3-12-8/h2-3H,4H2,1H3,(H,9,10,11,12)	-2.15
InChI=1S/C18H18O3/c1-2-3-12-21-17(19)18(20)15-10-6-4-8-13(15)14-9-5-7-11-16(14)18/h4-11,20H,2-3,12H2,1H3	-3.889
InChI=1S/C16H16O2/c1-3-7-13-10-11-15(16(12-13)17-2)18-14-8-5-4-6-9-14/h3-6,8-12H,1,7H2,2H3	-4.953
InChI=1S/C18H19NO2/c1-19-9-8-11-4-3-5-13-16(11)14(19)10-12-6-7-15(21-2)18(20)17(12)1h3-7,14,20H,8-10H2,1-2H3	-3.222
InChI=1S/C12H14N2O3/c1-3-17-12(16)11(9(2)15)14-13-10-7-5-4-6-8-10/h4-8,11H,3H2,1-2H3/b14-13+	-2.866
InChI=1S/C10H5Cl2NO2/c11-6-3-5-1-2-7(12)8(10(14)15)9(5)13-4-6/h1-4H,(H,14,15)	-3.57
InChI=1S/C10H13Cl2N5O6S2/c11-8-4(24(14,20)21)1-5(25(15,22)23)10(9(8)12)17-7(19)3-16-6(18)2-h1H,2-3,13H2,(H,16,18)(H,17,19)(H2,14,20,21)(H2,15,22,23)	-1.23
InChI=1S/C16H20N2O3/c1-9(2)16(4)15(20)17-13(18-16)11-7-6-10(3)8-12(11)14(19)21-5/h6-9H,1-5H3,(H,17,18,20)	-2.326
InChI=1S/C22H21N3O6/c1-30-9-10-31-8-4-7-25-21(28)15-16(22(25)29)18(24)14-13(17(15)23)h2-3,5-6H,4,7-10,23-24H2,1H3	-8.265
InChI=1S/C10H18O4/c1-3-5-9(11)13-7-8-14-10(12)6-4-2/h3-8H2,1-2H3	-2.607
InChI=1S/C15H12N2O/c1-10-7-8-13-12(9-10)14(17-15(18)16-13)11-5-3-2-4-6-11/h2-9H,1H3,(H,16,17,18)	-2.905
InChI=1S/C4H10O2/c1-4(5-2)6-3/h4H,1-3H3	1.045
InChI=1S/C5H13NO2/c1-2-5(6,3-7)4-8/h7-8H,2-4,6H2,1H3	0.902
InChI=1S/C15H14N4O4/c1-18(10-11-2-8-14(9-3-11)19(22)23)17-16-13-6-4-12(5-7-13)15(20)2h2-9H,10H2,1H3,(H,20,21)/b17-16+	-5.324

"InChi"	"logS(M)"
InChI=1S/C16H18N2O4S2/c17-24(20,21)15-9-14(11-23-15)16(19)13-3-1-2-12(8-13)10-18-4-6-22-h1-3,8-9,11H,4-7,10H2,(H2,17,20,21)	-1.92
InChI=1S/C7H5N3O5/c8-7(11)4-1-5(9(12)13)3-6(2-4)10(14)15/h1-3H,(H2,8,11)	-1.84
InChI=1S/C15H30O/c1-14(13-16)15-11-9-7-5-3-2-4-6-8-10-12-15/h14-16H,2-13H2,1H3	-5.452
InChI=1S/C4H6FN/c5-3-1-2-4-6/h1-3H2	-0.767
InChI=1S/C15H22N2O2/c1-11-6-4-7-12(2)14(11)16-15(18)19-13-8-5-9-17(3)10-13/h4,6-7,13H,5,8-10H2,1-3H3,(H,16,18)	-3.415
InChI=1S/C6H11ClO3/c1-6(4-7)9-3-5(2-8)10-6/h5,8H,2-4H2,1H3	-1.04
InChI=1S/C10H11FN2O/c11-7-1-3-8(4-2-7)13-6-5-9(12)10(13)14/h1-4,9H,5-6,12H2	-0.927
InChI=1S/C10H11ClO3/c1-10(2,9(12)13)14-8-5-3-4-7(11)6-8/h3-6H,1-2H3,(H,12,13)	-2.8
InChI=1S/C9H20N2/c1-8(2)6-5-7-9(3,4)11(8)10/h5-7,10H2,1-4H3	-1.974
InChI=1S/C7H14O3/c1-4-9-7(6(3)8)10-5-2/h7H,4-5H2,1-3H3	-0.206
InChI=1S/C20H40O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-4-2/h5-6H,3-4,7-20H2,1-2H3/b6-5+	-4.8
InChI=1S/C14H12O2/c1-11(15)16-14-9-7-13(8-10-14)12-5-3-2-4-6-12/h2-10H,1H3	-4.4
InChI=1S/C14H21N5O4/c1-11(2)18-7-5-17(6-8-18)10-13(20)16-15-9-12-3-4-14(23-12)19(21)2h3-4,9,11H,5-8,10H2,1-2H3,(H,16,20)/b15-9+	-3.402
InChI=1S/C17H21F3N2O4S2/c18-17(19,20)14-12-16(22-15-7-3-2-6-13(14)15)26-10-5-1-4-8-21-9-1h2-3,6-7,12,21H,1,4-5,8-11H2,(H,23,24,25)	-4.187
InChI=1S/C12H9NO/c14-12(10-6-2-1-3-7-10)11-8-4-5-9-13-11/h1-9H	-2.02
InChI=1S/C9H15Cl2N3O2/c10-5-6-14(13-16)9(15)12-8-4-2-1-3-7(8)11/h7-8H,1-6H2,(H,12,15)	-3.487
InChI=1S/C8H14N4O/c1-4-6-10-7(9-5-2)12-8(11-6)13-3/h4-5H2,1-3H3,(H,9,10,11,12)	-2.914
InChI=1S/C8H8O4/c1-12-7-3-2-5(8(10)11)4-6(7)9/h2-4,9H,1H3,(H,10,11)	-1.469
InChI=1S/C10H16N2O3/c1-11-5-7-2-3-8(6-11)12(7)9(13)4-10(14)15/h7-8H,2-6H2,1H3,(H,14,15)	-1.27
InChI=1S/C20H33NO4/c1-12(2)17-9-8-15(7)18(20(23)25-14(5)6)19(17)24-11-16(22)10-21-13h8-9,12-14,16,21-22H,10-11H2,1-7H3	-4.315
InChI=1S/C9H9NO4/c11-8(12)6-14-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)	-0.95
InChI=1S/C11H14N4O2S/c1-2-3-4-8(16)17-7-18-11-9-10(13-5-12-9)14-6-15-11/h5-6H,2-4,7H2,1H3,(H,12,13,14,15)	-3.1
InChI=1S/C15H16/c1-12(2)13-8-10-15(11-9-13)14-6-4-3-5-7-14/h3-12H,1-2H3	-5.61
InChI=1S/C7H5NOS/c9-7-3-1-2-6(4-7)8-5-10/h1-4,9H	-1.99

"InChi"	"logS(M)"
InChI=1S/C21H22O9/c22-6-8-4-10-14(21-20(29)19(28)17(26)13(7-23)30-21)9-2-1-3-11(24)h1-5,13-14,17,19-26,28-29H,6-7H2	-1.702
InChI=1S/C7H14N2O3/c1-4(2)6(8)7(12)9-3-5(10)11/h4,6H,3,8H2,1-2H3,(H,9,12)(H,10,11)	0.458
InChI=1S/C15H12I2O3/c16-12-7-9(8-13(17)14(12)18)6-11(15(19)20)10-4-2-1-3-5-10/h1-5,7-8,11,18H,6H2,(H,19,20)	-5.718
InChI=1S/C4H5F3O/c1-2-8-3-4(5,6)7/h2H,1,3H2	-1.478
InChI=1S/C7H14N2O4S2/c8-7(5-13-15(10,11)14)9-4-6-2-1-3-12-6/h6H,1-5H2,(H2,8,9)(H,10,11,14)	-0.704
InChI=1S/C12H20N2/c1-10(2)13-14-11(3)9-12-7-5-4-6-8-12/h4-8,10-11,13-14H,9H2,1-3H3	-2.966
InChI=1S/C9H10N4O2S/c1-2-6(14)15-5-16-9-7-8(11-3-10-7)12-4-13-9/h3-4H,2,5H2,1H3,(H,10,11,12,13)	-2.39
InChI=1S/C9H17NO/c1-8(2)5-7(11)6-9(3,4)10-8/h10H,5-6H2,1-4H3	0.529
InChI=1S/C16H17NO2/c1-10-8-14(18)19-16-12-5-3-7-17-6-2-4-11(15(12)17)9-13(10)16/h8-9H,2-7H2,1H3	-3.89
InChI=1S/C10H14Cl2NO2PS/c1-7(2)13-16(17,14-3)15-10-5-4-8(11)6-9(10)12/h4-7H,1-3H3,(H,13,17)	-4.798
InChI=1S/C8H5I3O3/c9-4-1-5(10)8(6(11)2-4)14-3-7(12)13/h1-2H,3H2,(H,12,13)	-6.791
InChI=1S/C12H15N2O3PS/c1-3-15-18(19,16-4-2)17-12-9-13-10-7-5-6-8-11(10)14-12/h5-9H,3-4H2,1-2H3	-4.132
InChI=1S/C9H22N2/c1-5-10(6-2)9-11(7-3)8-4/h5-9H2,1-4H3	-0.2
InChI=1S/C6H7N3O2/c1-11-6(10)4-5(7)9-3-2-8-4/h2-3H,1H3,(H2,7,9)	-1.642
InChI=1S/C14H12N2O4S/c17-9-15-11-1-5-13(6-2-11)21(19,20)14-7-3-12(4-8-14)16-10-18/h1-10H,(H,15,17)(H,16,18)	-2.176
InChI=1S/C12H11NO4S2/c1-17-10-4-2-8(3-5-10)12(14)9-6-11(18-7-9)19(13,15)16/h2-7H,1H3,(H2,13,15,16)	-4.473
InChI=1S/C3H5N3OS/c1-7-3-5-2(4)8-6-3/h1H3,(H2,4,5,6)	-1.243
InChI=1S/C12H17NO4S/c1-13(10-6-5-9-12(14)15)18(16,17)11-7-3-2-4-8-11/h2-4,7-8H,5-6,9-10H2,1H3,(H,14,15)	-1.558
InChI=1S/C14H10Cl4/c1-8-6-10(13(17)14(18)12(8)16)7-9-2-4-11(15)5-3-9/h2-6H,7H2,1H3	-8.18
InChI=1S/C20H17N3O5/c1-28-8-4-7-23-19(26)13-14(20(23)27)16(22)12-11(15(13)21)17(24)9-h2-3,5-6H,4,7-8,21-22H2,1H3	-7.324
InChI=1S/C12H8Cl5N3O2/c1-2-22-10(21)9-18-11(12(15,16)17)20(19-9)8-4-3-6(13)5-7(8)14/h3-5H,2H2,1H3	-5.652
InChI=1S/C9H13N/c1-6-5-7(2)10-9(4)8(6)3/h5H,1-4H3	-1.307

"InChi"	"logS(M)"
InChI=1S/C9H7FO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,(H,11,12)/b6-5+	-1.958
InChI=1S/C12H6Cl4O/c13-7-2-1-3-8(6-7)17-10-5-4-9(14)11(15)12(10)16/h1-6H	-7.09
InChI=1S/C10H20N2O/c1-5-10(13)12-6-8(2)11(4)9(3)7-12/h8-9H,5-7H2,1-4H3	-0.909
InChI=1S/C11H14N4O3/c1-11(2,3)10(17)18-6-15-4-7-8(14-15)12-5-13-9(7)16/h4-5H,6H2,1-3H3,(H,12,13,14,16)	-2.17
InChI=1S/C5H12O2/c6-4-2-1-3-5-7/h6-7H,1-5H2	0.982
InChI=1S/C16H27N3O/c1-18(2)12-10-16(15(17)20,11-13-19(3)4)14-8-6-5-7-9-14/h5-9H,10-13H2,1-4H3,(H2,17,20)	-1.917
InChI=1S/C8H4N4O6/c13-7-4-1-3(11(15)16)2-5(12(17)18)6(4)9-8(14)10-7/h1-2H,(H2,9,10,13,14)	-3.206
InChI=1S/C12H15N3O3/c1-4-7-13-10(16)14(8-5-2)12(18)15(9-6-3)11(13)17/h4-6H,1-3,7-9H2	-1.853
InChI=1S/C3H5ClO2/c1-6-3(5)2-4/h2H2,1H3	-0.373
InChI=1S/C11H13NO4/c1-8(2)7-11(13)16-10-5-3-9(4-6-10)12(14)15/h3-6,8H,7H2,1-2H3	-4.394
InChI=1S/C17H23N3O3/c1-10(2)7-13(18)16(21)20-15(17(22)23)8-11-9-19-14-6-4-3-5-12(11)19-h3-6,9-10,13,15,19H,7-8,18H2,1-2H3,(H,20,21)(H,22,23)	-1.12
InChI=1S/C12H20N2O/c1-3-9(2)14-8-12(15)10-4-6-11(13)7-5-10/h4-7,9,12,14-15H,3,8,13H2,1-2H3	-0.352
InChI=1S/C20H26O3/c1-4-5-6-7-12-23-20(21)15(2)16-8-9-18-14-19(22-3)11-10-17(18)13-1h8-11,13-15H,4-7,12H2,1-3H3	-7.54
InChI=1S/C22H23F2NO2/c23-19-7-3-16(4-8-19)21(26)2-1-13-25-14-11-18(12-15-25)22(27)17-5h3-10,18H,1-2,11-15H2	-4.65
InChI=1S/C8H6O5/c9-6-4(7(10)11)2-1-3-5(6)8(12)13/h1-3,9H,(H,10,11)(H,12,13)	-2.11
InChI=1S/C8H10O2/c1-2-10-8-6-4-3-5-7(8)9/h3-6,9H,2H2,1H3	-1.171
InChI=1S/C16H15N3O2/c1-17-16(20)21-19-15-12-6-3-2-5-11(12)8-9-14-13(15)7-4-10-18-14/h2-7,10H,8-9H2,1H3,(H,17,20)/b19-15+	-4.869
InChI=1S/C11H22O3/c1-3-5-8-13-10-7-11(12)14-9-6-4-2/h3-10H2,1-2H3	-2.403
InChI=1S/C17H23N3O3/c1-10(2)7-15(17(22)23)20-16(21)13(18)8-11-9-19-14-6-4-3-5-12(11)1h3-6,9-10,13,15,19H,7-8,18H2,1-2H3,(H,20,21)(H,22,23)	-1.76
InChI=1S/C19H18N2/c1-21(2)17-11-8-15(9-12-17)7-10-16-13-14-20-19-6-4-3-5-18(16)19/h3-14H,1-2H3/b10-7+	-5.345
InChI=1S/C13H9N3O2/c14-13-8-4-1-2-5-9(8)15-10-6-3-7-11(12(10)13)16(17)18/h1-7H,(H2,14,15)	-1.84
InChI=1S/C7H14N2O2S/c1-5(6(2)12-4)9-11-7(10)8-3/h6H,1-4H3,(H,8,10)/b9-5-	-0.735

"InChi"	"logS(M)"
InChI=1S/C8H7ClN2O/c1-10-8-11-6-4-5(9)2-3-7(6)12-8/h2-4H,1H3,(H,10,11)	-2.763
InChI=1S/C13H17N/c1-4-10-14(3)12(2)11-13-8-6-5-7-9-13/h1,5-9,12H,10-11H2,2-3H3	-2.51
InChI=1S/C19H23BrN2O2/c1-3-22(4-2)12-13-24-18-11-10-15(20)14-17(18)19(23)21-16-8-6-5-7-h5-11,14H,3-4,12-13H2,1-2H3,(H,21,23)	-4.806
InChI=1S/C9H12N4O2/c1-2-3-4-13-7-6(10-5-11-7)8(14)12-9(13)15/h5H,2-4H2,1H3,(H,10,11)(H,12,14,15)	-1.437
InChI=1S/C15H10O6/c16-8-4-11(19)15-12(20)6-13(21-14(15)5-8)7-1-2-9(17)10(18)3-7/h1-6,16-19H	-3.61
InChI=1S/C9H10N2O/c1-10-9-11(2)7-5-3-4-6-8(7)12-9/h3-6H,1-2H3/b10-9-	-2.67
InChI=1S/C2H8N2/c1-3-4-2/h3-4H,1-2H3	1.221
InChI=1S/C12H14N2S/c1-9-4-5-11(10(2)8-9)13-12-14(3)6-7-15-12/h4-8H,1-3H3/b13-12-	-3.163
InChI=1S/C16H17NO4/c18-11-3-8-1-2-17-6-9-4-12-13(21-7-20-12)5-10(9)14(15(8)17)16(11)h3-5,11,14-16,18-19H,1-2,6-7H2	-2.613
InChI=1S/C19H23NO2S/c1-20(2)12-6-11-19(21)15-7-4-5-8-17(15)23-18-10-9-14(22-3)13-16(1h4-5,7-10,13,21H,6,11-12H2,1-3H3	-5.091
InChI=1S/C35H44O16/c1-8-15(2)24(38)49-18-12-19(48-16(3)36)32(26(39)43-6)13-46-21-22(h8-10,17-23,25,28,37,41-42H,11-14H2,1-7H3/b15-8+	-3.443
InChI=1S/C19H14N2/c20-19-15-8-4-5-9-17(15)21-18-11-10-14(12-16(18)19)13-6-2-1-3-7-1h1-12H,(H2,20,21)	-5.84
InChI=1S/C12H8Cl2/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h1-8H	-5.299
InChI=1S/C13H10O3/c1-7-3-13(14)16-12-6-11-9(5-10(7)12)4-8(2)15-11/h3-6H,1-2H3	-5.23
InChI=1S/C12H10O2/c1-9(13)14-12-7-6-10-4-2-3-5-11(10)8-12/h2-8H,1H3	-3.44
InChI=1S/C10H20N2S2/c1-5-7(3)11-9(13)10(14)12-8(4)6-2/h7-8H,5-6H2,1-4H3,(H,11,13)(H,12,14)	-1.537
InChI=1S/C24H38O4/c1-5-9-11-19(7-3)17-27-23(25)21-13-15-22(16-14-21)24(26)28-18-20(h13-16,19-20H,5-12,17-18H2,1-4H3	-8.99
InChI=1S/C8H16NO3PS2/c1-4-11-13(10,12-5-2)9-8-14-6-7(3)15-8/h7H,4-6H2,1-3H3/b9-8+	-3.674
InChI=1S/C12H14N2O2/c15-12(11-4-2-1-3-5-11)10-13-14-6-8-16-9-7-14/h1-5,10H,6-9H2/b13-10+	-1.101
InChI=1S/C7H12ClN3O6S2/c8-1-2-11(10-13)7(12)9-6-3-18(14,15)5-19(16,17)4-6/h6H,1-5H2,(H,9,12)	-2.141
InChI=1S/C12H5Cl5O/c13-6-1-3-7(4-2-6)18-12-10(16)8(14)5-9(15)11(12)17/h1-5H	-7.76
InChI=1S/C10H13NO2/c1-7-4-5-10(13-3)9(6-7)11-8(2)12/h4-6H,1-3H3,(H,11,12)	-1.931

"InChi"	"logS(M)"
InChI=1S/C16H20N2O3S2/c1-11(2)8-18-9-12-3-5-13(6-4-12)16(19)14-7-15(22-10-14)23(17,20)2h3-7,10-11,18H,8-9H2,1-2H3,(H2,17,20,21)	-2.05
InChI=1S/C6H5NO4/c1-4(8)5-2-3-6(11-5)7(9)10/h2-3H,1H3	-1.247
InChI=1S/C14H14N2O2/c1-18-13-8-7-10(9-12(13)15)14(17)16-11-5-3-2-4-6-11/h2-9H,15H2,1H3,(H,16,17)	-3.866
InChI=1S/C6H18N3OP/c1-7(2)11(10,8(3)4)9(5)6/h1-6H3	0.747
InChI=1S/C13H24O4/c1-2-3-4-5-6-7-8-9-10-11(12(14)15)13(16)17/h11H,2-10H2,1H3,(H,14,15)(H,16,17)	-3.99
InChI=1S/C23H30ClN3O/c1-5-27(6-2)13-7-8-16(3)25-23-19-11-9-17(24)14-22(19)26-21-12-10-h9-12,14-16H,5-8,13H2,1-4H3,(H,25,26)	-2.64
InChI=1S/C36H60O6/c1-4-7-10-13-16-19-22-27-40-34(37)31-25-26-32(35(38)41-28-23-20-h25-26,30H,4-24,27-29H2,1-3H3	-6.757
InChI=1S/C26H28N2O4/c1-30-21-10-7-18(8-11-21)16-28-14-13-22-20(17-28)5-4-6-23(22)27-2h4-12,15H,13-14,16-17H2,1-3H3,(H,27,29)	-5.371
InChI=1S/C12H15N3O4/c13-10(16)6-14-11(17)7-15-12(18)19-8-9-4-2-1-3-5-9/h1-5H,6-8H2,(H2,13,16)(H,14,17)(H,15,18)	-2.35
InChI=1S/C7H7FN2O/c8-5-1-3-6(4-2-5)10-7(9)11/h1-4H,(H3,9,10,11)	-1.214
InChI=1S/C11H17N3O3/c1-3-17-10-9(8-12-13(2)11(10)15)14-4-6-16-7-5-14/h8H,3-7H2,1-2H3	0.621
InChI=1S/C10H20N2O4/c1-3-4-5-10(2,6-15-8(11)13)7-16-9(12)14/h3-7H2,1-2H3,(H2,11,13)(H2,12,14)	-2.154
InChI=1S/C6H12O/c1-7-6-4-2-3-5-6/h6H,2-5H2,1H3	-0.904
InChI=1S/C21H24O2/c1-5-7-15-13-17(9-11-19(15)22)21(3,4)18-10-12-20(23)16(14-18)8-6-h5-6,9-14,22-23H,1-2,7-8H2,3-4H3	-3.996
InChI=1S/C14H24O4/c1-2-12(6-16-8-14-10-18-14)4-3-11(1)5-15-7-13-9-17-13/h11-14H,1-10H2	-1.836
InChI=1S/C13H10N2S/c16-13-9-5-1-2-6-10(9)14-11-7-3-4-8-12(11)15-13/h1-8,14H,(H,15,16)	-4.074
InChI=1S/C12H24N2O4/c1-6-9(2)12(3,7-17-10(13)15)8-18-11(16)14(4)5/h9H,6-8H2,1-5H3,(H2,13,15)	-3.043
InChI=1S/C9H10O/c1-7-6-8-4-2-3-5-9(8)10-7/h2-5,7H,6H2,1H3	-2.68
InChI=1S/C25H46N10O9/c26-5-1-3-11(27)7-15(38)30-6-2-4-12(28)8-16(39)32-19-20(40)21(44-h11-14,17-21,23,36-37,40H,1-10,26-28H2,(H2,29,42)(H,30,38)(H,31,41)(H,32,39)(H2,33,34,35)	0.2
InChI=1S/C11H16O4/c1-14-11-4-2-9(3-5-11)7-15-8-10(13)6-12/h2-5,10,12-13H,6-8H2,1H3	-1.297
InChI=1S/C8H10NO6P/c1-13-16(12,14-2)15-8-5-3-7(4-6-8)9(10)11/h3-6H,1-2H3	-2.529

"InChi"	"logS(M)"
InChI=1S/C8H11NO3/c1-5-8(12)7(4-11)6(3-10)2-9-5/h2,10-12H,3-4H2,1H3	0.222
InChI=1S/C14H17NO3/c16-13(15-9-5-2-6-10-15)11-18-14(17)12-7-3-1-4-8-12/h1,3-4,7-8H,2,5-6,9-11H2	-2.501
InChI=1S/C12H4Cl6/c13-5-3-8(15)10(9(16)4-5)6-1-2-7(14)12(18)11(6)17/h1-4H	-8.24
InChI=1S/C21H12ClNO3/c22-15-10-11-16(23-21(26)12-6-2-1-3-7-12)18-17(15)19(24)13-8-4-5-h1-11H,(H,23,26)	-7.843
InChI=1S/C40H22Cl6N6O4/c41-21-9-11-27(43)33(15-21)49-51-35-23-7-3-1-5-19(23)13-25(37(35)h1-18,49-50H,(H,47,55)(H,48,56)/b51-35-,52-36+	-8.151
InChI=1S/C17H18F2N4O3/c1-6-9(20)5-22(6)15-11(18)13(21)10-14(12(15)19)23(7-2-3-7)4-8(16(h4,6-7,9H,2-3,5,20-21H2,1H3,(H,25,26)	-3.98
InChI=1S/C9H12O2/c1-9(2,11-10)8-6-4-3-5-7-8/h3-7,10H,1-2H3	-1.039
InChI=1S/C12H8N2O5/c15-10-7-6-9(13(16)17)11(12(10)14(18)19)8-4-2-1-3-5-8/h1-7,15H	-3.716
InChI=1S/C15H23NO2/c1-3-5-6-12(4-2)11-18-15(17)13-7-9-14(16)10-8-13/h7-10,12H,3-6,11,16H2,1-2H3	-5.054
InChI=1S/C13H16N4O5/c1-8(2)7-14-13(18)9-5-11(15-3-4-15)12(17(21)22)6-10(9)16(19)20/h5-6,8H,3-4,7H2,1-2H3,(H,14,18)	-3.85
InChI=1S/C20H27N5O5S/c1-15-14-18(23-30-15)19(26)21-11-10-16-6-8-17(9-7-16)31(28,29)24-h6-9,14H,2-5,10-13H2,1H3,(H,21,26)(H2,22,24,27)	-4.632
InChI=1S/C9H6N2O4/c12-9-6-4-2-1-3-5(6)7(10-13)8(9)11(14)15/h1-4,8,13H/b10-7+	-2.68
InChI=1S/C11H16N2O4S2/c1-2-16-4-3-13-7-9-5-8-6-10(19(12,14)15)17-11(8)18-9/h5-6,13H,2-4,7H2,1H3,(H2,12,14,15)	-0.92
InChI=1S/C21H30FN3O2/c22-18-8-6-17(7-9-18)19(26)5-4-12-24-15-10-21(11-16-24,20(23)27)2h6-9H,1-5,10-16H2,(H2,23,27)	-3.663
InChI=1S/C13H12N4O2/c1-16-11-9(12(18)17(2)13(16)19)14-10(15-11)8-6-4-3-5-7-8/h3-7H,1-2H3,(H,14,15)	-5
InChI=1S/C10H13NO2/c1-7(11)4-8-2-3-9-10(5-8)13-6-12-9/h2-3,5,7H,4,6,11H2,1H3	-0.901
InChI=1S/C11H12N2O2/c1-8(14)11(9(2)15)13-12-10-6-4-3-5-7-10/h3-7,11H,1-2H3/b13-12+	-2.866
InChI=1S/C11H22N2O4/c1-5-6-11(2,7-16-9(12)14)8-17-10(15)13(3)4/h5-8H2,1-4H3,(H2,12,14)	-2.584
InChI=1S/C10H16O2/c1-6-3-4-8-7(2)10(11)12-5-9(6)8/h6-9H,3-5H2,1-2H3	-1.925
InChI=1S/C11H18N2O6/c1-4-11(5-2,8(15)13-10(12)17)9(16)19-6-7(14)18-3/h4-6H2,1-3H3,(H3,12,13,15,17)	-2.01
InChI=1S/C4H10ClN/c1-6(2)4-3-5/h3-4H2,1-2H3	0.352

"InChi"	"logS(M)"
InChI=1S/C15H15ClF3N3O/c1-2-7-23-9-14(22-6-5-20-10-22)21-13-4-3-11(16)8-12(13)15(17,18)1h3-6,8,10H,2,7,9H2,1H3/b21-14-	-4.44
InChI=1S/C8H15N5O/c1-5(2)10-7-11-6(9-3)12-8(13-7)14-4/h5H,1-4H3,(H2,9,10,11,12,13)	-1.751
InChI=1S/C8H5NO6/c10-7(11)4-2-1-3-5(8(12)13)6(4)9(14)15/h1-3H,(H,10,11)(H,12,13)	-1.99
InChI=1S/C18H27NO2/c1-14-9-11-19(12-10-14)13-15(2)16(3)21-18(20)17-7-5-4-6-8-17/h4-8,14-16H,9-13H2,1-3H3	-4.257
InChI=1S/C13H10N2O3S/c14-10-2-1-8-5-9-6-11(19(16,17)18)3-4-12(9)15-13(8)7-10/h1-7H,14H2,(H,16,17,18)	-3.665
InChI=1S/C10H14N4O2/c1-5(2)7-11-6-8(12-7)13(3)10(16)14(4)9(6)15/h5H,1-4H3,(H,11,12)	-1.732
InChI=1S/C10H13NO3/c1-3-7(2)8-4-5-10(12)9(6-8)11(13)14/h4-7,12H,3H2,1-2H3	-3.84
InChI=1S/C22H18N2O4/c1-22(16-12-14-19(15-13-16)27-18-10-6-3-7-11-18)20(25)24(21(26)2h2-15,23H,1H3	-6.857
InChI=1S/C10H15NO/c1-8(11-2)7-9-3-5-10(12)6-4-9/h3-6,8,11-12H,7H2,1-2H3	-0.95
InChI=1S/C22H22ClN3O5/c1-14(2)26-29-11-10-28-22(27)15(3)30-17-5-7-18(8-6-17)31-21-13-24h4-9,12-13,15H,10-11H2,1-3H3	-5.848
InChI=1S/C17H24O4S/c1-13(2)21-16(18)17(11-5-4-6-12-17)22(19,20)15-9-7-14(3)8-10-15/h7-10,13H,4-6,11-12H2,1-3H3	-4.62
InChI=1S/C8H16N2O2S2/c1-7(11)9-3-5-13-14-6-4-10-8(2)12/h3-6H2,1-2H3,(H,9,11)(H,10,12)	-2.062
InChI=1S/C2H6O4S/c3-1-2-7(4,5)6/h3H,1-2H2,(H,4,5,6)	0.899
InChI=1S/C7H6O3/c8-4-5-1-2-6(9)7(10)3-5/h1-4,9-10H	-1.34
InChI=1S/C9H16N2O4/c10-7(12)14-5-9(3-1-2-4-9)6-15-8(11)13/h1-6H2,(H2,10,12)(H2,11,13)	-1.521
InChI=1S/C15H13N3O5/c1-23-13-7-4-10(8-12(13)18(21)22)15(20)17-11-5-2-9(3-6-11)14(16)1h2-8H,1H3,(H2,16,19)(H,17,20)	-4.654
InChI=1S/C17H16Br2ClNO2/c18-9-11-21(12-10-19)15-5-7-16(8-6-15)23-17(22)13-1-3-14(20)4-2-1h1-8H,9-12H2	-7.291
InChI=1S/C11H9NO4S2/c12-18(15,16)10-5-8(6-17-10)11(14)7-1-3-9(13)4-2-7/h1-6,13H,(H2,12,15,16)	-2.861
InChI=1S/C15H31N/c1-2-3-4-5-6-7-8-10-13-16-14-11-9-12-15-16/h2-15H2,1H3	-1.53
InChI=1S/C19H41NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18-19-24-25(21,22)2h20H,2-19H2,1H3,(H,21,22,23)	-6.511
InChI=1S/C5H13NO3S2/c1-5(2)6-3-4-10-11(7,8)9/h5-6H,3-4H2,1-2H3,(H,7,8,9)	0.701
InChI=1S/C8H5BrO4/c9-6-3-4(7(10)11)1-2-5(6)8(12)13/h1-3H,(H,10,11)(H,12,13)	-2.134

"InChi"	"logS(M)"
InChI=1S/C12H6Cl4/c13-9-4-2-1-3-7(9)8-5-11(15)12(16)6-10(8)14/h1-6H	-7.25
InChI=1S/C10H22O/c1-3-5-6-8-10(9-11)7-4-2/h10-11H,3-9H2,1-2H3	-3.518
InChI=1S/C16H22O4S/c1-12(2)20-15(17)16(10-4-5-11-16)21(18,19)14-8-6-13(3)7-9-14/h6-9,12H,4-5,10-11H2,1-3H3	-3.91
InChI=1S/C20H23ClO6/c1-5-6-7-26-12-8-11(2)20(15(22)9-12)19(23)16-13(24-3)10-14(25-4)1h9-11H,5-8H2,1-4H3	-5.4
InChI=1S/C20H12O5/c21-11-5-7-15-17(9-11)25-18-10-12(22)6-8-16(18)19(15)13-3-1-2-4-1h1-10,21H,(H,23,24)	-3.82
InChI=1S/C18H28N2O/c1-15(2)18(17(19)21,16-9-5-3-6-10-16)11-14-20-12-7-4-8-13-20/h3,5-6,9-10,15H,4,7-8,11-14H2,1-2H3,(H2,19,21)	-4.193
InChI=1S/C8H6O4/c9-4-5-2-1-3-6(7(5)10)8(11)12/h1-4,10H,(H,11,12)	-2.442
InChI=1S/C12H27N/c1-3-5-7-9-11-13-12-10-8-6-4-2/h13H,3-12H2,1-2H3	-3.157
InChI=1S/C11H16/c1-9-5-7-10(8-6-9)11(2,3)4/h5-8H,1-4H3	-4.472
InChI=1S/C10H16O5/c1-4-5-13-6-10(15-9(3)12)7-14-8(2)11/h4,10H,1,5-7H2,2-3H3	-1.549
InChI=1S/C11H11BrO4S/c1-16-10(13)11(6-7-11)17(14,15)9-4-2-8(12)3-5-9/h2-5H,6-7H2,1H3	-3.67
InChI=1S/C5H4N4S/c10-5-3-4(7-1-6-3)8-2-9-5/h1-2H,(H2,6,7,8,9,10)	-2.95
InChI=1S/C9H7NO3/c11-8-7(13-9(12)10-8)6-4-2-1-3-5-6/h1-5,7H,(H,10,11,12)	-1.424
InChI=1S/C6H7ClN6/c1-13-2-9-4-3(13)5(12-8)11-6(7)10-4/h2H,8H2,1H3,(H,10,11,12)	-1.143
InChI=1S/C14H24O2/c1-7-14(6,10-8-9-11(2)3)16-13(15)12(4)5/h7,9,12H,1,8,10H2,2-6H3	-4.811
InChI=1S/C18H14O8/c19-15(20)11-5-1-3-7-13(11)17(23)25-9-10-26-18(24)14-8-4-2-6-12(1h1-8H,9-10H2,(H,19,20)(H,21,22)	-2.83
InChI=1S/C12H23NO3/c1-3-6-10(7-4-2)12(16)13-9-5-8-11(14)15/h10H,3-9H2,1-2H3,(H,13,16)(H,14,15)	-1.5
InChI=1S/C22H27ClN2O/c1-17(2)24-14-12-21(13-15-24)25(20-10-8-19(23)9-11-20)22(26)16-1h3-11,17,21H,12-16H2,1-2H3	-6.046
InChI=1S/C9H12O3/c1-6-2-7(4-10)9(12)8(3-6)5-11/h2-3,10-12H,4-5H2,1H3	-0.388
InChI=1S/C17H16BrCl2NO2/c18-14-3-1-2-13(12-14)17(22)23-16-6-4-15(5-7-16)21(10-8-19)11-9-2h1-7,12H,8-11H2	-7.026
InChI=1S/C10H17NO3/c1-3-10(4-2)6-5-8(13)11(7-12)9(10)14/h12H,3-7H2,1-2H3	-3.96
InChI=1S/C10H14N2O4S2/c1-16-9-4-2-8(3-5-9)6-12-10(11)7-17-18(13,14)15/h2-5H,6-7H2,1H3,(H2,11,12)(H,13,14,15)	-2.048

"InChi"	"logS(M)"
InChI=1S/C9H10N4/c1-13(2)12-11-9-5-3-8(7-10)4-6-9/h3-6H,1-2H3/b12-11+	-2.778
InChI=1S/C14H13NO2/c15-14(16)17-13-8-6-12(7-9-13)10-11-4-2-1-3-5-11/h1-9H,10H2,(H2,15,16)	-3.777
InChI=1S/C11H15NO3S/c1-9(11(13)12(2)3)16(14,15)10-7-5-4-6-8-10/h4-9H,1-3H3	-0.87
InChI=1S/C6H9NOS/c1-5(8)4-6-7-2-3-9-6/h2-4H2,1H3	-1.156
InChI=1S/C19H38N2S4/c1-5-9-13-20(14-10-6-2)18(22)24-17-25-19(23)21(15-11-7-3)16-12-8-h5-17H2,1-4H3	-6.241
InChI=1S/C3H10N2/c1-5-3-2-4/h5H,2-4H2,1H3	1.13
InChI=1S/C13H16N10O5S/c1-22-11(7(6-14-22)10-18-21-23(2)19-10)29(25,26)20-13(24)17-12-15h5-6H,1-4H3,(H2,15,16,17,20,24)	-2.607
InChI=1S/C9H8N2S/c10-9-11-8(6-12-9)7-4-2-1-3-5-7/h1-6H,(H2,10,11)	-2.698
InChI=1S/C18H19ClO6/c1-5-24-13-7-10(20)6-9(2)18(13)17(21)14-11(22-3)8-12(23-4)15(19)1h7-9H,5-6H2,1-4H3	-5
InChI=1S/C7H5IN2O/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3H,(H2,9,10)	-3.304
InChI=1S/C9H10O2/c1-2-7-3-5-8(6-4-7)9(10)11/h3-6H,2H2,1H3,(H,10,11)	-2.52
InChI=1S/C13H16BrN4O2P/c14-11-1-3-12(4-2-11)16-13(19)15-5-10-21(20,17-6-7-17)18-8-9-18/h1-5,10H,6-9H2,(H2,15,16,19)/b10-5+	-2.717
InChI=1S/C18H15N3O4S/c22-21(23)18-13-16(26(24,25)20-15-9-5-2-6-10-15)11-12-17(18)19-14h1-13,19-20H	-6.269
InChI=1S/C5H12N2O6/c1-2-3-5(13-7(10)11)4-12-6(8)9/h5H,2-4H2,1H3,(H,8,9)(H,10,11)/q+2	-2.5
InChI=1S/C19H23NO4/c1-20-7-6-19-10-14(21)16(24-3)9-12(19)13(20)8-11-4-5-15(23-2)18(2h4-5,9,12-13,22H,6-8,10H2,1-3H3	-1.768
InChI=1S/C16H22N4O3/c1-16(2,21)13-11(22-3)6-9(7-12(13)23-4)5-10-8-19-15(18)20-14(10)1h6-8,21H,5H2,1-4H3,(H4,17,18,19,20)	-2.794
InChI=1S/C17H30O2/c1-6-19-17(18)13-16(5)12-8-11-15(4)10-7-9-14(2)3/h8,12-15H,6-7,9-11H2,1-5H3/b12-8+,16-13-	-5.693
InChI=1S/C11H14O4/c1-8(13)10-4-2-3-5-11(10)15-7-9(14)6-12/h2-5,9,12,14H,6-7H2,1H3	-1.196
InChI=1S/C9H13N/c1-7(2)8-3-5-9(10)6-4-8/h3-7H,10H2,1-2H3	-1.786
InChI=1S/C28H37NO9/c1-26(2,32)8-9-28(33,15-22(30)35-4)25(31)38-24-21(34-3)14-27-7-5-h12-14,23-24,32-33H,5-11,15-16H2,1-4H3	-3.817
InChI=1S/C10H10O4/c1-7(11)14-9-6-4-3-5-8(9)10(12)13-2/h3-6H,1-2H3	-1.84
InChI=1S/C9H19N/c1-8(2)6-7-9(3,4)10(8)5/h6-7H2,1-5H3	-1.105
InChI=1S/C8H13NO2/c1-3-8(2)4-6(10)9-7(11)5-8/h3-5H2,1-2H3,(H,9,10,11)	-1.228

"InChi"	"logS(M)"
InChI=1S/C12H4Cl6O/c13-5-1-2-9(6(14)3-5)19-12-10(17)7(15)4-8(16)11(12)18/h1-4H	-8.42
InChI=1S/C4H9ClO/c1-3(5)4(2)6/h3-4,6H,1-2H3	-0.212
InChI=1S/C16H16O2/c17-16(13-15-9-5-2-6-10-15)18-12-11-14-7-3-1-4-8-14/h1-10H,11-13H2	-4.189
InChI=1S/C15H14N4/c1-19(12-14-5-3-2-4-6-14)18-17-15-9-7-13(11-16)8-10-15/h2-10H,12H2,1H3/b18-17+	-4.553
InChI=1S/C11H14O2/c1-9(8-12)7-10-3-5-11(13-2)6-4-10/h3-6,8-9H,7H2,1-2H3	-2.247
InChI=1S/C20H24ClN3O2/c1-26-19-12-18(22)17(21)11-16(19)20(25)23-15-7-9-24(10-8-15)13-14-2-6,11-12,15H,7-10,13,22H2,1H3,(H,23,25)	-4.983
InChI=1S/C8H16O3/c1-3-4-6-11-8(9)5-7-10-2/h3-7H2,1-2H3	-1.214
InChI=1S/C5H10N2O/c6-5(8)4-2-1-3-7-4/h4,7H,1-3H2,(H2,6,8)/p+1	0.785
InChI=1S/C10H18O2/c1-3-5-6-7-8-10(11)12-9-4-2/h4H,2-3,5-9H2,1H3	-3.598
InChI=1S/C14H16F3N3O4/c1-2-5-18(8-9-3-4-9)13-11(19(21)22)6-10(14(15,16)17)7-12(13)20(23h6-7,9H,2-5,8H2,1H3	-6.541
InChI=1S/C23H28O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14,2)h6,8,10,16-17,20,28H,4-5,7,9,11-12H2,1-3H3	-4.24
InChI=1S/C23H26N4O/c28-23(17-6-2-1-3-7-17)24-10-11-26-12-13-27-16-22-20(14-18(27)15-h1-9,18,25H,10-16H2,(H,24,28)	-3.228
InChI=1S/C11H18O2/c1-8-6-5-7-11(2,3)9(8)10(12)13-4/h6,9H,5,7H2,1-4H3	-2.909
InChI=1S/C12H16N2O/c1-14(2)6-5-9-8-13-12-4-3-10(15)7-11(9)12/h3-4,7-8,13,15H,5-6H2,1-2H3	-0.672
InChI=1S/C10H16NO3PS/c1-3-12-15(16,13-4-2)14-10-7-5-9(11)6-8-10/h5-8H,3-4,11H2,1-2H3	-2.826
InChI=1S/C7H4N2O6/c10-7(11)4-1-2-5(8(12)13)6(3-4)9(14)15/h1-3H,(H,10,11)	-1.5
InChI=1S/C26H26N2O2S/c1-25(2,3)15-7-9-19-17(13-15)27-23(29-19)21-11-12-22(31-21)24-28-h7-14H,1-6H3	-5.634
InChI=1S/C9H2Cl6O3/c10-3-4(11)8(13)2-1(5(16)18-6(2)17)7(3,12)9(8,14)15/h1-2H	-5.171
InChI=1S/C10H22O6S3/c1-4-7-17(11,12)10(18(13,14)8-5-2)19(15,16)9-6-3/h10H,4-9H2,1-3H3	-1.95
InChI=1S/C2H3BrO2/c3-1-2(4)5/h1H2,(H,4,5)	1.1
InChI=1S/C12H7NO2/c14-11-8-5-1-3-7-4-2-6-9(10(7)8)12(15)13-11/h1-6H,(H,13,14,15)	-4.693
InChI=1S/C14H26O4/c1-3-17-13(15)11-9-7-5-6-8-10-12-14(16)18-4-2/h3-12H2,1-2H3	-3.509
InChI=1S/C5H6/c1-2-4-5-3-1/h1-4H,5H2	-1.565

"InChi"	"logS(M)"
InChI=1S/C9H11BrN2O5/c10-4-2-12(9(16)11-8(4)15)7-1-5(14)6(3-13)17-7/h2,5-7,13-14H,1,3H2,(H,11,15,16)	-2.502
InChI=1S/C4H6Cl2O2S/c5-3-1-9(7,8)2-4(3)6/h3-4H,1-2H2	-0.687
InChI=1S/C9H9N3O7/c10-5(9(14)15)1-4-2-6(11(16)17)8(13)7(3-4)12(18)19/h2-3,5,13H,1,10H2,(H,14,15)	-1.512
InChI=1S/C16H18N2OS/c1-12-6-8-13(9-7-12)20-11-10-18-15-5-3-2-4-14(15)16(17)19/h2-9,18H,10-11H2,1H3,(H2,17,19)	-3.978
InChI=1S/C8H17N3O4/c1-4(9)8(15)11-6(3-13)7(14)5(10)2-12/h2,4-7,13-14H,3,9-10H2,1H3,(H,11,15)	0.659
InChI=1S/C5H13N3O3S2/c6-5(7)8-3-1-2-4-12-13(9,10)11/h1-4H2,(H4,6,7,8)(H,9,10,11)	0.356
InChI=1S/C12H19BrN2O4S2/c13-11-4-5-12(15-10-11)19-8-3-1-2-6-14-7-9-20-21(16,17)18/h4-5,10,14H,1-3,6-9H2,(H,16,17,18)	-2.697
InChI=1S/C9H5I2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H	-5.131
InChI=1S/C22H27N3O/c1-3-25(4-2)17-11-16-23-22-24-20(18-12-7-5-8-13-18)21(26-22)19-14h5-10,12-15H,3-4,11,16-17H2,1-2H3,(H,23,24)	-5.147
InChI=1S/C10H20O2/c1-9(2,11)8-4-6-10(3,12)7-5-8/h8,11-12H,4-7H2,1-3H3	-1.634
InChI=1S/C12H26O5/c1-3-11(5-13,6-14)9-17-10-12(4-2,7-15)8-16/h13-16H,3-10H2,1-2H3	-1.076
InChI=1S/C18H16N2/c1-3-7-15(8-4-1)19-17-11-13-18(14-12-17)20-16-9-5-2-6-10-16/h1-14,19-20H	-6.239
InChI=1S/C18H22N2/c1-3-7-16(8-4-1)15-20-13-11-18(12-14-20)19-17-9-5-2-6-10-17/h1-10,18-19H,11-15H2	-3.954
InChI=1S/C22H22N6O7S2/c1-22(2,20(33)34)35-26-13(12-10-37-21(23)24-12)16(29)25-14-17(30h3-7,10,14,18H,8-9H2,1-2H3,(H4-,23,24,25,29,31,32,33,34)/b26-13+	-3.14
InChI=1S/C7H7N3/c1-5-3-2-4-6-7(5)9-10-8-6/h2-4H,1H3,(H,8,9,10)	-1.517
InChI=1S/C20H22O6/c1-11(12-3-4-14-8-15(23-2)6-5-13(14)7-12)20(22)26-17-10-25-18-16(h3-8,11,16-19,21H,9-10H2,1-2H3	-3.98
InChI=1S/C10H7F/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H	-3.453
InChI=1S/C13H9Cl2NO4/c1-19-13-7-9(3-4-11(13)16(17)18)20-12-5-2-8(14)6-10(12)15/h2-7H,1H3	-5.91
InChI=1S/C12H14O3/c1-10(2)12(13)15-9-8-14-11-6-4-3-5-7-11/h3-7H,1,8-9H2,2H3	-2.953
InChI=1S/C7H5ClN2O2/c8-3-1-5-6(2-4(3)9)12-7(11)10-5/h1-2H,9H2,(H,10,11)	-1.123
InChI=1S/C16H22INO2/c1-13-7-4-5-10-18(13)11-6-12-20-16(19)14-8-2-3-9-15(14)17/h2-3,8-9,13H,4-7,10-12H2,1H3	-5.254
InChI=1S/C13H16N4O6S2/c14-6-11(18)16-7-12(19)23-4-3-22-8-1-2-9-10(5-8)24-13(17-9)25(15,2h1-2,5H,3-4,6-7,14H2,(H,16,18)(H2,15,20,21)	-1.3

"InChi"	"logS(M)"
InChI=1S/C10H19N/c1-11(2)10-8-6-4-3-5-7-9-10/h3-4,10H,5-9H2,1-2H3/b4-3-	-1.6
InChI=1S/C18H36N2O6/c1-13(21)9-19(10-14(2)22)17(25)7-5-6-8-18(26)20(11-15(3)23)12-16(h13-16,21-24H,5-12H2,1-4H3	0.211
InChI=1S/C14H10Cl4/c1-8-11(15)6-5-9(14(8)18)7-10-12(16)3-2-4-13(10)17/h2-6H,7H2,1H3	-7.99
InChI=1S/C20H37N3O13/c1-23-7-2-5(21)9(26)15(10(7)27)33-19-17-16(11(28)8(4-25)32-19)35-h5-19,23-31H,2-4,21-22H2,1H3	0.278
InChI=1S/C14H16N2O4S/c1-19-12-9-14(13(20-2)8-11(12)15)21(17,18)16-10-6-4-3-5-7-10/h3-9,16H,15H2,1-2H3	-4.058
InChI=1S/C21H26N2O3/c1-4-11-23-12-10-17-16(14-23)6-5-7-18(17)22-21(24)15-8-9-19(25-2)h5-9,13H,4,10-12,14H2,1-3H3,(H,22,24)	-4.115
InChI=1S/C34H30Cl2N6O4/c1-19-9-5-7-11-27(19)37-33(45)31(21(3)43)41-39-29-15-13-23(17-25(h5-18,31-32H,1-4H3,(H,37,45)(H,38,46)/b41-39+,42-40+	-8.915
InChI=1S/C21H25N5O2/c1-15(2)25(14-23-20(27)17-9-8-12-22-13-17)19-16(3)24(4)26(21(19)2h5-13,15H,14H2,1-4H3,(H,23,27)	-2.562
InChI=1S/C8H14N2O4/c1-2-3-6(4-13-7(9)11)5-14-8(10)12/h3H,2,4-5H2,1H3,(H2,9,11)(H2,10,12)	-1.055
InChI=1S/C7H14N2O4S/c1-7(2,14(4,11)12)5-9-13-6(10)8-3/h5H,1-4H3,(H,8,10)/b9-5+	-1.347
InChI=1S/C9H9N3/c1-2-4-9(5-3-1)6-12-8-10-7-11-12/h1-5,7-8H,6H2	-1.148
InChI=1S/C18H21N3O9/c1-4-13(22)28-10-7-19-16(25)20(8-11-29-14(23)5-2)18(27)21(17(19)2h4-6H,1-3,7-12H2	-2.451
InChI=1S/C11H10O6/c1-6(12)16-9-5-3-4-8(11(14)15)10(9)17-7(2)13/h3-5H,1-2H3,(H,14,15)	-1.647
InChI=1S/C12H15N3O2S2/c1-12(2,3)10-13-14-11(18-10)15-19(16,17)9-7-5-4-6-8-9/h4-8H,1-3H3,(H,14,15)	-4.094
InChI=1S/C7H12O4/c1-4-10-7(9)5(2)11-6(3)8/h5H,4H2,1-3H3	-0.699
InChI=1S/C41H48N2O8/c1-42-12-10-23-16-32(44-3)34(46-5)20-27(23)29(42)15-26-19-33(45-4h16-22,29-30H,10-15H2,1-9H3	-7.727
InChI=1S/C12H15ClO2/c1-7(2)9-5-10(12(15)6-13)8(3)4-11(9)14/h4-5,7,14H,6H2,1-3H3	-2.58
InChI=1S/C18H24I3N3O8/c1-8(30)24(2-3-25)16-14(20)11(17(31)22-9(4-26)5-27)13(19)12(15(16h9-10,25-29H,2-7H2,1H3,(H,22,31)(H,23,32)	-4.135
InChI=1S/C28H23F3N6/c1-17-8-12-20(13-9-17)33-26-22(16-32)19(3)25(27(35-26)34-21-14-1h4-15H,1-3H3,(H2,33,34,35)/b37-36+	-7.717
InChI=1S/C16H30N4O5/c1-8(2)6-11(15(23)20-13(9(3)4)16(24)25)19-14(22)10(5)18-12(21)7-1h8-11,13H,6-7,17H2,1-5H3,(H,18,21)(H,19,22)(H,20,23)(H,24,25)	-2.13

"InChi"	"logS(M)"
InChI=1S/C6H10O7/c7-1-2(8)3(9)4(10)5(11)6(12)13/h2-4,7-10H,1H2,(H,12,13)	0.237
InChI=1S/C10H10Cl2FNO2/c11-9(12)10(16)14-8(15)5-6-1-3-7(13)4-2-6/h1-4,9-10,16H,5H2,(H,14,15)	-1.653
InChI=1S/C8H8O3/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)	-0.399
InChI=1S/C8H14/c1-2-4-6-8-7-5-3-1/h1-2H,3-8H2/b2-1-	-3.77
InChI=1S/C7H7IO/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2	-2.746
InChI=1S/C17H26N2O/c1-17(2,20)9-10-18-11-12-19-15(13-18)8-7-14-5-3-4-6-16(14)19/h3-6,15,20H,7-13H2,1-2H3	-2.753
InChI=1S/C29H37N3O6/c1-15-10-11-29(17(3)13-16(2)27(38-29)18(4)26(33)20-7-6-12-31-20)3h6-9,12,15-18,22,27,30-31H,10-11,13-14H2,1-5H3,(H,34,35)	-9.405
InChI=1S/C6H9N3O3/c1-8-5(2-3-10)4-7-6(8)9(11)12/h4,10H,2-3H2,1H3	-0.837
InChI=1S/C23H35NO5/c1-16(2)19-10-9-18(5)21(23(26)29-17(3)4)22(19)28-15-20(25)27-14-1h9-10,16-17H,6-8,11-15H2,1-5H3	-5.777
InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h8-9H,1,4-6H2,2-3H3	-4.292
InChI=1S/C15H30N2/c1-10-7-12(3-5-14(10)16)9-13-4-6-15(17)11(2)8-13/h10-15H,3-9,16-17H2,1-2H3	-1.821
InChI=1S/C10H14N4O4/c1-12-5-11-8-7(12)9(17)14(3-6(16)4-15)10(18)13(8)2/h5-6,15-16H,3-4H2,1-2H3	-1.12
InChI=1S/C15H12O3/c16-14(17)10-12-8-4-5-9-13(12)15(18)11-6-2-1-3-7-11/h1-9H,10H2,(H,16,17)	-2.764
InChI=1S/C33H34O3/c1-3-33(36-31(35)24-11-9-23(10-12-24)22-7-5-4-6-8-22)20-18-30-29-h1,4-12,21,27-30H,13-20H2,2H3	-8.11
InChI=1S/C21H30O2/c1-5-6-7-8-15-12-18(22)20-16-11-14(2)9-10-17(16)21(3,4)23-19(20)1h9,12-13,16-17,22H,5-8,10-11H2,1-4H3	-7.242
InChI=1S/C13H18O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-8H,9H2,1-4H3/b7-5+	-3.005
InChI=1S/C4H3F7O/c5-1-12-2(3(6,7)8)4(9,10)11/h2H,1H2	-1.613
InChI=1S/C22H29NO4/c1-17(18-5-6-20-16-21(25-2)8-7-19(20)15-18)22(24)27-12-4-3-9-23-1h5-8,15-17H,3-4,9-14H2,1-2H3	-3.7
InChI=1S/C5H4N2O4/c8-4(9)2-3(5(10)11)7-1-6-2/h1H,(H,6,7)(H,8,9)(H,10,11)	-2.494
InChI=1S/C18H24O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h10,13-16H,2-9H2,1H3	-3.157
InChI=1S/C7H7Cl/c1-6-3-2-4-7(8)5-6/h2-5H,1H3	-3.523
InChI=1S/C12H6Cl4/c13-8-6-9(14)12(16)10(11(8)15)7-4-2-1-3-5-7/h1-6H	-7.25

"InChi"	"logS(M)"
InChI=1S/C11H15NO3/c1-2-3-9-4-6-12(10(13)8-9)7-5-11(14)15/h4,6,8H,2-3,5,7H2,1H3,(H,14,15)	-2.11
InChI=1S/C4H7NO3/c5-2-1-8-3(2)4(6)7/h2-3H,1,5H2,(H,6,7)	0.931
InChI=1S/C28H40N2O3/c1-4-33-26-17-13-12-16-25(26)30-28(32)27(31)29-24-20-18-23(19-21h12-13,16-22H,4-11,14-15H2,1-3H3,(H,29,31)(H,30,32)	-6.099
InChI=1S/C14H19ClN4O/c15-11-2-1-3-12(8-11)19-6-4-18(5-7-19)10-13-9-17-14(16)20-13/h1-3,8,13H,4-7,9-10H2,(H2,16,17)	-2.913
InChI=1S/C15H14N2O4/c18-13(16-11-7-3-1-4-8-11)15(20,21)14(19)17-12-9-5-2-6-10-12/h1-10,20-21H,(H,16,18)(H,17,19)	-2.457
InChI=1S/C16H23NO3/c1-13-6-2-3-9-17(13)10-5-11-20-16(19)14-7-4-8-15(18)12-14/h4,7-8,12-13,18H,2-3,5-6,9-11H2,1H3	-3.02
InChI=1S/C12H3Cl7O/c13-5-1-4(2-6(14)9(5)16)20-8-3-7(15)10(17)12(19)11(8)18/h1-3H	-9.54
InChI=1S/C14H12N2O/c1-16-13-9-5-4-8-12(13)15-11-7-3-2-6-10(11)14(16)17/h2-9,15H,1H3	-3.963
InChI=1S/C10H22O2/c1-4-5-6-7-8-9-10(11-2)12-3/h10H,4-9H2,1-3H3	-2.918
InChI=1S/C10H14NO5PS/c1-3-15-17(14,18-4-2)16-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3	-3.942
InChI=1S/C12H14/c1-9(2)11-6-5-7-12(8-11)10(3)4/h5-8H,1,3H2,2,4H3	-4.451
InChI=1S/C12H9NO3/c14-12-7-6-10(8-11(12)13(15)16)9-4-2-1-3-5-9/h1-8,14H	-4.41
InChI=1S/C6H14OS2/c1-3-5-8-9(7)6-4-2/h3-6H2,1-2H3/p+1	-0.92
InChI=1S/C10H14N2O3/c1-3-5-6-10(4-2)7(13)11-9(15)12-8(10)14/h3,5H,4,6H2,1-2H3,(H2,11,12,13,14,15)/b5-3+	-1.906
InChI=1S/C10H8O4/c11-10(12)4-2-7-1-3-8-9(5-7)14-6-13-8/h1-5H,6H2,(H,11,12)/b4-2+	-3.852
InChI=1S/C10H14O4/c1-13-9-2-4-10(5-3-9)14-7-8(12)6-11/h2-5,8,11-12H,6-7H2,1H3	-1.45
InChI=1S/C18H18O4/c19-16(20)12-7-13-18(17(21)22,14-8-3-1-4-9-14)15-10-5-2-6-11-15/h1-6,8-11H,7,12-13H2,(H,19,20)(H,21,22)	-3.174
InChI=1S/C8H14OS/c1-2-4-8(5-3-1)9-6-7-10-8/h1-7H2	-2.898
InChI=1S/C3H6S2/c1-2-5-3-4-1/h1-3H2	-1.259
InChI=1S/C9H8N4O6S3/c10-21(16,17)9-12-11-8(20-9)13-22(18,19)6-4-2-1-3-5(6)7(14)15/h1-4H,(H,11,13)(H,14,15)(H2,10,16,17)	-2.32
InChI=1S/C6H10FN/c7-5-3-1-2-4-6-8/h1-5H2	-1.811
InChI=1S/C8H7ClO3/c9-6-3-5(4-8(11)12)1-2-7(6)10/h1-3,10H,4H2,(H,11,12)	-0.947
InChI=1S/C6H6N2O2/c7-4-2-1-3-8-5(4)6(9)10/h1-3H,7H2,(H,9,10)	-0.358
InChI=1S/C17H24Cl2N2O/c1-14-5-6-15(17(22)21-9-3-2-4-10-21)13-16(14)20(11-7-18)12-8-19/h5-6,13H,2-4,7-12H2,1H3	-5.38

"InChi"	"logS(M)"
InChI=1S/C11H11N3O3/c1-6(15)4-10(16)12-7-2-3-8-9(5-7)14-11(17)13-8/h2-3,5H,4H2,1H3,(H,12,16)(H2,13,14,17)	-2.523
InChI=1S/C5H3IN4/c6-4-3-5(9-1-7-3)10-2-8-4/h1-2H,(H,7,8,9,10)	-2.91
InChI=1S/C8H16O2/c1-4-8(9)10-6-5-7(2)3/h7H,4-6H2,1-3H3	-2.87
InChI=1S/C3H4O3/c1-2(4)3(5)6/h1H3,(H,5,6)	1.055
InChI=1S/C12H6Cl4O/c13-7-1-3-8(4-2-7)17-12-6-10(15)9(14)5-11(12)16/h1-6H	-7.04
InChI=1S/C9H5Cl4NO2/c10-4-2-1-3(5(11)6(4)12)9(8(14)15)7(13)16-9/h1-2,7H,(H2,14,15)	-4.091
InChI=1S/C15H22N2O2/c1-13-6-2-3-9-17(13)10-5-11-19-15(18)14-7-4-8-16-12-14/h4,7-8,12-13H,2-3,5-6,9-11H2,1H3	-2.333
InChI=1S/C28H52N2O4/c1-25(2)17-29-18-26(3,4)23(25)33-21(31)15-13-11-9-10-12-14-16-22(h23-24,29-30H,9-20H2,1-8H3	-4.408
InChI=1S/C14H20O5/c1-2-4-14-13(3-1)18-11-9-16-7-5-15-6-8-17-10-12-19-14/h1-4H,5-12H2	-1.934
InChI=1S/C9H10O5/c1-13-8-6(10)3-5(4-7(8)11)9(12)14-2/h3-4,10-11H,1-2H3	-1.6
InChI=1S/C7H16/c1-4-6-7(3)5-2/h7H,4-6H2,1-3H3	-4.306
InChI=1S/C17H21N/c1-15(13-16-9-5-3-6-10-16)18(2)14-17-11-7-4-8-12-17/h3-12,15H,13-14H2,1-2H3	-3.474
InChI=1S/C8H12N2O4/c9-4-1-5-10-6(8(13)14)2-3-7(11)12/h6,10H,1-3,5H2,(H,11,12)(H,13,14)	-1.302
InChI=1S/C11H13NO4/c13-10(14)7-12-9(11(15)16)6-8-4-2-1-3-5-8/h1-5,9,12H,6-7H2,(H,13,14)(H,15,16)	-2.16
InChI=1S/C12H2Cl8/c13-3-1-5(15)9(17)11(19)7(3)8-4(14)2-6(16)10(18)12(8)20/h1-2H	-9.1
InChI=1S/C5H8N2O2/c1-2-3-4(8)7-5(9)6-3/h3H,2H2,1H3,(H2,6,7,8,9)	-0.06
InChI=1S/C4H13N3/c5-1-3-7-4-2-6/h7H,1-6H2	0.986
InChI=1S/C10H16O/c1-3-4-9-5-8(2)6-10(11)7-9/h6,9H,3-5,7H2,1-2H3	-1.773
InChI=1S/C20H27O4P/c1-2-3-4-5-6-13-18-22-25(21,23-19-14-9-7-10-15-19)24-20-16-11-8-12-17-20/h7-12,14-17H,2-6,13,18H2,1H3	-6.413
InChI=1S/C5H10O2/c1-2-3-4-5(6)7/h2-4H2,1H3,(H,6,7)	-0.491
InChI=1S/C12H15BrO3/c1-2-3-9-6-10(13)4-5-12(9)16-8-11(15)7-14/h2,4-6,11,14-15H,1,3,7-8H2	-3.978
InChI=1S/C7H8O2/c1-5-6(8)3-2-4-7(5)9/h2-4,8-9H,1H3	0.193
InChI=1S/C10H8N2O2/c13-12(14)7-9-6-5-8-3-1-2-4-10(8)11-9/h1-6H,7H2	-2.054
InChI=1S/C16H25NO/c1-11-8-12-9-15(18)14-5-3-7-17-6-2-4-13(12)16(14,17)10-11/h11-14H,2-10H2,1H3	-2.393
InChI=1S/C13H14N2O/c16-12(11-6-2-1-3-7-11)10-15-13-8-4-5-9-14-13/h1-9,12,16H,10H2,(H,14,15)	-2.186

"InChi"	"logS(M)"
InChI=1S/C20H23N5O3S/c1-26-17-10-15-16(11-18(17)27-2)22-13-23-19(15)24-5-7-25(8-6-24)2h3-4,9-11,13H,5-8,12H2,1-2H3,(H,21,29)	-5.63
InChI=1S/C10H10N2O2/c1-6-9(13)12-8-5-3-2-4-7(8)10(14)11-6/h2-6H,1H3,(H,11,14)(H,12,13)	-2.38
InChI=1S/C7H4ClNO/c8-5-1-2-7-6(3-5)9-4-10-7/h1-4H	-2.34
InChI=1S/C15H10ClF3N2O3/c16-12-4-2-1-3-11(12)13(22)21-14(23)20-9-5-7-10(8-6-9)24-15(17,18h1-8H,(H2,20,21,22,23)	-7.157
InChI=1S/C13H17ClN2O2/c1-9-4-3-5-11(14)12(9)15-13(17)18-10-6-7-16(2)8-10/h3-5,10H,6-8H2,1-2H3,(H,15,17)	-3.124
InChI=1S/C3H6N6O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H2	-3.571
InChI=1S/C6H4BrNO2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H	-1.305
InChI=1S/C12H8O4S/c13-17(14,15)8-5-6-12-10(7-8)9-3-1-2-4-11(9)16-12/h1-7H,(H,13,14,15)/p-1	-0.466
InChI=1S/C10H14O/c1-2-3-9-11-10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3	-3.613
InChI=1S/C3H4O4/c4-2(5)1-3(6)7/h1H2,(H,4,5)(H,6,7)	0.865
InChI=1S/C3H9N3/c1-6(2)3(4)5/h1-2H3,(H3,4,5)	-1.731
InChI=1S/C15H12O3/c1-18-15(17)13-10-6-5-9-12(13)14(16)11-7-3-2-4-8-11/h2-10H,1H3	-3.478
InChI=1S/C8H9FN2O5/c1-2-15-8(14)16-4-11-6(12)5(9)3-10-7(11)13/h3H,2,4H2,1H3,(H,10,13)	-1.46
InChI=1S/C14H19NO4/c1-17-11-8-10(9-12(18-2)13(11)19-3)14(16)15-6-4-5-7-15/h8-9H,4-7H2,1-3H3	-2.083
InChI=1S/C7H8O/c1-8-7-5-3-2-4-6-7/h2-6H,1H3	-1.85
InChI=1S/C8H14BrNO3/c1-4(2)6(9)7(11)10-5(3)8(12)13/h4-6H,1-3H3,(H,10,11)(H,12,13)	-0.482
InChI=1S/C10H11NO3/c1-12-8-4-7(6-11)5-9(13-2)10(8)14-3/h4-5H,1-3H3	-1.773
InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3	1.136
InChI=1S/C13H20N2O2/c16-11-13(17)10-14-6-8-15(9-7-14)12-4-2-1-3-5-12/h1-5,13,16-17H,6-11H2	-0.082
InChI=1S/C7H5BrO3/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,9H,(H,10,11)	-2.65
InChI=1S/C17H37NO4S/c1-4-5-6-7-8-9-10-11-12-13-14-18(2,3)15-17(19)16-23(20,21)22/h17,19H,4-16H2,1-3H3	0.287
InChI=1S/CH5N3S/c2-1(5)4-3/h3H2,(H3,2,4,5)	-0.846
InChI=1S/C11H16O/c12-6-9-3-4-10-7-1-2-8(5-7)11(9)10/h6-11H,1-5H2	-2.42
InChI=1S/C15H10O4S/c1-20-9-3-5-13-11(7-9)14(16)10-6-8(15(17)18)2-4-12(10)19-13/h2-7H,1H3,(H,17,18)	-5.32

"InChi"	"logS(M)"
InChI=1S/C19H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-2/h3-18H2,1-2H3	-8.998
InChI=1S/C7H7O6P/c8-7(9)5-3-1-2-4-6(5)13-14(10,11)12/h1-4H,(H,8,9)(H2,10,11,12)	-0.987
InChI=1S/C12H14O4/c1-3-4-9-5-6-10(11(7-9)15-2)16-8-12(13)14/h3-7H,8H2,1-2H3,(H,13,14)/p-1/b4-3+	-1.583
InChI=1S/C13H11NS/c1-14-10-6-2-4-8-12(10)15-13-9-5-3-7-11(13)14/h2-9H,1H3	-5.593
InChI=1S/C4H12N2O/c5-1-3-7-4-2-6/h1-6H2	0.982
InChI=1S/C7H6O3/c8-4-5-3-6(9)1-2-7(5)10/h1-4,9-10H	-1
InChI=1S/C9H20O/c1-8(2)6-5-7-9(3,4)10/h8,10H,5-7H2,1-4H3	-2.287
InChI=1S/C10H23O2PS2/c1-6-9(4)14-13(11,12-8-3)15-10(5)7-2/h9-10H,6-8H2,1-5H3	-3.038
InChI=1S/C9H19NO/c1-9(2,11)8-10-6-4-3-5-7-10/h11H,3-8H2,1-2H3	-0.448
InChI=1S/C6H14N4O2/c7-9-5(11)3-1-2-4-6(12)10-8/h1-4,7-8H2,(H,9,11)(H,10,12)	-0.232
InChI=1S/C8H13Cl3O2/c1-3-6(4-2)7(12)13-5-8(9,10)11/h6H,3-5H2,1-2H3	-4.517
InChI=1S/C20H36N2O/c1-6-7-11-17-14-19(2,3)22(20(4,5)15-17)18(23)16-21-12-9-8-10-13-21h14H,6-13,15-16H2,1-5H3	-6.14
InChI=1S/C7H12O/c1-5-7(3,6-2)8-4/h1H,6H2,2-4H3	-1.42
InChI=1S/C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)	0.92
InChI=1S/C24H32N2O/c1-18(2)12-15-26(16-13-19(3)4)17-14-23(24(25)27)22-11-7-9-20-8-5-h5-13,23H,14-17H2,1-4H3,(H2,25,27)	-6.509
InChI=1S/C13H15BrN2/c1-16-6-2-3-13(16)11-8-15-12-5-4-9(14)7-10(11)12/h4-5,7-8,13,15H,2-3,6H2,1H3	-2.908
InChI=1S/C24H17ClN4O4/c1-14-6-2-5-9-19(14)26-24(31)18-12-15-7-3-4-8-17(15)22(23(18)30)2h2-13,27H,1H3,(H,26,31)/b28-22-	-7.563
InChI=1S/C15H11NOS/c1-10(17)12-7-8-14-13(9-12)16-15(18-14)11-5-3-2-4-6-11/h2-9H,1H3	-4.134
InChI=1S/C7H4Cl2O2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,(H,10,11)	-2.6
InChI=1S/C12H5Cl5O/c13-6-2-1-3-8(10(6)15)18-9-5-4-7(14)11(16)12(9)17/h1-5H	-7.38
InChI=1S/C5H11N3O2/c1-2-4(5(9)10)7-3-8-6/h3-4H,2,6H2,1H3,(H,7,8)(H,9,10)	-0.861
InChI=1S/C8H16O2/c1-3-5-7-10-8(9)6-4-2/h3-7H2,1-2H3	-2.361
InChI=1S/C8H16O2/c1-7(2)5(9)8(3,4)6(7)10/h5-6,9-10H,1-4H3	-0.374
InChI=1S/C16H12ClFN2O2/c1-20-13-7-6-9(17)8-11(13)14(19-15(21)16(20)22)10-4-2-3-5-12(10)1h2-8,15,21H,1H3	-3.053
InChI=1S/C19H27NO/c1-13(2)7-9-20-10-8-19(4)14(3)18(20)11-15-5-6-16(21)12-17(15)19/h5-7,12,14,18,21H,8-11H2,1-4H3	-3.975

"InChi"	"logS(M)"
InChI=1S/C14H18N2/c1-10-14(13-8-5-9-16(13)2)11-6-3-4-7-12(11)15-10/h3-4,6-7,13,15H,5,8-9H2,1-2H3	-2.144
InChI=1S/C14H14N2O/c1-16(2)13-7-3-11(4-8-13)15-12-5-9-14(17)10-6-12/h3-10H,1-2H3	-2.576
InChI=1S/C7H6Cl2O/c8-6-2-1-5(4-10)3-7(6)9/h1-3,10H,4H2	-2.044
InChI=1S/C40H26N2O4/c43-37-29-15-11-25-27-13-17-31-36-32(40(46)42(39(31)45)22-20-24-h1-18H,19-22H2	-8.476
InChI=1S/C14H15N3O/c1-9-3-8-13(10(2)16-9)17-14(18)11-4-6-12(15)7-5-11/h3-8H,15H2,1-2H3,(H,17,18)	-2.401
InChI=1S/C16H11N5O4/c1-18-13(22)9(6-17)11-7-4-2-3-5-8(7)12(19-11)10-14(23)20-16(25)21h2-5,19H,1H3,(H,18,22)(H2,20,21,23,24,25)/b11-9+	-7.528
InChI=1S/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h4-5H,3,6-7H2,1-2H3/b5-4+	-2.112
InChI=1S/C12H6Cl4O/c13-7-3-1-2-4-9(7)17-10-6-5-8(14)11(15)12(10)16/h1-6H	-6.74
InChI=1S/C10H10N2/c1-2-4-10(5-3-1)8-12-7-6-11-9-12/h1-7,9H,8H2	-2.26
InChI=1S/C4H12N6/c1-5-6-3-10-4-8-7-2-9(1)10/h5-8H,1-4H2	-0.013
InChI=1S/C7H5Cl2NS/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H2,10,11)	-2.336
InChI=1S/C8H6FNO/c9-6-3-1-2-5-4-7(11)10-8(5)6/h1-3H,4H2,(H,10,11)	-2.225
InChI=1S/C5HCl3O3/c6-1-2(7)4(8)11-3(1)5(9)10/h(H,9,10)	-2.219
InChI=1S/C9H12N4S/c1-2-3-4-14-9-7-8(11-5-10-7)12-6-13-9/h5-6H,2-4H2,1H3,(H,10,11,12,13)	-2.182
InChI=1S/C18H13BrN4O2/c19-12-2-1-3-13(7-12)22-18-14-6-11-4-5-23(9-17(24)25)16(11)8-15(1h1-8,10H,9H2,(H,24,25)(H,20,21,22)	-1.96
InChI=1S/C10H16ClN3O4/c11-5-6-14(13-18)10(17)12-8-3-1-7(2-4-8)9(15)16/h7-8H,1-6H2,(H,12,17)(H,15,16)	-2.532
InChI=1S/C22H20O13/c1-4-8-5(2-6(24)9(4)22(33)34)13(25)10-11(15(8)27)16(28)12(18(30)1h2,7,14,19-21,23-24,26,28-32H,3H2,1H3,(H,33,34)	-2.578
InChI=1S/C16H12INO3/c1-9(16(19)20)11-4-7-14-13(8-11)18-15(21-14)10-2-5-12(17)6-3-10/h2-9H,1H3,(H,19,20)	-5.515
InChI=1S/C15H21NO2/c1-3-14(18)15(7-9-16(2)10-8-15)12-5-4-6-13(17)11-12/h4-6,11,17H,3,7-10H2,1-2H3	-0.474
InChI=1S/C28H14N2O4/c31-25-13-5-1-3-7-15(13)27(33)21-17(25)9-11-19-23(21)29-20-12-10-h1-12,29-30H	-7.947
InChI=1S/C15H26O4/c16-14-10-8-6-4-2-1-3-5-7-9-11-15(17)19-13-12-18-14/h1-13H2	-4.262
InChI=1S/C19H21ClO6/c1-5-6-25-14-8-11(21)7-10(2)19(14)18(22)15-12(23-3)9-13(24-4)16(2h8-10H,5-7H2,1-4H3	-4.52

"InChi"	"logS(M)"
InChI=1S/C15H10F2N2S/c16-9-4-3-5-10(17)14(9)15-19-12-7-2-1-6-11(12)18-13(19)8-20-15/h1-7,15H,8H2	-3.76
InChI=1S/C7H5NOS/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H,8,10)	-2.179
InChI=1S/C11H24O3/c1-2-3-4-5-6-7-8-14-10-11(13)9-12/h11-13H,2-10H2,1H3	-1.921
InChI=1S/C17H44N3O15P5/c21-36(22,23)13-18(9-5-1-3-7-11-19(14-37(24,25)26)15-38(27,28)29)h1-17H2,(H2,21,22,23)(H2,24,25,26)(H2,27,28,29)(H2,30,31,32)(H2,33,34,35)	-0.088
InChI=1S/C3H2BrF3/c1-2(4)3(5,6)7/h1H2	-2.239
InChI=1S/C24H44O4/c1-5-9-11-19(7-3)17-27-23(25)21-13-15-22(16-14-21)24(26)28-18-20(h19-22H,5-18H2,1-4H3	-6.926
InChI=1S/C26H33NO6/c1-8-31-24(29)21-16(3)27-17(4)22(25(30)32-9-2)23(21)19-13-11-10-1h10-15,23,27H,8-9H2,1-7H3/b15-14+	-5.953
InChI=1S/C4H10N4O2/c5-7-3(9)1-2-4(10)8-6/h1-2,5-6H2,(H,7,9)(H,8,10)	0.835
InChI=1S/C18H18FN3O3/c19-14-4-12-15(5-16(14)21-7-9-3-11(21)6-20-9)22(10-1-2-10)8-13(17h4-5,8-11,20H,1-3,6-7H2,(H,24,25)	-3.65
InChI=1S/C6H16N2/c1-6(5-8)3-2-4-7/h6H,2-5,7-8H2,1H3	-1.327
InChI=1S/C7H14O7/c8-1-3(10)5(12)7(14)6(13)4(11)2-9/h1,3-7,9-14H,2H2	-0.323
InChI=1S/C13H19FN2O4/c1-2-3-4-5-6-7-11(17)20-9-16-12(18)10(14)8-15-13(16)19/h8H,2-7,9H2,1H3,(H,15,19)	-3.29
InChI=1S/C13H12N2O/c14-11-8-6-10(7-9-11)13(16)15-12-4-2-1-3-5-12/h1-9H,14H2,(H,15,16)	-2.27
InChI=1S/C4H7NO2/c1-3(6)2-4(5)7/h2H2,1H3,(H2,5,7)	0.995
InChI=1S/C3H4Cl2/c1-3(5)2-4/h1-2H2	-1.713
InChI=1S/C7H12N2O6/c10-8(11)14-6-4-2-1-3-5-7(6)15-9(12)13/h6-7H,1-5H2	-3.02
InChI=1S/C14H12N2/c1-9-6-7-11-13(8-9)16-12-5-3-2-4-10(12)14(11)15/h2-8H,1H3,(H2,15,16)	-4.349
InChI=1S/C8H7NO4/c1-5-2-3-6(8(10)11)4-7(5)9(12)13/h2-4H,1H3,(H,10,11)	-2.848
InChI=1S/C14H13Cl3N2/c15-14(16,17)13(9-1-5-11(18)6-2-9)10-3-7-12(19)8-4-10/h1-8,13H,18-19H2	-4.637
InChI=1S/C12H14N4O3S/c1-2-19-12-8-7-11(14-15-12)16-20(17,18)10-5-3-9(13)4-6-10/h3-8H,2,13H2,1H3,(H,14,16)	-2.427
InChI=1S/C7H13NO/c1-6-4-2-3-5-7(6)8-9/h6,9H,2-5H2,1H3/b8-7+	-1.266
InChI=1S/C13H24O4/c14-12(15)10-8-6-4-2-1-3-5-7-9-11-13(16)17/h1-11H2,(H,14,15)(H,16,17)	-3.79
InChI=1S/C6H3ClN4/c7-6-10-3-4-5(11-6)9-2-1-8-4/h1-3H	-0.71

"InChi"	"logS(M)"
InChI=1S/C12H4Cl6O/c13-6-1-2-9(12(18)11(6)17)19-5-3-7(14)10(16)8(15)4-5/h1-4H	-8.49
InChI=1S/C7H6INO/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H2,9,10)	-1.797
InChI=1S/C34H66O6/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-37-33(35)39-40-34(36)h3-32H2,1-2H3	-5.757
InChI=1S/C8H19O4P/c1-4-7-11-13(9,10-6-3)12-8-5-2/h4-8H2,1-3H3	-0.98
InChI=1S/C21H33NO2/c1-17(2)8-9-19-10-12-20(13-11-19)21(23)24-16-6-15-22-14-5-4-7-18(h10-13,17-18H,4-9,14-16H2,1-3H3	-5.933
InChI=1S/C12H20O2/c1-8(13)14-10-7-9-5-6-12(10,4)11(9,2)3/h9-10H,5-7H2,1-4H3	-3.089
InChI=1S/C21H33NO2/c1-2-3-4-8-14-20-15-9-10-16-22(20)17-11-18-24-21(23)19-12-6-5-7-1h5-7,12-13,20H,2-4,8-11,14-18H2,1H3	-5.948
InChI=1S/C16H21N3O8S/c1-7(20)27-5-8-6-28-14-11(13(22)19(14)12(8)16(25)26)18-10(21)4-2-h9,11,14H,2-6,17H2,1H3,(H,18,21)(H,23,24)(H,25,26)	-1.513
InChI=1S/C10H12O/c1-8(2)10(11)9-6-4-3-5-7-9/h3-8H,1-2H3	-2.357
InChI=1S/C15H17N3O3/c16-7-1-9-18(10-2-8-17)14(15(20)21)11-12-3-5-13(19)6-4-12/h3-6,14,19H,1-2,9-11H2,(H,20,21)	-1.68
InChI=1S/C14H14N2O2/c1-9-5-3-6-10(2)12(9)16-14(18)11-7-4-8-15-13(11)17/h3-8H,1-2H3,(H,15,17)(H,16,18)	-3.262
InChI=1S/C7H8/c1-3-5-7-6-4-2/h1-2H,5-7H2	-1.747
InChI=1S/C14H29NO2/c1-4-7-8-9-12-14(10-5-2,11-6-3)13(16)15-17/h17H,4-12H2,1-3H3,(H,15,16)	-2.82
InChI=1S/C22H29N7O5/c1-28(2)19-17-20(25-10-24-19)29(11-26-17)22-18(31)16(15(9-30)34-2h4-7,10-11,14-16,18,22,30-31H,8-9,23H2,1-3H3,(H,27,32)	-3.972
InChI=1S/C12H20ClN5S/c1-4-14-12-15-10(13)9(19-3)11(16-12)18-7-5-17(2)6-8-18/h4-8H2,1-3H3,(H,14,15,16)	-2.037
InChI=1S/C14H11N3/c15-14-11-6-2-1-5-10(11)9-13(17-14)12-7-3-4-8-16-12/h1-9H,(H2,15,17)	-3.155
InChI=1S/C12H15IN2O6/c1-2-10(17)20-5-8-7(16)3-9(21-8)15-4-6(13)11(18)14-12(15)19/h4,7-9,16H,2-3,5H2,1H3,(H,14,18,19)	-2.46
InChI=1S/C19H29NO3/c1-3-14-22-18-10-8-17(9-11-18)19(21)23-15-6-13-20-12-5-4-7-16(20)h8-11,16H,3-7,12-15H2,1-2H3	-4.671
InChI=1S/C10H18O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h5,8,11H,1,6-7H2,2-4H3	-1.8
InChI=1S/C13H15Cl2N3/c1-2-3-10(7-18-9-16-8-17-18)12-5-4-11(14)6-13(12)15/h4-6,8-10H,2-3,7H2,1H3	-3.59
InChI=1S/C7H12O4/c8-6(9)4-2-1-3-5-7(10)11/h1-5H2,(H,8,9)(H,10,11)	-0.506
InChI=1S/C9H12O3/c1-5-2-3-6-7(4-5)9(11)12-8(6)10/h5-7H,2-4H2,1H3	-1.302

"InChi"	"logS(M)"
InChI=1S/C21H41NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(24)22-19-20(2)23/h10-11,20,23H,3-9,12-19H2,1-2H3,(H,22,24)/b11-10+	-5.531
InChI=1S/C14H22N2O2/c1-4-16(5-2)10-11(3)18-14(17)12-6-8-13(15)9-7-12/h6-9,11H,4-5,10,15H2,1-3H3	-2.35
InChI=1S/C13H20O3/c1-3-4-11-7-10(2)5-6-13(11)16-9-12(15)8-14/h5-7,12,14-15H,3-4,8-9H2,1-2H3	-3.342
InChI=1S/C9H10N2O/c12-9-6-7-11(10-9)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,12)	-1.145
InChI=1S/C13H11ClN2O3/c1-2-10-12(13(18)19)11(17)7-15-16(10)9-5-3-8(14)4-6-9/h3-7H,2H2,1H3,(H,18,19)	0.4
InChI=1S/C10H13FN2O4/c1-10(2,3)8(15)17-5-13-4-6(11)7(14)12-9(13)16/h4H,5H2,1-3H3,(H,12,14,16)	-2.03
InChI=1S/C36H73NO/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-36(38)34-32-h3-35H2,1-2H3,(H,37,38)	-7.729
InChI=1S/C12H3Cl7/c13-4-1-5(9(16)7(14)2-4)6-3-8(15)11(18)12(19)10(6)17/h1-3H	-9.1
InChI=1S/C7H7FN2O4/c1-4(11)14-3-10-6(12)5(8)2-9-7(10)13/h2H,3H2,1H3,(H,9,13)	-1.2
InChI=1S/C11H12N2O2/c1-2-13-10(14)9(12-11(13)15)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H,12,15)	-1.587
InChI=1S/C4H2/c1-3-4-2/h1-2H	-0.724
InChI=1S/C16H36N2O/c1-16(2)10-6-4-3-5-7-14-19-15-9-13-18-12-8-11-17/h16,18H,3-15,17H2,1-2H3	-3.205
InChI=1S/C12H18O/c1-5-13-12-8-10(4)6-7-11(12)9(2)3/h6-9H,5H2,1-4H3	-4.403
InChI=1S/C11H16N2O3/c1-3-5-7-11(6-4-2)8(14)12-10(16)13-9(11)15/h4H,2-3,5-7H2,1H3,(H2,12,13,14,15,16)	-2.17
InChI=1S/C8H11N7S/c9-7(10)14-12-5-1-3-6(4-2-5)13-15-8(11)16/h1-4,12H,(H2,11,16)(H4,9,10,14)/b15-13+	-1.982
InChI=1S/C9H9NO2/c11-9(10-12)7-6-8-4-2-1-3-5-8/h1-7,12H,(H,10,11)/b7-6+	-0.987
InChI=1S/C10H12N4O/c1-3-6-7(4-2)13-9-8(12-6)5-11-10(15)14-9/h5H,3-4H2,1-2H3,(H,11,13,14,15)	-2.264
InChI=1S/C11H22O2/c1-9(2)7-8-11(3,4)10(12-5)13-6/h7,10H,8H2,1-6H3	-3.34
InChI=1S/C12H15NO2/c1-2-15-12(14)13-9-5-7-10-6-3-4-8-11(10)13/h3-4,6,8H,2,5,7,9H2,1H3	-4.04
InChI=1S/C10H13NO4S2/c1-7-5-8-3-2-4-16(12,13)10(8)6-9(7)17(11,14)15/h5-6H,2-4H2,1H3,(H2,11,14,15)	-4.195
InChI=1S/C4H10O2/c1-4(5)3-6-2/h4-5H,3H2,1-2H3	1.045
InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3	0.397

"InChi"	"logS(M)"
InChI=1S/C15H19NO4/c1-3-12(17-9-15-10-20-15)4-2-11(1)16(5-13-7-18-13)6-14-8-19-14/h1-4,13-15H,5-10H2	-1.919
InChI=1S/C16H18N2O4S/c1-16(2)12(15(21)22)18-13(20)11(14(18)23-16)17-10(19)8-9-6-4-3-5-h3-7,11-12,14H,8H2,1-2H3,(H,17,19)(H,21,22)	-1.63
InChI=1S/C9H13N3S/c1-12(2)11-10-8-5-4-6-9(7-8)13-3/h4-7H,1-3H3/b11-10+	-3.171
InChI=1S/C13H18O2/c1-3-4-7-10-15-13-9-6-5-8-12(13)11(2)14/h5-6,8-9H,3-4,7,10H2,1-2H3	-3.881
InChI=1S/C11H7NS/c13-8-12-11-6-5-9-3-1-2-4-10(9)7-11/h1-7H	-4.44
InChI=1S/C12H14O4S/c1-9-3-5-10(6-4-9)17(14,15)12(7-8-12)11(13)16-2/h3-6H,7-8H2,1-2H3	-2.88
InChI=1S/C20H21N/c1-21(2)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(17)20/h3-6,8-14H,7,15H2,1-2H3	-5.401
InChI=1S/C14H12N2O2/c17-15-13(11-7-3-1-4-8-11)14(16-18)12-9-5-2-6-10-12/h1-10,17-18H/b15-13-,16-14+	-5.9
InChI=1S/C8H15NOS2/c9-8(10)4-2-1-3-7-5-6-11-12-7/h7H,1-6H2,(H2,9,10)	-2.534
InChI=1S/C18H25NO6/c1-3-12-8-11(2)18(23,10-20)17(22)24-9-13-4-6-19-7-5-14(15(13)19)2h3-4,11,14-15,20,23H,5-10H2,1-2H3/b12-3+	-1.057
InChI=1S/C12H5Cl5/c13-7-4-2-1-3-6(7)10-11(16)8(14)5-9(15)12(10)17/h1-5H	-7.4
InChI=1S/C4H8Cl3N/c5-1-3-8(7)4-2-6/h1-4H2	-1.92
InChI=1S/C11H12O4S/c1-15-10(12)11(7-8-11)16(13,14)9-5-3-2-4-6-9/h2-6H,7-8H2,1H3	-2.26
InChI=1S/C13H11NO2/c15-13(12-7-4-8-14-9-12)16-10-11-5-2-1-3-6-11/h1-9H,10H2	-2.806
InChI=1S/C7H7N3O2S/c8-7(13)9-5-2-1-3-6(4-5)10(11)12/h1-4H,(H3,8,9,13)	-1.45
InChI=1S/C17H16ClN5O2/c1-2-22(11-3-10-19)14-6-4-13(5-7-14)20-21-17-9-8-15(23(24)25)12-1h4-9,12H,2-3,11H2,1H3/b21-20+	-4.253
InChI=1S/C11H15ClN2O2/c1-6(2)5-16-11(15)7-3-8(13)10(12)9(14)4-7/h3-4,6H,5,13-14H2,1-2H3	-2.738
InChI=1S/C5H11NO2/c1-2-3-4-5-6(7)8/h2-5H2,1H3	-1.955
InChI=1S/C22H28N2O4/c1-5-10-24-11-9-17-15(14-24)7-6-8-18(17)23-22(25)16-12-19(26-2)21h6-8,12-13H,5,9-11,14H2,1-4H3,(H,23,25)	-4.219
InChI=1S/C10H13NO3/c1-2-14-9-5-3-8(4-6-9)11-10(13)7-12/h3-6,12H,2,7H2,1H3,(H,11,13)	-2.106
InChI=1S/C14H12N2O4/c1-20-13-8-7-10(9-12(13)16(18)19)14(17)15-11-5-3-2-4-6-11/h2-9H,1H3,(H,15,17)	-4.988
InChI=1S/C12H14ClNO3/c1-2-7-17-11-5-3-9(8-10(11)13)4-6-12(15)14-16/h3-6,8,16H,2,7H2,1H3,(H,14,15)/b6-4+	-3.575

"InChi"	"logS(M)"
InChI=1S/C22H12N2O4/c25-21-15-5-1-3-7-17(15)23-19(27-21)13-9-11-14(12-10-13)20-24-18-h1-12H	-6.517
InChI=1S/C18H17NO3/c1-2-15(18(21)22)12-7-9-14(10-8-12)19-11-13-5-3-4-6-16(13)17(19)2h3-10,15H,2,11H2,1H3,(H,21,22)	-4.39
InChI=1S/C10H10Cl2O2/c1-2-10(13)14-6-7-3-4-8(11)5-9(7)12/h3-5H,2,6H2,1H3	-3.067
InChI=1S/C5H7N3O4/c6-3(5(10)11)2-12-4(9)1-8-7/h1,3H,2,6H2,(H-,9,10,11)/b4-1-	-0.826
InChI=1S/C5H7NOS2/c1-2-6-4(7)3-9-5(6)8/h2-3H2,1H3	-0.121
InChI=1S/C10H15NO/c1-2-11(8-9-12)10-6-4-3-5-7-10/h3-7,12H,2,8-9H2,1H3	-1.917
InChI=1S/C11H22N2S/c1-3-5-7-12-9-10-13(11(12)14)8-6-4-2/h3-10H2,1-2H3	-2.214
InChI=1S/C10H10O3/c1-7(11)9-3-5-10(6-4-9)13-8(2)12/h3-6H,1-2H3	-1.52
InChI=1S/C7H8O3/c1-4-5(7(9)10)2-3-6(4)8/h5H,1-3H2,(H,9,10)	0.408
InChI=1S/C12H17NO3/c1-4-13(5-2)12(15)9-6-7-10(14)11(8-9)16-3/h6-8,14H,4-5H2,1-3H3	-1.665
InChI=1S/C10H9NO/c1-7(12)9-6-11-10-5-3-2-4-8(9)10/h2-6,11H,1H3	-3.324
InChI=1S/C5H4N4/c1-4-5(8-2-6-1)9-3-7-4/h1-3H,(H,6,7,8,9)	0.619
InChI=1S/C20H22O5/c21-19(17-9-3-1-4-10-17)24-15-7-13-23-14-8-16-25-20(22)18-11-5-2-h1-6,9-12H,7-8,13-16H2	-4.596
InChI=1S/C13H27NO2/c1-3-4-5-6-7-8-9-10-11-14-13(16)12(2)15/h12,15H,3-11H2,1-2H3,(H,14,16)	-3.361
InChI=1S/C16H20ClN5O2/c1-2-20(12-8-4-3-5-9-12)15(23)22-16(24)21(18-19-22)14-11-7-6-10-1h6-7,10-12H,2-5,8-9H2,1H3	-5.182
InChI=1S/C12H18/c1-9(2)11-5-7-12(8-6-11)10(3)4/h5-10H,1-4H3	-6.603
InChI=1S/C11H18N2O2S/c1-4-11(6-5-7(2)3)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(H2,12,13,14,15,16)	-3.513
InChI=1S/C5H9NO4/c1-10-5(7)3-2-4-6(8)9/h2-4H2,1H3	-1.081
InChI=1S/C12H12N2O2S/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(12)16/h3-7H,2H2,1H3,(H2,13,14,15,16,17)	-3.58
InChI=1S/C11H12O4/c1-15-9-4-2-8(3-5-9)10(12)6-7-11(13)14/h2-5H,6-7H2,1H3,(H,13,14)	-1.063
InChI=1S/C13H8Cl4O2/c14-8-2-6(12(18)10(16)4-8)1-7-3-9(15)5-11(17)13(7)19/h2-5,18-19H,1H2	-5.895
InChI=1S/C9H20N2O4S/c1-3-5-6-8(4-2)7-15-9(12)11-16(10,13)14/h8H,3-7H2,1-2H3,(H,11,12)(H2,10,13,14)	-2.402
InChI=1S/C13H12ClN3O/c14-11-5-4-9-7-17(13(15)16-18)6-8-2-1-3-10(11)12(8)9/h1-5,18H,6-7H2,(H2,15,16)	-2

"InChi"	"logS(M)"
InChI=1S/C16H20O2/c1-15(2,17)11-16(3,18)14-10-6-8-12-7-4-5-9-13(12)14/h4-10,17-18H,11H2,1-3H3	-3.242
InChI=1S/C8H8BrNO2/c1-4-2-5(9)3-6(7(4)11)8(10)12/h2-3,11H,1H3,(H2,10,12)	-2.656
InChI=1S/C3H2F4/c1-2(4)3(5,6)7/h1H2	-2.76
InChI=1S/C7H8ClN/c1-5-2-3-6(9)4-7(5)8/h2-4H,9H2,1H3	-1.753
InChI=1S/C12H16O4S2/c1-7(2)15-10(13)9(11(14)16-8(3)4)12-17-5-6-18-12/h5-8H,1-4H3	-4.506
InChI=1S/C8H5ClFN/c9-7-2-1-6(3-4-11)8(10)5-7/h1-2,5H,3H2	-2.594
InChI=1S/C12H24N2O6/c15-7-9-19-11(17)13-5-3-1-2-4-6-14-12(18)20-10-8-16/h15-16H,1-10H2,(H,13,17)(H,14,18)	-0.92
InChI=1S/C5H9NO2/c1-2-8-5(7)6-3-4-6/h2-4H2,1H3	-0.677
InChI=1S/C10H11ClO3/c1-2-5-14-10(13)7-3-4-9(12)8(11)6-7/h3-4,6,12H,2,5H2,1H3	-3.38
InChI=1S/C28H37ClO7/c1-6-23(33)35-15-22(32)28(36-24(34)7-2)16(3)12-20-19-9-8-17-13-18h10-11,13,16,19-21,31H,6-9,12,14-15H2,1-5H3	-5.88
InChI=1S/C12H22O6/c1(13-3-5-15-7-11-9-17-11)2-14-4-6-16-8-12-10-18-12/h11-12H,1-10H2	0.581
InChI=1S/C9H9NO6/c1-15-7-3-5(9(11)12)6(10(13)14)4-8(7)16-2/h3-4H,1-2H3,(H,11,12)/p-1	-0.754
InChI=1S/C10H14NO6P/c1-7-5-9(17-18(14,15-3)16-4)6-8(2)10(7)11(12)13/h5-6H,1-4H3	-3.792
InChI=1S/C18H27NO3/c1-19(2)12-13-21-14-15-22-17(20)18(10-6-7-11-18)16-8-4-3-5-9-16/h3-5,8-9H,6-7,10-15H2,1-2H3	-3.19
InChI=1S/C9H14ClN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h2,4,8H,1,3,5-7H2,(H,11,14)	-2.983
InChI=1S/C10H9NO3S/c11-10-3-1-2-7-4-5-8(6-9(7)10)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-1.682
InChI=1S/C16H26O4/c1-3-15(17)19-13-11-9-7-5-6-8-10-12-14-20-16(18)4-2/h3-4H,1-2,5-14H2	-4.961
InChI=1S/C8H14N2OS/c1-5(2)4-6-7(11)10(3)8(12)9-6/h5-6H,4H2,1-3H3,(H,9,12)	-1.926
InChI=1S/C5H9NO4S/c6-3(5(9)10)1-11-2-4(7)8/h3H,1-2,6H2,(H,7,8)(H,9,10)	0.747
InChI=1S/C8H17N/c1-2-4-8-5-3-6-9-7-8/h8-9H,2-7H2,1H3	-1.011
InChI=1S/C2H4O3/c3-1-2(4)5/h3H,1H2,(H,4,5)	0.596
InChI=1S/C7H6ClNO/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H2,9,10)	-1.626
InChI=1S/C12H19NO/c1-3-13(4-2)10-11-14-12-8-6-5-7-9-12/h5-9H,3-4,10-11H2,1-2H3	-1.954
InChI=1S/C16H14O4/c1-20-13-8-6-11(7-9-13)15(17)10-12-4-2-3-5-14(12)16(18)19/h2-9H,10H2,1H3,(H,18,19)	-3.735
InChI=1S/C19H30N2O3/c1-5-19(18(23)24-8-4,16-12-10-9-11-13-16)17(22)20-14-15-21(6-2)7-9-13H,5-8,14-15H2,1-4H3,(H,20,22)	-3.854

"InChi"	"logS(M)"
InChI=1S/C10H13NO3/c1-3-14-8-4-5-9(10(13)6-8)11-7(2)12/h4-6,13H,3H2,1-2H3,(H,11,12)	-1.643
InChI=1S/C32H48O5/c1-19(33)37-24-10-11-30(6)23(27(24,2)3)9-12-32(8)25(30)22(34)17-21-23-25H,9-16,18H2,1-8H3,(H,35,36)	-10.596
InChI=1S/C15H21ClN2O2/c1-10(2)18-8-7-12(9-18)20-15(19)17-14-11(3)5-4-6-13(14)16/h4-6,10,12H,7-9H2,1-3H3,(H,17,19)	-4.105
InChI=1S/C16H17N3O3/c1-19(11-12-3-9-15(22-2)10-4-12)18-17-14-7-5-13(6-8-14)16(20)21/h3-10H,11H2,1-2H3,(H,20,21)/b18-17+	-5.166
InChI=1S/C16H26N2O2/c1-11(9-13(3)19)17-15-7-5-6-8-16(15)18-12(2)10-14(4)20/h9-10,15-18H,5-8H2,1-4H3/b11-9+,12-10+	-2.11
InChI=1S/C18H21NO5/c1-12(18(21)24-8-7-23-17(20)11-19)13-3-4-15-10-16(22-2)6-5-14(15)h3-6,9-10,12H,7-8,11,19H2,1-2H3	-1.98
InChI=1S/C6H13NO2/c1-6(8)9-5-4-7(2)3/h4-5H2,1-3H3	0.789
InChI=1S/C6H10O2/c1-2-3-7-4-6-5-8-6/h2,6H,1,3-5H2	0.05
InChI=1S/C10H20O/c1-7(2)10-8(3)5-4-6-9(10)11/h7-11H,4-6H2,1-3H3	-0.29
InChI=1S/C7H8ClNO/c1-4-2-3-5(9)6(8)7(4)10/h2-3,10H,9H2,1H3	-1.482
InChI=1S/C9H16O3/c10-8-6-4-2-1-3-5-7-9(11)12/h8H,1-7H2,(H,11,12)	-0.957
InChI=1S/C15H26O/c16-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-15/h7,9H,1-6,8,10-14H2/b9-7-	-4.883
InChI=1S/C15H23NO3/c1-9(2)11-7-12(10(3)4)14(18)13(8-11)15(19)16-5-6-17/h7-10,17-18H,5-6H2,1-4H3,(H,16,19)	-3.493
InChI=1S/C9H9N3S/c1-12-8(10-11-9(12)13)7-5-3-2-4-6-7/h2-6H,1H3,(H,11,13)	-2.511
InChI=1S/C11H15NO3/c1-8-5-3-4-6-10(8)14-7-9(2)15-11(12)13/h3-6,9H,7H2,1-2H3,(H2,12,13)	-2.595
InChI=1S/C15H12BrClF4N2O2/c1-6(2)25-14(24)7-4-8(10(18)5-9(7)17)12-11(16)13(15(19,20)21)23(3h4-6H,1-3H3	-6.923
InChI=1S/C7H6N2O5/c1-4-2-5(8(11)12)3-6(7(4)10)9(13)14/h2-3,10H,1H3	-3
InChI=1S/C14H12O4/c1-18-9-6-7-11(13(16)8-9)14(17)10-4-2-3-5-12(10)15/h2-8,15-16H,1H3	-7.274
InChI=1S/C8H12/c1-2-4-6-8-7-5-3-1/h1-2,7-8H,3-6H2/b2-1-,8-7-	-2.966
InChI=1S/C11H14O2/c1-11(2,8-10(12)13)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H,12,13)	-2.569
InChI=1S/C9H21NO2/c1-4-5-9(7-11,8-12)6-10(2)3/h11-12H,4-8H2,1-3H3	0.229
InChI=1S/C10H9Cl3/c1-8(7-10(11,12)13)9-5-3-2-4-6-9/h2-6H,1,7H2	-4.282
InChI=1S/C6H3Cl2NO2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H	-3.364
InChI=1S/C16H13ClN2O4S/c17-13-8-11(24(22,23)9-12(16(19)21)10-4-2-1h1-8,12H,9H2,(H2,18,22,23)	-2.777

"InChi"	"logS(M)"
InChI=1S/C16H12ClNO3/c1-9(16(19)20)10-6-7-14-13(8-10)18-15(21-14)11-4-2-3-5-12(11)17/h2-9H,1H3,(H,19,20)	-4.404
InChI=1S/C8H6ClNO2/c1-11-8-10-6-4-5(9)2-3-7(6)12-8/h2-4H,1H3	-3.016
InChI=1S/C6H4ClF/c7-5-2-1-3-6(8)4-5/h1-4H	-2.346
InChI=1S/C15H19N3O3/c1-5-9-6-10(13(19)20)11(16-7-9)12-17-14(21)15(4,18-12)8(2)3/h6-8H,5H2,1-4H3,(H,19,20)(H,17,18,21)	-2.315
InChI=1S/C13H10O6/c14-7-4-10(17)12(11(18)5-7)13(19)6-1-2-8(15)9(16)3-6/h1-5,14-18H	-1.72
InChI=1S/C8H14O4S2/c1-13-5(7(9)10)3-4-6(14-2)8(11)12/h5-6H,3-4H2,1-2H3,(H,9,10)(H,11,12)	-2.89
InChI=1S/C9H8O5/c1-14-7-4-5(8(10)11)2-3-6(7)9(12)13/h2-4H,1H3,(H,10,11)(H,12,13)	-1.992
InChI=1S/C8H20O5P2S2/c1-5-9-14(16,10-6-2)13-15(17,11-7-3)12-8-4/h5-8H2,1-4H3	-4.031
InChI=1S/C10H8O4/c11-9(7-3-1-5-13-7)10(12)8-4-2-6-14-8/h1-6,9,11H	-0.554
InChI=1S/C9H12ClN3O2/c10-7-6(5-13-3-1-2-4-13)11-9(15)12-8(7)14/h1-5H2,(H2,11,12,14,15)	-1.54
InChI=1S/C14H12O3S/c1-9(14(16)17)11-7-8-12(18-11)13(15)10-5-3-2-4-6-10/h2-9H,1H3,(H,16,17)	-2.835
InChI=1S/C16H9NO2/c18-17(19)15-9-8-13-11-5-2-1-4-10(11)12-6-3-7-14(15)16(12)13/h1-9H	-7.103
InChI=1S/C17H23ClN2O4S2/c1-13-12-16(20-17-14(13)6-5-7-15(17)18)24-10-4-2-3-8-19-9-11-25-2h5-7,12,19H,2-4,8-11H2,1H3,(H,21,22,23)	-4.24
InChI=1S/C6H9NO6/c8-4(9)1-7(2-5(10)11)3-6(12)13/h1-3H2,(H,8,9)(H,10,11)(H,12,13)	-0.51
InChI=1S/C8H5NO6/c10-6(11)3-1-2-9-5(8(14)15)4(3)7(12)13/h1-2H,(H,10,11)(H,12,13)(H,14,15)	-1.245
InChI=1S/C48H69N3O6/c1-43(2,3)31-19-28(20-32(37(31)52)44(4,5)6)25-49-40(55)50(26-29-2h19-24,52-54H,25-27H2,1-18H3	-7.292
InChI=1S/C12H16O/c1-10(2)12-7-5-11(6-8-12)4-3-9-13/h5-10H,3-4H2,1-2H3	-3.303
InChI=1S/C13H11N3O2S/c14-9-10-1-5-12(6-2-10)16-19(17,18)13-7-3-11(15)4-8-13/h1-8,16H,15H2	-3.6
InChI=1S/C12H22O/c1-10(13)9-12(2,3)11-7-5-4-6-8-11/h11H,4-9H2,1-3H3	-3.548
InChI=1S/C31H15NO3/c33-29-19-6-2-1-5-15(19)16-13-14-24-26-17(9-11-22(29)25(16)26)18·h1-14,32H	-5.507
InChI=1S/C10H10N2O4/c1-6-4-8(13)12(3-2-9(14)15)10(16)7(6)5-11/h4,13H,2-3H2,1H3,(H,14,15)	-1.444
InChI=1S/C2H3N3S/c6-2-3-1-4-5-2/h1H,(H2,3,4,5,6)	0.119

"InChi"	"logS(M)"
InChI=1S/C18H26O6/c1-8-18(9-22-15(19)12(2)3,10-23-16(20)13(4)5)11-24-17(21)14(6)7/h2,4,6,8-11H2,1,3,5,7H3	-4.226
InChI=1S/C2H2Br2O2/c3-1(4)2(5)6/h1H,(H,5,6)	0.986
InChI=1S/C12H6Cl4O/c13-7-1-2-12(11(16)6-7)17-10-4-8(14)3-9(15)5-10/h1-6H	-7.14
InChI=1S/C7H6Cl2N2O/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2H,10H2,(H2,11,12)	-2.081
InChI=1S/C8H20NO3PS/c1-5-11-13(10,12-6-2)14-8-7-9(3)4/h5-8H2,1-4H3	-0.568
InChI=1S/C12H15NO4/c1-8(17-2)10(12(15)16)13-11(14)9-6-4-3-5-7-9/h3-8,10H,1-2H3,(H,13,14)(H,15,16)	-1.74
InChI=1S/C17H22N2O/c1-17(16(18)20,11-12-19(2)3)15-10-6-8-13-7-4-5-9-14(13)15/h4-10H,11-12H2,1-3H3,(H2,18,20)	-3.129
InChI=1S/C21H20N6O7/c1-13(28)23-19-9-15(26(11-20(29)33-2)12-21(30)34-3)4-7-18(19)25-2h4-9H,11-12H2,1-3H3,(H,23,28)/b25-24+	-5.194
InChI=1S/C13H16N4O2/c1-18-10-4-8(5-11(6-10)19-2)3-9-7-16-13(15)17-12(9)14/h4-7H,3H2,1-2H3,(H4,14,15,16,17)	-2.44
InChI=1S/C6H12O2/c1-5(7)8-6(2,3)4/h1-4H3	-1.144
InChI=1S/C15H19F13N2O4S/c1-30(2,8-9(31)32)6-3-5-29-35(33,34)7-4-10(16,17)11(18,19)12(20,21h29H,3-8H2,1-2H3	-4.057
InChI=1S/C7H8O3S/c1-10-11(8,9)7-5-3-2-4-6-7/h2-6H,1H3	-1.742
InChI=1S/C10H8N2O/c11-7-9(10(12)13)6-8-4-2-1-3-5-8/h1-6H,(H2,12,13)/b9-6-	-2.055
InChI=1S/C20H26N2/c1-22(2)16-8-14-20(18-10-4-3-5-11-18)19-12-7-6-9-17(19)13-15-21-2h3-7,9-12,21H,8,13-16H2,1-2H3	-3.39
InChI=1S/C15H14Cl2N2O3/c1-5-6-21-12-8-11(9(16)7-10(12)17)19-14(20)22-13(18-19)15(2,3)4/h1,7-8H,6H2,2-4H3	-5.965
InChI=1S/C7H12N2/c1-6(2)5-7-8-3-4-9-7/h3-4,6H,5H2,1-2H3,(H,8,9)	-1.049
InChI=1S/C23H26Cl2O6/c1-22(2,30-18-10-6-16(24)7-11-18)20(26)28-14-5-15-29-21(27)23(3,4h6-13H,5,14-15H2,1-4H3	-7.183
InChI=1S/C18H27NO3/c1-3-21-17-10-8-16(9-11-17)18(20)22-14-6-13-19-12-5-4-7-15(19)2/h8-11,15H,3-7,12-14H2,1-2H3	-4.148
InChI=1S/C6H8N2/c7-5-2-1-3-6(8)4-5/h1-4H,7-8H2	0.51
InChI=1S/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3	0.43
InChI=1S/C20H35NOS/c1-5-6-7-8-9-10-15-21-17(4)20(22)18-11-13-19(14-12-18)23-16(2)3/h11-14,16-17,20-22H,5-10,15H2,1-4H3	-5.46
InChI=1S/C9H11NO3/c1-10-5-9(13)6-2-3-7(11)8(12)4-6/h2-4,10-12H,5H2,1H3	-0.464
InChI=1S/C7H8N2O2/c1-5-4-6(9(10)11)2-3-7(5)8/h2-4H,8H2,1H3	-3.036

"InChi"	"logS(M)"
InChI=1S/C9H16O4/c1-6(8(12)13)9(2,3)5-4-7(10)11/h6H,4-5H2,1-3H3,(H,10,11)(H,12,13)	-1.526
InChI=1S/C12H16N4O4/c1-4-5-6-20-12(19)16-7-13-9-8(16)10(17)15(3)11(18)14(9)2/h7H,4-6H2,1-3H3	-1.93
InChI=1S/C25H35N5O4S/c1-5-8-10-19(7-3)17-27-35(33,34)21-13-11-20(12-14-21)28-29-23-18(h11-14,19,27,32H,5-10,15,17H2,1-4H3/b29-28+	-8.797
InChI=1S/C6H4Br3NO3S/c7-2-1-3(8)6(14(11,12)13)4(9)5(2)10/h1H,10H2,(H,11,12,13)	-0.489
InChI=1S/C16H30O4/c1-13(2,3)17-19-15(7,8)11-12-16(9,10)20-18-14(4,5)6/h1-10H3	-5.115
InChI=1S/C21H28N7O17P3/c22-17-12-19(25-7-24-17)28(8-26-12)21-16(44-46(33,34)35)14(30)11h1-4,7-8,10-11,13-16,20-21,29-31H,5-6H2,(H7-,22,23,24,25,32,33,34,35,36,37,38,39)	-2.743
InChI=1S/C7H9NO/c1-5-4-6(9)2-3-7(5)8/h2-4,9H,8H2,1H3	-1.789
InChI=1S/C11H13ClF3N3O4S3/c1-18-10(4-23-5-11(13,14)15)17-7-2-6(12)8(24(16,19)20)3-9(7)25(18,h2-3,10,17H,4-5H2,1H3,(H2,16,19,20)	-5.08
InChI=1S/C18H22O3/c1-4-5-10-21-18(19)13(2)14-6-7-16-12-17(20-3)9-8-15(16)11-14/h6-9,11-13H,4-5,10H2,1-3H3	-7.53
InChI=1S/C9H11ClO3/c10-8-3-1-2-4-9(8)13-6-7(12)5-11/h1-4,7,11-12H,5-6H2	-1.815
InChI=1S/C4H10N4O2/c1-2(7-3(5)9)8-4(6)10/h2H,1H3,(H3,5,7,9)(H3,6,8,10)	-0.592
InChI=1S/C7H16NO2/c1-7(9)10-6-5-8(2,3)4/h5-6H2,1-4H3/q+1	0.835
InChI=1S/C4H10O3/c5-1-3-7-4-2-6/h5-6H,1-4H2	0.974
InChI=1S/C16H11ClN2O/c1-10(9-18)12-4-7-15-14(8-12)19-16(20-15)11-2-5-13(17)6-3-11/h2-8,10H,1H3	-5.04
InChI=1S/C17H16N2O/c1-19(2)17-18-15(13-9-5-3-6-10-13)16(20-17)14-11-7-4-8-12-14/h3-12H,1-2H3	-5.004
InChI=1S/C17H15NO2S/c1-2-20-16(19)11-12-8-9-15-14(10-12)18-17(21-15)13-6-4-3-5-7-13/h3-10H,2,11H2,1H3	-5.223
InChI=1S/C6H7NO/c1-6-3-2-4-7(8)5-6/h2-5H,1H3	0.962
InChI=1S/C13H9N3O5/c17-12-6-5-8(7-9(12)13(18)19)14-15-10-3-1-2-4-11(10)16(20)21/h1-7,15H,(H,18,19)/b14-8-	-2.01
InChI=1S/C5H4N2O/c1-4-5(2-6)8-3-7-4/h3H,1H3	-0.325
InChI=1S/C22H42N4O2/c1-3-5-13-25(21(27)23-15-9-7-10-16-23)19-20-26(14-6-4-2)22(28)24-h3-20H2,1-2H3	-6.282
InChI=1S/C14H24O2/c1-7-16-10(2)12-13(3,4)8-11(15)9-14(12,5)6/h12H,2,7-9H2,1,3-6H3	-3.643
InChI=1S/C12H12N4O2/c13-11-8(5-15-12(14)16-11)3-7-1-2-9-10(4-7)18-6-17-9/h1-2,4-5H,3,6H2,(H4,13,14,15,16)	-2.272

"InChi"	"logS(M)"
InChI=1S/C8H18N6/c1-5-3-14(8(11)12)6(2)4-13(5)7(9)10/h5-6H,3-4H2,1-2H3,(H3,9,10)(H3,11,12)	0.02
InChI=1S/C18H23ClN2O/c1-2-18(22)21-16-8-9-17(21)13-20(12-16)10-4-6-14-5-3-7-15(19)11-1h3-7,11,16-17H,2,8-10,12-13H2,1H3/b6-4+	-4.458
InChI=1S/C14H19N3O/c1-9-5-6-11-8-17(14(15)16-18)7-10-3-2-4-12(9)13(10)11/h5-6,10,18H,2-4,7-8H2,1H3,(H2,15,16)	-1.2
InChI=1S/C14H18Cl2N2O3/c15-5-7-18(8-6-16)12-3-1-11(2-4-12)9-13(14(20)21)17-10-19/h1-4,10,13H,5-9H2,(H,17,19)(H,20,21)	-2.86
InChI=1S/C11H15NO2/c1-3-8-14-11-6-4-10(5-7-11)12-9(2)13/h4-7H,3,8H2,1-2H3,(H,12,13)	-3.056
InChI=1S/C10H9NO3S/c11-8-5-1-3-7-4-2-6-9(10(7)8)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-3.07
InChI=1S/C9H15Br6O4P/c10-1-7(13)4-17-20(16,18-5-8(14)2-11)19-6-9(15)3-12/h7-9H,1-6H2	-4.941
InChI=1S/C16H21N3O/c1-4-9-18-10-11(2)19-15(12(18)3)17-14-8-6-5-7-13(14)16(19)20/h5-8,11-12H,4,9-10H2,1-3H3	-2.24
InChI=1S/C16H18ClNO2S/c1-11-5-4-6-12(2)16(11)18(15(19)9-17)10-14-13(20-3)7-8-21-14/h4-8H,9-10H2,1-3H3	-4.469
InChI=1S/C4H2Cl2N2/c5-3-1-4(6)8-2-7-3/h1-2H	-1.417
InChI=1S/C5H9ClFN3O2/c6-1-3-8-5(11)10(9-12)4-2-7/h1-4H2,(H,8,11)	-1.462
InChI=1S/C8H11N5/c9-7(10)13-8(11)12-6-4-2-1-3-5-6/h1-5H,(H6,9,10,11,12,13)	-1.433
InChI=1S/C16H22O8/c1-22-11-7-9(3-2-6-17)4-5-10(11)23-16-15(21)14(20)13(19)12(8-18)2h2-5,7,12-21H,6,8H2,1H3/b3-2+	-1.87
InChI=1S/C13H12N2/c14-15-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H,14H2	-3.015
InChI=1S/C14H18O4S/c1-3-18-13(15)14(9-4-10-14)19(16,17)12-7-5-11(2)6-8-12/h5-8H,3-4,9-10H2,1-2H3	-2.959
InChI=1S/C16H17BrFN3O3/c1-4-24-20-15(22)11-8-21(3)16(23)9(2)14(11)19-13-6-5-10(17)7-12(1h5-8,19H,4H2,1-3H3,(H,20,22)	-3.82
InChI=1S/C10H6Cl2/c11-8-5-4-7-2-1-3-10(12)9(7)6-8/h1-6H	-5.92
InChI=1S/C21H25NO2/c23-20(18-8-3-1-4-9-18)12-7-15-22-16-13-21(24,14-17-22)19-10-5-2-h1-6,8-11,24H,7,12-17H2	-2.68
InChI=1S/C12H16N4O3/c1-4-5-6-8(17)16-7-13-10-9(16)11(18)15(3)12(19)14(10)2/h7H,4-6H2,1-3H3	-2.12
InChI=1S/C10H14N2O2/c1-7(12-11)4-8-2-3-9-10(5-8)14-6-13-9/h2-3,5,7,12H,4,6,11H2,1H3	-1.86
InChI=1S/C14H18O10/c15-11(16)1-3-13(19)23-9-7-21-5-6-22-8-10-24-14(20)4-2-12(17)18/h1-4H,5-10H2,(H,15,16)(H,17,18)/b3-1+,4-2+	0.16

"InChi"	"logS(M)"
InChI=1S/C13H24O4/c1-3-16-12(14)10-8-6-5-7-9-11-13(15)17-4-2/h3-11H2,1-2H3	-2.99
InChI=1S/C8H8Cl2O2/c1-11-7-3-5(9)6(10)4-8(7)12-2/h3-4H,1-2H3	-3.459
InChI=1S/C20H42O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h21H,2-20H2,1H3	-5.475
InChI=1S/C5H10N2O2/c8-4-3-7-2-1-6-5(7)9/h8H,1-4H2,(H,6,9)	0.878
InChI=1S/C12H20N4OS/c1-8(2)7-13-16-10(17)9(12(3,4)5)14-15-11(16)18-6/h7-8H,1-6H3/b13-7+	-4.429
InChI=1S/C5H10O/c1-5-2-3-6-4-5/h5H,2-4H2,1H3	0.09
InChI=1S/C8H6Cl2O3/c1-13-7-5(10)3-2-4(9)6(7)8(11)12/h2-3H,1H3,(H,11,12)	-1.7
InChI=1S/C15H12ClN3O/c16-11-6-7-13-12(8-11)15(10-4-2-1-3-5-10)19(20)9-14(17)18-13/h1-8,17,20H,9H2/b17-14+	-2.095
InChI=1S/C9H13NO2/c1-7-2-3-8(6-9(7)12)10-4-5-11/h2-3,6,10-12H,4-5H2,1H3	-0.655
InChI=1S/C9H15Cl6O4P/c10-1-7(2-11)17-20(16,18-8(3-12)4-13)19-9(5-14)6-15/h7-9H,1-6H2	-4.377
InChI=1S/C13H16O4S/c1-17-12(14)13(9-5-6-10-13)18(15,16)11-7-3-2-4-8-11/h2-4,7-8H,5-6,9-10H2,1H3	-2.55
InChI=1S/C42H62N8O7/c1-26(2)16-32(36(51)21-37(52)47-33(17-27(3)4)38(53)45-23-30-15-1h8-15,18,24-27,32-36,51H,16-17,19-23,43H2,1-7H3,(H,44,46)(H,45,53)(H,47,52)(H,48,55)(H,49,54)(H,50,56)	-2.85
InChI=1S/C3H7ClO/c1-5-3-2-4/h2-3H2,1H3	-0.072
InChI=1S/C14H20O2/c1-4-13(14(15)16)12-7-5-11(6-8-12)9-10(2)3/h5-8,10,13H,4,9H2,1-3H3,(H,15,16)	-3.71
InChI=1S/C10H16N4/c1-5-9(3,7-11)13-14-10(4,6-2)8-12/h5-6H2,1-4H3/b14-13+	-2.696
InChI=1S/C2H8O7P2/c1-2(3,10(4,5)6)11(7,8)9/h3H,1H3,(H2,4,5,6)(H2,7,8,9)	0.525
InChI=1S/C16H12ClNO3/c1-9(16(19)20)11-4-7-14-13(8-11)18-15(21-14)10-2-5-12(17)6-3-10/h2-9H,1H3,(H,19,20)	-3.764
InChI=1S/C11H16O4/c1-11(13,7-12)8-15-10-6-4-3-5-9(10)14-2/h3-6,12-13H,7-8H2,1-2H3	-1.157
InChI=1S/CHBrCl2/c2-1(3)4/h1H	-1.54
InChI=1S/C36H20O4/c1-39-27-15-25-17-7-3-5-9-21(17)35(37)23-13-11-19-20-12-14-24-30h3-16H,1-2H3	-5.599
InChI=1S/C9H9NO3/c1-6(11)10-9(13)7-4-2-3-5-8(7)12/h2-5,12H,1H3,(H,10,11,13)	-0.978
InChI=1S/C6H12N4O2/c1-3-2-4(9-5(7)11)10-6(12)8-3/h3-4H,2H2,1H3,(H3,7,9,11)(H2,8,10,12)	-1.531
InChI=1S/C16H13ClN2O/c17-12-7-5-11(6-8-12)16(20)14-4-2-1-3-13(14)15-18-9-10-19(15)16/h1-8,20H,9-10H2	-5.267

"InChi"	"logS(M)"
InChI=1S/C14H12N6O6/c15-14(16)18-17-9(1-3-10-5-7-12(25-10)19(21)22)2-4-11-6-8-13(26-1h1-8H,(H4,15,16,18)/b3-1+,4-2+	-5.51
InChI=1S/C11H14Cl2N2O2/c1-9-2-3-10(15(16)17)8-11(9)14(6-4-12)7-5-13/h2-3,8H,4-7H2,1H3	-5.153
InChI=1S/C23H27N3O7/c1-25(2)12-5-6-13(27)15-10(12)7-9-8-11-17(26(3)4)19(29)16(22(24)3h5-6,9,11,17,27,29-30,33H,7-8H2,1-4H3,(H2,24,32)	-0.94
InChI=1S/C35H58O11/c1-4-5-11-16-31(42)34-33(44)22-29(40)20-27(38)18-25(36)17-26(37)h6-10,12-15,24-34,36-44H,4-5,11,16-22H2,1-3H3/b7-6-,10-8-,12-9-,15-13-,23-14-	-5.013
InChI=1S/C4H10N2O6/c1-4(12-6(9)10)2-3-11-5(7)8/h4H,2-3H2,1H3,(H,7,8)(H,9,10)/q+2	-1.66
InChI=1S/CH2Cl2/c2-1-3/h1H2	-0.63
InChI=1S/C14H20O4/c15-14(9-2-4-11-13(6-9)18-11)16-7-8-1-3-10-12(5-8)17-10/h8-13H,1-7H2	-1.26
InChI=1S/C12H19N3O2/c1-10(2)9-11(12(16)17)15(7-3-5-13)8-4-6-14/h10-11H,3-4,7-9H2,1-2H3,(H,16,17)	-1.14
InChI=1S/C12H5Br5/c13-6-1-2-9(14)7(3-6)8-4-11(16)12(17)5-10(8)15/h1-5H	-9.726
InChI=1S/C14H15NO/c1-4-10-15-14(16)12(3)11(2)13-8-6-5-7-9-13/h1,5-9H,10H2,2-3H3,(H,15,16)/b12-11-	-2.971
InChI=1S/C6H13N/c7-6-4-2-1-3-5-6/h6H,1-5,7H2	1.004
InChI=1S/C4H8Cl3FNOP/c5-1-3-9(4-2-8)11(6,7)10/h1-4H2	-1.96
InChI=1S/C2H2ClN3O6/c3-1-2(4(7)8,5(9)10)6(11)12/h1H2	-0.259
InChI=1S/C18H19NO3S/c1-19(2)16-12-17(23(20,21)22)18(13-8-4-3-5-9-13)15-11-7-6-10-14(1h3-11,16H,12H2,1-2H3,(H,20,21,22)	-1.173
InChI=1S/C22H42O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-22(23)21(2)3/h2,4-20H2,1,3H3	-8.53
InChI=1S/C7H15N/c1-2-8-6-4-3-5-7-8/h2-7H2,1H3	-1.276
InChI=1S/C9H18O2/c1-9(2,3)7-5-4-6-8(10)11/h4-7H2,1-3H3,(H,10,11)	-2.475
InChI=1S/C7H9NO5S3/c8-16(12,13)6-3-4-5(9)1-2-15(10,11)7(4)14-6/h3,5,9H,1-2H2,(H2,8,12,13)	-1.65
InChI=1S/C30H48N2O2/c1-7-29(25-13-17-27(18-14-25)33-23-21-31(9-3)10-4)30(8-2)26-15-19h13-20,29-30H,7-12,21-24H2,1-6H3	-10.251
InChI=1S/C15H12/c1-11-14-8-4-2-6-12(14)10-13-7-3-5-9-15(11)13/h2-10H,1H3	-5.89
InChI=1S/C24H27NO4/c1-26-20-8-7-15-19-13-25-9-5-6-14(25)10-16(19)17-11-21(27-2)22(28h7-8,11-12,14H,5-6,9-10,13H2,1-4H3	-5.72
InChI=1S/C2H7NS/c3-1-2-4/h4H,1-3H2	0.799

"InChi"	"logS(M)"
InChI=1S/C15H10Br2ClNO2S/c1-8(20)21-14-12(6-10(18)7-13(14)17)15(22)19-11-4-2-9(16)3-5-11/h2-7H,1H3,(H,19,22)	-6.815
InChI=1S/C10H10O3/c1-7-2-3-9-10(4-7)13-6-8(11)5-12-9/h2-4H,5-6H2,1H3	-1.114
InChI=1S/C14H14N2O6S2/c15-11-5-3-9(13(7-11)23(17,18)19)1-2-10-4-6-12(16)8-14(10)24(20,2 h1-8H,15-16H2,(H,17,18,19)(H,20,21,22)/b2-1+	-4.064
InChI=1S/C6H6O3/c1-8-6(7)5-3-2-4-9-5/h2-4H,1H3	-0.976
InChI=1S/C17H26O/c1-10-6-7-15-16(4,5)14-9-17(10,15)8-13(11(14)2)12(3)18/h10,14-15H,6-9H2,1-5H3	-4.613
InChI=1S/C5H5NO3/c1-3-4(5(7)8)2-6-9-3/h2H,1H3,(H,7,8)/p-1	-1.055
InChI=1S/C7H10N2/c1-9(2)7-3-5-8-6-4-7/h3-6H,1-2H3/p+1	-0.206
InChI=1S/C18H18O5/c19-17(15-7-3-1-4-8-15)22-13-11-21-12-14-23-18(20)16-9-5-2-6-10-1 h1-10H,11-14H2	-3.937
InChI=1S/C14H16ClN5O5S/c1-9-16-12(19-14(17-9)24-2)18-13(21)20-26(22,23)11-6-4-3-5-10(11) h3-6H,7-8H2,1-2H3,(H2,16,17,18,19,20,21)	-4.099
InChI=1S/C4H8Cl2S/c5-1-3-7-4-2-6/h1-4H2	-2.367
InChI=1S/C12H18N2O2/c1-11(2)4-10(14-9-16)5-12(3,6-11)7-13-8-15/h10H,4-7H2,1-3H3	-4.171
InChI=1S/C11H16O/c1-3-11(2,12)9-10-7-5-4-6-8-10/h4-8,12H,3,9H2,1-2H3	-2.391
InChI=1S/C8H6N2O/c11-7-3-1-2-6-8(7)10-5-4-9-6/h1-5,11H	-1.347
InChI=1S/C17H22N2O3S2/c1-12(2)6-7-19-10-13-4-3-5-14(8-13)17(20)15-9-16(23-11-15)24(18,2 h3-5,8-9,11-12,19H,6-7,10H2,1-2H3,(H2,18,21,22)	-1.5
InChI=1S/C10H19Cl2N/c11-6-8-13(9-7-12)10-4-2-1-3-5-10/h10H,1-9H2	-3.072
InChI=1S/C13H19N3O4/c1-4-6-14(7-5-2)13-11(15(17)18)8-10(3)9-12(13)16(19)20/h8-9H,4-7H2,1-3H3	-2.966
InChI=1S/C6H5Br2NO2S/c7-9(8)12(10,11)6-4-2-1-3-5-6/h1-5H	-3.28
InChI=1S/C17H17Cl2NO2/c18-10-12-20(13-11-19)15-6-8-16(9-7-15)22-17(21)14-4-2-1-3-5-14/h1-9H,10-13H2	-5.691
InChI=1S/C7H7IO/c1-5-3-2-4-6(8)7(5)9/h2-4,9H,1H3	-1.838
InChI=1S/C8H12O6/c1-4(5(9)10)3-8(2,6(11)12)7(13)14/h4H,3H2,1-2H3,(H,9,10)(H,11,12)(H,13,14)	-0.109
InChI=1S/C14H26N4O11P2/c1-18(2,3)6-7-26-30(22,23)29-31(24,25)27-8-9-11(19)12(20)13(28-9) h4-5,9,11-13,19-20H,6-8H2,1-3H3,(H3-,15,16,21,22,23,24,25)	0.311
InChI=1S/C12H10O3/c13-12(14)8-15-11-6-5-9-3-1-2-4-10(9)7-11/h1-7H,8H2,(H,13,14)	-3.36
InChI=1S/C14H18O4S/c1-10(2)18-13(15)14(8-9-14)19(16,17)12-6-4-11(3)5-7-12/h4-7,10H,8-9H2,1-3H3	-3.231
InChI=1S/C7H7NO3/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4,9H,1H3	-2.185
InChI=1S/C3H7NO3/c1-2-3-7-4(5)6/h2-3H2,1H3	-1.504

"InChi"	"logS(M)"
InChI=1S/C12H6Cl2O/c13-7-1-3-11-9(5-7)10-6-8(14)2-4-12(10)15-11/h1-6H	-7.213
InChI=1S/C40H24Cl4N6O4/c41-31-19-35(45-49-47-39(53)29-13-23-5-1-3-7-25(23)15-37(29)51)33h1-20,51-52H,(H,45,47,53)(H,46,48,54)	-8.087
InChI=1S/C12H6Cl4O/c13-8-6-9(11(15)12(16)10(8)14)17-7-4-2-1-3-5-7/h1-6H	-7.52
InChI=1S/C13H20N4O4/c1-3-7-16(8-4-2)10-12(18)15-14-9-11-5-6-13(21-11)17(19)20/h5-6,9H,3-4,7-8,10H2,1-2H3,(H,15,18)/b14-9+	-3.152
InChI=1S/C9H14N2O/c1-3-5-10-7-8-11(6-4-2)9(10)12/h3-6H,7-8H2,1-2H3/b5-3+,6-4+	-1.457
InChI=1S/C22H22N2O7/c1-8-9-5-4-6-12(25)13(9)17(26)14-10(8)7-11-16(24(2)3)18(27)15(21(2h4-6,11,16,25-26,29,31H,7H2,1-3H3,(H2,23,30)	-2.268
InChI=1S/C4H6N6O/c5-2-1(10-11)3(6)9-4(7)8-2/h(H6,5,6,7,8,9)	-3.845
InChI=1S/C13H17N3O5/c14-10(5-8-1-3-9(17)4-2-8)13(21)16-6-11(18)15-7-12(19)20/h1-4,10,17H,5-7,14H2,(H,15,18)(H,16,21)(H,19,20)	-1.47
InChI=1S/C11H13NO3S/c1-8(2)12-11(13)10-6-4-3-5-9(10)7-16(12,14)15/h3-6,8H,7H2,1-2H3	-2.511
InChI=1S/C12H16/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10H2	-4.342
InChI=1S/C3H8O3S3/c4-9(5,6)2-3(8)1-7/h3,7-8H,1-2H2,(H,4,5,6)	0.725
InChI=1S/C4H9N5O4S3/c1-9(2)16(12,13)8-3-6-7-4(14-3)15(5,10)11/h1-2H3,(H,6,8)(H2,5,10,11)	-2.68
InChI=1S/C4H4N2O3/c7-2-1-3(8)6-4(9)5-2/h1H2,(H2,5,6,7,8,9)	-1.049
InChI=1S/C8H9NO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,9H2,1H3	-1.28
InChI=1S/C6H5Cl2N/c7-4-1-2-6(9)5(8)3-4/h1-3H,9H2	-2.417
InChI=1S/C14H24N4O6/c1-9(19)17(23)7-3-5-11-13(21)16-12(14(22)15-11)6-4-8-18(24)10(2)2h11-12,23-24H,3-8H2,1-2H3,(H,15,22)(H,16,21)	0.262
InChI=1S/C10H13NO6/c12-4-6-8(15)9(16)10(17-6)11-2-1-5(13)3-7(11)14/h1-2,6,8-10,12,15-16H,3-4H2	-0.77
InChI=1S/C16H14O4/c1-11-3-7-13(8-4-11)15(17)19-20-16(18)14-9-5-12(2)6-10-14/h3-10H,1-2H3	-6.798
InChI=1S/C12H15NO3/c1-13-4-3-8-5-10-12(16-7-15-10)11(14-2)9(8)6-13/h5H,3-4,6-7H2,1-2H3	-1.466
InChI=1S/C4H6O2S/c1-3-7(5,6)4-2/h3-4H,1-2H2	0.274
InChI=1S/C7H13N3O2/c8-6(11)4-2-1-3-5(10-4)7(9)12/h4-5,10H,1-3H2,(H2,8,11)(H2,9,12)	0.289
InChI=1S/C18H24ClN/c1-20-13-12-15-4-2-3-5-17(15)18(20)11-8-14-6-9-16(19)10-7-14/h6-7,9-10,18H,2-5,8,11-13H2,1H3	-5.462
InChI=1S/C8H8Cl3N3O4S2/c9-7(8(10)11)3-1-4(12)6(20(14,17)18)2-5(3)19(13,15)16/h1-2H,12H2,(H2,13,15,16)(H2,14,17,18)	-4.054

"InChi"	"logS(M)"
InChI=1S/C9H11NO3/c10-9(12)13-6-8(11)7-4-2-1-3-5-7/h1-5,8,11H,6H2,(H2,10,12)	-0.816
InChI=1S/C15H11IN2O/c1-10-17-14-8-7-11(16)9-13(14)15(19)18(10)12-5-3-2-4-6-12/h2-9H,1H3	-6.068
InChI=1S/C15H13NO/c1-10(17)16-13-6-7-15-12(9-13)8-11-4-2-3-5-14(11)15/h2-7,9H,8H2,1H3,(H,16,17)	-4.24
InChI=1S/C13H15BrN4O2/c1-19-9-4-7(5-10(20-2)11(9)14)3-8-6-17-13(16)18-12(8)15/h4-6H,3H2,1-2H3,(H4,15,16,17,18)	-3.39
InChI=1S/C4H10N2O/c1-2-3-6-4(5)7/h2-3H2,1H3,(H3,5,6,7)	-1.166
InChI=1S/C17H19N3O3/c1-23-17-8-6-15(7-9-17)19-12-10-18(11-13-19)14-2-4-16(5-3-14)20(2h2-9H,10-13H2,1H3	-6.929
InChI=1S/C20H16OS/c1-15-7-11-18(12-8-15)22-19-13-9-17(10-14-19)20(21)16-5-3-2-4-6-1h2-14H,1H3	-7.615
InChI=1S/C10H19N/c1-10(2)8-5-4-7(6-8)9(10)11-3/h7-9,11H,4-6H2,1-3H3	-1.752
InChI=1S/C11H12O2/c1-9(2)11(12)13-8-10-6-4-3-5-7-10/h3-7H,1,8H2,2H3	-2.968
InChI=1S/C5H3BrO3/c6-3-1-4(5(7)8)9-2-3/h1-2H,(H,7,8)	-1.184
InChI=1S/C13H9ClN2/c14-9-5-3-7-11-12(9)13(15)8-4-1-2-6-10(8)16-11/h1-7H,(H2,15,16)	-1.58
InChI=1S/C8H8O5S/c1-13-14(11,12)7-4-2-6(3-5-7)8(9)10/h2-5H,1H3,(H,9,10)	-3.05
InChI=1S/C13H13ClN2O2S/c1-9-2-5-11(8-13(9)14)16-19(17,18)12-6-3-10(15)4-7-12/h2-8,16H,15H2,1H3	-4.91
InChI=1S/C8H9NO2/c1-5-2-3-6(8(9)11)7(10)4-5/h2-4,10H,1H3,(H2,9,11)	-2.917
InChI=1S/C10H11N5O5S3/c1-6(16)12-7-2-4-8(5-3-7)23(19,20)15-9-13-14-10(21-9)22(11,17)18/h2-5H,1H3,(H,12,16)(H,13,15)(H2,11,17,18)	-1.62
InChI=1S/C11H16N4O2/c1-4-5-6-15-7-12-9-8(15)10(16)14(3)11(17)13(9)2/h7H,4-6H2,1-3H3	-1.807
InChI=1S/C6H10O4S/c7-5(8)1-3-11-4-2-6(9)10/h1-4H2,(H,7,8)(H,9,10)	-0.799
InChI=1S/C9H16O2/c1-3-5-6-7-9(10)11-8-4-2/h4H,2-3,5-8H2,1H3	-2.611
InChI=1S/C12H12N2O4S/c15-11-9(5-3-7-13-11)14-12(16)8-4-1-2-6-10(8)19(14,17)18/h1-2,4,6,9H,3,5,7H2,(H,13,15)	-2.64
InChI=1S/C12H14O4/c1-2-8-15-12(14)11(13)9-16-10-6-4-3-5-7-10/h3-7,9,13H,2,8H2,1H3/b11-9-	-1.623
InChI=1S/C9H15N/c1-4-7-10(8-5-2)9-6-3/h4-6H,1-3,7-9H2	-1.74
InChI=1S/C4H9NO2/c1-5-3-2-4(6)7/h5H,2-3H2,1H3,(H,6,7)	-0.054
InChI=1S/C19H30O3/c1-2-3-4-5-6-7-8-9-10-11-16-22-19(21)17-12-14-18(20)15-13-17/h12-15,20H,2-11,16H2,1H3	-7.172
InChI=1S/C3H6O2/c1-3(5)2-4/h4H,2H2,1H3	1.13

"InChi"	"logS(M)"
InChI=1S/C7H6N2O5/c1-14-7-3-2-5(8(10)11)4-6(7)9(12)13/h2-4H,1H3	-3.107
InChI=1S/C24H34O4/c1-22-10-7-17(25)13-16(22)4-5-20-19(22)8-11-23(2)18(9-12-24(20,23h3,6,14,16-20,25,27H,4-5,7-13H2,1-2H3	-5.801
InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,5,7H2,1-2H3	-2.769
InChI=1S/C12H18ClN5O/c1-8-10(13)15-12(14-9(2)19)16-11(8)18-6-4-17(3)5-7-18/h4-7H2,1-3H3,(H,14,15,16,19)	-1.945
InChI=1S/C11H17ClN2O4S2/c12-10-3-4-11(14-9-10)18-7-2-1-5-13-6-8-19-20(15,16)17/h3-4,9,13H,1-2,5-8H2,(H,15,16,17)	-1.642
InChI=1S/C19H16O/c20-19(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15,20H	-2.26
InChI=1S/C10H11NO3/c1-7(12)11-9-4-2-8(3-5-9)6-10(13)14/h2-5H,6H2,1H3,(H,11,12)(H,13,14)	-1.789
InChI=1S/C7H8OS/c1-5-3-4-7(9-5)6(2)8/h3-4H,1-2H3	-1.73
InChI=1S/C14H9NO2/c15-8-5-6-11-12(7-8)14(17)10-4-2-1-3-9(10)13(11)16/h1-7H,15H2	-6.137
InChI=1S/C4HCl5/c5-2(4(8)9)1-3(6)7/h4H	-4.23
InChI=1S/C7H4I3NO2/c8-2-1-3(9)6(11)5(10)4(2)7(12)13/h1H,11H2,(H,12,13)	-5.821
InChI=1S/C6H9F/c1-2-3-4-5-6-7/h1H,3-6H2	-2.031
InChI=1S/C12H9Cl3N2O2S/c13-9-5-11(15)12(6-10(9)14)17-20(18,19)8-3-1-7(16)2-4-8/h1-6,17H,16H2	-4.83
InChI=1S/C3H6O/c1-3(2)4/h1-2H3	1.236
InChI=1S/C13H17NO3/c1-4-17-12(16)13(2,3)14-11(15)10-8-6-5-7-9-10/h5-9H,4H2,1-3H3,(H,14,15)	-1.19
InChI=1S/C12H4Cl6O/c13-5-3-7(15)12(8(16)4-5)19-9-2-1-6(14)10(17)11(9)18/h1-4H	-8.1
InChI=1S/C7H8O3S/c8-11(9,10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H,8,9,10)	0.118
InChI=1S/C16H20ClN5S/c1-21-8-10-22(11-9-21)15-13(23-2)14(17)19-16(20-15)18-12-6-4-3-5-7H,8-11H2,1-2H3,(H,18,19,20)	-3.392
InChI=1S/C19H15ClO4/c1-19(22)10-14(11-6-8-12(20)9-7-11)16-17(24-19)13-4-2-3-5-15(13)22-9,14,22H,10H2,1H3	-5.84
InChI=1S/C10H16O4/c1-13-9(11)7-3-5-8(6-4-7)10(12)14-2/h7-8H,3-6H2,1-2H3	-1.387
InChI=1S/C12H20N2O2S/c1-3-5-6-7-8-12(4-2)9(15)13-11(17)14-10(12)16/h3-8H2,1-2H3,(H2,13,14,15,16,17)	-4.08
InChI=1S/C7H4Cl4O/c1-12-7-4(9)2-3(8)5(10)6(7)11/h2H,1H3	-5.13
InChI=1S/C13H14O5/c1-5-7(3)18-4-8-9(5)6(2)11(14)10(12(8)15)13(16)17/h4-5,7,14H,1-3H3,(H,16,17)	-1.288

"InChi"	"logS(M)"
InChI=1S/C17H22O3/c1-4-14-11(2)15(17(18)19)9-10-16(14)12-5-7-13(20-3)8-6-12/h5-8,11,15H,4,9-10H2,1-3H3,(H,18,19)	-5.454
InChI=1S/C11H12O2/c1-2-4-10-8(3-1)5-9-6-12-7-13-11(9)10/h1-4,9,11H,5-7H2	-1.656
InChI=1S/C15H23N3O2/c1-2-3-4-5-6-7-8-14(19)17-18-15(20)13-9-11-16-12-10-13/h9-12H,2-8H2,1H3,(H,17,19)(H,18,20)	-3.52
InChI=1S/C7H6INO/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H2,9,10)	-2.702
InChI=1S/C6H15N/c1-5(2)7-6(3)4/h5-7H,1-4H3	0.036
InChI=1S/C12H14N2O3/c1-2-7-12(8-5-3-4-6-8)9(15)13-11(17)14-10(12)16/h2-3,5,8H,1,4,6-7H2,(H2,13,14,15,16,17)	-2.199
InChI=1S/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h3,13-17,20-21H,4-11H2,1-2H3	-4.35
InChI=1S/C13H26N2O4/c1-5-8-13(4,9-18-11(16)14-6-2)10-19-12(17)15-7-3/h5-10H2,1-4H3,(H,14,16)(H,15,17)	-3.675
InChI=1S/C7H11NO4/c9-6(10)4-1-2-8-3-5(4)7(11)12/h4-5,8H,1-3H2,(H,9,10)(H,11,12)	-0.539
InChI=1S/C10H9N3O/c11-9-5-8(6-13-10(9)14)7-1-3-12-4-2-7/h1-6H,11H2,(H,13,14)	-2.047
InChI=1S/C7H4BrNS/c8-6-2-1-3-7(4-6)9-5-10/h1-4H	-4.085
InChI=1S/C8H7BrO2/c1-6(10)11-8-4-2-7(9)3-5-8/h2-5H,1H3	-2.417
InChI=1S/C8H16N2O/c1-3-8(11)10-6-4-9(2)5-7-10/h3-7H2,1-2H3	-1.302
InChI=1S/C27H29NO10/c1-10-22(30)14(28)7-17(37-10)38-16-9-27(35,11(2)29)8-13-19(16)26(h4-6,10,14,16-17,22,30,32,34-35H,7-9,28H2,1-3H3	-4.129
InChI=1S/C8H19N/c1-2-3-4-5-6-7-8-9/h2-9H2,1H3	-2.75
InChI=1S/C11H18N2O8/c14-8(15)4-12(5-9(16)17)2-1-3-13(6-10(18)19)7-11(20)21/h1-7H2,(H,14,15)(H,16,17)(H,18,19)(H,20,21)	-1.469
InChI=1S/C9H9NO2/c1-7(11)9(10-12)8-5-3-2-4-6-8/h2-6,12H,1H3/b10-9+	-2.368
InChI=1S/C13H10N2/c14-11-6-5-10-7-9-3-1-2-4-12(9)15-13(10)8-11/h1-8H,14H2	-4.094
InChI=1S/C15H21NO4/c1-12(17)13-3-2-4-15(9-13)20-11-14(18)10-16-5-7-19-8-6-16/h2-4,9,14,18H,5-8,10-11H2,1H3	-0.245
InChI=1S/C16H16O2/c1-2-15(16(17)18)14-10-8-13(9-11-14)12-6-4-3-5-7-12/h3-11,15H,2H2,1H3,(H,17,18)	-4.26
InChI=1S/C15H22N2O3/c1-3-17-10-4-5-14(11-17)20-15(18)16-12-6-8-13(19-2)9-7-12/h6-9,14H,3-5,10-11H2,1-2H3,(H,16,18)	-3.085
InChI=1S/C6H5N3O5/c7-3-1-4(8(11)12)6(10)5(2-3)9(13)14/h1-2,10H,7H2	-2.385
InChI=1S/C14H18O4S/c1-18-13(15)14(10-6-3-7-11-14)19(16,17)12-8-4-2-5-9-12/h2,4-5,8-9H,3,6-7,10-11H2,1H3	-3.85

"InChi"	"logS(M)"
InChI=1S/C9H8O/c1-2-9(10)8-6-4-3-5-7-8/h1,3-7,9-10H	-0.462
InChI=1S/C11H9NO2/c1-8(13)14-10-6-2-4-9-5-3-7-12-11(9)10/h2-7H,1H3	-2.3
InChI=1S/C7H4BrClN2O/c8-3-1-6-5(2-4(3)9)11-7(10)12-6/h1-2H,(H2,10,11)	-3.528
InChI=1S/C8H9Cl/c1-7-4-2-3-5-8(7)6-9/h2-5H,6H2,1H3	-3.081
InChI=1S/C10H16N2/c1-8-5-3-4-6-10(8)7-9(2)12-11/h3-6,9,12H,7,11H2,1-2H3	-2.057
InChI=1S/C3H10NO3PS/c4-2-1-3-9-8(5,6)7/h1-4H2,(H2,5,6,7)	0.767
InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h7-9,13H,5-6,10H2,1-4H3/b9-8+	-3.992
InChI=1S/C8H3F5N4O4S3/c9-1-2(10)4(12)6(5(13)3(1)11)24(20,21)17-7-15-16-8(22-7)23(14,18)1h(H,15,17)(H2,14,18,19)	-1.21
InChI=1S/C6H5FN2O4/c1-13-6(12)9-2-3(7)4(10)8-5(9)11/h2H,1H3,(H,8,10,11)	-0.91
InChI=1S/C11H11NO6S2/c1-17-8-2-4-9(5-3-8)19(13,14)10-6-11(18-7-10)20(12,15)16/h2-7H,1H3,(H2,12,15,16)	-3.02
InChI=1S/C19H15FN2O4/c1-2-7-21-15-9-14(13(20)8-16(15)26-10-17(21)23)22-18(24)11-5-3-4-h1,8-9H,3-7,10H2	-5.297
InChI=1S/C18H24I3N3O9/c19-13-11(17(32)22-3-8(29)5-26)14(20)16(24(1-2-25)10(31)7-28)15(2h8-9,25-30H,1-7H2,(H,22,32)(H,23,33)	-3.845
InChI=1S/C8H8O2/c1-7(9)10-8-5-3-2-4-6-8/h2-6H,1H3	-1.374
InChI=1S/C18H20N2O6/c1-5-26-18(22)15-11(3)19-10(2)14(17(21)25-4)16(15)12-7-6-8-13(9-1h6-9,16,19H,5H2,1-4H3	-3.669
InChI=1S/C4H9NO3/c1-4(2,3-6)5(7)8/h6H,3H2,1-2H3	1.468
InChI=1S/C12H27O2P/c1-4-7-10-14-15(13,11-8-5-2)12-9-6-3/h4-12H2,1-3H3	-1.717
InChI=1S/C14H10N2O3/c17-13(18)9-5-1-2-6-10(9)15-14-16-11-7-3-4-8-12(11)19-14/h1-8H,(H,15,16)(H,17,18)	-3.133
InChI=1S/C5H10O/c1-3-5(2)4-6/h4-5H,3H2,1-2H3	-0.821
InChI=1S/CH4O6S2/c2-8(3,4)1-9(5,6)7/h1H2,(H,2,3,4)(H,5,6,7)	0.754
InChI=1S/C6H12O2/c1-2-8-6-4-3-5-7/h2,7H,1,3-6H2	-0.19
InChI=1S/C19H22N2O4/c1-3-20(4-2)14-18(15-8-6-5-7-9-15)25-19(22)16-10-12-17(13-11-16)2h5-13,18H,3-4,14H2,1-2H3	-2.84
InChI=1S/C21H30N2O2/c1-22-14-17-10-11-18(15-22)23(17)12-13-25-21(24)20-9-5-8-19(20)1h2-4,6-7,17-20H,5,8-15H2,1H3	-3.926
InChI=1S/C10H13N5O5/c11-10-13-7-4(8(19)14-10)12-2-15(7)9-6(18)5(17)3(1-16)20-9/h2-3,5-6,9,16-18H,1H2,(H3,11,13,14,19)	-2.74
InChI=1S/C21H27BrN2O2/c1-3-10-24(11-4-2)12-13-26-20-18(16-8-6-5-7-9-16)14-17(22)15-19(2h5-9,14-15H,3-4,10-13H2,1-2H3,(H2,23,25)	-6.059

"InChi"	"logS(M)"
InChI=1S/C42H63O3P/c1-37(2,3)28-19-22-34(31(25-28)40(10,11)12)43-46(44-35-23-20-29(3h19-27H,1-18H3	-8.112
InChI=1S/C13H18F3N3O4S2/c1-2-3-4-5-12-18-9-6-8(13(14,15)16)10(24(17,20)21)7-11(9)25(22,23)h6-7,12,18-19H,2-5H2,1H3,(H2,17,20,21)	-5.449
InChI=1S/C8H16O/c1-3-5-6-7-8(9)4-2/h4,8-9H,2-3,5-7H2,1H3	-1.822
InChI=1S/C11H16NO6P/c1-8(2)10-7-9(5-6-11(10)12(13)14)18-19(15,16-3)17-4/h5-8H,1-4H3	-3.894
InChI=1S/C15H13N5O4/c1-3-19-14(21)10(8-16)9(2)13(15(19)22)18-17-11-6-4-5-7-12(11)20(2h4-7,17H,3H2,1-2H3/b18-13-	-6.816
InChI=1S/C6H12Cl2/c7-5-3-1-2-4-6-8/h1-6H2	-3.435
InChI=1S/C12H5Cl5O/c13-8-2-1-6(3-9(8)14)18-7-4-10(15)12(17)11(16)5-7/h1-5H	-8.25
InChI=1S/C23H23NO/c1-4-10-20(11-5-1)23(21-12-6-2-7-13-21,22-14-8-3-9-15-22)24-16-18h1-15H,16-19H2	-7.217
InChI=1S/C25H34O3/c1-6-25(28-22(27)23(2,3)4)14-12-21-20-9-7-16-15-17(26)8-10-18(16)h1,15,18-21H,7-14H2,2-5H3	-7.16
InChI=1S/C8H16O3/c1-6(2)7(9)10-11-8(3,4)5/h6H,1-5H3	-1.607
InChI=1S/C24H32O4/c1-22-9-7-16(25)11-15(22)4-5-18-17(22)8-10-23(2)19(12-20-24(18,23h3,6,13,15-20,25H,4-5,7-12H2,1-2H3	-4.197
InChI=1S/C9H10O2/c1-7-2-4-8(5-3-7)6-9(10)11/h2-5H,6H2,1H3,(H,10,11)	-1.491
InChI=1S/C16H21NO2/c17-15-9-13-11(6-7-12(13)16(18)19)8-14(15)10-4-2-1-3-5-10/h8-10,12H,1-7,17H2,(H,18,19)	-4.268
InChI=1S/C12H4Cl6O/c13-6-3-8(15)11(4-7(6)14)19-5-1-9(16)12(18)10(17)2-5/h1-4H	-8.72
InChI=1S/C17H37NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16-17-22-23(19,20)21/h18H,2-17H2,1H3,(H,19,20,21)	-5.465
InChI=1S/C14H14/c1-12(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-12H,1H3	-4.693
InChI=1S/C10H18N2O2/c1-5-9(3)7(13)12-10(4,6-2)8(14)11-9/h5-6H2,1-4H3,(H,11,14)(H,12,13)	-1.92
InChI=1S/C22H42O4/c1-3-5-7-9-11-15-19-25-21(23)17-13-14-18-22(24)26-20-16-12-10-8-6h3-20H2,1-2H3	-5.677
InChI=1S/C20H20N2O2/c1-2-4-17(5-3-1)19-14-21-20(24-19)18-8-6-16(7-9-18)15-22-10-12-23h1-9,14H,10-13,15H2	-4.35
InChI=1S/C8H18O3P/c1-3-5-7-10-12(9)11-8-6-4-2/h3-8H2,1-2H3/q+1	-1.425
InChI=1S/C9H7N3O2/c13-11-7-3-4-8(12-14)9-6(7)2-1-5-10-9/h1-5,13-14H/b11-7+,12-8+	-3.8
InChI=1S/C7H11NO/c9-8-7(5-1-2-5)6-3-4-6/h5-6,9H,1-4H2	-2.502

"InChi"	"logS(M)"
InChI=1S/C10H16O2/c1-6(2)5-7-8(9(11)12)10(7,3)4/h5,7-8H,1-4H3,(H,11,12)	-3.011
InChI=1S/C18H16ClNO5/c1-3-22-17(21)11(2)23-13-5-7-14(8-6-13)24-18-20-15-9-4-12(19)10-16(15)18/h4-11H,3H2,1-2H3	-5.604
InChI=1S/C12H20O2/c1-2-10-14-12(13)9-8-11-6-4-3-5-7-11/h2,11H,1,3-10H2	-4.062
InChI=1S/C13H9ClN2/c14-8-5-6-10-12(7-8)16-11-4-2-1-3-9(11)13(10)15/h1-7H,(H2,15,16)	-1.73
InChI=1S/C10H18O/c1-5-10(4)8-6-7-9(2,3)11-10/h5H,1,6-8H2,2-4H3	-2.536
InChI=1S/C14H9ClO3/c15-10-7-5-9(6-8-10)13(16)11-3-1-2-4-12(11)14(17)18/h1-8H,(H,17,18)	-2.717
InChI=1S/C11H16O/c1-2-3-4-7-10-8-5-6-9-11(10)12/h5-6,8-9,12H,2-4,7H2,1H3	-3.256
InChI=1S/C5H6N2/c1-5-4-6-2-3-7-5/h2-4H,1H3	1.026
InChI=1S/C13H11N3O3S2/c1-9-2-4-10(5-3-9)21(18,19)11(6-14)7-16-8-12(17)15-13(16)20/h2-5,7H,8H2,1H3,(H,15,17,20)/b11-7+	-3.529
InChI=1S/C8H11N/c1-6-4-8(3)9-5-7(6)2/h4-5H,1-3H3	-0.782
InChI=1S/C10H14N6/c1-3-5-6(4-2)14-9-7(13-5)8(11)15-10(12)16-9/h3-4H2,1-2H3,(H4,11,12,14,15,16)	-3.267
InChI=1S/C10H24N2/c1-11(2)9-7-5-6-8-10-12(3)4/h5-10H2,1-4H3	-0.902
InChI=1S/C16H17N3O4S/c1-8-7-24-15-11(14(21)19(15)12(8)16(22)23)18-13(20)10(17)9-5-3-2-6,10-11,15H,7,17H2,1H3,(H,18,20)(H,22,23)	-1.58
InChI=1S/C4H5BrO4/c5-2(4(8)9)1-3(6)7/h2H,1H2,(H,6,7)(H,8,9)	-0.215
InChI=1S/C4H4N2O2/c7-3-1-2-5-4(8)6-3/h1-2H,(H2,5,6,7,8)	-1.48
InChI=1S/C11H18N2O3/c1-5-11(6-2)8(14)12-10(15)13-9(11)16-7(3)4/h7H,5-6H2,1-4H3,(H,12,14,15)	-2.44
InChI=1S/C16H26N2O4S/c1-4-5-6-7-8-9-10(19)17-11-13(20)18-12(15(21)22)16(2,3)23-14(11)1h11-12,14H,4-9H2,1-3H3,(H,17,19)(H,21,22)	-4.532
InChI=1S/C21H25N/c1-21(2,3)15-8-5-9-16-22(4)17-19-13-10-12-18-11-6-7-14-20(18)19/h5-7,9-14H,16-17H2,1-4H3/b9-5+	-4.465
InChI=1S/C11H16N2O3S3/c12-11(9-18-19(14,15)16)13-6-7-17-8-10-4-2-1-3-5-10/h1-5H,6-9H2,(H2,12,13)(H,14,15,16)	-2.691
InChI=1S/C13H18O2/c1-13(2,3)12(14)15-10-9-11-7-5-4-6-8-11/h4-8H,9-10H2,1-3H3	-3.675
InChI=1S/C10H22OS/c1-3-5-7-9-12(11)10-8-6-4-2/h3-10H2,1-2H3/p+1	-2.901
InChI=1S/C21H25N3O3/c1-22(17-8-4-3-5-9-17)21(26)18-10-6-7-11-19(18)23(2)20(25)16-24-13h3-11H,12-16H2,1-2H3	-3.407
InChI=1S/C18H37N5O9/c19-3-9-8(25)2-7(22)17(29-9)31-15-5(20)1-6(21)16(14(15)28)32-18-1h5-18,24-28H,1-4,19-23H2	0.33

"InChi"	"logS(M)"
InChI=1S/C7H16N2O/c1-3-5-9(6-4-2)7(8)10/h3-6H2,1-2H3,(H2,8,10)	-1.181
InChI=1S/C12H8N2O/c15-14-11-7-3-1-5-9(11)13-10-6-2-4-8-12(10)14/h1-8H	-3.28
InChI=1S/C7H8N2O3S/c1-2-12-6(11)4-3-8-7(13)9-5(4)10/h3H,2H2,1H3,(H2,8,9,10,13)	-2.099
InChI=1S/C7H14N2O3/c8-7(12)9-5-3-1-2-4-6(10)11/h1-5H2,(H,10,11)(H3,8,9,12)	-2.16
InChI=1S/C10H12/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,4-5,7-10H,3,6H2	-3.82
InChI=1S/C24H51O4P/c1-7-13-16-22(10-4)19-26-29(25,27-20-23(11-5)17-14-8-2)28-21-24(1h22-24H,7-21H2,1-6H3	-8.86
InChI=1S/C12H13N3O3S2/c1-8-7-19-12(13-8)15-20(17,18)11-5-3-10(4-6-11)14-9(2)16/h3-7H,1-2H3,(H,13,15)(H,14,16)	-4.15
InChI=1S/C7H9NO3/c1-3-4-8-6(9)5(2)11-7(8)10/h3,5H,1,4H2,2H3	-0.738
InChI=1S/C7H14O4/c1-2-3-7(10)11-5-6(9)4-8/h6,8-9H,2-5H2,1H3	-1.335
InChI=1S/C21H26N2O3/c1-3-20-10-6-11-22-12-9-15-14-7-4-5-8-16(14)23(17(15)18(20)22)21(h4-5,7-8,18,25H,3,6,9-13H2,1-2H3	-4.834
InChI=1S/C3H9O3PS/c1-4-7(8,5-2)6-3/h1-3H3	-1.334
InChI=1S/C15H32OS/c1-14(16)13-17-12-10-8-6-5-7-9-11-15(2,3)4/h14,16H,5-13H2,1-4H3	-4.731
InChI=1S/C11H22N2O4/c1-5-11(4,6-16-9(12)14)7-17-10(15)13-8(2)3/h8H,5-7H2,1-4H3,(H2,12,14)(H,13,15)	-2.591
InChI=1S/C2HF3O2/c3-2(4,5)1(6)7/h(H,6,7)	0.943
InChI=1S/C21H21O4P/c1-16-10-4-7-13-19(16)23-26(22,24-20-14-8-5-11-17(20)2)25-21-15-9h4-15H,1-3H3	-6.558
InChI=1S/C20H21NO3/c1-23-17-10-9-15-19(22)14-7-3-4-8-18(14)24-20(15)16(17)13-21-11-5h3-4,7-10H,2,5-6,11-13H2,1H3	-5.559
InChI=1S/C22H16F2N2/c23-19-12-10-18(11-13-19)22(26-15-14-25-16-26,17-6-2-1-3-7-17)20-h1-16H	-8.4
InChI=1S/C16H23NO4/c18-10-13(19)11-21-15-9-5-4-8-14(15)16(20)17-12-6-2-1-3-7-12/h4-5,8-9,12-13,18-19H,1-3,6-7,10-11H2,(H,17,20)	-3.337
InChI=1S/C3H5N3O/c4-2-1-3(7)6-5/h1,5H2,(H,6,7)	0.419
InChI=1S/C23H27N3O7/c1-25(2)12-5-6-13(27)15-10(12)7-9-8-11-17(26(3)4)19(29)16(22(24)3h5-6,9,11,17,27-28,31,33H,7-8H2,1-4H3,(H2,24,32)	-0.944
InChI=1S/C11H12O3/c1-8(12)3-4-9-5-6-10(13)11(7-9)14-2/h3-7,13H,1-2H3/b4-3+	-1.784
InChI=1S/C30H48O3/c1-25(2)14-16-30(24(32)33)17-15-28(6)19(20(30)18-25)8-9-22-27(5)1h8,20-23,31H,9-18H2,1-7H3,(H,32,33)	-9.926

"InChi"	"logS(M)"
InChI=1S/C18H18ClNO5/c1-4-20(25-18(22)12-8-6-5-7-9-12)17(21)15-14(23-2)11-10-13(19)16(h5-11H,4H2,1-3H3	-4.084
InChI=1S/C8H10O2/c1-6-2-3-8(10)7(4-6)5-9/h2-4,9-10H,5H2,1H3	-0.314
InChI=1S/C22H30O4/c1-13(23)22(26-14(2)24)11-9-20-19-6-4-15-12-16(25)5-7-17(15)18(19h12,17-20H,4-11H2,1-3H3	-4.996
InChI=1S/C9H11BrO3/c10-7-1-3-9(4-2-7)13-6-8(12)5-11/h1-4,8,11-12H,5-6H2	-2.497
InChI=1S/C15H11NO2S/c17-14(18)9-10-6-7-13-12(8-10)16-15(19-13)11-4-2-1-3-5-11/h1-8H,9H2,(H,17,18)	-3.646
InChI=1S/C17H16N4O4/c1-11-8-9-14(15(10-11)21(24)25)19-20-16(12(2)22)17(23)18-13-6-4-3h3-10,16H,1-2H3,(H,18,23)/b20-19+	-7.418
InChI=1S/C10H10N2O3/c11-9(13)6-12-5-7-3-1-2-4-8(7)15-10(12)14/h1-4H,5-6H2,(H2,11,13)	-0.903
InChI=1S/C5H8Br4/c6-1-5(2-7,3-8)4-9/h1-4H2	-5.384
InChI=1S/C3H9N3O3S2/c4-3(5)6-1-2-10-11(7,8)9/h1-2H2,(H4,4,5,6)(H,7,8,9)	0.701
InChI=1S/C12H16O2/c13-12(14)10-6-2-5-9-11-7-3-1-4-8-11/h1,3-4,7-8H,2,5-6,9-10H2,(H,13,14)	-2.603
InChI=1S/C7H7NO3/c1-5-3-2-4-6(9)7(5)8(10)11/h2-4,9H,1H3	-1.64
InChI=1S/C8H18N2O4S2/c9-8(7-15-16(12,13)14)10-5-3-1-2-4-6-11/h11H,1-7H2,(H2,9,10)(H,12,13,14)	-1.22
InChI=1S/C18H23N3O3/c1-2-18(14-9-5-3-6-10-14)15(22)19-17(24)21(16(18)23)13-20-11-7-4-h3,5-6,9-10H,2,4,7-8,11-13H2,1H3,(H,19,22,24)	-3.404
InChI=1S/C13H22N2O3/c1-3-5-6-7-8-9-13(4-2)10(16)14-12(18)15-11(13)17/h3-9H2,1-2H3,(H2,14,15,16,17,18)	-3.43
InChI=1S/C12H18N2O3/c1-4-6-8(3)12(7-5-2)9(15)13-11(17)14-10(12)16/h6H,4-5,7H2,1-3H3,(H2,13,14,15,16,17)/b8-6+	-2.997
InChI=1S/C11H9NO2/c12-11(14)9-5-7-3-1-2-4-8(7)6-10(9)13/h1-6,13H,(H2,12,14)	-1.874
InChI=1S/C12H16NO4PS2/c1-3-15-18(19,16-4-2)20-9-13-10-7-5-6-8-11(10)17-12(13)14/h5-8H,3-4,9H2,1-2H3	-5.191
InChI=1S/C24H32O6/c1-22-9-7-15(25)11-14(22)4-5-17-19(22)20(27)21(28)23(2)16(8-10-2h3,6,12,14-17,19-20,25,27,29H,4-5,7-11H2,1-2H3	-3.474
InChI=1S/C12H21NO3/c1-5-7-13-11(15)16-9-12(4,8-14)10(3)6-2/h1,10,14H,6-9H2,2-4H3,(H,13,15)	-2.528
InChI=1S/C9H10O3/c1-7-2-4-8(5-3-7)12-6-9(10)11/h2-5H,6H2,1H3,(H,10,11)	-2.141
InChI=1S/C20H29N3O/c1-22(2)14-12-20(19(21)24,13-15-23(3)4)18-11-7-9-16-8-5-6-10-17(1h5-11H,12-15H2,1-4H3,(H2,21,24)	-3.285
InChI=1S/C7H6N4O/c1-11-4-10-6-5(7(11)12)8-2-3-9-6/h2-4H,1H3	-1.07

"InChi"	"logS(M)"
InChI=1S/C18H19F2N3O3/c1-8-13(21-2)7-22(8)16-12(19)5-10-15(14(16)20)23(9-3-4-9)6-11(17(1h5-6,8-9,13,21H,3-4,7H2,1-2H3,(H,25,26)	-4.44
InChI=1S/C12H14O4/c1-2-9(11(13)14)10(12(15)16)8-6-4-3-5-7-8/h3-7,9-10H,2H2,1H3,(H,13,14)(H,15,16)	-2.326
InChI=1S/C9H19NO/c1-8(2)5-10(7-11)6-9(3)4/h7-9H,5-6H2,1-4H3	-1.083
InChI=1S/C24H20N4O/c1-16-7-3-6-10-21(16)26-25-19-12-13-22(17(2)15-19)27-28-24-20-9-5h3-15,27H,1-2H3/b26-25+,28-24-	-9.733
InChI=1S/C7H12O4/c1-6(8)10-4-3-5-11-7(2)9/h3-5H2,1-2H3	-0.205
InChI=1S/C12H14O5/c1-15-9-6-8(4-5-11(13)14)7-10(16-2)12(9)17-3/h4-7H,1-3H3,(H,13,14)/b5-4+	-2.83
InChI=1S/C9H13N3O2/c1-8(9(13)14)12(6-2-4-10)7-3-5-11/h8H,2-3,6-7H2,1H3,(H,13,14)	-0.17
InChI=1S/C4H6O4/c1-2(3(5)6)4(7)8/h2H,1H3,(H,5,6)(H,7,8)	0.76
InChI=1S/C7H7ClO/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2	-1.756
InChI=1S/C19H38N2O3/c1-4-5-6-7-8-9-10-11-12-14-18(22)20-15-13-16-21(2,3)17-19(23)24/h4-17H2,1-3H3,(H-,20,22,23,24)	-3.137
InChI=1S/C15H23N3O4S/c1-14(2)9(12(20)21)18-10(19)8(11(18)23-14)17-13(22)15(16)6-4-3-5-h8-9,11H,3-7,16H2,1-2H3,(H,17,22)(H,20,21)	-1.04
InChI=1S/C16H23NO4/c1-3-5-6-11-21-14-9-7-13(8-10-16(18)17-19)12-15(14)20-4-2/h7-10,12,19H,3-6,11H2,1-2H3,(H,17,18)/b10-8+	-4.184
InChI=1S/C8H18OS/c1-7(2)5-10(9)6-8(3)4/h7-8H,5-6H2,1-4H3/p+1	-1.732
InChI=1S/C11H15NO2/c1-3-12(11(13)14-4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3	0.867
InChI=1S/C12H11NO2/c1-9-12(15)11(14)7-8-13(9)10-5-3-2-4-6-10/h2-8,15H,1H3	-2.03
InChI=1S/C9H11NO3/c11-6-5-10-8-4-2-1-3-7(8)9(12)13/h1-4,10-11H,5-6H2,(H,12,13)	-1.676
InChI=1S/C18H27NO4/c1-13(2)15-6-5-14(3)16(18(20)21-4)17(15)23-12-9-19-7-10-22-11-8-1h5-6,13H,7-12H2,1-4H3	-3.287
InChI=1S/C17H26ClNO2/c1-4-11-21-12-10-19(16(20)13-18)17-14(5-2)8-7-9-15(17)6-3/h7-9H,4-6,10-13H2,1-3H3	-3.795
InChI=1S/C9H12O3S/c1-7(2)8-3-5-9(6-4-8)13(10,11)12/h3-7H,1-2H3,(H,10,11,12)	0.613
InChI=1S/C3H5N3/c4-3-1-5-6-2-3/h1-2H,4H2,(H,5,6)	1.08
InChI=1S/C9H14ClN5O2/c1-3-11-8-13-7(10)14-9(15-8)12-5-6(16)17-4-2/h3-5H2,1-2H3,(H2,11,12,13,14,15)	-2.937
InChI=1S/C18H17N3S4/c1-18(2,3)21(24-16-19-12-8-4-6-10-14(12)22-16)25-17-20-13-9-5-7-1h4-11H,1-3H3	-8.363
InChI=1S/C14H11Cl2NO3/c15-10-6-9(18)7-11(16)14(10)17-12-4-2-1-3-8(12)5-13(19)20/h1-4,6-7,17-18H,5H2,(H,19,20)	-4.241

"InChi"	"logS(M)"
InChI=1S/C10H24N2/c11-9-7-5-3-1-2-4-6-8-10-12/h1-12H2	1.528
InChI=1S/C7H8N2O3/c1-12-5-2-3-6(8)7(4-5)9(10)11/h2-4H,8H2,1H3	-1.226
InChI=1S/C4H4N2O4/c7-1-2(8)5-4(10)6-3(1)9/h1,7H,(H2,5,6,8,9,10)	-0.843
InChI=1S/C14H8O3/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7,15H	-4.421
InChI=1S/C7H12O4/c1-4(2)5(7(10)11)3-6(8)9/h4-5H,3H2,1-2H3,(H,8,9)(H,10,11)	-0.407
InChI=1S/C25H31NOS/c1-28-21-9-5-18(6-10-21)11-14-26-15-13-25-12-3-2-4-22(25)24(26)16h5-10,17,22,24,27H,2-4,11-16H2,1H3	-5.591
InChI=1S/C9H5BrClN3O2/c10-7-4-6(9(15)16)14(13-7)8-5(11)2-1-3-12-8/h1-4H,(H,15,16)	-1.449
InChI=1S/C7H6N2OS/c10-6-4-11-7-5(9-6)2-1-3-8-7/h1-3H,4H2,(H,9,10)	-1.204
InChI=1S/C12H17NO/c1-10-12(14-9-8-13(10)2)11-6-4-3-5-7-11/h3-7,10,12H,8-9H2,1-2H3	-1.043
InChI=1S/C7H7IO3/c9-7(10)5-3-1-2-4-6(5)8-11/h1-4H,8H2,(H,9,10)	0.512
InChI=1S/C9H9FN4O4S3/c1-14-8(19-9(12-14)20(11,15)16)13-21(17,18)7-4-2-6(10)3-5-7/h2-5H,1H3,(H2,11,15,16)/b13-8+	-2.03
InChI=1S/C3H5N3S/c1-6-2-4-5-3(6)7/h2H,1H3,(H,5,7)	-1.65
InChI=1S/C4H9NO2/c1-2-3-4-5(6)7/h2-4H2,1H3	-1.351
InChI=1S/C7H11NO2/c1-2-7(9)8-3-5-10-6-4-8/h2H,1,3-6H2	0.85
InChI=1S/C21H28N2O2/c1-16(2)21(20(22)24,10-11-23-12-14-25-15-13-23)19-9-5-7-17-6-3-4-h3-9,16H,10-15H2,1-2H3,(H2,22,24)	-4.083
InChI=1S/C22H30N2O/c1-17(2)22(21(23)25,13-16-24-14-6-3-7-15-24)20-12-8-10-18-9-4-5-1h4-5,8-12,17H,3,6-7,13-16H2,1-2H3,(H2,23,25)	-5.562
InChI=1S/C12H2Cl8/c13-3-1-4(14)6(5(15)2-3)7-8(16)10(18)12(20)11(19)9(7)17/h1-2H	-9.48
InChI=1S/C18H14/c1-3-9-15(10-4-1)17-13-7-8-14-18(17)16-11-5-2-6-12-16/h1-14H	-5.269
InChI=1S/C10H10ClNO2/c1-7(13)6-10(14)12-9-5-3-2-4-8(9)11/h2-5H,6H2,1H3,(H,12,14)	-2.407
InChI=1S/C18H21NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18)9-1h3,6,11-12,17H,4-5,7-9H2,1-2H3	-1.64
InChI=1S/C12H12N2O3/c1-2-17-12(16)10-8-11(15)14(13-10)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3	-3.255
InChI=1S/C9H24N2O6P2S2/c12-18(13,14)20-8-2-6-10-4-1-5-11-7-3-9-21-19(15,16)17/h10-11H,1-9H2,(H2,12,13,14)(H2,15,16,17)	-0.948
InChI=1S/C20H21NO3/c1-13-18(22)15-10-11-17(23-4)16(12-21(2)3)20(15)24-19(13)14-8-6-5h5-11H,12H2,1-4H3	-3.667
InChI=1S/C15H24O/c1-11-6-8-13(9-7-11)12(2)10-14-4-3-5-15(14)16/h6,12-14H,3-5,7-10H2,1-2H3	-4.68

"InChi"	"logS(M)"
InChI=1S/C13H12N2O/c14-11-6-2-1-5-10(11)9-15-12-7-3-4-8-13(12)16/h1-9,16H,14H2/b15-9+	-3.64
InChI=1S/C11H10O3/c1-8(12)2-3-9-4-5-10-11(6-9)14-7-13-10/h2-6H,7H2,1H3/b3-2+	-2.382
InChI=1S/C15H12N2O3/c1-8-14(9(2)20-17-8)16-12-7-13(18)15(19)11-6-4-3-5-10(11)12/h3-7,18H,1-2H3/b16-12+	-3.89
InChI=1S/C10H4Cl4/c11-5-1-7-8(10(14)3-5)2-6(12)4-9(7)13/h1-4H	-7.823
InChI=1S/C11H12ClN5/c1-16-4-5-17(11(16)15-8-13)7-9-2-3-10(12)14-6-9/h2-3,6H,4-5,7H2,1H3/b15-11+	-2.13
InChI=1S/C20H23N3O2/c1-20(2,3)18(24)19(23-14-21-13-22-23)25-17-11-9-16(10-12-17)15-7-h4-14,18-19,24H,1-3H3	-4.829
InChI=1S/C9H17NOS/c1-4-7-12-9(5-2,6-3)8(10)11/h4H,1,5-7H2,2-3H3,(H2,10,11)	-2.509
InChI=1S/C10H18ClN3O2/c1-8-2-4-9(5-3-8)12-10(15)14(13-16)7-6-11/h8-9H,2-7H2,1H3,(H,12,15)	-3.826
InChI=1S/C10H16N6O2/c17-5-7(6-18)11-8-12-9(15-1-2-15)14-10(13-8)16-3-4-16/h7,17-18H,1-6H2,(H,11,12,13,14)	-2.082
InChI=1S/C10H14O4/c1-7(2)9(11)13-5-6-14-10(12)8(3)4/h1,3,5-6H2,2,4H3	-2.261
InChI=1S/C11H20N2O4/c1-4-6-11(3,7-16-9(12)14)8-17-10(15)13-5-2/h5H,2,4,6-8H2,1,3H3,(H2,12,14)(H,13,15)	-2.522
InChI=1S/C18H20N4O2/c1-21(2)12-6-11-19-18-13-7-3-4-8-14(13)20-15-9-5-10-16(17(15)18)2h3-5,7-10H,6,11-12H2,1-2H3,(H,19,20)	-3.837
InChI=1S/C12H13NO6/c1-3-7(2)19-12(16)8-5-4-6-9(13(17)18)10(8)11(14)15/h4-7H,3H2,1-2H3,(H,14,15)/p-1	-2.719
InChI=1S/C12H24O3/c1-6-8-9-10(7-2)11(13)14-15-12(3,4)5/h10H,6-9H2,1-5H3	-3.67
InChI=1S/C10H20N2O4/c13-7-5-11-9(15)3-1-2-4-10(16)12-6-8-14/h13-14H,1-8H2,(H,11,15)(H,12,16)	0.412
InChI=1S/C11H22N2O4/c1-4-8(5-2)11(3,6-16-9(12)14)7-17-10(13)15/h8H,4-7H2,1-3H3,(H2,12,14)(H2,13,15)	-2.613
InChI=1S/C3H6O/c1-2-3-4/h2,4H,1,3H2	1.236
InChI=1S/C21H25NO5/c1-22-15-8-6-12-10-18(25-3)20(26-4)21(27-5)19(12)13-7-9-17(24-2)1h7,9-11,15,22H,6,8H2,1-5H3	-2.07
InChI=1S/C17H14N4O4/c1-18-17(23)20-14-8-7-12(21(24)25)9-13(14)16(19-10-15(20)22)11-5-h2-9H,10H2,1H3,(H,18,23)	-3.56
InChI=1S/C9H17N5O/c1-5(2)10-7-12-8(11-6(3)4)14-9(15)13-7/h5-6H,1-4H3,(H3,10,11,12,13,14,15)	-2.81
InChI=1S/C12H5Cl5O/c13-6-2-1-3-10(12(6)17)18-11-5-8(15)7(14)4-9(11)16/h1-5H	-7.48

"InChi"	"logS(M)"
InChI=1S/C8H16N2O2S2/c1-5-11-6-2-9(1)13-14-10-3-7-12-8-4-10/h1-8H2	-3.26
InChI=1S/C13H9FN2/c14-8-5-6-10-12(7-8)16-11-4-2-1-3-9(11)13(10)15/h1-7H,(H2,15,16)	-2.12
InChI=1S/C42H59N7O9/c1-25(2)18-30(34(50)22-35(51)45-31(19-26(3)4)39(54)49-36(40(55)5(h8-17,23-26,30-34,36,50H,18-22H2,1-7H3,(H,43,44)(H,45,51)(H,46,53)(H,47,52)(H,48,57)(H,49,54)(H,55,56)	-3.13
InChI=1S/C9H5N5O2/c10-5-8(6-11)13-12-7-1-3-9(4-2-7)14(15)16/h1-4,12H	-3.184
InChI=1S/C14H22N2O3/c1-2-3-9-11-12(17)15-14(19)16(13(11)18)10-7-5-4-6-8-10/h10-11H,2-9H2,1H3,(H,15,17,19)	-3.684
InChI=1S/C32H24Cl2N8O2/c1-19-29(31(43)41(39-19)23-9-5-3-6-10-23)37-35-27-15-13-21(17-25(h3-18,35-36H,1-2H3/b37-29-,38-30+	-8.142
InChI=1S/C18H15P/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H	-6.201
InChI=1S/C7H8O3/c1-9-5-7-3-2-6(4-8)10-7/h2-4H,5H2,1H3	-0.499
InChI=1S/C11H16O3/c1-9-5-3-4-6-10(9)14-8-11(2,13)7-12/h3-6,12-13H,7-8H2,1-2H3	-1.88
InChI=1S/C49H96O6/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-47(52)h50-51H,3-46H2,1-2H3	-8.349
InChI=1S/C13H7Cl3O5/c14-9-4-3-8(21-9)13(19)6-1-2-7(12(16)11(6)15)20-5-10(17)18/h1-4H,5H2,(H,17,18)	-4.376
InChI=1S/C7H4N2O7/c10-6-4(7(11)12)1-3(8(13)14)2-5(6)9(15)16/h1-2,10H,(H,11,12)	-1.057
InChI=1S/C18H27NO5/c1-5-10-23-18(21)12-14-8-9-15(16(11-14)22-4)24-13-17(20)19(6-2)7-h8-9,11H,5-7,10,12-13H2,1-4H3	-2.644
InChI=1S/C15H21NO3/c1-3-4-5-10-19-14-8-6-13(7-9-14)11-12(2)15(17)16-18/h6-9,11,18H,3-5,10H2,1-2H3,(H,16,17)/b12-11-	-4.387
InChI=1S/C10H7Cl2NO/c1-5-2-3-6-7(11)4-8(12)10(14)9(6)13-5/h2-4,14H,1H3	-3.244
InChI=1S/C11H17NO2/c1-8(2)12-7-11(14)9-4-3-5-10(13)6-9/h3-6,8,11-14H,7H2,1-2H3	0.37
InChI=1S/C7H5ClF3N/c8-4-1-2-6(12)5(3-4)7(9,10)11/h1-3H,12H2	-2.293
InChI=1S/C19H23NO5/c1-13(19(23)25-12-18(22)20(2)8-9-21)14-4-5-16-11-17(24-3)7-6-15(1h4-7,10-11,13,21H,8-9,12H2,1-3H3	-3.39
InChI=1S/C7H5I2NO2/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2H,10H2,(H,11,12)	-5.192
InChI=1S/C20H38O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h4H,2-3,5-19H2,1H3	-6.15
InChI=1S/C34H56N4O4/c1-5-9-15-27(7-3)25-41-23-13-21-35-33(39)37-31-19-11-18-30-29(31h11-12,17-20,27-28H,5-10,13-16,21-26H2,1-4H3,(H2,35,37,39)(H2,36,38,40)	-8.068

"InChi"	"logS(M)"
InChI=1S/C31H25NO2/c33-30(24-14-5-1-6-15-24,25-16-7-2-8-17-25)28-22-13-23-29(32-28)3h1-23,33-34H	-7.543
InChI=1S/C22H26O8/c1-5-27-19(23)17(20(24)28-6-2)13-15-9-11-16(12-10-15)14-18(21(25)h9-14H,5-8H2,1-4H3	-5.622
InChI=1S/C14H22O/c1-10-6-7-11(2)14(4,5)13(10)9-8-12(3)15/h6,8-9,11,13H,7H2,1-5H3/b9-8+	-3.803
InChI=1S/C5H12N2O4S/c1-2-3-4-11-5(8)7-12(6,9)10/h2-4H2,1H3,(H,7,8)(H2,6,9,10)	-1.038
InChI=1S/C25H20N4O4/c1-15-7-3-6-10-21(15)26-25(31)20-14-17-8-4-5-9-19(17)23(24(20)30)h3-14,27H,1-2H3,(H,26,31)/b28-23-	-7.981
InChI=1S/C15H17N3O3/c19-13-10-12(15(20)11-2-1-3-17-14(11)13)16-4-5-18-6-8-21-9-7-18/h1-3,10,16H,4-9H2	0.058
InChI=1S/C4H4ClN3O2/c1-7-2-6-3(5)4(7)8(9)10/h2H,1H3	-1.359
InChI=1S/C12H18O4S2/c1-7(2)15-10(13)9(11(14)16-8(3)4)12-17-5-6-18-12/h7-8H,5-6H2,1-4H3	-3.731
InChI=1S/C19H16O3/c20-18-15-9-3-4-11-16(15)22-19(21)17(18)14-10-5-7-12-6-1-2-8-13(1h1-4,6,8-9,11,14,21H,5,7,10H2	-4.864
InChI=1S/C12H15Cl2N5O/c1-12(2)18-10(15)17-11(16)19(12)20-6-7-3-4-8(13)9(14)5-7/h3-5H,6H2,1-2H3,(H4,15,16,17,18)	-2.715
InChI=1S/C19H20F3NO4/c1-3-4-11-25-18(24)13(2)26-15-6-8-16(9-7-15)27-17-10-5-14(12-23-1h5-10,12-13H,3-4,11H2,1-2H3	-5.584
InChI=1S/C10H9NO3/c1-6(12)11-8-3-2-7-5-14-10(13)9(7)4-8/h2-4H,5H2,1H3,(H,11,12)	-2.6
InChI=1S/C13H9ClN2O3/c14-10-2-1-3-11(12(10)13(18)19)16-15-8-4-6-9(17)7-5-8/h1-7,17H,(H,18,19)/b16-15+	-3
InChI=1S/C17H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h2-16H2,1H3,(H,18,19)	-4.69
InChI=1S/C8H8N4O6/c1-2-9-8-6(11(15)16)3-5(10(13)14)4-7(8)12(17)18/h3-4,9H,2H2,1H3	-3.409
InChI=1S/C11H15NO3/c1-9-5-2-3-6-10(9)14-7-4-8-15-11(12)13/h2-3,5-6H,4,7-8H2,1H3,(H2,12,13)	-2.658
InChI=1S/C8H12O4/c1-6(4-11-7(2)9)5-12-8(3)10/h1,4-5H2,2-3H3	-0.78
InChI=1S/C18H16N6O2/c1-2-23(11-3-10-19)16-6-4-15(5-7-16)21-22-18-9-8-17(24(25)26)12-1h4-9,12H,2-3,11H2,1H3/b22-21+	-6.053
InChI=1S/C12H12N4O3S/c1-9(17)15-10-3-5-11(6-4-10)20(18,19)16-12-13-7-2-8-14-12/h2-8H,1H3,(H,15,17)(H,13,14,16)	-3.59
InChI=1S/C13H18O/c1-10(2)12-4-6-13(7-5-12)11(3)8-9-14/h4-7,9-11H,8H2,1-3H3	-3.46
InChI=1S/C3H5Cl3O/c1-2(7)3(4,5)6/h2,7H,1H3	-0.757

"InChi"	"logS(M)"
InChI=1S/C9H15NOS/c1-4-7-12-9(5-2,6-3)8(10)11/h1H, 5-7H2,2-3H3,(H2,10,11)	-1.952
InChI=1S/C8H15N2O4P/c1-4-12-15(11,13-5-2)14-8-6-7(3)9-10-8/ h6H,4-5H2,1-3H3,(H,9,10)	-2.37
InChI=1S/C13H20N2O4/ c1-13(11(17)19-3,9-7-5-4-6-8-9)10(16)15-12(18)14-2/h7H, 4-6,8H2,1-3H3,(H2,14,15,16,18)	-2.68
InChI=1S/C20H26O3/ c1-3-20(18(21)9-10-19(20)22)12-11-14-5-4-6-15-13-16(23-2)7-8-17(1 h7-8,11,13,18,21H,3-6,9-10,12H2,1-2H3/b14-11+	-4.123
InChI=1S/C15H28O3/ c16-15-11-7-4-2-1-3-5-8-12-17-13-9-6-10-14-18-15/h1-14H2	-3.884
InChI=1S/C8H14O2/c1-4-7(3)6-10-8(9)5-2/h5,7H,2,4,6H2,1,3H3	-2.653
InChI=1S/C12H18O/c1-8-6-9(2)11(13)10(7-8)12(3,4)5/h6-7,13H, 1-5H3	-3.172
InChI=1S/C11H13NO2/c1-8(7-9(2)13)12-10-3-5-11(14)6-4-10/ h3-6,14H,7H2,1-2H3/b12-8-	-3.59
InChI=1S/C13H24N2O4/ c1-5-6-13(4,8-18-11(14)16)9-19-12(17)15-7-10(2)3/ h2,5-9H2,1,3-4H3,(H2,14,16)(H,15,17)	-3.614
InChI=1S/C19H27NO3/ c1-3-14-22-18-10-8-17(9-11-18)19(21)23-15-6-13-20-12-5-4-7-16(20) h3,8-11,16H,1,4-7,12-15H2,2H3	-4.539
InChI=1S/C18H25N3/ c19-16-18(21-11-5-2-6-12-21)9-13-20(14-10-18)15-17-7-3-1-4-8-17/ h1,3-4,7-8H,2,5-6,9-15H2/p+2	-2.246
InChI=1S/C3H7ClO/c4-2-1-3-5/h5H,1-3H2	0.422
InChI=1S/C11H10N2O2/c1-8(14)12-11-13-10(7-15-11)9-5-3-2-4-6-9/ h2-7H,1H3,(H,12,13,14)	-2.13
InChI=1S/C14H21Br2NO2/ c1-4-17(5-2)6-7-19-10-11-8-12(15)9-13(16)14(11)18-3/h8-9H, 4-7,10H2,1-3H3	-3.852
InChI=1S/C12H22N2O3S2/ c1-11(2)8-4-5-12(11,3)9(6-8)14-10(13)7-18-19(15,16)17/h8-9H, 4-7H2,1-3H3,(H2,13,14)(H,15,16,17)	-3.612
InChI=1S/C8H16O2/c1-4-8(5-2)6-10-7(3)9/h8H,4-6H2,1-3H3	-1.353
InChI=1S/C20H23N3O/ c24-19(10-9-18-6-2-1-3-7-18)11-13-22-14-16-23(17-15-22)20-8-4-5-1 h1-10,12H,11,13-17H2/b10-9+	-3.017
InChI=1S/C17H12Br2O3/ c1-2-13-15(10-5-3-4-6-14(10)22-13)16(20)9-7-11(18)17(21)12(19)8-9 h3-8,21H,2H2,1H3	-6.627
InChI=1S/C5H3F7/c6-2-1-3(7,8)5(11,12)4(2,9)10/h2H,1H2	-2.437
InChI=1S/C7H6N4O/c1-4-2-8-5-6(11-4)9-3-10-7(5)12/h2-3H,1H3, (H,9,10,11,12)	-1.56
InChI=1S/C14H15N3O/ c1-9-7-10(2)16-13(8-9)17-14(18)11-3-5-12(15)6-4-11/h3-8H, 15H2,1-2H3,(H,16,17,18)	-2.881
InChI=1S/C2H4Cl3O4P/c3-2(4,5)1-9-10(6,7)8/h1H2,(H2,6,7,8)	-1.841

"InChi"	"logS(M)"
InChI=1S/C11H14N4O2/c1-14-9-7(10(16)15(2)11(14)17)12-8(13-9)6-4-3-5-6/h6H,3-5H2,1-2H3,(H,12,13)	-2.142
InChI=1S/C8H18O3/c1-7(2)3-4-11-6-8(10)5-9/h7-10H,3-6H2,1-2H3	-1.21
InChI=1S/C3H2F6O/c4-2(5,6)1(10)3(7,8)9/h1,10H	0.02
InChI=1S/C14H20O2/c1-4-8-13(15)16-14(2,3)11-12-9-6-5-7-10-12/h5-7,9-10H,4,8,11H2,1-3H3	-4.136
InChI=1S/C20H24BrN3O/c1-4-24(5-2)20(25)12-9-14-13-7-6-8-16-18(13)15(19(21)22-16)10-17(h6-9,12,17,22H,4-5,10-11H2,1-3H3	-4.505
InChI=1S/C9H9Br2NO3/c10-5-1-4(2-6(11)8(5)13)3-7(12)9(14)15/h1-2,7,13H,3,12H2,(H,14,15)	-1.928
InChI=1S/C32H64O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-34-32(33)30-28-26-24-h3-31H2,1-2H3	-8.755
InChI=1S/C9H10ClNO/c1-11-5-8-4-9(10)3-2-7(8)6-12-11/h2-4H,5-6H2,1H3	-2.735
InChI=1S/C11H14N2O6/c14-8-3-1-6(10(16)17)12(8)5-13-7(11(18)19)2-4-9(13)15/h6-7H,1-5H2,(H,16,17)(H,18,19)	-1.31
InChI=1S/C12H20N2O2/c1-5-9(4)11-7-13-10(6-8(2)3)12(15)14(11)16/h7-9,16H,5-6H2,1-4H3	-4.007
InChI=1S/C21H28N2O/c1-16(2)12-13-21(20(22)24,14-15-23(3)4)19-11-7-9-17-8-5-6-10-18(1h5-12H,13-15H2,1-4H3,(H2,22,24)	-5.064
InChI=1S/C18H11NO3/c20-14-9-10-5-1-4-8-13(10)19-16(14)15-17(21)11-6-2-3-7-12(11)18(1h1-9,19-20H	-7.046
InChI=1S/C5H10O2/c1-2-4-7-5-6-3-1/h1-5H2	0.411
InChI=1S/C17H14N4O3/c1-11-15(16(22)21(20-11)14-5-3-2-4-6-14)19-18-13-9-7-12(8-10-13)1h2-10,15H,1H3,(H,23,24)/b19-18+	-5.767
InChI=1S/C13H22ClN5S/c1-9(2)15-13-16-11(14)10(20-4)12(17-13)19-7-5-18(3)6-8-19/h9H,5-8H2,1-4H3,(H,15,16,17)	-2.495
InChI=1S/C24H33N3O3/c25-23(28)24(8-10-26-12-16-29-17-13-26,9-11-27-14-18-30-19-15-27h1-7H,8-19H2,(H2,25,28)	-3.236
InChI=1S/C26H20ClN5O4/c1-14(33)29-17-7-9-18(10-8-17)30-26(36)20-12-15-4-2-3-5-19(15)23(h2-13,31H,1H3,(H2,28,35)(H,29,33)(H,30,36)/b32-23-	-7.304
InChI=1S/C9H11FN2O5/c1-3-5(13)6(14)8(17-3)12-2-4(10)7(15)11-9(12)16/h2-3,5-6,8,13-14H,1H3,(H,11,15,16)	-0.252
InChI=1S/C11H20N2O/c1-3-11(14)13-9-5-4-6-10(13)8-12(2)7-9/h9-10H,3-8H2,1-2H3	-1.32
InChI=1S/C11H9ClN2O2S/c12-11-10(7-4-8-13-11)14-17(15,16)9-5-2-1-3-6-9/h1-8,14H	-3.76
InChI=1S/C12H9N3O3/c16-12(14-10-5-7-13-8-6-10)9-1-3-11(4-2-9)15(17)18/h1-8H,(H,13,14,16)	-2.978

"InChi"	"logS(M)"
InChI=1S/C10H5ClN2O4/c11-10-7-4-2-1-3-6(7)8(12(14)15)5-9(10)13(16)17/h1-5H	-5.4
InChI=1S/C12H15IO3/c1-2-3-4-7-16-12(15)9-5-6-11(14)10(13)8-9/h5-6,8,14H,2-4,7H2,1H3	-4.22
InChI=1S/C12H3Cl7/c13-5-2-7(15)6(14)1-4(5)10-8(16)3-9(17)11(18)12(10)19/h1-3H	-7.92
InChI=1S/C11H16N2O4S2/c1-17-10-4-2-9(3-5-10)6-7-13-11(12)8-18-19(14,15)16/h2-5H,6-8H2,1H3,(H2,12,13)(H,14,15,16)	-2.569
InChI=1S/C10H16O/c1-8(2)6-10-7-9(3)4-5-11-10/h6,10H,3-5,7H2,1-2H3	-2.51
InChI=1S/C3H2ClF5/c4-1(5)3(8,9)2(6)7/h1-2H	-3.068
InChI=1S/C10H12BrNO2/c1-3-12-10(14)8-5-7(11)4-6(2)9(8)13/h4-5,13H,3H2,1-2H3,(H,12,14)	-3.586
InChI=1S/C18H30N2/c1-15(2)20(16(3)4)14-13-19-12-8-7-10-17-9-5-6-11-18(17)19/h5-6,9,11,15-16H,7-8,10,12-14H2,1-4H3	-4.551
InChI=1S/C15H29N3O/c1-4-15(19)18-13-7-8-14(18)12-17(11-13)10-9-16(5-2)6-3/h13-14H,4-12H2,1-3H3	-1.999
InChI=1S/C11H16O/c1-8(2)10-6-5-9(3)7-11(10)12-4/h5-8H,1-4H3	-3.881
InChI=1S/C9H10F3NO2/c1-6-7(4-14)13-3-2-8(6)15-5-9(10,11)12/h2-3,14H,4-5H2,1H3	-1.792
InChI=1S/C17H18N2O2/c1-13(19-12-15-7-3-5-9-17(15)21)10-18-11-14-6-2-4-8-16(14)20/h2-9,11-13,18-19H,10H2,1H3/b14-11-,15-12+	-3.172
InChI=1S/C15H20N2O4S3/c1-3-11(2)17-9-12-5-4-6-13(7-12)23(18,19)14-8-15(22-10-14)24(16,2(	-1.33
InChI=1S/C12H15NO3/c1-9(2)13-11(14)8-16-12(15)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3,(H,13,14)	-2.732
InChI=1S/C34H46N2O3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-25-39-32-24-19-18-23-29(32)3	-4.847
InChI=1S/C18H24O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h14-16H,2-10H2,1H3	-4.055
InChI=1S/C10H11N5O/c1-16-7-4-2-6(3-5-7)8-13-9(11)15-10(12)14-8/h2-5H,1H3,(H4,11,12,13,14,15)	-2.087
InChI=1S/C11H7FN2O4/c12-8-6-13-10(16)14(9(8)15)11(17)18-7-4-2-1-3-5-7/h1-6H,(H,13,16)	-3.22
InChI=1S/C19H29NO5/c1-12(2)15-9-8-13(3)17(19(22)23-7)18(15)24-11-16(21)25-14(4)10-2(	-3.802
InChI=1S/C5H11NO2/c1-6(2)4-5(7)8-3/h4H2,1-3H3	0.931
InChI=1S/C19H24N4O6/c1-6-22(7-2)17(25)13(11-20)8-12-9-14(23(27)28)16(24)15(10-12)29-1	-3.53
InChI=1S/C8H16O3/c1-3-4-6-11-7-5-8(9)10-2/h3-7H2,1-2H3	-1.291

"InChi"	"logS(M)"
InChI=1S/C24H50O/c1-3-5-7-9-11-13-14-16-18-20-22-24(23-25)21-19-17-15-12-10-8-6-4-h24-25H,3-23H2,1-2H3	-5.55
InChI=1S/C10H13NO/c1-3-10(12)8-4-6-9(11-2)7-5-8/h4-7,11H,3H2,1-2H3	-1.925
InChI=1S/C12H3Cl7O/c13-4-1-2-7(11(19)8(4)16)20-12-9(17)5(14)3-6(15)10(12)18/h1-3H	-9.09
InChI=1S/C11H17NO3/c1-13-9-6-8(4-5-12)7-10(14-2)11(9)15-3/h6-7H,4-5,12H2,1-3H3	-0.4
InChI=1S/C12H5Cl5O/c13-6-1-4-10(9(16)5-6)18-12-8(15)3-2-7(14)11(12)17/h1-5H	-7.24
InChI=1S/C6H7N3O/c7-5-2-1-4(3-9-5)6(8)10/h1-3H,(H2,7,9)(H2,8,10)	-0.892
InChI=1S/C10H23NO3S2/c1-3-4-5-6-7-10(2)11-8-9-15-16(12,13)14/h10-11H,3-9H2,1-2H3,(H,12,13,14)	-1.753
InChI=1S/C10H16O4/c1-9(2)6(7(11)12)4-5-10(9,3)8(13)14/h6H,4-5H2,1-3H3,(H,11,12)(H,13,14)	-1.42
InChI=1S/C9H16N8O4S2/c1-17(7(10)11)4-6(19)13-3-2-5(18)14-8-15-16-9(22-8)23(12,20)21/h2-4H2,1H3,(H3,10,11)(H,13,19)(H2,12,20,21)(H,14,15,18)	-1.13
InChI=1S/C14H21N3O4S/c1-6-10-9(7(2)18)13(19)17(10)11(14(20)21)12(6)22-5-8(15)16(3)4/h6-7,9-10,15,18H,5H2,1-4H3,(H,20,21)/b15-8-	-0.28
InChI=1S/C35H61NO12/c1-16-14-35(15-43-35)32(40)19(4)27(37)18(3)22(7)46-33(41)21(6)31(h16-31,34,37-39H,12-15H2,1-11H3	-4.647
InChI=1S/C9H18Cl3O4P/c1-7(4-10)14-17(13,15-8(2)5-11)16-9(3)6-12/h7-9H,4-6H2,1-3H3	-2.436
InChI=1S/C15H10O4/c16-14(17)11-7-3-1-5-9(11)13-10-6-2-4-8-12(10)15(18)19-13/h1-8,13H,(H,16,17)	-3.104
InChI=1S/C20H14O2/c21-19-17-13-7-8-14-18(17)20(22-19,15-9-3-1-4-10-15)16-11-5-2-6-1h1-14H	-3.85
InChI=1S/C14H19NO/c16-14(11-12-7-3-1-4-8-12)15-13-9-5-2-6-10-13/h1,3-4,7-8,13H,2,5-6,9-11H2,(H,15,16)	-3.588
InChI=1S/C5H10Cl2O2/c6-1-5(2-7,3-8)4-9/h8-9H,1-4H2	-1.028
InChI=1S/C16H24N2/c1-11-8-13(16(3,4)5)9-12(2)14(11)10-15-17-6-7-18-15/h8-9H,6-7,10H2,1-5H3,(H,17,18)	-6.191
InChI=1S/C15H17FN4O3/c1-2-19-8-10(15(22)23)12(21)9-7-11(16)14(18-13(9)19)20-5-3-17-4-6h7-8,17H,2-6H2,1H3,(H,22,23)	-2.92
InChI=1S/C9H7NS/c1-2-4-8(5-3-1)9-6-11-7-10-9/h1-7H	-2.732
InChI=1S/C15H10O2/c1-9-6-7-12-13(8-9)15(17)11-5-3-2-4-10(11)14(12)16/h2-8H,1H3	-6.117
InChI=1S/C20H34N2O2S2/c1-17(2,11-23)9-19(5,6)15-21-13-14(25-15)22-16(26-13)20(7,8)10-18h23-24H,9-12H2,1-8H3	-7.375
InChI=1S/C8H9ClO2/c1-10-6-3-4-8(11-2)7(9)5-6/h3-5H,1-2H3	-2.672

"InChi"	"logS(M)"
InChI=1S/C14H28N2O3/c1-2-3-4-5-6-10-13(17)16-11-8-7-9-12(15)14(18)19/h12H,2-11,15H2,1H3,(H,16,17)(H,18,19)	0.058
InChI=1S/C5H6N2/c6-5-1-3-7-4-2-5/h1-4H,(H2,6,7)	-0.053
InChI=1S/C19H23ClN2O2/c1-3-22(4-2)12-13-24-18-11-10-15(20)14-17(18)19(23)21-16-8-6-5-7-h5-11,14H,3-4,12-13H2,1-2H3,(H,21,23)	-5.235
InChI=1S/C13H26N2O4/c1-5-13(6-2,9-14-11(16)18-7-3)10-15-12(17)19-8-4/h5-10H2,1-4H3,(H,14,16)(H,15,17)	-3.675
InChI=1S/C18H22O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h3-5,10,14,16-17,19-20H,2,6-9H2,1H3	-4.4
InChI=1S/C14H16N2O3S/c15-11-1-5-13(6-2-11)20(18,19)14-7-3-12(4-8-14)16-9-10-17/h1-8,16-17H,9-10,15H2	-2.597
InChI=1S/C9H9BrN4O4S3/c1-14-8(19-9(12-14)20(11,15)16)13-21(17,18)7-4-2-6(10)3-5-7/h2-5H,1H3,(H2,11,15,16)/b13-8+	-2.51
InChI=1S/C7H6N2O2/c8-4-1-2-6-5(3-4)9-7(10)11-6/h1-3H,8H2,(H,9,10)	-1.631
InChI=1S/C19H17Cl2N3O3/c1-13-9-25-19(27-13,10-24-12-22-11-23-24)17-7-6-16(8-18(17)21)26-h2-8,11-13H,9-10H2,1H3	-4.91
InChI=1S/C16H19N3S/c1-18(2)11-6-12-19-13-7-3-4-8-14(13)20-15-9-5-10-17-16(15)19/h3-5,7-10H,6,11-12H2,1-2H3	-3.219
InChI=1S/C7H4ClF3/c8-6-3-1-5(2-4-6)7(9,10)11/h1-4H	-3.728
InChI=1S/C15H18N2O6/c1-5-10(4)12-7-11(16(19)20)8-13(17(21)22)15(12)23-14(18)6-9(2)3/h6-8,10H,5H2,1-4H3	-5.508
InChI=1S/C8H16N2O4S2/c9-5(7(11)12)3-15-1-2-16-4-6(10)8(13)14/h5-6H,1-4,9-10H2,(H,11,12)(H,13,14)	-2.85
InChI=1S/C36H38N2O2/c1-7-23-17-21(5)18-24(8-2)33(23)37-29-15-16-30(38-34-25(9-3)19-22h11-20,37-38H,7-10H2,1-6H3	-7.424
InChI=1S/C7H11NO4S2/c1-2-12-7(13)14-4(6(10)11)3-5(8)9/h4H,2-3H2,1H3,(H2,8,9)(H,10,11)	-1.7
InChI=1S/C10H12N3O3PS2/c1-15-17(18,16-2)19-7-13-10(14)8-5-3-4-6-9(8)11-12-13/h3-6H,7H2,1-2H3	-4.04
InChI=1S/C14H24O/c1-11-7-5-9-14(3,4)13(11)12(2)8-6-10-15/h7,10,12-13H,5-6,8-9H2,1-4H3	-4.653
InChI=1S/C11H15NO4/c1-8(14)12-10-4-2-3-5-11(10)16-7-9(15)6-13/h2-5,9,13,15H,6-7H2,1H3,(H,12,14)	-0.331
InChI=1S/C14H12ClNO3/c1-19-11-5-3-10(4-6-11)16-13-8-9(15)2-7-12(13)14(17)18/h2-8,16H,1H3,(H,17,18)	-5.418
InChI=1S/C4H11N3O3S2/c1-6-4(5)7-2-3-11-12(8,9)10/h2-3H2,1H3,(H3,5,6,7)(H,8,9,10)	0.671

"InChi"	"logS(M)"
InChI=1S/C24H29N5O3/c1-4-5-10-21(30)29(22(16(2)3)24(31)32)15-17-11-13-18(14-12-17)19-h6-9,11-14,16,22H,4-5,10,15H2,1-3H3,(H,31,32)(H,25,26,27,28)	-2.736
InChI=1S/C14H14O3/c1-16-13-9-12(17-14(15)10-13)8-7-11-5-3-2-4-6-11/h2-8,10,12H,9H2,1H3/b8-7+	-2.367
InChI=1S/C15H17N3/c1-12-5-4-6-14(11-12)17-16-13-7-9-15(10-8-13)18(2)3/h4-11H,1-3H3/b17-16+	-5.777
InChI=1S/C6H8N2/c7-8-6-4-2-1-3-5-6/h1-5,8H,7H2	0.07
InChI=1S/C13H10N2O3/c16-12(10-2-1-7-14-8-10)15-11-5-3-9(4-6-11)13(17)18/h1-8H,(H,15,16)(H,17,18)	-3.083
InChI=1S/C10H8OS3/c1-11-8-4-2-7(3-5-8)9-6-10(12)14-13-9/h2-6H,1H3	-4.216
InChI=1S/C8H7ClO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2,(H,10,11)	-1.861
InChI=1S/C8H16N2S/c1-3-9-6-5-7-10(4-2)8(9)11/h3-7H2,1-2H3	-0.65
InChI=1S/C16H28N2O/c1-2-16(19)18-14-7-8-15(18)12-17(11-14)10-9-13-5-3-4-6-13/h13-15H,2-12H2,1H3	-3.755
InChI=1S/C8H8O3/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3,(H,10,11)	-2.76
InChI=1S/C2H3NS/c1-3-2-4/h1H3	-0.983
InChI=1S/C14H23NO3/c1-14(2,13(16)11-15-9-10-17-3)18-12-7-5-4-6-8-12/h4-8,13,15-16H,9-11H2,1-3H3	-0.987
InChI=1S/C13H15ClN2/c1-16-6-2-3-13(16)11-8-15-12-5-4-9(14)7-10(11)12/h4-5,7-8,13,15H,2-3,6H2,1H3	-2.375
InChI=1S/C6H10N2O2/c7-5(9)4-8-3-1-2-6(8)10/h1-4H2,(H2,7,9)	-0.234
InChI=1S/C10H12N4O2/c1-3-5-6(4-2)12-8-7(11-5)9(15)14-10(16)13-8/h3-4H2,1-2H3,(H2,12,13,14,15,16)	-2.39
InChI=1S/C25H24F6N4/c1-23(2)15-32-22(33-16-23)35-34-21(13-7-17-3-9-19(10-4-17)24(26,2h3-14H,15-16H2,1-2H3,(H2,32,33,35)/b13-7+,14-8+	-7.916
InChI=1S/C13H10FNO2/c14-11-6-4-5-10(9-11)13(16)15(17)12-7-2-1-3-8-12/h1-9,17H	-2.6
InChI=1S/C16H23NO4/c1-16(2,21-14-6-4-3-5-7-14)15(18)20-13-10-17-8-11-19-12-9-17/h3-7H,8-13H2,1-2H3	-1.865
InChI=1S/C16H22Cl2O3/c1-3-5-6-12(4-2)10-21-16(19)11-20-15-8-7-13(17)9-14(15)18/h7-9,12H,3-6,10-11H2,1-2H3	-7.012
InChI=1S/C15H19NO5/c1-18-12-9-11(10-13(19-2)15(12)20-3)5-6-14(17)16-7-4-8-21-16/h5-6,9-10H,4,7-8H2,1-3H3/b6-5+	-1.529
InChI=1S/C33H54O6/c1-7-13-16-25(10-4)22-37-31(34)28-19-20-29(32(35)38-23-26(11-5)1h19-21,25-27H,7-18,22-24H2,1-6H3	-8.252

"InChi"	"logS(M)"
InChI=1S/C24H27BrN6O10/c1-5-39-23-13-19(27-28-20-10-17(30(35)36)11-22(24(20)25)31(37)38h10-13H,5-9H2,1-4H3,(H,26,32)/b28-27+	-8.834
InChI=1S/C6H9N2O2P/c7-11(8,9)10-6-4-2-1-3-5-6/h1-5H,(H4,7,8,9)	-1.488
InChI=1S/C13H18ClN3O2/c1-13(2,10-11-6-4-3-5-7-11)15-12(18)17(16-19)9-8-14/h3-7H,8-10H2,1-2H3,(H,15,18)	-4.455
InChI=1S/C21H40O4/c1-7-11-13-17(9-3)19(22)24-15-21(5,6)16-25-20(23)18(10-4)14-12-8-h17-18H,7-16H2,1-6H3	-5.021
InChI=1S/C14H28N2O2/c1-3-5-7-9-13(17)15-11-12-16-14(18)10-8-6-4-2/h3-12H2,1-2H3,(H,15,17)(H,16,18)	-3.108
InChI=1S/C18H18ClNO5/c1-4-24-20-17(25-18(21)12-8-6-5-7-9-12)15-14(22-2)11-10-13(19)16(h5-11H,4H2,1-3H3/b20-17-	-4.08
InChI=1S/C9H11NO/c1-10(2)9-5-3-8(7-11)4-6-9/h3-7H,1-2H3	-2.283
InChI=1S/C8H7N3S/c12-8-9-7(10-11-8)6-4-2-1-3-5-6/h1-5H,(H2,9,10,11,12)	-2.54
InChI=1S/C7H9N3O3S/c8-5-1-3-6(4-2-5)14(12,13)10-7(9)11/h1-4H,8H2,(H3,9,10,11)	-1.97
InChI=1S/C38H72O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-35-41-37(39)33-34-38(h33-34H,3-32,35-36H2,1-2H3/b34-33+	-7.074
InChI=1S/C7H4Br2O5/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h10-12H,(H,13,14)	-0.419
InChI=1S/C17H34N2O4/c1-7-12-17(6,13-22-15(20)18(8-2)9-3)14-23-16(21)19(10-4)11-5/h7-14H2,1-6H3	-5.622
InChI=1S/C8H7Cl3O/c9-8(10,11)7(12)6-4-2-1-3-5-6/h1-5,7,12H	-2.769
InChI=1S/C21H31N3O5/c22-13-5-4-9-16(19(25)24-14-6-10-18(24)21(28)29)23-17(20(26)27)1h1-3,7-8,16-18,23H,4-6,9-14,22H2,(H,26,27)(H,28,29)	-4.494
InChI=1S/C7H19N3/c1-10(6-2-4-8)7-3-5-9/h2-9H2,1H3	0.838
InChI=1S/C18H34O6/c1-5-9-11-15(7-3)13-21-17(19)23-24-18(20)22-14-16(8-4)12-10-6-2/h15-16H,5-14H2,1-4H3	-2.595
InChI=1S/C14H15N3O3S/c1-17(2)13-7-3-11(4-8-13)15-16-12-5-9-14(10-6-12)21(18,19)20/h3-10H,1-2H3,(H,18,19,20)/b16-15+	-3.86
InChI=1S/C21H31ClN2O/c1-5-16(3)24(17(4)6-2)15-21(25)20-12-9-13-23(20)14-18-10-7-8-11-1h7-13,16-17,21,25H,5-6,14-15H2,1-4H3	-5.351
InChI=1S/C12H15NO/c14-12-6-8-13(9-7-12)10-11-4-2-1-3-5-11/h1-5H,6-10H2	-1.017
InChI=1S/C15H28N4O4/c1-7-8-15(6,9-22-13(20)18-16-11(2)3)10-23-14(21)19-17-12(4)5/h7-10H2,1-6H3,(H,18,20)(H,19,21)	-5.824
InChI=1S/C15H28N2O4/c1-5-8-10-17-14(19)21-12-15(4,9-6-2)11-20-13(18)16-7-3/h5,8H,6-7,9-12H2,1-4H3,(H,16,18)(H,17,19)/b8-5+	-4.52

"InChi"	"logS(M)"
InChI=1S/C19H20O4/c1-19(2,13-22-17(20)15-9-5-3-6-10-15)14-23-18(21)16-11-7-4-8-12-1h3-12H,13-14H2,1-2H3	-5.423
InChI=1S/C15H26N2O/c1-2-15(18)17-13-7-8-14(17)11-16(10-13)9-12-5-3-4-6-12/h12-14H,2-11H2,1H3	-3.234
InChI=1S/C42H70O11/c1-11-29(38(46)47)31-15-14-23(4)36(50-31)27(8)34(44)26(7)35(45)3(h16,19,23-34,36-37,43-44,48H,11-15,17-18,20-22H2,1-10H3,(H,46,47)	-10.01
InChI=1S/C11H15NO4/c1-8(14)12-9-2-4-11(5-3-9)16-7-10(15)6-13/h2-5,10,13,15H,6-7H2,1H3,(H,12,14)	-0.815
InChI=1S/C16H15NO2/c1-2-19-16(18)17-11-12-7-3-4-8-13(12)14-9-5-6-10-15(14)17/h3-10H,2,11H2,1H3	-5.261
InChI=1S/C21H24N2O2/c24-18-10-16-19-13-9-17-21(6-7-22(17)11-12(13)5-8-25-16)14-3-1-2-h1-4,12-13,16-17,19-20H,5-11H2	-3.037
InChI=1S/C12H10O4/c13-8-3-5-12(16,6-4-8)10-7-9(14)1-2-11(10)15/h1-7,14-16H	-1.73
InChI=1S/C19H36N2O/c1-8-11-12-16-13-18(4,5)21(19(6,7)14-16)17(22)15-20(9-2)10-3/h13H,8-12,14-15H2,1-7H3	-5.73
InChI=1S/C11H21NO/c1-7-9(13)12-11(5,6)8-10(2,3)4/h7H,1,8H2,2-6H3,(H,12,13)	-2.259
InChI=1S/C11H22N2O4/c1-2-3-4-5-6-9(7-16-10(12)14)8-17-11(13)15/h9H,2-8H2,1H3,(H2,12,14)(H2,13,15)	-2.708
InChI=1S/C15H30N2/c1-14(2)11-13(9-8-10-16(5)6)12-15(3,4)17(14)7/h11H,8-10,12H2,1-7H3	-2.675
InChI=1S/C3H4O2/c4-3-1-2-5-3/h1-2H2	0.71
InChI=1S/C7H6N2O5/c8-5-2-3(9(13)14)1-4(6(5)10)7(11)12/h1-2,10H,8H2,(H,11,12)	-2.491
InChI=1S/C15H26O/c1-6-16-15(5)10-8-12-11(2)13(15)7-9-14(12,3)4/h12-13H,2,6-10H2,1,3-5H3	-4.734
InChI=1S/C20H25N3O/c1-3-22(4-2)14-9-15-23-18-12-7-5-10-16(18)20(24)21-17-11-6-8-13-1h5-8,10-13H,3-4,9,14-15H2,1-2H3,(H,21,24)	-6.3
InChI=1S/C5H9NO3/c7-3-1-4(5(8)9)6-2-3/h3-4,6-7H,1-2H2,(H,8,9)	0.44
InChI=1S/C13H10N2O/c14-13-9-3-1-2-4-11(9)15-12-7-8(16)5-6-10(12)13/h1-7,15H,14H2	-2.906
InChI=1S/C11H20O2/c1-2-3-4-5-6-7-10-8-9-11(12)13-10/h10H,2-9H2,1H3	-3.067
InChI=1S/C6H8IN3O2/c1-5-8-6(10(11)12)4-9(5)3-2-7/h4H,2-3H2,1H3	-3.536
InChI=1S/C26H43NO5/c1-15(4-7-22(30)27-14-23(31)32)18-5-6-19-24-20(9-11-26(18,19)3)25h15-21,24,28-29H,4-14H2,1-3H3,(H,27,30)(H,31,32)	-5.155
InChI=1S/C6H3Cl2NO2/c7-3-1-2-4(8)9-5(3)6(10)11/h1-2H,(H,10,11)	-1.388
InChI=1S/C9H9N5/c10-8-12-7(13-9(11)14-8)6-4-2-1-3-5-6/h1-5H,(H4,10,11,12,13,14)	-2.494

"InChi"	"logS(M)"
InChI=1S/C6H14N4O2/c7-4(5(11)12)2-1-3-10-6(8)9/h4H,1-3,7H2,(H,11,12)(H4,8,9,10)	0
InChI=1S/C12H16O2/c1-7(13)14-11-5-4-10-8-2-3-9(6-8)12(10)11/h5,8-10,12H,2-4,6H2,1H3	-3.01
InChI=1S/C7H4O7/c8-2-1-3(6(10)11)14-5(4(2)9)7(12)13/h1,12-13H,(H,10,11)	-1.377
InChI=1S/C12H15NO6S/c1-8-2-4-9(5-3-8)20(18,19)13-10(12(16)17)6-7-11(14)15/h2-5,10,13H,6-7H2,1H3,(H,14,15)(H,16,17)	-0.93
InChI=1S/C9H12N2O/c1-2-10-9(12)11-8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H2,10,11,12)	-1.8
InChI=1S/C4H6O2S/c5-7(6)3-1-2-4-7/h1-2H,3-4H2	0.321
InChI=1S/C12H15NO/c1-9(10(2)12(14)13-3)11-7-5-4-6-8-11/h4-8H,1-3H3,(H,13,14)/b10-9-	-2.616
InChI=1S/C10H13N/c1-11-7-6-9-4-2-3-5-10(9)8-11/h2-5H,6-8H2,1H3	-0.94
InChI=1S/C11H16N2O/c12-8-4-5-9-13-11(14)10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9,12H2,(H,13,14)	-1.099
InChI=1S/C20H23N/c1-21(2)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(17)20/h3-6,8-11,13-14,20H,7,12,15H2,1-2H3	-5.686
InChI=1S/C16H16O2/c1-11-5-4-6-13(9-11)16(17)14-7-8-15(18-3)12(2)10-14/h4-10H,1-3H3	-5.08
InChI=1S/C17H13Cl3N4S/c18-13-3-1-12(2-4-13)9-25-17(8-24-11-21-10-22-24)23-16-6-5-14(19)h1-7,10-11H,8-9H2/b23-17+	-5.384
InChI=1S/C18H25NO/c1-12-17-9-14-5-6-15(20)10-16(14)18(12,2)7-8-19(17)11-13-3-4-13/h5-6,10,12-13,17,20H,3-4,7-9,11H2,1-2H3	-4.322
InChI=1S/C33H34O4/c1-3-33(37-31(35)22-9-13-26(14-10-22)36-25-7-5-4-6-8-25)20-18-30-h1,4-10,13-14,21,27-30H,11-12,15-20H2,2H3	-6.84
InChI=1S/C2H6N2O/c1-4(2)3-5/h1-2H3	1.13
InChI=1S/C10H19N/c1-3-10(11-2)7-8-4-5-9(10)6-8/h8-9,11H,3-7H2,1-2H3	-1.814
InChI=1S/C16H17N3O2/c1-12-3-5-13(6-4-12)11-19(2)18-17-15-9-7-14(8-10-15)16(20)21/h3-10H,11H2,1-2H3,(H,20,21)/b18-17+	-5.323
InChI=1S/C18H27Cl2NO9/c1-10(22)26-9-14-16(27-11(2)23)17(28-12(3)24)15(18(30-14)29-13(4)h14-18H,5-9H2,1-4H3	-2.498
InChI=1S/C10H14N2O2/c1-7(13)6-12-9-5-3-2-4-8(9)10(11)14/h2-5,7,12-13H,6H2,1H3,(H2,11,14)	-1.148
InChI=1S/C7H5NO2/c9-7-8-5-3-1-2-4-6(5)10-7/h1-4H,(H,8,9)	-1.178
InChI=1S/C15H20O4/c1-8-9-4-6-14(2)10(16)5-7-15(3,18)12(14)11(9)19-13(8)17/h5,7-9,11-12,18H,4,6H2,1-3H3	-0.815
InChI=1S/C9H16O3/c1-3-8-5-10-9(4-2,11-6-8)12-7-8/h3-7H2,1-2H3	-2.523
InChI=1S/C16H19N3O2/c1-5-11-18-12(2)14(17(3)4)15(20)19(16(18)21)13-9-7-6-8-10-13/h5-10H,1,11H2,2-4H3	-2.511

"InChi"	"logS(M)"
InChI=1S/C14H16N4O5/c19-14(16-4-2-1-3-5-16)10-8-12(15-6-7-15)13(18(22)23)9-11(10)17(2h8-9H,1-7H2	-3.17
InChI=1S/C10H6N2O8S/c13-10-7-3-5(21(18,19)20)1-2-6(7)8(11(14)15)4-9(10)12(16)17/h1-4,13H,(H,18,19,20)	-2.54
InChI=1S/C3H3N3O2/c7-6(8)3-1-2-4-5-3/h1-2H,(H,4,5)	-1.285
InChI=1S/C9H16ClN5/c1-4-5-11-8-13-7(10)14-9(15-8)12-6(2)3/h6H,4-5H2,1-3H3,(H2,11,12,13,14,15)	-3.74
InChI=1S/C6H6N2O3/c7-5-3-4(8(10)11)1-2-6(5)9/h1-3,9H,7H2	-2.206
InChI=1S/C15H13Cl2F3N2O4/c1-3-24-11(23)6-25-10-4-7(9(18)5-8(10)16)13-12(17)14(22(2)21-13)2h4-5,15H,3,6H2,1-2H3	-5.616
InChI=1S/C6H8O3/c1-3-5(7)6(8)4(2)9-3/h3,8H,1-2H3	0.391
InChI=1S/C8H14N2O2/c1-2-6-3-4-7(9-11)8(5-6)10-12/h6,11-12H,2-5H2,1H3/b9-7+,10-8+	-1.83
InChI=1S/C10H18O2/c1-8(12-9(2)11)10-6-4-3-5-7-10/h8,10H,3-7H2,1-2H3	-3.598
InChI=1S/C14H15N3/c1-10-5-3-4-6-14(10)17-16-12-7-8-13(15)11(2)9-12/h3-9H,15H2,1-2H3/b17-16+	-4.05
InChI=1S/C9H10F3N3/c1-15(2)14-13-8-5-3-4-7(6-8)9(10,11)12/h3-6H,1-2H3/b14-13+	-4.013
InChI=1S/C10H10O/c1-3-8-5-6-10(11)9(4-2)7-8/h3-7,11H,1-2H2	-3.394
InChI=1S/C18H22BrNO/c1-18(21-14-13-20(2)3,15-7-5-4-6-8-15)16-9-11-17(19)12-10-16/h4-12H,13-14H2,1-3H3	-5.603
InChI=1S/C21H16ClF3N4O3/c1-26-19(30)18-11-15(8-9-27-18)32-14-5-2-12(3-6-14)28-20(31)29-13h2-11H,1H3,(H,26,30)(H2,28,29,31)	-6.667
InChI=1S/C4H8N2O3/c1-2(3(7)8)6-4(5)9/h2H,1H3,(H,7,8)(H3,5,6,9)	-0.784
InChI=1S/C19H17NOS/c1-14-6-5-9-17(12-14)20(2)19(22)21-18-11-10-15-7-3-4-8-16(15)13-1h3-13H,1-2H3	-6.642
InChI=1S/C11H23NO/c1-5-7-11(8-6-2)9(3)12-10(4)13/h9,11H,5-8H2,1-4H3,(H,12,13)	-3.189
InChI=1S/C22H23N3O3/c1-2-27-22(26)25-15-13-24(14-16-25)21-23-19(17-9-5-3-6-10-17)20(2h3-12H,2,13-16H2,1H3	-6.17
InChI=1S/C6H4ClNO3/c7-4-1-2-6(9)5(3-4)8(10)11/h1-3,9H	-3.09
InChI=1S/C10H17N/c1-9(2)5-4-6-10(3)7-8-11/h5,10H,4,6-7H2,1-3H3	-3.104
InChI=1S/C20H29FO3/c1-17-8-6-13(22)10-12(17)4-5-15-14-7-9-19(3,24)18(14,2)11-16(23)2h10,14-16,23-24H,4-9,11H2,1-3H3	-3.698
InChI=1S/C11H14N2O/c1-9-4-6-10(7-5-9)11(14)8-12-13(2)3/h4-8H,1-3H3/b12-8+	-1.696
InChI=1S/C11H11N3O3S2/c1-8(15)13-9-2-4-10(5-3-9)19(16,17)14-11-12-6-7-18-11/h2-7H,1H3,(H,12,14)(H,13,15)	-3.43

"InChi"	"logS(M)"
InChI=1S/C15H18N4O3/c1-8(20)13-11(21-2)5-9(6-12(13)22-3)4-10-7-18-15(17)19-14(10)16/h5-7H,4H2,1-3H3,(H4,16,17,18,19)	-2.344
InChI=1S/C13H15N3O3/c1-7(2)13(3)12(19)15-10(16-13)9-8(11(17)18)5-4-6-14-9/h4-7H,1-3H3,(H,17,18)(H,15,16,19)	-1.364
InChI=1S/C33H36O7/c1-17(2)8-9-21-27-20(11-12-30(4,5)38-27)25(35)24-26(36)22-14-19-1h8,10-12,14,16,19,23,35H,9,13,15H2,1-7H3/b18-10-	-10.05
InChI=1S/C15H19NO3/c1-3-4-11-19-15(17)16-13-8-6-5-7-12(13)9-10-14(16)18-2/h5-10,14H,3-4,11H2,1-2H3	-4.857
InChI=1S/C16H26O2/c1-7-15(3,4)11-9-14(18)12(10-13(11)17)16(5,6)8-2/h9-10,17-18H,7-8H2,1-6H3	-6.496
InChI=1S/C15H16N4O/c1-3-18-12-8-6-10-17-14(12)19(4-2)13-11(15(18)20)7-5-9-16-13/h5-10H,3-4H2,1-2H3	-2.86
InChI=1S/C15H12Cl2O3/c16-12-6-7-14(13(17)10-12)19-8-9-20-15(18)11-4-2-1-3-5-11/h1-7,10H,8-9H2	-3.812
InChI=1S/C15H12O2/c16-15(17)12-7-8-14-11(9-12)6-5-10-3-1-2-4-13(10)14/h1-4,7-9H,5-6H2,(H,16,17)	-5.893
InChI=1S/C7H6ClNO2/c1-5-6(8)3-2-4-7(5)9(10)11/h2-4H,1H3	-3.271
InChI=1S/C10H23NO/c1-3-5-7-11(9-10-12)8-6-4-2/h12H,3-10H2,1-2H3	-1.637
InChI=1S/C9H12N2S/c1-2-3-8-6-7(9(10)12)4-5-11-8/h4-6H,2-3H2,1H3,(H2,10,12)	-1.997
InChI=1S/C15H17Cl2N3OS/c1-11-2-3-12(14(21)19-15-18-6-9-22-15)10-13(11)20(7-4-16)8-5-17/h2-3,6,9-10H,4-5,7-8H2,1H3,(H,18,19,21)	-5.796
InChI=1S/C8H11NO3S2/c9-14(11,12)8-3-1-7(2-4-8)13-6-5-10/h1-4,10H,5-6H2,(H2,9,11,12)	-1.824
InChI=1S/C5H7NO2/c7-4-2-1-3-5(8)6-4/h1-3H2,(H,6,7,8)	0.691
InChI=1S/C8H14I2/c9-5-7-1-2-8(6-10)4-3-7/h7-8H,1-6H2	-5.748
InChI=1S/C11H8ClNO2/c1-6-4-7-2-3-8(12)9(11(14)15)10(7)13-5-6/h2-5H,1H3,(H,14,15)	-2.997
InChI=1S/C8H5NO2S/c9-5-12-7-3-1-6(2-4-7)8(10)11/h1-4H,(H,10,11)	-2.457
InChI=1S/C6H5FN2O3/c1-3(10)9-2-4(7)5(11)8-6(9)12/h2H,1H3,(H,8,11,12)	-0.6
InChI=1S/C14H23NO3S2/c16-20(17,18)19-13-12-15-11-7-2-1-4-8-14-9-5-3-6-10-14/h3,5-6,9-10,15H,1-2,4,7-8,11-13H2,(H,16,17,18)	-2.785
InChI=1S/C7H6O5/c8-3-1-4(9)6(7(11)12)5(10)2-3/h1-2,8-10H,(H,11,12)	-0.959
InChI=1S/C22H28N2O3/c1-14-11-15(2)13-17(12-14)21(26)24(22(27)23-20(25)18-9-8-10-19h8-13H,1-7H3,(H,23,25)	-5.566

"InChi"	"logS(M)"
InChI=1S/C20H13NS/c1-3-7-15-13(5-1)9-11-17-19(15)21-20-16-8-4-2-6-14(16)10-12-18(20)h1-12,21H	-7.908
InChI=1S/C8H5F13O/c9-3(10,1-2-22)4(11,12)5(13,14)6(15,16)7(17,18)8(19,20)21/h22H,1-2H2	-4.287
InChI=1S/C10H12OS2/c1-11-9-4-2-8(3-5-9)10-12-6-7-13-10/h2-5,10H,6-7H2,1H3	-3.655
InChI=1S/C28H46O4/c1-3-5-7-9-11-13-15-19-23-31-27(29)25-21-17-18-22-26(25)28(30)32-h17-18,21-22H,3-16,19-20,23-24H2,1-2H3	-9.308
InChI=1S/C7H6ClF/c8-5-6-2-1-3-7(9)4-6/h1-4H,5H2	-2.544
InChI=1S/C7H7NO5S/c8-5-1-4(7(9)10)2-6(3-5)14(11,12)13/h1-3H,8H2,(H,9,10)(H,11,12,13)	-0.94
InChI=1S/C10H7BrClNO/c11-6-9-5-10(13-14-9)7-1-3-8(12)4-2-7/h1-5H,6H2	-4.19
InChI=1S/C2H4FNO/c3-1-2(4)5/h1H2,(H2,4,5)	1.113
InChI=1S/C23H46N6O13/c24-2-7-13(32)15(34)10(28)21(37-7)40-18-6(27)1-5(26)12(31)20(18)4h5-23,30-36H,1-4,24-29H2	0.211
InChI=1S/C16H23NO2/c1-4-15(18)19-16(14-8-6-5-7-9-14)10-11-17(3)12-13(16)2/h5-9,13H,4,10-12H2,1-3H3	-2.516
InChI=1S/C5H13N/c1-2-3-4-5-6/h2-6H2,1H3	1.06
InChI=1S/C20H25NO4/c1-5-21(6-2)19(22)13-25-20(23)14(3)15-7-8-17-12-18(24-4)10-9-16(17h7-12,14H,5-6,13H2,1-4H3	-4.46
InChI=1S/C16H22Cl2O3/c1-2-3-4-5-6-7-10-20-16(19)12-21-15-9-8-13(17)11-14(15)18/h8-9,11H,2-7,10,12H2,1H3	-7.022
InChI=1S/C17H19NO2/c1-3-18(4-2)17(20)15-12-8-11-14(16(15)19)13-9-6-5-7-10-13/h5-12,19H,3-4H2,1-2H3	-3.806
InChI=1S/C17H16O2/c1-11(17(18)19)13-8-9-16-14(10-13)7-6-12-4-2-3-5-15(12)16/h2-5,8-11H,6-7H2,1H3,(H,18,19)	-5.678
InChI=1S/C11H11ClN2O/c12-10-3-1-9(2-4-10)11(15)7-14-6-5-13-8-14/h1-6,8,11,15H,7H2	-2.457
InChI=1S/C3H8N2/c1-3-5-4-2/h3-4H,1-2H3/b5-3+	0.11
InChI=1S/C18H20O5/c1-21-14-7-9-17(22-2)13(11-14)6-4-12-5-8-16(19)15(10-12)18(20)23-h5,7-11,19H,4,6H2,1-3H3	-6.39
InChI=1S/C9H10O/c10-9-5-4-7-2-1-3-8(7)6-9/h4-6,10H,1-3H2	-1.329
InChI=1S/C3H3NO2/c4-2-1-3(5)6/h1H2,(H,5,6)	1.07
InChI=1S/C4H9NO2/c1-3-4(2)5(6)7/h4H,3H2,1-2H3	-0.62
InChI=1S/C14H21N3O2/c1-2-3-4-5-6-7-13(18)16-17-14(19)12-8-10-15-11-9-12/h8-11H,2-7H2,1H3,(H,16,18)(H,17,19)	-2.91
InChI=1S/C10H20N2O4S2/c11-7(9(13)14)5-17-3-1-2-4-18-6-8(12)10(15)16/h7-8H,1-6,11-12H2,(H,13,14)(H,15,16)	-3.62

"InChi"	"logS(M)"
InChI=1S/C10H14N4O2/c1-5-6-11-8-7(12(6)2)9(15)14(4)10(16)13(8)3/h5H2,1-4H3	-1.569
InChI=1S/C5H11NO3/c1-3-4-5(2)9-6(7)8/h5H,3-4H2,1-2H3	-2.481
InChI=1S/C19H14O5S/c20-15-9-5-13(6-10-15)19(14-7-11-16(21)12-8-14)17-3-1-2-4-18(17)24-h1-12,20-21H	-3.07
InChI=1S/C8H14O4/c1-2-12-8(11)6-4-3-5-7(9)10/h2-6H2,1H3,(H,9,10)	-0.36
InChI=1S/C21H30N2O/c1-5-23(6-2)15-14-21(16(3)4,20(22)24)19-13-9-11-17-10-7-8-12-18(1h7-13,16H,5-6,14-15H2,1-4H3,(H2,22,24)	-5.152
InChI=1S/C9H10O4/c1-12-6-13-9(11)7-4-2-3-5-8(7)10/h2-5,10H,6H2,1H3	-2.3
InChI=1S/C8H8O3/c1-5(9)6-2-3-7(10)8(11)4-6/h2-4,10-11H,1H3	-0.341
InChI=1S/C14H10F3NO2/c15-14(16,17)9-4-3-5-10(8-9)18-13(20)11-6-1-2-7-12(11)19/h1-8,19H,(H,18,20)	-4.309
InChI=1S/C6H12N2O6/c9-7(10)13-5-3-1-2-4-6(5)14-8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)/q+2	-2.35
InChI=1S/C5H4N4S/c10-5-6-1-3-4(9-5)8-2-7-3/h1-2H,(H2,6,7,8,9,10)	-2.58
InChI=1S/C14H27N5O3P/c1-13(2)9-11(10-14(3,4)19(13)21)15-12(20)16-23(22,17-5-6-17)18-7-h11H,5-10H2,1-4H3,(H2,15,16,20,22)	-2.662
InChI=1S/C16H20N2O3/c1-17-9-13-6-7-14(10-17)18(13)16(21)12-4-2-11(3-5-12)8-15(19)20/h2-5,13-14H,6-10H2,1H3,(H,19,20)	-2.54
InChI=1S/C8H3N3O2/c9-4-6-1-2-8(11(12)13)3-7(6)5-10/h1-3H	-1.892
InChI=1S/C4H9NO2/c1-4(2,5)3(6)7/h5H2,1-2H3,(H,6,7)	0.245
InChI=1S/C12H16N4O2S2/c1-8(2)7-11-14-15-12(19-11)16-20(17,18)10-5-3-9(13)4-6-10/h3-6,8H,7,13H2,1-2H3,(H,15,16)	-3.823
InChI=1S/C14H12N2/c1-9-5-4-7-11-13(15)10-6-2-3-8-12(10)16-14(9)11/h2-8H,1H3,(H2,15,16)	-4.349
InChI=1S/C17H12ClFN2O/c18-16-4-2-1-3-15(16)17(22,13-9-20-11-21-10-13)12-5-7-14(19)8-6-1h1-11,22H	-4.083
InChI=1S/C3H7NO/c1-4(2)3-5/h3H,1-2H3	1.136
InChI=1S/C14H22N2O4/c1-4-20-12(18)14(2,10-8-6-5-7-9-10)11(17)16-13(19)15-3/h8H,4-7,9H2,1-3H3,(H2,15,16,17,19)	-3
InChI=1S/C10H10O5/c1-6(11)15-8-4-3-7(10(12)13)5-9(8)14-2/h3-5H,1-2H3,(H,12,13)	-2.06
InChI=1S/C10H16ClN5S/c1-15-3-5-16(6-4-15)9-7(17-2)8(11)13-10(12)14-9/h3-6H2,1-2H3,(H2,12,13,14)	-0.947
InChI=1S/C7H14O2/c1-6(2)5-7-8-3-4-9-7/h6-7H,3-5H2,1-2H3	-0.369
InChI=1S/C6H8N2O2/c1-4-3-10-6(7-4)8-5(2)9/h3H,1-2H3,(H,7,8,9)	-0.639
InChI=1S/C12H4Br4O/c13-7-1-5-6-2-8(14)10(16)4-12(6)17-11(5)3-9(7)15/h1-4H	-6.84

"InChi"	"logS(M)"
InChI=1S/C10H14O/c1-7(2)10-5-4-9(11)6-8(10)3/h4-7,11H,1-3H3	-2.855
InChI=1S/C9H10N2O3/c1-10(2)9(12)7-3-5-8(6-4-7)11(13)14/h3-6H,1-2H3	-1.27
InChI=1S/C22H22N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(h4-6,10,14-15,17,25-27,31-32H,1,23H2,2-3H3/b21-13+	-1.768
InChI=1S/C7H12O4/c1-3-10-6(8)5-7(9)11-4-2/h3-5H2,1-2H3	-0.82
InChI=1S/C11H20N2O2/c1-2-11(15)13-9-3-4-10(13)8-12(7-9)5-6-14/h9-10,14H,2-8H2,1H3	-1.496
InChI=1S/C18H21N5O4/c24-17(20-19-12-16-6-7-18(27-16)23(25)26)14-22-10-8-21(9-11-22)1h1-7,12H,8-11,13-14H2,(H,20,24)/b19-12+	-3.124
InChI=1S/C7H10O4S3/c1-3(5(8)9)13-7(12)14-4(2)6(10)11/h3-4H,1-2H3,(H,8,9)(H,10,11)	-1.41
InChI=1S/C13H20O/c1-12(2)8-10-14-11-9-13-6-4-3-5-7-13/h3-7,12H,8-11H2,1-2H3	-3.934
InChI=1S/C11H14N2O2/c1-3-4-5-13-10(14)6-8(2)9(7-12)11(13)15/h6,15H,3-5H2,1-2H3	-2.273
InChI=1S/C4H4O5/c5-2(4(8)9)1-3(6)7/h1H2,(H,6,7)(H,8,9)	0.879
InChI=1S/C13H16O3/c1-2-3-4-7-10-16-13(15)11-8-5-6-9-12(11)14/h3-6,8-9,14H,2,7,10H2,1H3/b4-3+	-4.644
InChI=1S/C8H18O2S/c1-7(2,3)11(9,10)8(4,5)6/h1-6H3	-1.218
InChI=1S/C17H15NO4S/c1-21-13-6-4-11(9-14(13)22-2)17-18-12-5-3-10(8-16(19)20)7-15(12)2h3-7,9H,8H2,1-2H3,(H,19,20)	-3.78
InChI=1S/C7H14N2O3S2/c1-7(2,9-5-3-4-8)6-13-14(10,11)12/h9H,3,5-6H2,1-2H3,(H,10,11,12)	0.623
InChI=1S/C15H26N2O3S2/c1-13-3-11-4-14(2,7-13)9-15(5-11,8-13)10-17-12(16)6-21-22(18,19)2(h11H,3-10H2,1-2H3,(H2,16,17)(H,18,19,20)	-4.742
InChI=1S/C19H24O2/c1-11-7-15(8-12(2)17(11)20)19(5,6)16-9-13(3)18(21)14(4)10-16/h7-10,20-21H,1-6H3	-4.953
InChI=1S/C10H13NO2/c1-7(2)13-10(12)8-3-5-9(11)6-4-8/h3-7H,11H2,1-2H3	-2.61
InChI=1S/C14H8O3/c15-8-5-6-11-12(7-8)14(17)10-4-2-1-3-9(10)13(11)16/h1-7,15H	-5.309
InChI=1S/C12H22O4/c1-11(2,7-9(13)14)5-6-12(3,4)8-10(15)16/h5-8H2,1-4H3,(H,13,14)(H,15,16)	-3.132
InChI=1S/C10H10O4/c1-14-9-4-2-7(6-8(9)11)3-5-10(12)13/h2-6,11H,1H3,(H,12,13)/b5-3+	-1.431
InChI=1S/C8H10N2O3/c11-6-5-9-7-3-1-2-4-8(7)10(12)13/h1-4,9,11H,5-6H2	-1.993
InChI=1S/C28H56O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-30-28(29)26-24-22-20-18-16-h3-27H2,1-2H3	-7.327
InChI=1S/C23H24N4O2/c1-16-20(22(28)26(24(16)3)18-11-7-5-8-12-18)15-21-17(2)25(4)27(23h5-14H,15H2,1-4H3	-2.955

"InChi"	"logS(M)"
InChI=1S/C16H14ClN3O/c1-18-15-10-20(21)16(11-5-3-2-4-6-11)13-9-12(17)7-8-14(13)19-15/h2-9H,10H2,1H3,(H,18,19)	-4.48
InChI=1S/C6H3Cl2NO2/c7-4-1-5(8)3-6(2-4)9(10)11/h1-3H	-3.584
InChI=1S/C12H7Cl3/c13-8-5-6-12(15)10(7-8)9-3-1-2-4-11(9)14/h1-7H	-6.02
InChI=1S/C8H7ClO3/c1-12-7-3-5(4-10)2-6(9)8(7)11/h2-4,11H,1H3	-2.875
InChI=1S/C23H31NO2/c1-4-17-23(20-13-9-7-10-14-20,21-15-11-8-12-16-21)22(25)26-19-18-h7-16H,4-6,17-19H2,1-3H3	-5.748
InChI=1S/C8H9NO/c1-9(7-10)8-5-3-2-4-6-8/h2-7H,1H3	-1.495
InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h6-7,9H,4-5H2,1-3H3	-1.788
InChI=1S/C3H6BrCl/c1-3(4)2-5/h3H,2H2,1H3	-1.848
InChI=1S/C21H33N5O4/c1-17(2)5-4-6-18(3)9-10-24-11-13-25(14-12-24)16-20(27)23-22-15-19h5,7-8,15,18H,4,6,9-14,16H2,1-3H3,(H,23,27)/b22-15+	-5.593
InChI=1S/C51H88N4O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-43-52-50(56)54-48-h35-42H,3-34,43-45H2,1-2H3,(H2,52,54,56)(H2,53,55,57)	-5.943
InChI=1S/C4H9N3O2/c1-7(4(5)6)2-3(8)9/h2H2,1H3,(H3,5,6)(H,8,9)	-0.939
InChI=1S/C14H12N2O3S2/c1-8-2-7-11-12(13(8)21(17,18)19)20-14(16-11)9-3-5-10(15)6-4-9/h2-7H,15H2,1H3,(H,17,18,19)	-4.332
InChI=1S/C11H12O2/c1-9(8-11(12)13)7-10-5-3-2-4-6-10/h2-7H,8H2,1H3,(H,12,13)/b9-7-	-2.746
InChI=1S/C18H24O/c1-5-18(4,13-6-7-15(2)3)14-12-16-8-10-17(19)11-9-16/h5,7-12,14,19H,1,6,13H2,2-4H3/b14-12+	-6.337
InChI=1S/C10H8ClN3O2/c11-7-2-1-3-8(6-7)13-9(15)14-10-12-4-5-16-10/h1-6H,(H2,12,13,14,15)	-3.028
InChI=1S/C9H13NO/c10-9(7-11)6-8-4-2-1-3-5-8/h1-5,9,11H,6-7,10H2	0.455
InChI=1S/C20H43NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-19-20-25-26(22,2h21H,2-20H2,1H3,(H,22,23,24)	-7.03
InChI=1S/C11H22N2O2/c1-3-5-6-12-7-9-13(10-8-12)11(14)15-4-2/h3-10H2,1-2H3	-1.391
InChI=1S/C17H21NO/c1-18(2)12-13-19-17-11-7-6-10-16(17)14-15-8-4-3-5-9-15/h3-11H,12-14H2,1-2H3	-2.913
InChI=1S/C4H9NO3/c1-8-2-3(5)4(6)7/h3H,2,5H2,1H3,(H,6,7)	0.652
InChI=1S/C13H18ClNO3/c1-2-3-4-7-18-12-6-5-10(8-11(12)14)9-13(16)15-17/h5-6,8,17H,2-4,7,9H2,1H3,(H,15,16)	-3.84
InChI=1S/C12H2Cl8/c13-4-2-6(15)9(17)11(19)7(4)3-1-5(14)10(18)12(20)8(3)16/h1-2H	-9.42
InChI=1S/C8H10O/c1-7-4-2-3-5-8(7)6-9/h2-5,9H,6H2,1H3	-1.09

"InChi"	"logS(M)"
InChI=1S/C14H26O4/c15-13(16)11-9-7-5-3-1-2-4-6-8-10-12-14(17)18/h1-12H2,(H,15,16)(H,17,18)	-3.111
InChI=1S/C15H10O5/c16-9-3-1-8(2-4-9)11-7-20-13-6-10(17)5-12(18)14(13)15(11)19/h1-7,16-18H	-4.469
InChI=1S/C18H20N2OS/c1-3-19(4-2)13-18(21)20-14-9-5-7-11-16(14)22-17-12-8-6-10-15(17)20/h5-12H,3-4,13H2,1-2H3	-5.146
InChI=1S/C25H27NO/c27-21-12-11-20-17-24-22-10-4-5-13-25(22,23(20)18-21)14-16-26(24)h1-3,7-8,11-12,18,22,24,27H,4-5,10,13-17H2	-4.814
InChI=1S/C6H7NO2S2/c1-4-3-11-6(10)7(4)2-5(8)9/h3H,2H2,1H3,(H,8,9)	-1.963
InChI=1S/C9H16N4OS/c1-9(2,3)6-11-12-8(15-6)13(5)7(14)10-4/h1-5H3,(H,10,14)	-1.997
InChI=1S/C15H19N3O2/c1-11-13(16(2)3)14(19)18(15(20)17(11)4)10-12-8-6-5-7-9-12/h5-9H,10H2,1-4H3	-2.75
InChI=1S/C15H18N2O5/c1-2-15(10-6-4-3-5-7-10)12(20)16-14(22)17(13(15)21)8-11(19)9-18/h3-7,11,18-19H,2,8-9H2,1H3,(H,16,20,22)	-1.787
InChI=1S/C20H27FN2O3/c1-2-16-14-22-19(25)26-20(16)9-12-23(13-10-20)11-3-4-18(24)15-5-7h5-8,16H,2-4,9-14H2,1H3,(H,22,25)	-4.014
InChI=1S/C8H5NO6/c10-7(11)4-1-2-6(9(14)15)5(3-4)8(12)13/h1-3H,(H,10,11)(H,12,13)	-1.339
InChI=1S/C7H12O4/c1-5(11-7(3)9)4-10-6(2)8/h5H,4H2,1-3H3	-0.205
InChI=1S/C12H18/c1-4-10-7-11(5-2)9-12(6-3)8-10/h7-9H,4-6H2,1-3H3	-7.064
InChI=1S/C8H3F3N2O2/c9-8(10,11)6-2-1-5(4-12)7(3-6)13(14)15/h1-3H	-2.471
InChI=1S/CH4N2O2/c1-2-3(4)5/h2H,1H3	1.119
InChI=1S/C14H20N2/c1-3-16(4-2)10-9-12-11-15-14-8-6-5-7-13(12)14/h5-8,11,15H,3-4,9-10H2,1-2H3	-2.271
InChI=1S/C10H14O/c1-3-8(2)9-6-4-5-7-10(9)11/h4-8,11H,3H2,1-2H3	-2.012
InChI=1S/C16H14O4/c17-15(13-7-3-1-4-8-13)19-11-12-20-16(18)14-9-5-2-6-10-14/h1-10H,11-12H2	-5.07
InChI=1S/C13H10Cl2O3S/c14-12-8(6-9-2-1-5-19-9)3-4-10(13(12)15)18-7-11(16)17/h1-5H,6-7H2,(H,16,17)	-5.125
InChI=1S/C23H35Cl2NO/c1-22-9-7-17(27)15-16(22)3-4-18-19-5-6-21(26(13-11-24)14-12-25)23h15,18-21H,3-14H2,1-2H3	-5.836
InChI=1S/C8H7N5O8/c1-2-9(13(20)21)8-6(11(16)17)3-5(10(14)15)4-7(8)12(18)19/h3-4H,2H2,1H3	-3.701

"InChi"	"logS(M)"
InChI=1S/C12H18N4O2/ c1-4-5-6-7-8-13-9-10(14-8)15(2)12(18)16(3)11(9)17/h4-7H2,1-3H3, (H,13,14)	-2.837
InChI=1S/C21H26N2O4/ c24-20(25)18(16-10-4-1-5-11-16)22-14-8-3-9-15-23-19(21(26)27)17-1 h1-2,4-7,10-13,18-19,22-23H,3,8-9,14-15H2,(H,24,25)(H,26,27)	-2.02
InChI=1S/C18H28O3/ c1-17(2,3)13-10-12(8-9-15(19)21-7)11-14(16(13)20)18(4,5)6/ h10-11,20H,8-9H2,1-7H3	-5.124
InChI=1S/C3H6N2O2/c1-3(5-7)2-4-6/h2,6-7H,1H3/b4-2+,5-3-	-0.35
InChI=1S/C15H9BrO2/ c16-10-6-7-11-12(8-10)15(18)13(14(11)17)9-4-2-1-3-5-9/h1-8,13H	-4.56
InChI=1S/C18H30O2/ c1-15(2)8-5-9-16(3)13(15)7-11-18-12-19-17(4,20-18)10-6-14(16)18/ h13-14H,5-12H2,1-4H3	-5.645
InChI=1S/C8H11NO/c1-6-3-4-8(10-2)7(9)5-6/h3-5H,9H2,1-2H3	-1.66
InChI=1S/C17H21N3O2/ c1-14-13-16(20(9-11-21)10-12-22)7-8-17(14)19-18-15-5-3-2-4-6-15/ h2-8,13,21-22H,9-12H2,1H3/b19-18+	-4.125
InChI=1S/C10H14ClN/c1-10(2,12)7-8-3-5-9(11)6-4-8/h3-6H, 7,12H2,1-2H3	-1.754
InChI=1S/C21H32O2/ c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-21(h14,16-19H,4-12H2,1-3H3	-5.236
InChI=1S/C9H7NO6/c1-16-9(13)7-5(8(11)12)3-2-4-6(7)10(14)15/ h2-4H,1H3,(H,11,12)	-2.085
InChI=1S/C14H22O/c1-13(2,3)10-8-7-9-11(12(10)15)14(4,5)6/ h7-9,15H,1-6H3	-4.714
InChI=1S/C21H22N6O5/ c1-31-18-11-16-17(12-19(18)32-2)22-13-23-20(16)25-7-9-26(10-8-25 h3-6,11-13H,7-10H2,1-2H3,(H,24,28)	-6.95
InChI=1S/C18H13Cl2NO/ c19-16-7-3-13(4-8-16)18(22,15-2-1-11-21-12-15)14-5-9-17(20)10-6-1 h1-12,22H	-4.924
InChI=1S/C6H13NOS/c1-4-7-6(9)8-5(2)3/h5H,4H2,1-3H3,(H,7,9)	-1.745
InChI=1S/C6H8ClN3O2/c1-5-8-4-6(10(11)12)9(5)3-2-7/h4H, 2-3H2,1H3	-1.725
InChI=1S/C4H5F3N4O4S3/ c1-11-2(10-18(14,15)4(5,6)7)16-3(9-11)17(8,12)13/h1H3, (H2,8,12,13)/b10-2+	-1.16
InChI=1S/C5H10O/c1-3-4-5(2)6/h3-6H,1-2H3/b4-3+	0.015
InChI=1S/C10H13NO2/c1-2-10(13,9(11)12)8-6-4-3-5-7-8/h3-7,13H, 2H2,1H3,(H2,11,12)	-1.534
InChI=1S/C36H34Cl2N6O6/ c1-5-49-27-13-9-25(10-14-27)39-35(47)33(21(3)45)43-41-31-17-7-23(h7-20,33-34H,5-6H2,1-4H3,(H,39,47)(H,40,48)/b43-41+,44-42+	-7.831
InChI=1S/C18H25N3O5/ c1-19-18(22)20-13-14(23-2)12-6-10-25-15(12)17(24-3)16(13)26-11-9- h6,10H,4-5,7-9,11H2,1-3H3,(H2,19,20,22)	-3.028
InChI=1S/C12H13N3O/ c16-12(10-4-2-1-3-5-10)14-7-6-11-8-13-9-15-11/h1-5,8-9H,6-7H2,(H, 13,15)(H,14,16)	-0.634

"InChi"	"logS(M)"
InChI=1S/C27H32N4O4/c32-24-7-3-1-5-17-30(24)26(34)28-22-13-9-20(10-14-22)19-21-11-15-h9-16H,1-8,17-19H2,(H,28,34)(H,29,35)	-7.763
InChI=1S/C13H17N4O2P/c18-13(15-12-4-2-1-3-5-12)14-6-11-20(19,16-7-8-16)17-9-10-17/h1-6,11H,7-10H2,(H2,14,15,18)/b11-6+	-2.693
InChI=1S/C13H16N2O4/c1-3-13(11(17)19-2,10(16)15-12(14)18)9-7-5-4-6-8-9/h4-8H,3H2,1-2H3,(H3,14,15,16,18)	-2.75
InChI=1S/C7H5FO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)	-1.97
InChI=1S/C12H24N9P3/c1-2-16(1)22(17-3-4-17)13-23(18-5-6-18,19-7-8-19)15-24(14-22,20-9-h1-12H2	-3.754
InChI=1S/C11H15NO2/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h4-7H,2-3,8,12H2,1H3	-3.383
InChI=1S/C6H7N/c1-6-2-4-7-5-3-6/h2-5H,1H3	1.031
InChI=1S/C10H11N3O5S/c1-19-6-8-5-12(10(14)18-8)11-4-7-2-3-9(17-7)13(15)16/h2-4,8H,5-6H2,1H3/b11-4+	-3.621
InChI=1S/C6H10O4/c1-3-5(7)9-10-6(8)4-2/h3-4H2,1-2H3	-0.963
InChI=1S/C12H16N2O/c1-14(2)7-6-9-8-13-10-4-3-5-11(15)12(9)10/h3-5,8,13,15H,6-7H2,1-2H3	-0.929
InChI=1S/C10H19N/c1-7-8-4-5-9(6-8)10(2,3)11-7/h7-9,11H,4-6H2,1-3H3	-1.368
InChI=1S/C8H11N5O3S/c14-4-3-12-2-1-9-7(12)11-8-10-5-6(17-8)13(15)16/h5,14H,1-4H2,(H,9,10,11)	-1.509
InChI=1S/C16H12O3/c1-19-11-8-6-10(7-9-11)14-15(17)12-4-2-3-5-13(12)16(14)18/h2-9,14H,1H3	-3.5
InChI=1S/C8H14O3/c1-5(2)7(9)11-8(10)6(3)4/h5-6H,1-4H3	0.592
InChI=1S/C14H19ClN2O2/c1-2-17-9-3-4-13(10-17)19-14(18)16-12-7-5-11(15)6-8-12/h5-8,13H,2-4,9-10H2,1H3,(H,16,18)	-3.598
InChI=1S/C7H14O2/c1-7(4-6-9)3-2-5-8/h5,7,9H,2-4,6H2,1H3	-1.073
InChI=1S/C13H18O3/c14-8-12(15)9-16-13-6-5-10-3-1-2-4-11(10)7-13/h5-7,12,14-15H,1-4,8-9H2	-3.233
InChI=1S/C15H26O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h6,9,11,16H,1,7-8,10,12H2,2-5H3/b14-11-	-3.985
InChI=1S/C9H10N4O4/c1-11-4-10-7-6(11)8(16)13(3-5(14)15)9(17)12(7)2/h4H,3H2,1-2H3,(H,14,15)/p-1	-1.377
InChI=1S/C12H16N3O3PS2/c1-3-17-19(20,18-4-2)21-9-15-12(16)10-7-5-6-8-11(10)13-14-15/h5-8H,3-4,9H2,1-2H3	-4.517
InChI=1S/C7H4N2O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)	-2.208
InChI=1S/C10H8O3/c1-6-4-10(12)13-9-5-7(11)2-3-8(6)9/h2-5,11H,1H3	-1.529

"InChi"	"logS(M)"
InChI=1S/C11H23N3O/c1-14(2)9-8-12-11(15)13-10-6-4-3-5-7-10/h10H,3-9H2,1-2H3,(H2,12,13,15)	-0.66
InChI=1S/C8H12F3N5/c1-3-12-6-14-5(8(9,10)11)15-7(16-6)13-4-2/h3-4H2,1-2H3,(H2,12,13,14,15,16)	-3.238
InChI=1S/C6H4Cl2O/c7-4-2-1-3-5(8)6(4)9/h1-3,9H	-1.79
InChI=1S/C18H23NO/c1-4-19(5-2)15(3)16-11-13-18(14-12-16)20-17-9-7-6-8-10-17/h6-15H,4-5H2,1-3H3	-4.6
InChI=1S/C3H7I/c1-2-3-4/h2-3H2,1H3	-2.29
InChI=1S/C17H21NO2/c1-18-8-7-17-11-3-2-4-14(17)20-16-13(19)6-5-10(15(16)17)9-12(11)1h5-6,11-12,14,19H,2-4,7-9H2,1H3	-2.28
InChI=1S/C9H15N3O2/c1-3-5-12-8(13)6-7(10)11(4-2)9(12)14/h6H,3-5,10H2,1-2H3	-2.134
InChI=1S/C11H25NO/c1-3-5-7-11(4-2)10-13-9-6-8-12/h11H,3-10,12H2,1-2H3	-1.097
InChI=1S/C7H4Br2O/c8-6-1-2-7(9)5(3-6)4-10/h1-4H	-3.8
InChI=1S/C6H9N3O4/c10-4-5(11)3-8-2-1-7-6(8)9(12)13/h1-2,5,10-11H,3-4H2	-0.137
InChI=1S/C13H12O2/c14-10-11-5-4-8-13(9-11)15-12-6-2-1-3-7-12/h1-9,14H,10H2	-2.826
InChI=1S/C6H15NO/c1-3-6(2)7-4-5-8/h6-8H,3-5H2,1-2H3	0.667
InChI=1S/C8H4I3NO4/c9-3-1(7(13)14)4(10)6(12)5(11)2(3)8(15)16/h12H2,(H,13,14)(H,15,16)/p-2	-1.57
InChI=1S/C2H6O3P/c1-4-6(3)5-2/h1-2H3/q+1	-0.038
InChI=1S/C41H61N9O7/c1-25(2)17-31(35(51)21-36(52)47-32(18-26(3)4)37(53)45-23-29(42)3(h8-16,22,24-26,29,31-35,51H,17-21,23,42H2,1-7H3,(H,43,46)(H,45,53)(H,47,52)(H,48,55)(H,49,54)(H,50,56)	-3.4
InChI=1S/C4H8N2O2/c1-3(5-7)4(2)6-8/h5,7H,1-2H3/b4-3+	-2.287
InChI=1S/C10H9NO3S/c11-9-3-1-8-6-10(15(12,13)14)4-2-7(8)5-9/h1-6H,11H2,(H,12,13,14)	-3.27
InChI=1S/C8H10N2O/c1-10-8(11)6-2-4-7(9)5-3-6/h2-5H,9H2,1H3,(H,10,11)	-1.24
InChI=1S/C12H16N2O2/c1-13(2)11(15)9-5-7-10(8-6-9)12(16)14(3)4/h5-8H,1-4H3	0.266
InChI=1S/C12H16BrNO3/c1-2-3-6-17-11-5-4-9(7-10(11)13)8-12(15)14-16/h4-5,7,16H,2-3,6,8H2,1H3,(H,14,15)	-3.851
InChI=1S/C9H10/c1-3-9-6-4-5-8(2)7-9/h3-7H,1H2,2H3	-3.123
InChI=1S/C28H44O/c1-19(2)20(3)9-10-22(5)26-15-16-27-23(8-7-17-28(26,27)6)12-13-24-h9-10,12-13,19-20,22,25-27,29H,4,7-8,11,14-18H2,1-3,5-6H3/b10-9+,23-12+,24-13+	-3.899
InChI=1S/C6H10OS2/c1-5(7)6(2)8-3-4-9-6/h3-4H2,1-2H3	-1.839
InChI=1S/C10H12O3/c1-7-4-3-5-8(2)10(7)13-6-9(11)12/h3-5H,6H2,1-2H3,(H,11,12)	-2.257
InChI=1S/C5H11ClO/c1-4(6)5(2,3)7/h4,7H,1-3H3	-0.293

"InChi"	"logS(M)"
InChI=1S/C13H26N2O4/c1-6-13(9(2)3,7-18-11(14)16)8-19-12(17)15-10(4)5/h9-10H,6-8H2,1-5H3,(H2,14,16)(H,15,17)	-3.571
InChI=1S/C14H26N2O/c1-7-15(8-2)11-12(17)16-13(3,4)9-10-14(16,5)6/h9-10H,7-8,11H2,1-6H3	-2.691
InChI=1S/C16H22O11/c1-7(17)22-6-12-13(23-8(2)18)14(24-9(3)19)15(25-10(4)20)16(27-12)h12-16H,6H2,1-5H3	-2.415
InChI=1S/C14H29NO2/c1-5-9-10-12(6-2)11-14(7-3,8-4)13(16)15-17/h12,17H,5-11H2,1-4H3,(H,15,16)	-3.35
InChI=1S/C12H4Cl6O/c13-5-3-7(15)10(16)9(4-5)19-8-2-1-6(14)11(17)12(8)18/h1-4H	-8.55
InChI=1S/C4H9NO2/c1-2-3-7-4(5)6/h2-3H2,1H3,(H2,5,6)	-0.13
InChI=1S/C11H16ClN5/c1-7(2)15-10(13)17-11(14)16-9-5-3-8(12)4-6-9/h3-7H,1-2H3,(H5,13,14,15,16,17)	-3.212
InChI=1S/C6H14/c1-5-6(2,3)4/h5H2,1-4H3	-3.55
InChI=1S/C23H29NO2/c1-3-22(25)23(20-10-6-4-7-11-20,21-12-8-5-9-13-21)18-19(2)24-14-1h4-13,19H,3,14-18H2,1-2H3	-3.666
InChI=1S/C10H16N2O2S/c1-4-6(3)10(5-2)7(13)11-9(15)12-8(10)14/h6H,4-5H2,1-3H3,(H2,11,12,13,14,15)	-3.637
InChI=1S/C11H22O2/c1-6-13-10(12)7-9(2)8-11(3,4)5/h9H,6-8H2,1-5H3	-3.823
InChI=1S/C20H23Cl2NO2/c1-23-10-9-13-11-19(24-2)20(25-3)12-15(13)18(23)8-7-14-16(21)5-4-h4-6,11-12,18H,7-10H2,1-3H3	-5.67
InChI=1S/C23H30N2O3/c1-15(2)9-12-28-23(27)19-14-25-11-8-16(19)13-21(25)22(26)18-7-10-h3-7,10,15-16,19,21-22,26H,8-9,11-14H2,1-2H3	-1.41
InChI=1S/C14H18Cl2N4O/c15-12-2-1-10(7-13(12)16)20-5-3-19(4-6-20)9-11-8-18-14(17)21-11/h1-2,7,11H,3-6,8-9H2,(H2,17,18)	-3.65
InChI=1S/C14H19NO4/c1-17-12-7-9-5-4-6-10(15-16)8-11(9)13(18-2)14(12)19-3/h7,16H,4-6,8H2,1-3H3/b15-10+	-2.093
InChI=1S/C13H10O4/c14-9-6-10(15)12(11(16)7-9)13(17)8-4-2-1-3-5-8/h1-7,14-16H	-1.871
InChI=1S/C9H10O2/c1-11-9(10)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3	-2.211
InChI=1S/C5H11NO2/c1-4(7)5(8)6(2)3/h4,7H,1-3H3	1.63
InChI=1S/C19H29NO2/c1-17-11-7-9-15-20(17)14-8-2-3-10-16-22-19(21)18-12-5-4-6-13-18/h4-6,12-13,17H,2-3,7-11,14-16H2,1H3	-4.905
InChI=1S/C10H14N4O2/c15-10(9-7-11-1-2-12-9)13-8-14-3-5-16-6-4-14/h1-2,7H,3-6,8H2,(H,13,15)	0.176
InChI=1S/C15H20N2O2/c18-13-6-4-12(5-7-13)17-11-8-14(15(17)19)16-9-2-1-3-10-16/h4-7,14,18H,1-3,8-11H2	-2.567

"InChi"	"logS(M)"
InChI=1S/C19H24O3/c1-7-8-13-12(4)16(10-15(13)20)22-18(21)17-14(9-11(2)3)19(17,5)6/h1,9,14,16-17H,8,10H2,2-6H3	-4.575
InChI=1S/C7H5N3O3/c8-7-9-5-3-4(10(11)12)1-2-6(5)13-7/h1-3H,(H2,8,9)	-1.954
InChI=1S/C10H17N3O2/c1-10(2,3)7-6-8(12-15-7)11-9(14)13(4)5/h6H,1-5H3,(H,11,12,14)	-2.427
InChI=1S/C19H18N2O2/c1-3-7-15(8-4-1)17-18(16-9-5-2-6-10-16)23-19(20-17)21-11-13-22-14h1-10H,11-14H2	-4.978
InChI=1S/C14H21NO/c1-2-3-4-5-6-7-14(16)12-8-10-13(15)11-9-12/h8-11H,2-7,15H2,1H3	-3.963
InChI=1S/C6H4N2/c7-4-6-2-1-3-8-5-6/h1-3,5H	0.113
InChI=1S/C6H12N2O4/c9-3-1-7-5(11)6(12)8-2-4-10/h9-10H,1-4H2,(H,7,11)(H,8,12)	-0.112
InChI=1S/C6H7NO/c7-5-2-1-3-6(8)4-5/h1-4,8H,7H2	-0.623
InChI=1S/C5H10N2O3S2/c6-5(7-4-1-2-4)3-11-12(8,9)10/h4H,1-3H2,(H2,6,7)(H,8,9,10)	-0.617
InChI=1S/C6H12O3/c7-3-5-1-2-6(4-8)9-5/h5-8H,1-4H2	0.879
InChI=1S/C10H11ClN4O4/c11-8-5-9(13-2-12-8)15(3-14-5)10-7(18)6(17)4(1-16)19-10/h2-4,6-7,10,16-18H,1H2	-1.895
InChI=1S/C8H6O2/c9-5-7-1-2-8(6-10)4-3-7/h1-6H	-2.826
InChI=1S/C13H14/c1-10(2)12-8-7-11-5-3-4-6-13(11)9-12/h3-10H,1-2H3	-5.298
InChI=1S/C19H17Cl2N5O4/c1-13(27)30-10-9-25(8-2-7-22)15-5-3-14(4-6-15)23-24-19-17(20)11-1h3-6,11-12H,2,8-10H2,1H3/b24-23+	-7.051
InChI=1S/C11H7Cl2FN2O2/c12-7-2-1-6(8(13)3-7)4-16-5-9(14)10(17)15-11(16)18/h1-3,5H,4H2,(H,15,17,18)	-3.94
InChI=1S/C11H13N3O3S/c1-7-8(2)17-13-11(7)14-18(15,16)10-5-3-9(12)4-6-10/h3-6H,12H2,1-2H3,(H,13,14)	-2.19
InChI=1S/C15H22N4O2/c1-20-13-4-2-3-12(9-13)19-7-5-18(6-8-19)11-14-10-17-15(16)21-14/h2-4,9,14H,5-8,10-11H2,1H3,(H2,16,17)	-2.061
InChI=1S/C16H30N2O3/c1-2-3-7-13-21-15(19)11-8-12-17-16(20)18-14-9-5-4-6-10-14/h14H,2-13H2,1H3,(H2,17,18,20)	-2.3
InChI=1S/C19H28O4/c1-3-7-15(8-4-1)17-20-11-19(12-21-17)13-22-18(23-14-19)16-9-5-2-6h1-3,5,15-18H,4,6-14H2	-5.24
InChI=1S/C12H18N2O2/c1-3-14(4-2)8-9-16-12(15)11-6-5-7-13-10-11/h5-7,10H,3-4,8-9H2,1-2H3	-0.433
InChI=1S/C12H15ClO3/c1-2-3-9-6-10(13)4-5-12(9)16-8-11(15)7-14/h2,4-6,11,14-15H,1,3,7-8H2	-3.445
InChI=1S/C9H13N/c1-2-3-8-4-6-9(10)7-5-8/h4-7H,2-3,10H2,1H3	-2.238
InChI=1S/C7H16O7/c8-1-3(10)5(12)7(14)6(13)4(11)2-9/h3-14H,1-2H2	0.372

"InChi"	"logS(M)"
InChI=1S/C25H36O6/c1-4-5-21(29)31-14-20(28)25(30)11-9-18-17-7-6-15-12-16(26)8-10-23h12,17-19,22,27,30H,4-11,13-14H2,1-3H3	-5.069
InChI=1S/C13H17NO3/c1-13(2,3)14-11(15)9-17-12(16)10-7-5-4-6-8-10/h4-8H,9H2,1-3H3,(H,14,15)	-2.866
InChI=1S/C10H13N5/c1-3-6-7(4-2)15-10-8(14-6)9(11)12-5-13-10/h5H,3-4H2,1-2H3,(H2,11,12,13,15)	-2.93
InChI=1S/C5H6N2O4/c8-3(9)1-2-4(10)7-5(11)6-2/h2H,1H2,(H,8,9)(H2,6,7,10,11)	-1.152
InChI=1S/C10H12O3/c11-7-4-8-13-10(12)9-5-2-1-3-6-9/h1-3,5-6,11H,4,7-8H2	-1.256
InChI=1S/C13H15NO2/c1-10(2)16-13(15)14-9-5-7-11-6-3-4-8-12(11)14/h3-8,10H,9H2,1-2H3	-4.3
InChI=1S/C6H17N2O3PS/c7-3-1-4-8-5-2-6-13-12(9,10)11/h8H,1-7H2,(H2,9,10,11)	0.64
InChI=1S/C11H9NO2/c1-8-6-7-9-4-2-3-5-10(9)11(8)12(13)14/h2-7H,1H3	-4.27
InChI=1S/C10H12N4O5/c15-1-3-7(16)8(17)9(19-3)5-4-6(14-13-5)10(18)12-2-11-4/h2-3,7-9,15-17H,1H2,(H,13,14)(H,11,12,18)	0.571
InChI=1S/C16H17NO/c1-13(15-10-6-3-7-11-15)17-16(18)12-14-8-4-2-5-9-14/h2-11,13H,12H2,1H3,(H,17,18)	-3.19
InChI=1S/C14H16N2/c1-9-7-11(3-5-13(9)15)12-4-6-14(16)10(2)8-12/h3-8H,15-16H2,1-2H3	-2.213
InChI=1S/C13H16IN4O2P/c14-11-1-3-12(4-2-11)16-13(19)15-5-10-21(20,17-6-7-17)18-8-9-18/h1-5,10H,6-9H2,(H2,15,16,19)/b10-5+	-3.295
InChI=1S/C19H21NO4/c1-22-16-11-14(12-17(23-2)18(16)24-3)19(21)20-10-6-8-13-7-4-5-9-14h4-5,7,9,11-12H,6,8,10H2,1-3H3	-4.119
InChI=1S/C12H25NO3/c1-4-7-8-12(5-2,9-14)10-16-11(15)13-6-3/h14H,4-10H2,1-3H3,(H,13,15)	-3.278
InChI=1S/C10H12O2/c1-10(2,12)9(11)8-6-4-3-5-7-8/h3-7,12H,1-2H3	-1.092
InChI=1S/C8H17N/c1-7(2)5-4-6-8(3)9/h5,8H,4,6,9H2,1-3H3	-1.314
InChI=1S/C6H14O3/c1-2-8-5-6-9-4-3-7/h7H,2-6H2,1H3	0.872
InChI=1S/C8H14O2S2/c9-7(11)5-3-1-2-4-6-8(10)12/h1-6H2,(H,9,11)(H,10,12)	-2.24
InChI=1S/C14H19NO/c1-5-16-11-6-7-13-12(8-11)10(2)9-14(3,4)15-13/h6-9,15H,5H2,1-4H3	-3.333
InChI=1S/C15H30N6O6/c1-22-7-19(8-23-2)13-16-14(20(9-24-3)10-25-4)18-15(17-13)21(11-26h7-12H2,1-6H3	-3.418
InChI=1S/C19H16N2O3/c1-12(22)20-15-6-8-16(9-7-15)21-19(24)17-10-13-4-2-3-5-14(13)11-1h2-11,23H,1H3,(H,20,22)(H,21,24)	-5.25
InChI=1S/C12H16O2/c1-12(2,3)10-7-5-9(6-8-10)11(13)14-4/h5-8H,1-4H3	-3.74

"InChi"	"logS(M)"
InChI=1S/C14H18N2O/c1-10(2)13-11(3)15(4)16(14(13)17)12-8-6-5-7-9-12/h5-10H,1-4H3	-1.91
InChI=1S/C12H15NO3/c1-10(14)13(2)8-9-16-12(15)11-6-4-3-5-7-11/h3-7H,8-9H2,1-2H3	-0.849
InChI=1S/C16H32O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16(2)17/h3-15H2,1-2H3	-6.205
InChI=1S/C8H12BrCl3O2/c1-4(2)6(9)7(13)14-5(3)8(10,11)12/h4-6H,1-3H3	-5.259
InChI=1S/C20H18N6O4S/c1-14(27)30-12-11-25(10-2-9-21)16-5-3-15(4-6-16)23-24-20-22-18-8-h3-8,13H,2,10-12H2,1H3/b24-23+	-4.341
InChI=1S/C8H8N4O/c9-7-10-8(13)11-12(7)6-4-2-1-3-5-6/h1-5H,(H3,9,10,11,13)	-1.7
InChI=1S/C18H23N5O5/c1-21-16-15(17(27)22(2)18(21)28)23(10-20-16)5-3-4-19-9-14(26)11-6h6-8,10,14,19,24-26H,3-5,9H2,1-2H3	-2.437
InChI=1S/C29H30N4/c1-4-11-25(12-5-1)29(26-13-6-2-7-14-26,27-15-8-3-9-16-27)17-20-32h1-16,18-19H,17,20-24H2	-6.518
InChI=1S/C14H15NO4/c16-9-8-15-7-6-11(17)14(19)12(15)13(18)10-4-2-1-3-5-10/h1-7,13,16,18-19H,8-9H2	-2.82
InChI=1S/C12H17NO2/c1-2-3-8-15-11-6-4-10(5-7-11)9-12(13)14/h4-7H,2-3,8-9H2,1H3,(H2,13,14)	-2.506
InChI=1S/C11H13NO4/c1-11(10(15)16)7-5-9(14)8(13)4-6(7)2-3-12-11/h4-5,12-14H,2-3H2,1H3,(H,15,16)	-0.75
InChI=1S/C12H13N/c1-13-9-11-7-4-6-10-5-2-3-8-12(10)11/h2-8,13H,9H2,1H3	-1.715
InChI=1S/C9H15NO3S/c1-6(5-14)8(11)10-4-2-3-7(10)9(12)13/h6-7,14H,2-5H2,1H3,(H,12,13)	-1.076
InChI=1S/C4H10N2O6/c7-5(8)11-3-1-2-4-12-6(9)10/h1-4H2,(H,7,8)(H,9,10)/q+2	-1.68
InChI=1S/C38H72N2O12/c1-15-27-38(10,46)31(42)24(6)40(13)19-20(2)17-36(8,45)33(52-35-29h20-33,35,41-43,45-46H,15-19H2,1-14H3	-5.024
InChI=1S/C16H11ClN4/c17-12-6-7-14-13(8-12)16(11-4-2-1-3-5-11)18-9-15-20-19-10-21(14)15h1-8,10H,9H2	-5.295
InChI=1S/C9H15NO3/c1-4-13-9(12)6-10-7(2)5-8(3)11/h5,10H,4,6H2,1-3H3/b7-5+	-0.59
InChI=1S/C2HBrClF3/c3-2(6,7)1(4)5/h1H	-3.316
InChI=1S/C7H4O6/c8-3-1-4(6(9)10)13-5(2-3)7(11)12/h1-2H,(H,9,10)(H,11,12)	-1.11
InChI=1S/C10H12N4O3/c1-7(2)12-13-10(15)11-8-3-5-9(6-4-8)14(16)17/h3-6H,1-2H3,(H2,11,13,15)	-3.595
InChI=1S/C8H3N3O2/c9-4-6-2-1-3-8(11(12)13)7(6)5-10/h1-3H	-2.937
InChI=1S/C12H22O2/c1-6-10(2)8-7-9-12(4,5)14-11(3)13/h6,10H,1,7-9H2,2-5H3	-4.03
InChI=1S/C5H11NO2/c1-3-5(2,6)4(7)8/h3,6H2,1-2H3,(H,7,8)	0.38

"InChi"	"logS(M)"
InChI=1S/C7H14O3/c1-3-9-6-5-7(8)10-4-2/h3-6H2,1-2H3	-0.432
InChI=1S/C32H60O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-29-35-31(33)27-28-32(34)36-30-h27-28H,3-26,29-30H2,1-2H3/b28-27+	-7.008
InChI=1S/C23H22ClN3/c1-26(2)14-15-27-21-13-12-18(24)16-19(21)23(17-8-4-3-5-9-17)25-2(h3-13,16H,14-15H2,1-2H3	-5.842
InChI=1S/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h1-5,8-10H	0.164
InChI=1S/C5H7N/c1-2-3-4-5-6/h3-4H,2H2,1H3/b4-3+	-0.86
InChI=1S/C7H5NO4/c9-4-5-1-2-7(10)6(3-5)8(11)12/h1-4,10H	-2.951
InChI=1S/C7H7NO3/c9-5-6-3-1-2-4-7(6)8(10)11/h1-4,9H,5H2	-1.486
InChI=1S/C12H12N4O7/c1-2-22-11(18)7-14-9(17)6-15(12(14)19)13-5-8-3-4-10(23-8)16(20)21h3-5H,2,6-7H2,1H3/b13-5+	-2.446
InChI=1S/C25H30N2O/c1-19(2)25(24(26)28,16-17-27(3)18-20-10-5-4-6-11-20)23-15-9-13-21h4-15,19H,16-18H2,1-3H3,(H2,26,28)	-6.12
InChI=1S/C25H36O5/c1-15(26)30-18-6-9-23(2)17(13-18)4-5-21-20(23)7-10-24(3)19(8-11-2h12,17-21,28H,4-11,13-14H2,1-3H3	-4.92
InChI=1S/C12H15Cl2NO2/c1-9-2-3-10(12(16)17)8-11(9)15(6-4-13)7-5-14/h2-3,8H,4-7H2,1H3,(H,16,17)	-4.707
InChI=1S/C7H9N5/c1-12(2)7-10-5-3-8-4-9-6(5)11-7/h3-4H,1-2H3,(H,8,9,10,11)	-1.389
InChI=1S/C17H23N5O3/c23-16-13(12-18-22-10-11-25-17(22)24)15(20-7-3-1-4-8-20)19-14-6-2h12H,1-11H2/b18-12+	-3.231
InChI=1S/C22H45NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24/h2-21H2,1H3,(H2,23,24)	-6.832
InChI=1S/C12H3Cl7O/c13-4-1-2-6(5(14)3-4)20-12-10(18)8(16)7(15)9(17)11(12)19/h1-3H	-9.64
InChI=1S/C12H14N4O/c1-9-11(12(17)15(2)3)13-14-16(9)10-7-5-4-6-8-10/h4-8H,1-3H3	-1.822
InChI=1S/C10H12N4O2/c1-7-4-10(16-3)14(13-7)8-5-9(15-2)12-6-11-8/h4-6H,1-3H3	-2.114
InChI=1S/C9H15BrN2O3/c1-4-9(10,5-2)7(14)12-8(15)11-6(3)13/h4-5H2,1-3H3,(H2,11,12,13,14,15)	-2.759
InChI=1S/C27H33O4P/c1-19(2)22-7-13-25(14-8-22)29-32(28,30-26-15-9-23(10-16-26)20(3)4h7-21H,1-6H3	-6.137
InChI=1S/C18H14N4O2/c23-22(24)18-12-10-17(11-13-18)21-20-16-8-6-15(7-9-16)19-14-4-2-1h1-13,19H/b21-20+	-7.523
InChI=1S/C10H19N3O4/c1-6(2)3-7(10(16)17)13-9(15)5-12-8(14)4-11/h6-7H,3-5,11H2,1-2H3,(H,12,14)(H,13,15)(H,16,17)	-0.11
InChI=1S/C7H8N2O2/c10-5-9-7(11)6-2-1-3-8-4-6/h1-4,10H,5H2,(H,9,11)	0.535

"InChi"	"logS(M)"
InChI=1S/C14H13Cl2N5O4S/c1-7-4-5-8(15)12(11(7)16)20-26(22,23)14-18-13-17-9(24-2)6-10(25-3)h4-6,20H,1-3H3	-3.32
InChI=1S/C8H20N4/c1-2-10-5-6-12-8-7-11-4-3-9-1/h9-12H,1-8H2	-0.031
InChI=1S/C28H27ClN2O7/c1-4-38-28(35)24-21(15-37-14-13-31-25(32)17-9-5-6-10-18(17)26(31)h5-12,23,30H,4,13-15H2,1-3H3	-4.501
InChI=1S/C13H26N2O3/c1-4-5-6-7-8-9-10-15(17)14-13(11-18-3)12(2)16/h9-10,12-13,16H,4-8,11H2,1-3H3/b10-9+,15-14-	-4.076
InChI=1S/C12H17NO2/c1-9(13(3)10(2)14)12(15)11-7-5-4-6-8-11/h4-9,12,15H,1-3H3	-1.22
InChI=1S/C14H23N3O2/c1-10-12(15(2)3)13(18)17(14(19)16(10)4)11-8-6-5-7-9-11/h11H,5-9H2,1-4H3	-3.171
InChI=1S/C10H10O4/c1-7(11)14-9(10(12)13)8-5-3-2-4-6-8/h2-6,9H,1H3,(H,12,13)	-1.231
InChI=1S/C4H9/c1-4(2)3/h1-3H3	-4.377
InChI=1S/C7H14N2O2S/c1-7(2,12-4)5-9-11-6(10)8-3/h5H,1-4H3,(H,8,10)/b9-5+	-1.499
InChI=1S/C17H16ClFN2O2/c18-12-5-3-11(4-6-12)17(21-9-1-2-16(20)23)14-10-13(19)7-8-15(14)2h3-8,10,21H,1-2,9H2,(H2,20,23)/b17-14-	-3.674
InChI=1S/C27H43NO2/c1-15-5-8-22-16(2)25-23(28(22)14-15)12-21-19-7-6-17-11-18(29)9-10h6,15-16,18-25,29-30H,5,7-14H2,1-4H3	-7.696
InChI=1S/C23H30N2O2/c1-4-23(24(2)3,18-19-8-6-5-7-9-19)22(26)20-10-12-21(13-11-20)25-1h5-13H,4,14-18H2,1-3H3	-4.793
InChI=1S/C16H13NO/c18-16(14-8-2-1-3-9-14)17-12-6-10-13-7-4-5-11-15(13)17/h1-11H,12H2	-3.682
InChI=1S/C10H20N2O3/c1-5(2)7(11)9(13)12-8(6(3)4)10(14)15/h5-8H,11H2,1-4H3,(H,12,13)(H,14,15)	-0.4
InChI=1S/C9H12N2O3/c1-4-9(5(2)3)6(12)10-8(14)11-7(9)13/h4-5H,1H2,2-3H3,(H2,10,11,12,13,14)	-1.71
InChI=1S/C9H12O2/c1-5-4-8(10)6(2)7(3)9(5)11/h4,10-11H,1-3H3	-1.638
InChI=1S/C8H9NO4/c1-4-7(11)6(8(12)13)5(3-10)2-9-4/h2,10-11H,3H2,1H3,(H,12,13)	-0.538
InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)	-0.197
InChI=1S/C12H28O5P2S2/c1-5-9-13-18(20,14-10-6-2)17-19(21,15-11-7-3)16-12-8-4/h5-12H2,1-4H3	-4.101
InChI=1S/C12H15N5O5/c13-9-6-4(10(14)21)1-17(11(6)16-3-15-9)12-8(20)7(19)5(2-18)22-12/h1,3,5,7-8,12,18-20H,2H2,(H2,14,21)(H2,13,15,16)	-0.131
InChI=1S/C4H10OS2/c1-3-6-7(5)4-2/h3-4H2,1-2H3/p+1	-0.099
InChI=1S/C12H14N4O5S2/c13-15-22(17,18)11-5-1-9(2-6-11)21-10-3-7-12(8-4-10)23(19,20)16-14h1-8,15-16H,13-14H2	-3.758

"InChi"	"logS(M)"
InChI=1S/C22H24ClN5O7/c1-14(29)24-22-13-17(27(8-10-34-15(2)30)9-11-35-16(3)31)4-7-21(22h4-7,12-13H,8-11H2,1-3H3,(H,24,29)/b26-25+	-6.964
InChI=1S/C2H2Cl2O2/c3-1(4)2(5)6/h1H,(H,5,6)	0.89
InChI=1S/C13H10N2O3/c16-12-7-6-10(8-11(12)13(17)18)15-14-9-4-2-1-3-5-9/h1-8,14H,(H,17,18)/b15-10-	-3.056
InChI=1S/C12H17N2O4P/c1-14(2)7-6-9-8-13-10-4-3-5-11(12(9)10)18-19(15,16)17/h3-5,8,13H,6-7H2,1-2H3,(H2,15,16,17)	-2.156
InChI=1S/C43H66N12O12S2/c1-5-22(4)35-42(66)49-26(12-13-32(45)57)38(62)51-29(17-33(46)58)3h8-11,21-22,25-31,35,56H,5-7,12-20,44H2,1-4H3,(H2,45,57)(H2,46,58)(H2,47,59)(H,48,61)(H,49,66)(H,50,60)(H,51,62)(H,52,65)(H,53,63)(H,54,64)	-1.916
InChI=1S/C6H6N4O2/c1-5-8-4-6(10(11)12)9(5)3-2-7/h4H,3H2,1H3	-1.008
InChI=1S/C12H7Cl3/c13-9-5-2-1-4-8(9)12-10(14)6-3-7-11(12)15/h1-7H	-5.9
InChI=1S/C24H30O8/c1-6-8-14(25)16-19(28)11(3)18(27)12(20(16)29)10-13-21(30)17(15(2h27-31H,6-10H2,1-5H3	-5.383
InChI=1S/C17H16O2/c18-17(12-11-15-7-3-1-4-8-15)19-14-13-16-9-5-2-6-10-16/h1-12H,13-14H2/b12-11+	-5.402
InChI=1S/C13H10O3/c14-13(15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H	-4.217
InChI=1S/C12H8Cl2/c13-10-5-3-4-9(8-10)11-6-1-2-7-12(11)14/h1-8H	-5.585
InChI=1S/C6H5Cl2N3O2/c1-13-6(12)2-5(9)11-4(8)3(7)10-2/h1H3,(H2,9,11)	-4.535
InChI=1S/C30H58O6/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-33-29(31)35-36-30(32)34-28h3-28H2,1-2H3	-4.35
InChI=1S/C11H11N3O2/c1-2-8-9(14-11(16)13-8)10(15)7-3-5-12-6-4-7/h3-6H,2H2,1H3,(H2,13,14,16)	-1.99
InChI=1S/C12H15ClO3/c1-2-3-4-7-16-12(15)9-5-6-11(14)10(13)8-9/h5-6,8,14H,2-4,7H2,1H3	-3.95
InChI=1S/C9H4Cl3NO2S/c10-9(11,12)16-13-7(14)5-3-1-2-4-6(5)8(13)15/h1-4H	-5.569
InChI=1S/C15H16Cl2N2O8/c16-14(17)15(24)18-10(7-27-12(22)6-5-11(20)21)13(23)8-1-3-9(4-2-8h1-4,10,13-14,23H,5-7H2,(H,18,24)(H,20,21)	-2.082
InChI=1S/C5H7N3O2/c1-4-3-6-5(7(4)2)8(9)10/h3H,1-2H3	-1.451
InChI=1S/C13H19N5O4/c1-16-6-8-17(9-7-16)5-4-12(19)15-14-10-11-2-3-13(22-11)18(20)21/h2-3,10H,4-9H2,1H3,(H,15,19)/b14-10+	-2.601
InChI=1S/C8H5NO6/c10-7(11)4-2-1-3-5(9(14)15)6(4)8(12)13/h1-3H,(H,10,11)(H,12,13)	-1.021
InChI=1S/C12H15NO3/c1-2-9-16-11-6-4-3-5-10(11)12(15)13-7-8-14/h2-6,14H,1,7-9H2,(H,13,15)	-1.803

"InChi"	"logS(M)"
InChI=1S/C10H20N2O4/c1-9(2,3)10(4,5-15-7(11)13)6-16-8(12)14/h5-6H2,1-4H3,(H2,11,13)(H2,12,14)	-2.059
InChI=1S/C21H23N3OS/c22-15-16-6-7-21-19(14-16)24(18-4-1-2-5-20(18)26-21)11-3-10-23-12h1-2,4-7,14,17,25H,3,8-13H2	-3.98
InChI=1S/C11H8O2/c12-7-10-9-4-2-1-3-8(9)5-6-11(10)13/h1-7,13H	-3.894
InChI=1S/C3H7ClOS/c4-1-3(5)2-6/h3,5-6H,1-2H2	-0.531
InChI=1S/C11H10O/c12-8-10-6-3-5-9-4-1-2-7-11(9)10/h1-7,12H,8H2	-1.744
InChI=1S/C12H8INS/c13-8-5-6-10-12(7-8)15-11-4-2-1-3-9(11)14-10/h1-7,14H	-6.928
InChI=1S/C11H12O2/c1-2-10(11(12)13)8-9-6-4-3-5-7-9/h2-7H,8H2,1H3,(H,12,13)/b10-2-	-2.565
InChI=1S/C11H15NO3/c1-2-7-15-10-5-3-9(4-6-10)8-11(13)12-14/h3-6,14H,2,7-8H2,1H3,(H,12,13)	-1.994
InChI=1S/C9H18O3/c1-3-4-5-6-7-12-9(11)8(2)10/h8,10H,3-7H2,1-2H3	-1.14
InChI=1S/C23H24Br8O2/c1-21(2,13-5-15(26)19(16(27)6-13)32-11-22(3,30)9-24)14-7-17(28)20(h5-8H,9-12H2,1-4H3	-7.686
InChI=1S/C8H14N2O2/c1-5(2)3-6-8(12)9-4-7(11)10-6/h5-6H,3-4H2,1-2H3,(H,9,12)(H,10,11)	-1.25
InChI=1S/C15H9FO2/c16-10-7-5-9(6-8-10)13-14(17)11-3-1-2-4-12(11)15(13)18/h1-8,13H	-3.83
InChI=1S/C5H11N5O4S3/c1-9(2)17(13,14)8-4-10(3)7-5(15-4)16(6,11)12/h1-3H3,(H2,6,11,12)/b8-4+	-2.7
InChI=1S/C14H24N2O2S/c1-3-5-6-12(4-2)11-16-19(17,18)14-9-7-13(15)8-10-14/h7-10,12,16H,3-6,11,15H2,1-2H3	-5.454
InChI=1S/C6H12Cl3N/c7-1-4-10(5-2-8)6-3-9/h1-6H2	-3.107
InChI=1S/C12H16O4/c1-12(2,15)11(14)9-3-5-10(6-4-9)16-8-7-13/h3-6,13,15H,7-8H2,1-2H3	-1.47
InChI=1S/C9H8N2O2/c12-8-5-10-9(13)6-3-1-2-4-7(6)11-8/h1-4H,5H2,(H,10,13)(H,11,12)	-2.85
InChI=1S/C15H22O3/c1-11-6-7-12(2)13(10-11)18-9-5-8-15(3,4)14(16)17/h6-7,10H,5,8-9H2,1-4H3,(H,16,17)	-4.36
InChI=1S/C28H38N4O8/c1-15-9-7-12-20(35)21(15)24(36)40-14-27(39)23(30-19-11-8-10-18(1h7-13,17,22-23,30,34-35,38-39H,14,29H2,1-6H3,(H,31,37)	-3.447
InChI=1S/C18H38S3/c1-13(15(3,4)5)17(9,10)19-21-20-18(11,12)14(2)16(6,7)8/h13-14H,1-12H3	-9.13
InChI=1S/C11H20N2O/c1-3-4-11(14)13-9-5-6-10(13)8-12(2)7-9/h9-10H,3-8H2,1-2H3	-1.32
InChI=1S/C12H7Cl3O/c13-8-1-3-9(4-2-8)16-10-5-6-11(14)12(15)7-10/h1-7H	-5.66

"InChi"	"logS(M)"
InChI=1S/C6H18O24P6/c7-31(8,9)25-1-2(26-32(10,11)12)4(28-34(16,17)18)6(30-36(22,23)24)5(29-35(19,20)21)3(27-33(13,14)15)h1-6H,(H2,7,8,9)(H2,10,11,12)(H2,13,14,15)(H2,16,17,18)(H2,19,20,21)(H2,22,23,24)	0.18
InChI=1S/C3H4N2OS/c6-2-1-4-3(7)5-2/h1H2,(H2,4,5,6,7)	-0.993
InChI=1S/C21H21O4P/c1-16-4-10-19(11-5-16)23-26(22,24-20-12-6-17(2)7-13-20)25-21-14-8-18(3)9-15-21/h4-15H,1-3H3	-6.089
InChI=1S/C18H24N2O2/c1-19-13-12-15-4-2-3-5-17(15)18(19)11-8-14-6-9-16(10-7-14)20(21)22/h6-7,9-10,18H,2-5,8,11-13H2,1H3	-5.222
InChI=1S/C8H14O3/c1-3-4-5-6-7-11-8(9)10-2/h4-5H,3,6-7H2,1-2H3/b5-4+	-3.07
InChI=1S/C13H17NO4/c1-3-14(4-2)12(16)9-18-13(17)10-7-5-6-8-11(10)15/h5-8,15H,3-4,9H2,1-2H3	-2.56
InChI=1S/C13H21BrN2O4S2/c14-12-5-6-13(16-11-12)20-9-4-2-1-3-7-15-8-10-21-22(17,18)19/h5-6,11,15H,1-4,7-10H2,(H,17,18,19)	-3.218
InChI=1S/C18H17N3O/c1-13-17-19-16-10-6-5-9-15(16)18(22)21(17)12-20(13)11-14-7-3-2-4-8-14/h2-10,13H,11-12H2,1H3	-4
InChI=1S/C13H15BrO4S/c1-18-12(15)13(8-2-3-9-13)19(16,17)11-6-4-10(14)5-7-11/h4-7H,2-3,8-9H2,1H3	-4.01
InChI=1S/C6H4N4O2/c11-3-1-7-5-4(10-3)6(12)9-2-8-5/h1-2H,(H,10,11)(H,7,8,9,12)	-2.96
InChI=1S/C9H11FN2O4/c1-2-3-4-16-9(15)12-5-6(10)7(13)11-8(12)14/h5H,2-4H2,1H3,(H,11,13,14)	-1.59
InChI=1S/C12H4Cl6/c13-6-4-2-1-3-5(6)7-8(14)10(16)12(18)11(17)9(7)15/h1-4H	-8.013
InChI=1S/C17H23ClN2O4S2/c1-13-11-17(20-16-6-5-14(18)12-15(13)16)24-9-4-2-3-7-19-8-10-25-26(21,22)23/h5-6,11-12,19H,2-4,7-10H2,1H3,(H,21,22,23)	-4.24
InChI=1S/C9H10ClNO/c1-11-5-7-2-3-9(10)4-8(7)6-12-11/h2-4H,5-6H2,1H3	-2.735
InChI=1S/C21H28N2O2/c24-16-18-25-17-15-22-11-13-23(14-12-22)21(19-7-3-1-4-8-19)20-9-5-2-6-10-21/h1-10,21,24H,11-18H2	-2.141
InChI=1S/C10H11NO3/c1-14-9-5-2-8(3-6-9)4-7-10(12)11-13/h2-7,13H,1H3,(H,11,12)/b7-4+	-1.73
InChI=1S/C15H14O2/c16-15(11-13-7-3-1-4-8-13)17-12-14-9-5-2-6-10-14/h1-10H,11-12H2	-3.863
InChI=1S/C24H32N2O2/c1-5-24(25(3)4,18-20-8-6-19(2)7-9-20)23(27)21-10-12-22(13-11-21)26-14-16-28-17-15-26/h6-13H,5,14-18H2,1-4H3	-5.133
InChI=1S/C21H22N4O5/c1-10-15(23-11-6-4-3-5-7-11)18(27)14-12(9-30-20(22)28)21(29-2)19-13(17(14)26)8-24-25(19)16(10)23/h3-7,12-13,19,23-24H,8-9H2,1-2H3,(H2,22,28)	-2.294

"InChi"	"logS(M)"
InChI=1S/C14H21NO2/c1-4-10-15-14(2,3)11-17-13(16)12-8-6-5-7-9-12/h5-9,15H,4,10-11H2,1-3H3	-2.249
InChI=1S/C5H7F3O2/c1-3(2)10-4(9)5(6,7)8/h3H,1-2H3	-1.336
InChI=1S/C15H13F3N4O/c1-3-22-12-9(5-4-6-19-12)14(23)21-11-10(15(16,17)18)7-8(2)20-13(1h4-7H,3H2,1-2H3,(H,21,23)	-4.207
InChI=1S/C10H9NO6/c1-16-9(12)6-3-7(10(13)17-2)5-8(4-6)11(14)15/h3-5H,1-2H3	-2.6
InChI=1S/C7H7BrO2/c8-6-1-2-7(10)5(3-6)4-9/h1-3,9-10H,4H2	-0.207
InChI=1S/C11H21N3O4/c1-6(2)4-8(12)11(18)14-7(3)10(17)13-5-9(15)16/h6-8H,4-5,12H2,1-3H3,(H,13,17)(H,14,18)(H,15,16)	-0.895
InChI=1S/C10H17NO4/c1-3-5-6-11-10(13)15-8-7-14-9(12)4-2/h4H,2-3,5-8H2,1H3,(H,11,13)	-1.635
InChI=1S/C7H6Cl2O2/c1-11-7-3-5(9)4(8)2-6(7)10/h2-3,10H,1H3	-2.53
InChI=1S/C13H20N2O3/c16-10-13(11(17)15-12(18)14-10)8-6-4-2-1-3-5-7-9-13/h1-9H2,(H2,14,15,16,17,18)	-4.59
InChI=1S/C23H22ClF3O2/c1-14-16(10-7-11-17(14)15-8-5-4-6-9-15)13-29-21(28)20-18(22(20,2)h4-12,18,20H,13H2,1-3H3/b19-12-	-6.626
InChI=1S/C4H8O2S/c1-4(5)6-2-3-7/h7H,2-3H2,1H3	-1.5
InChI=1S/C21H28O4/c1-19-9-12(11-22)16(23)8-13(19)4-5-14-15-6-7-21(3,25)20(15,2)10-1'h8-9,11,14-15,17-18,24-25H,4-7,10H2,1-3H3	-3.472
InChI=1S/C18H26N2O4S2/c1-14-6-7-17-16(12-14)15(2)13-18(20-17)24-10-5-3-4-8-19-9-11-25-2h6-7,12-13,19H,3-5,8-11H2,1-2H3,(H,21,22,23)	-4.008
InChI=1S/C13H27N3O4/c1-5-6-7-13(4,8-19-11(14)17)9-20-12(18)16-15-10(2)3/h10,15H,5-9H2,1-4H3,(H2,14,17)(H,16,18)	-3.432
InChI=1S/C15H28O/c1-6-15(5,16)12-8-11-14(4)10-7-9-13(2)3/h1,13-14,16H,7-12H2,2-5H3	-4.953
InChI=1S/C16H22N6O4/c17-14(24)12-2-1-5-22(12)16(26)11(6-9-7-18-8-19-9)21-15(25)10-3-4h7-8,10-12H,1-6H2,(H2,17,24)(H,18,19)(H,20,23)(H,21,25)	-1.051
InChI=1S/C5H5NO/c7-6-4-2-1-3-5-6/h1-5H	1.022
InChI=1S/C19H27NO2/c21-18-14-8-7-13-17(18)19(22)20(15-9-3-1-4-10-15)16-11-5-2-6-12-1h7-8,13-16,21H,1-6,9-12H2	-5.57
InChI=1S/C10H12N2O2/c1-8(13)11-7-10(14)12-9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,11,13)(H,12,14)	-1.568
InChI=1S/C13H10INO2/c14-12-9-5-4-8-11(12)13(16)15(17)10-6-2-1-3-7-10/h1-9,17H	-3.53
InChI=1S/C10H19N/c1-9(2)7-6-8-10(3,4)11(9)5/h6-7H,8H2,1-5H3	-1.427
InChI=1S/C16H15Cl2NO2/c1-10-13(17)8-9-14(15(10)18)21-11(2)16(20)19-12-6-4-3-5-7-12/h3-9,11H,1-2H3,(H,19,20)	-7.006
InChI=1S/C3H2BrIO2/c4-1-2(5)3(6)7/h1H,(H,6,7)/b2-1-	-1.212

"InChi"	"logS(M)"
InChI=1S/C14H17ClO4S/c1-13(2,3)19-12(16)14(8-9-14)20(17,18)11-6-4-10(15)5-7-11/h4-7H,8-9H2,1-3H3	-4.121
InChI=1S/C35H41N5O5/c1-20(2)34(37-31(41)23-16-25-24-11-7-12-26-30(24)22(18-36-26)17-3h4-7,9-12,18,20,23,25,27-29,36,44H,8,13-17,19H2,1-3H3,(H,37,41)	-5.27
InChI=1S/C8H6O4/c9-8(10)5-1-2-6-7(3-5)12-4-11-6/h1-3H,4H2,(H,9,10)	-2.666
InChI=1S/C7H4N2O6/c10-7(11)5-2-1-4(8(12)13)3-6(5)9(14)15/h1-3H,(H,10,11)	-1.067
InChI=1S/C8H6BrClO/c9-5-8(11)6-1-3-7(10)4-2-6/h1-4H,5H2	-3.253
InChI=1S/C5H8O/c1-3-5(2)4-6/h3-4H,1-2H3/b5-3-	-0.527
InChI=1S/C19H11F5N2O2/c20-12-6-7-16(15(21)10-12)26-17(27)14-5-2-8-25-18(14)28-13-4-1-3-h1-10H,(H,26,27)	-6.897
InChI=1S/C10H14O7/c1-4-5(10(15)16)2-7(17-4)9(14)8(13)6(12)3-11/h2,6,8-9,11-14H,3H2,1H3,(H,15,16)	-1.28
InChI=1S/C14H18N2O4/c1-10-5-4-6-11(2)13(10)16(12(17)9-19-3)15-7-8-20-14(15)18/h4-6H,7-9H2,1-3H3	-1.913
InChI=1S/C8H16O4/c1-7(9-3)5-12-8(2,10-4)6-11-7/h5-6H2,1-4H3	-1.246
InChI=1S/C4H8O2S/c1-6-4(5)2-3-7/h7H,2-3H2,1H3	-0.758
InChI=1S/C11H11NO3S/c1-2-7-12-11(13)8-9-5-3-4-6-10(9)16(12,14)15/h2-6H,1,7-8H2	-2.053
InChI=1S/C20H21N3O/c1-13-12-16(6-11-19(13)23)20(24,14-2-7-17(21)8-3-14)15-4-9-18(22)h2-12,24H,21-23H2,1H3	-3.027
InChI=1S/C11H12N2O/c1-11(2)10(14)12-9(13-11)8-6-4-3-5-7-8/h3-7H,1-2H3,(H,12,13,14)	-0.85
InChI=1S/C12H10N2O/c15-12-8-6-11(7-9-12)14-13-10-4-2-1-3-5-10/h1-9,13H	-3.343
InChI=1S/C21H28N2O/c1-2-21(20(22)24,13-16-23-14-6-3-7-15-23)19-12-8-10-17-9-4-5-11-1h4-5,8-12H,2-3,6-7,13-16H2,1H3,(H2,22,24)	-5.103
InChI=1S/C17H15NO2/c18-17(19)16(11-13-7-4-10-20-13)15-9-3-6-12-5-1-2-8-14(12)15/h1-10,16H,11H2,(H2,18,19)	-2.856
InChI=1S/C19H22N2O5/c1-12(19(24)26-11-18(23)21(2)10-17(20)22)13-4-5-15-9-16(25-3)7-6-h4-9,12H,10-11H2,1-3H3,(H2,20,22)	-3.78
InChI=1S/C24H31N3O/c1-18(2)23-22(17-25(4)19(3)16-20-12-8-6-9-13-20)26(5)27(24(23)28)h6-15,18-19H,16-17H2,1-5H3	-5.068
InChI=1S/C12H7Cl3O/c13-8-1-4-10(5-2-8)16-12-6-3-9(14)7-11(12)15/h1-7H	-6.22
InChI=1S/C12H23N/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-11H2,1H3	-5.29
InChI=1S/C18H18N2O4/c1-12(21)24-15-9-7-13(8-10-15)11-16(17(19)22)20-18(23)14-5-3-2-4-h2-10,16H,11H2,1H3,(H2,19,22)(H,20,23)	-3.89

"InChi"	"logS(M)"
InChI=1S/C17H16Cl2FNO2/c18-9-11-21(12-10-19)15-5-7-16(8-6-15)23-17(22)13-1-3-14(20)4-2-1h1-8H,9-12H2	-5.993
InChI=1S/C20H32N2O4/c1-7-22(8-2)12-11-21-17(23)13-26-19-16(14(3)4)10-9-15(5)18(19)20(h9-10,14H,7-8,11-13H2,1-6H3,(H,21,23)	-4.89
InChI=1S/C10H8O3S/c11-14(12,13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H,11,12,13)	0.23
InChI=1S/C14H19NO/c1-4-10-15-14(16)12(3)11(2)13-8-6-5-7-9-13/h5-9H,4,10H2,1-3H3,(H,15,16)/b12-11-	-3.659
InChI=1S/C12H21N3O5S3/c1-3-14-10-8-15(5-4-6-20-2)23(18,19)12-9(10)7-11(21-12)22(13,16)1'h7,10,14H,3-6,8H2,1-2H3,(H2,13,16,17)	-2.95
InChI=1S/C26H38O4/c1-4-5-6-7-24(29)30-26(17(2)27)15-13-23-22-10-8-18-16-19(28)9-11-h16,20-23H,4-15H2,1-3H3	-6.488
InChI=1S/C12H18Br6/c13-7-1-8(14)3-10(16)5-12(18)6-11(17)4-9(15)2-7/h7-12H,1-6H2	-6.99
InChI=1S/C14H17BrO4S/c1-19-13(16)14(9-3-2-4-10-14)20(17,18)12-7-5-11(15)6-8-12/h5-8H,2-4,9-10H2,1H3	-4.479
InChI=1S/C14H22O/c1-9-13(2,3)10-7-6-8-11(15)12(10)14(9,4)5/h9H,6-8H2,1-5H3	-3.265
InChI=1S/C15H16N4O5S/c1-9-8-10(2)17-14(16-9)18-15(21)19-25(22,23)12-7-5-4-6-11(12)13(2h4-8H,1-3H3,(H2,16,17,18,19,21)	-3.174
InChI=1S/C36H71NO3/c1-3-5-7-9-11-13-15-17-18-20-22-24-26-28-30-32-36(40)37-34(33-38)h17-18,34-35,38-39H,3-16,19-33H2,1-2H3,(H,37,40)/b18-17+	-6.452
InChI=1S/C13H9FN2/c14-10-6-3-5-9-12(15)8-4-1-2-7-11(8)16-13(9)10/h1-7H,(H2,15,16)	-1.66
InChI=1S/C7H13Cl2N/c1-2-5-10(6-3-8)7-4-9/h2H,1,3-7H2	-1.549
InChI=1S/C12H9FN2O5/c13-9-6-14-11(17)15(10(9)16)7-19-12(18)20-8-4-2-1-3-5-8/h1-6H,7H2,(H,14,17)	-2.45
InChI=1S/C10H9I3O3/c1-2-8(10(14)15)16-9-6(12)3-5(11)4-7(9)13/h3-4,8H,2H2,1H3,(H,14,15)	-6.833
InChI=1S/C3H2Br2N2O/c4-3(5,1-6)2(7)8/h(H2,7,8)	-1.208
InChI=1S/C14H18N6O7S/c1-5-27-12(21)8-7-15-20(2)11(8)28(23,24)19-14(22)18-13-16-9(25-3)h6-7H,5H2,1-4H3,(H2,16,17,18,19,22)	-4.456
InChI=1S/C9H9ClN2O2/c10-8-2-1-6-4-12(9(11)13)14-5-7(6)3-8/h1-3H,4-5H2,(H2,11,13)	-2.163
InChI=1S/C11H18O2/c1-10(2)8-4-5-11(10,3)9(13)7(8)6-12/h7-8,12H,4-6H2,1-3H3	-0.215
InChI=1S/C15H19ClN2O/c16-12-4-6-13(7-5-12)18-11-8-14(15(18)19)17-9-2-1-3-10-17/h4-7,14H,1-3,8-11H2	-3.662
InChI=1S/C12H18Cl2N2O4S2/c13-10-8-11(14)12(16-9-10)20-6-3-1-2-4-15-5-7-21-22(17,18)19/h8-9,15H,1-7H2,(H,17,18,19)	-2.965

"InChi"	"logS(M)"
InChI=1S/C15H22N2O2/c1-3-17-10-4-5-14(11-17)19-15(18)16-13-8-6-12(2)7-9-13/h6-9,14H,3-5,10-11H2,1-2H3,(H,16,18)	-3.366
InChI=1S/C8H4N2O4S2/c11-8(12)4-3-15-7(9-4)5-1-2-6(16-5)10(13)14/h1-3H,(H,11,12)	-3.404
InChI=1S/C20H28N4O2/c1-3-5-23-16-15(17(25)24(6-4-2)19(23)26)21-18(22-16)20-10-12-7-13-h12-14H,3-11H2,1-2H3,(H,21,22)	-5.85
InChI=1S/C8H17NOS/c1-4-5-6-11-8(2,3)7(9)10/h4-6H2,1-3H3,(H2,9,10)	-2.026
InChI=1S/C10H18N2O3S2/c11-10(6-15-17(13,14)16)12-5-9-4-7-1-2-8(9)3-7/h7-9H,1-6H2,(H2,11,12)(H,13,14,16)	-2.696
InChI=1S/C27H35N3O4S/c1-26(2,3)29-24(33)22-27(4,5)35-17-30(22)25(34)21(31)20(16-18-12-h6-15,20-22,31H,16-17H2,1-5H3,(H,28,32)(H,29,33)	-3.62
InChI=1S/C15H22ClNO2/c1-11(2)9-19-10-17(14(18)8-16)15-12(3)6-5-7-13(15)4/h5-7,11H,8-10H2,1-4H3	-3.682
InChI=1S/C27H30N4O/c32-27-28-24-14-7-8-15-25(24)31(27)17-9-16-29-18-20-30(21-19-29)h1-8,10-15,26H,9,16-21H2,(H,28,32)	-5.81
InChI=1S/C16H14Cl2O3/c1-2-21-15(19)16(20,11-3-7-13(17)8-4-11)12-5-9-14(18)10-6-12/h3-10,20H,2H2,1H3	-4.512
InChI=1S/C30H52O3S/c1-23(2)17-15-13-11-9-10-12-14-16-18-33-27(31)22-34-21-24-19-25(h19-20,23,32H,9-18,21-22H2,1-8H3	-6.79
InChI=1S/C17H13ClFNO4/c1-3-8-22-17(21)11(2)23-13-4-6-14(7-5-13)24-16-15(19)9-12(18)10-2h1,4-7,9-11H,8H2,2H3	-4.942
InChI=1S/C3H5Cl3/c1-2-3(4,5)6/h2H2,1H3	-1.89
InChI=1S/C11H22N6/c1-7-17(8-2)11-13-9(15(3)4)12-10(14-11)16(5)6/h7-8H2,1-6H3	-3.885
InChI=1S/C14H17N3O3S/c1-15-7-6-10-8-12(15)16(9-10)13(18)4-2-11-3-5-14(21-11)17(19)20/h2-5,10,12H,6-9H2,1H3/b4-2+	-3.064
InChI=1S/C12H2Cl8/c13-3-1-6(16)11(19)12(20)7(3)8-9(17)4(14)2-5(15)10(8)18/h1-2H	-9.2
InChI=1S/C13H11N3O3/c14-9-5-3-8(4-6-9)12(17)16-11-10(13(18)19)2-1-7-15-11/h1-7H,14H2,(H,18,19)(H,15,16,17)	-2.826
InChI=1S/C6H11Cl/c7-6-4-2-1-3-5-6/h6H,1-5H2	-2.375
InChI=1S/C19H31NO/c1-20(2)15-10-16-21-19(13-8-3-4-9-14-19)17-18-11-6-5-7-12-18/h5-7,11-12H,3-4,8-10,13-17H2,1-2H3	-1.62
InChI=1S/C22H20Cl2N2O3/c1-12-5-7-15(8-6-12)18(27)11-29-22-19(14(3)25-26(22)4)21(28)16-9-h5-10H,11H2,1-4H3	-6.521
InChI=1S/C24H31NO3/c1-22(2)17-16-20(23(3,4)25(22)5)28-21(26)24(27,18-12-8-6-9-13-18)h6-15,20,27H,16-17H2,1-5H3	-4.388

"InChi"	"logS(M)"
InChI=1S/C13H26N2O4/c1-5-6-7-15-12(17)19-9-13(4,10(2)3)8-18-11(14)16/h10H,5-9H2,1-4H3,(H2,14,16)(H,15,17)	-3.634
InChI=1S/C9H7ClO2/c10-8(6-9(11)12)7-4-2-1-3-5-7/h1-6H,(H,11,12)/b8-6-	-2.77
InChI=1S/C4H6N2O3S/c1-3-4(6-2-5-3)10(7,8)9/h2H,1H3,(H,5,6)(H,7,8,9)	0.188
InChI=1S/C15H13NO5/c1-20-14-7-10(4-5-12(14)17)13(18)9-21-15(19)11-3-2-6-16-8-11/h2-8,17H,9H2,1H3	-2
InChI=1S/C8H5NO2/c9-5-6-2-1-3-7(4-6)8(10)11/h1-4H,(H,10,11)	-2.63
InChI=1S/C13H31N3O/c1-13(17)12-16(10-6-8-14(2)3)11-7-9-15(4)5/h13,17H,6-12H2,1-5H3	0.61
InChI=1S/C13H24N3O5P/c1-7-20-11(18)16(21-10(2)17)22(19,14-8-12(14,3)4)15-9-13(15,5)6/h7-9H2,1-6H3	-2.056
InChI=1S/C7H8O2/c1-9-7-4-2-6(8)3-5-7/h2-5,8H,1H3	-0.492
InChI=1S/C16H15N3O3S/c1-23(21,22)12-7-5-11(6-8-12)16-13(10-14(17)20)19-9-3-2-4-15(19)1	-2.154
InChI=1S/C26H28N2/c1-4-11-23(12-5-1)13-10-18-27-19-21-28(22-20-27)26(24-14-6-2-7-15	-4.2
InChI=1S/C9H7NOS/c1-7(11)8-2-4-9(5-3-8)10-6-12/h2-5H,1H3	-4.02
InChI=1S/C22H24ClN5O2/c23-15-6-7-20-18(14-15)25-22(30)28(20)16-8-12-26(13-9-16)10-3-11	-5.635
InChI=1S/C4H7BrO2/c1-2-3(5)4(6)7/h3H,2H2,1H3,(H,6,7)	-0.378
InChI=1S/C19H21N5O3S/c1-12-15(23-10-22-12)9-28-5-4-20-19-21-8-14(18(25)24-19)6-13-2-3-	-3.914
InChI=1S/C13H19N3O2/c1-2-3-4-5-6-12(17)15-16-13(18)11-7-9-14-10-8-11/h7-10H,2-6H2,1H3,(H,15,17)(H,16,18)	-2.1
InChI=1S/C6H5IO/c7-5-1-3-6(8)4-2-5/h1-4,8H	-1.71
InChI=1S/CH5N5O2/c2-1(4-3)5-6(7)8/h3H2,(H3,2,4,5)	-1.646
InChI=1S/C10H18O5/c1-4-5-6-14-10(13)8(3)15-9(12)7(2)11/h7-8,11H,4-6H2,1-3H3	-1.375
InChI=1S/C37H49N7O9S/c1-37(2,3)53-36(52)39-16-14-30(45)41-28(19-23-21-40-25-13-9-8-12-	-5.015
InChI=1S/C9H11NO2/c1-7(11)10-8-5-3-4-6-9(8)12-2/h3-6H,1-2H3,(H,10,11)	-0.979
InChI=1S/C10H6Cl2N2O2/c11-8-3-1-2-6(10(8)14(15)16)7-4-13-5-9(7)12/h1-5,13H	-5.134
InChI=1S/C46H58N4O9/c1-8-42(54)23-28-24-45(40(52)57-6,36-30(15-19-49(25-28)26-42)29-	-7.26

"InChi"	"logS(M)"
InChI=1S/C21H20BrN7O6/c1-4-7-27(8-5-6-23)18-11-16(24-13(2)30)17(12-20(18)35-3)25-26-21-h4,9-12H,1,5,7-8H2,2-3H3,(H,24,30)/b26-25+	-8.9
InChI=1S/C8H4N2S2/c11-5-9-7-2-1-3-8(4-7)10-6-12/h1-4H	-4.7
InChI=1S/C16H26O/c1-5-12(2)14(4)13(3)6-7-15-8-10-16(17)11-9-15/h8-14,17H,5-7H2,1-4H3	-5.182
InChI=1S/C5H12O5/c6-1-3(8)5(10)4(9)2-7/h3-10H,1-2H2	0.625
InChI=1S/C13H17NO2/c1-9(2)8-14-12-6-4-11(5-7-12)10(3)13(15)16/h4-7,10,14H,1,8H2,2-3H3,(H,15,16)	-2.855
InChI=1S/C13H8F2O/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8H	-4.397
InChI=1S/C2H5F2N/c3-2(4)1-5/h2H,1,5H2	0.523
InChI=1S/C18H21NO3/c1-19-8-7-18-10-12(20)4-5-13(18)14(19)9-11-3-6-15(22-2)17(21)16(1h3-6,13-14,21H,7-10H2,1-2H3	-1.87
InChI=1S/C28H37N3O4S/c1-27(2,3)30-25(34)24-28(4,5)36-18-31(24)26(35)23(33)21(16-19-12-h6-15,21,23-24,33H,16-18H2,1-5H3,(H,29,32)(H,30,34)	-3.72
InChI=1S/C16H24N2/c1-13(2)16(12-17,11-14(3)18(4)5)15-9-7-6-8-10-15/h6-10,13-14H,11H2,1-5H3	-3.192
InChI=1S/C12H22N2O2/c1-5-11(6-2)9(15)14-12(7-3,8-4)10(16)13-11/h5-8H2,1-4H3,(H,13,16)(H,14,15)	-2.31
InChI=1S/C24H42O/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21(3)23-19-20(2)18-22(4)24(2h18-19,21,25H,5-17H2,1-4H3	-7.336
InChI=1S/C9H8N2O/c1-6-5-10-11-9-7(6)3-2-4-8(9)12/h2-5,12H,1H3	-2.678
InChI=1S/C31H44O7/c1-18-7-6-8-23-17-35-28-27(32)21(4)14-26(31(23,28)34)29(33)36-25-h6-9,14,18,20,22,24-28,32,34H,10-13,15-17H2,1-5H3/b7-6-,19-9-,23-8-	-5.779
InChI=1S/C29H42O9/c1-16-25(33)22(31)12-24(37-16)38-18-3-8-27(15-30)20-4-7-26(2)19(1h11,15-16,18-22,24-25,31,33-35H,3-10,12-14H2,1-2H3	-3.352
InChI=1S/C7H12O4/c1-4(6(8)9)3-5(2)7(10)11/h4-5H,3H2,1-2H3,(H,8,9)(H,10,11)/p-2	-0.456
InChI=1S/C19H21Br2NO2/c1-14-4-3-5-15(2)18(14)19(23)24-17-8-6-16(7-9-17)22(12-10-20)13-1h3-9H,10-13H2,1-2H3	-7.629
InChI=1S/C27H27NO6/c1-31-22-13-11-18-19(15-21(22)29)20(28-27(30)16-8-6-5-7-9-16)12-1h5-9,11,13-15,20H,10,12H2,1-4H3,(H,28,30)	-5.651
InChI=1S/C8H11NO2/c9-5-8(11)6-2-1-3-7(10)4-6/h1-4,8,10-11H,5,9H2	0.815
InChI=1S/C19H18N2O3/c1-19(2)8-7-11-13(24-19)10-14(23-4)15-16(11)21(17(15)22)6h5-10H,1-4H3	-3.96
InChI=1S/C8H18N2O6/c11-9(12)15-7-5-3-1-2-4-6-8-16-10(13)14/h1-8H2,(H,11,12)(H,13,14)/q+2	-4.14
InChI=1S/C5H5N5/c6-4-3-1-9-10-5(3)8-2-7-4/h1-2H,(H3,6,7,8,9,10)	-0.878

"InChi"	"logS(M)"
InChI=1S/C7H6O4/c8-6-3-4-5(11-6)1-2-10-7(4)9/h1,3,7,9H,2H2	0.812
InChI=1S/C13H12N2O4S/ c14-9-5-7-10(8-6-9)20(18,19)15-12-4-2-1-3-11(12)13(16)17/ h1-8,15H,14H2,(H,16,17)	-0.8
InChI=1S/C18H26N2O4/ c1-3-12-20(13-4-2)18(24)15(10-11-16(21)22)19-17(23)14-8-6-5-7-9-1 h5-9,15H,3-4,10-13H2,1-2H3,(H,19,23)(H,21,22)	-3.381
InChI=1S/C6H5N5O3/c7-6-10-2-1(3(12)11-6)8-4(13)5(14)9-2/h(H, 8,13)(H4,7,9,10,11,12,14)	-5.165
InChI=1S/C14H9F3N2/ c15-14(16,17)9-5-3-7-11-12(9)13(18)8-4-1-2-6-10(8)19-11/h1-7H, (H2,18,19)	-2.48
InChI=1S/C6H12O3/c1-2-3-9-6(4-7)5-8/h2,6-8H,1,3-5H2	0.481
InChI=1S/C8H7N5O6S3/ c9-21(16,17)8-11-10-7(20-8)12-22(18,19)6-4-2-1-3-5(6)13(14)15/ h1-4H,(H,10,12)(H2,9,16,17)	-1.82
InChI=1S/C20H31NO5/ c1-7-21(8-2)11-12-25-17(22)13-26-19-16(14(3)4)10-9-15(5)18(19)20(h9-10,14H,7-8,11-13H2,1-6H3	-4.387
InChI=1S/C5H8FNS/c6-3-1-2-4-8-5-7/h1-4H2	-2.001
InChI=1S/C20H27NO2/ c1-15(12-17-8-7-10-19(14-17)22-3)21-16(2)13-18-9-5-6-11-20(18)23- h5-11,14-16,21H,12-13H2,1-4H3	-3
InChI=1S/C12H24N2O4/ c1-4-6-7-12(5-2,8-17-10(13)15)9-18-11(16)14-3/h4-9H2,1-3H3, (H2,13,15)(H,14,16)	-3.175
InChI=1S/C14H8O8S2/ c15-13-7-3-1-5-9(23(17,18)19)11(7)14(16)8-4-2-6-10(12(8)13)24(20,2 h1-6H,(H,17,18,19)(H,20,21,22)	0.257
InChI=1S/C25H33ClN2O/ c1-18(2)27(19(3)4)16-7-17-28-24-9-6-5-8-21(24)12-15-23(25(28)29)2 h5-6,8-11,13-14,18-19,23H,7,12,15-17H2,1-4H3	-7.452
InChI=1S/C9H11NO5/c10-7(9(14)15)8(13)4-1-2-5(11)6(12)3-4/ h1-3,7-8,11-13H,10H2,(H,14,15)	0.131
InChI=1S/C7H11N3O2/c1-9-6(11)4-2-3-5(7(9)12)10(4)8/h4-5H, 2-3,8H2,1H3	0.743
InChI=1S/C17H24O3/ c1-12-9-14(11-17(2,3)10-12)20-16(19)15(18)13-7-5-4-6-8-13/ h4-8,12,14-15,18H,9-11H2,1-3H3	-3.973
InChI=1S/C6H6N2O/c7-6(9)5-3-1-2-4-8-5/h1-4H,(H2,7,9)	0.169
InChI=1S/C7H12ClN3O2S2/ c8-1-2-11(10-13)7(12)9-6-3-14-5-15-4-6/h6H,1-5H2,(H,9,12)	-2.944
InChI=1S/C8H7NO5/c10-8(11)5-14-7-4-2-1-3-6(7)9(12)13/h1-4H, 5H2,(H,10,11)	-2.016
InChI=1S/C17H21N3O4/ c1-2-17(13-6-4-3-5-7-13)14(21)18-16(23)20(15(17)22)12-19-8-10-24- h3-7H,2,8-12H2,1H3,(H,18,21,23)	-1.925
InChI=1S/C17H16N4O2/ c22-15-10-14(17(23)13-2-1-5-21-16(13)15)20-9-8-19-11-12-3-6-18-7- h1-7,10,19-20H,8-9,11H2	0.511

"InChi"	"logS(M)"
InChI=1S/C18H24N2O/c1-4-18(17(19)21,12-13-20(2)3)16-11-7-9-14-8-5-6-10-15(14)16/h5-11H,4,12-13H2,1-3H3,(H2,19,21)	-3.65
InChI=1S/C8H8N4O2/c1-11-6-5(9-3-4-10-6)7(13)12(2)8(11)14/h3-4H,1-2H3	-1.46
InChI=1S/C11H13NO3/c1-2-12-10(13)8-15-11(14)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,12,13)	-2.237
InChI=1S/C15H14O5/c1-17-12-7-11(20-15(16)8-12)4-2-10-3-5-13-14(6-10)19-9-18-13/h2-6,8,11H,7,9H2,1H3/b4-2+	-2.854
InChI=1S/C10H16/c1-7-8-4-5-9(6-8)10(7,2)3/h8-9H,1,4-6H2,2-3H3	-4.472
InChI=1S/C23H45N5O14/c24-2-7-13(32)15(34)10(27)21(37-7)41-19-9(4-30)39-23(17(19)36)42-h5-23,29-36H,1-4,24-28H2	0.211
InChI=1S/C9H16N2O3/c1-6(2)7(8(12)13)11-5-3-4-10-9(11)14/h6-7H,3-5H2,1-2H3,(H,10,14)(H,12,13)	-1.103
InChI=1S/C3H3N3O4/c1-2-3(5(7)8)4-10-6(2)9/h1H3	-1.316
InChI=1S/C13H20N2O5/c1-6-7-9(11(17)14-8-10(16)19-5)15-12(18)20-13(2,3)4/h1,9H,7-8H2,2-5H3,(H,14,17)(H,15,18)	-1.45
InChI=1S/C18H16Br2F3NO2/c19-9-11-24(12-10-20)15-5-7-16(8-6-15)26-17(25)13-1-3-14(4-2-13)1h1-8H,9-12H2	-7.808
InChI=1S/CHClF2/c2-1(3)4/h1H	-1.46
InChI=1S/C10H14/c1-4-6-7-9-10(3)8-5-2/h4-9H,2H2,1,3H3/b6-4+,9-7+,10-8-	-2.09
InChI=1S/C21H41N7O12/c1-5-21(36,4-30)16(40-17-9(26-2)13(34)10(31)6(3-29)38-17)18(37-5)h5-18,26,29-36H,3-4H2,1-2H3,(H4,22,23,27)(H4,24,25,28)	0.234
InChI=1S/C12H7Cl3/c13-9-5-8(6-10(14)7-9)11-3-1-2-4-12(11)15/h1-7H	-6.3
InChI=1S/C12H9NO2/c14-13(15)12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H	-5.209
InChI=1S/C24H29NO/c1-16(2)24(26)12-13-25-15-21-19-8-4-3-6-17(19)10-11-18-7-5-9-20(2h3-9,16,21-22,26H,10-15H2,1-2H3	-3.81
InChI=1S/C10H4Cl4/c11-7-5-3-1-2-4-6(5)8(12)10(14)9(7)13/h1-4H	-7.795
InChI=1S/C10H14N2O3S3/c11-10(8-17-18(13,14)15)12-6-7-16-9-4-2-1-3-5-9/h1-5H,6-8H2,(H2,11,12)(H,13,14,15)	-2.56
InChI=1S/C10H22OS2/c1-3-5-7-9-12-13(11)10-8-6-4-2/h3-10H2,1-2H3/p+1	-3.171
InChI=1S/C12H14N2O6/c1-4-7(2)10-5-9(13(16)17)6-11(14(18)19)12(10)20-8(3)15/h5-7H,4H2,1-3H3	-2.25
InChI=1S/C7H10O/c1-4-7(8,5-2)6-3/h1,5,8H,2,6H2,3H3	-0.603
InChI=1S/C13H19NO2S/c1-2-3-4-9-17-12-7-5-11(6-8-12)10-13(15)14-16/h5-8,16H,2-4,9-10H2,1H3,(H,14,15)	-3.599

"InChi"	"logS(M)"
InChI=1S/C9H12N2O5S/c10-8(15)3-2-17-9(11-3)7-6(14)5(13)4(1-12)16-7/h2,4-7,12-14H,1H2,(H2,10,15)	-0.931
InChI=1S/C14H11N/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10,14H	-2.944
InChI=1S/C11H15ClO3/c1-8-5-9(3-4-10(8)12)15-7-11(2,14)6-13/h3-5,13-14H,6-7H2,1-2H3	-2.681
InChI=1S/C13H16O2/c1-2-12(14)15-11-6-5-10-8-3-4-9(7-8)13(10)11/h2,5-6,8-11,13H,1,3-4,7H2	-3.708
InChI=1S/C18H23NO3/c1-13(12-22-17-6-4-3-5-7-17)19-14(2)18(21)15-8-10-16(20)11-9-15/h3-11,13-14,18-21H,12H2,1-2H3	-1.53
InChI=1S/C11H14N4O/c1-7-5-8(2)13-11(12-7)16-10-6-9(3)15(4)14-10/h5-6H,1-4H3	-1.52
InChI=1S/C32H25ClN4O5/c1-41-27-15-13-21(33)18-25(27)35-32(40)24-16-19-8-6-7-11-23(19)29h3-18,36H,1-2H3,(H,34,39)(H,35,40)/b37-29-	-8.184
InChI=1S/C41H84N4O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-36-42-40(46)44-38h3-39H2,1-2H3,(H2,42,44,46)(H2,43,45,47)	-5.823
InChI=1S/C5H7NO3/c7-4-2-1-3(6-4)5(8)9/h3H,1-2H2,(H,6,7)(H,8,9)	-0.404
InChI=1S/C20H34N2O3/c1-2-3-4-8-25-18(23)6-5-7-21-19(24)22-20-12-15-9-16(13-20)11-17(1h15-17H,2-14H2,1H3,(H2,21,22,24)	-2.32
InChI=1S/C16H20ClN3/c1-19(2)11-12-20(16-5-3-4-10-18-16)13-14-6-8-15(17)9-7-14/h3-10H,11-13H2,1-2H3	-2.618
InChI=1S/C36H74O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-36-34-32-30h3-36H2,1-2H3	-7.02
InChI=1S/C4H5NOS/c6-2-4-1-5-3-7-4/h1,3,6H,2H2	0.526
InChI=1S/C17H36N2O2/c18-14-10-6-8-12-16-19-15-11-7-4-2-1-3-5-9-13-17(20)21/h19H,1-16,18H2,(H,20,21)	-2.302
InChI=1S/C40H62O19/c1-18(2)33(43)50-16-27-29(54-35(45)20(5)6)32(57-38(48)23(11)12)4h18-23,26-32,39H,15-17H2,1-14H3	-6.074
InChI=1S/C28H48O2/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-28(7)18-16-25-19-26(29h19-22,29H,8-18H2,1-7H3	-8.506
InChI=1S/C11H15NO2/c1-4-14-10-5-6-11(8(2)7-10)12-9(3)13/h5-7H,4H2,1-3H3,(H,12,13)	-1.839
InChI=1S/C8H11N/c1-3-8-5-4-7(2)9-6-8/h4-6H,3H2,1-2H3	-1.004
InChI=1S/C10H20N2O4/c1-3-5-10(4-2,6-15-8(11)13)7-16-9(12)14/h3-7H2,1-2H3,(H2,11,13)(H2,12,14)	-2.154
InChI=1S/C11H13NO4/c1-3-15-10(13)8-5-6-12-9(7-8)11(14)16-4-2/h5-7H,3-4H2,1-2H3	-1.218
InChI=1S/C41H37ClN6O/c1-2-3-23-38-43-39(42)37(29-49)47(38)28-30-24-26-31(27-25-30)35-3h4-22,24-27,49H,2-3,23,28-29H2,1H3	-6.461

"InChi"	"logS(M)"
InChI=1S/C14H17NO3/c1-2-14(11-6-4-3-5-7-11)9-8-12(17)15(10-16)13(14)18/h3-7,16H,2,8-10H2,1H3	-1.66
InChI=1S/C15H21FN2O5S/c1-9(2)13(14(19)17-12-7-8-23-15(12)20)18-24(21,22)11-5-3-10(16)4-h3-6,9,12-13,15,18,20H,7-8H2,1-2H3,(H,17,19)	-2.38
InChI=1S/C13H20O2/c1-12(2,3)14-15-13(4,5)11-9-7-6-8-10-11/h6-10H,1-5H3	-4.291
InChI=1S/C10H11BrO3/c1-6-3-7(2)10(8(11)4-6)14-5-9(12)13/h3-4H,5H2,1-2H3,(H,12,13)	-3.123
InChI=1S/C8H15NO/c1-2-9-7-5-3-4-6-8(9)10/h2-7H2,1H3	-0.787
InChI=1S/C6H11Cl4O3PS/c1-3-11-14(15,12-4-2)13-5(7)6(8,9)10/h5H,3-4H2,1-2H3	-5.526
InChI=1S/C27H27N3O2/c1-2-3-4-11-18-32-22-16-17-23(24(31)19-22)27-29-25(20-12-7-5-8-13h5-10,12-17,19,31H,2-4,11,18H2,1H3	-9.152
InChI=1S/C8H7NO4/c1-13-8(10)6-2-4-7(5-3-6)9(11)12/h2-5H,1H3	-3.04
InChI=1S/C15H18N4O4/c1-21-10-5-8(4-9-7-18-15(17)19-13(9)16)6-11(22-2)12(10)14(20)23-3h5-7H,4H2,1-3H3,(H4,16,17,18,19)	-2.333
InChI=1S/C8H14O4/c1-2-3-4-5-6(7(9)10)8(11)12/h6H,2-5H2,1H3,(H,9,10)(H,11,12)	0.592
InChI=1S/C4H5NS/c1-2-3-5-4-6/h2H,1,3H2	-1.695
InChI=1S/C12H16N2/c1-3-14(4-2)12(10-13)11-8-6-5-7-9-11/h5-9,12H,3-4H2,1-2H3	-0.974
InChI=1S/C4H6N2O2/c5-2-3-1-4(7)6-8-3/h1H,2,5H2,(H,6,7)	0.696
InChI=1S/C22H23ClN2O8/c1-21(32)7-6-8-15(25(2)3)17(28)13(20(24)31)19(30)22(8,33)18(29)11h4-5,7-8,15,26-27,30,32-33H,6H2,1-3H3,(H2,24,31)	-2.881
InChI=1S/C4H11NO/c1-2-4(5)3-6/h4,6H,2-3,5H2,1H3	1.05
InChI=1S/C19H38O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19(22)23-17-18(21)16-20/h18,20-21H,2-17H2,1H3	-4.727
InChI=1S/C12H14N2O5/c15-12-10(8-4-2-1-3-5-8)6-9(13(16)17)7-11(12)14(18)19/h6-8,15H,1-5H2	-4.249
InChI=1S/C8H7ClO2/c1-5-3-2-4-6(9)7(5)8(10)11/h2-4H,1H3,(H,10,11)	-2.419
InChI=1S/C15H19N3O2/c1-17-9-12-7-8-13(10-17)18(12)15(20)14(19)16-11-5-3-2-4-6-11/h2-6,12-13H,7-10H2,1H3,(H,16,19)	-1.876
InChI=1S/C21H26N2OS/c1-4-8-19(24)16-11-12-21-18(15-16)23(14-7-13-22(2)3)17-9-5-6-10-2h5-6,9-12,15H,4,7-8,13-14H2,1-3H3	-6.852
InChI=1S/C8H6N2O/c11-8-6-3-1-2-4-7(6)9-5-10-8/h1-5H,(H,9,10,11)	-0.925
InChI=1S/C5H8O2/c1-2-3-4-5(6)7/h3-4H,2H2,1H3,(H,6,7)/b4-3+	-0.202
InChI=1S/C5H11NO2/c1-2-3-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)	-0.069
InChI=1S/C7H16O/c1-4-5-7(8)6(2)3/h6-8H,4-5H2,1-3H3	-1.309
InChI=1S/C2H3N3S/c3-1-5-2(4)6/h(H3,4,5,6)	-0.005

"InChi"	"logS(M)"
InChI=1S/C30H22N4O4/c35-27-25(28(36)32(22-15-7-2-8-16-22)31(27)21-13-5-1-6-14-21)26-2h1-20,25-26H	-5.233
InChI=1S/C4H9NO/c1-3(2)4(5)6/h3H,1-2H3,(H2,5,6)	-0.285
InChI=1S/C18H14O/c19-18-16(14-8-3-1-4-9-14)12-7-13-17(18)15-10-5-2-6-11-15/h1-13,19H	-5.684
InChI=1S/C11H16O/c1-2-3-9-11(12)10-7-5-4-6-8-10/h4-8,11-12H,2-3,9H2,1H3	-2.247
InChI=1S/C8H18O2/c1-7(2,3)8(4,5-9)6-10/h9-10H,5-6H2,1-4H3	-1.571
InChI=1S/C21H26N2O3/c1-17(24)20-9-5-6-10-21(20)26-16-19(25)15-22-11-13-23(14-12-22)1h2-10,19,25H,11-16H2,1H3	-2.588
InChI=1S/C34H46ClN3O10/c1-18-11-10-12-26(45-9)34(43)17-25(46-32(42)36-34)19(2)30-33(5,4h10-12,14-15,19-20,25-27,30,43H,13,16-17H2,1-9H3,(H,36,42)/b12-10-,18-11-	-5.943
InChI=1S/C7H13O6P/c1-6(5-7(8)10-2)13-14(9,11-3)12-4/h5H,1-4H3/b6-5-	0.428
InChI=1S/C13H14N4O3S/c1-2-8-17-9-7-12(15-13(17)18)16-21(19,20)11-5-3-10(14)4-6-11/h2-7,9H,1,8,14H2,(H,15,16,18)	-3.11
InChI=1S/C12H15NO3S/c1-2-3-8-13-12(14)11-7-5-4-6-10(11)9-17(13,15)16/h4-7H,2-3,8-9H2,1H3	-3.096
InChI=1S/C15H15NO2/c1-2-18-15(17)16(13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12H,2H2,1H3	-3.969
InChI=1S/C26H34O7/c1-14(27)32-21-20(15-4-5-19(29)31-13-15)24(3)10-7-17-18(26(24)22(h4-5,13,16-18,20-22,28,30H,6-12H2,1-3H3	-4.261
InChI=1S/C17H24N2O5S2/c1-23-16-13-17(19-15-8-4-3-7-14(15)16)24-11-6-2-5-9-18-10-12-25-2h3-4,7-8,13,18H,2,5-6,9-12H2,1H3,(H,20,21,22)	-3.157
InChI=1S/C19H18ClN3O3/c1-22(2)19(25)26-17-18(24)23(3)15-10-9-13(20)11-14(15)16(21-17)1h4-11,17H,1-3H3	-4.393
InChI=1S/C12H9ClN2/c13-10-6-8-12(9-7-10)15-14-11-4-2-1-3-5-11/h1-9H/b15-14+	-5.702
InChI=1S/C23H16O3/c24-21-17-13-7-8-14-18(17)22(25)20(21)23(26)19(15-9-3-1-4-10-15)1h1-14,19-20H	-6.055
InChI=1S/C7H6O3/c8-4-5-1-2-6(9)3-7(5)10/h1-4,9-10H	-1.257
InChI=1S/C12H13N5O7S2/c1-22-8(18)7-6(4-5-25-7)26(20,21)17-10(19)13-9-14-11(23-2)16-12(1h4-5H,1-3H3,(H2,13,14,15,16,17,19)	-3.19
InChI=1S/C12H9NO3/c14-10-6-7-12(13(15)16)11(8-10)9-4-2-1-3-5-9/h1-8,14H	-3.63
InChI=1S/C10H13N5/c1-3-6-7(4-2)14-9-8(13-6)5-12-10(11)15-9/h5H,3-4H2,1-2H3,(H2,11,12,14,15)	-3.04
InChI=1S/C9H16N2O/c1-2-9(12)11-7-3-4-8(11)6-10-5-7/h7-8,10H,2-6H2,1H3	-1.826

"InChi"	"logS(M)"
InChI=1S/C22H20/c1-2-3-10-21-19-11-6-5-9-17(19)15-18-14-13-16-8-4-7-12-20(16)22(1h4-9,11-15H,2-3,10H2,1H3	-7.524
InChI=1S/C21H24FNO2/c22-19-10-8-17(9-11-19)20(24)7-4-14-23-15-12-21(25,13-16-23)18-5-h1-3,5-6,8-11,25H,4,7,12-16H2	-4.118
InChI=1S/C13H10O2/c14-13(15)12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H,(H,14,15)	-2.73
InChI=1S/C7H16O3/c1-4-8-7(9-5-2)10-6-3/h7H,4-6H2,1-3H3	-2.041
InChI=1S/C11H10O4/c1-13-9-5-7-3-4-11(12)15-8(7)6-10(9)14-2/h3-6H,1-2H3	-2.174
InChI=1S/C20H24N2/c1-2-3-4-5-10-15-21-20-16-11-6-8-13-18(16)22-19-14-9-7-12-17(19)2h6-9,11-14H,2-5,10,15H2,1H3,(H,21,22)	-7.477
InChI=1S/C8H6O5/c9-5-3-1-2-4(7(10)11)6(5)8(12)13/h1-3,9H,(H,10,11)(H,12,13)	-2.11
InChI=1S/C17H19F3N6O6S/c1-9-6-5-7-10(12(27)31-4)11(9)33(29,30)25-15(28)22-13-21-14(26(2)h5-7H,8H2,1-4H3,(H2,21,22,23,24,25,28)	-5.69
InChI=1S/C7H9NO3S/c1-5-2-3-6(8)4-7(5)12(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)	-1.62
InChI=1S/C12H6Cl2O2/c13-7-5-11-12(6-8(7)14)16-10-4-2-1-3-9(10)15-11/h1-6H	-7.23
InChI=1S/C9H10N2O2/c10-9(13)11-8(12)6-7-4-2-1-3-5-7/h1-5H,6H2,(H3,10,11,12,13)	-1.244
InChI=1S/C7H6N2O/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H,(H2,8,9)	-1.487
InChI=1S/C16H14O3/c1-2-19-16(18)14-11-7-6-10-13(14)15(17)12-8-4-3-5-9-12/h3-11H,2H2,1H3	-3.405
InChI=1S/C12H14N4O/c1-17-10-4-2-8(3-5-10)6-9-7-15-12(14)16-11(9)13/h2-5,7H,6H2,1H3,(H4,13,14,15,16)	-2.025
InChI=1S/C16H22N2O/c1-13-5-7-14(8-6-13)18-12-9-15(16(18)19)17-10-3-2-4-11-17/h5-8,15H,2-4,9-12H2,1H3	-3.43
InChI=1S/C12H13NO4/c14-12(13-3-5-15-6-4-13)9-1-2-10-11(7-9)17-8-16-10/h1-2,7H,3-6,8H2	-1.261
InChI=1S/C23H29N3OS/c27-15-14-24-16-18-10-11-19(17-24)25(18)12-5-13-26-20-6-1-3-8-22(h1-4,6-9,18-19,27H,5,10-17H2	-5.511
InChI=1S/C9H14O2/c10-8-6-9(7-11-8)4-2-1-3-5-9/h1-7H2	-1.971
InChI=1S/C9H8O5/c1-14-7-3-2-5(8(10)11)4-6(7)9(12)13/h2-4H,1H3,(H,10,11)(H,12,13)	-3.116
InChI=1S/C15H11ClN2O/c16-11-6-7-13-12(8-11)15(17-9-14(19)18-13)10-4-2-1-3-5-10/h1-8H,9H2,(H,18,19)	-3.677
InChI=1S/C21H42O5/c1-2-3-4-11-14-19(23)15-12-9-7-5-6-8-10-13-16-21(25)26-18-20(24)1h19-20,22-24H,2-18H2,1H3	-3.397

"InChi"	"logS(M)"
InChI=1S/C16H14BrN5O4S2/c17-11-1-5-14(6-2-11)28(25,26)22-16-19-10-9-15(21-16)20-12-3-7-13h1-10H,(H2,18,23,24)(H2,19,20,21,22)	-2.62
InChI=1S/C19H20FN3O3/c1-21-7-12-4-11(21)8-22(12)17-6-16-13(5-15(17)20)18(24)14(19(25)2h5-6,9-12H,2-4,7-8H2,1H3,(H,25,26)	-2.9
InChI=1S/C12H11N5O/c1-8-16-11(10(5-13)12(18)17-8)15-7-9-3-2-4-14-6-9/h2-4,6H,7H2,1H3,(H2,15,16,17,18)	-2.35
InChI=1S/C14H6Cl4O4/c15-7-1-3-9(11(17)5-7)13(19)21-22-14(20)10-4-2-8(16)6-12(10)18/h1-6H	-8.279
InChI=1S/C22H43N5O12/c1-22(35)6-36-20(15(33)18(22)26-2)39-17-8(27-19(34)9(28)4-23)3-7(h7-18,20-21,26,28-33,35H,3-6,23-25H2,1-2H3,(H,27,34)	0.244
InChI=1S/C18H13ClN2O/c1-2-10-21-16-9-8-14(19)11-15(16)18(20-12-17(21)22)13-6-4-3-5-7-1h1,3-9,11H,10,12H2	-4.138
InChI=1S/C16H23NO3/c1-3-4-5-6-7-8-16(19)20-15-11-9-14(10-12-15)17-13(2)18/h9-12H,3-8H2,1-2H3,(H,17,18)	-4.44
InChI=1S/C15H11ClF3NO3/c16-7-2-1-6(15(17,18)19)5-8(7)20-13(21)11-9-3-4-10(23-9)12(11)14(2h1-2,5,9-12H,3-4H2	-2.526
InChI=1S/C11H22N2O3S2/c12-11(9-17-18(14,15)16)13-8-10-6-4-2-1-3-5-7-10/h10H,1-9H2,(H2,12,13)(H,14,15,16)	-3.746
InChI=1S/C16H20N2O5/c1-15(2,3)22-23-16(10-9-11-7-5-4-6-8-11)12(19)17-14(21)18-13(16)2h4-8H,9-10H2,1-3H3,(H2,17,18,19,20,21)	-3.742
InChI=1S/C8H22N2O5P2/c1-7-13-17(12,14-8-2)15-16(11,9(3)4)10(5)6/h7-8H2,1-6H3	-1.064
InChI=1S/C18H16IN3O3/c1-23-8-13-9-24-16-7-15-14(6-17(16)25-13)18(21-10-20-15)22-12-4-2h2-7,10,13H,8-9H2,1H3,(H,20,21,22)	-3.52
InChI=1S/C15H20N4O5/c1-3-5-12(20)23-9-18-8-16-14-11(15(18)22)7-17-19(14)10-24-13(21)6h7-8H,3-6,9-10H2,1-2H3	-3.83
InChI=1S/C11H8O3/c1-14-10-6-9(12)7-4-2-3-5-8(7)11(10)13/h2-6H,1H3	-1.727
InChI=1S/C21H23NO6/c1-20(27)11-7-5-4-6-10(11)18(25)16-12(20)8-13-17(22(2)3)14(23)9-1h4-7,9,12-13,17,23,26-28H,8H2,1-3H3	-1.42
InChI=1S/C14H16O/c1-11(2)10-15-14-8-7-12-5-3-4-6-13(12)9-14/h3-9,11H,10H2,1-2H3	-5.212
InChI=1S/C7H6O4/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,8-9H,(H,10,11)	-0.85
InChI=1S/C14H26O/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15/h7,11,13-14H,5-6,8-10H2,1-4H3	-5.497
InChI=1S/C17H14O2/c1-11(17(18)19)14-9-8-13-7-6-12-4-2-3-5-15(12)16(13)10-14/h2-11H,1H3,(H,18,19)	-5.327
InChI=1S/C6H13NO2/c1-4-7(3)6(8)9-5-2/h4-5H2,1-3H3	-0.419

"InChi"	"logS(M)"
InChI=1S/C15H15N3S/ c1-3-18-13-9-5-4-8-12(13)17(2)15(19)11-7-6-10-16-14(11)18/ h4-10H,3H2,1-2H3	-4.706
InChI=1S/C6H4ClI/c7-5-3-1-2-4-6(5)8/h1-4H	-3.54
InChI=1S/C12H4Cl6/ c13-5-1-7(15)11(8(16)2-5)12-9(17)3-6(14)4-10(12)18/h1-4H	-8.71
InChI=1S/C11H11NO3/c1-15-8-2-3-10-9(5-8)7(6-12-10)4-11(13)14/ h2-3,5-6,12H,4H2,1H3,(H,13,14)	-1.645
InChI=1S/C13H18O4/ c1-13(2)7-16-11(14)9-5-3-4-6-10(9)12(15)17-8-13/h3-4,9-10H, 5-8H2,1-2H3	-3.004
InChI=1S/C20H24ClNO2/ c1-22-11-10-15-12-19(23-2)20(24-3)13-17(15)18(22)9-6-14-4-7-16(21 h4-5,7-8,12-13,18H,6,9-11H2,1-3H3	-5.012
InChI=1S/C16H22N4O2/ c1-4-5-11-17-16(22)18-14-12(2)19(3)20(15(14)21)13-9-7-6-8-10-13/ h6-10H,4-5,11H2,1-3H3,(H2,17,18,22)	-1.63
InChI=1S/C8H7Cl2FN2O3/ c1-15-3(14)2-16-8-5(10)6(12)4(9)7(11)13-8/h2H2,1H3,(H2,12,13)	-3.951
InChI=1S/C6H14N2O6/c7-8-6(14)5(13)4(12)3(11)2(10)1-9/ h2-5,9-13H,1,7H2,(H,8,14)	-0.498
InChI=1S/C7H6N2OS/c8-7-9-6-4(10)2-1-3-5(6)11-7/h1-3,10H, (H2,8,9)	-1.92
InChI=1S/C6H12O3/c1-3-9-5-4-6(7)8-2/h3-5H2,1-2H3	-0.072
InChI=1S/C8H18O/c1-4-6-8(3,9)7-5-2/h9H,4-7H2,1-3H3	-1.587
InChI=1S/C9H12O3/c1-10-7-4-8(11-2)6-9(5-7)12-3/h4-6H,1-3H3	-2.68
InChI=1S/C13H12BrCl2N3O/ c14-9-4-13(20-5-9,6-19-8-17-7-18-19)11-2-1-10(15)3-12(11)16/ h1-3,7-9H,4-6H2	-3.877
InChI=1S/C4H5N3O3/c1-2-3(4(5)8)7(9)10-6-2/h1H3,(H2,5,8)	-0.553
InChI=1S/C17H28N2O3S/ c1-5-6-7-8-9-10-17(20)19(4)15-11-13-16(14-12-15)23(21,22)18(2)3/ h11-14H,5-10H2,1-4H3	-3.59
InChI=1S/C8H8O4/c1-4-3-6(10)7(5(2)9)8(11)12-4/h3,7H,1-2H3	-1.226
InChI=1S/C14H11N3O4/ c15-13(18)9-1-5-11(6-2-9)16-14(19)10-3-7-12(8-4-10)17(20)21/ h1-8H,(H2,15,18)(H,16,19)	-4.937
InChI=1S/C19H23NO3/ c1-3-22-18-11-9-17(10-12-18)19(21)23-14-13-20-15(2)16-7-5-4-6-8-1 h4-12,15,20H,3,13-14H2,1-2H3	-1.49
InChI=1S/C21H16N2O4S/ c24-19-21(16-10-4-1-5-11-16,17-12-6-2-7-13-17)23(20(25)22-19)28(2 h1-15H,(H,22,24,25)	-5.511
InChI=1S/C20H9Cl3F5N3O3/ c21-10-5-9(30-19(33)31-17(32)15-13(24)2-1-3-14(15)25)6-11(22)16(1 h1-7H,(H2,30,31,32,33)	-8.65
InChI=1S/C23H22/ c1-2-3-4-13-21-20-12-8-6-10-18(20)16-23-19-11-7-5-9-17(19)14-15-2 h5-12,14-16H,2-4,13H2,1H3	-8.57

"InChi"	"logS(M)"
InChI=1S/C25H27NO5/c1-16(19-9-10-21-15-22(29-3)12-11-20(21)14-19)24(27)30-17(2)31-25-h4-12,14-17,23H,13,26H2,1-3H3	-3.5
InChI=1S/C10H9NO6S2/c11-9-3-4-10(19(15,16)17)8-5-6(18(12,13)14)1-2-7(8)9/h1-5H,11H2,(H,12,13,14)(H,15,16,17)	-0.259
InChI=1S/C16H24N2O4/c1-10(2)8-13(16(21)22)18-15(20)14(19)12(17)9-11-6-4-3-5-7-11/h3-7,10,12-14,19H,8-9,17H2,1-2H3,(H,18,20)(H,21,22)	-2.375
InChI=1S/C14H18O3/c1-14(2,3)13(15)7-5-10-4-6-11-12(8-10)17-9-16-11/h4-8,13,15H,9H2,1-3H3/b7-5+	-3.546
InChI=1S/C13H19NO2/c1-2-3-4-7-10-16-12-9-6-5-8-11(12)13(14)15/h5-6,8-9H,2-4,7,10H2,1H3,(H2,14,15)	-3.055
InChI=1S/C11H16N2O3S2/c1-7(2)5-13-6-9-3-8-4-10(18(12,14)15)16-11(8)17-9/h3-4,7,13H,5-6H2,1-2H3,(H2,12,14,15)	-1.33
InChI=1S/C9H13NO3/c10-8-3-1-2-4-9(8)13-6-7(12)5-11/h1-4,7,11-12H,5-6,10H2	-0.488
InChI=1S/C15H10O2/c16-15(17)12-8-7-11-6-5-10-3-1-2-4-13(10)14(11)9-12/h1-9H,(H,16,17)	-5.541
InChI=1S/C11H15ClN4O2/c1-3-15(11(13-2)8-16(17)18)7-9-4-5-10(12)14-6-9/h4-6,8,13H,3,7H2,1-2H3/b11-8+	0.492
InChI=1S/C8H17N/c1-7-5-4-6-8(2,3)9-7/h7,9H,4-6H2,1-3H3	-1.029
InChI=1S/C13H23N/c1-3-12(4-2)10-13(11-14)8-6-5-7-9-13/h12H,3-10H2,1-2H3	-6.587
InChI=1S/C4H11NO3S2/c1-2-5-3-4-9-10(6,7)8/h5H,2-4H2,1H3,(H,6,7,8)	0.732
InChI=1S/C20H36O6/c1-2-6-18-17(5-1)23-13-9-21-11-15-25-19-7-3-4-8-20(19)26-16-12-22-h17-20H,1-16H2	-3.033
InChI=1S/C13H23N2O3PS/c1-7-16-19(20,17-10(2)3)18-11-8-14-12(15-9-11)13(4,5)6/h8-10H,7H2,1-6H3	-4.763
InChI=1S/C11H21N3O4/c1-6(2)5-7(12)10(16)14-8(11(17)18)3-4-9(13)15/h6-8H,3-5,12H2,1-2H3,(H2,13,15)(H,14,16)(H,17,18)	-1.569
InChI=1S/C15H20N4O3/c1-20-8-11-12(21-2)5-9(6-13(11)22-3)4-10-7-18-15(17)19-14(10)16/h5-7H,4,8H2,1-3H3,(H4,16,17,18,19)	-2.436
InChI=1S/C7H3IN2O3/c8-5-1-4(3-9)2-6(7(5)11)10(12)13/h1-2,11H	-4.661
InChI=1S/C8H8O3/c1-5-2-3-6(8(10)11)7(9)4-5/h2-4,9H,1H3,(H,10,11)	-1.182
InChI=1S/C16H20N4O4/c1-4-24-15(21)13-11(22-2)6-9(7-12(13)23-3)5-10-8-19-16(18)20-14(1h6-8H,4-5H2,1-3H3,(H4,17,18,19,20)	-2.691
InChI=1S/C19H31NO4/c1-7-23-19(22)17-14(6)8-9-16(12(2)3)18(17)24-11-15(21)10-20-13(4)h8-9,12-13,15,20-21H,7,10-11H2,1-6H3	-3.856

"InChi"	"logS(M)"
InChI=1S/C10H13N5O/c1-3-5-6(4-2)13-8-7(12-5)9(16)15-10(11)14-8/h3-4H2,1-2H3,(H3,11,13,14,15,16)	-4.28
InChI=1S/C14H22BrN3O2/c1-4-18(5-2)7-6-17-14(19)10-8-11(15)12(16)9-13(10)20-3/h8-9H,4-7,16H2,1-3H3,(H,17,19)	-4.127
InChI=1S/C14H21NO2/c1-4-14(5-2,13(16)15-17)10-12-8-6-11(3)7-9-12/h6-9,17H,4-5,10H2,1-3H3,(H,15,16)	-3.35
InChI=1S/C19H29IO2/c1-3-22-19(21)11-9-7-5-4-6-8-10-16(2)17-12-14-18(20)15-13-17/h12-16H,3-11H2,1-2H3	-8.376
InChI=1S/C12H9NO3/c14-11-8-4-7-10(12(11)13(15)16)9-5-2-1-3-6-9/h1-8,14H	-3.95
InChI=1S/C14H11NO2/c1-9-8-13(16)15(17)12-7-6-10-4-2-3-5-11(10)14(9)12/h2-8,17H,1H3	-4
InChI=1S/C3H5IO2/c4-2-1-3(5)6/h1-2H2,(H,5,6)	-0.43
InChI=1S/C10H7F3O4/c1-5(14)17-8-4-6(10(11,12)13)2-3-7(8)9(15)16/h2-4H,1H3,(H,15,16)	-2.079
InChI=1S/C6H8IN3O2/c1-5-8-4-6(10(11)12)9(5)3-2-7/h4H,2-3H2,1H3	-3.536
InChI=1S/C11H22N2O/c1-6-10(14)13-9(2)7-12(5)8-11(13,3)4/h9H,6-8H2,1-5H3	-1.399
InChI=1S/C14H19NO4/c1-3-4-9-19-13-10-11(5-7-12(13)18-2)6-8-14(16)15-17/h5-8,10,17H,3-4,9H2,1-2H3,(H,15,16)/b8-6+	-3.14
InChI=1S/C20H26N2O2/c1-2-20(19(21)23,10-11-22-12-14-24-15-13-22)18-9-5-7-16-6-3-4-8-1h3-9H,2,10-15H2,1H3,(H2,21,23)	-3.625
InChI=1S/C4H7N3O/c1-7-2-3(8)6-4(7)5/h2H2,1H3,(H2,5,6,8)	-0.15
InChI=1S/C12H8Cl2O/c13-9-5-7-10(8-6-9)15-12-4-2-1-3-11(12)14/h1-8H	-5.52
InChI=1S/C14H22N2O2/c1-4-16(5-2)11(3)10-18-14(17)12-6-8-13(15)9-7-12/h6-9,11H,4-5,10,15H2,1-3H3	-2.38
InChI=1S/C8H8N2O2/c1-11-5-2-3-7-6(4-5)10-8(9)12-7/h2-4H,1H3,(H2,9,10)	-1.68
InChI=1S/C11H22O3/c1-3-5-6-7-9-14-11(12)8-10-13-4-2/h3-10H2,1-2H3	-2.829
InChI=1S/C20H40O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h7,17-19,21H,1,8-16H2,2-6H3	-4.709
InChI=1S/C50H42Cl2N6O8/c1-27-16-17-33(49(63)65-20-18-51)26-41(27)55-57-43-34-13-7-5-11-h5-17,22-26,55-56H,18-21H2,1-4H3,(H,53,61)(H,54,62)/b57-43-,58-44+	-7.814
InChI=1S/C7H6N2O4/c1-5-2-3-6(8(10)11)7(4-5)9(12)13/h2-4H,1H3	-3.26
InChI=1S/C20H27NO2/c1-19-9-7-16-15-6-4-14(23-2)11-13(15)3-5-17(16)18(19)8-10-20(19,2h4,16-18,22H,3,5-11H2,1-2H3	-5.683
InChI=1S/C13H28O4/c1-4-15-7-5-6-13(3)17-9-8-16-11-12(2)10-14/h12-14H,4-11H2,1-3H3	-0.791

"InChi"	"logS(M)"
InChI=1S/C11H16O/c1-8-6-5-7-9(10(8)12)11(2,3)4/h5-7,12H,1-4H3	-2.728
InChI=1S/C8H16BrF/c9-7-5-3-1-2-4-6-8-10/h1-8H2	-4.631
InChI=1S/C12H17O4PS2/c1-4-16-12(13)11(10-8-6-5-7-9-10)19-17(18,14-2)15-3/h5-9,11H,4H2,1-3H3	-4.464
InChI=1S/C33H44O8/c1-17(2)10-9-11-21(30(38)39)26-22-12-13-25-31(6)15-14-23(36)18(3)h10,14-15,18,22,24-25,27-28H,9,11-13,16H2,1-8H3,(H,38,39)/b26-21+	-7.538
InChI=1S/C12H19NO/c1-2-3-4-5-10-14-12-8-6-11(13)7-9-12/h6-9H,2-5,10,13H2,1H3	-3.696
InChI=1S/C13H17NO/c1-10(11(2)13(15)14(3)4)12-8-6-5-7-9-12/h5-9H,1-4H3/b11-10-	-2.898
InChI=1S/C6H9N3O2S/c1-8-4(10)3(7)5(12)9(2)6(8)11/h3H,7H2,1-2H3	-1.117
InChI=1S/C15H10BrClFNO2/c16-8-14(20)19-13-6-5-9(17)7-11(13)15(21)10-3-1-2-4-12(10)18/h1-7H,8H2,(H,19,20)	-5.569
InChI=1S/C10H12N4/c1-3-7-8(4-2)14-10-9(13-7)5-11-6-12-10/h5-6H,3-4H2,1-2H3	-0.18
InChI=1S/C19H21N5O3S/c1-26-16-9-14-15(10-17(16)27-2)20-12-21-18(14)23-4-6-24(7-5-23)19h3,8-12H,4-7H2,1-2H3,(H,22,25)	-5.3
InChI=1S/C13H15N3O4S/c1-8-9(2)15-20-13(8)16(10(3)17)21(18,19)12-6-4-11(14)5-7-12/h4-7H,14H2,1-3H3	-3.59
InChI=1S/C3H2Br2O2/c4-2(5)1-3(6)7/h1H,(H,6,7)	-0.836
InChI=1S/C18H22N2OS/c1-19(2)11-6-12-20-15-7-4-5-8-17(15)22-18-10-9-14(21-3)13-16(18)2h4-5,7-10,13H,6,11-12H2,1-3H3	-5.78
InChI=1S/C10H22N4O2S2/c11-3-1-9(15)13-5-7-17-18-8-6-14-10(16)2-4-12/h1-8,11-12H2,(H,13,15)(H,14,16)	-0.811
InChI=1S/C10H14N4S/c1-14(2)9-5-3-8(4-6-9)7-12-13-10(11)15/h3-7H,1-2H3,(H3,11,13,15)/b12-7+	-2.668
InChI=1S/C19H18N6O2/c1-4-24(5-2)16-6-7-18(13(3)8-16)22-23-19-14(11-20)9-17(25(26)27)1h6-10H,4-5H2,1-3H3/b23-22+	-7.473
InChI=1S/C12H16N2S/c1-9-5-3-6-10(2)11(9)14-12-13-7-4-8-15-12/h3,5-6H,4,7-8H2,1-2H3,(H,13,14)	-5.391
InChI=1S/C14H22O7/c1-3-13(15)20-11-9-18-7-5-17-6-8-19-10-12-21-14(16)4-2/h3-4H,1-2,5-12H2	-0.5
InChI=1S/C10H12N4O2/c1-13-8-6(9(15)14(2)10(13)16)11-7(12-8)5-3-4-5/h5H,3-4H2,1-2H3,(H,11,12)	-1.621
InChI=1S/C19H29NO5/c1-13(2)16-6-5-14(3)17(19(22)23-4)18(16)25-12-15(21)11-20-7-9-24-h5-6,13,15,21H,7-12H2,1-4H3	-2.914
InChI=1S/C6H14NO3PS2/c1-4-7-6(8)5-13-11(12,9-2)10-3/h4-5H2,1-3H3,(H,7,8)	-1.457

"InChi"	"logS(M)"
InChI=1S/C18H14Cl2N6O2/c19-16-11-15(26(27)28)12-17(20)18(16)24-23-13-3-5-14(6-4-13)25(9-h3-6,11-12H,1-2,9-10H2/b24-23+	-7.115
InChI=1S/C47H51NO14/c1-25-31(60-43(56)36(52)35(28-16-10-7-11-17-28)48-41(54)29-18-12h7-21,31-33,35-38,40,51-52,57H,22-24H2,1-6H3,(H,48,54)	-6.33
InChI=1S/C9H10N2S/c1-11(2)9-5-3-8(4-6-9)10-7-12/h3-6H,1-2H3	-4.13
InChI=1S/C11H15BrN2O2/c1-7-9(12)10(15)14(11(16)13(7)2)8-5-3-4-6-8/h8H,3-6H2,1-2H3	-3.238
InChI=1S/C16H21NO4/c18-15(19)14(13-9-5-2-6-10-13)17-16(20)21-11-12-7-3-1-4-8-12/h1,3-4,7-8,13-14H,2,5-6,9-11H2,(H,17,20)(H,18,19)	-3.285
InChI=1S/C14H23NO4S2/c1-19-14-8-6-13(7-9-14)5-2-3-10-15-11-4-12-20-21(16,17)18/h6-9,15H,2-5,10-12H2,1H3,(H,16,17,18)	-2.551
InChI=1S/C11H13NO4/c1-14-9-4-2-3-5-10(9)15-7-8-6-12-11(13)16-8/h2-5,8H,6-7H2,1H3,(H,12,13)	-2.406
InChI=1S/C8H10O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1,6H,2-4H2,(H,9,10)(H,11,12)	-2.93
InChI=1S/C14H28O2/c1-5-11(15)10-16-13-9-7-6-8-12(13)14(2,3)4/h11-13,15H,5-10H2,1-4H3	-3.699
InChI=1S/C7H10O4/c1-4-7(10-5(2)8)11-6(3)9/h4,7H,1H2,2-3H3	-1.245
InChI=1S/C7H6N2/c8-5-6-2-1-3-7(9)4-6/h1-4H,9H2	-1.169
InChI=1S/C18H20O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h2-5,10,16-17,19-20H,6-9H2,1H3	-4.64
InChI=1S/C4H6N4O/c5-2-1-3(9)8-4(6)7-2/h1H,(H5,5,6,7,8,9)	-1.378
InChI=1S/C19H29NO3/c1-14(2)16-9-8-15(3)17(19(21)22-4)18(16)23-13-12-20-10-6-5-7-11-2h8-9,14H,5-7,10-13H2,1-4H3	-4.766
InChI=1S/C40H23Cl5N6O4/c41-22-9-12-29(43)33(17-22)48-50-35-25-7-3-1-5-20(25)15-27(37(35h1-19,48-49H,(H,46,54)(H,47,55)/b50-35-,51-36-	-7.869
InChI=1S/C16H11Cl2NO3/c1-8(16(20)21)9-3-5-14-13(7-9)19-15(22-14)10-2-4-11(17)12(18)6-10h2-8H,1H3,(H,20,21)	-5.206
InChI=1S/C14H22ClNO2/c1-10-5-6-12(15)13(7-10)18-9-11(17)8-16-14(2,3)4/h5-7,11,16-17H,8-9H2,1-4H3	-2.566
InChI=1S/C11H21NO5S/c1-10(2)11(13)17-8-7-12(3,4)6-5-9-18(14,15)16/h1,5-9H2,2-4H3	0.963
InChI=1S/C21H44N2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-21-18-19-22/h9-10,23H,2-8,11-22H2,1H3/b10-9+	-3.955
InChI=1S/C7H11N3O2/c1-2-3-8-6(11)10-7-9-4-5-12-7/h4-5H,2-3H2,1H3,(H2,8,9,10,11)	-1.284
InChI=1S/C17H20N2O4/c20-12-16(22)17(23)15(21)11-18-19(13-7-3-1-4-8-13)14-9-5-2-6-10-1h1-11,15-17,20-23H,12H2/b18-11+	-3.1

"InChi"	"logS(M)"
InChI=1S/C12H27NO4S2/c1-3-5-7-9-11-18(14,15)13-19(16,17)12-10-8-6-4-2/h13H,3-12H2,1-2H3	-2.2
InChI=1S/C12H18/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,7-10H,3-6,11-12H2/b2-1-,9-7-,10-8-	-5.365
InChI=1S/C8H6N2O/c11-7-5-9-4-6-2-1-3-10-8(6)7/h1-5,11H	-1.658
InChI=1S/C9H9ClO/c10-8-4-5-9(11)7-3-1-2-6(7)8/h4-5,11H,1-3H2	-2.977
InChI=1S/C8H12O4/c1-3-11-7(9)5-6-8(10)12-4-2/h5-6H,3-4H2,1-2H3/b6-5+	-1.09
InChI=1S/C4H7Cl/c1-4(2)3-5/h1,3H2,2H3	-1.811
InChI=1S/C26H42O4/c1-21(2)15-9-5-7-13-19-29-25(27)23-17-11-12-18-24(23)26(28)30-20-h11-12,17-18,21-22H,5-10,13-16,19-20H2,1-4H3	-6.622
InChI=1S/C11H15NO3/c1-7(2)12-6-11(15)8-3-4-9(13)10(14)5-8/h3-5,7,12-14H,6H2,1-2H3	-0.316
InChI=1S/C6H11N3O4/c7-1-4(10)8-2-5(11)9-3-6(12)13/h1-3,7H2,(H,8,10)(H,9,11)(H,12,13)	-0.53
InChI=1S/C14H14O/c1-11-3-7-13(8-4-11)15-14-9-5-12(2)6-10-14/h3-10H,1-2H3	-4.85
InChI=1S/C12H6Br4/c13-7-1-3-11(15)9(5-7)10-6-8(14)2-4-12(10)16/h1-6H	-8.06
InChI=1S/C11H15NO2S/c13-15(14,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8H,2,5-6,9-10H2	-2.537
InChI=1S/C22H30N6O3S/c1-26(2)32(29,30)15-17-4-5-20-19(12-17)18(13-24-20)6-7-27-8-10-28h4-5,12-14,16,24H,6-11,15H2,1-3H3	-3.76
InChI=1S/C19H23N5O4/c25-18(21-20-14-17-6-7-19(28-17)24(26)27)15-23-12-10-22(11-13-23h1-7,14H,8-13,15H2,(H,21,25)/b20-14+	-3.456
InChI=1S/C17H31NO/c1-5-18(6-2)10-12-19-11-9-14-7-8-15-13-16(14)17(15,3)4/h7,15-16H,5-6,8-13H2,1-4H3	-3.789
InChI=1S/C9H13N3O2/c1-2-14-8-5-3-7(4-6-8)11-9(13)12-10/h3-6H,2,10H2,1H3,(H2,11,12,13)	-1.647
InChI=1S/C14H19ClN2O2/c1-10-4-3-5-12(15)13(10)16-14(18)19-11-6-8-17(2)9-7-11/h3-5,11H,6-9H2,1-2H3,(H,16,18)	-3.646
InChI=1S/C7H15NO2/c1-2-3-4-5-6(8)7(9)10/h6H,2-5,8H2,1H3,(H,9,10)	-0.94
InChI=1S/C15H20N4O5/c1-3-5-12(20)23-9-18-8-16-14-11(15(18)22)7-19(17-14)10-24-13(21)6h7-8H,3-6,9-10H2,1-2H3	-3.55
InChI=1S/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5-8,10,12H,9H2,1-4H3/b7-5+	-3.396
InChI=1S/C8H6N2OS2/c1-12-8(11)5-3-2-4-6-7(5)13-10-9-6/h2-4H,1H3	-4.436
InChI=1S/C8H5ClO2/c9-6-2-1-5-4-11-8(10)7(5)3-6/h1-3H,4H2	-2.482
InChI=1S/C12H3Cl7/c13-5-2-1-4(3-6(5)14)7-8(15)10(17)12(19)11(18)9(7)16/h1-3H	-8.9

"InChi"	"logS(M)"
InChI=1S/C18H24N2O6/c1-7-8-15(21)26-16-13(18(5,6)11-17(2,3)4)9-12(19(22)23)10-14(16)2(h7-10H,11H2,1-6H3/b8-7+	-4.96
InChI=1S/C26H37N3O/c27-25(30)26(14-20-28-16-5-1-6-17-28,15-21-29-18-7-2-8-19-29)24-1 h3-4,9-13H,1-2,5-8,14-21H2,(H2,27,30)	-6.192
InChI=1S/C10H7NO3/c12-9-6-5-7-3-1-2-4-8(7)10(9)11(13)14/h1-6,12H	-2.976
InChI=1S/C11H16O/c1-11(2,12)9-8-10-6-4-3-5-7-10/h3-7,12H,8-9H2,1-2H3	-1.556
InChI=1S/C18H35NO2/c1-6-12-19(7-2)13-16-14-20-18(21-16)10-8-15(9-11-18)17(3,4)5/h15-16H,6-14H2,1-5H3	-2.801
InChI=1S/C5H12N2O6/c8-6(9)12-4-2-1-3-5-13-7(10)11/h1-5H2,(H,8,9)(H,10,11)/q+2	-2.19
InChI=1S/C13H7F3N2O5/c14-13(15,16)8-1-6-12(11(7-8)18(21)22)23-10-4-2-9(3-5-10)17(19)20 h1-7H	-5.215
InChI=1S/C56H112O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-28-29-30-31-33-35-37-39-41- h3-55H2,1-2H3	-5.703
InChI=1S/C18H29NO4/c1-11(2)15-8-7-13(5)16(18(21)22-6)17(15)23-10-14(20)9-19-12(3)4/h7-8,11-12,14,19-20H,9-10H2,1-6H3	-3.334
InChI=1S/C17H20N2O/c1-13-9-11-15(12-10-13)18-16(20)19-17(2,3)14-7-5-4-6-8-14/h4-12H,1-3H3,(H2,18,19,20)	-5.349
InChI=1S/C13H17NO2/c15-12-9-5-4-8-11(12)13(16)14-10-6-2-1-3-7-10/h4-5,8-10,15H,1-3,6-7H2,(H,14,16)	-3.44
InChI=1S/C9H16O2/c1-7-3-5-9(10-7)6-4-8(2)11-9/h7-8H,3-6H2,1-2H3	-0.449
InChI=1S/C9H10ClNO2/c1-6(9(12)13)11-8-5-3-2-4-7(8)10/h2-6,11H,1H3,(H,12,13)	-2.327
InChI=1S/C3H7NO3/c1-3(2)7-4(5)6/h3H,1-2H3	-1.459
InChI=1S/C12H17NO2/c1-8-10-7-12(15-3)11(14-2)6-9(10)4-5-13-8/h6-8,13H,4-5H2,1-3H3	-3.054
InChI=1S/C29H28O9/c1-3-10-35-18-6-7-19-21(12-18)27(20-8-5-17(34-2)13-23(20)36-14-25 h4-9,11-13,26-28H,3,10,14-15H2,1-2H3,(H,30,31)(H,32,33)	-6.77
InChI=1S/C3H7FO2/c4-1-3(6)2-5/h3,5-6H,1-2H2	0.829
InChI=1S/C15H13N/c16-15-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)15/h1-10,15H,16H2	-3.779
InChI=1S/C13H20N4O4/c1-9(2)16(10(3)4)8-12(18)15-14-7-11-5-6-13(21-11)17(19)20/h5-7,9-10H,8H2,1-4H3,(H,15,18)/b14-7+	-3.025
InChI=1S/C4H12N2/c1-5-3-4-6-2/h5-6H,3-4H2,1-2H3	1.055
InChI=1S/C6H7N/c1-6-3-2-4-7-5-6/h2-5H,1H3	1.031
InChI=1S/C6H10N6O/c1-12(2)11-10-6-4(5(7)13)8-3-9-6/h3,11H,1-2H3,(H2,7,13)/b10-6-	-1.635

"InChi"	"logS(M)"
InChI=1S/C11H13NO3S/c1-2-7-12-11(13)8-9-5-3-4-6-10(9)16(12,14)15/h3-6H,2,7-8H2,1H3	-2.183
InChI=1S/C17H17N5O2/c1-2-21(13-3-12-18)16-8-4-14(5-9-16)19-20-15-6-10-17(11-7-15)22(2h4-11H,2-3,13H2,1H3/b20-19+	-7.209
InChI=1S/C10H7NO2/c12-10(13)9-6-5-7-3-1-2-4-8(7)11-9/h1-6H,(H,12,13)	-1.091
InChI=1S/C7H14O3/c1-3-5-10-7(8)4-6-9-2/h3-6H2,1-2H3	-0.66
InChI=1S/C10H11BrO3/c1-2-5-14-10(13)7-3-4-9(12)8(11)6-7/h3-4,6,12H,2,5H2,1H3	-3.51
InChI=1S/C9H10ClNS/c10-8-3-1-2-7(6-8)9-11-4-5-12-9/h1-3,6,9,11H,4-5H2	-1.392
InChI=1S/C29H24N4O8/c34-25(21-5-1-9-30-13-21)38-17-29(18-39-26(35)22-6-2-10-31-14-22,h1-16H,17-20H2	-4.153
InChI=1S/C11H15NO/c1-2-3-4-11(13)9-5-7-10(12)8-6-9/h5-8H,2-4,12H2,1H3	-2.46
InChI=1S/C17H28N4O4/c1-3-5-7-11-20(12-8-6-4-2)14-16(22)19-18-13-15-9-10-17(25-15)21(2h9-10,13H,3-8,11-12,14H2,1-2H3,(H,19,22)/b18-13+	-5.237
InChI=1S/C6H12N2S3/c1-7(2)5(9)11-6(10)8(3)4/h1-4H3	-2.83
InChI=1S/C19H29NO3/c1-15(2)23-18-10-8-17(9-11-18)19(21)22-14-6-13-20-12-5-4-7-16(20)h8-11,15-16H,4-7,12-14H2,1-3H3	-4.608
InChI=1S/C11H16O3/c1-9-2-4-10(5-3-9)7-14-8-11(13)6-12/h2-5,11-13H,6-8H2,1H3	-1.578
InChI=1S/C11H20O2/c1-3-13-11(12)9(2)10-7-5-4-6-8-10/h9-10H,3-8H2,1-2H3	-3.327
InChI=1S/C9H10N4O4/c1-11-7-6(8(16)12(2)9(11)17)13(4-10-7)3-5(14)15/h4H,3H2,1-2H3,(H,14,15)	-2.366
InChI=1S/C7H5N3O3/c11-7-8-5-2-1-4(10(12)13)3-6(5)9-7/h1-3H,(H2,8,9,11)	-3.274
InChI=1S/C7H17O4PS2/c1-4-10-12(8,11-5-2)13-7-14(9)6-3/h4-7H2,1-3H3/p+1	-1.512
InChI=1S/C11H6F3NO3/c12-11(13,14)5-1-2-6-8(3-5)15-4-7(9(6)16)10(17)18/h1-4H,(H,15,16)(H,17,18)	-3.943
InChI=1S/C8H3Cl2F3N2/c9-3-1-2-4-6(5(3)10)15-7(14-4)8(11,12)13/h1-2H,(H,14,15)	-3.568
InChI=1S/C10H20O3/c1-4-5-8(2)10(3)12-7-9(6-11)13-10/h8-9,11H,4-7H2,1-3H3	-2.594
InChI=1S/C3H2N2/c4-2-1-3-5/h1H2	0.25
InChI=1S/C9H9N3O3S2/c1-5(13)11-6-2-3-7-8(4-6)16-9(12-7)17(10,14)15/h2-4H,1H3,(H,11,13)(H2,10,14,15)	-3.16
InChI=1S/C9H8Cl6O2/c10-5-6(11)8(13)4(2-17)3(1-16)7(5,12)9(8,14)15/h3-4,16-17H,1-2H2	-3.08
InChI=1S/C13H13N3O4S/c1-9-8-10(14)6-7-13(9)21(19,20)15-11-4-2-3-5-12(11)16(17)18/h2-8,15H,14H2,1H3	-4.51

"InChi"	"logS(M)"
InChI=1S/C38H58O6S/c1-35(2,3)27-21-25(22-28(33(27)41)36(4,5)6)13-15-31(39)43-17-19-4h21-24,41-42H,13-20H2,1-12H3	-5.808
InChI=1S/C7H9ClN2OS/c1-3-5(11)10-7-9-4(2)6(8)12-7/h3H2,1-2H3,(H,9,10,11)	-3.06
InChI=1S/C18H34O6/c1-3-21-13-15-23-17(19)11-9-7-5-6-8-10-12-18(20)24-16-14-22-4-2/h3-16H2,1-2H3	-3.197
InChI=1S/C14H17NO/c1-10(12-6-4-3-5-7-12)11(2)14(16)15-13-8-9-13/h3-7,13H,8-9H2,1-2H3,(H,15,16)/b11-10-	-3.486
InChI=1S/C20H21ClO4/c1-13(2)24-19(23)20(3,4)25-17-11-7-15(8-12-17)18(22)14-5-9-16(21)h5-13H,1-4H3	-5.936
InChI=1S/C8H9NO2/c10-6-8(11)9-7-4-2-1-3-5-7/h1-5,10H,6H2,(H,9,11)	-0.447
InChI=1S/C23H32O3/c1-23-11-10-18-17-9-7-16(26-15-4-2-3-5-15)12-14(17)6-8-19(18)20(2h7,9,12,15,18-22,24-25H,2-6,8,10-11,13H2,1H3	-6.052
InChI=1S/C20H25NO3/c1-3-21(4-2)15-16-24-19(22)20(23,17-11-7-5-8-12-17)18-13-9-6-10-1h5-14,23H,3-4,15-16H2,1-2H3	-2.513
InChI=1S/C8H15NO2/c1-3-5-6-11-7-9-8(10)4-2/h4H,2-3,5-7H2,1H3,(H,9,10)	-0.654
InChI=1S/C8H10N2O3/c1-3-4-8(2)5(11)9-7(13)10-6(8)12/h3H,1,4H2,2H3,(H2,9,10,11,12,13)	-1.16
InChI=1S/C18H26O/c1-11-8-16-15(9-14(11)13(3)19)17(4,5)10-12(2)18(16,6)7/h8-9,12H,10H2,1-7H3	-5.315
InChI=1S/C7H12O4/c1-2-3-4-5(6(8)9)7(10)11/h5H,2-4H2,1H3,(H,8,9)(H,10,11)	0.437
InChI=1S/C5H12NO4PS/c1-6-5(7)4-12-11(8,9-2)10-3/h4H2,1-3H3,(H,6,7)	0.671
InChI=1S/C12H19NO3/c1-15-8-7-13-9-11(14)10-16-12-5-3-2-4-6-12/h2-6,11,13-14H,7-10H2,1H3	-0.039
InChI=1S/C18H12O4/c19-15-13(11-7-3-1-4-8-11)16(20)18(22)14(17(15)21)12-9-5-2-6-10-1h1-10,19,22H	-3.39
InChI=1S/C6H11BrN2O2/c1-2-3-4(7)5(10)9-6(8)11/h4H,2-3H2,1H3,(H3,8,9,10,11)	-1.428
InChI=1S/C8H14O4/c1-9-5-3-11-8-6(10-2)4-12-7(5)8/h5-8H,3-4H2,1-2H3	1.06
InChI=1S/C12H18N2O4S2/c13-12(10-19-20(15,16)17)14-7-4-8-18-9-11-5-2-1-3-6-11/h1-3,5-6H,4,7-10H2,(H2,13,14)(H,15,16,17)	-2.366
InChI=1S/C19H14/c1-13-16-8-4-3-7-15(16)12-19-17(13)11-10-14-6-2-5-9-18(14)19/h2-12H,1H3	-7.343
InChI=1S/C16H8O6/c17-13-7-3-1-2-4-8(7)14(18)11-9(13)5-6-10(15(19)20)12(11)16(21)22h1-6H,(H,19,20)(H,21,22)	-2.814

"InChi"	"logS(M)"
InChI=1S/C21H23NO5/c1-11(23)25-16-6-4-13-10-15-14-5-7-17(26-12(2)24)20-21(14,8-9-22(h4-7,14-15,17,20H,8-10H2,1-3H3	-2.789
InChI=1S/C3H3Cl5/c4-1(2(5)6)3(7)8/h1-3H	-2.722
InChI=1S/C28H37ClN4O/c29-24-12-11-23-10-9-22-7-2-3-8-25(22)33(26(23)21-24)18-6-15-31-1h2-3,7-8,11-12,21H,1,4-6,9-10,13-20H2,(H2,30,34)	-7.729
InChI=1S/C14H22N2O3/c1-10(2)15-8-13(18)9-19-14-6-4-12(5-7-14)16-11(3)17/h4-7,10,13,15,18H,8-9H2,1-3H3,(H,16,17)	-1.775
InChI=1S/C8H5NO3/c10-7-5-3-1-2-4-6(5)9-8(11)12-7/h1-4H,(H,9,11)	-2.735
InChI=1S/C13H17NO5/c15-8-11(16)9-19-12-5-3-10(4-6-12)13(17)2-1-7-14-18/h3-7,11,15-16,18H,1-2,8-9H2/b14-7+	-0.802
InChI=1S/C8H8Cl2O2/c1-11-7-3-6(10)8(12-2)4-5(7)9/h3-4H,1-2H3	-4.413
InChI=1S/C10H20O2/c1-4-6-7-10(5-2)8-12-9(3)11/h10H,4-8H2,1-3H3	-4.645
InChI=1S/C12H15NO4/c1-3-8-16-12(15)17-11-6-4-10(5-7-11)13-9(2)14/h4-7H,3,8H2,1-2H3,(H,13,14)	-2.57
InChI=1S/C11H18N2O2/c1-8(13-12)6-9-4-5-10(14-2)11(7-9)15-3/h4-5,7-8,13H,6,12H2,1-3H3	-1.62
InChI=1S/C12H18O4/c1-10-3-2-4-11(5-10)16-9-12(6-13,7-14)8-15/h2-5,13-15H,6-9H2,1H3	-2.122
InChI=1S/C32H32O14/c1-10-8-9-15-18-16(10)29(38)45-26-17-13(23(35)20(19(18)26)30(39)h5-9,11-12,21-22,24-25,27-28,31-37H,1-4H3	-2.147
InChI=1S/C17H12ClF3N2O/c18-12-6-7-14-13(8-12)16(11-4-2-1-3-5-11)22-9-15(24)23(14)10-17(1h1-8H,9-10H2	-5.165
InChI=1S/C8H8O3/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)	0.818
InChI=1S/C9H12N2O3/c1-2-5-14-9-4-3-7(11(12)13)6-8(9)10/h3-4,6H,2,5,10H2,1H3	-3.159
InChI=1S/C10H12O4/c1-12-8-4-7(6-11)5-9(13-2)10(8)14-3/h4-6H,1-3H3	-2.119
InChI=1S/C15H15N3O/c1-3-18-13-9-5-4-8-12(13)17(2)15(19)11-7-6-10-16-14(11)18/h4-10H,3H2,1-2H3	-3.324
InChI=1S/C12H5Cl5O/c13-6-1-3-7(4-2-6)18-12-9(15)5-8(14)10(16)11(12)17/h1-5H	-7.77
InChI=1S/C6H14O3/c1-5(8)4-9-6(2)3-7/h5-8H,3-4H2,1-2H3	0.872
InChI=1S/C7H4ClNOS/c8-4-1-2-6-5(3-4)9-7(11)10-6/h1-3H,(H,9,11)	-3.165
InChI=1S/C9H13NO2/c1-9(2,3)7-5-4-6(12-7)8(10)11/h4-5H,1-3H3,(H2,10,11)	-1.933
InChI=1S/C7H15NOS/c1-4-8(5-2)7(9)10-6-3/h4-6H2,1-3H3	-1.692
InChI=1S/C16H33NO3/c1-2-3-4-5-6-7-8-9-10-11-16(20)17(12-14-18)13-15-19/h18-19H,2-15H2,1H3	-3.104

"InChi"	"logS(M)"
InChI=1S/C16H17NO/c1-17(2)16(18)15(13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12,15H,1-2H3	-2.98
InChI=1S/C12H19NO3/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-8H,5,13H2,1-4H3	-1.323
InChI=1S/C8H8O3/c1-11-8-4-6(5-9)2-3-7(8)10/h2-5,10H,1H3	-1.228
InChI=1S/C4H11N/c1-2-3-4-5/h2-5H2,1H3	1.136
InChI=1S/C16H22N2O3/c1-3-18-10-4-5-15(11-18)21-16(20)17-14-8-6-13(7-9-14)12(2)19/h6-9,15H,3-5,10-11H2,1-2H3,(H,17,20)	-2.83
InChI=1S/C14H11NO/c1-2-6-11(7-3-1)10-14-15-12-8-4-5-9-13(12)16-14/h1-9H,10H2	-4.122
InChI=1S/C5H12N2S/c1-3-6-5(8)7-4-2/h3-4H2,1-2H3,(H2,6,7,8)	-1.46
InChI=1S/C13H19N3O2/c1-4-10(2)9-16(3)15-14-12-7-5-11(6-8-12)13(17)18/h5-8,10H,4,9H2,1-3H3,(H,17,18)/b15-14+	-1.79
InChI=1S/C8H8Cl2O3/c1-12-7-4(9)3-5(10)8(13-2)6(7)11/h3,11H,1-2H3	-2.96
InChI=1S/C21H22N2O5S/c1-4-28-13-10-9-11-7-5-6-8-12(11)14(13)17(24)22-15-18(25)23-16(2(h5-10,15-16,19H,4H2,1-3H3,(H,22,24)(H,26,27)	-5.456
InChI=1S/C12H10O2/c13-11-5-1-3-9(7-11)10-4-2-6-12(14)8-10/h1-8,13-14H	-2.368
InChI=1S/C15H22O5/c1-8-4-5-11-9(2)12(16)17-13-15(11)10(8)6-7-14(3,18-13)19-20-15/h8-11,13H,4-7H2,1-3H3	-3.736
InChI=1S/C10H8ClN3O2/c1-16-10(15)9(6-12)14-13-8-4-2-3-7(11)5-8/h2-5,13H,1H3/b14-9-	-4.008
InChI=1S/C8H8ClNO/c9-8-2-1-6-4-10-11-5-7(6)3-8/h1-3,10H,4-5H2	-2.453
InChI=1S/C20H24N2/c1-21-18-12-13-19(21)15-22(14-18)20(16-8-4-2-5-9-16)17-10-6-3-7-1 h2-11,18-20H,12-15H2,1H3	-3.475
InChI=1S/C13H24O3/c1-5-15-12(14)16-11-9-7-6-8-10(11)13(2,3)4/h10-11H,5-9H2,1-4H3	-4.321
InChI=1S/C25H28O3/c1-25-14-13-20-19-10-8-18(28-24(27)16-5-3-2-4-6-16)15-17(19)7-9-2 h2-6,8,10,15,20-23,26H,7,9,11-14H2,1H3	-6.894
InChI=1S/C5H9NO/c1-4(2)5(7)3-6/h4-5,7H,1-2H3	0.305
InChI=1S/C8H7NO4/c1-6(10)13-8-4-2-7(3-5-8)9(11)12/h2-5H,1H3	-2.599
InChI=1S/C12H22O2/c1-10(2)6-5-7-11(3)8-9-14-12(4)13/h6,11H,5,7-9H2,1-4H3	-4.096
InChI=1S/C12H6Cl4/c13-8-4-2-1-3-7(8)11-9(14)5-6-10(15)12(11)16/h1-6H	-6.3
InChI=1S/C13H15NO5/c1-9(15)19-11-7-5-4-6-10(11)13(17)18-8-12(16)14(2)3/h4-7H,8H2,1-3H3	-1.55
InChI=1S/C12H6Cl4/c13-8-3-1-7(2-4-8)9-5-11(15)12(16)6-10(9)14/h1-6H	-7.77
InChI=1S/C17H29NO/c1-16(2,3)13-9-12(11-18(7)8)10-14(15(13)19)17(4,5)6/h9-10,19H,11H2,1-8H3	-2.711

"InChi"	"logS(M)"
InChI=1S/C18H13ClFN3/c1-11-21-9-13-10-22-18(14-4-2-3-5-16(14)20)15-8-12(19)6-7-17(15)2h2-9H,10H2,1H3	-4.13
InChI=1S/C13H24O/c1-5-6-7-8-13(4)10-9-12(2,3)11(13)14/h5-10H2,1-4H3	-4.017
InChI=1S/C12H6Cl4/c13-7-4-5-8(11(16)6-7)12-9(14)2-1-3-10(12)15/h1-6H	-6.65
InChI=1S/C6H2ClN3O6/c7-6-4(9(13)14)1-3(8(11)12)2-5(6)10(15)16/h1-2H	-2.669
InChI=1S/C11H12N2/c1-8-7-9(2)13-11-6-4-3-5-10(11)12-8/h3-6H,7H2,1-2H3	-1.37
InChI=1S/C14H10Cl4/c1-8-5-9(14(18)7-13(8)17)6-10-11(15)3-2-4-12(10)16/h2-5,7H,6H2,1H3	-8.36
InChI=1S/C17H25NO3/c1-14-6-3-4-11-18(14)12-5-13-21-17(19)15-7-9-16(20-2)10-8-15/h7-10,14H,3-6,11-13H2,1-2H3	-3.628
InChI=1S/C19H20N2/c1-2-8-14(9-3-1)20-19-15-10-4-6-12-17(15)21-18-13-7-5-11-16(18)19h4-7,10-14H,1-3,8-9H2,(H,20,21)	-6.783
InChI=1S/C9H10O/c1-8(10)7-9-5-3-2-4-6-9/h2-6H,7H2,1H3	-1.411
InChI=1S/C12H2Cl8/c13-4-1-3(8(16)12(20)11(4)19)7-9(17)5(14)2-6(15)10(7)18/h1-2H	-9.29
InChI=1S/C15H21NO5/c1-11(17)8-16(9-12(2)18)14(19)10-21-15(20)13-6-4-3-5-7-13/h3-7,11-12,17-18H,8-10H2,1-2H3	-1.18
InChI=1S/C10H17NO3S/c11-9(12)13-6-8-7-15-10(14-8)4-2-1-3-5-10/h8H,1-7H2,(H2,11,12)	-2.82
InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3	0.553
InChI=1S/C8H11N/c1-2-7-3-5-8(9)6-4-7/h3-6H,2,9H2,1H3	-1.76
InChI=1S/C13H24O/c1-10(9-14)5-7-12-8-6-11(2)13(12,3)4/h6,10,12,14H,5,7-9H2,1-4H3	-3.843
InChI=1S/C6H15O2PS2/c1-5(2)7-9(10,11)8-6(3)4/h5-6H,1-4H3,(H,10,11)	-0.553
InChI=1S/C9H7NOS2/c11-8-6-13-9(12)10(8)7-4-2-1-3-5-7/h1-5H,6H2	-1.256
InChI=1S/C7H4BrN/c8-7-3-1-6(5-9)2-4-7/h1-4H	-2.869
InChI=1S/C15H10/c1-3-10-7-8-11-4-2-6-13-9-12(5-1)14(10)15(11)13/h1-8H,9H2	-5.238
InChI=1S/C13H26N2O4/c1-7-13(8-2,9-18-11(16)14(3)4)10-19-12(17)15(5)6/h7-10H2,1-6H3	-3.536
InChI=1S/C16H14O3/c1-19-13-9-6-12(7-10-13)8-11-16(18)14-4-2-3-5-15(14)17/h2-11,17H,1H3/b11-8+	-5.7
InChI=1S/C10H15N3O6S2/c14-13(15)9-3-1-5-12-10(9)19-7-2-4-11-6-8-20-21(16,17)18/h1,3,5,11H,2,4,6-8H2,(H,16,17,18)	-0.882
InChI=1S/C5H8N4/c1-3-4(2)8-9-5(6)7-3/h1-2H3,(H2,6,7,9)	-1.094
InChI=1S/C6H8BrN3O2/c1-5-8-6(10(11)12)4-9(5)3-2-7/h4H,2-3H2,1H3	-2.839

"InChi"	"logS(M)"
InChI=1S/C16H21NO2/c1-2-12-19-15-11-7-6-10-14(15)16(18)17-13-8-4-3-5-9-13/h2,6-7,10-11,13H,1,3-5,8-9,12H2,(H,17,18)	-4.85
InChI=1S/C11H14N4O3/c1-4-5-7(16)15-6-12-9-8(15)10(17)14(3)11(18)13(9)2/h6H,4-5H2,1-3H3	-1.53
InChI=1S/C12H14N4O5/c1-2-3-13-12(17)8-6-10(14-4-5-14)11(16(20)21)7-9(8)15(18)19/h6-7H,2-5H2,1H3,(H,13,17)	-3.89
InChI=1S/C8H15NO2/c1-3-5-6-8(4-2,11-6)7(9)10/h6H,3-5H2,1-2H3,(H2,9,10)	-1.175
InChI=1S/C10H22N2O6/c1-2-3-4-5-6-7-8-10(18-12(15)16)9-17-11(13)14/h10H,2-9H2,1H3,(H,13,14)(H,15,16)/q+2	-5.72
InChI=1S/C20H17ClN2O3/c1-3-23(4-2)14-7-5-12-9-15(20(24)26-18(12)11-14)19-22-16-10-13(21)h5-11H,3-4H2,1-2H3	-7.488
InChI=1S/C10H14O/c1-10(2,3)8-5-4-6-9(11)7-8/h4-7,11H,1-3H3	-1.861
InChI=1S/C8H16O2/c1-6(2)5-10-8(9)7(3)4/h6-7H,5H2,1-4H3	-2.159
InChI=1S/C10H10O4/c1-7(11)14-9-5-3-8(4-6-9)10(12)13-2/h3-6H,1-2H3	-2.5
InChI=1S/C8H10N2O4S/c1-5(11)10-6-2-3-7(9)8(4-6)15(12,13)14/h2-4H,9H2,1H3,(H,10,11)(H,12,13,14)	-1.232
InChI=1S/C7H3N3O4S/c8-4-15-7-2-1-5(9(11)12)3-6(7)10(13)14/h1-3H	-2.972
InChI=1S/C14H26O2/c1-3-5-6-7-8-9-10-11-12-13-14(15)16-4-2/h4H,2-3,5-13H2,1H3	-5.355
InChI=1S/C19H22N2O3/c1-20-12-11-15-13-17(24-2)8-9-18(15)19(20)10-5-14-3-6-16(7-4-14)2h3-4,6-9,13,19H,5,10-12H2,1-2H3	-4.783
InChI=1S/C16H23NO2/c1-3-19-15(18)16(14-8-5-4-6-9-14)10-7-12-17(2)13-11-16/h4-6,8-9H,3,7,10-13H2,1-2H3	-2.668
InChI=1S/C15H20O4/c1-6-4-11-13(8(3)15(18)19-11)14(17)12-7(2)10(16)5-9(6)12/h6,8-9,11,13-14,17H,4-5H2,1-3H3	-1.945
InChI=1S/C20H43N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(2)3/h4-20H2,1-3H3	-7.455
InChI=1S/C7H11NO2/c1-7(2)3-5(9)8-6(10)4-7/h3-4H2,1-2H3,(H,8,9,10)	-0.257
InChI=1S/C4H7N/c1-2-3-4-5/h2-3H2,1H3	-0.321
InChI=1S/C12H2Cl8O/c13-3-1-5(15)6(2-4(3)14)21-12-10(19)8(17)7(16)9(18)11(12)20/h1-2H	-10.1
InChI=1S/C11H17NO/c1-12(2)9-11(13-3)10-7-5-4-6-8-10/h4-8,11H,9H2,1-3H3	-0.695
InChI=1S/C18H22ClNO/c1-18(21-14-13-20(2)3,15-7-5-4-6-8-15)16-9-11-17(19)12-10-16/h4-12H,13-14H2,1-3H3	-3.998

"InChi"	"logS(M)"
InChI=1S/C8H7ClN4O4S3/c9-5-1-3-6(4-2-5)20(16,17)13-7-11-12-8(18-7)19(10,14)15/h1-4H,(H,11,13)(H2,10,14,15)	-2.01
InChI=1S/C13H15NO3/c15-12(14-8-4-5-9-14)10-17-13(16)11-6-2-1-3-7-11/h1-3,6-7H,4-5,8-10H2	-1.57
InChI=1S/C15H10N6/c16-10-15(11-17)21-20-14-8-6-13(7-9-14)19-18-12-4-2-1-3-5-12/h1-9,20H/b19-18+	-4.92
InChI=1S/C13H10OS/c14-10-11-6-8-13(9-7-11)15-12-4-2-1-3-5-12/h1-10H	-4.185
InChI=1S/C25H21ClN2O6/c1-31-19-11-15(12-20(32-2)22(19)33-3)25(30)34-24-23(29)27-18-10-9h4-13,24H,1-3H3,(H,27,29)	-5.908
InChI=1S/C15H16N4O/c1-4-19-13-11(6-5-7-16-13)15(20)18-12-9(2)8-10(3)17-14(12)19/h5-8H,4H2,1-3H3,(H,18,20)	-4.554
InChI=1S/C12H6N2O6/c15-11(7-3-1-5-18-7)9-10(14(17)20-13-9)12(16)8-4-2-6-19-8/h1-6H	-3.85
InChI=1S/C21H18N4O2/c1-14-18(20(26)24(22-14)16-9-5-3-6-10-16)13-19-15(2)23-25(21(19)2h3-13,18H,1-2H3/b19-13+	-7.882
InChI=1S/C5H7N7/c6-2-1-3(11-4(7)9-1)12-5(8)10-2/h(H7,6,7,8,9,10,11,12)	-1.52
InChI=1S/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)	0.86
InChI=1S/C9H9NO4/c1-4-6(8(11)12)3-7(9(13)14)5(2)10-4/h3H,1-2H3,(H,11,12)(H,13,14)	-2.809
InChI=1S/C23H22ClN3O2S/c1-16(28)26-10-12-27(13-11-26)23(29)7-3-17-2-6-22(20(24)14-17)30h2-9,14-15,25H,10-13H2,1H3/b7-3+	-2.74
InChI=1S/C13H20O2/c1-5-11(14)15-10-8-9-6-7-13(10,4)12(9,2)3/h5,9-10H,1,6-8H2,2-4H3	-4.583
InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h4,8-9H,5-6H2,1-3H3	-4.67
InChI=1S/C14H26O2/c1-7-14(6,11-9-10-12(3)4)16-13(5)15-8-2/h7,10,13H,1,8-9,11H2,2-6H3	-3.976
InChI=1S/C19H24N2/c1-20-14-12-19(13-15-20)21(18-10-6-3-7-11-18)16-17-8-4-2-5-9-17/h2-11,19H,12-16H2,1H3	-4.086
InChI=1S/C5H8ClN5/c1-2-8-5-10-3(6)9-4(7)11-5/h2H2,1H3,(H3,7,8,9,10,11)	-2.413
InChI=1S/C15H19FN2O/c16-12-4-6-13(7-5-12)18-11-8-14(15(18)19)17-9-2-1-3-10-17/h4-7,14H,1-3,8-11H2	-2.57
InChI=1S/C12H9ClO/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9H	-4.793
InChI=1S/C22H32O2/c1-17(9-7-10-18(2)14-16-24-20(4)23)12-13-21-19(3)11-8-15-22(21,5)h7,9-10,12-14H,8,11,15-16H2,1-6H3/b10-7+,13-12+,17-9+,18-14+	-7.517
InChI=1S/C17H28N2O/c1-6-12-19(8-3)15(7-2)17(20)18-16-13(4)10-9-11-14(16)5/h9-11,15H,6-8,12H2,1-5H3,(H,18,20)	-4.367

"InChi"	"logS(M)"
InChI=1S/C12H22O11/c13-1-3-5(14)8(17)10(19)12(23-3)21-2-4-6(15)7(16)9(18)11(20)22-4/h3-20H,1-2H2	0.466
InChI=1S/C7H15NO3/c1-8(2,3)5-6(9)4-7(10)11/h6,9H,4-5H2,1-3H3	0.793
InChI=1S/C9H13N3O2/c1-7-6-8(13)9(11-10-7)12-2-4-14-5-3-12/h6H,2-5H2,1H3,(H,10,13)	-1.183
InChI=1S/C23H29N3O2/c1-2-26-22(20-8-4-5-9-21(20)23(26)27)24-18-10-12-19(13-11-18)28-1h4-5,8-13,22,24H,2-3,6-7,14-17H2,1H3	-3.859
InChI=1S/CH4Cl2O6P2/c2-1(3,10(4,5)6)11(7,8)9/h(H2,4,5,6)(H2,7,8,9)	-2.793
InChI=1S/C18H22ClN3/c1-21(2)10-5-11-22-17-7-4-3-6-16(17)20-13-14-8-9-15(19)12-18(14)2h3-4,6-9,12,20H,5,10-11,13H2,1-2H3	-5.109
InChI=1S/C15H17F3N2O4S2/c16-15(17,18)12-10-14(20-13-5-2-1-4-11(12)13)24-8-3-6-19-7-9-25-2h1-2,4-5,10,19H,3,6-9H2,(H,21,22,23)	-3.143
InChI=1S/C14H26N2O2/c1-3-15(4-2)9-10-18-14(17)13-11-12-5-7-16(13)8-6-12/h12-13H,3-11H2,1-2H3	-1.629
InChI=1S/C6H13O5P/c1-6(7)11-4-5-12(8,9-2)10-3/h4-5H2,1-3H3	-0.159
InChI=1S/C9H11NO4/c1-13-6-3-5(9(10)12)4-7(14-2)8(6)11/h3-4,11H,1-2H3,(H2,10,12)	-0.561
InChI=1S/C15H10O2/c16-15-13-9-5-4-8-12(13)14(17-15)10-11-6-2-1-3-7-11/h1-10H/b14-10-	-3.174
InChI=1S/C12H8N2O5/c15-12-6-9(8-4-2-1-3-5-8)10(13(16)17)7-11(12)14(18)19/h1-7,15H	-4.461
InChI=1S/C10H13NO2/c1-7-4-5-9(6-8(7)2)13-10(12)11-3/h4-6H,1-3H3,(H,11,12)	-2.49
InChI=1S/C20H19NO5/c1-21-7-13-11(2-3-15-20(13)26-9-23-15)18-14(22)4-10-5-16-17(25-8-h2-3,5-6,14,18-19,22H,4,7-9H2,1H3	-3.39
InChI=1S/C9H18N2O/c1-3-10-4-2-9(1)11-5-7-12-8-6-11/h9-10H,1-8H2	-2.903
InChI=1S/C19H27NO2/c1-5-20(6-2)14-13-19(3,21)17-11-12-18(22-4)16-10-8-7-9-15(16)17/h7-12,21H,5-6,13-14H2,1-4H3	-1.68
InChI=1S/C4H10N2O/c5-3-1-2-4(6)7/h1-3,5H2,(H2,6,7)	0.152
InChI=1S/C10H19N/c1-3-10-9-5-4-8(6-9)7-11(10)2/h8-10H,3-7H2,1-2H3	-1.608
InChI=1S/C5H3ClO3/c6-4-2-1-3(9-4)5(7)8/h1-2H,(H,7,8)/p-1	-1.719
InChI=1S/C8H16O/c9-8-6-4-2-1-3-5-7-8/h8-9H,1-7H2	-1.29
InChI=1S/C20H22N6O3/c1-12-21-11-14(18(28)22-12)19(29)26-24-15-9-20(2,3)10-16(27)17(15h4-8,11,23H,9-10H2,1-3H3,(H,26,29)(H,21,22,28)/b24-15-,25-17-	-5.965
InChI=1S/C13H15NO2/c15-12-9-5-2-6-10-14(12)13(16)11-7-3-1-4-8-11/h1,3-4,7-8H,2,5-6,9-10H2	-2.167
InChI=1S/C7H6N4S/c1-12-6-3-9-5-2-8-4-10-7(5)11-6/h2-4H,1H3	-1.55
InChI=1S/C7H3Cl2NS/c8-6-2-1-5(10-4-11)3-7(6)9/h1-3H	-4.634

"InChi"	"logS(M)"
InChI=1S/C10H15NO2/c1-7(11-2)10(13)8-5-3-4-6-9(8)12/h3-7,10-13H,1-2H3	0.742
InChI=1S/C9H20N2/c1-8(2)6-10-7-9(3,4)11(8)5/h10H,6-7H2,1-5H3	0.064
InChI=1S/C3H3N3O2/c7-2-1-4-6-3(8)5-2/h1H,(H2,5,6,7,8)	-0.833
InChI=1S/C9H9NO4/c1-2-9(11)14-8-5-3-7(4-6-8)10(12)13/h3-6H,2H2,1H3	-3.893
InChI=1S/C7H9N3O2/c1-4-3-6(12)7(10-9-4)8-5(2)11/h3H,1-2H3,(H,9,12)(H,8,10,11)	-0.971
InChI=1S/C12H17NO/c1-4-10(2)12(14)13(3)11-8-6-5-7-9-11/h5-10H,4H2,1-3H3	-1.581
InChI=1S/C13H19N3O4/c1-5-10(6-2)14-12-11(15(17)18)7-8(3)9(4)13(12)16(19)20/h7,10,14H,5-6H2,1-4H3	-5.972
InChI=1S/C3H6N2O/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)	0.84
InChI=1S/C18H29NO3/c1-3-4-5-6-7-8-9-10-13-22-16-11-12-17(15(2)19-21)18(20)14-16/h11-12,14,20-21H,3-10,13H2,1-2H3/b19-15+	-4.89
InChI=1S/C7H4Cl2O2/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3H,(H,10,11)	-3.495
InChI=1S/C7H4BrClN2O/c8-3-1-5-6(2-4(3)9)12-7(10)11-5/h1-2H,(H2,10,11)	-3.528
InChI=1S/C10H11NO3/c1-14-9(12)7-11-10(13)8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,11,13)	-1.056
InChI=1S/C16H15NO2S/c1-13-8-10-15(11-9-13)20(18,19)17-12-4-6-14-5-2-3-7-16(14)17/h2-11H,12H2,1H3	-5.072
InChI=1S/C10H18O2/c1-4-5-6-7-8-12-10(11)9(2)3/h2,4-8H2,1,3H3	-3.755
InChI=1S/C14H13NO3/c16-13-11-9-6-7-10(18-9)12(11)14(17)15(13)8-4-2-1-3-5-8/h1-5,9-12H,6-7H2	-0.687
InChI=1S/C20H24O3/c1-4-5-6-7-12-23-20(21)15(2)16-8-9-18-14-19(22-3)11-10-17(18)13-1h5-6,8-11,13-15H,4,7,12H2,1-3H3/b6-5+	-7.36
InChI=1S/C10H12O3/c1-11-9-4-2-3-5-10(9)13-7-8-6-12-8/h2-5,8H,6-7H2,1H3	-1.522
InChI=1S/C13H12N4S/c18-13(16-14-11-7-3-1-4-8-11)17-15-12-9-5-2-6-10-12/h1-10,14H,(H,16,18)/b17-15+	-6.61
InChI=1S/C12H26OS/c1-2-3-4-5-6-7-8-9-11-14-12-10-13/h13H,2-12H2,1H3	-4.522
InChI=1S/C9H10N2O3/c1-10-5-7-2-3-9(11(12)13)4-8(7)6-14-10/h2-4H,5-6H2,1H3	-2.497
InChI=1S/C18H23FN2O3/c19-15-5-3-14(4-6-15)16(22)2-1-11-21-12-8-18(9-13-21)7-10-20-17(23)h3-6H,1-2,7-13H2,(H,20,23)	-3.033
InChI=1S/C8H9NO5/c1-2-8(10)13-5-6-3-4-7(14-6)9(11)12/h3-4H,2,5H2,1H3	-2.546
InChI=1S/C12H4Cl4O/c13-7-1-5-6-2-8(14)10(16)4-12(6)17-11(5)3-9(7)15/h1-4H	-8.646
InChI=1S/C15H16N2O/c1-16(13-9-5-3-6-10-13)15(18)17(2)14-11-7-4-8-12-14/h3-12H,1-2H3	-3.498

"InChi"	"logS(M)"
InChI=1S/C10H16ClN5S/c1-12-10-14-8(11)7(17-2)9(15-10)16-5-3-13-4-6-16/h13H,3-6H2,1-2H3,(H,12,14,15)	-1.233
InChI=1S/C8H14O2/c9-8(10)6-5-7-3-1-2-4-7/h7H,1-6H2,(H,9,10)	-1.769
InChI=1S/C7H13N/c1-4-7-8(5-2)6-3/h1H,5-7H2,2-3H3	-0.602
InChI=1S/C11H20O/c1-9-5-7-10(8-6-9)11(2,3)12-4/h5,10H,6-8H2,1-4H3	-3.297
InChI=1S/C16H22N4O2/c1-11-14(17-15(21)12(2)18(3)4)16(22)20(19(11)5)13-9-7-6-8-10-13/h6-10,12H,1-5H3,(H,17,21)	-2.673
InChI=1S/C9H6O6/c10-7(11)4-2-1-3-5(8(12)13)6(4)9(14)15/h1-3H,(H,10,11)(H,12,13)(H,14,15)	-0.837
InChI=1S/C20H28ClN3O2/c1-5-17-19(21)20(24-13-23-17)22-10-12-26-18-8-7-16(9-11-25-6-2)14h7-8,13H,5-6,9-12H2,1-4H3,(H,22,23,24)	-5.241
InChI=1S/C54H106O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-39-43-47-51-57-h3-52H2,1-2H3	-6.406
InChI=1S/C12H13NO2/c1-2-15-12(14)13-9-5-7-10-6-3-4-8-11(10)13/h3-8H,2,9H2,1H3	-3.843
InChI=1S/C14H17NO3/c1-3-10-18-14(16)15-12-7-5-4-6-11(12)8-9-13(15)17-2/h4-9,13H,3,10H2,1-2H3	-4.336
InChI=1S/C21H26O3/c1-21(2,3)14-10-8-13(9-11-14)12-17-18(22)15-6-4-5-7-16(15)19(23)24h4-7,13-14,24H,8-12H2,1-3H3	-7.04
InChI=1S/C13H16N2/c1-3-10-9(2)13(8-14)15-12-7-5-4-6-11(10)12/h4-7H,3,8,14H2,1-2H3	-1.48
InChI=1S/C6H15NO/c1-2-3-4-7-5-6-8/h7-8H,2-6H2,1H3	0.931
InChI=1S/C20H20N6O3/c21-11-1-13-25(14-16-29-15-2-12-22)19-7-3-17(4-8-19)23-24-18-5-9-h3-10H,1-2,13-16H2/b24-23+	-4.594
InChI=1S/C11H15NO2/c1-7-5-8(2)9(3)10(6-7)14-11(13)12-4/h5-6H,1-4H3,(H,12,13)	-1.985
InChI=1S/C17H15NO3/c1-10-4-3-5-13(8-10)16-18-14-9-12(11(2)17(19)20)6-7-15(14)21-16/h3-9,11H,1-2H3,(H,19,20)	-4.173
InChI=1S/C12H20N2O3S/c1-9(2)13-8-12(15)10-4-6-11(7-5-10)14-18(3,16)17/h4-7,9,12-15H,8H2,1-3H3	-1.694
InChI=1S/C11H16O4/c12-6-11(7-13,8-14)9-15-10-4-2-1-3-5-10/h1-5,12-14H,6-9H2	-1.551
InChI=1S/C12H4Cl6O/c13-5-1-2-9(12(18)11(5)17)19-10-4-7(15)6(14)3-8(10)16/h1-4H	-8.31
InChI=1S/C9H13O6PS/c1-12-9-5-15-7(4-8(9)10)6-17-16(11,13-2)14-3/h4-5H,6H2,1-3H3	0.729
InChI=1S/C5H12O3/c1-2-8-4-5(7)3-6/h5-7H,2-4H2,1H3	0.481
InChI=1S/C9H11N3O4/c10-5-1-2-12-8-7(16-9(12)11-5)6(14)4(3-13)15-8/h1-2,4,6-8,10,13-14H,3H2/b10-5+	0.647

"InChi"	"logS(M)"
InChI=1S/C9H12O3/c1-2-3-6-12-9(10)8-5-4-7-11-8/h4-5,7H,2-3,6H2,1H3	-2.498
InChI=1S/C10H20N2O4/c1-3-5-12-10(14)16-7-8(4-2)6-15-9(11)13/h8H,3-7H2,1-2H3,(H2,11,13)(H,12,14)	-2.165
InChI=1S/C16H22O4/c1-3-5-10-19-15(17)13-8-7-9-14(12-13)16(18)20-11-6-4-2/h7-9,12H,3-6,10-11H2,1-2H3	-4.868
InChI=1S/C16H18N4O3/c1-2-19(11-12-21)15-7-3-13(4-8-15)17-18-14-5-9-16(10-6-14)20(22)2h3-10,21H,2,11-12H2,1H3/b18-17+	-6.293
InChI=1S/C21H23F2NO2/c1-5-25-18-11-13(21(2,3)4)9-10-14(18)17-12-26-20(24-17)19-15(22)7h6-11,17H,5,12H2,1-4H3	-6.678
InChI=1S/C8H9NO4S/c1-13-8(10)6-4-2-3-5-7(6)14(9,11)12/h2-5H,1H3,(H2,9,11,12)	-0.779
InChI=1S/C8H10ClN3/c1-12(2)11-10-8-5-3-7(9)4-6-8/h3-6H,1-2H3/b11-10+	-3.143
InChI=1S/C6H13NO2/c1-2-3-4-5-9-6(7)8/h2-5H2,1H3,(H2,7,8)	-1.47
InChI=1S/C8H6Cl4O2/c1-13-7-5(11)3(9)4(10)6(12)8(7)14-2/h1-2H3	-5.239
InChI=1S/C14H32N2O4/c1-11(17)7-15(8-12(2)18)5-6-16(9-13(3)19)10-14(4)20/h11-14,17-20H,5-10H2,1-4H3	0.534
InChI=1S/C14H9NO2/c16-15(17)14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H	-6.292
InChI=1S/C12H24N2O4/c1-5-6-14-11(16)18-8-12(4,9(2)3)7-17-10(13)15/h9H,5-8H2,1-4H3,(H2,13,15)(H,14,16)	-3.112
InChI=1S/C17H21N3O2/c21-15-12-14(17(22)13-6-4-7-19-16(13)15)18-8-5-11-20-9-2-1-3-10-2h4,6-7,12,18H,1-3,5,8-11H2	-1.942
InChI=1S/C13H21NO/c1-11(15)10-14-13(2,3)9-12-7-5-4-6-8-12/h4-8,11,14-15H,9-10H2,1-3H3	-1.515
InChI=1S/C6H9N3/c7-3-1-5-9-6-2-4-8/h9H,1-2,5-6H2	0.91
InChI=1S/C11H21N5/c1-6-9-14-10(12-7(2)3)16-11(15-9)13-8(4)5/h7-8H,6H2,1-5H3,(H2,12,13,14,15,16)	-3.929
InChI=1S/C17H22N2OS/c1-13-4-5-16-15(10-13)14(2)11-17(18-16)20-8-3-6-19-7-9-21-12-19/h4-5,10-11H,3,6-9,12H2,1-2H3	-3.759
InChI=1S/C16H18N4O7S/c1-25-12-8-13(26-2)18-15(17-12)19-16(22)20-28(23,24)9-10-6-4-5-7-h4-8H,9H2,1-3H3,(H2,17,18,19,20,22)	-3.534
InChI=1S/C6H4N4O2/c11-5-6(12)10-4-3(9-5)1-7-2-8-4/h1-2H,(H,9,11)(H,7,8,10,12)	-2.69
InChI=1S/C10H19N5O/c1-5-7(3)12-9-13-8(11-6-2)14-10(15-9)16-4/h7H,5-6H2,1-4H3,(H2,11,12,13,14,15)	-2.575
InChI=1S/C12H5Cl5O/c13-6-1-2-7(14)10(5-6)18-9-4-3-8(15)11(16)12(9)17/h1-5H	-7.7
InChI=1S/C7H16O/c1-6(2)8-7(3,4)5/h6H,1-5H3	-2.366
InChI=1S/C16H21N3O2/c1-4-5-11-17-14-12(2)18(3)16(21)19(15(14)20)13-9-7-6-8-10-13/h6-10,17H,4-5,11H2,1-3H3	-2.739

"InChi"	"logS(M)"
InChI=1S/C22H25NO6/c1-12(24)23-16-8-6-13-10-19(27-3)21(28-4)22(29-5)20(13)14-7-9-17(h7,9-11,16H,6,8H2,1-5H3,(H,23,24)	-2.966
InChI=1S/C6H4N4O3S/c7-6-9-8-5(14-6)3-1-2-4(13-3)10(11)12/h1-2H,(H2,7,9)	-2.994
InChI=1S/C15H18N6O6S/c1-4-27-15-19-12(16-2)17-13(20-15)18-14(23)21-28(24,25)10-8-6-5-7h5-8H,4H2,1-3H3,(H3,16,17,18,19,20,21,23)	-4.388
InChI=1S/C12H26O4/c1-9-12(8,15-13-10(2,3)4)16-14-11(5,6)7/h9H2,1-8H3	-4.451
InChI=1S/C9H13NO2/c1-6(10)9(12)7-3-2-4-8(11)5-7/h2-6,9,11-12H,10H2,1H3	0.777
InChI=1S/C22H29NO2/c1-5-21(24)25-22(18(2)17-23(3)4,20-14-10-7-11-15-20)16-19-12-8-6-h6-15,18H,5,16-17H2,1-4H3	-5.01
InChI=1S/C16H34O/c1-3-5-7-9-10-12-14-16(15-17)13-11-8-6-4-2/h16-17H,3-15H2,1-2H3	-5.385
InChI=1S/C22H28O5/c1-7-8-9-10-15-14(3)18(12-17(15)23)27-21(25)19-16(22(19,4)5)11-13h7-9,11,16,18-19H,1,10,12H2,2-6H3/b9-8+,13-11-	-4.617
InChI=1S/C7H6Cl2O/c1-4-2-5(8)3-6(9)7(4)10/h2-3,10H,1H3	-2.044
InChI=1S/C16H32O3/c1-8-10-11-13(9-2)14(17)18-19-16(6,7)12-15(3,4)5/h13H,8-12H2,1-7H3	-5.95
InChI=1S/C24H36O3/c1-4-5-6-22(26)27-21-10-9-19-18-8-7-16-15-17(25)11-13-23(16,2)20(h15,18-21H,4-14H2,1-3H3	-6.19
InChI=1S/C6H6N4O3/c1-10-3-2(7-6(10)13)4(11)9-5(12)8-3/h1H3,(H,7,13)(H2,8,9,11,12)	-3.94
InChI=1S/C10H16O4/c1-9(2)6(7(11)12)4-5-10(9,3)8(13)14/h6H,4-5H2,1-3H3,(H,11,12)(H,13,14)/p-2	-1.421
InChI=1S/C9H7NO4/c11-9(12)5-4-7-2-1-3-8(6-7)10(13)14/h1-6H,(H,11,12)/b5-4+	-2.998
InChI=1S/C15H15ClFN3O3S2/c1-23-13(21)8-24-12-7-11(10(17)6-9(12)16)18-14-19-4-2-3-5-20(19)1h6-7H,2-5,8H2,1H3/b18-14-	-5.677
InChI=1S/C8H7N3O/c9-8-10-7(11-12-8)6-4-2-1-3-5-6/h1-5H,(H2,9,10,11)	-1.39
InChI=1S/C10H18O4/c1-7(2)13-9(11)5-6-10(12)14-8(3)4/h7-8H,5-6H2,1-4H3	-1.729
InChI=1S/C9H12O/c1-6-4-7(2)8(3)9(10)5-6/h4-5,10H,1-3H3	-2.252
InChI=1S/C12H3Cl5O/c13-6-1-4-5-2-8(15)10(16)11(17)12(5)18-9(4)3-7(6)14/h1-3H	-9.161
InChI=1S/C6H4N4O/c11-6-4-5(9-3-10-6)8-2-1-7-4/h1-3H,(H,8,9,10,11)	-1.472
InChI=1S/C17H17NO2/c1-3-20-16-12-8-4-5-9-13(12)17(19)18(2)15-11-7-6-10-14(15)16/h4-11,16H,3H2,1-2H3	-4.541
InChI=1S/C5H11NO3/c1-3(9-2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)	0.485
InChI=1S/C10H10N2O4/c13-5-9-10(6-14)12(16)8-4-2-1-3-7(8)11(9)15/h1-4,13-14H,5-6H2	0.653

"InChi"	"logS(M)"
InChI=1S/C17H16O3/c1-9-8-14(18)20-17-12(9)7-10(2)16-15(17)11-5-3-4-6-13(11)19-16/h7-8H,3-6H2,1-2H3	-5.09
InChI=1S/C5H6O2/c6-4-5-2-1-3-7-5/h1-3,6H,4H2	1.008
InChI=1S/C5H12N2S/c1-6-5(8-4)7(2)3/h1-4H3/b6-5-	-0.44
InChI=1S/C2H5N5/c3-1-5-2(4)7-6-1/h(H5,3,4,5,6,7)	1.004
InChI=1S/C13H10Cl2O/c14-11-7-10(13(16)12(15)8-11)6-9-4-2-1-3-5-9/h1-5,7-8,16H,6H2	-4.64
InChI=1S/C41H63NO14/c1-10-20(4)34(46)55-33-28(45)27-23(18-42-17-19(3)12-13-25(42)38(3 h19-20,23-33,45,48-51H,10-18H2,1-9H3	-5.538
InChI=1S/C8H18O/c1-4-6-7(3)8(9)5-2/h7-9H,4-6H2,1-3H3	-1.964
InChI=1S/C12H18O2/c1-5-14-11(13)10-9(2)7-6-8-12(10,3)4/h6-7H,5,8H2,1-4H3	-3.412
InChI=1S/C29H40N2O/c1-22(2)14-17-29(28(30)32,27-13-9-11-25-10-7-8-12-26(25)27)18-21-h7-16H,17-21H2,1-6H3,(H2,30,32)	-8.935
InChI=1S/C14H18N4O2/c1-3-20-11-5-4-9(7-12(11)19-2)6-10-8-17-14(16)18-13(10)15/h4-5,7-8H,3,6H2,1-2H3,(H4,15,16,17,18)	-2.346
InChI=1S/C7H14O2/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3,(H,8,9)	-1.665
InChI=1S/C6H5N5O2/c7-6-10-4-3(5(13)11-6)9-2(12)1-8-4/h1H,(H,9,12)(H3,7,8,10,11,13)	-3.86
InChI=1S/C6H5IN2O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,8H2	-4.422
InChI=1S/C10H18N2O4/c1-3-5-10(4-2,6-15-8(11)13)7-16-9(12)14/h3H,1,4-7H2,2H3,(H2,11,13)(H2,12,14)	-2.022
InChI=1S/C10H16N2/c1-9(12-11-2)8-10-6-4-3-5-7-10/h3-7,9,11-12H,8H2,1-2H3	-1.988
InChI=1S/C14H16N2O2/c17-13-7-6-11(15-13)14(18)16-12-8-10(12)9-4-2-1-3-5-9/h1-5,10-12H,6-8H2,(H,15,17)(H,16,18)	-1.419
InChI=1S/C9H9NO4/c1-5(11)10-6-2-3-7(9(13)14)8(12)4-6/h2-4,12H,1H3,(H,10,11)(H,13,14)	-2.008
InChI=1S/C11H14N4O4/c1-4-7(16)19-6-15-5-12-9-8(15)10(17)14(3)11(18)13(9)2/h5H,4,6H2,1-3H3	-2.3
InChI=1S/C16H8Cl2F6N2O3/c17-7-4-6(5-8(18)12(7)29-16(23,24)14(21)22)25-15(28)26-13(27)11-9 h1-5,14H,(H2,25,26,27,28)	-5.82
InChI=1S/C13H21N3O2/c1-9-11(15(2)3)12(17)14-13(18)16(9)10-7-5-4-6-8-10/h10H,4-8H2,1-3H3,(H,14,17,18)	-2.89
InChI=1S/C13H22N2O3/c1-6-8-9(3)13(7-2)10(16)14(4)12(18)15(5)11(13)17/h9H,6-8H2,1-5H3	-3.129
InChI=1S/C6H8N2/c7-5-6-3-1-2-4-8-6/h1-4H,5,7H2	0.966
InChI=1S/C11H11F3N2O4/c1-10(2,18)9(17)15-6-3-4-8(16(19)20)7(5-6)11(12,13)14/h3-5,18H,1-2H3,(H,15,17)	-4.027

"InChi"	"logS(M)"
InChI=1S/C21H14/c1-13-16-7-2-3-8-18(16)19-12-10-15-6-4-5-14-9-11-17(13)21(19)20(1h2-12H,1H3	-8.523
InChI=1S/C18H15NO2/c1-12-6-2-5-9-16(12)19-18(21)15-10-13-7-3-4-8-14(13)11-17(15)20/h2-11,20H,1H3,(H,19,21)	-4.623
InChI=1S/C12H18O/c1-12(2)10-6-5-9(4-3-7-13)11(12)8-10/h5,7,10-11H,3-4,6,8H2,1-2H3	-3.466
InChI=1S/C6H10O4/c1-5(7)9-3-4-10-6(2)8/h3-4H2,1-2H3	0.068
InChI=1S/C6H5Cl2N3O/c7-4-1-3(6(12)11-9)2-5(8)10-4/h1-2H,9H2,(H,11,12)	-1.11
InChI=1S/C7H12ClNO3/c1-3-12-7(11)5(2)9-6(10)4-8/h5H,3-4H2,1-2H3,(H,9,10)	-0.463
InChI=1S/C12H19N5O2/c1-10-13-11(16-2-6-18-7-3-16)15-12(14-10)17-4-8-19-9-5-17/h2-9H2,1H3	-2.537
InChI=1S/C5H8O/c1-2-4-6-5-3-1/h2,4H,1,3,5H2	-1.038
InChI=1S/C7H15NO2/c1-4-10-7(9)5-6-8(2)3/h4-6H2,1-3H3	0.268
InChI=1S/C6H9N3O2/c1-3-8-5(2)4-7-6(8)9(10)11/h4H,3H2,1-2H3	-1.971
InChI=1S/C31H44O8/c1-17-27(36-4)25(33)26(34)28(38-17)39-20-9-12-29(2)19(15-20)6-7-2h5,8,15-17,20-23,25-28,33-35H,6-7,9-14H2,1-4H3	-6.036
InChI=1S/C10H13NO2/c11-10(12)13-8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H2,11,12)	-2.183
InChI=1S/C17H28O2/c1-11-6-7-13-15(3,4)14-10-17(11,13)9-8-16(14,5)19-12(2)18/h11,13-14H,6-10H2,1-5H3	-5.427
InChI=1S/C38H69NO13/c1-15-26-38(10,45)31(42)21(4)28(40)19(2)17-37(9,47-14)33(52-35-29h19-27,29-33,35,41-43,45H,15-18H2,1-14H3	-2.2
InChI=1S/C11H13NO3/c1-2-15-10-6-3-9(4-7-10)5-8-11(13)12-14/h3-8,14H,2H2,1H3,(H,12,13)/b8-5+	-2.252
InChI=1S/C6H7N3O3/c1-2-8-5(11)3(4(7)10)6(12)9-2/h3H,1H3,(H2,7,10)(H,8,9,11,12)	-2.41
InChI=1S/C12H18O3/c1-9-4-10(2)6-11(5-9)15-8-12(3,14)7-13/h4-6,13-14H,7-8H2,1-3H3	-2.449
InChI=1S/C19H28O2/c1-18-8-3-4-14(18)13-6-5-12-10-16(20)17(21)11-19(12,2)15(13)7-9-1h12-15H,3-11H2,1-2H3	-3.76
InChI=1S/C14H28N2O4/c1-5-6-7-16-13(18)20-10-14(4,8-11(2)3)9-19-12(15)17/h11H,5-10H2,1-4H3,(H2,15,17)(H,16,18)	-4.155
InChI=1S/C18H41N3/c1-2-3-4-5-6-7-8-9-10-11-16-21(17-12-14-19)18-13-15-20/h2-20H2,1H3	-0.198
InChI=1S/C20H23ClO6/c1-5-6-7-26-15-9-12(22)8-11(2)20(15)19(23)16-13(24-3)10-14(25-4)1h9-11H,5-8H2,1-4H3	-4.7
InChI=1S/C7H16N2O6/c10-8(11)14-6-4-2-1-3-5-7-15-9(12)13/h1-7H2,(H,10,11)(H,12,13)/q+2	-3.4

"InChi"	"logS(M)"
InChI=1S/C15H13N3O3S/c1-21-15(19)18-14-16-12-8-7-11(9-13(12)17-14)22(20)10-5-3-2-4-6-1h2-9H,1H3,(H2,16,17,18,19)/p+1	-3.956
InChI=1S/C9H10O2/c1-6-3-4-8(9(10)11)5-7(6)2/h3-5H,1-2H3,(H,10,11)/p-1	-3.065
InChI=1S/C6H11FOS/c1-6(8)9-5-3-2-4-7/h2-5H2,1H3	-1.697
InChI=1S/C7H9NO2S/c1-6-3-2-4-7(5-6)11(8,9)10/h2-5H,1H3,(H2,8,9,10)	-1.341
InChI=1S/C6H10O3/c1-3-9-5(2)6(8)4-7/h4-5H,3H2,1-2H3	-0.155
InChI=1S/C20H24N2S2/c1-23-16-9-10-20-18(14-16)22(13-11-15-6-4-5-12-21-15)17-7-2-3-8-1h2-3,7-10,14-15,21H,4-6,11-13H2,1H3	-7.228
InChI=1S/C5H7NO2/c1-2-8-5(7)3-4-6/h2-3H2,1H3	-0.328
InChI=1S/C26H51NO/c1-4-7-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26(28)27(24-8-5-h15-16H,4-14,17-25H2,1-3H3/b16-15+	-4.789
InChI=1S/C41H67NO11/c1-10-32(43)29(8)36(45)26(5)20-28(7)38-27(6)19-23(2)15-16-31(50-3h13,15-17,23,26-31,33,35-39,45-46,48H,10-12,14,18-22H2,1-9H3,(H2,42,47)/b16-15-,24-13-	-8.527
InChI=1S/C5H6O5/c6-3(5(9)10)1-2-4(7)8/h1-2H2,(H,7,8)(H,9,10)	0.615
InChI=1S/C14H17NO4/c16-12-6-8-15(9-7-12)13(17)10-19-14(18)11-4-2-1-3-5-11/h1-5,12,16H,6-10H2	-1.349
InChI=1S/C23H30N2O3/c1-17-8-9-20(14-18(17)2)25-12-10-24(11-13-25)15-21(27)16-28-23-7-h4-9,14,21,27H,10-13,15-16H2,1-3H3	-3.727
InChI=1S/C40H60N2O8/c1-37(2,3)27-21-25(22-28(33(27)45)38(4,5)6)13-15-31(43)49-19-17-4h21-24,45-46H,13-20H2,1-12H3,(H,41,47)(H,42,48)	-8.667
InChI=1S/C14H26O6/c1-3-5-13(15)19-11-9-17-7-8-18-10-12-20-14(16)6-4-2/h3-12H2,1-2H3	-1.56
InChI=1S/C6H14N2O6/c9-7(10)13-5-3-1-2-4-6-14-8(11)12/h1-6H2,(H,9,10)(H,11,12)/q+2	-2.77
InChI=1S/C8H18O2/c1-3-5-8(4-2,6-9)7-10/h9-10H,3-7H2,1-2H3	-1.665
InChI=1S/C42H57N3O6/c1-22-16-31(40(7,8)9)34(46)25(4)28(22)19-43-37(49)44(20-29-23(2)1h16-18,46-48H,19-21H2,1-15H3	-7.544
InChI=1S/C21H28Cl2N2/c1-5-12-9-14(18(22)16(7-3)20(12)24)11-15-10-13(6-2)21(25)17(8-4)1h9-10H,5-8,11,24-25H2,1-4H3	-7.278
InChI=1S/C12H12N6O4/c1-15-7-5(9(19)17(3)11(15)21)13-6-8(14-7)16(2)12(22)18(4)10(6)20/h1-4H3	-3.31
InChI=1S/C7H5NO3/c9-5-6-2-1-3-7(4-6)8(10)11/h1-5H	-1.98
InChI=1S/C12H16N4O2/c1-15-10-8(11(17)16(2)12(15)18)13-9(14-10)7-5-3-4-6-7/h7H,3-6H2,1-2H3,(H,13,14)	-2.664
InChI=1S/C6H12O2/c1-6(8)4-2-3-5-7/h5-6,8H,2-4H2,1H3	-0.463

"InChi"	"logS(M)"
InChI=1S/C21H29NO/c23-21(19-7-3-1-4-8-19,11-14-22-12-5-2-6-13-22)20-16-17-9-10-18(2h1,3-4,7-10,17-18,20,23H,2,5-6,11-16H2	-4.093
InChI=1S/C9H16N2O/c1-7(12)11-8-3-4-9(11)6-10(2)5-8/h8-9H,3-6H2,1-2H3	-1.587
InChI=1S/C11H20O4/c1-2-3-4-5-6-7-8-9(10(12)13)11(14)15/h9H,2-8H2,1H3,(H,12,13)(H,14,15)	-2.92
InChI=1S/C8H8ClN3O4S2/c1-4-11-6-2-5(9)7(17(10,13)14)3-8(6)18(15,16)12-4/h2-3H,1H3,(H,11,12)(H2,10,13,14)	-2.536
InChI=1S/C10H16N2O3/c1-5-10(9(2,3)4)6(13)11-8(15)12-7(10)14/h5H2,1-4H3,(H2,11,12,13,14,15)	-1.928
InChI=1S/C12H12N2O3/c1-3-17-12(16)9-6-13-10-5-4-8(2)7-14(10)11(9)15/h4-7H,3H2,1-2H3	-1.663
InChI=1S/C4H6N2O2/c7-4-2-1-3-6(4)5-8/h1-3H2	0.052
InChI=1S/C8H10N4O2/c9-11-7(13)5-1-2-6(4-3-5)8(14)12-10/h1-4H,9-10H2,(H,11,13)(H,12,14)	-2.29
InChI=1S/C17H16O3/c1-2-17(18)20-13-12-19-16-11-7-6-10-15(16)14-8-4-3-5-9-14/h2-11H,1,12-13H2	-3.952
InChI=1S/C14H15N3O5/c1-3-16(4-2)14(20)10(8-15)5-9-6-11(17(21)22)13(19)12(18)7-9/h5-7,18-19H,3-4H2,1-2H3/b10-5-	-4.26
InChI=1S/C9H11BrO3/c10-8-3-1-2-4-9(8)13-6-7(12)5-11/h1-4,7,11-12H,5-6H2	-2.497
InChI=1S/C5H3N5/c6-4-3-5(9-1-7-3)10-2-8-4/h1H,6H2	-2.12
InChI=1S/C14H8Cl2N4/c15-11-7-3-1-5-9(11)13-17-19-14(20-18-13)10-6-2-4-8-12(10)16/h1-8H	-5.482
InChI=1S/C7H12O2/c1-5-6(8)9-7(2,3)4/h5H,1H2,2-4H3	-1.805
InChI=1S/C22H23F3N2S/c1-3-12-26(13-4-2)14-7-15-27-18-8-5-6-9-20(18)28-21-11-10-17(16-1h3-6,8-11,16H,1-2,7,12-15H2	-8.411
InChI=1S/C14H19NO4/c15-14(17)19-9-12(16)8-18-13-6-5-10-3-1-2-4-11(10)7-13/h5-7,12,16H,1-4,8-9H2,(H2,15,17)	-3.271
InChI=1S/C11H19NO2/c13-11(9-5-4-6-9)12(14)10-7-2-1-3-8-10/h9-10,14H,1-8H2	-2.7
InChI=1S/C5H6N2O2S/c1-3(8)7-2-4(9)6-5(7)10/h2H2,1H3,(H,6,9,10)	-0.234
InChI=1S/C4H8ClF/c5-3-1-2-4-6/h1-4H2	-2.144
InChI=1S/C8H11ClN2O/c1-2-3-4-7-10-6(5-12)8(9)11-7/h5H,2-4H2,1H3,(H,10,11)	-2.199
InChI=1S/C14H17N3O2/c1-10-12(15(2)3)13(18)17(14(19)16(10)4)11-8-6-5-7-9-11/h5-9H,1-4H3	-2.663
InChI=1S/C12H20O2/c13-5-7-1-2-10-11-4-8(12(7)10)3-9(11)6-14/h7-14H,1-6H2	-1.252
InChI=1S/C16H29NO2/c1-14-8-5-6-11-17(14)12-7-13-19-16(18)15-9-3-2-4-10-15/h14-15H,2-13H2,1H3	-4.079

"InChi"	"logS(M)"
InChI=1S/C8H8O3/c9-5-6-3-1-2-4-7(6)8(10)11/h1-4,9H,5H2,(H,10,11)	-1.551
InChI=1S/C8H16O/c1-2-3-4-5-6-7-8-9/h2,9H,1,3-8H2	-1.744
InChI=1S/C12H19BrN2O4S2/c13-11-10-15-6-4-12(11)19-8-3-1-2-5-14-7-9-20-21(16,17)18/h4,6,10,14H,1-3,5,7-9H2,(H,16,17,18)	-2.309
InChI=1S/C19H26NO4P/c1-2-10-20-11-9-19-8-4-3-5-16(19)18(20)12-14-6-7-15(13-17(14)19)2h2,6-7,13,16,18H,1,3-5,8-12H2,(H2,21,22,23)	-4.082
InChI=1S/C17H19NO3/c1-18-16(20)21-13-17(12-19,14-8-4-2-5-9-14)15-10-6-3-7-11-15/h2-11,19H,12-13H2,1H3,(H,18,20)	-3.212
InChI=1S/C14H10Cl2N4O2/c1-7-9(6-17)13(21)20(2)14(22)12(7)19-18-8-3-4-10(15)11(16)5-8/h3-5,18H,1-2H3/b19-12-	-6.926
InChI=1S/C8H9NO5/c10-2-1-4-7(8(12)13)9-5(11)3-6(9)14-4/h1,6-7,10H,2-3H2,(H,12,13)/b4-1-	0.701
InChI=1S/C11H12ClNO2/c1-2-11(14)13-6-8-3-4-10(12)5-9(8)7-15-13/h3-5H,2,6-7H2,1H3	-3.013
InChI=1S/C8H19O4P/c1-4-7-8-12-13(9,10-5-2)11-6-3/h4-8H2,1-3H3	-1.147
InChI=1S/C8H10O2/c1-2-10-8-5-3-7(9)4-6-8/h3-6,9H,2H2,1H3	-1.29
InChI=1S/C46H62Cl2O6/c1-26(2)9-7-10-27(3)35-14-15-36-32-13-12-30-25-44(4,19-20-45(30,5h11,21-24,26-27,30,32,35-37,49-50H,7-10,12-20,25H2,1-6H3,(H,51,52)(H,53,54)	-8.46
InChI=1S/C10H12O/c11-8-10(6-7-10)9-4-2-1-3-5-9/h1-5,11H,6-8H2	-1.759
InChI=1S/C10H8ClNOS2/c1-6-9(13)12(10(14)15-6)8-4-2-7(11)3-5-8/h2-6H,1H3	-2.516
InChI=1S/C10H18O2/c1-2-8-3-4-9(7-8)5-6-10(11)12/h8-9H,2-7H2,1H3,(H,11,12)	-3.286
InChI=1S/C3H5Cl2NO/c4-1-2(5)3(6)7/h2H,1H2,(H2,6,7)	-0.514
InChI=1S/C20H22ClN3O2/c21-17-4-7-19(8-5-17)24-13-11-23(12-14-24)15-16-26-20(25)9-6-18-3h1-10H,11-16H2/b9-6+	-3.659
InChI=1S/C10H7NOS2/c12-9-8(14-10(13)11-9)6-7-4-2-1-3-5-7/h1-6H,(H,11,12,13)/b8-6-	-1.783
InChI=1S/C13H12FNO/c1-15(13(16)9-14)12-8-4-6-10-5-2-3-7-11(10)12/h2-8H,9H2,1H3	-2.809
InChI=1S/C19H30N2O/c1-15(2)20(16(3)4)13-8-14-21-18-11-6-5-9-17(18)10-7-12-19(21)22/h5-6,9,11,15-16H,7-8,10,12-14H2,1-4H3	-4.701
InChI=1S/C8H11N3O2/c1-3-4-11-6(9)5-7(12)10(2)8(11)13/h3,5H,1,4,9H2,2H3	-1.48
InChI=1S/CH2ClNO2/c2-1-3(4)5/h1H2	-0.281
InChI=1S/C17H21NO3/c1-18-7-6-17-10-3-5-13(20)16(17)21-15-12(19)4-2-9(14(15)17)8-11(1h2,4,10-11,13,16,19-20H,3,5-8H2,1H3	-1.479
InChI=1S/C11H9NO3S/c1-2-7-12-11(13)10-6-4-3-5-9(10)8-16(12,14)15/h1,3-6H,7-8H2	-1.886
InChI=1S/C12H25NO2/c13-11-9-7-5-3-1-2-4-6-8-10-12(14)15/h1-11,13H2,(H,14,15)	-3.196

"InChi"	"logS(M)"
InChI=1S/C6H4Cl2O/c7-4-1-2-5(8)6(9)3-4/h1-3,9H	-1.911
InChI=1S/C21H19N3/c1-12-8-15-19(10-17(12)22)24-20-11-18(23)13(2)9-16(20)21(15)14-6-h3-11H,22-23H2,1-2H3	-6.306
InChI=1S/C8H18O/c1-4-5-7(2)6-8(3)9/h7-9H,4-6H2,1-3H3	-1.878
InChI=1S/C11H9N3O2/c15-10(8-4-2-1-3-5-8)13-9-6-7-12-11(16)14-9/h1-7H,(H2,12,13,14,15,16)	-5.16
InChI=1S/C18H21O3P/c1-5-21-22(20,16-9-7-6-8-10-16)18(19)17-14(3)11-13(2)12-15(17)4/h6-12H,5H2,1-4H3	-3.956
InChI=1S/C14H18O4/c1-7-8(2)12-10(9(3)11(7)15)5-6-14(4,18-12)13(16)17/h15H,5-6H2,1-4H3,(H,16,17)	-3.078
InChI=1S/C6H12O4/c1-3-10-4(2)5(7)6(8)9/h4,6,8-9H,3H2,1-2H3	-0.171
InChI=1S/C8H12N2/c1-7(10-9)8-5-3-2-4-6-8/h2-7,10H,9H2,1H3	-1.155
InChI=1S/C11H16N2O2/c1-3-10-8(6-15-11(10)14)4-9-5-12-7-13(9)2/h5,7-8,10H,3-4,6H2,1-2H3	-0.823
InChI=1S/C9H7Cl3O3/c1-4(9(13)14)15-8-3-6(11)5(10)2-7(8)12/h2-4H,1H3,(H,13,14)	-3.13
InChI=1S/C12H22O2/c1-4-12(13)14-11-7-5-10(6-8-11)9(2)3/h9-11H,4-8H2,1-3H3	-4.173
InChI=1S/C12H8N6O3/c19-12(7-1-3-8(4-2-7)18(20)21)17-11-9-10(14-5-13-9)15-6-16-11/h1-6H,(H2,13,14,15,16,17,19)	-2.086
InChI=1S/C12H7Br3/c13-9-6-10(14)12(11(15)7-9)8-4-2-1-3-5-8/h1-7H	-7.3
InChI=1S/C25H34O6/c1-4-5-21-30-20-11-17-16-7-6-14-10-15(27)8-9-23(14,2)22(16)18(28)h8-10,16-18,20-22,26,28H,4-7,11-13H2,1-3H3	-4.603
InChI=1S/C19H25ClN2O3/c1-14-13-21-18(24)25-19(14)8-11-22(12-9-19)10-2-3-17(23)15-4-6-16h4-7,14H,2-3,8-13H2,1H3,(H,21,24)	-3.992
InChI=1S/C9H20O/c1-7(2)5-9(10)6-8(3)4/h7-10H,5-6H2,1-4H3	-2.159
InChI=1S/C16H13N3O3/c1-18-14-8-7-12(19(21)22)9-13(14)16(17-10-15(18)20)11-5-3-2-4-6-1h2-9H,10H2,1H3	-3.8
InChI=1S/C12H5Cl5O/c13-7-2-1-6(3-8(7)14)18-12-5-10(16)9(15)4-11(12)17/h1-5H	-7.83
InChI=1S/C8H9NO3/c1-12-5-2-3-7(10)6(4-5)8(9)11/h2-4,10H,1H3,(H2,9,11)	-0.793
InChI=1S/C9H20O/c1-5-7(3)9(10)8(4)6-2/h7-10H,5-6H2,1-4H3	-2.511
InChI=1S/C19H32O3/c1-2-3-4-5-6-7-8-9-18-10-12-19(13-11-18)22-17-16-21-15-14-20/h10-13,20H,2-9,14-17H2,1H3	-0.305
InChI=1S/C12H8ClNO2/c13-10-7-5-9(6-8-10)11-3-1-2-4-12(11)14(15)16/h1-8H	-4.937
InChI=1S/C12H17NO2/c1-3-4-9-15-12-8-6-5-7-11(12)13-10(2)14/h5-8H,3-4,9H2,1-2H3,(H,13,14)	-2.498

"InChi"	"logS(M)"
InChI=1S/C20H26N2O3/c1-15(20(23)25-12-11-22-9-7-21-8-10-22)16-3-4-18-14-19(24-2)6-5-17h3-6,13-15,21H,7-12H2,1-2H3	-1.52
InChI=1S/C17H36N2O/c1-5-9-13-18(14-10-6-2)17(20)19(15-11-7-3)16-12-8-4/h5-16H2,1-4H3	-4.821
InChI=1S/C10H9NO5S3/c11-19(15,16)10-5-9(6-17-10)18(13,14)8-3-1-7(12)2-4-8/h1-6,12H,(H2,11,15,16)	-3.03
InChI=1S/C16H27NO5/c1-10(2)16(20,11(3)21-4)15(19)22-9-12-5-7-17-8-6-13(18)14(12)17/h5,10-11,13-14,18,20H,6-9H2,1-4H3	-0.83
InChI=1S/C9H11ClN4O2/c1-12-7-6(8(15)13(2)9(12)16)14(4-3-10)5-11-7/h5H,3-4H2,1-2H3	-1.741
InChI=1S/C7H5NO5/c9-3-4-1-5(8(12)13)7(11)6(10)2-4/h1-3,10-11H	-1.938
InChI=1S/C17H18O4/c1-2-5-12-11-7-4-3-6-10(11)8-13-14(18)9-15(17(19)20)21-16(12)13/h8-9H,2-7H2,1H3,(H,19,20)	-1.9
InChI=1S/C10H13ClO/c1-6(2)8-5-9(11)7(3)4-10(8)12/h4-6,12H,1-3H3	-2.266
InChI=1S/C19H17O4P/c1-16-12-14-19(15-13-16)23-24(20,21-17-8-4-2-5-9-17)22-18-10-6-3-h2-15H,1H3	-6.152
InChI=1S/C10H10N2/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h1-6H,11-12H2	-2.307
InChI=1S/C16H11NO3/c18-15-13(16(19)20)11-8-4-5-9-12(11)17-14(15)10-6-2-1-3-7-10/h1-9,18H,(H,19,20)	-4.904
InChI=1S/C7H12N2S/c1-5-4-7(2,3)9-6(10)8-5/h4H,1-3H3,(H2,8,9,10)	0.024
InChI=1S/C17H21ClN2O2S/c1-11-15(12-7-9-13(18)10-8-12)23-17(22)20(11)16(21)19-14-5-3-2-4-h7-11,14-15H,2-6H2,1H3,(H,19,21)	-5.849
InChI=1S/C10H13Cl2N/c11-6-8-13(9-7-12)10-4-2-1-3-5-10/h1-5H,6-9H2	-3.269
InChI=1S/CH5O3P/c1-5(2,3)4/h1H3,(H2,2,3,4)	-0.681
InChI=1S/C9H18O3/c1-3-6-11-8-5-9(10)12-7-4-2/h3-8H2,1-2H3	-1.685
InChI=1S/C26H32O4/c1-23(2)15-26(7,18-11-8-16(9-12-18)21(27)24(3,4)29)19-13-10-17(14h8-14,29-30H,15H2,1-7H3	-5.937
InChI=1S/C14H14N2O4S/c1-2-20-14(17)11-8-9-13(15-10-11)16-21(18,19)12-6-4-3-5-7-12/h3-10H,2H2,1H3,(H,15,16)	-4.24
InChI=1S/C13H19NO/c1-2-3-4-5-6-13(15)11-7-9-12(14)10-8-11/h7-10H,2-6,14H2,1H3	-4.871
InChI=1S/C6H15N/c1-3-5-6-7-4-2/h7H,3-6H2,1-2H3	-0.441
InChI=1S/C11H12O3/c12-11(13)7-14-10-5-4-8-2-1-3-9(8)6-10/h4-6H,1-3,7H2,(H,12,13)	-2.198
InChI=1S/C16H16N6O5/c1-9-7-22(16(25)19-14(9)23)13-6-11(20-21-17)12(27-13)8-26-15(24)1h2-5,7,11-13H,6,8H2,1H3,(H,19,23,25)	-2.72

"InChi"	"logS(M)"
InChI=1S/C12H11NO2/c14-11-5-1-9(2-6-11)13-10-3-7-12(15)8-4-10/h1-8,13-15H	-2.061
InChI=1S/C14H16Cl6O5/c1-8-4-2-3-5-10(8)23-6-9(25-12(22)14(18,19)20)7-24-11(21)13(15,16)h2-5,9,11-12,21-22H,6-7H2,1H3	-5.257
InChI=1S/C6H10O4/c1-2-3-4(5(7)8)6(9)10/h4H,2-3H2,1H3,(H,7,8)(H,9,10)	0.68
InChI=1S/C11H15ClN2/c1-13-7-8-14(2)11(13)9-3-5-10(12)6-4-9/h3-6,11H,7-8H2,1-2H3	-0.935
InChI=1S/C16H14N2O3/c19-11-18-14(20)16(17-15(18)21,12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10,19H,11H2,(H,17,21)	-3.3
InChI=1S/C8H14O2/c1-7(2,9)5-6-8(3,4)10/h9-10H,1-4H3	-0.93
InChI=1S/C11H22O2S/c1-10(2)6-4-3-5-8-13-11(12)7-9-14/h10,14H,3-9H2,1-2H3	-4.454
InChI=1S/C14H13N/c1-2-15-13-9-5-3-7-11(13)12-8-4-6-10-14(12)15/h3-10H,2H2,1H3	-6.814
InChI=1S/C7H4Cl2O3/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2,10H,(H,11,12)	-2.422
InChI=1S/C15H21NO4/c1-3-4-5-10-20-14-11-12(6-8-13(14)19-2)7-9-15(17)16-18/h6-9,11,18H,3-5,10H2,1-2H3,(H,16,17)/b9-7+	-3.662
InChI=1S/C7H4ClNS/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H	-2.733
InChI=1S/C6H8ClN3O2/c1-9-5(2-3-7)4-8-6(9)10(11)12/h4H,2-3H2,1H3	-2.44
InChI=1S/C7H6N4O/c1-11-6(12)3-9-5-2-8-4-10-7(5)11/h2-4H,1H3	-0.92
InChI=1S/C14H15ClO/c1-14(2)8-7-11(13(14)16)9-10-3-5-12(15)6-4-10/h3-6,9H,7-8H2,1-2H3/b11-9+	-5.672
InChI=1S/C19H20N2O3/c1-24-15-7-8-18-16(10-15)14(9-17(20)19(22)23)12-21(18)11-13-5-3-2h2-8,10,12,17H,9,11,20H2,1H3,(H,22,23)	-4.588
InChI=1S/C10H9NO5S3/c11-19(15,16)10-5-9(6-17-10)18(13,14)8-3-1-2-7(12)4-8/h1-6,12H,(H2,11,15,16)	-2.72
InChI=1S/C5H7NO4S2/c7-3(8)1-6-5(11)12-2-4(9)10/h1-2H2,(H,6,11)(H,7,8)(H,9,10)	-1.301
InChI=1S/C6H14O3/c1-3-5(7)9-6(8)4-2/h5-8H,3-4H2,1-2H3	0.872
InChI=1S/C16H13NO/c17-12-15(13-7-3-1-4-8-13)11-16(18)14-9-5-2-6-10-14/h1-10,15H,11H2	-3.591
InChI=1S/C13H10F2/c14-12-5-1-10(2-6-12)9-11-3-7-13(15)8-4-11/h1-8H,9H2	-6.912
InChI=1S/C10H12N6O5S3/c11-5-8(17)13-6-1-3-7(4-2-6)24(20,21)16-9-14-15-10(22-9)23(12,18)1h1-4H,5,11H2,(H,13,17)(H,14,16)(H2,12,18,19)	-1.19
InChI=1S/C12H5Cl5O/c13-6-1-2-11(9(16)3-6)18-12-5-8(15)7(14)4-10(12)17/h1-5H	-7.61
InChI=1S/C10H12O2/c1-2-12-10(11)8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3	-2.136

"InChi"	"logS(M)"
InChI=1S/C7H15ClFN2O2P/c8-2-5-11(6-3-9)14(12)10-4-1-7-13-14/h1-7H2,(H,10,12)	-1.549
InChI=1S/C21H32N2O/c1-7-22(8-2)16-19(24)23-20(3,4)14-18(15-21(23,5)6)17-12-10-9-11-1 h9-14H,7-8,15-16H2,1-6H3	-5.657
InChI=1S/C12H13N3O3S2/c16-15(17)11-2-1-10(20-11)12-13-9(8-19-12)7-14-3-5-18-6-4-14/h1-2,8H,3-7H2	-2.052
InChI=1S/C10H12O/c1-8(2)10-5-3-9(7-11)4-6-10/h3-8H,1-2H3	-2.785
InChI=1S/C10H9NO3S/c11-10-6-8(15(12,13)14)5-7-3-1-2-4-9(7)10/h1-6H,11H2,(H,12,13,14)	-2.34
InChI=1S/C11H11NS2/c1-2-4-10-8(3-1)9(7-12-10)11-13-5-6-14-11/h1-4,7,11-12H,5-6H2	-3.704
InChI=1S/C4H9NO4/c1-4(2-6,3-7)5(8)9/h6-7H,2-3H2,1H3	0.772
InChI=1S/C13H9Cl3N2O/c14-8-1-3-9(4-2-8)17-13(19)18-10-5-6-11(15)12(16)7-10/h1-7H,(H2,17,18,19)	-6.458
InChI=1S/C9H6ClNO2/c10-6-1-2-7-5(3-6)4-8(11-7)9(12)13/h1-4,11H,(H,12,13)	-2.832
InChI=1S/C9H12O3/c1-11-6-7-3-4-8(10)9(5-7)12-2/h3-5,10H,6H2,1-2H3	-1.893
InChI=1S/C25H22O10/c1-32-17-6-11(2-4-14(17)28)24-20(10-26)33-16-5-3-12(7-18(16)34-24 h2-9,20,23-29,31H,10H2,1H3	-3.795
InChI=1S/C11H14O3/c1-4-10(12)9-7-8(13-2)5-6-11(9)14-3/h5-7H,4H2,1-3H3	-2.604
InChI=1S/C11H12O3/c1-8(6-12)4-9-2-3-10-11(5-9)14-7-13-10/h2-3,5-6,8H,4,7H2,1H3	-2.313
InChI=1S/C3H6N4O4S3/c1-13(8,9)7-2-5-6-3(12-2)14(4,10)11/h1H3,(H,5,7)(H2,4,10,11)	-1.68
InChI=1S/C9H6N4/c10-6-9(7-11)13-12-8-4-2-1-3-5-8/h1-5,12H	-3.36
InChI=1S/C20H32N2O/c1-4-7-9-14-19(17-18-12-10-8-11-13-18)20(23)21-15-16-22(5-2)6-3/h8,10-13,17H,4-7,9,14-16H2,1-3H3,(H,21,23)/b19-17-	-5.333
InChI=1S/C13H18N2O/c1-9(14)13(16)15-12-7-6-10-4-2-3-5-11(10)8-12/h2-5,9,12H,6-8,14H2,1H3,(H,15,16)	-2.143
InChI=1S/C7H6N2O4/c10-7(8-11)5-1-3-6(4-2-5)9(12)13/h1-4,11H,(H,8,10)	-1.94
InChI=1S/C42H82O4S/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-37-45-41(43)35-39 h3-40H2,1-2H3	-8.232
InChI=1S/C5H8O2/c1-4(2)7-5(3)6/h1H2,2-3H3	-0.528
InChI=1S/C17H13NO5/c1-9(17(19)20)10-2-4-13-12(6-10)18-16(23-13)11-3-5-14-15(7-11)22-h2-7,9H,8H2,1H3,(H,19,20)	-3.976
InChI=1S/C17H20Cl6O4/c1-3-5-7-26-13(24)9-10(14(25)27-8-6-4-2)16(21)12(19)11(18)15(9,20 h9-10H,3-8H2,1-2H3	-7.51

"InChi"	"logS(M)"
InChI=1S/C21H11ClF6N2O3/c22-12-8-10(21(26,27)28)4-7-17(12)33-11-5-6-16(15(25)9-11)29-20(3h1-9H,(H2,29,30,31,32)	-8.09
InChI=1S/C10H7NO2/c11-8-5-9(12)10(13)7-4-2-1-3-6(7)8/h1-5H,11H2	-3.84
InChI=1S/C9H18N2O4/c1-6(2)9(3,4-14-7(10)12)5-15-8(11)13/h6H,4-5H2,1-3H3,(H2,10,12)(H2,11,13)	-1.57
InChI=1S/C18H25NO4/c1-19-13-5-6-14(19)10-16(9-13)23-18(21)17(11-20)12-3-7-15(22-2)8-h3-4,7-8,13-14,16-17,20H,5-6,9-11H2,1-2H3	-2.219
InChI=1S/C2H6N2O/c1-4(3)2-5/h2H,3H2,1H3	1.13
InChI=1S/C12H16O4/c1-2-12(15)9-3-5-11(6-4-9)16-8-10(14)7-13/h3-6,10,13-14H,2,7-8H2,1H3	-1.717
InChI=1S/C7H4Cl3NO3/c8-3-1-4(9)7(11-6(3)10)14-2-5(12)13/h1H,2H2,(H,12,13)	-2.766
InChI=1S/C16H11Cl2NO3/c1-8(16(20)21)9-2-3-14-13(6-9)19-15(22-14)10-4-11(17)7-12(18)5-10h2-8H,1H3,(H,20,21)	-5.206
InChI=1S/C30H53NO11/c1-3-4-9-31-29-7-5-28(6-8-29)30(32)42-27-26-41-25-24-40-23-22-39-h5-8,31H,3-4,9-27H2,1-2H3	-5.692
InChI=1S/C9H10O2/c1-7-3-5-8(6-4-7)9(10)11-2/h3-6H,1-2H3	-2.577
InChI=1S/C8H18O6/c1-5-7(3,11-9)13-14-8(4,6-2)12-10/h9-10H,5-6H2,1-4H3	-1.508
InChI=1S/C5H8O4/c1-3(5(8)9)2-4(6)7/h3H,2H2,1H3,(H,6,7)(H,8,9)	0.631
InChI=1S/C7H7Br/c1-6-4-2-3-5-7(6)8/h2-5H,1H3	-2.23
InChI=1S/C10H20N2O4/c1-4-10(7(2)3,5-15-8(11)13)6-16-9(12)14/h7H,4-6H2,1-3H3,(H2,11,13)(H2,12,14)	-2.09
InChI=1S/C18H24N2O2/c1-19-12-11-15-6-2-3-8-17(15)18(19)10-9-14-5-4-7-16(13-14)20(21)2h4-5,7,13,18H,2-3,6,8-12H2,1H3	-5.222
InChI=1S/C7H14O/c1-6-3-2-4-7(8)5-6/h6-8H,2-5H2,1H3	-1.28
InChI=1S/C9H8Cl4FNO2S2/c1-19(16,17)15(7-5-3-2-4-6-7)18-9(12,13)8(10,11)14/h2-6H,1H3	-5.149
InChI=1S/C10H11N3O2/c1-14-7-5-6-9(13-4-3-12-6)8(11)10(7)15-2/h3-5H,11H2,1-2H3	-1.71
InChI=1S/C18H34N2O6S/c1-5-6-10-7-11(20(3)8-10)17(25)19-12(9(2)21)16-14(23)13(22)15(24)h9-16,18,21-24H,5-8H2,1-4H3,(H,19,25)	-2.642
InChI=1S/C10H14/c1-8(2)10-6-4-5-9(3)7-10/h4-8H,1-3H3	-3.499
InChI=1S/C7H7FN2O4/c1-2-14-7(13)10-3-4(8)5(11)9-6(10)12/h3H,2H2,1H3,(H,9,11,12)	-1.47
InChI=1S/C8H16N2O3S2/c9-8(6-14-15(11,12)13)10-7-4-2-1-3-5-7/h7H,1-6H2,(H2,9,10)(H,11,12,13)	-2.182
InChI=1S/C11H13NO2/c13-9-8-12-11(14)7-6-10-4-2-1-3-5-10/h1-7,13H,8-9H2,(H,12,14)/b7-6+	-0.908
InChI=1S/C20H22N2O2/c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6-8-21-18-5-4-15(24-2)1h3-6,8,11,13-14,19H,1,7,9-10,12H2,2H3	-5.031
InChI=1S/C7H8O3/c8-4-5-3-6(9)1-2-7(5)10/h1-3,8-10H,4H2	0.853

"InChi"	"logS(M)"
InChI=1S/CHCl2F/c2-1(3)4/h1H	-0.738
InChI=1S/C10H19N2O4PS/c1-5-15-17(14,16-6-2)18-7-9(13)12-10(3,4)8-11/h5-7H2,1-4H3,(H,12,13)	-0.624
InChI=1S/C10H9NO5/c1-4-7(5(2)12)8(10(15)16)6(3-11-4)9(13)14/h3H,1-2H3,(H,13,14)(H,15,16)	-1.35
InChI=1S/C8H13NO3/c1-3-8(4-2)5-12-7(11)9-6(8)10/h3-5H2,1-2H3,(H,9,10,11)	-1.638
InChI=1S/C20H41O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-20-18-21/h2-20H2,1H3	-6.496
InChI=1S/C24H23BrF2O3/c1-23(2,19-11-13-21(14-12-19)30-24(25,26)27)17-28-16-18-7-6-10-22h3-15H,16-17H2,1-2H3	-9.98
InChI=1S/C14H19ClN2O2/c1-10-5-3-7-12(15)13(10)16-14(18)19-11-6-4-8-17(2)9-11/h3,5,7,11H,4,6,8-9H2,1-2H3,(H,16,18)	-3.646
InChI=1S/C12H4Cl6O/c13-5-1-3-6(4-2-5)19-12-10(17)8(15)7(14)9(16)11(12)18/h1-4H	-8.94
InChI=1S/C25H27ClN2O8/c1-13-17(10-22(32)27-19(11-29)23(33)24(34)21(31)12-30)18-9-16(36h3-9,11,19,21,23-24,30-31,33-34H,10,12H2,1-2H3,(H,27,32)	-4.906
InChI=1S/C27H33NO10S/c1-12(30)28-16-7-5-13-9-18(37-27-24(34)23(33)22(32)19(11-29)38-2'h6,8-10,16,19,22-24,27,29,32-34H,5,7,11H2,1-4H3,(H,28,30)	-3.63
InChI=1S/C12H4Cl6/c13-7-2-1-6(10(16)12(7)18)5-3-8(14)11(17)9(15)4-5/h1-4H	-9.1
InChI=1S/C20H28O2/c1-3-20-11-10-16-15-7-5-14(22-2)12-13(15)4-6-17(16)18(20)8-9-19(2h5,16-18H,3-4,6-12H2,1-2H3	-5.364
InChI=1S/C10H22O3/c1-2-3-4-5-7-12-9-10-13-8-6-11/h11H,2-10H2,1H3	-1.049
InChI=1S/C8H11NO/c1-5-4-9-6(2)8(5)7(3)10/h4,9H,1-3H3	-1.615
InChI=1S/C10H13ClO3/c1-10(13,6-12)7-14-9-5-3-2-4-8(9)11/h2-5,12-13H,6-7H2,1H3	-2.11
InChI=1S/C15H14O3/c1-11(15(16)17)12-6-5-9-14(10-12)18-13-7-3-2-4-8-13/h2-11H,1H3,(H,16,17)	-3.7
InChI=1S/C8H11BrN2O2/c1-4(2)11-7(12)6(9)5(3)10-8(11)13/h4H,1-3H3,(H,10,13)	-2.06
InChI=1S/C8H3Cl5O3/c9-3-4(10)6(12)8(7(13)5(3)11)16-1-2(14)15/h1H2,(H,14,15)	-3.75
InChI=1S/C2H6N2O2/c3-2(6)4-1-5/h5H,1H2,(H3,3,4,6)	-0.346
InChI=1S/C17H28O5/c1-5-18-14-11(3)13-7-6-10(2)12-8-9-16(4)20-15(19-14)17(12,13)22-2h10-15H,5-9H2,1-4H3	-4.8
InChI=1S/C10H15NO/c1-9(2)4-8(12)5-10(3,6-9)7-11/h4-6H2,1-3H3	-1.54
InChI=1S/C12H7Cl3/c13-9-6-7-10(14)12(15)11(9)8-4-2-1-3-5-8/h1-7H	-6.29

"InChi"	"logS(M)"
InChI=1S/C15H20O6/c1-7-3-9-14(5-16,11(19)10(7)18)13(2)4-8(17)12(21-9)15(13)6-20-15/h3,8-9,11-12,16-17,19H,4-6H2,1-2H3	-0.728
InChI=1S/C11H16O3/c1-2-9-5-3-4-6-11(9)14-8-10(13)7-12/h3-6,10,12-13H,2,7-8H2,1H3	-2.251
InChI=1S/C7H12ClN5/c1-4(2)10-7-12-5(8)11-6(9-3)13-7/h4H,1-3H3,(H2,9,10,11,12,13)	-2.89
InChI=1S/C7H12N4O2/c1-6-3-7(2,10-4(12)8-6)11-5(13)9-6/h3H2,1-2H3,(H2,8,10,12)(H2,9,11,13)	-2.09
InChI=1S/C8H14O4/c1-5-4-8(11-6(2)9)12-7(3)10-5/h5,7-8H,4H2,1-3H3	0.759
InChI=1S/C17H12F3NO3/c1-9(16(22)23)10-5-6-14-13(8-10)21-15(24-14)11-3-2-4-12(7-11)17(1h2-9H,1H3,(H,22,23)	-4.921
InChI=1S/C14H22N2O/c1-4-14(13(15)17,10-11-16(2)3)12-8-6-5-7-9-12/h5-9H,4,10-11H2,1-3H3,(H2,15,17)	-2.28
InChI=1S/C10H7NO3S2/c12-6-2-1-5(3-7(6)13)4-8-9(14)11-10(15)16-8/h1-4,12-13H,(H,11,14,15)/b8-4-	-3.34
InChI=1S/C29H56O4/c1-26(2)20-14-8-6-12-18-24-32-28(30)22-16-10-5-11-17-23-29(31)33-h26-27H,5-25H2,1-4H3	-6.972
InChI=1S/C10H16O2/c1-8(2)10-6-4-9(3,5-7-10)11-12-10/h4,6,8H,5,7H2,1-3H3	-3.267
InChI=1S/C10H13ClO3/c1-10(13,6-12)7-14-9-4-2-8(11)3-5-9/h2-5,12-13H,6-7H2,1H3	-2.11
InChI=1S/C30H33N5/c1-31-28-17-19-32-29(33-28)35-23-21-34(22-24-35)20-18-30(25-11-5h2-17,19H,18,20-24H2,1H3,(H,31,32,33)	-6.411
InChI=1S/C16H16N2O2/c1-18(2)13-9-7-12(8-10-13)11-17-15-6-4-3-5-14(15)16(19)20/h3-11H,1-2H3,(H,19,20)/b17-11+	-3.649
InChI=1S/C19H25N5O4/c1-26-15-10-12-13(11-16(15)27-2)21-19(22-17(12)20)24-7-5-23(6-8-2h10-11,14H,3-9H2,1-2H3,(H2,20,21,22)	-1.8
InChI=1S/C8H9ClNO6P/c1-14-17(13,15-2)16-8-4-3-6(10(11)12)5-7(8)9/h3-5H,1-2H3	-3.207
InChI=1S/C11H14ClNO2/c1-3-8(2)15-11(14)13-10-6-4-5-9(12)7-10/h4-8H,3H2,1-2H3,(H,13,14)	-3.173
InChI=1S/C13H21N3O2/c1-9-11(14(2)3)12(17)15(4)13(18)16(9)10-7-5-6-8-10/h10H,5-8H2,1-4H3	-2.651
InChI=1S/C13H21N3O/c1-5-16(6-2)15-13(17)14-12-10(3)8-7-9-11(12)4/h7-9H,5-6H2,1-4H3,(H2,14,15,17)	-1.09
InChI=1S/C11H13N5O2/c12-11-14-9-8(10(18)15-11)13-5-16(9)7-2-1-6(3-7)4-17/h1-2,5-7,17H,3-4H2,(H3,12,14,15,18)	-2.3
InChI=1S/C13H19NO2/c1-3-4-7-16-12-6-5-11(8-10(12)2)9-13(14)15/h5-6,8H,3-4,7,9H2,1-2H3,(H2,14,15)	-5.481

"InChi"	"logS(M)"
InChI=1S/C15H24/c1-10-11-6-7-12-13(11)14(2,3)8-5-9-15(10,12)4/h11-13H,1,5-9H2,2-4H3	-4.413
InChI=1S/C18H24O5/c1-22-16-11-17(23-2)14(15(19)8-9-18(20)21)10-13(16)12-6-4-3-5-7-12h10-12H,3-9H2,1-2H3,(H,20,21)	-4.897
InChI=1S/C4H7N3OS/c1-2-8-4-6-3(5)9-7-4/h2H2,1H3,(H2,5,6,7)	-0.651
InChI=1S/C28H58O/c1-3-5-7-9-11-13-15-16-18-20-22-24-26-28(27-29)25-23-21-19-17-14-h28-29H,3-27H2,1-2H3	-5.614
InChI=1S/C8H11NO/c9-6-7-10-8-4-2-1-3-5-8/h1-5H,6-7,9H2	-0.129
InChI=1S/C14H19NO2/c1-11(16)14(6-8-15(2)9-7-14)12-4-3-5-13(17)10-12/h3-5,10,17H,6-9H2,1-2H3	-1.172
InChI=1S/C6H9ClN2O4/c7-2-5(11)9-3(6(12)13)1-4(8)10/h3H,1-2H2,(H2,8,10)(H,9,11)(H,12,13)	-0.319
InChI=1S/C18H34O6/c1-5-15(6-2)17(19)23-13-11-21-9-10-22-12-14-24-18(20)16(7-3)8-4/h15-16H,5-14H2,1-4H3	-3.239
InChI=1S/C23H29N3O/c27-19-18-25-16-14-24(15-17-25)12-5-13-26-22-8-3-1-6-20(22)10-11-h1-4,6-11,27H,5,12-19H2	-3.574
InChI=1S/C16H21NO5/c1-5-17(6-2)15(19)11(3)21-16(20)13-9-7-8-10-14(13)22-12(4)18/h7-11H,5-6H2,1-4H3	-1.6
InChI=1S/C8H7ClO3/c1-12-8(11)5-2-3-7(10)6(9)4-5/h2-4,10H,1H3	-2.873
InChI=1S/C10H16O/c1-5-10(4,11)8-6-7-9(2)3/h1,7,11H,6,8H2,2-4H3	-1.772
InChI=1S/C2H6N4S2/c3-1(7)5-6-2(4)8/h(H3,3,5,7)(H3,4,6,8)	-1.796
InChI=1S/C11H16O3/c1-9-3-5-10(6-4-9)14-8-11(2,13)7-12/h3-6,12-13H,7-8H2,1-2H3	-1.88
InChI=1S/C7H7N3O/c8-4-1-2-5-6(3-4)10-7(11)9-5/h1-3H,8H2,(H2,9,10,11)	-2.335
InChI=1S/C12H20O/c1-4-11(2)7-5-8-12(3)9-6-10-13/h4,8,10-11H,1,5-7,9H2,2-3H3/b12-8-	-3.794
InChI=1S/C4H10N4O2/c5-3(9)7-1-2-8-4(6)10/h1-2H2,(H3,5,7,9)(H3,6,8,10)	0.574
InChI=1S/C14H11ClN2O/c1-18-9-3-5-12-11(7-9)14(16)10-4-2-8(15)6-13(10)17-12/h2-7H,1H3,(H2,16,17)	-4.867
InChI=1S/C17H14O/c1-12(11-18)14-8-9-17-15(10-14)7-6-13-4-2-3-5-16(13)17/h2-12H,1H3	-5.701
InChI=1S/C6H13N/c1-2-4-6-7-5-3-1/h7H,1-6H2	-0.49
InChI=1S/C11H11ClN2O2/c1-6(2)10(15)14-11-13-8-5-7(12)3-4-9(8)16-11/h3-6H,1-2H3,(H,13,14,15)	-3.5
InChI=1S/C16H17ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)20)11-5-3-2-4-6-11/h5,7-9H,2-4,6,10H2,1H3	-4.039
InChI=1S/C16H18O4/c1-11(16(18)20-8-7-17)12-3-4-14-10-15(19-2)6-5-13(14)9-12/h3-6,9-11,17H,7-8H2,1-2H3	-3.33

"InChi"	"logS(M)"
InChI=1S/C5H13NO/c1-5(7)4-6(2)3/h5,7H,4H2,1-3H3	0.793
InChI=1S/C15H10O4/ c16-10-3-1-9(2-4-10)14-8-13(18)12-6-5-11(17)7-15(12)19-14/ h1-8,16-17H	-2.651
InChI=1S/C21H19ClN2O5/ c1-13(21(25)29-20-3-2-10-26-20)27-15-5-7-16(8-6-15)28-19-12-23-18 h4-9,11-13,20H,2-3,10H2,1H3	-5.02
InChI=1S/C29H44O2/ c1-26(2,3)20-14-18(15-21(24(20)30)27(4,5)6)13-19-16-22(28(7,8)9)25 h14-17,30-31H,13H2,1-12H3	-8.628
InChI=1S/C10H20N2O/c1-5-10(13)12-8(2)6-11(4)7-9(12)3/h8-9H, 5-7H2,1-4H3	-0.909
InChI=1S/C9H10O3/c1-6-3-8(11)9(12-2)4-7(6)5-10/h3-5,11H,1-2H3	-2.744
InChI=1S/C16H16O3S/ c1-18-13-8-6-12(7-9-13)16(17)11-20-15-5-3-4-14(10-15)19-2/ h3-10H,11H2,1-2H3	-5.285
InChI=1S/C6H12O/c1-3-5-6(7)4-2/h3,5-7H,4H2,1-2H3/b5-3+	-0.42
InChI=1S/C8H8Cl2O5S/c9-6-1-2-8(7(10)5-6)14-3-4-15-16(11,12)13/ h1-2,5H,3-4H2,(H,11,12,13)	-0.06
InChI=1S/C7H6N4O/c1-11-4-5-6(10-7(11)12)9-3-2-8-5/h2-4H,1H3	-0.909
InChI=1S/C10H12N2O3/c1-6-3-2-4-8-11-5-7(10(14)15)9(13)12(6)8/ h5-6H,2-4H2,1H3,(H,14,15)	-1.606
InChI=1S/C10H14O/c1-3-10(2,11)9-7-5-4-6-8-9/h4-8,11H, 3H2,1-2H3	-1.869
InChI=1S/C10H12N2/c1-2-5-10-11-8-6-3-4-7-9(8)12-10/h3-4,6-7H, 2,5H2,1H3,(H,11,12)	-2.731
InChI=1S/C9H12FN3O3/ c10-5-3-8(16-6(5)4-14)13-2-1-7(11)12-9(13)15/h1-2,5-6,8,14H, 3-4H2,(H2,11,12,15)	-1.18
InChI=1S/C17H22N2O4/ c1-6-7-18-9-13(20)19(16(18)22)10-23-15(21)14-12(8-11(2)3)17(14,4) h1,8,12,14H,7,9-10H2,2-5H3	-3.532
InChI=1S/C25H30N2O4/ c1-5-20(26(10-22-14-28-22)11-23-15-29-23)6-2-18(1)9-19-3-7-21(8-4 h1-8,22-25H,9-17H2	-4.662
InChI=1S/C10H15NO/c1-3-11(4-2)9-6-5-7-10(12)8-9/h5-8,12H, 3-4H2,1-2H3	-2.011
InChI=1S/C22H18O11/ c23-10-5-12(24)11-7-18(33-22(31)9-3-15(27)20(30)16(28)4-9)21(32-1 h1-6,18,21,23-30H,7H2	-1.059
InChI=1S/C11H16N2O/c1-3-13(4-2)11(14)12-10-8-6-5-7-9-10/ h5-9H,3-4H2,1-2H3,(H,12,14)	-2.624
InChI=1S/C17H23NO6S/ c1-13(2)24-16(19)17(11-5-3-4-6-12-17)25(22,23)15-9-7-14(8-10-15)1 h7-10,13H,3-6,11-12H2,1-2H3	-5.071
InChI=1S/C9H9ClO3/c1-6(9(11)12)13-8-4-2-7(10)3-5-8/h2-6H,1H3, (H,11,12)	-2.135
InChI=1S/C10H9N5O/c1-7-2-3-13-10(14-7)15-9(16)8-6-11-4-5-12-8/ h2-6H,1H3,(H,13,14,15,16)	-0.731
InChI=1S/C10H13NO4/c1-13-7-4-6(10(11)12)5-8(14-2)9(7)15-3/ h4-5H,1-3H3,(H2,11,12)	-0.954

"InChi"	"logS(M)"
InChI=1S/C14H17N3O2/c1-10-12(15(2)3)13(18)16(4)14(19)17(10)11-8-6-5-7-9-11/h5-9H,1-4H3	-1.877
InChI=1S/C15H10O7/c16-7-4-10(19)12-11(5-7)22-15(14(21)13(12)20)6-1-2-8(17)9(18)3-6/h1-5,16-19,21H	-1.99
InChI=1S/C31H32N4O2/c1-2-29(36)35-28-16-10-9-15-27(28)34(30(35)37)26-17-20-33(21-18-2 h3-16,26H,2,17-22H2,1H3	-6.73
InChI=1S/C21H27NO4/c1-22-9-8-15-12-20(25-4)21(26-5)13-16(15)17(22)10-14-6-7-18(23-2)h6-7,11-13,17H,8-10H2,1-5H3	-3.68
InChI=1S/C8H8O4/c1-4-6(9)3-2-5(7(4)10)8(11)12/h2-3,9-10H,1H3,(H,11,12)	-1.823
InChI=1S/C6H10O3/c1-3-6(8)9-4-5(2)7/h3,5,7H,1,4H2,2H3	0.886
InChI=1S/C18H36N4O11/c19-2-6-10(25)12(27)13(28)18(30-6)33-16-5(21)1-4(20)15(14(16)29)3 h4-18,23-29H,1-3,19-22H2	0.315
InChI=1S/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/b3-2+	0.038
InChI=1S/C10H12N2/c11-6-5-8-7-12-10-4-2-1-3-9(8)10/h1-4,7,12H,5-6,11H2	-3.3
InChI=1S/C13H16N2O4/c1-8(16)15-12(13(14)18)7-10-3-5-11(6-4-10)19-9(2)17/h3-6,12H,7H2,1-2H3,(H2,14,18)(H,15,16)	-1.9
InChI=1S/C10H18O4/c1(3-11-5-9-7-13-9)2-4-12-6-10-8-14-10/h9-10H,1-8H2	-0.561
InChI=1S/C11H16O/c1-3-4-5-6-10-9(2)7-8-11(10)12/h4-5H,3,6-8H2,1-2H3/b5-4+	-2.045
InChI=1S/C11H10O4/c1-8(12)15-10-5-3-2-4-9(10)6-7-11(13)14/h2-7H,1H3,(H,13,14)/b7-6+	-3.156
InChI=1S/C14H19NO3/c1-4-15(5-2)13(16)11(3)18-14(17)12-9-7-6-8-10-12/h6-11H,4-5H2,1-3H3	-2.28
InChI=1S/C19H25NO4/c1-13(9-14-3-6-17(24-2)7-4-14)20-11-19(23)15-5-8-18(22)16(10-15)1h3-8,10,13,19-23H,9,11-12H2,1-2H3	-1.522
InChI=1S/C10H13NO4S/c1-7(2)15-10(12)8-5-3-4-6-9(8)16(11,13)14/h3-7H,1-2H3,(H2,11,13,14)	-2.396
InChI=1S/C9H6O5S/c10-7-5-3-1-2-4-6(5)8(11)9(7)15(12,13)14/h1-4,10H,(H,12,13,14)	-2.23
InChI=1S/C9H9NO3/c1-6(11)13-8-5-3-2-4-7(8)9(10)12/h2-5H,1H3,(H2,10,12)	-0.167
InChI=1S/C7H6N4S/c1-12-6-3-9-7-5(11-6)2-8-4-10-7/h2-4H,1H3	-1.55
InChI=1S/C6H9ClO3/c1-3-10-6(9)5(7)4(2)8/h5H,3H2,1-2H3	-0.986
InChI=1S/C9H8O4/c1-5(10)6-2-3-8(11)7(4-6)9(12)13/h2-4,11H,1H3,(H,12,13)/p-1	-2.23
InChI=1S/C12H11N3O4S/c1-9-2-7-12(13-8-9)14-20(18,19)11-5-3-10(4-6-11)15(16)17/h2-8H,1H3,(H,13,14)	-4.29

"InChi"	"logS(M)"
InChI=1S/C21H26N2O7/c1-12(2)30-21(25)18-14(4)22-13(3)17(20(24)29-10-9-28-5)19(18)15-7h6-8,11-12,19,22H,9-10H2,1-5H3	-4.237
InChI=1S/C9H10O4/c10-7(8(11)9(12)13)6-4-2-1-3-5-6/h1-5,7-8,10-11H,(H,12,13)	-0.306
InChI=1S/C12H13N3O4S2/c13-9-1-5-12(6-2-9)21(18,19)15-10-3-7-11(8-4-10)20(14,16)17/h1-8,15H,13H2,(H2,14,16,17)	-2.759
InChI=1S/C6H13NO4/c8-3-1-7(2-4-9)6(11)5-10/h8-10H,1-5H2	0.787
InChI=1S/C10H9NO3/c12-9(6-7-10(13)14)11-8-4-2-1-3-5-8/h1-7H,(H,11,12)(H,13,14)/b7-6+	-2.281
InChI=1S/C11H11N3O2/c1-14-7-5-3-2-4-6(7)8(10(12)15)9(14)11(13)16/h2-5H,1H3,(H2,12,15)(H2,13,16)	-1.818
InChI=1S/C7H10N2O2S/c8-5-6-1-3-7(4-2-6)12(9,10)11/h1-4H,5,8H2,(H2,9,10,11)	0.321
InChI=1S/C13H10N2/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H,(H,14,15)	-3.385
InChI=1S/C14H11Cl4O4P/c1-2-20-23(19,21-13-5-3-9(15)7-11(13)17)22-14-6-4-10(16)8-12(14)1h3-8H,2H2,1H3	-5.774
InChI=1S/C6H6O3/c1-4-2-3-5(9-4)6(7)8/h2-3H,1H3,(H,7,8)	-0.824
InChI=1S/C8H10O2/c1-9-7-5-3-4-6-8(7)10-2/h3-6H,1-2H3	-1.315
InChI=1S/C13H14/c1-9-4-5-12-7-10(2)11(3)8-13(12)6-9/h4-8H,1-3H3	-5.001
InChI=1S/C17H27N3O4S/c1-4-20-8-6-7-12(20)11-19-17(21)13-9-16(25(22,23)5-2)14(18)10-15(h9-10,12H,4-8,11,18H2,1-3H3,(H,19,21)	-2.833
InChI=1S/C16H18N4O2/c1-4-17-16(18-5-1)20-8-6-19(7-9-20)11-13-2-3-14-15(10-13)22-12-21h1-5,10H,6-9,11-12H2	-2.313
InChI=1S/C8H9NO2/c1-11-8(10)6-4-2-3-5-7(6)9/h2-5H,9H2,1H3	-1.734
InChI=1S/C7H15Cl2N/c1-7(2)10(5-3-8)6-4-9/h7H,3-6H2,1-2H3	-1.618
InChI=1S/C18H29NO3/c1-12(2)15-9-8-14(5)16(18(20)22-13(3)4)17(15)21-11-10-19(6)7/h8-9,12-13H,10-11H2,1-7H3	-4.292
InChI=1S/C6H10N4O/c1-3-7-5-8-4(2)9-6(11)10-5/h3H2,1-2H3,(H2,7,8,9,10,11)	-1.388
InChI=1S/C9H10O/c10-9-6-5-7-3-1-2-4-8(7)9/h1-4,9-10H,5-6H2	-1.317
InChI=1S/C14H19N/c1-10-8-12(14(3,4)5)9-11(2)13(10)6-7-15/h8-9H,6H2,1-5H3	-4.702
InChI=1S/C12H6Cl4/c13-7-4-5-8(11(15)6-7)9-2-1-3-10(14)12(9)16/h1-6H	-6.681
InChI=1S/C20H26N2O/c23-15-14-22(13-12-17-6-2-1-3-7-17)16-19-11-10-18-8-4-5-9-20(18)21h1-9,19,21,23H,10-16H2	-3.168
InChI=1S/C8H5NO2/c9-8(11)6-4-2-1-3-5-7-10/h10H,7H2,(H2,9,11)	-0.097
InChI=1S/C23H15Cl2N3O2/c24-15-10-11-19(25)20(13-15)27-28-21-17-9-5-4-6-14(17)12-18(22(2h1-13,27H,(H,26,30)/b28-21-	-7.907

"InChi"	"logS(M)"
InChI=1S/C12H6O2/c13-11-8-5-1-3-7-4-2-6-9(10(7)8)12(11)14/h1-6H	-3.306
InChI=1S/C20H26N2O/c1-20(19(21)23,12-15-22-13-5-2-6-14-22)18-11-7-9-16-8-3-4-10-17(1h3-4,7-11H,2,5-6,12-15H2,1H3,(H2,21,23)	-4.582
InChI=1S/C14H9Cl2NO5/c1-21-14(18)10-7-9(3-4-12(10)17(19)20)22-13-5-2-8(15)6-11(13)16/h2-7H,1H3	-5.934
InChI=1S/C2H5NO3/c4-2-1-3(5)6/h4H,1-2H2	1.041
InChI=1S/C11H8N4O/c1-8(16)9-2-4-10(5-3-9)14-15-11(6-12)7-13/h2-5,14H,1H3	-2.71
InChI=1S/C22H42O4/c1-3-5-7-15-19-25-21(23)17-13-11-9-10-12-14-18-22(24)26-20-16-8-(h3-20H2,1-2H3	-4.57
InChI=1S/C16H14N2O3/c19-15(20)11-21-16-13-8-4-5-9-14(13)18(17-16)10-12-6-2-1-3-7-12/h1-9H,10-11H2,(H,19,20)	-3.934
InChI=1S/C8H14O6/c1-7(13,5(9)10)3-4-8(2,14)6(11)12/h13-14H,3-4H2,1-2H3,(H,9,10)(H,11,12)	-0.837
InChI=1S/C7H4ClNOS/c8-4-1-2-6-5(3-4)7(10)9-11-6/h1-3H,(H,9,10)	-1.65
InChI=1S/C16H13ClN2O2/c1-18-13-8-7-11(17)9-14(13)19(16(21)10-15(18)20)12-5-3-2-4-6-12/h2-9H,10H2,1H3	-3.204
InChI=1S/C11H11NO6/c1-6(2)18-11(15)9-7(10(13)14)4-3-5-8(9)12(16)17/h3-6H,1-2H3,(H,13,14)/p-1	-2.49
InChI=1S/C8H16N6/c1-9-6-10-7(13(2)3)12-8(11-6)14(4)5/h1-5H3,(H,9,10,11,12)	-2.196
InChI=1S/C22H24N2O8/c1-21(31)8-5-4-6-11(25)12(8)16(26)13-9(21)7-10-15(24(2)3)17(27)14h4-6,9-10,15,25-26,30-32H,7,23H2,1-3H3/b20-14-	-3.284
InChI=1S/C24H32O5/c1-22-9-7-15(25)11-14(22)4-5-17-16(22)8-10-23(2)19(13-3-6-18(26)2h3,6,12,14-17,19-21,25,27H,4-5,7-11H2,1-2H3	-4.469
InChI=1S/C8H9NO2/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H,9H2,(H,10,11)	-1.508
InChI=1S/C11H22N2O4/c1-7(2)11(8(3)4,5-16-9(12)14)6-17-10(13)15/h7-8H,5-6H2,1-4H3,(H2,12,14)(H2,13,15)	-2.549
InChI=1S/C15H13ClFN5O5S/c1-3-27-15-18-10(17)7-11-19-14(20-22(11)15)28(24,25)21-12-8(13(2h4-7,21H,3H2,1-2H3	-4.429
InChI=1S/C7H15NO3/c1-2-3-4-10-5-6-11-7(8)9/h2-6H2,1H3,(H2,8,9)	-0.508
InChI=1S/C9H11N/c10-9-6-8(9)7-4-2-1-3-5-7/h1-5,8-9H,6,10H2	-0.438
InChI=1S/C12H7Cl3/c13-9-4-1-3-8(7-9)12-10(14)5-2-6-11(12)15/h1-7H	-6.824
InChI=1S/C13H9ClN2O3/c14-12-7-9(3-6-11(12)13(18)19)16-15-8-1-4-10(17)5-2-8/h1-7,17H,(H,18,19)/b16-15+	-2.62

"InChi"	"logS(M)"
InChI=1S/C14H11FN2O5/c1-9(18)22-8-16-7-11(15)13(20)17(14(16)21)12(19)10-5-3-2-4-6-10/h2-7H,8H2,1H3	-3.34
InChI=1S/C7H9NO/c1-9-7-5-3-2-4-6(7)8/h2-5H,8H2,1H3	-0.944
InChI=1S/C9H10O3/c1-7-3-2-4-8(5-7)12-6-9(10)11/h2-5H,6H2,1H3,(H,10,11)	-1.539
InChI=1S/C40H76O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-37-43-39(41)35-36-h35-36H,3-34,37-38H2,1-2H3/b36-35+	-7.094
InChI=1S/C17H14N2O2/c1-21-16-9-5-4-8-14(16)18-19-17-13-7-3-2-6-12(13)10-11-15(17)20/h2-11,18H,1H3/b19-17-	-8.926
InChI=1S/C14H10O4/c15-13(11-7-3-1-4-8-11)17-18-14(16)12-9-5-2-6-10-12/h1-10H	-4.425
InChI=1S/C10H13N3O2/c1-2-3-9(14)12-13-10(15)8-4-6-11-7-5-8/h4-7H,2-3H2,1H3,(H,12,14)(H,13,15)	-0.32
InChI=1S/C6H2BrF3/c7-3-1-4(8)6(10)5(9)2-3/h1-2H	-3.21
InChI=1S/C6H15O4PS3/c1-4-14(7,8)6-5-13-11(12,9-2)10-3/h4-6H2,1-3H3	-2.542
InChI=1S/C13H17N3O/c1-15-11-2-3-12(15)9-16(8-11)13(17)10-4-6-14-7-5-10/h4-7,11-12H,2-3,8-9H2,1H3	-2.083
InChI=1S/C13H17NO6/c15-7-13(8-16,9-17)14-11(18)6-20-12(19)10-4-2-1-3-5-10/h1-5,15-17H,6-9H2,(H,14,18)	-1.27
InChI=1S/C21H20/c1-17-9-8-14-20(15-18-10-4-2-5-11-18)21(17)16-19-12-6-3-7-13-19/h2-14H,15-16H2,1H3	-7.18
InChI=1S/C9H8O2/c10-7-9(11)6-8-4-2-1-3-5-8/h1-5,7H,6H2	-2.171
InChI=1S/C10H10O4/c1-7(11)13-9-4-3-5-10(6-9)14-8(2)12/h3-6H,1-2H3	-2.213
InChI=1S/C7H17NO/c1-4-8(5-2)6-7(3)9/h7,9H,4-6H2,1-3H3	0.102
InChI=1S/C6H8N2O4S2/c7-13(9,10)5-1-2-6(4-3-5)14(8,11)12/h1-4H,(H2,7,9,10)(H2,8,11,12)	-2.528
InChI=1S/C10H14Br2N2O2S/c11-5-7-14(8-6-12)9-1-3-10(4-2-9)17(13,15)16/h1-4H,5-8H2,(H2,13,15,16)	-3.908
InChI=1S/C12H10ClNO2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H,14H2	-4.127
InChI=1S/C7H14N2O3/c1-4(2)6(7(11)12)9-5(10)3-8/h4,6H,3,8H2,1-2H3,(H,9,10)(H,11,12)	0.458
InChI=1S/C10H11N3O/c11-10(12-14)7-13-6-5-8-3-1-2-4-9(8)13/h1-6,14H,7H2,(H2,11,12)	-1.444
InChI=1S/C9H9ClO4S/c1-14-9(11)6-15(12,13)8-4-2-7(10)3-5-8/h2-5H,6H2,1H3	-2.38
InChI=1S/C22H14/c1-3-7-19-15(5-1)9-11-17-13-18-12-10-16-6-2-4-8-20(16)22(18)14-21h1-14H	-8.432
InChI=1S/C10H20ClF/c11-9-7-5-3-1-2-4-6-8-10-12/h1-10H2	-5.272

"InChi"	"logS(M)"
InChI=1S/C8H11ClN4O4/c9-3-4-13(12-17)8(16)10-5-1-2-6(14)11-7(5)15/h5H,1-4H2,(H,10,16)(H,11,14,15)	-1.432
InChI=1S/C36H32N10O8/c1-19(47)31(33(49)37-21-11-13-23-27(17-21)41-35(51)39-23)45-43-2h3-14,17-18,31-32H,15-16H2,1-2H3,(H,37,49)(H,38,50)(H2,39,41,51)(H2,40,42,52)/b45-43+,46-44+	-7.634
InChI=1S/C10H14O6/c1-7(11)5-9(13)15-3-4-16-10(14)6-8(2)12/h3-6H2,1-2H3	-0.034
InChI=1S/C11H15NO3/c13-10-6-3-5-9-12(10)8-4-1-2-7-11(14)15/h3,5-6,9H,1-2,4,7-8H2,(H,14,15)	-0.64
InChI=1S/C12H20N2/c1-9(2)12-6-4-11(5-7-12)8-10(3)14-13/h4-7,9-10,14H,8,13H2,1-3H3	-2.966
InChI=1S/C14H20N2O3/c1-3-9-7-5-6-8-10(9)14(4-2)11(17)15-13(19)16-12(14)18/h3-8H2,1-2H3,(H2,15,16,17,18,19)	-3.53
InChI=1S/C8H6ClNO3/c1-12-6-3-7-5(2-4(6)9)10-8(11)13-7/h2-3H,1H3,(H,10,11)	-2.085
InChI=1S/C10H21NO3/c1-5-6-10(2,7-12)8-14-9(13)11(3)4/h12H,5-8H2,1-4H3	-2.165
InChI=1S/C12H18O4/c1-3-11(13)15-9-7-5-6-8-10-16-12(14)4-2/h3-4H,1-2,5-10H2	-2.819
InChI=1S/C13H19NO3/c1-3-4-7-17-12-6-5-11(8-10(12)2)9-13(15)14-16/h5-6,8,16H,3-4,7,9H2,1-2H3,(H,14,15)	-3.085
InChI=1S/C19H14ClF5N4O2/c20-14-7-6-13(8-12(14)9-31-10-18(21,22)19(23,24)25)29-17(11-4-2-1h1-8H,9-10H2,(H2,26,30)	-5.663
InChI=1S/C15H21NO/c1-13(12-16-10-6-3-7-11-16)15(17)14-8-4-2-5-9-14/h2,4-5,8-9,13H,3,6-7,10-12H2,1H3	-2.878
InChI=1S/C12H11I3N2O4/c1-4(18)16-10-7(13)6(12(20)21)8(14)11(9(10)15)17(3)5(2)19/h1-3H3,(H,16,18)(H,20,21)	-5.158
InChI=1S/C10H18O/c1-10(2,3)8-4-6-9(11)7-5-8/h8H,4-7H2,1-3H3	-2.417
InChI=1S/C15H18/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h5-10H,1-4H3	-5.475
InChI=1S/C6H10O2/c1-6(2)3-5(7)8-4-6/h3-4H2,1-2H3	-0.517
InChI=1S/C20H34O4/c1-17(2,3)21-23-19(7,8)15-11-13-16(14-12-15)20(9,10)24-22-18(4,5)h11-14H,1-10H3	-5.737
InChI=1S/C8H7Cl3O2/c1-12-5-3-4(9)6(10)7(11)8(5)13-2/h3H,1-2H3	-4.37
InChI=1S/C6H11O4P/c1-2-6-3-8-11(7,9-4-6)10-5-6/h2-5H2,1H3	0.425
InChI=1S/C12H8Cl6O/c13-8-5-3(2-19)1-4-6(5)9(14,12(8,17)18)11(16)7(4)10(8,11)15/h2-7H,1H2	-7.201
InChI=1S/C7H15NO2/c1-4-7(3,5-2)10-6(8)9/h4-5H2,1-3H3,(H2,8,9)	-1.56
InChI=1S/C40H78O5/c1-36(2)31-27-23-19-15-11-7-5-9-13-17-21-25-29-33-44-39(42)35-38h36-38,41H,5-35H2,1-4H3	-7.993

"InChi"	"logS(M)"
InChI=1S/C27H58N4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-29-24-19-26-31-27-2h9-10,29-31H,2-8,11-28H2,1H3/b10-9+	-3.836
InChI=1S/C4H8FI/c5-3-1-2-4-6/h1-4H2	-3.241
InChI=1S/C11H9NO3/c1-15-11-7-6-10(12(13)14)8-4-2-3-5-9(8)11/h2-7H,1H3	-4.36
InChI=1S/C12H20O2/c1-9(13)14-12-7-6-10-4-2-3-5-11(10)8-12/h10-12H,2-8H2,1H3	-3.561
InChI=1S/C17H15ClFNO3/c1-11(17(22)23-2)20(13-8-9-15(19)14(18)10-13)16(21)12-6-4-3-5-7-1h3-11H,1-2H3	-3.982
InChI=1S/C13H24O4S2/c1-3-5-7-16-12(14)9-18-11-19-10-13(15)17-8-6-4-2/h3-11H2,1-2H3	-4.343
InChI=1S/C4H8N2S/c7-4-5-2-1-3-6-4/h1-3H2,(H2,5,6,7)	0.229
InChI=1S/C17H18O4/c1-11(18)10-21-17(19)12(2)13-4-5-15-9-16(20-3)7-6-14(15)8-13/h4-9,12H,10H2,1-3H3	-4.65
InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)	1.129
InChI=1S/C10H15N5O2/c11-10-12-3-8-9(14-10)15(6-13-8)2-1-7(4-16)5-17/h3,6-7,16-17H,1-2,4-5H2,(H2,11,12,14)	-0.3
InChI=1S/C21H24ClNO2/c22-19-10-8-18(9-11-19)21(25)12-15-23(16-13-21)14-4-7-20(24)17-5-h1-3,5-6,8-11,25H,4,7,12-16H2	-3.35
InChI=1S/C8H4N2S/c9-5-7-2-1-3-8(4-7)10-6-11/h1-4H	-3.19
InChI=1S/C10H25N3/c1-12(2)9-5-7-11-8-6-10-13(3)4/h11H,5-10H2,1-4H3	0.356
InChI=1S/C21H15NO6S/c1-29(26,27)28-13-8-6-12(7-9-13)22-16-10-11-17(23)19-18(16)20(24)h2-11,22-23H,1H3	-6.214
InChI=1S/C48H26N6O4/c55-45-37-23-19-33-35-21-25-39-44-40(48(58)54(47(39)57)32-17-13-h1-26H/b51-49+,52-50+	-7.876
InChI=1S/C42H72N2O5/c1-18-19-20-42(34(46)48-29-24-38(8,9)43(16)39(10,11)25-29,35(47)4h21-22,29-30,45H,18-20,23-27H2,1-17H3	-5.836
InChI=1S/C14H14O6/c15-13(19-7-11-5-17-11)9-1-2-10(4-3-9)14(16)20-8-12-6-18-12/h1-4,11-12H,5-8H2	-3.558
InChI=1S/C16H28O/c1-14(2)8-5-9-15(3)12(14)6-10-16(4)13(15)7-11-17-16/h12-13H,5-11H2,1-4H3	-5.099
InChI=1S/C8H9ClNO5PS/c1-13-16(17,14-2)15-6-3-4-8(10(11)12)7(9)5-6/h3-5H,1-2H3	-3.872
InChI=1S/C18H34O6S/c1-2-3-4-11-14-17(24-25(21,22)23)15-12-9-7-5-6-8-10-13-16-18(19)2h9,12,17H,2-8,10-11,13-16H2,1H3,(H,19,20)(H,21,22,23)/b12-9+	-0.578
InChI=1S/C24H40O3/c1-15(7-10-21(26)27)17-8-9-18-22-19(11-13-24(17,18)3)23(2)12-5-4-h15-20,22,25H,4-14H2,1-3H3,(H,26,27)	-6.46
InChI=1S/C2H6O4S/c1-5-7(3,4)6-2/h1-2H3	-0.654

"InChi"	"logS(M)"
InChI=1S/C15H11ClN2O2/c16-11-6-7-13-12(8-11)15(10-4-2-1-3-5-10)18(20)9-14(19)17-13/h1-8,20H,9H2	-2.564
InChI=1S/C12H18O3/c1-2-3-4-5-6-7-8-10-9-11(13)15-12(10)14/h7-8,10H,2-6,9H2,1H3/b8-7+	-4.022
InChI=1S/C15H12O3/c16-12-8-5-11(6-9-12)7-10-15(18)13-3-1-2-4-14(13)17/h1-10,16-17H/b10-7+	-3.339
InChI=1S/C13H21NO2/c1-10(2)14-8-12(15)9-16-13-6-4-5-11(3)7-13/h4-7,10,12,14-15H,8-9H2,1-3H3	-1.492
InChI=1S/C10H20BrN/c1-9(2)6-8(11)7-10(3,4)12(9)5/h8H,6-7H2,1-5H3	-2.43
InChI=1S/C4H6N2O/c1-4(2-5)6-3-7/h3-4H,1H3,(H,6,7)	1.008
InChI=1S/C17H28N2O3/c1-4-7-11-21-16-13-14(18)8-9-15(16)17(20)22-12-10-19(5-2)6-3/h8-9,13H,4-7,10-12,18H2,1-3H3	-3.465
InChI=1S/C6H4Cl2N2O2/c7-3-1-2(9)4(8)5(10-3)6(11)12/h1H,(H2,9,10)(H,11,12)	-0.004
InChI=1S/C14H21NO4/c1-5-17-12-8-7-11(9-13(12)18-6-2)15-14(16)19-10(3)4/h7-10H,5-6H2,1-4H3,(H,15,16)	-4.002
InChI=1S/C24H31FO6/c1-13-9-18-17-6-5-15-10-16(27)7-8-21(15,3)23(17,25)19(28)11-22(18h7-8,10,13,17-19,28,30H,5-6,9,11-12H2,1-4H3	-4.9
InChI=1S/C5H9NS/c7-5-3-1-2-4-6-5/h1-4H2,(H,6,7)	-0.154
InChI=1S/C10H22O2/c1-2-3-4-5-6-7-9-12-10-8-11/h11H,2-10H2,1H3	-2.125
InChI=1S/C11H13N3O3/c1-8(2-3-10(15)16)13-14-11(17)9-4-6-12-7-5-9/h4-7H,2-3H2,1H3,(H,14,17)(H,15,16)/b13-8-	-1.59
InChI=1S/C14H19IN2O6/c1-14(2,3)12(20)22-6-9-8(18)4-10(23-9)17-5-7(15)11(19)16-13(17)21h5,8-10,18H,4,6H2,1-3H3,(H,16,19,21)	-3.36
InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2-5,7H,6H2,1H3/b3-2+,5-4+	-0.579
InChI=1S/C44H88O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-46h3-43H2,1-2H3	-7.113
InChI=1S/C14H18N4O/c1-4-17(5-2)14(19)13-11(3)18(16-15-13)12-9-7-6-8-10-12/h6-10H,4-5H2,1-3H3	-2.866
InChI=1S/C7H13NO/c9-7-3-5-1-2-6(4-7)8-5/h5-9H,1-4H2	0.852
InChI=1S/C25H34N2O8/c1-5-10-32-12-14-34-24(28)21-17(3)26-18(4)22(25(29)35-15-13-33-1h7-9,16,23,26H,5-6,10-15H2,1-4H3	-5.5
InChI=1S/C3H7NO/c1-3(5)4-2/h1-2H3,(H,4,5)	1.136
InChI=1S/C12H7NOS/c14-8-5-6-10-12(7-8)15-11-4-2-1-3-9(11)13-10/h1-7H	-3.72
InChI=1S/C7H4ClN3O2/c8-7-5-3-4(11(12)13)1-2-6(5)9-10-7/h1-3H,(H,9,10)	-2.481

"InChi"	"logS(M)"
InChI=1S/C10H18Cl2N2O2S2/c11-1-5-17-7-9(15)13-3-4-14-10(16)8-18-6-2-12/h1-8H2,(H,13,15)(H,14,16)	-2.68
InChI=1S/C11H7N3O3/c15-14(16)10-6-5-9(17-10)11-12-7-3-1-2-4-8(7)13-11/h1-6H,(H,12,13)	-3.89
InChI=1S/C19H30N2O2/c1-14(2)20(15(3)4)11-12-21-18-13-17(23-5)10-9-16(18)7-6-8-19(21)2h9-10,13-15H,6-8,11-12H2,1-5H3	-4.466
InChI=1S/C10H10N2O3/c13-6-5-12-9(14)7-3-1-2-4-8(7)11-10(12)15/h1-4,13H,5-6H2,(H,11,15)	-3.113
InChI=1S/C5H3FN2O4/c6-1-2(4(10)11)7-5(12)8-3(1)9/h(H,10,11)(H2,7,8,9,12)	-1.731
InChI=1S/C13H16N4O2/c1-18-10-4-3-8(6-11(10)19-2)5-9-7-16-13(15)17-12(9)14/h3-4,6-7H,5H2,1-2H3,(H4,14,15,16,17)	-1.927
InChI=1S/C6H14N2O/c1-5(2)8(7-9)6(3)4/h5-6H,1-4H3	-1.001
InChI=1S/C16H23ClN2O2/c1-3-9-19-10-5-7-13(11-19)21-16(20)18-15-12(2)6-4-8-14(15)17/h4,6,8,13H,3,5,7,9-11H2,1-2H3,(H,18,20)	-4.689
InChI=1S/C8H10O2S/c1-7-3-5-8(6-4-7)11(2,9)10/h3-6H,1-2H3	-1.987
InChI=1S/C10H18O2/c1-7(2)10-5-4-9(3,12-10)8(11)6-10/h7-8,11H,4-6H2,1-3H3	-0.288
InChI=1S/C18H19NO4/c1-13-8-4-7-11-16(13)23-12-14-9-5-6-10-15(14)17(19-22-3)18(20)21-h4-11H,12H2,1-3H3/b19-17-	-5.195
InChI=1S/C16H17NO2/c1-11-7-6-10-14(12(11)2)17-15-9-5-4-8-13(15)16(18)19-3/h4-10,17H,1-3H3	-5.824
InChI=1S/C13H11N/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,14H	-2.781
InChI=1S/C7H9BrN2O3/c1-3(2)7(8)4(11)9-6(13)10-5(7)12/h3H,1-2H3,(H2,9,10,11,12,13)	-2.209
InChI=1S/C8H6N2O2S/c9-6-13-5-7-1-3-8(4-2-7)10(11)12/h1-4H,5H2	-2.93
InChI=1S/C17H16Cl2N2O4/c18-8-10-20(11-9-19)14-4-6-16(7-5-14)25-17(22)13-2-1-3-15(12-13)2h1-7,12H,8-11H2	-6.253
InChI=1S/C19H21NO5/c1-23-16-8-10-4-6-13(20)12-9-15(22)14(21)7-5-11(12)17(10)19(25-3)h5,7-9,13H,4,6,20H2,1-3H3,(H,21,22)	-1.39
InChI=1S/C12H3Cl7O/c13-5-2-1-4(3-6(5)14)20-12-10(18)8(16)7(15)9(17)11(12)19/h1-3H	-9.46
InChI=1S/C9H9NO3/c1-6(11)13-8-4-2-7(3-5-8)9(10)12/h2-5H,1H3,(H2,10,12)	-1.64
InChI=1S/C12H14O6/c1-4-18-12(15)7-5-6-8(16-2)10(17-3)9(7)11(13)14/h5-6H,4H2,1-3H3,(H,13,14)/p-1	-2.253
InChI=1S/C16H22N4O2/c1-9(2)14-12(21-3)6-10(7-13(14)22-4)5-11-8-19-16(18)20-15(11)17/h6-9H,5H2,1-4H3,(H4,17,18,19,20)	-4.283
InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h4,8H,1,5-7H2,2-3H3	-4.459

"InChi"	"logS(M)"
InChI=1S/C5H6N2/c6-5-3-1-2-4-7-5/h1-4H,(H2,6,7)	0.976
InChI=1S/C7H7NO5S/c8-6-3-4(14(11,12)13)1-2-5(6)7(9)10/h1-3H,8H2,(H,9,10)(H,11,12,13)	-1.316
InChI=1S/C14H14N4S/c1-3-18-12-10(6-4-8-15-12)14(19)17(2)11-7-5-9-16-13(11)18/h4-9H,3H2,1-2H3	-4.634
InChI=1S/C6H4N4/c1-2-9-6-5(8-1)3-7-4-10-6/h1-4H	0.02
InChI=1S/C8H16Cl2N2/c9-1-3-11-5-7-12(4-2-10)8-6-11/h1-8H2	-0.684
InChI=1S/C6H5N5/c7-5-4-6(11-3-10-5)9-2-1-8-4/h1-3H,(H2,7,9,10,11)	-2.31
InChI=1S/C8H12N4O5/c13-5-6(14)3-10-7(15)4-11-2-1-9-8(11)12(16)17/h1-2,6,13-14H,3-5H2,(H,10,15)	-1.102
InChI=1S/C11H23NO3/c1-5-6-11(4,7-13)8-15-10(14)12-9(2)3/h9,13H,5-8H2,1-4H3,(H,12,14)	-2.695
InChI=1S/C9H8INO3/c10-7-3-1-6(2-4-7)9(14)11-5-8(12)13/h1-4H,5H2,(H,11,14)(H,12,13)	-3.082
InChI=1S/C8H17NO3/c1-3-5-6-8(4-2)7-12-9(10)11/h8H,3-7H2,1-2H3	-4.147
InChI=1S/C12H26N2O3/c1-5-6-7-12(4,8-15)9-17-11(16)14-13-10(2)3/h10,13,15H,5-9H2,1-4H3,(H,14,16)	-3.015
InChI=1S/C9H10O3/c1-2-12-8-5-3-7(4-6-8)9(10)11/h3-6H,2H2,1H3,(H,10,11)	-2.455
InChI=1S/C7H9NO5S3/c8-16(12,13)6-2-4-1-5(9)3-15(10,11)7(4)14-6/h2,5,9H,1,3H2,(H2,8,12,13)	-1.54
InChI=1S/C9H10O4/c1-12-7-4-2-3-5-8(7)13-6-9(10)11/h2-5H,6H2,1H3,(H,10,11)	-0.972
InChI=1S/C5H7N3O2/c1-4-6-3-5(7(4)2)8(9)10/h3H,1-2H3	-1.16
InChI=1S/C34H67NO/c1-3-5-7-9-11-13-15-17-18-19-21-23-25-27-29-31-33-35-34(36)32-30-h17-18H,3-16,19-33H2,1-2H3,(H,35,36)/b18-17+	-7.704
InChI=1S/C10H19N/c1-7-8-4-5-9(6-8)10(7,2)11-3/h7-9,11H,4-6H2,1-3H3	-1.752
InChI=1S/C8H8N2O4/c11-8(12)5-9-6-1-3-7(4-2-6)10(13)14/h1-4,9H,5H2,(H,11,12)	-1.324
InChI=1S/C6H6O4S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4,7H,(H,8,9,10)	0.759
InChI=1S/C17H18N4O6S/c1-10-7-11(2)19-16(18-10)20-17(23)21-28(24,25)14-6-4-3-5-13(14)15h3-7,12H,8-9H2,1-2H3,(H2,18,19,20,21,23)	-3.893
InChI=1S/C14H16ClO6P/c1-4-18-22(17,19-5-2)21-10-6-7-11-9(3)13(15)14(16)20-12(11)8-10/h6-8H,4-5H2,1-3H3	-3.18
InChI=1S/C7H17N/c1-3-4-5-6-7(2)8/h7H,3-6,8H2,1-2H3	-1.084
InChI=1S/C6H14O2/c1-3-8-6(2)4-5-7/h6-7H,3-5H2,1-2H3	-0.374
InChI=1S/C12H9NO2/c14-13(15)11-7-6-9-5-4-8-2-1-3-10(11)12(8)9/h1-3,6-7H,4-5H2	-5.34

"InChi"	"logS(M)"
InChI=1S/C72H139N/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45-h23,25,29,31,42,44,48,50,73H,3-22,24,26-28,30,32-41,43,45-47,49,51-72H2,1-2H3/b25-23+,31-29+,44-42+,50-48+	-9.707
InChI=1S/C8H6N2/c1-2-4-8-7(3-1)9-5-6-10-8/h1-6H	0.705
InChI=1S/C8H8INO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)	-3.25
InChI=1S/C21H21N5O6/c1-15(27)31-11-9-25(10-12-32-16(2)28)19-5-3-18(4-6-19)23-24-21-8-h3-8,13H,9-12H2,1-2H3/b24-23+	-7.3
InChI=1S/C12H12N4/c1-8-7-9(2)16(15-8)12-13-10-5-3-4-6-11(10)14-12/h3-7H,1-2H3,(H,13,14)	-2.081
InChI=1S/C15H15N3O2/c1-18(11-12-5-3-2-4-6-12)17-16-14-9-7-13(8-10-14)15(19)20/h2-10H,11H2,1H3,(H,19,20)/b17-16+	-4.615
InChI=1S/C8H7N3O2/c9-8-11-10-7(13-8)5-1-3-6(12)4-2-5/h1-4,12H,(H2,9,11)	-0.77
InChI=1S/C14H13N3O5S/c1-8-7-11(16-22-8)15-14(19)12-13(18)9-5-3-4-6-10(9)23(20,21)17(12h3-7,18H,1-2H3,(H,15,16,19)	-4.062
InChI=1S/C12H6Cl4O/c13-7-2-1-3-8(4-7)17-12-6-10(15)9(14)5-11(12)16/h1-6H	-7.27
InChI=1S/C10H9N/c1-2-5-9(6-3-1)10-7-4-8-11-10/h1-8,11H	-2.603
InChI=1S/C8H18O2/c1-2-3-4-5-6-8(10)7-9/h8-10H,2-7H2,1H3	-1.29
InChI=1S/C42H66O14/c1-20-37(49-6)29(43)16-35(51-20)55-39-22(3)53-36(18-31(39)45)56-h13,20-22,24-32,34-39,43-46,48H,7-12,14-19H2,1-6H3	-6.529
InChI=1S/C4H9Cl/c1-4(2,3)5/h1-3H3	-1.507
InChI=1S/C31H48O2S2/c1-27(2,3)21-15-19(32)16-22(28(4,5)6)25(21)34-31(13,14)35-26-23(2h15-18,32-33H,1-14H3	-8.17
InChI=1S/C9H12O/c1-6-4-8(3)9(10)5-7(6)2/h4-5,10H,1-3H3	-2.31
InChI=1S/C10H10O2/c1-12-10-7-3-2-5-9(10)6-4-8-11/h2-8H,1H3/b6-4+	-2.006
InChI=1S/C14H15NO2S/c16-13-11-8-4-5-9-12(11)14(17)15(13)18-10-6-2-1-3-7-10/h4-5,8-10H,1-3,6-7H2	-4.324
InChI=1S/C10H20O2/c1-7(2)9-5-4-8(3)6-10(9)12-11/h7-11H,4-6H2,1-3H3	-2.589
InChI=1S/C8H9NO3/c1-9-8(12)6-4-5(10)2-3-7(6)11/h2-4,10-11H,1H3,(H,9,12)	-0.713
InChI=1S/C24H32N2O/c1-19(2)13-14-24(23(25)27,15-18-26-16-6-3-7-17-26)22-12-8-10-20-9h4-5,8-13H,3,6-7,14-18H2,1-2H3,(H2,25,27)	-6.516
InChI=1S/C13H8N2O3/c16-15(17)10-7-5-9(6-8-10)13-14-11-3-1-2-4-12(11)18-13/h1-8H	-4.16
InChI=1S/C13H10BrF2N3O2/c1-19-5-7(12(17)20)11(10(16)13(19)21)18-9-3-2-6(14)4-8(9)15/h2-5,18H,1H3,(H2,17,20)	-4.14

"InChi"	"logS(M)"
InChI=1S/C11H9ClO2S/c1-6-8-3-2-7(12)4-10(8)15-9(6)5-11(13)14/h2-4H,5H2,1H3,(H,13,14)	-3.84
InChI=1S/C12H3Cl7/c13-5-1-4(2-6(14)3-5)7-8(15)10(17)12(19)11(18)9(7)16/h1-3H	-9.1
InChI=1S/C26H21Cl2NO4/c1-2-31-20-13-11-19(12-14-20)25(17-26(25,27)28)24(30)33-23(16-29h3-15,23H,2,17H2,1H3	-6.724
InChI=1S/C8H7NO/c10-7-1-2-8-6(5-7)3-4-9-8/h1-5,9-10H	-0.541
InChI=1S/C7H12FN3O2S2/c8-1-2-11(10-13)7(12)9-6-3-14-5-15-4-6/h6H,1-5H2,(H,9,12)	-2.363
InChI=1S/C9H9Cl2N3/c10-6-2-1-3-7(11)8(6)14-9-12-4-5-13-9/h1-3H,4-5H2,(H2,12,13,14)	-1.229
InChI=1S/C14H10Cl4/c1-8-6-12(16)14(18)13(17)10(8)7-9-4-2-3-5-11(9)15/h2-6H,7H2,1H3	-7.24
InChI=1S/C13H21NO3S2/c15-19(16,17)18-12-11-14-10-6-2-5-9-13-7-3-1-4-8-13/h1,3-4,7-8,14H,2,5-6,9-12H2,(H,15,16,17)	-2.265
InChI=1S/C16H19ClN2/c1-19(2)12-10-15(16-5-3-4-11-18-16)13-6-8-14(17)9-7-13/h3-9,11,15H,10,12H2,1-2H3	-2.67
InChI=1S/C8H12O4/c1-2-3-6-12-8(11)5-4-7(9)10/h4-5H,2-3,6H2,1H3,(H,9,10)/b5-4+	-0.668
InChI=1S/C12H16N2O/c1-14(2)6-5-9-8-13-12-7-10(15)3-4-11(9)12/h3-4,7-8,13,15H,5-6H2,1-2H3	-0.353
InChI=1S/C26H18N2O4/c27-21-19-20(24(30)18-14-8-7-13-17(18)23(19)29)22(28)26(32-16-11h1-14H,27-28H2	-8.272
InChI=1S/C23H48N2O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23(26)24-21-19-22-25h4-22H2,1-3H3,(H,24,26)	-4.567
InChI=1S/C7H5NO4/c9-6(10)4-1-2-5(7(11)12)8-3-4/h1-3H,(H,9,10)(H,11,12)	-2.13
InChI=1S/C8H8O2/c1-2-4-8-7(3-1)9-5-6-10-8/h1-4H,5-6H2	-1.912
InChI=1S/C14H8O2/c15-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(13)16/h1-8H	-4.444
InChI=1S/C15H22O2/c1-3-5-9-13(4-2)12-17-15(16)14-10-7-6-8-11-14/h6-8,10-11,13H,3-5,9,12H2,1-2H3	-5.768
InChI=1S/C5H7N3/c6-4-2-1-3-5(7)8-4/h1-3H,(H4,6,7,8)	-0.08
InChI=1S/C11H22O2/c1-3-5-6-10(4-2)7-12-8-11-9-13-11/h10-11H,3-9H2,1-2H3	-3.115
InChI=1S/C23H23ClN2O4S/c1-16(27)25-8-10-26(11-9-25)23(28)7-3-17-2-6-22(19(24)14-17)31-18h2-7,14-15H,8-13H2,1H3/b7-3+	-2.05
InChI=1S/C4H7NO3/c1-3(6)5-2-4(7)8/h2H2,1H3,(H,5,6)(H,7,8)	-0.649
InChI=1S/C12H27NO3/c1-4-10(14)7-13(8-11(15)5-2)9-12(16)6-3/h10-12,14-16H,4-9H2,1-3H3	-0.523
InChI=1S/C26H34O8/c1-14-10-16-17-7-9-26(33,20(29)13-34-22(32)5-4-21(30)31)25(17,3)1h6,8,11,14,16-17,19,23,28,33H,4-5,7,9-10,12-13H2,1-3H3,(H,30,31)	-4.2

"InChi"	"logS(M)"
InChI=1S/C24H29N/c1-23(2,3)18-24(4,5)25(20-14-7-6-8-15-20)22-17-11-13-19-12-9-10-16-21(19)22/h6-17H,18H2,1-5H3	-8.29
InChI=1S/C12H13NO2/c1-9(14)13-11-6-4-3-5-10(11)7-8-12(13)15-2/h3-8,12H,1-2H3	-1.835
InChI=1S/C8H4Cl2O2/c9-7(11)5-1-2-6(4-3-5)8(10)12/h1-4H	-4.029
InChI=1S/C7H4F3NO3/c8-7(9,10)5-3-4(12)1-2-6(5)11(13)14/h1-3,12H	-1.617
InChI=1S/C7H9NO/c1-6-3-7(2)5-8(9)4-6/h3-5H,1-2H3	0.909
InChI=1S/C16H25NO2/c1-2-3-4-5-6-7-8-13-19-16(18)14-9-11-15(17)12-10-14/h9-12H,2-8,13,17H2,1H3	-6
InChI=1S/C20H18ClF3N2O6/c1-5-8-31-17(29)19(2,3)32-16(28)12-9-11(6-7-13(12)21)26-15(27)10-h5-7,9-10H,1,8H2,2-4H3	-4.677
InChI=1S/C10H20N2/c1-9(2)7-6-8-10(3,4)12(9)11-5/h5-8H2,1-4H3	-3.661
InChI=1S/C19H21N5O2/c1-26-18-8-6-16(7-9-18)23-12-10-22(11-13-23)15-2-4-17(5-3-15)24-1h2-9,14H,10-13H2,1H3,(H,21,25)	-6.489
InChI=1S/C24H34O5/c1-21-9-5-16(25)13-23(21,27)11-7-19-18(21)6-10-22(2)17(8-12-24(19h3-4,14,16-19,25,27-28H,5-13H2,1-2H3	-3.768
InChI=1S/C9H10O2/c1-11-7-9(10)8-5-3-2-4-6-8/h2-6H,7H2,1H3	-0.762
InChI=1S/C10H7Cl5O2/c1-5(16)17-9(10(13,14)15)6-2-3-7(11)8(12)4-6/h2-4,9H,1H3	-3.828
InChI=1S/C17H24N2O2/c1-3-21-16-8-4-13(5-9-16)10-17(20)19-11-14-6-7-15(12-19)18(14)2/h4-5,8-9,14-15H,3,6-7,10-12H2,1-2H3	-3.098
InChI=1S/C6H11Cl4O4P/c1-3-12-15(11,13-4-2)14-5(7)6(8,9)10/h5H,3-4H2,1-2H3	-3.589
InChI=1S/C13H17N3O3S2/c1-9(2)8-12-14-15-13(20-12)16-21(17,18)11-6-4-10(19-3)5-7-11/h4-7,9H,8H2,1-3H3,(H,15,16)	-3.987
InChI=1S/C7H19N2O4PS/c10-6-4-8-2-1-3-9-5-7-15-14(11,12)13/h8-10H,1-7H2,(H2,11,12,13)	0.588
InChI=1S/C42H23N3O6/c46-37-23-15-7-9-17-25(23)39(48)33-31(37)29(43-41(50)21-11-3-1-4h1-20,45H,(H,43,50)(H,44,51)	-4.522
InChI=1S/C4H7ClO/c1-4(2-5)3-6-4/h2-3H2,1H3	-0.55
InChI=1S/C27H33NO11/c1-12(30)28-16-7-5-13-9-19(38-27-24(34)23(33)22(32)20(11-29)39-2h6,8-10,16,20,22-24,27,29,32-34H,5,7,11H2,1-4H3,(H,28,30)	-2.955
InChI=1S/C9H9NO5/c1-2-14-9(11)6-4-7-3-5-8(15-7)10(12)13/h3-6H,2H2,1H3/b6-4+	-2.925
InChI=1S/C12H5Cl5/c13-7-2-1-6(5-10(7)16)11-8(14)3-4-9(15)12(11)17/h1-5H	-7.65
InChI=1S/C8H11N5O2S/c1-2-12-4-3-9-7(12)11-8-10-5-6(16-8)13(14)15/h5H,2-4H2,1H3,(H,9,10,11)	-3.298
InChI=1S/C12H24N3OP/c1-10(2)7-13(10)17(16,14-8-11(14,3)4)15-9-12(15,5)6/h7-9H2,1-6H3	-1.679

"InChi"	"logS(M)"
InChI=1S/C7H8N4S/c8-7(12)11-10-5-6-1-3-9-4-2-6/h1-5H,(H3,8,11,12)/b10-5+	0.106
InChI=1S/C22H28N2O4/c1-2-22(26)28-21-10-8-20(9-11-21)27-17-19(25)16-23-12-14-24(15-1h3-11,19,25H,2,12-17H2,1H3	-3.155
InChI=1S/C14H21NO4/c1-10(2)17-8-12(19-14(15)16)9-18-13-7-5-4-6-11(13)3/h4-7,10,12H,8-9H2,1-3H3,(H2,15,16)	-3.139
InChI=1S/C8H11NO3/c9-4-8(12)5-1-2-6(10)7(11)3-5/h1-3,8,10-12H,4,9H2	0.772
InChI=1S/C12H7Cl3/c13-10-7-6-9(11(14)12(10)15)8-4-2-1-3-5-8/h1-7H	-6.18
InChI=1S/C14H8O4/c15-9-5-1-3-7-11(9)14(18)12-8(13(7)17)4-2-6-10(12)16/h1-6,15-16H	-5.19
InChI=1S/C16H23NO3/c1-5-8-13-9-10-14(15(11-13)19-4)20-12-16(18)17(6-2)7-3/h5,9-11H,1,6-8,12H2,2-4H3	-2.766
InChI=1S/C13H26O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h11-12H,5-10H2,1-4H3	-4.005
InChI=1S/C6H15N/c1-2-3-4-5-6-7/h2-7H2,1H3	-1.1
InChI=1S/C4H7Cl2NO2/c5-1-3(2-6)9-4(7)8/h3H,1-2H2,(H2,7,8)	-1.361
InChI=1S/C4H2N4O3/c5-8-1-2(9)6-4(11)7-3(1)10/h(H2,6,7,9,10,11)	-1.472
InChI=1S/C13H10N2O/c14-13-9-3-1-2-4-11(9)15-12-6-5-8(16)7-10(12)13/h1-7,16H,(H2,14,15)	-2.906
InChI=1S/C20H34O5/c1-2-3-6-9-15(21)12-13-17-16(18(22)14-19(17)23)10-7-4-5-8-11-20(2h12-13,15-17,19,21,23H,2-11,14H2,1H3,(H,24,25)/b13-12+	-3.67
InChI=1S/C7H7N3/c8-6-3-1-2-5-4-9-10-7(5)6/h1-4H,8H2,(H,9,10)	-1.128
InChI=1S/C10H15ClN2O4S2/c11-9-2-3-10(13-8-9)17-6-1-4-12-5-7-18-19(14,15)16/h2-3,8,12H,1,4-7H2,(H,14,15,16)	-1.12
InChI=1S/C10H13N5O4/c1-6(16)19-3-2-18-5-15-4-12-7-8(15)13-10(11)14-9(7)17/h4H,2-3,5H2,1H3,(H3,11,13,14,17)	-2.7
InChI=1S/C10H22O3/c1-4-5-6-12-8-10(3)13-7-9(2)11/h9-11H,4-8H2,1-3H3	-0.653
InChI=1S/C9H7NS/c11-9-6-5-7-3-1-2-4-8(7)10-9/h1-6H,(H,10,11)	-2.799
InChI=1S/C14H22O/c1-13(2,3)10-7-8-12(15)11(9-10)14(4,5)6/h7-9,15H,1-6H3	-3.796
InChI=1S/C4H9NO/c1-3-4(2)5-6/h6H,3H2,1-2H3/b5-4+	0.06
InChI=1S/C15H20O4/c1-10(7-13(17)18)5-6-15(19)11(2)8-12(16)9-14(15,3)4/h5-8,19H,9H2,1-4H3,(H,17,18)/b6-5+,10-7+	-2.588
InChI=1S/C15H22O2/c1-14(2,3)11-7-10(9-16)8-12(13(11)17)15(4,5)6/h7-9,17H,1-6H3	-3.917
InChI=1S/C10H12N4O4S3/c1-14-9(19-10(12-14)21(11,17)18)13-20(15,16)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H2,11,17,18)/b13-9-	-2.48

"InChi"	"logS(M)"
InChI=1S/C14H17N3O3/c1-7(2)14(4)13(20)16-11(17-14)10-9(12(18)19)5-8(3)6-15-10/h5-7H,1-4H3,(H,18,19)(H,16,17,20)	-2.091
InChI=1S/C16H23NO3/c1-13-7-4-5-10-17(13)11-6-12-20-16(19)14-8-2-3-9-15(14)18/h2-3,8-9,13,18H,4-7,10-12H2,1H3	-3.538
InChI=1S/C13H6Br2F6N2O2S/c1-4-22-10(12(16,17)18)9(26-4)11(24)23-8-6(14)2-5(3-7(8)15)25-13(1h2-3H,1H3,(H,23,24)	-5.519
InChI=1S/C8H6Cl2O2S/c9-5-1-2-7(6(10)3-5)12-4-8(11)13/h1-3H,4H2,(H,11,13)	-2.69
InChI=1S/C7H8N2O3/c1-12-7-3-2-5(9(10)11)4-6(7)8/h2-4H,8H2,1H3	-1.883
InChI=1S/C23H45NO2/c1-3-4-5-6-7-8-9-10-11-12-13-18-23(25)26-21-16-20-24-19-15-14-17-h22H,3-21H2,1-2H3	-7.904
InChI=1S/C5H12O3/c1-7-4-5-8-3-2-6/h6H,2-5H2,1H3	0.92
InChI=1S/C11H12ClNO4/c12-7-1-2-10-9(3-7)13(4-8(15)5-14)11(16)6-17-10/h1-3,8,14-15H,4-6H2	-0.597
InChI=1S/C8H10O2/c9-5-7-2-1-3-8(4-7)6-10/h1-4,9-10H,5-6H2	-0.233
InChI=1S/C7H9ClO/c1-3-7(9,4-2)5-6-8/h1,5-6,9H,4H2,2H3/b6-5+	-0.924
InChI=1S/C9H16N2O4/c1-4-9(5-2,7(13)15-3)6(12)11-8(10)14/h4-5H2,1-3H3,(H3,10,11,12,14)	-1.96
InChI=1S/C14H19NO3/c1-3-4-5-6-14(17)18-13-9-7-12(8-10-13)15-11(2)16/h7-10H,3-6H2,1-2H3,(H,15,16)	-4.14
InChI=1S/C12H11ClN2O2S/c13-9-1-5-11(6-2-9)15-18(16,17)12-7-3-10(14)4-8-12/h1-8,15H,14H2	-4.13
InChI=1S/C13H16N2O4/c14-11(16)7-6-10(13(18)19)15-12(17)8-9-4-2-1-3-5-9/h1-5,10H,6-8H2,(H2,14,16)(H,15,17)(H,18,19)	-2.096
InChI=1S/C11H14N4O5/c1-4-19-11(18)20-6-15-5-12-8-7(15)9(16)14(3)10(17)13(8)2/h5H,4,6H2,1-3H3	-1.86
InChI=1S/C40H79NO/c1-3-5-7-9-11-13-15-17-19-21-22-23-24-26-28-30-32-34-36-38-40(42)h17,19H,3-16,18,20-39H2,1-2H3,(H,41,42)/b19-17+	-7.771
InChI=1S/C17H16N2O4/c1-11(20)18-14-5-3-13(4-6-14)17(22)19-15-7-9-16(10-8-15)23-12(2)2h3-10H,1-2H3,(H,18,20)(H,19,22)	-4.41
InChI=1S/C4H12N2O/c5-1-2-6-3-4-7/h6-7H,1-5H2	0.982
InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h8-10H,4-7H2,1-3H3	-3.806
InChI=1S/C4H8Cl2O/c1-4(7,2-5)3-6/h7H,2-3H2,1H3	-0.182
InChI=1S/C19H31NO4/c1-7-20(8-2)11-15(21)12-24-18-16(13(3)4)10-9-14(5)17(18)19(22)23-h9-10,13,15,21H,7-8,11-12H2,1-6H3	-3.68
InChI=1S/C12H5Cl5/c13-7-3-1-6(2-4-7)10-8(14)5-9(15)11(16)12(10)17/h1-5H	-7.95
InChI=1S/C4H8N2O4/c5-1(3(6)8)2(7)4(9)10/h1-2,7H,5H2,(H2,6,8)(H,9,10)	-1.149

"InChi"	"logS(M)"
InChI=1S/C29H34O6/c1-2-32-29-26(30)28(34-20-24-16-10-5-11-17-24)27(35-29)25(33-19-2 h3-17,25-30H,2,18-21H2,1H3	-6.399
InChI=1S/C11H18N2O3S/c1-7(2)3-4-11(5-6-14)8(15)12-10(17)13-9(11)16/h7,14H, 3-6H2,1-2H3,(H2,12,13,15,16,17)	-2.56
InChI=1S/C13H19NO2S/c1-3-4-7-17-12-6-5-11(8-10(12)2)9-13(15)14-16/h5-6,8,16H, 3-4,7,9H2,1-2H3,(H,14,15)	-3.647
InChI=1S/C11H12O6S/c1-8(12)17-10-6-4-3-5-9(10)11(13)16-7-18(2,14)15/h3-6H, 7H2,1-2H3	-3.394
InChI=1S/C10H8O2/c11-9-3-1-7-5-10(12)4-2-8(7)6-9/h1-6,11-12H	-2.205
InChI=1S/C11H8O3/c1-6-9(12)7-4-2-3-5-8(7)11(14)10(6)13/ h2-5,12H,1H3	-1.599
InChI=1S/C12H13NO6/c1-12(2,3)19-11(16)7-5-4-6-8(13(17)18)9(7)10(14)15/h4-6H,1-3H3, (H,14,15)/p-1	-3.047
InChI=1S/C13H13NO2/c1-9-3-5-11(6-4-9)14-8-7-12(15)13(16)10(14)2/h3-8,16H,1-2H3	-3.22
InChI=1S/C10H8N2/c1-2-7-12-10(5-1)9-4-3-6-11-8-9/h1-8H	-0.592
InChI=1S/C16H18N2O/c1-12(13-8-4-2-5-9-13)18-16(19)15(17)14-10-6-3-7-11-14/ h2-12,15H,17H2,1H3,(H,18,19)	-1.66
InChI=1S/C12H20N2S4/c15-11(13-7-3-1-4-8-13)17-18-12(16)14-9-5-2-6-10-14/h1-10H2	-4.598
InChI=1S/C10H15NO2/c1-8-2-4-9(5-3-8)11-6-10(13)7-12/ h2-5,10-13H,6-7H2,1H3	-0.998
InChI=1S/C14H9F3N2/c15-14(16,17)8-5-6-10-12(7-8)19-11-4-2-1-3-9(11)13(10)18/h1-7H, (H2,18,19)	-2.17
InChI=1S/C15H30N2O4/c1-7-8-15(4,11-21-14(19)17(5)6)10-20-13(18)16-9-12(2)3/h12H, 7-11H2,1-6H3,(H,16,18)	-4.586
InChI=1S/C7H5Cl3/c8-4-5-1-2-6(9)3-7(5)10/h1-3H,4H2	-3.513
InChI=1S/C12H13NO4S2/c1-2-18(14,15)11-7-8-12(19(13,16)17)10-6-4-3-5-9(10)11/h3-8H, 2H2,1H3,(H2,13,16,17)	-3.493
InChI=1S/C8H13N2O3PS/c1-3-11-14(15,12-4-2)13-8-7-9-5-6-10-8/ h5-7H,3-4H2,1-2H3	-2.338
InChI=1S/C18H22N2O2S/c1-18(2,3)13-8-6-9-14(12-13)22-17(23)20(4)15-10-7-11-16(19-15)21- h6-12H,1-5H3	-6.014
InChI=1S/C4H8N2S/c1-2-3-6-4(5)7/h2H,1,3H2,(H3,5,6,7)	-0.294
InChI=1S/C16H15N5O7S2/c1-2-6-4-29-14-10(13(25)21(14)11(6)15(26)27)19-12(24)9(20-28-3-8(h2,5,10,14H,1,3-4H2,(H2,17,18)(H,19,24)(H,22,23)(H,26,27)/b20-9+	-3.915
InChI=1S/C11H10O6/c1-6(12)16-9-4-3-8(11(14)15)5-10(9)17-7(2)13/h3-5H,1-2H3,(H, 14,15)	-2.431

"InChi"	"logS(M)"
InChI=1S/C21H20ClNO5/c1-23-7-6-12(17(27)10-23)19-14(24)8-15(25)20-16(26)9-18(28-21(19)h2-5,8-9,12,17,24-25,27H,6-7,10H2,1H3	-4.26
InChI=1S/C5H7BrN2/c1-3-5(6)4(2)8-7-3/h1-2H3,(H,7,8)	-2.222
InChI=1S/C14H11N3/c1-3-7-11(8-4-1)13-15-14(17-16-13)12-9-5-2-6-10-12/h1-10H,(H,15,16,17)	-3.178
InChI=1S/C10H28N6/c11-1-3-13-5-7-15-9-10-16-8-6-14-4-2-12/h13-16H,1-12H2	0.333
InChI=1S/C22H42O4/c1-19(2)13-7-5-11-17-25-21(23)15-9-10-16-22(24)26-18-12-6-8-14-20(h19-20H,5-18H2,1-4H3	-6.87
InChI=1S/C15H12BrN3O/c16-10-6-7-12-13(8-10)19(11-4-2-1-3-5-11)15(20)9-14(17)18-12/h1-8H,9H2,(H2,17,18)	-2.76
InChI=1S/C10H20O2/c1-3-5-6-9(4-2)10-11-7-8-12-10/h9-10H,3-8H2,1-2H3	-3.12
InChI=1S/C13H19NO2/c1-4-13(2,3)11-7-5-10(6-8-11)9-12(15)14-16/h5-8,16H,4,9H2,1-3H3,(H,14,15)	-3.259
InChI=1S/C13H15NO6/c1-9(15)19-8-12(14(17)18)13(20-10(2)16)11-6-4-3-5-7-11/h3-7,12-13H,8H2,1-2H3	-3.972
InChI=1S/C23H32O6/c1-5-6-7-8-9-10-14(24)28-18-15-13(11-20(18,2)3)16(25)23-19(29-23)h13,15,18-19H,5-12H2,1-4H3	-5.299
InChI=1S/C7H9ClO/c1-3-7(9,4-2)5-6-8/h3,9H,1,4H2,2H3	-1.119
InChI=1S/C13H8Cl2O4S/c14-11-8(13(18)7-3-4-20-6-7)1-2-9(12(11)15)19-5-10(16)17/h1-4,6H,5H2,(H,16,17)	-4.287
InChI=1S/C13H9N3O6/c17-13(14(18)10-4-2-1-3-5-10)9-6-11(15(19)20)8-12(7-9)16(21)22/h1-8,18H	-3.637
InChI=1S/C18H24ClN3O/c1-13(2)17-8-5-15(9-14-3-6-16(19)7-4-14)18(17,23)10-22-12-20-11-2h3-4,6-7,11-13,15,17,23H,5,8-10H2,1-2H3	-4.683
InChI=1S/C12H4Cl6/c13-6-3-1-2-5(10(6)16)9-7(14)4-8(15)11(17)12(9)18/h1-4H	-8.48
InChI=1S/C6H15NO2/c1-5(8)3-7-4-6(2)9/h5-9H,3-4H2,1-2H3	0.815
InChI=1S/C9H20NO3PS2/c1-5-12-14(15,13-6-2)16-7-9(11)10-8(3)4/h8H,5-7H2,1-4H3,(H,10,11)	-2.058
InChI=1S/C11H14N4O4S3/c1-6-4-7(2)9(8(3)5-6)22(18,19)15-10-13-14-11(20-10)21(12,16)17/h4-5H,1-3H3,(H,13,15)(H2,12,16,17)	-2.7
InChI=1S/C14H17N2O4PS/c1-3-18-21(22,19-4-2)20-13-10-11-14(17)16(15-13)12-8-6-5-7-9-12/h5-11H,3-4H2,1-2H3	-3.532
InChI=1S/C18H21NO3/c1-19-10-9-17-11-13(20)6-8-18(17,19)7-5-12-3-4-14(22-2)16(21)15(1h3-4,6,8,21H,5,7,9-11H2,1-2H3	-1.87
InChI=1S/C19H21N3O/c1-13-5-8-15(9-6-13)19-16(11-18(23)21(3)4)22-12-14(2)7-10-17(22)2h5-10,12H,11H2,1-4H3	-1.3

"InChi"	"logS(M)"
InChI=1S/C16H12O6/c17-14(18)11-7-3-1-5-9(11)13(16(21)22)10-6-2-4-8-12(10)15(19)20/h1-8,13H,(H,17,18)(H,19,20)(H,21,22)	-2.5
InChI=1S/C8H16N2O4S2/c9-5(7(11)12)1-3-15-16-4-2-6(10)8(13)14/h5-6H,1-4,9-10H2,(H,11,12)(H,13,14)	-3.12
InChI=1S/C22H29NO5/c1-5-14(2)20(23)22(25)28-11-10-27-21(24)15(3)16-6-7-18-13-19(26-4)h6-9,12-15,20H,5,10-11,23H2,1-4H3	-3.82
InChI=1S/C14H22O8/c1-5-19-11(16)8-14(22-10(4)15,13(18)21-7-3)9-12(17)20-6-2/h5-9H2,1-4H3	-2.665
InChI=1S/C21H21ClN2O8/c1-24(2)14-7-5-6-10(16(27)12-9(25)4-3-8(22)11(12)15(6)26)18(29)21h3-4,6-7,14-15,25-27,30,32H,5H2,1-2H3,(H2,23,31)	-2.487
InChI=1S/C14H17N3O2/c1-10(8-12-6-4-3-5-7-12)15-16-14(18)13-9-11(2)19-17-13/h3-7,9-10,15H,8H2,1-2H3,(H,16,18)	-2.803
InChI=1S/C12H18O3/c1-2-4-10-5-3-6-12(7-10)15-9-11(14)8-13/h3,5-7,11,13-14H,2,4,8-9H2,1H3	-2.775
InChI=1S/C12H11NOS/c14-12(8-15)13-11-6-5-9-3-1-2-4-10(9)7-11/h1-7,15H,8H2,(H,13,14)	-3.34
InChI=1S/C11H22N2O2/c1-4-10(3)12-6-8-13(9-7-12)11(14)15-5-2/h10H,4-9H2,1-3H3	-1.327
InChI=1S/C6H8N2O2S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H,7H2,(H2,8,9,10)	-0.645
InChI=1S/C7H6ClF/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2	-2.541
InChI=1S/C18H23N3O4/c1-3-5-6-11-25-17(22)16(4-2)21(13-15-8-7-12-24-15)18(23)20-10-9-1h3,7-10,12,14,16H,1,4-6,11,13H2,2H3	-2.892
InChI=1S/C8H12O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)	-1.935
InChI=1S/C13H16N2S2/c1-2-6-10(7-3-1)15-17-13-14-11-8-4-5-9-12(11)16-13/h4-5,8-10,15H,1-3,6-7H2	-5.917
InChI=1S/C4H7Cl/c1-4(2)3-5/h3H,1-2H3	-1.957
InChI=1S/C16H22O2/c1-2-3-4-5-9-12-15(17)13-16(18)14-10-7-6-8-11-14/h6-8,10-11H,2-5,9,12-13H2,1H3	-5.884
InChI=1S/C9H11FN2O5/c10-4-2-12(9(16)11-8(4)15)7-1-5(14)6(3-13)17-7/h2,5-7,13-14H,1,3H2,(H,11,15,16)	-1.316
InChI=1S/C6H6O6/c7-4(8)1-3(6(11)12)2-5(9)10/h1H,2H2,(H,7,8)(H,9,10)(H,11,12)/b3-1-	0.361
InChI=1S/C16H14ClFN3O6PS/c1-27-14-7-2-10(8-13(14)18)15-16(17)19-9-21(15)11-3-5-12(6-4-11)2h2-9H,1H3,(H3,20,22,23,24)	-2.55
InChI=1S/C5H9N3O4/c6-5(12)8-1-3(9)7-2-4(10)11/h1-2H2,(H,7,9)(H,10,11)(H3,6,8,12)	-0.9
InChI=1S/C9H13N/c1-10(2)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3	-1.228
InChI=1S/C11H12N4O5/c1-12(2)11(16)7-5-9(13-3-4-13)10(15(19)20)6-8(7)14(17)18/h5-6H,3-4H2,1-2H3	-2.48

"InChi"	"logS(M)"
InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3,5-9,11-12H,1-2H2	0.635
InChI=1S/C13H22O2/c1-13(2,15)9-3-4-11-5-7-12(10-14)8-6-11/h5,10,12,15H,3-4,6-9H2,1-2H3	-1.538
InChI=1S/C16H12N2O2S/c1-9(19)12-6-7-14-13(8-12)18-16(21-14)11-4-2-10(3-5-11)15(17)20/h2-8H,1H3,(H2,17,20)	-3.375
InChI=1S/C10H18N2O2/c1-3-10(13)14-12-8-4-5-9(12)7-11(2)6-8/h8-9H,3-7H2,1-2H3	0.257
InChI=1S/C8H4Cl6/c9-7(10,11)5-1-2-6(4-3-5)8(12,13)14/h1-4H	-5.427
InChI=1S/C2H8N2/c3-1-2-4/h1-4H2	1.221
InChI=1S/C13H16N2O3/c1-3-11(10-7-5-4-6-8-10)12(17)15-13(18)14-9(2)16/h4-8,11H,3H2,1-2H3,(H2,14,15,16,17,18)	-2.674
InChI=1S/C16H12O3S/c1-2-19-16(18)10-7-8-14-12(9-10)15(17)11-5-3-4-6-13(11)20-14/h3-9H,2H2,1H3	-6.757
InChI=1S/C18H16Br2F3NO2/c19-8-10-24(11-9-20)15-4-6-16(7-5-15)26-17(25)13-2-1-3-14(12-13)1h1-7,12H,8-11H2	-7.808
InChI=1S/C9H20O2/c1-4-9(6-10,7-11)5-8(2)3/h8,10-11H,4-7H2,1-3H3	-2.126
InChI=1S/C19H18/c1-13-16-8-4-3-7-15(16)12-19-17(13)11-10-14-6-2-5-9-18(14)19/h2,5-6,9-12H,3-4,7-8H2,1H3	-6.75
InChI=1S/C12H22O2/c1-3-4-5-6-7-8-9-10-11-12(13)14-2/h3H,1,4-11H2,2H3	-5.398
InChI=1S/C21H20N4O2S/c1-22-20-13-14(25-28(2,26)27)11-12-19(20)24-21-15-7-3-5-9-17(15)2h3-13,22,25H,1-2H3,(H,23,24)	-2.94
InChI=1S/C12H26/c1-3-5-7-9-11-12-10-8-6-4-2/h3-12H2,1-2H3	-6.41
InChI=1S/C9H17N/c1-6-7-3-4-8(5-7)9(6,2)10/h6-8H,3-5,10H2,1-2H3	-1.252
InChI=1S/C24H14/c1-2-8-17-15(6-1)12-13-21-22(17)14-16-7-5-11-19-18-9-3-4-10-20(18h1-14H	-8.481
InChI=1S/C20H30O3/c1-19-9-7-14(22)11-13(19)3-4-15-16-5-6-18(23-12-21)20(16,2)10-8-1h12-13,15-18H,3-11H2,1-2H3	-5.32
InChI=1S/C10H14N2O3/c1-4-5-6-10(2)7(13)11-9(15)12(3)8(10)14/h4-5H,6H2,1-3H3,(H,11,13,15)/b5-4+	-1.544
InChI=1S/C15H23N5O4/c1-2-3-6-18-7-9-19(10-8-18)12-14(21)17-16-11-13-4-5-15(24-13)20(2h4-5,11H,2-3,6-10,12H2,1H3,(H,17,21)/b16-11+	-2.676
InChI=1S/C29H38O3/c1-28-17-15-22(30)19-21(28)11-12-23-24-13-14-26(29(24,2)18-16-25h3-5,7-8,19,23-26H,6,9-18H2,1-2H3	-5.43
InChI=1S/C18H27NO2/c1-3-19(4-2)14-15-21-17(20)18(12-8-9-13-18)16-10-6-5-7-11-16/h5-7,10-11H,3-4,8-9,12-15H2,1-2H3	-4.147
InChI=1S/C9H9NO3/c1-6(11)10-8-5-3-2-4-7(8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)	-2.114

"InChi"	"logS(M)"
InChI=1S/C10H12N2/c1-2-7-12-10(5-1)9-4-3-6-11-8-9/h1-4,6,8,10,12H,5,7H2	0.795
InChI=1S/C5H10ClN3O3/c6-1-3-9(8-12)5(11)7-2-4-10/h10H,1-4H2,(H,7,11)	-2.194
InChI=1S/C6H12O3/c1-2-3-4-9-6(8)5-7/h7H,2-5H2,1H3	-0.458
InChI=1S/C8H11Cl2N3O2/c9-1-3-13(4-2-10)6-5-11-8(15)12-7(6)14/h5H,1-4H2,(H2,11,12,14,15)	-2.374
InChI=1S/C4H10O2/c1-5-3-4-6-2/h3-4H2,1-2H3	1.045
InChI=1S/C4H4N2O2/c5-3(7)1-2-4(6)8/h(H2,5,7)(H2,6,8)	0.95
InChI=1S/C9H14N2O2/c1-11-7(12)9(10-8(11)13)5-3-2-4-6-9/h2-6H2,1H3,(H,10,13)	-1.64
InChI=1S/C23H44O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23(24)25-21-20-22(2)h11-12,22H,4-10,13-21H2,1-3H3/b12-11+	-8.07
InChI=1S/C10H7Cl5O/c11-7-1-6(2-8(12)3-7)9(5-16-9)4-10(13,14)15/h1-3H,4-5H2	-5.25
InChI=1S/C16H22N4O3/c1-3-7-19-14-12(15(22)20(8-4-2)16(19)23)17-13(18-14)10-5-6-11(21)h10H,3-9H2,1-2H3,(H,17,18)	-3.16
InChI=1S/C22H24N2O9/c1-21(32)7-5-4-6-8(25)9(7)15(26)10-12(21)17(28)13-14(24(2)3)16(27h4-6,12-14,17,25-28,32-33H,1-3H3,(H2,23,31)	-3.09
InChI=1S/C14H21NO6/c1-19-11-8-10(9-12(20-2)13(11)21-3)14(18)15(4-6-16)5-7-17/h8-9,16-17H,4-7H2,1-3H3	-0.272
InChI=1S/C9H13ClN2O4S2/c10-8-1-2-9(12-7-8)16-5-3-11-4-6-17-18(13,14)15/h1-2,7,11H,3-6H2,(H,13,14,15)	-0.599
InChI=1S/C17H16N2O/c1-11-8-9-16(12(2)10-11)19-13(3)18-15-7-5-4-6-14(15)17(19)20/h4-10H,1-3H3	-5.292
InChI=1S/C23H22N2O6S/c1-23(2)17(21(28)29)25-19(27)16(20(25)32-23)24-18(26)15(13-9-5-3-h3-12,15-17,20H,1-2H3,(H,24,26)(H,28,29)	-5.194
InChI=1S/C23H21Br2NO2/c24-14-16-26(17-15-25)21-10-12-22(13-11-21)28-23(27)20-8-6-19(7-h1-13H,14-17H2	-8.553
InChI=1S/C10H5Cl3/c11-8-2-1-6-4-9(12)10(13)5-7(6)3-8/h1-5H	-7.142
InChI=1S/C7H4N2O2/c8-5-6-1-3-7(4-2-6)9(10)11/h1-4H	-1.954
InChI=1S/C5H8N4O6/c6-2(12)7-5(15)4(14,1(10)11)8-3(13)9-5/h14-15H,(H,10,11)(H3,6,7,12)(H2,8,9,13)	-0.37
InChI=1S/C10H16N2O3S2/c13-17(14,15)16-9-8-11-6-7-12-10-4-2-1-3-5-10/h1-5,11-12H,6-9H2,(H,13,14,15)	-2.025
InChI=1S/C23H46N2O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23(26)24-21-19-22-25h11-12H,4-10,13-22H2,1-3H3,(H,24,26)/b12-11+	-4.149
InChI=1S/C8H9N5O4S3/c9-5-1-3-6(4-2-5)20(16,17)13-7-11-12-8(18-7)19(10,14)15/h1-4H,9H2,(H,11,13)(H2,10,14,15)	-1.5

"InChi"	"logS(M)"
InChI=1S/C15H17NO3/c17-15(16-8-2-1-3-9-16)7-5-12-4-6-13-14(10-12)19-11-18-13/h4-7,10H,1-3,8-9,11H2/b7-5+	-3.5
InChI=1S/C10H23O3P/c1-4-7-8-9-10-14(11,12-5-2)13-6-3/h4-10H2,1-3H3	-2.569
InChI=1S/C13H12Cl2O4/c1-3-7(2)13(18)8-4-5-9(12(15)11(8)14)19-6-10(16)17/h4-5H,2-3,6H2,1H3,(H,16,17)	-4.049
InChI=1S/C15H25N3O3/c1-4-6-8-20-13-10-12(15(19)18(3)16)11-14(17-13)21-9-7-5-2/h10-11H,4-9,16H2,1-3H3	-3.928
InChI=1S/C9H8O2S/c10-9(11)8(12)6-7-4-2-1-3-5-7/h1-6,12H,(H,10,11)/b8-6-	-2.96
InChI=1S/C21H17N3O2S/c1-3-24(4-2)13-9-10-14-15(12-22)19(21(25)26-17(14)11-13)20-23-16-5-11H,3-4H2,1-2H3	-8.097
InChI=1S/C16H24O6/c1-8(2)10-5-4-9(3)6-11(10)21-16-15(20)14(19)13(18)12(7-17)22-16/h4-6,8,12-20H,7H2,1-3H3	-2.392
InChI=1S/C20H26N2/c1-20(2)16-10-5-7-12-18(16)22(15-9-14-21(3)4)19-13-8-6-11-17(19)2h5-8,10-13H,9,14-15H2,1-4H3	-5.611
InChI=1S/C14H26O2/c1-9(2)11(4)12(5)14(16)8-7-10(3)13(6)15/h9-16H,1-6H3	-2.276
InChI=1S/C10H14O2/c1-6-3-4-8-7(2)5-12-10(11)9(6)8/h5-6,8-9H,3-4H2,1-2H3	-1.564
InChI=1S/C12H2Br8/c13-4-2-1-3(6(14)7(4)15)5-8(16)10(18)12(20)11(19)9(5)17/h1-2H	-9.351
InChI=1S/C22H30N2/c1-3-23(4-2)15-10-16-24(21-13-6-5-7-14-21)22-17-19-11-8-9-12-20(1h5-9,11-14,22H,3-4,10,15-18H2,1-2H3	-4.694
InChI=1S/C15H14N4O3/c16-15-18-12-11(13(20)19-15)10(7-17-12)6-3-8-1-4-9(5-2-8)14(21)22h1-2,4-5,7H,3,6H2,(H,21,22)(H4,16,17,18,19,20)	-3.574
InChI=1S/C13H11N3/c14-9-5-4-8-6-10-11(15)2-1-3-12(10)16-13(8)7-9/h1-7H,14-15H2	-3.106
InChI=1S/C11H11F3N2O3/c1-6(2)10(17)15-7-3-4-9(16(18)19)8(5-7)11(12,13)14/h3-6H,1-2H3,(H,15,17)	-4.466
InChI=1S/C9H18N2O3S2/c10-9(7-15-16(12,13)14)11-6-8-4-2-1-3-5-8/h8H,1-7H2,(H2,10,11)(H,12,13,14)	-2.703
InChI=1S/C17H12ClNO2/c18-15-7-9-16(10-8-15)19(21)17(20)14-6-5-12-3-1-2-4-13(12)11-14/h1-11,21H	-5.47
InChI=1S/C26H29N3O6/c1-17-22(25(30)34-4)24(20-11-8-12-21(15-20)29(32)33)23(18(2)27-1'h5-12,15,24,27H,13-14,16H2,1-4H3	-5.339
InChI=1S/C12H6Cl4/c13-8-3-1-2-7(6-8)9-4-5-10(14)12(16)11(9)15/h1-6H	-6.77
InChI=1S/C11H17NO2/c1-8(12)6-9-4-5-10(13-2)11(7-9)14-3/h4-5,7-8H,6,12H2,1-3H3	-0.642

"InChi"	"logS(M)"
InChI=1S/C14H20O/c15-7-2-1-4-10-8-11-9-14(10)13-6-3-5-12(11)13/h4,7,11-14H,1-3,5-6,8-9H2/b10-4+	-4.09
InChI=1S/C4H7NO2/c1-3(5-7)4(2)6/h7H,1-2H3/b5-3+	-1.775
InChI=1S/C6H12O6/c7-2-4(9)1-6(12,3-8)5(10)11/h4,7-9,12H,1-3H2,(H,10,11)	0.61
InChI=1S/C13H24O2/c1-3-11(4-2)10-13(12(14)15)8-6-5-7-9-13/h11H,3-10H2,1-2H3,(H,14,15)	-4.282
InChI=1S/C4H7Cl/c1-2-3-4-5/h2-3H,4H2,1H3/b3-2+	-1.957
InChI=1S/C14H10Cl4/c1-8-4-14(18)10(7-13(8)17)5-9-6-11(15)2-3-12(9)16/h2-4,6-7H,5H2,1H3	-8.03
InChI=1S/C12H13BrO4S/c1-17-11(14)12(7-2-8-12)18(15,16)10-5-3-9(13)4-6-10/h3-6H,2,7-8H2,1H3	-3.55
InChI=1S/C42H18N2O6/c45-37-17-7-1-3-9-19(17)39(47)29-25(37)15-13-23-27-28-24-14-16-2(h1-16,43-44H	-4.51
InChI=1S/C20H31N3O3/c21-19(24)20(18-4-2-1-3-5-18,6-8-22-10-14-25-15-11-22)7-9-23-12-1 h1-5H,6-17H2,(H2,21,24)	-3.178
InChI=1S/C15H20ClN3O/c1-15(2,3)14(20)13(19-10-17-9-18-19)8-11-4-6-12(16)7-5-11/h4-7,9-10,13-14,20H,8H2,1-3H3	-4.05
InChI=1S/C9H15NO2/c1-7(11)12-9-6-10-4-2-8(9)3-5-10/h8-9H,2-6H2,1H3	-0.428
InChI=1S/C6H6OS/c1-5(7)6-3-2-4-8-6/h2-4H,1H3	-0.955
InChI=1S/C8H8O3/c1-6(9)11-8-4-2-3-7(10)5-8/h2-5,10H,1H3	-0.782
InChI=1S/C26H36N2O9/c1-6-7-9-18-23(37-20(30)12-14(2)3)16(5)36-26(34)21(15(4)35-25(18) h8,10-11,13-16,18,21,23,31H,6-7,9,12H2,1-5H3,(H,27,29)(H,28,32)	-5.44
InChI=1S/C6H4N4O/c11-5-2-8-4-1-7-3-9-6(4)10-5/h1-3H,(H,7,9,10,11)	-2.12
InChI=1S/C20H38O4/c1-5-9-11-17(7-3)15-23-19(21)13-14-20(22)24-16-18(8-4)12-10-6-2/h17-18H,5-16H2,1-4H3	-7.836
InChI=1S/C16H32O2/c1-4-5-6-7-8-9-10-11-12-13-16(17)18-14-15(2)3/h15H,4-14H2,1-3H3	-7.932
InChI=1S/C2H3ClF2/c1-2(3,4)5/h1H3	-1.723
InChI=1S/C19H21Br2NO2/c1-2-15-5-3-4-6-18(15)19(23)24-17-9-7-16(8-10-17)22(13-11-20)14-1 h3-10H,2,11-14H2,1H3	-7.583
InChI=1S/C12H20O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h5-8H,3-4,9-11H2,1-2H3/b7-5+,8-6+	-4.51
InChI=1S/C6H3F3N4/c7-6(8,9)5-12-3-1-10-2-11-4(3)13-5/h1-2H,(H,10,11,12,13)	-0.451
InChI=1S/C18H20N2O6/c21-13-7-3-1-5-11(13)15(17(23)24)19-9-10-20-16(18(25)26)12-6-2-4- h1-8,15-16,19-22H,9-10H2,(H,23,24)(H,25,26)	-1.199

"InChi"	"logS(M)"
InChI=1S/C19H13F/c1-12-14-7-3-2-6-13(14)10-18-15-8-4-5-9-16(15)19(20)11-17(12)18/h2-11H,1H3	-7.31
InChI=1S/C13H9ClN2O/c14-9-6-7-11-12(8-9)16(13(17)15-11)10-4-2-1-3-5-10/h1-8H,(H,15,17)	-3.224
InChI=1S/C10H10O3/c1-13-9-5-3-2-4-8(9)6-7-10(11)12/h2-7H,1H3,(H,11,12)/b7-6+	-1.652
InChI=1S/C9H18N2O4/c1-3-4-7(5-14-8(10)12)6(2)15-9(11)13/h6-7H,3-5H2,1-2H3,(H2,10,12)(H2,11,13)	-1.601
InChI=1S/C6H4ClIO2S/c7-11(9,10)6-3-1-5(8)2-4-6/h1-4H	-4.269
InChI=1S/C12H12N2O3/c13-8-11(10-4-2-1-3-5-10)14-17-9-12-15-6-7-16-12/h1-5,12H,6-7,9H2/b14-11+	-4.065
InChI=1S/C13H20N2O2/c1-2-3-9-17-10-8-15-12-7-5-4-6-11(12)13(14)16/h4-7,15H,2-3,8-10H2,1H3,(H2,14,16)	-2.863
InChI=1S/C12H12N2O2/c15-10-12(14-11(16)13-10)6-5-8-3-1-2-4-9(8)7-12/h1-4H,5-7H2,(H2,13,14,15,16)	-4.013
InChI=1S/C21H41N5O11/c1-26-11-14(30)18-8(33-20(11)37-21-16(32)13(29)10(25)9(4-27)34-2 h5-21,26-32H,2-4,22-25H2,1H3	0.268
InChI=1S/C9H4F6O2/c10-8(11,12)5-1-4(7(16)17)2-6(3-5)9(13,14)15/h1-3H,(H,16,17)	-4.329
InChI=1S/C19H25NO/c1-2-10-20-11-9-19-8-4-3-5-16(19)18(20)12-14-6-7-15(21)13-17(14)1 h2,6-7,13,16,18,21H,1,3-5,8-12H2	-2.651
InChI=1S/C4H6O4S/c5-3(6)1-2(9)4(7)8/h2,9H,1H2,(H,5,6)(H,7,8)	0.522
InChI=1S/C9H10N2O2S/c10-9(13)14-6-8(12)11-7-4-2-1-3-5-7/h1-5H,6H2,(H2,10,13)(H,11,12)	-1.323
InChI=1S/C15H15NO2/c1-16-15(17)13-10-6-9-12(14(13)18-2)11-7-4-3-5-8-11/h3-10H,1-2H3,(H,16,17)	-3.361
InChI=1S/C3H7NOS/c1-2-5-3(4)6/h2H2,1H3,(H2,4,6)	-0.315
InChI=1S/C16H12FNO3/c1-9(16(19)20)10-6-7-14-13(8-10)18-15(21-14)11-4-2-3-5-12(11)17/h2-9H,1H3,(H,19,20)	-3.905
InChI=1S/C12H20ClN3O4/c1-9(17)20-8-10-2-4-11(5-3-10)14-12(18)16(15-19)7-6-13/h10-11H,2-8H2,1H3,(H,14,18)	-3.343
InChI=1S/C8H11O3P/c1-6-3-4-8(7(2)5-6)12(9,10)11/h3-5H,1-2H3,(H2,9,10,11)	-1.094
InChI=1S/C12H18ClN/c1-11(14-9-5-8-13)10-12-6-3-2-4-7-12/h2-4,6-7,11,14H,5,8-10H2,1H3	-2.69
InChI=1S/C16H12ClNO2/c1-2-16(20-15(18)19,12-6-4-3-5-7-12)13-8-10-14(17)11-9-13/h1,3-11H,(H2,18,19)	-5.572
InChI=1S/C6H12N2O2/c1-5(9)7-3-4-8-6(2)10/h3-4H2,1-2H3,(H,7,9)(H,8,10)	0.675
InChI=1S/C9H8N2O2/c10-9-11-8(12)7(13-9)6-4-2-1-3-5-6/h1-5,7H,(H2,10,11,12)	-2.501

"InChi"	"logS(M)"
InChI=1S/C12H13N/c1-3-12(2,10-13)9-11-7-5-4-6-8-11/h3-8H,1,9H2,2H3	-3.001
InChI=1S/C13H10ClNO/c14-10-6-7-12(15)11(8-10)13(16)9-4-2-1-3-5-9/h1-8H,15H2	-4.255
InChI=1S/C15H11N3O/c19-15-17-13(11-7-3-1-4-8-11)16-14(18-15)12-9-5-2-6-10-12/h1-10H,(H,16,17,18,19)	-5.494
InChI=1S/C11H17O4PS2/c1-4-13-16(17,14-5-2)15-10-6-8-11(9-7-10)18(3)12/h6-9H,4-5H2,1-3H3/p+1	-2.3
InChI=1S/C7H12O2/c1-6(2)4-5-9-7(3)8/h4H,5H2,1-3H3	-1.474
InChI=1S/C5H9Br3O/c6-1-5(2-7,3-8)4-9/h9H,1-4H2	-2.226
InChI=1S/C12H18O5/c1-5-11(13)16-9(3)7-15-8-10(4)17-12(14)6-2/h5-6,9-10H,1-2,7-8H2,3-4H3	-1.668
InChI=1S/C24H50S2/c1-7-9-11-13-15-17-19-21-23(3,4)25-26-24(5,6)22-20-18-16-14-12-10h7-22H2,1-6H3	-7.128
InChI=1S/C16H22O4/c1-3-5-7-11-9-10-13(15(17)18)14(16(19)20)12(11)8-6-4-2/h9-10H,3-8H2,1-2H3,(H,17,18)(H,19,20)	-4.4
InChI=1S/C16H16N2O4/c1-2-9-17-13(19)8-7-12(16(17)22)18-14(20)10-5-3-4-6-11(10)15(18)2h3-6,12H,2,7-9H2,1H3	-3.72
InChI=1S/C11H8Cl2N2O/c1-6-8(12)4-7(5-9(6)13)10-2-3-11(16)15-14-10/h2-5H,1H3,(H,15,16)	-5.537
InChI=1S/C6H10FNS/c7-4-2-1-3-5-9-6-8/h1-5H2	-2.523
InChI=1S/C23H16O11/c24-11(9-31-14-3-1-5-16-20(14)12(25)7-18(33-16)22(27)28)10-32-15h1-8,11,24H,9-10H2,(H,27,28)(H,29,30)	-3.348
InChI=1S/C13H16O4/c1-8(14)11(9(2)15)6-10-4-5-12(16)13(7-10)17-3/h4-5,7,11,16H,6H2,1-3H3	-1.786
InChI=1S/C20H25ClN2O2/c1-24-19-8-7-16(15-20(19)25-2)9-10-22-11-13-23(14-12-22)18-6-4-3-h3-8,15H,9-14H2,1-2H3	-4.256
InChI=1S/C7H12O/c1-6-4-2-3-5-7(6)8/h6H,2-5H2,1H3	-0.94
InChI=1S/C6H11Cl3O2/c1-3-10-5(11-4-2)6(7,8)9/h5H,3-4H2,1-2H3	-1.646
InChI=1S/C12H17NO2/c1-8(2)10-5-9(3)6-11(7-10)15-12(14)13-4/h5-8H,1-4H3,(H,13,14)	-3.357
InChI=1S/C9H8O3/c10-4-3-7-1-2-8-9(5-7)12-6-11-8/h1-2,4-5H,3,6H2	-1.96
InChI=1S/C20H24O2/c1-14-12-16(6-8-18(14)21)20(10-4-3-5-11-20)17-7-9-19(22)15(2)13-1h6-9,12-13,21-22H,3-5,10-11H2,1-2H3	-5.372
InChI=1S/C20H32N6O12S2/c21-9(19(35)36)1-3-13(27)25-11(17(33)23-5-15(29)30)7-39-40-8-12(1h9-12H,1-8,21-22H2,(H,23,33)(H,24,34)(H,25,27)(H,26,28)(H,29,30)(H,31,32)(H,35,36)(H,37,38)	-0.31
InChI=1S/C6H9NS/c7-4-3-6-2-1-5-8-6/h1-2,5H,3-4,7H2	-0.301

"InChi"	"logS(M)"
InChI=1S/C18H14ClFN2O3/c1-2-25-18(24)16-17(23)21-14-8-7-10(19)9-12(14)15(22-16)11-5-3-4-h3-9,16H,2H2,1H3,(H,21,23)	-4.363
InChI=1S/C6H12ClF/c7-5-3-1-2-4-6-8/h1-6H2	-3.187
InChI=1S/C12H26OS/c1-3-5-7-9-11-14(13)12-10-8-6-4-2/h3-12H2,1-2H3/p+1	-3.945
InChI=1S/C20H21FN2O/c1-23(2)11-3-10-20(17-5-7-18(21)8-6-17)19-9-4-15(13-22)12-16(19)1h4-9,12H,3,10-11,14H2,1-2H3	-4.018
InChI=1S/C7H9Cl3O5/c8-7(9,10)6-14-4-3(12)2(1-11)13-5(4)15-6/h2-6,11-12H,1H2	-2.12
InChI=1S/C10H10O2/c11-10(12)9-6-5-7-3-1-2-4-8(7)9/h1-4,9H,5-6H2,(H,11,12)	-1.938
InChI=1S/C20H23N3O3/c1-22(16-7-3-2-4-8-16)20(25)17-9-5-6-10-18(17)21-19(24)15-23-11-1h2-10H,11-15H2,1H3,(H,21,24)	-3.291
InChI=1S/C6H8FN3O3/c7-3-5(11)4-9-2-1-8-6(9)10(12)13/h1-2,5,11H,3-4H2	-0.527
InChI=1S/C14H17NO3/c1-3-17-13-10-9-11-7-5-6-8-12(11)15(13)14(16)18-4-2/h5-10,13H,3-4H2,1-2H3	-4.118
InChI=1S/C15H24O/c1-12(2)7-6-11-15(16-11)13(3,4)10-5-8-14(12,15)9-10/h10-11H,5-9H2,1-4H3	-4.653
InChI=1S/C7H3Cl5O/c8-3-2(1-13)4(9)6(11)7(12)5(3)10/h13H,1H2	-5.147
InChI=1S/C6H14O/c1-3-4-6(2)5-7/h6-7H,3-5H2,1-2H3	-1.11
InChI=1S/C18H21NO4/c1-12(18(21)23-11-17(20)19(2)3)13-5-6-15-10-16(22-4)8-7-14(15)9-1h5-10,12H,11H2,1-4H3	-4.9
InChI=1S/C9H10N2O/c10-9-11-6-8(12-9)7-4-2-1-3-5-7/h1-5,8H,6H2,(H2,10,11)	-1.946
InChI=1S/C12H18O2/c1-11(2,13)9-6-5-7-10(8-9)12(3,4)14/h5-8,13-14H,1-4H3	-1.864
InChI=1S/C4H6O3/c1-3(5)2-4(6)7/h2H2,1H3,(H,6,7)	0.991
InChI=1S/C12H18O4/c1-2-7-15-11-5-3-4-6-12(11)16-9-10(14)8-13/h3-6,10,13-14H,2,7-9H2,1H3	-2.051
InChI=1S/C6H9N3O2/c1-4(2)6-7-3-5(8-6)9(10)11/h3-4H,1-2H3,(H,7,8)	-1.15
InChI=1S/C12H12N2O6S2/c13-7-1-3-9(11(5-7)21(15,16)17)10-4-2-8(14)6-12(10)22(18,19)20/h1-6H,13-14H2,(H,15,16,17)(H,18,19,20)	-2.692
InChI=1S/C8H18O3/c1-4-10-5-8(9)6-11-7(2)3/h7-9H,4-6H2,1-3H3	0.002
InChI=1S/C14H19N3O/c1-18-12-6-5-10-8-17(14(15)16)7-9-3-2-4-11(12)13(9)10/h5-6,9H,2-4,7-8H2,1H3,(H3,15,16)	-1.22
InChI=1S/C11H7NO4/c13-11(14)8-5-1-3-7-4-2-6-9(10(7)8)12(15)16/h1-6H,(H,13,14)	-2.75
InChI=1S/C13H17NO3/c1-3-17-13(16)12(14-10(2)15)9-11-7-5-4-6-8-11/h4-8,12H,3,9H2,1-2H3,(H,14,15)	-1.756
InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3	-0.095

"InChi"	"logS(M)"
InChI=1S/C3H5NS2/c5-3-4-1-2-6-3/h1-2H2,(H,4,5)	-0.081
InChI=1S/C8H7NO2/c10-8-9-7-4-2-1-3-6(7)5-11-8/h1-4H,5H2,(H,9,10)	-1.737
InChI=1S/C9H17N/c1-2-6-9-8(4-1)5-3-7-10-9/h8-10H,1-7H2	-1.083
InChI=1S/C18H26N2O4S2/c1-17(2,15(21)23-5)9-7-11-19-13-14(25-11)20-12(26-13)8-10-18(3,4)h7-10H2,1-6H3	-6.419
InChI=1S/C16H14N6O3S/c17-26(24,25)13-5-3-12(4-6-13)20-14-7-9-19-16(21-14)22-15(23)11-2h1-10H,(H2,17,24,25)(H2,19,20,21,22,23)	-1.27
InChI=1S/C5H12N2O/c1-3-4(2)7-5(6)8/h4H,3H2,1-2H3,(H3,6,7,8)	-1.625
InChI=1S/C19H22N2O4/c1-4-21(16-10-6-5-7-11-16)19(23)25-17-12-8-9-15(13-17)20-18(22)24h5-14H,4H2,1-3H3,(H,20,22)	-5.057
InChI=1S/C19H26O2/c1-19-10-9-15-14-6-4-13(21-2)11-12(14)3-5-16(15)17(19)7-8-18(19)2h4,15-17H,3,5-11H2,1-2H3	-4.98
InChI=1S/C12H22O4/c1-4-5-6-14-7-8-15-9-10-16-12(13)11(2)3/h2,4-10H2,1,3H3	-2.016
InChI=1S/C19H29NO/c1-16-7-6-8-17(15-16)19(21-2)11-9-18(10-12-19)20-13-4-3-5-14-20/h6-8,15,18H,3-5,9-14H2,1-2H3	-4.599
InChI=1S/C8H6O7S/c9-7(10)4-1-2-6(16(13,14)15)5(3-4)8(11)12/h1-3H,(H,9,10)(H,11,12)(H,13,14,15)	0.609
InChI=1S/C15H14O4/c1-19-14-8-6-11(13(16)7-9-15(17)18)10-4-2-3-5-12(10)14/h2-6,8H,7,9H2,1H3,(H,17,18)	-2.326
InChI=1S/C11H16N4O2/c1-6(2)5-7-12-8-9(13-7)14(3)11(17)15(4)10(8)16/h6H,5H2,1-4H3,(H,12,13)	-2.253
InChI=1S/C27H32F4/c1-2-3-17-4-6-18(7-5-17)19-8-10-20(11-9-19)21-12-13-23(24(28)14-2h12-20H,2-11H2,1H3	-6.636
InChI=1S/C13H18O2/c1-2-12(14)15-11-6-5-10-8-3-4-9(7-8)13(10)11/h5-6,8-11,13H,2-4,7H2,1H3	-3.559
InChI=1S/C16H14N2O/c19-16(17-14-9-2-1-3-10-14)18-12-6-8-13-7-4-5-11-15(13)18/h1-11H,12H2,(H,17,19)	-4.02
InChI=1S/C6H8N2O3S/c7-5-2-1-4(3-6(5)8)12(9,10)11/h1-3H,7-8H2,(H,9,10,11)	-1.181
InChI=1S/C5H11NO2/c6-4-2-1-3-5(7)8/h1-4,6H2,(H,7,8)	0.931
InChI=1S/C12H6Cl3NO3/c13-7-5-10(14)12(11(15)6-7)19-9-3-1-8(2-4-9)16(17)18/h1-6H	-5.62
InChI=1S/C14H18N4O3/c1-20-11-4-8(5-12(21-2)10(11)7-19)3-9-6-17-14(16)18-13(9)15/h4-6,19H,3,7H2,1-2H3,(H4,15,16,17,18)	-1.676
InChI=1S/C16H23NO2/c1-3-17(4-2)13-8-14-19-16(18)12-11-15-9-6-5-7-10-15/h5-7,9-12H,3-4,8,13-14H2,1-2H3/b12-11+	-3.112
InChI=1S/C5H7N3/c6-4-1-2-8-3-5(4)7/h1-3H,7H2,(H2,6,8)	-0.455

"InChi"	"logS(M)"
InChI=1S/C22H24N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(2h4-7,10,14-15,17,25-27,30,32H,1-3H3,(H2,23,31)	-2.848
InChI=1S/C27H36F2O6/c1-14-9-16-17-11-19(28)18-10-15(30)7-8-24(18,5)26(17,29)20(31)12-h7-8,10,14,16-17,19-20,31,34H,9,11-13H2,1-6H3	-6.101
InChI=1S/C6H12O2/c7-5-6-3-1-2-4-8-6/h6-7H,1-5H2	0.935
InChI=1S/C4H6Cl2/c1-2-4(6)3-5/h2,4H,1,3H2	-2.056
InChI=1S/C29H24O7/c30-21(17-35-22-11-13-24(26(31)15-22)28(33)19-7-3-1-4-8-19)18-36h1-16,21,30-32H,17-18H2	-7.139
InChI=1S/C14H10Cl2O4/c15-9-1-5-11(6-2-9)19-14(13(17)18)20-12-7-3-10(16)4-8-12/h1-8,14H,(H,17,18)	-4.751
InChI=1S/C9H8N2O/c1-12-9-7-4-2-3-5-8(7)10-6-11-9/h2-6H,1H3	-2.053
InChI=1S/C10H10N2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1-6H,11-12H2	-2.768
InChI=1S/C9H12/c1-2-8-5-7-3-4-9(8)6-7/h2-4,7-9H,1,5-6H2	-3.08
InChI=1S/C16H16O2/c17-16(15-11-5-2-6-12-15)18-13-7-10-14-8-3-1-4-9-14/h1-6,8-9,11-12H,7,10,13H2	-4.801
InChI=1S/C21H21ClN6O6/c1-5-7-26(8-6-2)18-11-16(23-13(3)29)17(12-20(18)34-4)24-25-21-15(h5-6,9-12H,1-2,7-8H2,3-4H3,(H,23,29)/b25-24+	-4.388
InChI=1S/C9H9N3/c10-9-8(6-11-12-9)7-4-2-1-3-5-7/h1-6H,(H3,10,11,12)	-1.137
InChI=1S/C13H22O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h10-11H,3-9H2,1-2H3	-2.908
InChI=1S/C10H15NO3S2/c12-16(13,14)15-9-8-11-7-6-10-4-2-1-3-5-10/h1-5,11H,6-9H2,(H,12,13,14)	-0.509
InChI=1S/C11H15N3O4/c12-5-1-7-14(8-2-6-13)9(11(17)18)3-4-10(15)16/h9H,1-4,7-8H2,(H,15,16)(H,17,18)	-0.228
InChI=1S/C12H4Cl6O/c13-6-2-1-5(3-7(6)14)19-9-4-8(15)10(16)12(18)11(9)17/h1-4H	-8.78
InChI=1S/C11H25N/c1-2-3-4-5-6-7-8-9-10-11-12/h2-12H2,1H3	-3.109
InChI=1S/C8H12N2O3S/c1-2-8(3-4-11)5(12)9-7(14)10-6(8)13/h11H,2-4H2,1H3,(H2,9,10,12,13,14)	-1.47
InChI=1S/C10H7NO2/c12-10(13)8-3-1-5-9-7(8)4-2-6-11-9/h1-6H,(H,12,13)	-2.677
InChI=1S/C8H8FNO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)	-1.78
InChI=1S/C11H19N3O2/c1-11(9(15)12-10(16)13-11)5-8-14-6-3-2-4-7-14/h2-8H2,1H3,(H2,12,13,15,16)	-0.821
InChI=1S/C15H23N3O2/c1-4-18(5-2)11-10-16-15(20)13-6-8-14(9-7-13)17-12(3)19/h6-9H,4-5,10-11H2,1-3H3,(H,16,20)(H,17,19)	-2.069

"InChi"	"logS(M)"
InChI=1S/C24H30N2O3/c1-3-22(27)26(21-12-8-5-9-13-21)24(23(28)29-2)15-18-25(19-16-24)1h4-13H,3,14-19H2,1-2H3	-4.972
InChI=1S/C10H13N5O3/c1-7(17)13-10-11-4-8-9(14-10)15(5-12-8)6-18-3-2-16/h4-5,16H,2-3,6H2,1H3,(H,11,13,14,17)	-0.86
InChI=1S/C12H18N2O4S2/c13-12(10-19-20(15,16)17)14-8-4-5-9-18-11-6-2-1-3-7-11/h1-3,6-7H,4-5,8-10H2,(H2,13,14)(H,15,16,17)	-3.042
InChI=1S/C16H16N4O2/c1-18-12(10-9-11-7-5-4-6-8-11)17-14-13(18)15(21)20(3)16(22)19(14)h4-10H,1-3H3/b10-9+	-5.55
InChI=1S/C6H4N4S/c11-5-2-8-6-4(10-5)1-7-3-9-6/h1-3H,(H,10,11)	-2.71
InChI=1S/C12H17NO4/c1-8(14)12(16)7-17-11-5-3-10(4-6-11)13-9(2)15/h3-6,8,12,14,16H,7H2,1-2H3,(H,13,15)	-0.932
InChI=1S/C6H7NO2S/c1-4-5(2-6(8)9)10-3-7-4/h3H,2H2,1H3,(H,8,9)	-0.786
InChI=1S/C9H13N/c1-2-5-8-6-3-4-7-9(8)10/h3-4,6-7H,2,5,10H2,1H3	-2.413
InChI=1S/C12H15NO3/c1-3-16-11-6-4-10(5-7-11)13-12(15)8-9(2)14/h4-7H,3,8H2,1-2H3,(H,13,15)	-2.163
InChI=1S/C9H15NO5/c1-9(2)7(13)10(8(14)15-9)4-3-6(12)5-11/h6,11-12H,3-5H2,1-2H3	0.663
InChI=1S/C7H11N3O3/c1-5(11)3-6-4-8-7(9(6)2)10(12)13/h4-5,11H,3H2,1-2H3	-1.296
InChI=1S/C40H58N8O7/c1-25(2)17-30(34(49)21-35(50)45-31(18-26(3)4)36(51)43-23-28-15-1h8-16,22,24-26,30-34,49H,17-21,23H2,1-7H3,(H,41,44)(H,43,51)(H,45,50)(H,46,53)(H,47,52)(H,48,54)	-3.42
InChI=1S/C21H31NO5/c1-15(2)17-9-8-16(3)19(21(24)25-4)20(17)27-14-18(23)26-13-12-22-1h8-9,15H,5-7,10-14H2,1-4H3	-4.797
InChI=1S/C8H8O2/c1-5-3-8(10)6(2)4-7(5)9/h3-4H,1-2H3	-1.288
InChI=1S/C40H58N8O7/c1-25(2)17-30(34(49)21-35(50)45-31(18-26(3)4)36(51)43-22-28-13-1h8-16,23-26,30-34,49H,17-22H2,1-7H3,(H,42,44)(H,43,51)(H,45,50)(H,46,53)(H,47,52)(H,48,54)	-3.36
InChI=1S/C54H32N4O6/c59-49-39-7-1-3-9-41(39)51(61)47-43(49)11-5-13-45(47)55-53(63)35-h1-30H,(H,55,63)(H,56,64)/b58-57+	-5.716
InChI=1S/C21H30O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)8-9-20(13,2)19(15)18(24)11-h10,15-19,24H,4-9,11H2,1-3H3	-3.82
InChI=1S/C15H25NO3/c1-12(2)16-10-14(17)11-19-15-6-4-13(5-7-15)8-9-18-3/h4-7,12,14,16-17H,8-11H2,1-3H3	-1.199
InChI=1S/C9H11NO4S2/c1-10-9(11)15-8-5-3-7(4-6-8)14-16(2,12)13/h3-6H,1-2H3,(H,10,11)	-2.736
InChI=1S/C7H15Cl2N2O2P/c8-2-4-10-14(12)11(6-3-9)5-1-7-13-14/h1-7H2,(H,10,12)	-1.839
InChI=1S/C8H12O2/c1-8(2)4-6(9)3-7(10)5-8/h3-5H2,1-2H3	-1.528

"InChi"	"logS(M)"
InChI=1S/C12H13N5/c13-11(14)17-12(15)16-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H6,13,14,15,16,17)	-2.315
InChI=1S/C17H27NO4/c1-11(2)14-8-7-12(3)15(17(20)21-6)16(14)22-10-13(19)9-18(4)5/h7-8,11,13,19H,9-10H2,1-6H3	-2.637
InChI=1S/C17H26N2O2/c1-14(2)17(16(18)20,15-6-4-3-5-7-15)8-9-19-10-12-21-13-11-19/h3-7,14H,8-13H2,1-2H3,(H2,18,20)	-2.715
InChI=1S/C9H18O4/c1-2-3-4-5-6-7(10)8(11)9(12)13/h7-8,10-11H,2-6H2,1H3,(H,12,13)	-1.547
InChI=1S/C12H24N2O4/c1-4-6-7-12(3,8-17-10(13)15)9-18-11(16)14-5-2/h4-9H2,1-3H3,(H2,13,15)(H,14,16)	-3.175
InChI=1S/C8H9NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-2,5-6H,3-4H2,(H,9,10,11)	-1.093
InChI=1S/C11H14ClNO/c1-2-13(8-7-12)11-5-3-10(9-14)4-6-11/h3-6,9H,2,7-8H2,1H3	-3.033
InChI=1S/C21H21O4P/c1-17(2)20-15-9-10-16-21(20)25-26(22,23-18-11-5-3-6-12-18)24-19-1h3-17H,1-2H3	-5.224
InChI=1S/C6H9NO/c8-7-6-4-2-1-3-5-6/h2,4,8H,1,3,5H2/b7-6-	-0.967
InChI=1S/C10H23NO3S2/c1-2-3-4-5-6-7-8-11-9-10-15-16(12,13)14/h11H,2-10H2,1H3,(H,12,13,14)	-1.816
InChI=1S/C15H24N2O/c1-12(2)15(14(16)18,10-11-17(3)4)13-8-6-5-7-9-13/h5-9,12H,10-11H2,1-4H3,(H2,16,18)	-2.739
InChI=1S/C10H9N/c1-9-4-6-10(7-5-9)3-2-8-11/h2-7H,1H3/b3-2+	-2.548
InChI=1S/C18H23NO3S/c1-18(9-3-2-4-10-18)12-22-14-7-5-13(6-8-14)11-15-16(20)19-17(21)2h5-8,15H,2-4,9-12H2,1H3,(H,19,20,21)	-4.964
InChI=1S/C12H4Cl6O/c13-5-1-9(17)12(10(18)2-5)19-11-4-7(15)6(14)3-8(11)16/h1-4H	-8.04
InChI=1S/C7H16O/c1-5-6(2)7(3,4)8/h6,8H,5H2,1-4H3	-0.89
InChI=1S/C10H12N2/c1-2-4-9(5-3-1)8-10-11-6-7-12-10/h1-5H,6-8H2,(H,11,12)	-2.633
InChI=1S/C18H23ClN2O/c1-2-18(22)21-16-9-10-17(21)13-20(12-16)11-3-4-14-5-7-15(19)8-6-1h3-8,16-17H,2,9-13H2,1H3/b4-3+	-4.458
InChI=1S/C8H7N3O5/c12-8-10(3-4-15-8)9-5-6-1-2-7(16-6)11(13)14/h1-2,5H,3-4H2/b9-5+	-3.75
InChI=1S/C3H2ClF5O/c4-1(3(7,8)9)10-2(5)6/h1-2H	-1.616
InChI=1S/C15H20N2/c1-15(2)9-8-14(17(15)3)12-10-16-13-7-5-4-6-11(12)13/h4-7,10,14,16H,8-9H2,1-3H3	-2.138
InChI=1S/C11H13NO2/c1-13-10-6-5-9(4-3-7-12)8-11(10)14-2/h5-6,8H,3-4H2,1-2H3	-1.901
InChI=1S/C22H22FN3O2/c23-17-9-7-16(8-10-17)21(27)6-3-13-25-14-11-18(12-15-25)26-20-5-2h1-2,4-5,7-11H,3,6,12-15H2,(H,24,28)	-4.955

"InChi"	"logS(M)"
InChI=1S/C7H15N3O2S2/c1-10(2)5(3-13-6(8)11)4-14-7(9)12/h5H,3-4H2,1-2H3,(H2,8,11)(H2,9,12)	-0.07
InChI=1S/C19H27FN2O3/c1-14(2)21-19(24)25-17-9-12-22(13-10-17)11-3-4-18(23)15-5-7-16(20h5-8,14,17H,3-4,9-13H2,1-2H3,(H,21,24)	-3.635
InChI=1S/C24H32O6/c1-21(2)29-19-10-16-15-6-5-13-9-14(26)7-8-22(13,3)20(15)17(27)11-h7-9,15-17,19-20,25,27H,5-6,10-12H2,1-4H3	-5.582
InChI=1S/C19H17N3O4S2/c23-14(9-13-5-4-8-27-13)20-15-17(24)22-16(19(25)26)12(11-28-18(1h1-8,15,18H,9-11H2,(H-,20,23,25,26)	-2.168
InChI=1S/C22H14Cl2I2N2O2/c1-11-6-15(17(10-27)12-2-4-13(23)5-3-12)18(24)9-20(11)28-22(30)16h2-9,17,29H,1H3,(H,28,30)	-10.347
InChI=1S/C45H54N4O8/c1-8-27-19-28-22-44(40(51)55-6,36-30(25-48(23-27)24-28)29-13-10-h10-15,19-21,28,37-39,46,53H,8-9,16-18,22-25H2,1-7H3	-7.969
InChI=1S/C2H3Br3/c3-1-2(4)5/h2H,1H2	-2.727
InChI=1S/C7H12O4/c1-5(4-7(10)11)2-3-6(8)9/h5H,2-4H2,1H3,(H,8,9)(H,10,11)	0.09
InChI=1S/C21H12N3O6PS/c25-13-22-16-1-7-19(8-2-16)28-31(32,29-20-9-3-17(4-10-20)23-14-26h1-12H	-6.492
InChI=1S/C14H16N4O2S/c15-11-5-7-12(8-6-11)21(19,20)18-14-16-9-10-3-1-2-4-13(10)17-14/h5-9H,1-4,15H2,(H,16,17,18)	-3.65
InChI=1S/C10H10N2O5S/c1-2-16-9-10(12(13)17-11-9)18(14,15)8-6-4-3-5-7-8/h3-7H,2H2,1H3	-4.24
InChI=1S/C11H16N4O4/c1-2-3-4-7-14(11(12)16)13-8-9-5-6-10(19-9)15(17)18/h5-6,8H,2-4,7H2,1H3,(H2,12,16)/b13-8+	-2.897
InChI=1S/C41H67NO15/c1-19-17-41(18-49-41)38(46)23(5)34(53-27(9)43)21(3)25(7)52-39(47)h19-26,30-37,40H,15-18H2,1-14H3	-6.292
InChI=1S/C4H11NO/c1-4(2,5)3-6/h6H,3,5H2,1-2H3	1.05
InChI=1S/C11H17BrN2O4S2/c12-10-3-4-11(14-9-10)18-7-2-1-5-13-6-8-19-20(15,16)17/h3-4,9,13H,1-2,5-8H2,(H,15,16,17)	-2.176
InChI=1S/C6H10O4/c1-9-5(7)3-4-6(8)10-2/h3-4H2,1-2H3	-0.075
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3/p+1	0.72
InChI=1S/C21H32N2O/c1-6-7-13-22-16-19(24)23-20(2,3)14-18(15-21(23,4)5)17-11-9-8-10-1h8-12,14,22H,6-7,13,15-16H2,1-5H3	-5.895
InChI=1S/C12H18O/c1-10(9-13)8-11(2)12-6-4-3-5-7-12/h3-7,10-11,13H,8-9H2,1-2H3	-2.347
InChI=1S/C21H24N2O4/c22-19(20(24)25)11-5-6-12-23-21(26)27-13-18-16-9-3-1-7-14(16)15-8h1-4,7-10,18-19H,5-6,11-13,22H2,(H,23,26)(H,24,25)	-3
InChI=1S/C21H23NO5S/c1-11(23)22-15-7-5-12-9-17(25)20(26-2)21(27-3)19(12)13-6-8-18(28-h6,8-10,15,25H,5,7H2,1-4H3,(H,22,23)	-3.98

"InChi"	"logS(M)"
InChI=1S/C20H40O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-4-2/h4H,2-3,5-20H2,1H3	-6.472
InChI=1S/C19H23ClN2O2S/c1-2-3-4-5-6-10-13-25-19(23)24-16-14-17(20)21-22-18(16)15-11-8-7-h7-9,11-12,14H,2-6,10,13H2,1H3	-5.402
InChI=1S/C17H25NO3/c1-13(2)10-18(11-14(3)4)16(19)12-21-17(20)15-8-6-5-7-9-15/h5-9,13-14H,10-12H2,1-4H3	-3.56
InChI=1S/C22H22N2O8/c1-7-8-5-4-6-9(25)11(8)16(26)12-10(7)17(27)14-15(24(2)3)18(28)13(h4-6,10,14-15,17,25-27,30,32H,1H2,2-3H3,(H2,23,31)	-1.768
InChI=1S/C9H12N2O/c1-2-6-12-11-8-9-4-3-5-10-7-9/h3-5,7-8H,2,6H2,1H3/b11-8+	-0.875
InChI=1S/C10H22O7/c11-1-9(2-12,3-13)7-17-8-10(4-14,5-15)6-16/h11-16H,1-8H2	-1.958
InChI=1S/C2H2N2S3/c5-1-3-4-2(6)7-1/h(H,3,5)(H,4,6)	-0.755
InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5-6H3	-7.242
InChI=1S/C9H14N2O3/c1-4-7(5-2)8(13)11-9(14)10-6(3)12/h4H,5H2,1-3H3,(H2,10,11,12,13,14)/b7-4-	-1.638
InChI=1S/C11H8O/c12-8-9-5-6-10-3-1-2-4-11(10)7-9/h1-8H	-2.909
InChI=1S/C14H18N2O4S2/c17-22(18,19)21-11-9-15-8-3-10-20-14-7-6-12-4-1-2-5-13(12)16-14/h1-2,4-7,15H,3,8-11H2,(H,17,18,19)	-1.827
InChI=1S/C11H13N/c1-3-10(2)12-9-11-7-5-4-6-8-11/h1,4-8,10,12H,9H2,2H3	-1.203
InChI=1S/C13H24N2O/c1-3-5-8-14-9-11-6-7-12(10-14)15(11)13(16)4-2/h11-12H,3-10H2,1-2H3	-2.363
InChI=1S/C15H11Cl2NO2/c16-9-14(19)18-13-7-6-11(17)8-12(13)15(20)10-4-2-1-3-5-10/h1-8H,9H2,(H,18,19)	-5.067
InChI=1S/C12H15N3O3S2/c13-12(8-19-20(16,17)18)14-6-5-9-7-15-11-4-2-1-3-10(9)11/h1-4,7,15H,5-6,8H2,(H2,13,14)(H,16,17,18)	-2.618
InChI=1S/C18H17Cl2NO3/c1-3-24-18(23)12(2)21(14-9-10-15(19)16(20)11-14)17(22)13-7-5-4-6-h4-12H,3H2,1-2H3	-4.263
InChI=1S/C14H23IN2O4S2/c15-13-6-7-14(17-12-13)21-10-5-3-1-2-4-8-16-9-11-22-23(18,19)20/h6-7,12,16H,1-5,8-11H2,(H,18,19,20)	-4.318
InChI=1S/C10H10N2O4/c1-7(13)11-5-8-2-3-10(12(14)15)4-9(8)6-16-11/h2-4H,5-6H2,1H3	-2.253
InChI=1S/C7H13ClO2/c1-5(2)4-10-7(9)6(3)8/h5-6H,4H2,1-3H3	-2.518
InChI=1S/C21H19N5O7/c1-10(27)17(18(28)22-13-4-5-15-16(9-13)24-21(31)23-15)26-25-14-7-h4-9,17H,1-3H3,(H,22,28)(H2,23,24,31)/b26-25+	-6.378
InChI=1S/C9H12N4O3/c1-10-5-6(11(2)8(10)15)12(3)9(16)13(4)7(5)14/h1-4H3	-0.953
InChI=1S/C14H21NO/c1-3-15(4-2)12-8-11-14(16)13-9-6-5-7-10-13/h5-7,9-10H,3-4,8,11-12H2,1-2H3	-2.221

"InChi"	"logS(M)"
InChI=1S/C12H20O2/c1-6-10(2)8-7-9-12(4,5)14-11(3)13/h6H,1-2,7-9H2,3-5H3	-3.597
InChI=1S/C6H6O3/c1-4-2-5(7)3-6(8)9-4/h2H,3H2,1H3	-1.119
InChI=1S/C8H12N4O4/c9-7-10-3-12(8(15)11-7)6-1-4(14)5(2-13)16-6/h3-6,13-14H,1-2H2,(H2,9,11,15)	-0.561
InChI=1S/C12H15N3O3/c1-3-6-18-8-4-5-9-10(7-8)14-11(13-9)15-12(16)17-2/h4-5,7H,3,6H2,1-2H3,(H2,13,14,15,16)	-4.487
InChI=1S/C9H9Cl3O3/c10-5-1-7(11)9(8(12)2-5)15-4-6(14)3-13/h1-2,6,13-14H,3-4H2	-3.566
InChI=1S/C13H9NO/c15-11-6-5-10-7-9-3-1-2-4-12(9)14-13(10)8-11/h1-8,14H	-3.58
InChI=1S/C7H3Cl2NO2/c8-3-1-5-6(2-4(3)9)12-7(11)10-5/h1-2H,(H,10,11)	-2.598
InChI=1S/C6H10O4/c1-3-9-5(7)6(8)10-4-2/h3-4H2,1-2H3	-0.609
InChI=1S/C6H9N5O2/c1-4-3-5(2)10(8-4)6(7)9-11(12)13/h3H,1-2H3,(H2,7,9)	-1.064
InChI=1S/C11H15NO3/c1-4-8-7(3)10(11(14)15-5-2)12-9(8)6-13/h6,12H,4-5H2,1-3H3	-2.719
InChI=1S/C12H22O2/c1-5-10(13)14-11-9(2)7-6-8-12(11,3)4/h9,11H,5-8H2,1-4H3	-3.803
InChI=1S/C9H10N2O3/c1-6(12)14-8-4-2-7(3-5-8)11-9(10)13/h2-5H,1H3,(H3,10,11,13)	-2.49
InChI=1S/C12H27O4P/c1-4-7-10-14-17(13,15-11-8-5-2)16-12-9-6-3/h4-12H2,1-3H3	-2.85
InChI=1S/C8H12N2O3/c1-3-8(4-2)5(11)9-7(13)10-6(8)12/h3-4H2,1-2H3,(H2,9,10,11,12,13)/p-1	-0.07
InChI=1S/C15H10O2/c16-13-10-15(11-6-2-1-3-7-11)17-14-9-5-4-8-12(13)14/h1-10H	-3.862
InChI=1S/C12H17NO2/c1-13(2)12(14)15-10-6-9-11-7-4-3-5-8-11/h3-5,7-8H,6,9-10H2,1-2H3	-3.215
InChI=1S/C12H17NO2/c1-4-9-6-10(5-2)8-11(7-9)15-12(14)13-3/h6-8H,4-5H2,1-3H3,(H,13,14)	-3.32
InChI=1S/C12H15O3P/c1-3-10-14-16(13,15-11-4-2)12-8-6-5-7-9-12/h3-9H,1-2,10-11H2	-2.9
InChI=1S/C13H15N3O3S/c1-8-9(2)15-19-13(8)16(10(3)17)20(18)12-6-4-11(14)5-7-12/h4-7H,14H2,1-3H3/p+1	-3.59
InChI=1S/C16H14O5/c17-9-1-2-10-14(4-9)21-7-16(20)6-8-3-12(18)13(19)5-11(8)15(10)16/h1-5,15,17-20H,6-7H2	-1.218
InChI=1S/C20H26N2O/c1-3-13-8-12-9-17-19-15(6-7-22(11-12)20(13)17)16-10-14(23-2)4-5-18(16)21(19)h4-5,10,12-13,17,20-21H,3,6-9,11H2,1-2H3	-4.082
InChI=1S/C19H21N/c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16-8-3-5-10-18(16)19/h2-5,7-10,12-13,19-20H,6,11,14H2,1H3	-5.404
InChI=1S/C3H4N2/c1-2-4-5-3-1/h1-3H,(H,4,5)	1.288
InChI=1S/C10H7NO2/c12-9-6-5-7-3-1-2-4-8(7)10(9)11-13/h1-6,13H/b11-10-	-2.94

"InChi"	"logS(M)"
InChI=1S/C12H24O6/c1-2-3-4-5-6-17-12-11(16)10(15)9(14)8(7-13)18-12/h8-16H,2-7H2,1H3	-0.659
InChI=1S/C15H26O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h6,8,13H,7,9-11H2,1-5H3/b14-6-	-5.792
InChI=1S/C6H6N2O2/c9-6(8-10)5-2-1-3-7-4-5/h1-4,10H,(H,8,9)	0.281
InChI=1S/C21H22O5/c1-12(2)4-9-15-16(23)10-19(25-3)20-17(24)11-18(26-21(15)20)13-5-7h4-8,10,18,22-23H,9,11H2,1-3H3	-5.44
InChI=1S/C13H17N3O/c1-15-8-11-2-3-12(9-15)16(11)13(17)10-4-6-14-7-5-10/h4-7,11-12H,2-3,8-9H2,1H3	-2.083
InChI=1S/C6H10O/c1-5(2)4-6(3)7/h4H,1-3H3	-0.561
InChI=1S/C37H70N2O12/c1-14-25-37(10,45)30(41)20(4)27(38)18(2)16-35(8,44)32(51-34-28(4(h18-32,34,40-42,44-45H,14-17,38H2,1-13H3	-6.109
InChI=1S/C17H19NO4/c1-12(18(19)20)17(13-4-8-15(21-2)9-5-13)14-6-10-16(22-3)11-7-14/h4-12,17H,1-3H3	-4.545
InChI=1S/C9H13N5/c1-6-4-2-3-5-7(6)13-9(12)14-8(10)11/h2-5H,1H3,(H6,10,11,12,13,14)	-1.842
InChI=1S/C6H7NO3S/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H,7H2,(H,8,9,10)	-1.205
InChI=1S/C14H12O3/c1-17-11-7-8-12(13(15)9-11)14(16)10-5-3-2-4-6-10/h2-9,15H,1H3	-4.58
InChI=1S/C18H25NO6/c1-10-8-18(11(2)25-18)16(21)24-13-5-7-19-6-4-12(14(13)19)9-23-15(h4,10-11,13-14,22H,5-9H2,1-3H3	-0.086
InChI=1S/C13H13N3O/c17-13(12-8-4-5-9-14-12)16-15-10-11-6-2-1-3-7-11/h1-9,15H,10H2,(H,16,17)	-2.02
InChI=1S/C17H26N4O4S/c1-4-7-21-8-5-6-12(21)11-20-17(22)13-9-16(26(23,24)19-2)14(18)10-h4,9-10,12,19H,1,5-8,11,18H2,2-3H3,(H,20,22)	-2.359
InChI=1S/C6H11ClO/c1-6(2,3)5(8)4-7/h4H2,1-3H3	-1.363
InChI=1S/C13H13N3O5S2/c17-11(5-6-12(18)19)15-9-1-3-10(4-2-9)23(20,21)16-13-14-7-8-22-13h1-4,7-8H,5-6H2,(H,14,16)(H,15,17)(H,18,19)	-3.11
InChI=1S/C16H18N2/c1-18-10-14(12-6-3-2-4-7-12)13-8-5-9-16(17)15(13)11-18/h2-9,14H,10-11,17H2,1H3	-2.931
InChI=1S/C14H18N2/c1-15-9-5-8-14(15)12-10-16(2)13-7-4-3-6-11(12)13/h3-4,6-7,10,14H,5,8-9H2,1-2H3	-2.144
InChI=1S/C16H19NO3/c1-19-13-3-2-12-5-7-17-6-4-11-10-20-15(18)8-14(11)16(12,17)9-13/h2-3,5,13H,4,6-10H2,1H3	-0.418
InChI=1S/C13H17NO3/c15-10-8-14(9-11-16)13(17)7-6-12-4-2-1-3-5-12/h1-7,15-16H,8-11H2/b7-6+	-0.88
InChI=1S/C14H8O4/c15-9-5-6-10(16)12-11(9)13(17)7-3-1-2-4-8(7)14(12)18/h1-6,15-16H	-6.253

"InChi"	"logS(M)"
InChI=1S/C17H23N3O2/c1-5-18(6-2)15-13(4)19(7-3)17(22)20(16(15)21)14-11-9-8-10-12-14/h8-12H,5-7H2,1-4H3	-2.917
InChI=1S/C5H8Cl3NO3/c1-2-12-4(11)9-3(10)5(6,7)8/h3,10H,2H2,1H3,(H,9,11)	-2.497
InChI=1S/C3H5N5O/c4-1-6-2(5)8-3(9)7-1/h(H5,4,5,6,7,8,9)	-3.229
InChI=1S/C13H16N4O5/c1-13(2,3)14-12(18)8-6-10(15-4-5-15)11(17(21)22)7-9(8)16(19)20/h6-7H,4-5H2,1-3H3,(H,14,18)	-3.17
InChI=1S/C14H19NO2/c1-4-11-17-13-10-8-7-9-12(13)14(16)15(5-2)6-3/h4,7-10H,1,5-6,11H2,2-3H3	-3.156
InChI=1S/C7H4N2/c1-2-4-7-6(3-1)5-8-9-7/h1-4H	-2.16
InChI=1S/C23H31FO6/c1-13(25)30-12-19(28)22(29)9-7-16-17-5-4-14-10-15(26)6-8-20(14,2)h10,16-18,27,29H,4-9,11-12H2,1-3H3	-4.209
InChI=1S/C7H6N4O/c1-12-6-3-9-7-5(11-6)2-8-4-10-7/h2-4H,1H3	-1.14
InChI=1S/C21H17N/c1-3-8-18(9-4-1)14-16-20-12-7-13-21(22-20)17-15-19-10-5-2-6-11-19h1-17H/b16-14+,17-15+	-6.276
InChI=1S/C60H116O6/c1-8-60(51-64-57(61)48-42-36-30-24-18-12-9-15-21-27-33-39-45-54(h54-56H,8-53H2,1-7H3	-7.271
InChI=1S/C11H11NO/c13-10-5-4-8-2-1-3-9-6-7-12(10)11(8)9/h1-3H,4-7H2	-1.637
InChI=1S/C7H6N2/c1-2-4-7-6(3-1)8-5-9-7/h1-5H,(H,8,9)	-1.769
InChI=1S/C9H5Cl2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H	-3.273
InChI=1S/C5H5N3O3S/c6-7-5(9)3-1-2-4(12-3)8(10)11/h1-2H,6H2,(H,7,9)	-1.97
InChI=1S/C10H10N2O4S/c1-7-5-10(13)12(11-7)8-3-2-4-9(6-8)17(14,15)16/h2-4,6H,5H2,1H3,(H,14,15,16)	-1.772
InChI=1S/C7H4ClN/c8-7-3-1-6(5-9)2-4-7/h1-4H	-2.749
InChI=1S/C6H10O3/c1-2-6(8)9-5-3-4-7/h2,7H,1,3-5H2	0.886
InChI=1S/C18H14N2O2/c1-11-3-5-15-13(9-11)19-17(21-15)7-8-18-20-14-10-12(2)4-6-16(14)2h3-10H,1-2H3/b8-7+	-6
InChI=1S/C9H13NO2/c1-3-9(4-2)7(11)5-6-10-8(9)12/h5-6H,3-4H2,1-2H3,(H,10,12)	-1.422
InChI=1S/C5H7NO/c6-4-5-2-1-3-7-5/h1-3H,4,6H2	1.013
InChI=1S/C13H18N2O3/c1-2-13(9-7-5-3-4-6-8-9)10(16)14-12(18)15-11(13)17/h7H,2-6,8H2,1H3,(H2,14,15,16,17,18)	-3
InChI=1S/C41H27N7O6/c1-18(49)25-16-27(29-31(33(25)42)37(53)23-14-8-6-12-21(23)35(29)h3-17H,42-43H2,1-2H3,(H2,44,45,46,47,48)	-4.95
InChI=1S/C10H20O/c1-8(2)6-10-7-9(3)4-5-11-10/h8-10H,4-7H2,1-3H3	-3.08
InChI=1S/C9H12O/c1-8(10)7-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3	-1.368

"InChi"	"logS(M)"
InChI=1S/C15H21ClN2O2/ c1-3-8-18-9-7-12(10-18)20-15(19)17-14-11(2)5-4-6-13(14)16/ h4-6,12H,3,7-10H2,1-2H3,(H,17,19)	-4.167
InChI=1S/C26H22BrF2NO4/ c1-16(2)24(17-6-10-21(11-7-17)33-26(28)29)25(31)34-23(15-30)18-4 h3-14,16,23-24,26H,1-2H3	-8.173
InChI=1S/C2H2N4O3/c7-2-3-1(4-5-2)6(8)9/h(H2,3,4,5,7)	-0.879
InChI=1S/C21H25N3O3S/ c25-21(27-16-15-26-14-13-23-11-4-1-5-12-23)24-17-7-2-3-8-18(17)28 h2-3,6-10H,1,4-5,11-16H2	-6.43
InChI=1S/C23H27NO3/ c1-3-24(4-2)14-16-27-23(25)22(17-19-11-8-15-26-19)21-13-7-10-18-9 h5-13,15,22H,3-4,14,16-17H2,1-2H3	-5.495
InChI=1S/C7H10O5/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1,4-6,8-10H, 2H2,(H,11,12)	0.01
InChI=1S/C16H17NO3/ c17-15(19)20-12-16(11-18,13-7-3-1-4-8-13)14-9-5-2-6-10-14/ h1-10,18H,11-12H2,(H2,17,19)	-2.712
InChI=1S/C5H12NO3PS2/c1-6-5(7)4-12-10(11,8-2)9-3/h4H2,1-3H3, (H,6,7)	-0.962
InChI=1S/C14H12/c1-12(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-11H, 1H2	-4.436
InChI=1S/C11H11ClN2O2/ c1-2-16-11(15)6-10-8-5-7(12)3-4-9(8)13-14-10/h3-5H,2,6H2,1H3,(H, 13,14)	-3.026
InChI=1S/C13H17NO/c15-13-7-10-14(11-8-13)9-6-12-4-2-1-3-5-12/ h1-5H,6-11H2	-0.808
InChI=1S/C19H24N2O/ c1-20-12-14-21(15-13-20)16-19(22,17-8-4-2-5-9-17)18-10-6-3-7-11-1 h2-11,22H,12-16H2,1H3	-2.023
InChI=1S/C8H10N6/c9-11-7-5-3-1-2-4-6(5)8(12-10)14-13-7/h1-4H, 9-10H2,(H,11,13)(H,12,14)	0.055
InChI=1S/C13H18O4/ c1-2-3-13(16)10-4-6-12(7-5-10)17-9-11(15)8-14/h4-7,11,14-15H, 2-3,8-9H2,1H3	-2.237
InChI=1S/C7H10O2/c1-4-5-9-7(8)6(2)3/h4H,1-2,5H2,3H3	-1.758
InChI=1S/C10H14FN3O4/ c1-12-9-5(11)3-14(10(17)13-9)8-2-6(16)7(4-15)18-8/h3,6-8,15-16H, 2,4H2,1H3,(H,12,13,17)	-1.317
InChI=1S/C11H15NO/c1-9(12-10(2)13)8-11-6-4-3-5-7-11/h3-7,9H, 8H2,1-2H3,(H,12,13)	-2.135
InChI=1S/C13H9N3O5/ c17-12(8-3-5-9(6-4-8)16(20)21)15-11-10(13(18)19)2-1-7-14-11/ h1-7H,(H,18,19)(H,14,15,17)	-4.06
InChI=1S/C9H16N2O6/ c12-3-4-6(14)7(15)8(17-4)11-2-1-5(13)10-9(11)16/h4-8,12-15H, 1-3H2,(H,10,16)	0.046
InChI=1S/C15H20N2/ c1-3-11-8-9-15(17(11)2)13-10-16-14-7-5-4-6-12(13)14/ h4-7,10-11,15-16H,3,8-9H2,1-2H3	-2.554
InChI=1S/C6H13N3/c1-5(2)3-4-9-6(7)8/h3H,4H2,1-2H3,(H4,7,8,9)	-0.668

"InChi"	"logS(M)"
InChI=1S/C8H8N2O3/c9-10-8(11)5-1-2-6-7(3-5)13-4-12-6/h1-3H,4,9H2,(H,10,11)	-0.6
InChI=1S/C12H5Cl5O/c13-6-3-10(16)12(11(17)4-6)18-7-1-2-8(14)9(15)5-7/h1-5H	-7.62
InChI=1S/C17H20N4O/c18-15(22)14-11-20-16-17(6-8-19-9-7-17)13-4-2-1-3-12(13)5-10-21(16)h1-4,11,19H,5-10H2,(H2,18,22)	-2.43
InChI=1S/C7H9N3O2/c8-4-1-2-5(6(11)3-4)7(12)10-9/h1-3,11H,8-9H2,(H,10,12)	-0.823
InChI=1S/C12H16O2/c1-8(2)6-12(14)10-4-5-11(13)9(3)7-10/h4-5,7-8,13H,6H2,1-3H3	-1.98
InChI=1S/C12H21N3/c1-4-7-10-9(6-3)12(13)15-11(14-10)8-5-2/h4-8H2,1-3H3,(H2,13,14,15)	-2.513
InChI=1S/C7H6ClNO4S/c8-5-2-1-4(7(10)11)3-6(5)14(9,12)13/h1-3H,(H,10,11)(H2,9,12,13)	-1.685
InChI=1S/C11H12O3/c1-2-13-11(12)10-9(14-10)8-6-4-3-5-7-8/h3-7,9-10H,2H2,1H3	-2.41
InChI=1S/C10H22/c1-5-7-9-10(3,4)8-6-2/h5-9H2,1-4H3	-4.811
InChI=1S/C8H19NO/c1-7(9)5-4-6-8(2,3)10/h7,10H,4-6,9H2,1-3H3	-0.029
InChI=1S/C5H13N/c1-3-5-6-4-2/h6H,3-5H2,1-2H3/p+1	1.055
InChI=1S/C12H19IN2O4S2/c13-11-4-5-12(15-10-11)19-8-3-1-2-6-14-7-9-20-21(16,17)18/h4-5,10,14H,1-3,6-9H2,(H,16,17,18)	-3.277
InChI=1S/C11H12Cl2N2O/c1-7(11-14-5-6-15-11)16-10-8(12)3-2-4-9(10)13/h2-4,7H,5-6H2,1H3,(H,14,15)	-4.497
InChI=1S/C6H12S/c7-6-4-2-1-3-5-6/h6-7H,1-5H2	-3.367
InChI=1S/C9H14N4O3/c10-2-1-8(14)13-7(9(15)16)3-6-4-11-5-12-6/h4-5,7H,1-3,10H2,(H,11,12)(H,13,14)(H,15,16)	-0.44
InChI=1S/C10H16ClN3O2/c11-3-4-14(13-16)10(15)12-9-6-7-1-2-8(9)5-7/h7-9H,1-6H2,(H,12,15)	-3.538
InChI=1S/C11H7ClN4O/c12-5-11(17)8-1-3-9(4-2-8)15-16-10(6-13)7-14/h1-4,15H,5H2	-3.19
InChI=1S/C17H25NO3/c1-3-4-9-15(19)13-14(2)8-5-6-10-16(20)18-12-7-11-17(18)21/h5-6,8,10,13,15,19H,3-4,7,9,11-12H2,1-2H3/b8-5+,10-6+,14-13+	-3.584
InChI=1S/C14H18N2O4S2/c17-22(18,19)21-11-9-15-7-3-10-20-14-13-5-2-1-4-12(13)6-8-16-14/h1-2,4-6,8,15H,3,7,9-11H2,(H,17,18,19)	-1.827
InChI=1S/C21H16/c1-13-5-8-17-15(11-13)7-9-18-19-10-6-14-3-2-4-16(21(14)19)12-20(1)h2-5,7-9,11-12H,6,10H2,1H3	-7.92
InChI=1S/C5H13N3O3S2/c1-2-7-5(6)8-3-4-12-13(9,10)11/h2-4H2,1H3,(H3,6,7,8)(H,9,10,11)	0.378
InChI=1S/C16H19N3O3/c1-12-14(18-8-10-22-11-9-18)15(20)19(16(21)17(12)2)13-6-4-3-5-7-13/h3-7H,8-11H2,1-2H3	-1.987
InChI=1S/C8H4F13I/c9-3(10,1-2-22)4(11,12)5(13,14)6(15,16)7(17,18)8(19,20)21/h1-2H2	-7.189
InChI=1S/C9H16O4/c1-2-3-4-5-6-7(8(10)11)9(12)13/h7H,2-6H2,1H3,(H,10,11)(H,12,13)	-1.657

"InChi"	"logS(M)"
InChI=1S/C14H14ClNO3/c15-10-2-1-3-11(8-10)16(13(17)9-4-5-9)12-6-7-19-14(12)18/h1-3,8-9,12H,4-7H2	-2.688
InChI=1S/C18H23N3O2/c22-17-12-23-18(13-20-17)6-9-21(10-7-18)8-5-14-11-19-16-4-2-1-3-15(14)16/h1-4,11,19H,5-10,12-13H2,(H,20,22)	-2.99
InChI=1S/C3H7NO/c1-2-3(4)5/h2H2,1H3,(H2,4,5)	-4.23
InChI=1S/C7H6N2S/c8-5-10-7-3-1-6(9)2-4-7/h1-4H,9H2	-2.602
InChI=1S/C12H18O2/c1-7(13)14-12-6-8-5-11(12)10-4-2-3-9(8)10/h8-12H,2-6H2,1H3	-3.338
InChI=1S/C15H24N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h11-14H,1-10H2	-2.475
InChI=1S/C4H7BrO2/c1-4(6)7-3-2-5/h2-3H2,1H3	-0.674
InChI=1S/C7H6ClNO3/c1-4-2-7(10)6(9(11)12)3-5(4)8/h2-3,10H,1H3	-4.39
InChI=1S/C8H6ClNOS/c1-12-8-10-6-4-5(9)2-3-7(6)11-8/h2-4H,1H3	-3.577
InChI=1S/C24H50O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25H,2-24H2,1H3	-5.55
InChI=1S/C6H9NO6/c8-3-1-11-6-4(13-7(9)10)2-12-5(3)6/h3-6,8H,1-2H2	-0.254
InChI=1S/C7H6O3/c8-7(9)4-3-6-2-1-5-10-6/h1-5H,(H,8,9)/b4-3+	-1.839
InChI=1S/C23H29NO/c1-2-22(25)23(20-12-5-3-6-13-20,21-14-7-4-8-15-21)16-11-19-24-17-h3-8,12-15H,2,9-11,16-19H2,1H3	-5.002
InChI=1S/C7H4ClNS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H	-3.778
InChI=1S/C8H8N4O2/c1-2-6(13)12-7-5(3-11-12)8(14)10-4-9-7/h3-4H,2H2,1H3,(H,9,10,14)	-2.81
InChI=1S/C13H20N2O3S/c1-3-18-11(16)9-10-14(2)12(17)13(19-10)15-7-5-4-6-8-15/h9,13H,3-8H2,1-2H3/b10-9-	-3.524
InChI=1S/C14H20N2O2/c1-14(2,3)16-9-12(17)10-18-13-7-5-4-6-11(13)8-15/h4-7,12,16-17H,9-10H2,1-3H3	-1.635
InChI=1S/C33H68O4/c1-5-9-13-17-21-25-34-29-33(30-35-26-22-18-14-10-6-2,31-36-27-23-h5-32H2,1-4H3	-7.945
InChI=1S/C14H13ClFN3O4S2/c15-10-6-11-13(7-12(10)24(17,20)21)25(22,23)19-14(18-11)5-8-1-3-9h1-4,6-7,14,18-19H,5H2,(H2,17,20,21)	-5.052
InChI=1S/C13H11N3/c14-8-5-6-10-12(7-8)16-11-4-2-1-3-9(11)13(10)15/h1-7H,14H2,(H2,15,16)	-3.4
InChI=1S/C21H30O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)8-9-20(13,2)19(15)18(24)11-h13,15-17,19H,4-11H2,1-3H3	-3.419
InChI=1S/C18H29NO3/c1-7-11-22-18(20)16-14(4)8-9-15(13(2)3)17(16)21-12-10-19(5)6/h8-9,13H,7,10-12H2,1-6H3	-4.354
InChI=1S/C9H6O2/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-6H	-1.446

"InChi"	"logS(M)"
InChI=1S/C19H35N3O8S4/c23-33(24,25)31-16-12-20-10-3-1-5-14-29-18-8-7-9-19(22-18)30-15-6h7-9,20-21H,1-6,10-17H2,(H,23,24,25)(H,26,27,28)	-5.154
InChI=1S/C10H20O5/c1-2-12-5-6-14-9-10-15-8-7-13-4-3-11-1/h1-10H2	-0.398
InChI=1S/C16H24N2O4/c1-10(2)17-8-14(21)9-22-16-6-5-13(18-12(4)20)7-15(16)11(3)19/h5-7,10,14,17,21H,8-9H2,1-4H3,(H,18,20)	-2.251
InChI=1S/C21H26ClN3O/c1-14(6-5-9-25(2)3)23-20-13-18(26-4)12-16-10-15-11-17(22)7-8-19(1h7-8,10-14,23H,5-6,9H2,1-4H3	-7.099
InChI=1S/C9H20O/c1-9(2)7-5-3-4-6-8-10/h9-10H,3-8H2,1-2H3	-2.487
InChI=1S/C10H10Cl3NO3/c11-7-3-1-6(2-4-7)8(15)10(12,13)5-17-9(14)16/h1-4,8,15H,5H2,(H2,14,16)	-3.418
InChI=1S/C8H9NO3/c1-12-8-6(11)3-2-5(4-10)7(8)9/h2-4,11H,9H2,1H3	-0.223
InChI=1S/C7H10N2O2/c1-3-6(10)8-5-9-7(11)4-2/h3-4H,1-2,5H2,(H,8,10)(H,9,11)	-0.655
InChI=1S/C16H21NO3/c1-17(14-10-6-3-7-11-14)15(18)12-20-16(19)13-8-4-2-5-9-13/h2,4-5,8-9,14H,3,6-7,10-12H2,1H3	-3.29
InChI=1S/C4HI4N/c5-1-2(6)4(8)9-3(1)7/h9H	-3.46
InChI=1S/C10H23NO3S2/c1-3-5-7-10(6-4-2)11-8-9-15-16(12,13)14/h10-11H,3-9H2,1-2H3,(H,12,13,14)	-1.753
InChI=1S/C16H17NO4/c1-10(16(19)21-9-15(17)18)11-3-4-13-8-14(20-2)6-5-12(13)7-11/h3-8,10H,9H2,1-2H3,(H2,17,18)	-3.93
InChI=1S/C14H22N2O5S2/c1-2-21-14(17)12-4-6-13(7-5-12)16-9-3-8-15-10-11-22-23(18,19)20/h4-7,15-16H,2-3,8-11H2,1H3,(H,18,19,20)	-3.688
InChI=1S/C15H28O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h11-14,16-17H,3-10H2,1-2H3	-3.098
InChI=1S/C23H32O4/c1-21-8-5-16(24)12-15(21)3-4-19-18(21)6-9-22(2)17(7-10-23(19,22)2h11,15,17-19,26H,3-10,12-13H2,1-2H3	-3.304
InChI=1S/C13H9ClN2O3/c14-11-6-1-8(13(18)19)7-12(11)16-15-9-2-4-10(17)5-3-9/h1-7,17H,(H,18,19)/b16-15+	-4.08
InChI=1S/C10H11N3O2S2/c1-7-6-10(16-12-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6,13H,11H2,1H3	-1.076
InChI=1S/C15H21ClN2O2/c1-3-18-9-7-12(8-10-18)20-15(19)17-14-11(2)5-4-6-13(14)16/h4-6,12H,3,7-10H2,1-2H3,(H,17,19)	-4.167
InChI=1S/C7H6ClNO3/c8-4-5-3-6(9(11)12)1-2-7(5)10/h1-3,10H,4H2	-2.303
InChI=1S/C8H5F3O/c9-8(10,11)7(12)6-4-2-1-3-5-6/h1-5H	-1.16
InChI=1S/C6H12O2/c1-3-4-5(2)6(7)8/h5H,3-4H2,1-2H3,(H,7,8)	-0.889
InChI=1S/C17H20ClNO/c18-16-9-8-15(13-6-2-3-7-14(13)16)17(20)12-19-10-4-1-5-11-19/h2-3,6-9,17,20H,1,4-5,10-12H2	-1.55

"InChi"	"logS(M)"
InChI=1S/C19H25N3OS/c1-4-5-14-23-18-12-8-16(9-13-18)21-19(24)20-15-6-10-17(11-7-15)22h6-13H,4-5,14H2,1-3H3,(H2,20,21,24)	-5.927
InChI=1S/C8H11NO6S2/c9-7-1-3-8(4-2-7)16(10,11)6-5-15-17(12,13)14/h1-4H,5-6,9H2,(H,12,13,14)	-1.905
InChI=1S/C20H27NO/c22-16-7-6-15-11-19-17-3-1-2-8-20(17,18(15)12-16)9-10-21(19)13-14h6-7,12,14,17,19,22H,1-5,8-11,13H2	-4.448
InChI=1S/C16H16N4O8S/c1-26-19-9(8-3-2-4-27-8)12(21)18-10-13(22)20-11(15(23)24)7(5-28-1h2-4,10,14H,5-6H2,1H3,(H2,17,25)(H,18,21)(H,23,24)/b19-9+	-3.467
InChI=1S/C21H20O12/c22-6-13-15(26)17(28)19(30)21(33-13)31-8-4-11(25)14-12(5-8)32-20(h1-5,13,15,17,19,21-26,28-30H,6H2	-1.346
InChI=1S/C4H5ClO2/c1-2-3(5)4(6)7/h2H,1H3,(H,6,7)/b3-2-	0.919
InChI=1S/C32H46O7/c1-6-27-21(4)12-13-31(39-27)17-25-16-24(38-31)11-10-20(3)14-19(2)h7-10,15,19,21,24-29,33,35H,6,11-14,16-18H2,1-5H3/b8-7-,20-10-,23-9-	-4.877
InChI=1S/C10H18O2/c1-4-7-8-9(5-2)10(11)12-6-3/h6,9H,3-5,7-8H2,1-2H3	-4.152
InChI=1S/C4H5N3/c5-1-3-7-4-2-6/h7H,3-4H2	1.022
InChI=1S/C12H7ClO2/c13-8-5-6-11-12(7-8)15-10-4-2-1-3-9(10)14-11/h1-7H	-5.836
InChI=1S/C13H11Cl2NO5/c1-3-20-11(18)13(2)10(17)16(12(19)21-13)9-5-7(14)4-8(15)6-9/h4-6H,3H2,1-2H3	-5.22
InChI=1S/C12H27NO2/c1-2-3-4-5-6-7-8-9-13-10-12(15)11-14/h12-15H,2-11H2,1H3	-2.64
InChI=1S/C13H19N5O5/c19-8-7-16-3-5-17(6-4-16)10-12(20)15-14-9-11-1-2-13(23-11)18(21)2h1-2,9,19H,3-8,10H2,(H,15,20)/b14-9+	-1.808
InChI=1S/C10H10O4/c1-13-9(11)7-3-5-8(6-4-7)10(12)14-2/h3-6H,1-2H3	-3.797
InChI=1S/C10H19N5O2/c1-6(2)7-13-15(9(17)14(7)11)8(16)12-10(3,4)5/h6H,11H2,1-5H3,(H,12,16)	-1.719
InChI=1S/C13H16N4O3S/c1-9(2)17-8-7-12(15-13(17)18)16-21(19,20)11-5-3-10(14)4-6-11/h3-9H,14H2,1-2H3,(H,15,16,18)	-3.17
InChI=1S/C20H22O4/c1-13(20(22)24-19-6-4-3-5-18(19)21)14-7-8-16-12-17(23-2)10-9-15(1h7-13,19H,3-6H2,1-2H3	-5.59
InChI=1S/C7H8FN3O3/c1-2-9-6(13)11-3-4(8)5(12)10-7(11)14/h3H,2H2,1H3,(H,9,13)(H,10,12,14)	-2.13
InChI=1S/C10H13NO3/c1-7(12)11-9-6-8(13-2)4-5-10(9)14-3/h4-6H,1-3H3,(H,11,12)	-1.592
InChI=1S/C15H11BrN2O/c1-10-17-14-8-7-11(16)9-13(14)15(19)18(10)12-5-3-2-4-6-12/h2-9H,1H3	-5.49

"InChi"	"logS(M)"
InChI=1S/C16H21ClN2/c1-18-15-8-9-16(18)12-19(11-15)10-2-3-13-4-6-14(17)7-5-13/h2-7,15-16H,8-12H2,1H3/b3-2+	-3.17
InChI=1S/C26H50O4/c1-23(2)17-11-7-5-9-15-21-29-25(27)19-13-14-20-26(28)30-22-16-10-h23-24H,5-22H2,1-4H3	-6.63
InChI=1S/C3H4S3/c4-3-5-1-2-6-3/h1-2H2	0.314
InChI=1S/C22H42O4/c1-5-9-13-19(7-3)17-25-21(23)15-11-12-16-22(24)26-18-20(8-4)14-10h19-20H,5-18H2,1-4H3	-6.569
InChI=1S/C12H7Cl3/c13-10-4-1-8(2-5-10)9-3-6-11(14)12(15)7-9/h1-7H	-6.554
InChI=1S/C20H22N2S/c1-3-7-19-17(5-1)22(18-6-2-4-8-20(18)23-19)14-16-13-21-11-9-15(16h1-8,15-16H,9-14H2	-5.888
InChI=1S/C11H16N4O4/c1-7(15-5-10(18)13-11(19)6-15)2-14-3-8(16)12-9(17)4-14/h7H,2-6H2,1H3,(H,12,16,17)(H,13,18,19)	-1.27
InChI=1S/C10H10N2/c1-12-7-3-5-10(12)9-4-2-6-11-8-9/h2-8H,1H3	-2.065
InChI=1S/C9H10O3/c1-6(10)8-4-3-7(12-2)5-9(8)11/h3-5,11H,1-2H3	-1.525
InChI=1S/C7H12O3/c8-7(9)5-10-6-3-1-2-4-6/h6H,1-5H2,(H,8,9)	-0.847
InChI=1S/C13H11NO6/c15-10(16)6-5-9(13(19)20)14-11(17)7-3-1-2-4-8(7)12(14)18/h1-4,9H,5-6H2,(H,15,16)(H,19,20)	-1.446
InChI=1S/C7H7NS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H2,8,9)	-1.92
InChI=1S/C10H12N4O4S3/c1-7-3-5-8(6-4-7)21(17,18)13-9-14(2)12-10(19-9)20(11,15)16/h3-6H,1-2H3,(H2,11,15,16)/b13-9+	-2.84
InChI=1S/C12H15NO8/c14-5-8-9(15)10(16)11(17)12(21-8)20-7-3-1-2-6(4-7)13(18)19/h1-4,8-12,14-17H,5H2	-1.28
InChI=1S/C26H52O2/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-22-24-26(27)28-25-23-21-h3-25H2,1-2H3	-6.899
InChI=1S/C3H5NO2S2/c4-3(7)8-1-2(5)6/h1H2,(H2,4,7)(H,5,6)	-0.748
InChI=1S/C14H14N4O2/c1-16-10-12(17(2)14(20)18(3)13(10)19)15-11(16)9-7-5-4-6-8-9/h4-8H,1-3H3	-3.31
InChI=1S/C2H2F2/c1-2(3)4/h1H2	-0.706
InChI=1S/C5H8O2/c6-5-3-1-2-4-7-5/h1-4H2	0.999
InChI=1S/C11H14ClNO4/c1-13-11(14)17-9-6-4-3-5-8(9)16-10(7-12)15-2/h3-6,10H,7H2,1-2H3,(H,13,14)	-2.3
InChI=1S/C4H8N2O3/c5-4(9)6-2-1-3(7)8/h1-2H2,(H,7,8)(H3,5,6,9)	-0.801
InChI=1S/C6H3F9/c1-2-3(7,8)4(9,10)5(11,12)6(13,14)15/h2H,1H2	-4.198
InChI=1S/C18H12/c1-2-7-15-12-18-16(11-14(15)6-1)10-9-13-5-3-4-8-17(13)18/h1-12H	-7.385
InChI=1S/C8H10N2S/c1-2-7-5-6(8(9)11)3-4-10-7/h3-5H,2H2,1H3,(H2,9,11)	-1.724

"InChi"	"logS(M)"
InChI=1S/C45H73NO15/c1-19-6-9-27-20(2)31-28(46(27)16-19)15-26-24-8-7-22-14-23(10-12-4h7,19-21,23-43,47-55H,6,8-18H2,1-5H3	-5.799
InChI=1S/C21H32O2/c1-13-11-14-12-15(22)5-8-19(14,2)16-6-9-20(3)17(18(13)16)7-10-21(h12-13,16-18,23H,5-11H2,1-4H3	-5.07
InChI=1S/C12H20N2O3/c1-5-7-8(3)12(6-2)9(15)13-11(17)14(4)10(12)16/h8H,5-7H2,1-4H3,(H,13,15,17)	-3.046
InChI=1S/C9H11NO2/c1-2-12-9(11)10-8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H,10,11)	-2.291
InChI=1S/C16H22O3/c1-2-14(15(17)18)16(19)10-8-13(9-11-16)12-6-4-3-5-7-12/h3-7,13-14,19H,2,8-11H2,1H3,(H,17,18)	-4.004
InChI=1S/C8H10N2O2/c1-12-7-4-2-6(3-5-7)8(11)10-9/h2-5H,9H2,1H3,(H,10,11)	-1.15
InChI=1S/C12H4Cl6/c13-5-3-6(11(17)9(16)4-5)10-7(14)1-2-8(15)12(10)18/h1-4H	-7.822
InChI=1S/C14H24O/c1-10(12(3)15)6-8-13-9-7-11(2)14(13,4)5/h6-8,10,12-13,15H,9H2,1-5H3/b8-6+	-3.786
InChI=1S/C7H9N3O2S2/c8-5-1-3-6(4-2-5)14(11,12)10-7(9)13/h1-4H,8H2,(H3,9,10,13)	-2.24
InChI=1S/C17H18O5/c1-2-5-11-9-6-3-4-7-10(9)15(19)14-12(18)8-13(17(20)21)22-16(11)14h8,19H,2-7H2,1H3,(H,20,21)	-2.68
InChI=1S/C7H4BrNO4/c8-5-2-1-4(7(10)11)3-6(5)9(12)13/h1-3H,(H,10,11)	-2.968
InChI=1S/C17H16ClNO4/c1-23-15-7-6-13(18)10-14(15)16(20)19-9-8-11-2-4-12(5-3-11)17(21)2h2-7,10H,8-9H2,1H3,(H,19,20)(H,21,22)	-4.537
InChI=1S/C9H17N/c1-2-3-4-5-6-7-8-9-10/h2-8H2,1H3	-3.299
InChI=1S/C17H18N2O/c1-19-11-10-15-14(12-19)8-5-9-16(15)18-17(20)13-6-3-2-4-7-13/h2-9H,10-12H2,1H3,(H,18,20)	-2.938
InChI=1S/C14H15N5O2/c1-20-11-4-8(5-12(21-2)10(11)6-15)3-9-7-18-14(17)19-13(9)16/h4-5,7H,3H2,1-2H3,(H4,16,17,18,19)	-2.733
InChI=1S/C16H26O/c1-11-9-13-7-6-8-15(3,4)14(13)10-16(11,5)12(2)17/h11H,6-10H2,1-5H3	-4.942
InChI=1S/C6H3BrCl2/c7-4-1-2-5(8)6(9)3-4/h1-3H	-1.011
InChI=1S/C18H19NO4/c1-2-23-18(22)16(12-13-8-10-15(20)11-9-13)19-17(21)14-6-4-3-5-7-1h3-11,16,20H,2,12H2,1H3,(H,19,21)	-3.33
InChI=1S/C15H20N2O5S2/c1-21-14-11-15(17-13-6-3-2-5-12(13)14)22-9-4-7-16-8-10-23-24(18,1h2-3,5-6,11,16H,4,7-10H2,1H3,(H,18,19,20)	-2.115
InChI=1S/C14H12ClNO3/c15-7-3-1-2-4-8(7)16-13(17)11-9-5-6-10(19-9)12(11)14(16)18/h1-4,9-12H,5-6H2	-1.208

"InChi"	"logS(M)"
InChI=1S/C17H20N2O/c1-18(2)15-9-5-13(6-10-15)17(20)14-7-11-16(12-8-14)19(3)4/h5-12H,1-4H3	-2.827
InChI=1S/C17H23NO2/c1-18-9-8-17-7-3-2-4-12(17)13(18)10-11-5-6-14(19)16(20)15(11)17/h5-6,12-13,19-20H,2-4,7-10H2,1H3	-2.106
InChI=1S/C19H24N2O2/c1-3-21(4-2)14-15-23-18-13-9-8-12-17(18)19(22)20-16-10-6-5-7-11-1h5-13H,3-4,14-15H2,1-2H3,(H,20,22)	-4.433
InChI=1S/C8H14O/c1-5-8(4,9)6-7(2)3/h1,7,9H,6H2,2-4H3	-1.037
InChI=1S/C19H20N2O2/c1-13-16(11-17(20)19(22)23)15-9-5-6-10-18(15)21(13)12-14-7-3-2-4-h2-10,17H,11-12,20H2,1H3,(H,22,23)	-4.87
InChI=1S/C4H6N2O2S/c5-4-6-2(1-9-4)3(7)8/h2H,1H2,(H2,5,6)(H,7,8)	0.257
InChI=1S/C6H4Cl2N2/c7-9-5-1-2-6(10-8)4-3-5/h1-4H/b9-5-,10-6+	-3.643
InChI=1S/C7H12O5/c8-1-5-7-6(11-4-10-5)2-9-3-12-7/h5-8H,1-4H2	-0.62
InChI=1S/C15H11NO2/c1-18-15(17)14-10-6-2-4-8-12(10)16-13-9-5-3-7-11(13)14/h2-9H,1H3	-4.735
InChI=1S/C7H10O/c8-7-4-5-1-2-6(7)3-5/h5-6H,1-4H2	-1.756
InChI=1S/C16H25NO2/c1-17(2)12-14-7-4-5-10-16(14,18)13-8-6-9-15(11-13)19-3/h6,8-9,11,14,18H,4-5,7,10,12H2,1-3H3	-2.36
InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2	1.236
InChI=1S/C11H6FN3O3/c12-6-1-2-7-8(5-6)14-11(13-7)9-3-4-10(18-9)15(16)17/h1-5H,(H,13,14)	-4
InChI=1S/C11H16O3/c1-8(12)6-9-4-5-10(13-2)11(7-9)14-3/h4-5,7-8,12H,6H2,1-3H3	-1.514
InChI=1S/C12H10O4S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8,13-14H	-2.357
InChI=1S/C13H16N2O2/c1-2-3-9-11-12(16)14-15(13(11)17)10-7-5-4-6-8-10/h4-8,11H,2-3,9H2,1H3,(H,14,16)	-2.574
InChI=1S/C14H30O/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h3-14H2,1-2H3	-5.855
InChI=1S/C21H18F3N3O3/c1-11-9-26(5-4-25-11)19-8-18-13(7-16(19)24)20(28)14(21(29)30)10-2h2-3,6-8,10-11,25H,4-5,9H2,1H3,(H,29,30)	-3.8
InChI=1S/C9H17Cl2NO2/c1-4-14-9(13)12(5-7(2)10)6-8(3)11/h7-8H,4-6H2,1-3H3	-3.81
InChI=1S/C4H8N2O2/c1-3(7)5-6-4(2)8/h1-2H3,(H,5,7)(H,6,8)	0.329
InChI=1S/C20H32O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(19,h13,15-17,22H,4-12H2,1-3H3	-4.759
InChI=1S/C29H38F3N3O2S/c1-2-3-4-5-11-28(36)37-21-20-34-18-16-33(17-19-34)14-8-15-35-24-9h6-7,9-10,12-13,22H,2-5,8,11,14-21H2,1H3	-9.794
InChI=1S/C17H34O2/c1-7-9-10-15(8-2)13-19-16(18)11-14(3)12-17(4,5)6/h14-15H,7-13H2,1-6H3	-5.955

"InChi"	"logS(M)"
InChI=1S/C4H6N4O2/c5-2-1(9)3(10)8-4(6)7-2/h2H,5H2,(H3,6,7,8,10)	-1.698
InChI=1S/C5H13N3/c1-7(2)5(6)8(3)4/h6H,1-4H3	0.939
InChI=1S/C10H10N4O/c1-7-12-13-9(10(15)14(7)11)8-5-3-2-4-6-8/h2-6H,11H2,1H3	-2.051
InChI=1S/C14H13NO2/c1-10-5-4-6-11(9-10)15-13-8-3-2-7-12(13)14(16)17/h2-9,15H,1H3,(H,16,17)	-5.06
InChI=1S/C16H18O3/c1-4-19-16(17)11(2)12-5-6-14-10-15(18-3)8-7-13(14)9-12/h5-11H,4H2,1-3H3	-5.24
InChI=1S/C14H26O6/c1-3-17-9-11-19-13(15)7-5-6-8-14(16)20-12-10-18-4-2/h3-12H2,1-2H3	-2.065
InChI=1S/C23H28O4/c1-2-3-4-5-6-12-17-26-22(24)20-15-10-11-16-21(20)23(25)27-18-19-1h7-11,13-16H,2-6,12,17-18H2,1H3	-8.288
InChI=1S/C13H10BrCl2O3P/c1-18-20(17,9-5-3-2-4-6-9)19-13-8-11(15)10(14)7-12(13)16/h2-8H,1H3	-4.99
InChI=1S/C20H18ClNO4/c1-12-16(11-19(23)26-3)17-10-15(25-2)8-9-18(17)22(12)20(24)13-4-6h4-10H,11H2,1-3H3	-6.078
InChI=1S/C21H26O3/c1-14(8-7-9-15(2)12-21(22)23)10-11-19-16(3)13-20(24-6)18(5)17(19)h7-13H,1-6H3,(H,22,23)/b9-7+,11-10+,14-8+,15-12+	-6.651
InChI=1S/C9H8O4/c1-13-9(12)7-4-2-6(3-5-7)8(10)11/h2-5H,1H3,(H,10,11)	-2.97
InChI=1S/C17H18O6/c1-9-5-10(18)6-14(22-4)17(9)16(19)15-12(21-3)7-11(20-2)8-13(15)23h6-9H,5H2,1-4H3	-3.699
InChI=1S/C5H10O2/c6-4-5-2-1-3-7-5/h5-6H,1-4H2	0.389
InChI=1S/C9H16O2S2/c10-8(12)6-4-2-1-3-5-7-9(11)13/h1-7H2,(H,10,12)(H,11,13)	-2.39
InChI=1S/C6H3ClN4/c7-5-2-9-6-4(11-5)1-8-3-10-6/h1-3H	-0.87
InChI=1S/C15H21NO5/c1-3-8-15(2,9-17)10-21-14(20)16-12-6-4-11(5-7-12)13(18)19/h4-7,17H,3,8-10H2,1-2H3,(H,16,20)(H,18,19)	-3.686
InChI=1S/C9H12ClO4P/c1-12-15(11,13-2)14-9-7-5-3-4-6(7)8(9)10/h3-4,6-7H,5H2,1-2H3	-2.001
InChI=1S/CH3FO2S/c1-5(2,3)4/h1H3	-0.514
InChI=1S/C13H13N3O/c1-9-3-2-4-12(15-9)16-13(17)10-5-7-11(14)8-6-10/h2-8H,14H2,1H3,(H,15,16,17)	-2.311
InChI=1S/C17H13ClN2O4/c1-10(17(21)22)23-12-3-5-13(6-4-12)24-16-9-19-15-8-11(18)2-7-14(1h2-10H,1H3,(H,21,22)	-6.06
InChI=1S/C37H67NO13/c1-14-25-37(10,45)30(41)20(4)27(39)18(2)16-35(8,44)32(51-34-28(4Ch18-26,28-32,34,40-42,44-45H,14-17H2,1-13H3	-1.27

"InChi"	"logS(M)"
InChI=1S/C10H12N2O5S/c1-4(13)17-2-5-3-18-9-6(11)8(14)12(9)7(5)10(15)16/h6,9H,2-3,11H2,1H3,(H,15,16)	-2.649
InChI=1S/C4H9NO3/c1-2(5)3(6)4(7)8/h2-3,6H,5H2,1H3,(H,7,8)	-0.353
InChI=1S/C23H30N2O3/c1-3-23(27)19-9-11-22(12-10-19)28-17-21(26)16-24-13-14-25(18(2)15 h4-12,18,21,26H,3,13-17H2,1-2H3	-3.57
InChI=1S/C7H7ClN2O/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H2,10,11)	-1.372
InChI=1S/C8H12N2/c9-7-5-3-1-2-4-6-8-10/h1-6H2	-1.081
InChI=1S/C22H34O4/c1-3-5-7-9-13-17-25-21(23)19-15-11-12-16-20(19)22(24)26-18-14-10- h11-12,15-16H,3-10,13-14,17-18H2,1-2H3	-8.56
InChI=1S/C11H16N2O3S/c1-9(14)13(4)10-5-7-11(8-6-10)17(15,16)12(2)3/h5-8H,1-4H3	-2.3
InChI=1S/C8H14O4/c9-3-7-11-5-1-2-6-12-8-4-10/h9-10H,3-8H2	0.759
InChI=1S/C4H7Cl3O2/c1-2(5)4(6,7)3(8)9/h2-3,8-9H,1H3	-0.867
InChI=1S/C22H21ClN2O5/c1-14(22(26)28-13-18-3-2-10-27-18)29-16-5-7-17(8-6-16)30-21-12-24 h4-9,11-12,14,18H,2-3,10,13H2,1H3	-5.03
InChI=1S/C5H13NO2/c1-6(2-4-7)3-5-8/h7-8H,2-5H2,1H3	0.924
InChI=1S/C26H50O10/c1-2-3-4-5-6-7-8-9-10-11-24(30)34-19-18-31-20-22(32-15-12-27)26-2 h22-23,25-29H,2-21H2,1H3	-6.417
InChI=1S/C10H20N2O/c1-3-6-11-8-5-9-12(7-4-2)10(11)13/h3-9H2,1-2H3	-2.375
InChI=1S/C13H24O4/c1-4-5-6-7-8-9-10-16-13(15)11(2)17-12(3)14/h11H,4-10H2,1-3H3	-3.39
InChI=1S/C8H16N2O3/c1-5(2)3-6(8(12)13)10-7(11)4-9/h5-6H,3-4,9H2,1-2H3,(H,10,11)(H,12,13)	-0.43
InChI=1S/C11H17N/c1-4-10(2)6-5-7-11(3)8-9-12/h6,8H,4-5,7H2,1-3H3/b10-6+,11-8+	-3.59
InChI=1S/C4H4BrNO2/c5-6-3(7)1-2-4(6)8/h1-2H2	-1.083
InChI=1S/C5H9NO/c7-6-5-3-1-2-4-5/h7H,1-4H2	-0.325
InChI=1S/C11H18N2O3/c1-3-16-11(15)10(14)13-8-4-5-9(13)7-12(2)6-8/h8-9H,3-7H2,1-2H3	-1.617
InChI=1S/C15H15N3O2S/c1-10(2)7-20-15(19)18-13-6-4-3-5-11(13)17-14(18)12-8-21-9-16-12/h3-6,8-10H,7H2,1-2H3	-4.17
InChI=1S/C6H3F7O/c1-14-3-2(7)4(8,9)6(12,13)5(3,10)11/h1H3	-2.449
InChI=1S/C12H24O2/c1-3-4-5-6-7-8-9-10-11-14-12(2)13/h3-11H2,1-2H3	-4.986
InChI=1S/C18H18ClNS/c1-20(2)11-5-7-14-15-6-3-4-8-17(15)21-18-10-9-13(19)12-16(14)18/h3-4,6-10,12H,5,11H2,1-2H3/b14-7+	-5.87
InChI=1S/C34H50O7/c1-29(2)23-10-13-34(7)27(32(23,5)12-11-24(29)41-26(38)9-8-25(36)3 h18,21,23-24,27H,8-17,19H2,1-7H3,(H,36,37)(H,39,40)	-9.69
InChI=1S/C8H17NO3/c1-2-3-4-7(5-10)6-12-8(9)11/h7,10H,2-6H2,1H3,(H2,9,11)	-1.247

"InChi"	"logS(M)"
InChI=1S/C11H16O4/c1-2-14-10-5-3-4-6-11(10)15-8-9(13)7-12/h3-6,9,12-13H,2,7-8H2,1H3	-1.53
InChI=1S/C11H22N2O3/c1-6(2)5-8(12)10(14)13-9(7(3)4)11(15)16/h6-9H,5,12H2,1-4H3,(H,13,14)(H,15,16)	-0.17
InChI=1S/C12H12N2O3/c1-2-9-10(15)13-12(17)14(11(9)16)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H,13,15,17)	-1.466
InChI=1S/C4H3Br3F3NO2/c5-3(6,7)1(12)11-2(13)4(8,9)10/h1,12H,(H,11,13)	-2.868
InChI=1S/C11H10IN3O2S/c12-11-6-3-9(7-14-11)15-18(16,17)10-4-1-8(13)2-5-10/h1-7,15H,13H2	-1.81
InChI=1S/C13H20O/c1-8(2)11-7-6-10(5)12(9(3)4)13(11)14/h6-9,14H,1-5H3	-3.544
InChI=1S/C22H30N2O2/c1-4-21-10-6-13-23-14-12-22(20(21)23)16-7-5-8-17(26-3)19(16)24(15h5,7-8,18,20H,4,6,9-14H2,1-3H3	-1.327
InChI=1S/C5H5N/c1-2-3-4-5-6/h2-4H,1H2/b4-3+	-0.722
InChI=1S/C13H11NO3/c14-9-6-7-11(12(15)8-9)13(16)17-10-4-2-1-3-5-10/h1-8,15H,14H2	-4.515
InChI=1S/C15H17NO5/c1-20-15(19)12-8-5-9-16(12)13(17)10-21-14(18)11-6-3-2-4-7-11/h2-4,6-7,12H,5,8-10H2,1H3	-2.084
InChI=1S/C16H19N5O2/c1-3-21-14-11(5-4-8-17-14)16(23)18-12-6-7-13(19-15(12)21)20(2)9-1h4-8,22H,3,9-10H2,1-2H3,(H,18,23)	-3.36
InChI=1S/C11H11NO/c1-9(13)12-8-4-6-10-5-2-3-7-11(10)12/h2-7H,8H2,1H3	-1.864
InChI=1S/C18H16N4O3/c23-10-14(24)17(25)15-16-18(20-13-9-5-4-8-12(13)19-16)22(21-15)1h1-9,14,17,23-25H,10H2	-3.13
InChI=1S/C6H7NO3S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H,7H2,(H,8,9,10)	-1.747
InChI=1S/C11H11N3O2/c1-8-4-2-3-5-9(8)13-10(15)14-11-12-6-7-16-11/h2-7H,1H3,(H2,12,13,14,15)	-2.797
InChI=1S/C7H12N2S/c10-7-8-5-3-1-2-4-6(5)9-7/h5-6H,1-4H2,(H2,8,9,10)	-0.077
InChI=1S/C11H15BrN2O2/c1-7-9(12)10(15)13(2)11(16)14(7)8-5-3-4-6-8/h8H,3-6H2,1-2H3	-3.238
InChI=1S/C15H26N2O3/c1-3-5-6-7-8-9-10-11-15(4-2)12(18)16-14(20)17-13(15)19/h3-11H2,1-2H3,(H2,16,17,18,19,20)	-4.46
InChI=1S/C9H21O4P/c1-4-7-8-9-13-14(10,11-5-2)12-6-3/h4-9H2,1-3H3	-1.476
InChI=1S/C11H22N2O4S2/c12-8(10(14)15)6-18-4-2-1-3-5-19-7-9(13)11(16)17/h8-9H,1-7,12-13H2,(H,14,15)(H,16,17)	-2.91
InChI=1S/C26H36O6/c1-4-5-6-22(31)32-26(21(30)15-27)12-10-19-18-8-7-16-13-17(28)9-11h9,11,13,18-20,23,27,29H,4-8,10,12,14-15H2,1-3H3	-5.889
InChI=1S/C7H5Cl3O2/c1-12-4-2-3(8)5(9)6(10)7(4)11/h2,11H,1H3	-3.66

"InChi"	"logS(M)"
InChI=1S/C11H10ClN3O2/c1-2-17-11(16)10(7-13)15-14-9-5-3-4-8(12)6-9/h3-6,14H,2H2,1H3/b15-10-	-4.401
InChI=1S/C15H14O4/c1-8(2)14-15(17-3)10-6-9-4-5-13(16)18-11(9)7-12(10)19-14/h4-8H,1-3H3	-4.122
InChI=1S/C22H34O3/c1-13-11-16(24)12-15-5-6-17-18-7-8-20(25-14(2)23)21(18,3)10-9-19(h13,15,17-20H,5-12H2,1-4H3	-5.093
InChI=1S/C5H10OS/c1-5(2)6-3-4-7-5/h3-4H2,1-2H3	-1.445
InChI=1S/C16H19NO3/c18-15-16(19)20-14(12-7-3-1-4-8-12)11-17(15)13-9-5-2-6-10-13/h1,3-4,7-8,13-14H,2,5-6,9-11H2	-3.847
InChI=1S/C7H9NO/c1-7(5-8)4-2-3-6(7)9/h2-4H2,1H3	0.909
InChI=1S/C7H8N2O/c1-10-9-6-7-2-4-8-5-3-7/h2-6H,1H3/b9-6+	0.167
InChI=1S/C9H7Cl5N2O/c10-6-2-1-5(3-7(6)11)16-8(15-4-17)9(12,13)14/h1-4,8,16H,(H,15,17)	-3.323
InChI=1S/C14H22O2/c1-3-10-14(16,11-4-2)13(15)12-8-6-5-7-9-12/h5-9,13,15-16H,3-4,10-11H2,1-2H3	-2.648
InChI=1S/C10H9NO3S/c11-8-4-5-9-7(6-8)2-1-3-10(9)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-2.75
InChI=1S/C20H28O3/c1-19-9-7-14(23-12-21)11-13(19)3-4-15-16-5-6-18(22)20(16,2)10-8-1h3,12,14-17H,4-11H2,1-2H3	-4.41
InChI=1S/C20H26N2O2/c1-16-8-4-5-13-22(16)14-7-15-24-20(23)21-19-12-6-10-17-9-2-3-11-1h2-3,6,9-12,16H,4-5,7-8,13-15H2,1H3,(H,21,23)	-4.753
InChI=1S/C21H31N5O4/c1-17(2)5-4-6-18(3)9-10-24-11-13-25(14-12-24)16-20(27)23-22-15-19h5,7-9,15H,4,6,10-14,16H2,1-3H3,(H,23,27)/b18-9-,22-15+	-5.503
InChI=1S/C4H8N2O3/c5-1-3(7)6-2-4(8)9/h1-2,5H2,(H,6,7)(H,8,9)	0.1
InChI=1S/C10H11IO3/c1-2-5-14-10(13)7-3-4-9(12)8(11)6-7/h3-4,6,12H,2,5H2,1H3	-3.687
InChI=1S/C13H17NO2/c1-2-16-13(15)14(12-8-9-12)10-11-6-4-3-5-7-11/h3-7,12H,2,8-10H2,1H3	-3.67
InChI=1S/C12H15N3O6/c1-7(2)5-10(12(16)17)13-9-4-3-8(14(18)19)6-11(9)15(20)21/h3-4,6-7,10,13H,5H2,1-2H3,(H,16,17)	-3.456
InChI=1S/C6H5NO2/c8-6(9)5-3-1-2-4-7-5/h1-4H,(H,8,9)	0.892
InChI=1S/C14H12N2/c1-9-6-7-13-11(8-9)14(15)10-4-2-3-5-12(10)16-13/h2-8H,1H3,(H2,15,16)	-2.39
InChI=1S/C6H8O/c1-4-6(3,7)5-2/h1,5,7H,2H2,3H3	-0.08
InChI=1S/C18H27ClO3/c1-4-5-6-7-8-9-12-21-18(20)15(3)22-17-11-10-16(19)13-14(17)2/h10-11,13,15H,4-9,12H2,1-3H3	-6.514
InChI=1S/C14H12N4O2/c15-5-1-2-6(16)10-9(5)13(19)11-7(17)3-4-8(18)12(11)14(10)20/h1-4H,15-18H2	-6.952

"InChi"	"logS(M)"
InChI=1S/C18H20FN3O3/c1-9-18(2,20)8-22(9)15-6-14-11(5-13(15)19)16(23)12(17(24)25)7-21(h5-7,9-10H,3-4,8,20H2,1-2H3,(H,24,25)	-5.42
InChI=1S/C29H36O6/c1-21(2)27(30)34-19-7-17-32-25-13-9-23(10-14-25)29(5,6)24-11-15-2h9-16H,1,3,7-8,17-20H2,2,4-6H3	-7.456
InChI=1S/C27H33N3O8/c1-26(37)13-7-6-8-16(31)17(13)21(32)18-14(26)11-15-20(29(2)3)22(3h6-8,14-15,20,31-32,35,37-38H,4-5,9-12H2,1-3H3,(H,28,36)	0.022
InChI=1S/C5H4N4O/c10-5-8-3-1-6-2-7-4(3)9-5/h1-2H,(H2,6,7,8,9,10)	-1.514
InChI=1S/C14H10N4O5/c19-12-9-16(14(20)17(12)10)4-2-1-3-5-10)15-8-11-6-7-13(23-11)18(2h1-8H,9H2/b15-8+	-2.601
InChI=1S/C25H35NO5/c1-6-26(19(2)17-20-9-12-22(28-3)13-10-20)15-7-8-16-31-25(27)21-11h9-14,18-19H,6-8,15-17H2,1-5H3	-5.694
InChI=1S/C14H8I4O4/c15-8-4-7(5-9(16)13(8)21)22-14-10(17)1-6(2-11(14)18)3-12(19)20/h1-2,4-5,21H,3H2,(H,19,20)	-9.508
InChI=1S/C12H20N2O4/c1-4-6-12(3,8-17-10(13)15)9-18-11(16)14-7-5-2/h2H,4,6-9H2,1,3H3,(H2,13,15)(H,14,16)	-2.487
InChI=1S/C8H14N4O/c1-4-9-7-10-6(3)11-8(12-7)13-5-2/h4-5H2,1-3H3,(H,9,10,11,12)	-2.914
InChI=1S/C8H14O4/c1-3-5(7(9)10)6(4-2)8(11)12/h5-6H,3-4H2,1-2H3,(H,9,10)(H,11,12)	-0.861
InChI=1S/C16H23ClN2O2/c1-11-6-5-7-13(17)14(11)18-15(20)21-12-8-9-19(10-12)16(2,3)4/h5-7,12H,8-10H2,1-4H3,(H,18,20)	-4.594
InChI=1S/C8H19NO3S2/c1-2-3-4-5-6-9-7-8-13-14(10,11)12/h9H,2-8H2,1H3,(H,10,11,12)	-0.773
InChI=1S/C9H11O4P/c10-9(11)6-7-14(12,13)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,11)(H,12,13)	-0.828
InChI=1S/C10H11NO2/c1-13-10-4-2-9(3-5-10)6-7-11-8-12/h2-8H,1H3,(H,11,12)/b7-6+	-2.151
InChI=1S/C20H24N2O4/c1-21-11-10-15-12-19(25-2)20(26-3)13-17(15)18(21)9-6-14-4-7-16(8-h4-5,7-8,12-13,18H,6,9-11H2,1-3H3	-4.629
InChI=1S/C16H12F3N3O/c17-16(18,19)10-6-7-12-13(8-10)22(11-4-2-1-3-5-11)15(23)9-14(20)2h1-8H,9H2,(H2,20,21)	-2.742
InChI=1S/C12H22N2O4/c1-4-6-12(3,8-17-10(13)15)9-18-11(16)14-7-5-2/h5H,2,4,6-9H2,1,3H3,(H2,13,15)(H,14,16)	-3.043
InChI=1S/C9H10BrNO2/c1-5-3-6(10)4-7(8(5)12)9(13)11-2/h3-4,12H,1-2H3,(H,11,13)	-3.398
InChI=1S/C13H11ClN2O/c1-9-3-2-8-15-12(9)16-13(17)10-4-6-11(14)7-5-10/h2-8H,1H3,(H,15,16,17)	-3.306

"InChi"	"logS(M)"
InChI=1S/C10H10N4O3S/c11-7-1-3-8(4-2-7)18(16,17)14-9-5-6-12-10(15)13-9/h1-6H,11H2,(H2,12,13,14,15)	-3.55
InChI=1S/C7H7N3/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H,(H3,8,9,10)	-0.951
InChI=1S/C13H24N3O3PS/c1-6-16(7-2)13-14-11(5)10-12(15-13)19-20(21,17-8-3)18-9-4/h10H,6-9H2,1-5H3	-4.924
InChI=1S/C17H13BrN4/c1-22-6-5-11-7-14-15(9-16(11)22)19-10-20-17(14)21-13-4-2-3-12(18)h2-10H,1H3,(H,19,20,21)	-3.31
InChI=1S/C11H18N2O4/c1-4-6-13-10(15)17-8-11(3,5-2)7-16-9(12)14/h1H,5-8H2,2-3H3,(H2,12,14)(H,13,15)	-1.964
InChI=1S/C6H12O2/c1-4-5(2)8-6(3)7/h5H,4H2,1-3H3	-1.273
InChI=1S/C7H10N2/c1-3-7-6(2)8-4-5-9-7/h4-5H,3H2,1-2H3	0.445
InChI=1S/C25H29BrF2O7/c1-12(29)34-11-21(33)24(35-13(2)30)6-5-14-15-7-18(27)16-8-19(31)1h8-9,14-15,18,20,32H,5-7,10-11H2,1-4H3	-5.506
InChI=1S/C17H13NO2/c19-17(14-8-2-1-3-9-14)18(20)16-12-6-10-13-7-4-5-11-15(13)16/h1-12,20H	-3.307
InChI=1S/C7H4ClF3/c8-6-3-1-2-5(4-6)7(9,10)11/h1-4H	-3.412
InChI=1S/C6H6N4O3S/c7-6(14)9-8-3-4-1-2-5(13-4)10(11)12/h1-3H,(H3,7,9,14)/b8-3+	-2.554
InChI=1S/C12H12Cl2N4/c1-2-9-10(11(15)18-12(16)17-9)6-3-4-7(13)8(14)5-6/h3-5H,2H2,1H3,(H4,15,16,17,18)	-3.853
InChI=1S/C16H28O/c17-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-16/h6,8H,1-5,7,9-15H2/b8-6-	-5.561
InChI=1S/C14H12ClNO3/c15-7-1-3-8(4-2-7)16-13(17)11-9-5-6-10(19-9)12(11)14(16)18/h1-4,9-12H,5-6H2	-1.488
InChI=1S/C9H20O/c1-4-7-9(5-2,6-3)8-10/h10H,4-8H2,1-3H3	-2.419
InChI=1S/C40H64O12/c1-21-17-29-9-13-34(49-29)26(6)38(42)46-23(3)19-31-11-15-36(51-3h21-36H,9-20H2,1-8H3	-9.248
InChI=1S/C13H14N2/c1-13(2)14-10-7-3-5-9-6-4-8-11(15-13)12(9)10/h3-8,14-15H,1-2H3	-2.93
InChI=1S/C18H18O4/c1-3-14(12-7-5-4-6-8-12)17(20)13-9-11(2)16(19)15(10-13)18(21)22/h4-10,14,19H,3H2,1-2H3,(H,21,22)	-5.205
InChI=1S/C8H5NO2/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4H,(H,10,11)	-2.088
InChI=1S/C13H17N5O8S2/c1-5-7(10(20)18(5)28(23,24)25)16-9(19)8(6-4-27-12(14)15-6)17-26-1h4-5,7H,1-3H3,(H2,14,15)(H,16,19)(H,21,22)(H,23,24,25)/b17-8-	-1.64
InChI=1S/C21H27N7O14P2/c22-17-12-19(25-7-24-17)28(8-26-12)21-16(32)14(30)11(41-21)6-39-4h1-4,7-8,10-11,13-16,20-21,29-32H,5-6H2,(H5-,22,23,24,25,33,34,35,36,37)	0.178

"InChi"	"logS(M)"
InChI=1S/C22H12N2O/c25-22-16-10-2-6-13-5-1-9-15(19(13)16)21-23-17-11-3-7-14-8-4-12-1h1-12H	-7.205
InChI=1S/C17H22I3N3O7/c1-8(27)23(6-9(28)7-26)15-13(19)10(16(29)21-2-4-24)12(18)11(14(15h9,24-26,28H,2-7H2,1H3,(H,21,29)(H,22,30)	-4.466
InChI=1S/C13H15NO6/c1-8(2)6-7-20-13(17)9-4-3-5-10(14(18)19)11(9)12(15)16/h3-5,8H,6-7H2,1-2H3,(H,15,16)/p-1	-3.069
InChI=1S/C17H9BrO/c18-15-9-8-11-10-4-1-2-5-12(10)17(19)14-7-3-6-13(15)16(11)14/h1-9H	-7.36
InChI=1S/C12H14N2O2/c1-3-12(9-7-5-4-6-8-9)10(15)14(2)11(16)13-12/h4-8H,3H2,1-2H3,(H,13,16)	-2.236
InChI=1S/C8H16NO5P/c1-7(6-8(10)9(2)3)14-15(11,12-4)13-5/h6H,1-5H3/b7-6+	0.625
InChI=1S/C24H51N/c1-4-7-10-13-16-19-22-25(23-20-17-14-11-8-5-2)24-21-18-15-12-9-6-h4-24H2,1-3H3	-6.85
InChI=1S/C18H15NO3/c20-16(21)12-11-15-19-17(13-7-3-1-4-8-13)18(22-15)14-9-5-2-6-10-1h1-10H,11-12H2,(H,20,21)	-2.24
InChI=1S/C36H62O11/c1-10-34(31-20(3)16-26(43-31)28-19(2)15-21(4)36(41,18-37)46-28)12h19-31,37-38,41H,10-18H2,1-9H3,(H,39,40)	-8.35
InChI=1S/C22H30O4/c1-20-9-5-15(23)13-14(20)3-4-16-17(20)6-10-21(2)18(16)7-11-22(21,h3-4,13,16-18,26H,5-12H2,1-2H3,(H,24,25)	-5.17
InChI=1S/C10H12N2O4/c1-7(2)11-9(13)5-3-8-4-6-10(16-8)12(14)15/h3-7H,1-2H3,(H,11,13)/b5-3+	-2.567
InChI=1S/C11H22N2O4/c1-4-6-11(3,7-16-9(12)14)8-17-10(15)13-5-2/h4-8H2,1-3H3,(H2,12,14)(H,13,15)	-2.653
InChI=1S/C15H19ClN2O4S2/c1-11-9-15(18-14-4-3-12(16)10-13(11)14)22-7-2-5-17-6-8-23-24(19,2h3-4,9-10,17H,2,5-8H2,1H3,(H,19,20,21)	-3.198
InChI=1S/C4H5N3O2/c1-3-5-2-4(6-3)7(8)9/h2H,1H3,(H,5,6)	-1.63
InChI=1S/C8H4N2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H	-1.085
InChI=1S/C10H14O2/c1-10(2,3)7-4-5-8(11)9(12)6-7/h4-6,11-12H,1-3H3	-1.92
InChI=1S/C20H20N2O6/c23-11-14(12-24)17(25)28-13-22-18(26)20(21-19(22)27,15-7-3-1-4-8-h1-10,14,23-24H,11-13H2,(H,21,27)	-2.21
InChI=1S/C4H9Br/c1-4(2,3)5/h1-3H3	-2.359
InChI=1S/C17H16Cl2N2O4/c1-11(17(22)21-7-2-8-23-21)24-13-3-5-14(6-4-13)25-16-15(19)9-12(1h3-6,9-11H,2,7-8H2,1H3	-4.592
InChI=1S/C6H13NO2/c1-4-9-6(8)5-7(2)3/h4-5H2,1-3H3	0.789
InChI=1S/C7H4Cl4O/c1-12-7-5(10)3(8)2-4(9)6(7)11/h2H,1H3	-5.131
InChI=1S/C6H12ClNO/c1-3-8(4-2)6(9)5-7/h3-5H2,1-2H3	-0.243

"InChi"	"logS(M)"
InChI=1S/C16H30Br2N2O2S2/c17-7-13-23-11-3-1-5-15(21)19-9-10-20-16(22)6-2-4-12-24-14-8-18/h1-14H2,(H,19,21)(H,20,22)	-6.555
InChI=1S/C20H15NO3/c22-15-9-5-13(6-10-15)20(14-7-11-16(23)12-8-14)17-3-1-2-4-18(17)21-19(24)h1-12,22-23H,(H,21,24)	-3.828
InChI=1S/C24H30O8/c1-6-8-14(25)18-16(27)11-17(32-5)12(20(18)28)10-13-21(29)19(15(2(h11,27-30H,6-10H2,1-5H3	-5.341
InChI=1S/C14H18N2O/c1-11(17)15-8-9-16-13(10-15)7-6-12-4-2-3-5-14(12)16/h2-5,13H,6-10H2,1H3	-2.661
InChI=1S/C8H16N2O3S2/c9-8(6-14-15(11,12)13)10-5-7-3-1-2-4-7/h7H,1-6H2,(H2,9,10)(H,11,12,13)	-2.182
InChI=1S/C21H20O8/c1-25-13-4-9(5-14(26-2)19(13)23)16-11-6-15-20(29-8-28-15)18(22)12h4-6,10,16-17,22-23H,3,7-8H2,1-2H3	-4.125
InChI=1S/C9H12N2O3/c1-3-5-9(4-2)6(12)10-8(14)11-7(9)13/h3H,1,4-5H2,2H3,(H2,10,11,12,13,14)	-1.61
InChI=1S/C19H30N2O/c1-3-16(2)19(18(20)22,17-10-6-4-7-11-17)12-15-21-13-8-5-9-14-21/h4,6-7,10-11,16H,3,5,8-9,12-15H2,1-2H3,(H2,20,22)	-4.715
InChI=1S/C12H3Cl7/c13-5-1-4(2-6(14)10(5)17)9-11(18)7(15)3-8(16)12(9)19/h1-3H	-9.1
InChI=1S/C17H26N2O4S/c1-4-19-10-6-7-13(19)12-18-17(20)15-11-14(24(21,22)5-2)8-9-16(15)h8-9,11,13H,4-7,10,12H2,1-3H3,(H,18,20)	-2.69
InChI=1S/C14H26N2S4/c1-4-5-6-7-8-9-10-11-14(2,3)20-19-13-16-15-12(17)18-13/h4-11H2,1-3H3,(H,15,17)	-3.989
InChI=1S/C9H12O2/c1-6-4-7(10)5-9(2,3)8(6)11/h4H,5H2,1-3H3	-0.878
InChI=1S/C18H16ClNO4S/c1-3-22-17(21)11(2)23-13-5-4-6-14(10-13)24-18-20-15-8-7-12(19)9-1h4-11H,3H2,1-2H3	-5.674
InChI=1S/C8H13NO2/c9-7(8(10)11)6-4-2-1-3-5-6/h1-2,6-7H,3-5,9H2,(H,10,11)	-1.604
InChI=1S/C8H6N2O/c1-2-4-7(5-3-1)8-10-9-6-11-8/h1-6H	-1.387
InChI=1S/C9H14N4O4/c1-2-16-9(14)10-8-7-13(11-17-8)12-3-5-15-6-4-12/h7H,2-6H2,1H3	0.616
InChI=1S/C8H8N2O4/c1-9(12)8(11)6-2-4-7(5-3-6)10(13)14/h2-5,12H,1H3	-2.87
InChI=1S/C20H32O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(19,h4,14-17,21-22H,5-12H2,1-3H3	-6.106
InChI=1S/C45H73NO16/c1-19-8-13-45(46-16-19)20(2)30-27(62-45)15-26-24-7-6-22-14-23(9-1h6,19-21,23-42,46-55H,7-18H2,1-5H3	-5.963
InChI=1S/C5H9NO/c7-5-3-1-2-4-6-5/h1-4H2,(H,6,7)	0.467
InChI=1S/C8H8N2O4/c1-14-9-8(11)6-2-4-7(5-3-6)10(12)13/h2-5H,1H3,(H,9,11)	-2.28
InChI=1S/C4H5N3O2/c1-2-3(8)5-4(9)7-6-2/h1H3,(H2,5,7,8,9)	-1.306

"InChi"	"logS(M)"
InChI=1S/C24H31NO4/c1-4-7-8-11-16-29-24(28)20-13-10-9-12-19(20)23(27)21-15-14-18(17-h9-10,12-15,17,26H,4-8,11,16H2,1-3H3	-7.395
InChI=1S/C7H16N2O2S/c8-4-7-12(10,11)9-5-2-1-3-6-9/h1-8H2	-0.893
InChI=1S/C8H16Cl2O5S2/c9-1-5-16(11,12)7-3-15-4-8-17(13,14)6-2-10/h1-8H2	-1.941
InChI=1S/C13H13NO5/c15-11(14-7-6-10(14)12(16)17)8-19-13(18)9-4-2-1-3-5-9/h1-5,10H,6-8H2,(H,16,17)	-2.14
InChI=1S/C4H5ClO4/c5-2(4(8)9)1-3(6)7/h2H,1H2,(H,6,7)(H,8,9)	-0.795
InChI=1S/C22H40N2O2/c1-19(2)16-21(17-20(3,4)24-19)18(25)23-22(26-21)14-12-10-8-6-5-7-h24H,5-17H2,1-4H3,(H,23,25)	-5.085
InChI=1S/C18H23ClN2O/c1-2-18(22)21-15-9-10-16(21)13-20(12-15)11-5-7-14-6-3-4-8-17(14)1h3-8,15-16H,2,9-13H2,1H3/b7-5+	-4.458
InChI=1S/C6H12N2O2/c1-3-5(7-9)6(4-2)8-10/h7,9H,3-4H2,1-2H3/b6-5+	-2.553
InChI=1S/C12H18O4S2/c1-3-7-17-9(11(13)14)5-6-10(12(15)16)18-8-4-2/h3-4,9-10H,1-2,5-8H2,(H,13,14)(H,15,16)	-2.2
InChI=1S/C15H26O/c1-11-7-8-13(15(11,5)6)9-10-14(3,4)12(2)16/h7,9-10,12-13,16H,8H2,1-6H3/b10-9+	-4.217
InChI=1S/C11H17O3PS/c1-3-13-15(12,14-4-2)16-10-11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-2H3	-2.416
InChI=1S/C11H11NO6S/c1-18-10(13)11(6-7-11)19(16,17)9-4-2-8(3-5-9)12(14)15/h2-5H,6-7H2,1H3	-3.38
InChI=1S/C6H14N2O6/c1-2-3-4-6(14-8(11)12)5-13-7(9)10/h6H,2-5H2,1H3,(H,9,10)(H,11,12)/q+2	-3.1
InChI=1S/C16H25NO2/c1-17(2)11-10-13-8-9-15(18)16(12-13)19-14-6-4-3-5-7-14/h8-9,12,14,18H,3-7,10-11H2,1-2H3	-3.214
InChI=1S/C31H35N5/c1-34(2)29-18-20-32-30(33-29)36-24-22-35(23-25-36)21-19-31(26-12h3-18,20H,19,21-25H2,1-2H3	-6.981
InChI=1S/C7H7NO3/c1-5-4-6(9)2-3-7(5)8(10)11/h2-4,9H,1H3	-2.11
InChI=1S/C6H10O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-5,7-10H,1H2	0.52
InChI=1S/C22H25NO4/c1-22(2,25)13-11-16-5-8-18(9-6-16)21(24)23-14-12-17-7-10-19(26-3)h5-10,15,25H,12,14H2,1-4H3,(H,23,24)	-2.203
InChI=1S/C9H10N2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-5H,6-7H2,(H,10,11)	-2.361
InChI=1S/C17H19N5O2/c1-9-11(6-10-7-12(23-2)4-5-13(10)24-3)8-20-16-14(9)15(18)21-17(19h4-5,7-8H,6H2,1-3H3,(H4,18,19,20,21,22)	-3.392
InChI=1S/C17H21NO4/c1-7-17(2,3)18-15(19)9-8-12-10-13(20-4)16(22-6)14(11-12)21-5/h1,8-11H,2-6H3,(H,18,19)/b9-8+	-3.018
InChI=1S/C15H10BrN5/c16-10-2-1-3-11(5-10)20-15-12-4-9-7-19-21-13(9)6-14(12)17-8-18-15h1-8H,(H,19,21)(H,17,18,20)	-3.96

"InChi"	"logS(M)"
InChI=1S/C10H11NO2/c1-7(12)9-5-3-4-6-10(9)11-8(2)13/h3-6H,1-2H3,(H,11,13)	-1.775
InChI=1S/C13H8Cl2O4S/c14-11-7(13(18)9-2-1-5-20-9)3-4-8(12(11)15)19-6-10(16)17/h1-5H,6H2,(H,16,17)	-4.286
InChI=1S/C10H13NO2/c1-8(13-10(11)12)7-9-5-3-2-4-6-9/h2-6,8H,7H2,1H3,(H2,11,12)	-2.307
InChI=1S/C12H15NO3/c1-3-16-11-6-4-10(8-9(11)2)5-7-12(14)13-15/h4-8,15H,3H2,1-2H3,(H,13,14)/b7-5+	-2.821
InChI=1S/C15H12/c1-11-5-4-8-14-9-12-6-2-3-7-13(12)10-15(11)14/h2-10H,1H3	-5.854
InChI=1S/C12H14N2O3/c1-2-16-11(15)7-8-14-9-5-3-4-6-10(9)17-12(14)13/h3-6,13H,2,7-8H2,1H3/b13-12+	-3.174
InChI=1S/C8H6Cl2O3/c9-6-2-1-5(3-7(6)10)13-4-8(11)12/h1-3H,4H2,(H,11,12)	-2.685
InChI=1S/C12H5Cl5O/c13-6-1-3-9(8(15)5-6)18-10-4-2-7(14)11(16)12(10)17/h1-5H	-7.44
InChI=1S/C17H19F2N3O3/c1-3-21-9-11(17(24)25)16(23)10-8-12(18)15(13(19)14(10)21)22-6-4-2h8-9H,3-7H2,1-2H3,(H,24,25)	-1.623
InChI=1S/C9H12N4S/c1-2-3-4-13-6-12-7-8(13)10-5-11-9(7)14/h5-6H,2-4H2,1H3,(H,10,11,14)	-2.339
InChI=1S/C16H15NO/c17-16(18)15-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)15/h1-8,15H,9-10H2,(H2,17,18)	-4.638
InChI=1S/C22H28N2O4/c1-4-14-12-24-10-9-22(17-7-5-6-8-18(17)23-21(22)26)19(24)11-15(14h5-8,13-15,19H,4,9-12H2,1-3H3,(H,23,26)/b16-13-	-4.892
InChI=1S/C2HClF2O2/c3-2(4,5)1(6)7/h(H,6,7)	0.884
InChI=1S/C12H17N5O4/c1-15-4-6-16(7-5-15)9-11(18)14-13-8-10-2-3-12(21-10)17(19)20/h2-3,8H,4-7,9H2,1H3,(H,14,18)/b13-8+	-2.968
InChI=1S/C15H17OP/c1-13(2)17(16,14-9-5-3-6-10-14)15-11-7-4-8-12-15/h3-13H,1-2H3	-3.363
InChI=1S/C16H25N3O/c1-3-16(20)19(15-9-5-6-10-17-15)14(2)13-18-11-7-4-8-12-18/h5-6,9-10,14H,3-4,7-8,11-13H2,1-2H3	-3.762
InChI=1S/C15H24O/c1-13(2)7-5-3-4-6-8-14-9-11-15(16)12-10-14/h9-13,16H,3-8H2,1-2H3	-4.587
InChI=1S/C9H10N4O5S3/c1-18-6-2-4-7(5-3-6)21(16,17)13-8-11-12-9(19-8)20(10,14)15/h2-5H,1H3,(H,11,13)(H2,10,14,15)	-2.25
InChI=1S/C9H19NO2/c1-2-3-4-5-6-7-8-12-9(10)11/h2-8H2,1H3,(H2,10,11)	-3.3
InChI=1S/C12H14O3/c1-2-10-7-9-5-8(6-12(13)14)3-4-11(9)15-10/h3-5,10H,2,6-7H2,1H3,(H,13,14)	-2.747
InChI=1S/C7H12N4O3S2/c1-4-16(13,14)7-10-9-6(15-7)11(3)5(12)8-2/h4H2,1-3H3,(H,8,12)	-1.945
InChI=1S/C11H20O2/c1-5-13-10(12)8-6-7-9-11(2,3)4/h5H,1,6-9H2,2-4H3	-7.122

"InChi"	"logS(M)"
InChI=1S/C20H10Cl2N2O2/c21-13-5-1-3-9-17(13)23-15-8-12-16(7-11(15)19(9)25)24-18-10(20(12h1-8H,(H,23,25)(H,24,26)	-6.457
InChI=1S/C15H14N2O3S2/c18-22(19,20)21-10-9-16-15-11-5-1-3-7-13(11)17-14-8-4-2-6-12(14)1h1-8H,9-10H2,(H,16,17)(H,18,19,20)	-6.137
InChI=1S/C10H22N2/c1-9(2)7-6-8-10(3,4)12(9)11-5/h11H,6-8H2,1-5H3	-2.473
InChI=1S/C16H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-15-17-16/h16H,2-15H2,1H3	-6.682
InChI=1S/C15H12F3NO4/c1-9(14(20)21)22-11-3-5-12(6-4-11)23-13-7-2-10(8-19-13)15(16,17)1h2-9H,1H3,(H,20,21)	-2.623
InChI=1S/C15H22N2O2/c1-11-5-4-6-12(2)14(11)16-15(18)19-13-7-9-17(3)10-8-13/h4-6,13H,7-10H2,1-3H3,(H,16,18)	-3.415
InChI=1S/C8H11N/c1-3-8-6-4-5-7(2)9-8/h4-6H,3H2,1-2H3	-0.823
InChI=1S/C16H26N2O3/c1-4-10-20-15-12-13(17)7-8-14(15)16(19)21-11-9-18(5-2)6-3/h7-8,12H,4-6,9-11,17H2,1-3H3	-2.943
InChI=1S/C14H26N2O/c1-14(2,3)16-13(17)12-8-10-6-4-5-7-11(10)9-15-12/h10-12,15H,4-9H2,1-3H3,(H,16,17)/p+1	-2.162
InChI=1S/C4H10O2S2/c1-3-7-8(5,6)4-2/h3-4H2,1-2H3	-1.109
InChI=1S/C9H11NO2/c1-2-6-12-9(11)8-4-3-5-10-7-8/h3-5,7H,2,6H2,1H3	-1.24
InChI=1S/C24H27N3O4S/c1-17(2)20-6-4-5-7-22(20)32-23-10-8-19(16-21(23)27(30)31)9-11-24(h4-11,16-17H,12-15H2,1-3H3/b11-9+	-2.7
InChI=1S/C15H12N2O2/c18-14-11-15(19)17(13-9-5-2-6-10-13)16(14)12-7-3-1-4-8-12/h1-10H,11H2	-2.279
InChI=1S/C2H8NO4P/c3-1-2-7-8(4,5)6/h1-3H2,(H2,4,5,6)	0.851
InChI=1S/C13H9ClN2O4/c14-8-1-3-9(4-2-8)15-13(18)11-7-10(16(19)20)5-6-12(11)17/h1-7,17H,(H,15,18)	-5.122
InChI=1S/C15H20N2O5S2/c1-11-9-15(17-14-4-3-12(21-2)10-13(11)14)22-7-5-16-6-8-23-24(18,1h3-4,9-10,16H,5-8H2,1-2H3,(H,18,19,20)	-2.163
InChI=1S/CH6N4O/c2-4-1(6)5-3/h2-3H2,(H2,4,5,6)	0.415
InChI=1S/C12H15BrO3/c1-2-3-4-7-16-12(15)9-5-6-11(14)10(13)8-9/h5-6,8,14H,2-4,7H2,1H3	-4.1
InChI=1S/C9H5F15O/c1-2-25-6(15,3(10,7(16,17)18)8(19,20)21)4(11,12)5(13,14)9(22,23)24h2H2,1H3	-7.289
InChI=1S/C19H16ClF3N2O7/c1-29-9-15(24-31-10-18(26)30-2)13-8-12(4-5-16(13)25(27)28)32-17-6h3-8H,9-10H2,1-2H3/b24-15+	-5.678
InChI=1S/C23H32N2OS/c1-15(2)19-13-18(26-17-11-9-8-10-12-17)14-20(16(3)4)21(19)24-22(2h8-16H,1-7H3,(H2,24,25,27)	-6.807

"InChi"	"logS(M)"
InChI=1S/C18H22N2/c1-2-6-15(7-3-1)12-13-19-14-17-11-10-16-8-4-5-9-18(16)20-17/h1-9,17,19-20H,10-14H2	-3.499
InChI=1S/C17H24N2O4S2/c1-2-6-14-13-17(19-16-8-4-3-7-15(14)16)23-11-5-9-18-10-12-24-25(2,22)21-18/h3-4,7-8,13,18H,2,5-6,9-12H2,1H3,(H,20,21,22)	-3.439
InChI=1S/C5H10O/c1-3-4-5(2)6/h3-4H2,1-2H3	-0.19
InChI=1S/C8H17NO/c10-8-4-7-9-5-2-1-3-6-9/h10H,1-8H2	-0.022
InChI=1S/C10H18O3/c1-2-8(9(11)12)10(13)6-4-3-5-7-10/h8,13H,2-7H2,1H3,(H,11,12)	-1.501
InChI=1S/C18H11NO2/c20-17-12-6-2-3-7-13(12)18(21)16(17)15-10-9-11-5-1-4-8-14(11)19-15/h1-10,16H	-4.701
InChI=1S/C8H7ClO3/c1-4-2-7(10)5(8(11)12)3-6(4)9/h2-3,10H,1H3,(H,11,12)	-3.125
InChI=1S/C12H9N3O3/c16-12-7-3-10(4-8-12)14-13-9-1-5-11(6-2-9)15(17)18/h1-8,13H	-4.796
InChI=1S/C5H8O4/c6-4(7)2-1-3-5(8)9/h1-3H2,(H,6,7)(H,8,9)	1
InChI=1S/C12H19NO3/c1-8(13)5-9-6-10(14-2)12(16-4)11(7-9)15-3/h6-8H,5,13H2,1-4H3	-0.869
InChI=1S/C14H23O4P/c1-3-5-12-16-19(15,17-13-6-4-2)18-14-10-8-7-9-11-14/h7-11H,3-6,12-13H2,1-2H3	-3.475
InChI=1S/C12H6Cl4O/c13-8-5-4-7(6-10(8)15)17-11-3-1-2-9(14)12(11)16/h1-6H	-6.9
InChI=1S/C16H16N2O5/c19-8-12-13(20)14(21)16(23-12)18-10-5-2-1-4-9(10)17-15(18)11-6-3-7,12-14,16,19-21H,8H2	-2.92
InChI=1S/C12H13NO4/c1-3-12(4-2)10-6-5-8(13(15)16)7-9(10)11(14)17-12/h5-7H,3-4H2,1-2H3	-3.66
InChI=1S/C12H2Cl8/c13-4-2-6(15)5(14)1-3(4)7-8(16)10(18)12(20)11(19)9(7)17/h1-2H	-9.5
InChI=1S/C11H21N/c1-8-11(2,3)9-5-6-10(7-9)12(8)4/h8-10H,5-7H2,1-4H3	-2.036
InChI=1S/C9H7NO2/c1-7(11)12-9-4-2-8(6-10)3-5-9/h2-5H,1H3	-1.799
InChI=1S/C4H6N2OS/c1-2-3(7)6-4(8)5-2/h2H,1H3,(H2,5,6,7,8)	-1.451
InChI=1S/C12H8Br2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H	-7.74
InChI=1S/C11H13N5O5/c12-15-13-5-10(18)14-9(6-17)11(19)7-1-3-8(4-2-7)16(20)21/h1-4,9,11,17,19H,5-6H2,(H,14,18)	-1.169
InChI=1S/C9H6ClNO/c10-8-4-2-1-3-7(8)9(12)5-6-11/h1-4H,5H2	-2.175
InChI=1S/C18H12N4O/c23-18-16-17(19-11-20-18)22-15(13-9-5-2-6-10-13)14(21-16)12-7-3-1-11H,(H,19,20,22,23)	-3.177
InChI=1S/C3H3ClN2/c4-3-1-5-6-2-3/h1-2H,(H,5,6)	-0.551
InChI=1S/C10H20O2S/c1-3-5-6-9(4-2)7-12-10(11)8-13/h9,13H,3-8H2,1-2H3	-4.635

"InChi"	"logS(M)"
InChI=1S/C8H8F3N3O4S2/c9-8(10,11)4-1-5-7(2-6(4)19(12,15)16)20(17,18)14-3-13-5/h1-2,13-14H,3H2,(H2,12,15,16)	-2.97
InChI=1S/C3H3N3O2S/c4-3-5-1-2(9-3)6(7)8/h1H,(H2,4,5)	-1.359
InChI=1S/C28H43N/c1-25(2,3)19-27(7,8)21-11-15-23(16-12-21)29-24-17-13-22(14-18-24)h11-18,29H,19-20H2,1-10H3	-6.595
InChI=1S/C6H3Cl2NO3/c7-3-1-4(8)6(10)5(2-3)9(11)12/h1-2,10H	-4.088
InChI=1S/C18H29NO4/c1-20-17-7-3-4-8-18(17)23-16-15-22-14-13-21-12-11-19-9-5-2-6-10-1h3-4,7-8H,2,5-6,9-16H2,1H3	-1.546
InChI=1S/C9H12NO5PS/c1-7-6-8(4-5-9(7)10(11)12)15-16(17,13-2)14-3/h4-6H,1-3H3	-4.04
InChI=1S/C11H8FN3O3/c12-8-6-15(11(18)14-9(8)16)10(17)13-7-4-2-1-3-5-7/h1-6H,(H,13,17)(H,14,16,18)	-1.618
InChI=1S/C5H12ClO2PS2/c1-3-7-9(10,8-4-2)11-5-6/h3-5H2,1-2H3	-3.592
InChI=1S/C9H6O4/c10-6-3-5-1-2-9(12)13-8(5)4-7(6)11/h1-4,10-11H	-1.745
InChI=1S/C14H16N2O4/c1-9(17)7-13(19)15-11-3-5-12(6-4-11)16-14(20)8-10(2)18/h3-6H,7-8H2,1-2H3,(H,15,19)(H,16,20)	-3.128
InChI=1S/C12H9N3O3/c16-12(14-10-2-1-7-13-8-10)9-3-5-11(6-4-9)15(17)18/h1-8H,(H,14,16)	-2.978
InChI=1S/C14H28O5S/c1-2-3-4-5-6-7-8-20-13-11(16)10(9-15)19-14(18)12(13)17/h10-18H,2-9H2,1H3	-2.91
InChI=1S/C21H24O4/c1-21(2,15-3-7-17(8-4-15)22-11-19-13-24-19)16-5-9-18(10-6-16)23-1h3-10,19-20H,11-14H2,1-2H3	-4.8
InChI=1S/C12H2Cl8O/c13-3-1-2-4(6(15)5(3)14)21-12-10(19)8(17)7(16)9(18)11(12)20/h1-2H	-10.6
InChI=1S/C5H11NS2/c1-6(2)5-3-7-8-4-5/h5H,3-4H2,1-2H3	-1.873
InChI=1S/C23H29N3O2/c1-17-19(20-15-22(27-2)23(28-3)16-21(20)24-17)9-10-25-11-13-26(1h4-8,15-16,24H,9-14H2,1-3H3	-4.249
InChI=1S/C4H7NO4/c1-3(6)5-9-2-4(7)8/h2H2,1H3,(H,5,6)(H,7,8)	0.858
InChI=1S/C13H29NO3S2/c1-2-3-4-5-6-7-8-9-10-11-14-12-13-18-19(15,16)17/h14H,2-13H2,1H3,(H,15,16,17)	-3.38
InChI=1S/C17H20O4/c1-12(17(19)21-9-3-8-18)13-4-5-15-11-16(20-2)7-6-14(15)10-13/h4-7,10-12,18H,3,8-9H2,1-2H3	-3.4
InChI=1S/C3H6O2/c4-1-3-2-5-3/h3-4H,1-2H2	1.13
InChI=1S/C12H16O/c1-10(13)9-12(2,3)11-7-5-4-6-8-11/h4-8H,9H2,1-3H3	-2.338
InChI=1S/C34H54O8/c1-9-25(31-21(6)18-34(11-3,42-31)26-16-17-33(40,10-2)23(8)41-26)3h13,15,19,21-23,25-26,28,31,35-36,40H,9-12,14,16-18H2,1-8H3,(H,38,39)	-8.679

"InChi"	"logS(M)"
InChI=1S/C6H7NOS/c1-5(7-8)6-3-2-4-9-6/h2-4,8H,1H3/b7-5+	-1.777
InChI=1S/C23H30N2O3/ c1-2-6-23(27)19-9-11-22(12-10-19)28-18-21(26)17-24-13-15-25(16-1 h3-5,7-12,21,26H,2,6,13-18H2,1H3	-5.238
InChI=1S/C17H34O3/ c1-5-9-11-15(7-3)13-19-17(18)20-14-16(8-4)12-10-6-2/h15-16H, 5-14H2,1-4H3	-6.98
InChI=1S/C5H11NO2/c1-6(7)2-4-8-5-3-6/h2-5H2,1H3	0.456
InChI=1S/C5H8O3/c1-4(6)3-5(7)8-2/h3H2,1-2H3	0.634
InChI=1S/C18H39N/ c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2)3/h4-18H2,1-3H3	-4.652
InChI=1S/C7H5ClO/c8-7-4-2-1-3-6(7)5-9/h1-5H	-1.981
InChI=1S/C17H14N2O2/ c20-15-17(19-16(21)18-15)13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)1 h1-8H,9-10H2,(H2,18,19,20,21)	-5.025
InChI=1S/C6H13Cl2NO/c1-2-9(10,5-3-7)6-4-8/h2-6H2,1H3	-1.628
InChI=1S/C10H9NO/c1-11-7-6-10(12)8-4-2-3-5-9(8)11/h2-7H,1H3	-0.982
InChI=1S/C13H26O4/c1-6-8-9-11(7-2)10-15-12(14)16-17-13(3,4)5/ h11H,6-10H2,1-5H3	-4.66
InChI=1S/C20H16/ c1-13-6-5-9-18-19-12-16-8-4-3-7-15(16)11-17(19)10-14(2)20(13)18/ h3-12H,1-2H3	-7.974
InChI=1S/C12H13N3O4S/ c1-8-7-12(14-19-8)15-20(17,18)11-5-3-10(4-6-11)13-9(2)16/h3-7H, 1-2H3,(H,13,16)(H,14,15)	-2.384
InChI=1S/C52H98N16O13/ c1-9-29(6)11-10-12-40(71)59-32(13-19-53)47(76)68-42(31(8)70)52(8 h27-39,41-42,69-70H,9-26,53-57H2,1-8H3,(H,58,80)(H,59,71)(H, 60,75)(H,61,72)(H,62,78)(H,63,73)(H,64,81)(H,65,74)(H,66,79)(H, 67,77)(H,68,76)	-0.311
InChI=1S/C14H22O/c1-10-7-6-8-14(4,5)13(10)9-11(2)12(3)15/ h7,9,13H,6,8H2,1-5H3/b11-9-	-3.992
InChI=1S/C21H27NO/ c1-16(15-22(2)3)14-21(23)19-10-6-4-8-17(19)12-13-18-9-5-7-11-20(1 h4-11,16,23H,12-15H2,1-3H3	-5.617
InChI=1S/C14H18N2O4S3/ c1-10(2)16-8-11-4-3-5-12(6-11)22(17,18)13-7-14(21-9-13)23(15,19)2 h3-7,9-10,16H,8H2,1-2H3,(H2,15,19,20)	-1.56
InChI=1S/C20H13NS/ c1-3-7-15-13(5-1)9-11-17-19(15)22-20-16-8-4-2-6-14(16)10-12-18(20 h1-12,21H	-6.879
InChI=1S/C15H12O2/ c16-14-9-5-4-8-13(14)15(17)11-10-12-6-2-1-3-7-12/h1-11,16H/ b11-10+	-3.634
InChI=1S/C27H32O14/ c1-10-20(32)22(34)24(36)26(37-10)41-25-23(35)21(33)18(9-28)40-27 h2-7,10,16,18,20-30,32-36H,8-9H2,1H3	-2.722
InChI=1S/C19H17OP/ c20-21(18-12-6-2-7-13-18,19-14-8-3-9-15-19)16-17-10-4-1-5-11-17/ h1-15H,16H2	-4.398

"InChi"	"logS(M)"
InChI=1S/C17H16N2O3/c1-11-7-3-5-9-13(11)18-16(21)15(20)17(22)19-14-10-6-4-8-12(14)2/h3-10H,1-2H3,(H,18,21)(H,19,22)	-2.2
InChI=1S/C11H9N5O/c17-10-8-9(13-6-12-8)15-11(16-10)14-7-4-2-1-3-5-7/h1-6H,(H3,12,13,14,15,16,17)	-4.12
InChI=1S/C19H17ClN2O4/c20-12-5-6-14-17(7-8-21-18(14)9-12)22-16-4-2-1-3-15(16)19(25)26-1h1-9,13,23-24H,10-11H2,(H,21,22)	-4.54
InChI=1S/C20H23NO5/c1-23-16-8-6-12-13(10-15(16)22)14(21)7-5-11-9-17(24-2)19(25-3)20(h6,8-10,14H,5,7,21H2,1-4H3	-1.737
InChI=1S/C3H6N2O5/c1-2(6)3(4(7)8)5(9)10/h2-3,6H,1H3	0.079
InChI=1S/C7H14O3/c1-2-3-6-10-7(9)4-5-8/h8H,2-6H2,1H3	-1.29
InChI=1S/C14H18N2O/c15-12-14(17)7-10-16(11-8-14)9-6-13-4-2-1-3-5-13/h1-5,17H,6-11H2	-1.441
InChI=1S/C12H8Cl2O/c13-10-7-4-8-11(14)12(10)15-9-5-2-1-3-6-9/h1-8H	-5.061
InChI=1S/C19H16ClNO4/c1-24-17-10-15(18(25-2)9-14(17)20)21-19(23)13-7-11-5-3-4-6-12(11)h3-10,22H,1-2H3,(H,21,23)	-5.062
InChI=1S/C9H21NO3/c1-7(11)4-10(5-8(2)12)6-9(3)13/h7-9,11-13H,4-6H2,1-3H3	0.417
InChI=1S/C7H5NO/c8-5-6-3-1-2-4-7(6)9/h1-4,9H	-0.775
InChI=1S/C31H35NO11/c1-14-26(34)18(32-7-9-41-10-8-32)11-21(42-14)43-20-13-31(39,15(2)h4-6,14,18,20-21,26,34,36,38-39H,7-13H2,1-3H3	-5.049
InChI=1S/C13H9N3O2/c14-13-9-3-1-2-4-11(9)15-12-7-8(16(17)18)5-6-10(12)13/h1-7H,(H2,14,15)	-4.341
InChI=1S/C18H23N3/c1-20(2)12-7-13-21-17-10-5-3-8-15(17)14-19-16-9-4-6-11-18(16)21/h3-6,8-11,19H,7,12-14H2,1-2H3	-4.306
InChI=1S/C6H10O2S2/c7-5(9)3-1-2-4-6(8)10/h1-4H2,(H,7,9)(H,8,10)	-1.733
InChI=1S/C6H10/c1-5-6(2,3)4/h1H,2-4H3	-2.614
InChI=1S/C12H4Cl4O2/c13-5-1-7(15)11-9(3-5)18-12-8(16)2-6(14)4-10(12)17-11/h1-4H	-9.003
InChI=1S/C8H9NO/c1-7(10)9-8-5-3-2-4-6-8/h2-6H,1H3,(H,9,10)	-1.33
InChI=1S/C10H18O2S2/c11-9(13)7-5-3-1-2-4-6-8-10(12)14/h1-8H2,(H,11,13)(H,12,14)	-3.07
InChI=1S/C13H9ClN2/c14-8-5-6-12-10(7-8)13(15)9-3-1-2-4-11(9)16-12/h1-7H,(H2,15,16)	-2.42
InChI=1S/C42H69NO15/c1-11-16-32(48)55-40-27(6)53-34(23-42(40,7)58-31(47)12-2)56-37-2(h13-15,18,20,24-30,34-41,45-46,50H,11-12,16-17,19,21-23H2,1-10H3/b14-13-,18-15-	-6.854
InChI=1S/C8H8N4O/c9-7-10-8(13)12(11-7)6-4-2-1-3-5-6/h1-5H,(H3,9,10,11,13)	-2.47
InChI=1S/C13H9NO/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H	-3.759

"InChi"	"logS(M)"
InChI=1S/C7H9NO4S/c1-12-7-3-2-5(4-6(7)8)13(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)	-0.9
InChI=1S/C9H12N6/c1-2-13(1)7-10-8(14-3-4-14)12-9(11-7)15-5-6-15/h1-6H2	0.292
InChI=1S/C7H11ClO4/c1-3-11-6(9)5(8)7(10)12-4-2/h5H,3-4H2,1-2H3	-1.721
InChI=1S/C10H14/c1-3-9-5-7-10(4-2)8-6-9/h5-8H,3-4H2,1-2H3	-3.75
InChI=1S/C13H22O2/c1-5-12(14)15-11-8-6-10(7-9-11)13(2,3)4/h5,10-11H,1,6-9H2,2-4H3	-3.539
InChI=1S/C10H11N3O/c1-8-7-10(12-13(8)2)14-9-5-3-4-6-11-9/h3-7H,1-2H3	-0.98
InChI=1S/C17H9ClF8N2O4/c18-8-6-7(4-5-11(8)31-16(22,23)14(21)32-17(24,25)26)27-15(30)28-1h1-6,14H,(H2,27,28,29,30)	-6.968
InChI=1S/C8H8N2O2S/c1-6-9-7-4-2-3-5-8(7)13(11,12)10-6/h2-5H,1H3,(H,9,10)	-0.88
InChI=1S/C9H11Cl2FN2O2S2/c1-13(2)18(15,16)14(17-9(10,11)12)8-6-4-3-5-7-8/h3-7H,1-2H3	-5.409
InChI=1S/C6H14N2O/c1-3-5-8(7-9)6-4-2/h3-6H2,1-2H3	-1.001
InChI=1S/C14H26N4S4/c1-15-5-3-7-17(11-9-15)13(19)21-22-14(20)18-8-4-6-16(2)10-12-18/h3-12H2,1-2H3	0.187
InChI=1S/C14H22ClNO/c1-11(10-16(3)4)14(2,17)9-12-5-7-13(15)8-6-12/h5-8,11,17H,9-10H2,1-4H3	-2.788
InChI=1S/C9H13NO2/c1-10-6-9(12)7-2-4-8(11)5-3-7/h2-5,9-12H,6H2,1H3	0.777
InChI=1S/C17H24N4O5/c1-16(2,3)14(23)25-9-20-8-18-12-11(13(20)22)7-19-21(12)10-26-15(2h7-8H,9-10H2,1-6H3	-4.26
InChI=1S/C9H13BrN2O4S2/c10-8-1-2-9(12-7-8)16-5-3-11-4-6-17-18(13,14)15/h1-2,7,11H,3-6H2,(H,13,14,15)	-1.133
InChI=1S/C2H2O2/c3-1-2-4/h1-2H	1.236
InChI=1S/C17H12O6/c1-20-10-6-11-14(8-4-5-21-17(8)22-11)15-13(10)7-2-3-9(18)12(7)16(h4-6,8,17H,2-3H2,1H3	-3.713
InChI=1S/C4H9NO/c1-2-3-4(5)6/h2-3H2,1H3,(H2,5,6)	0.272
InChI=1S/C16H21N5O2/c1-3-6-21-7-4-5-11(21)10-17-16(22)12-8-13-14(19-20-18-13)9-15(12)h3,8-9,11H,1,4-7,10H2,2H3,(H,17,22)(H,18,19,20)	-3.029
InChI=1S/C7H8N2O4/c1-3-4(2-5(10)11)6(12)9-7(13)8-3/h2H2,1H3,(H,10,11)(H2,8,9,12,13)	-2.31
InChI=1S/C20H26O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(18,h1,16-18,22H,4-12H2,2H3	-4.523
InChI=1S/C11H13NO4/c13-10(14)6-9(11(15)16)12-7-8-4-2-1-3-5-8/h1-5,9,12H,6-7H2,(H,13,14)(H,15,16)	-1.063
InChI=1S/C14H18O5/c1-10-6-4-5-7-14(10)18-9-13(19-12(3)16)8-17-11(2)15/h4-7,13H,8-9H2,1-3H3	-3.372

"InChi"	"logS(M)"
InChI=1S/C11H20O/c1-2-3-4-5-7-10-8-6-9-11(10)12/h10H, 2-9H2,1H3	-3.452
InChI=1S/C48H86N4O8/ c1-41(2)23-31(24-42(3,4)49(41)17)57-37(53)21-35(39(55)59-33-27-45 h31-36H,21-30H2,1-20H3	-4.673
InChI=1S/C6H13NO2/c1-4-7(5-2)6(8)9-3/h4-5H2,1-3H3	-0.292
InChI=1S/C12H7N3O2/ c16-15(17)10-7-8-3-1-5-13-11(8)12-9(10)4-2-6-14-12/h1-7H	-3.917
InChI=1S/C13H26O3/c1-3-4-5-6-7-8-9-10-11-16-13(15)12(2)14/ h12,14H,3-11H2,1-2H3	-3.06
InChI=1S/C10H12N2O5/ c1-5-4-6(13)12(3-2-7(14)15)10(17)8(5)9(11)16/h4,13H,2-3H2,1H3, (H2,11,16)(H,14,15)	-1.602
InChI=1S/C17H18N4O3/ c1-12(22)18-15-7-3-13(4-8-15)11-21(2)20-19-16-9-5-14(6-10-16)17(2 h3-10H,11H2,1-2H3,(H,18,22)(H,23,24)/b20-19+	-4.441
InChI=1S/C18H23NO2/ c1-19-10-9-18-8-4-3-5-14(18)16(19)17(20)13-7-6-12(21-2)11-15(13)1 h6-7,11,14,16H,3-5,8-10H2,1-2H3	-3.727
InChI=1S/C15H20N2O6/ c1-8-15(23)17(6-11(19)13(21)12(20)7-18)10-5-3-2-4-9(10)14(22)16-8 h2-5,8,11-13,18-21H,6-7H2,1H3,(H,16,22)	-1.51
InChI=1S/C19H31NO2/ c1-2-3-4-5-6-7-8-9-10-11-16-22-19(21)17-12-14-18(20)15-13-17/ h12-15H,2-11,16,20H2,1H3	-7.8
InChI=1S/C24H30N2O4/ c1-3-24(28)20-9-11-22(12-10-20)29-18-23(30-19(2)27)17-25-13-15-2 h4-12,23H,3,13-18H2,1-2H3	-4.275
InChI=1S/C20H23Br2NO2/ c1-15(2)18-5-3-4-6-19(18)20(24)25-17-9-7-16(8-10-17)23(13-11-21)1 h3-10,15H,11-14H2,1-2H3	-8.041
InChI=1S/C13H17N3O3/ c17-13(10-15-8-2-1-3-9-15)14-11-4-6-12(7-5-11)16(18)19/h4-7H, 1-3,8-10H2,(H,14,17)	-3.834
InChI=1S/C10H12S2/c1-2-5-9(6-3-1)10-11-7-4-8-12-10/ h1-3,5-6,10H,4,7-8H2	-3.888
InChI=1S/C4H11NO/c1-2-4(6)3-5/h4,6H,2-3,5H2,1H3	1.05
InChI=1S/C16H11Cl2NO3/ c1-8(16(20)21)9-2-5-14-13(6-9)19-15(22-14)11-4-3-10(17)7-12(11)18 h2-8H,1H3,(H,20,21)	-5.206
InChI=1S/C7HF5O2/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h(H, 13,14)	-1.479
InChI=1S/C4H8O/c1-2-3-4-5/h2-3,5H,4H2,1H3/b3-2+	0.362
InChI=1S/C17H27NO3/ c1-7-20-17(19)15-13(4)8-9-14(12(2)3)16(15)21-11-10-18(5)6/ h8-9,12H,7,10-11H2,1-6H3	-3.834
InChI=1S/C14H12N2/ c1-9-5-4-8-12-13(9)14(15)10-6-2-3-7-11(10)16-12/h2-8H,1H3, (H2,15,16)	-4.349
InChI=1S/C10H17N2O4PS/ c1-5-8-11-9(15-6-2)7-10(12-8)16-17(18,13-3)14-4/h7H,5-6H2,1-4H3	-3.864

"InChi"	"logS(M)"
InChI=1S/C12H27OPS3/c1-4-7-10-15-14(13,16-11-8-5-2)17-12-9-6-3/h4-12H2,1-3H3	-5.14
InChI=1S/C17H29BrN2O4S2/c18-16-9-10-17(20-15-16)24-13-8-6-4-2-1-3-5-7-11-19-12-14-25-26(2h9-10,15,19H,1-8,11-14H2,(H,21,22,23)	-5.304
InChI=1S/C10H11NO4/c1-7(2)10(12)15-9-5-3-8(4-6-9)11(13)14/h3-7H,1-2H3	-3.959
InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+	-1.939
InChI=1S/C5H8N2O2/c8-6-4-2-1-3-5(4)7-9/h6,8H,1-3H2	-1.994
InChI=1S/C3H10N2/c1-3(5)2-4/h3H,2,4-5H2,1H3	1.13
InChI=1S/C9H17NO5/c1-9(2,5-11)7(14)8(15)10-4-3-6(12)13/h7,11,14H,3-5H2,1-2H3,(H,10,15)(H,12,13)	0.659
InChI=1S/C8H8ClNO4/c1-13-7-4-6(10(11)12)8(14-2)3-5(7)9/h3-4H,1-2H3	-3.179
InChI=1S/C36H34Cl2N6O4/c1-19-7-11-29(21(3)15-19)39-35(47)33(23(5)45)43-41-31-13-9-25(17-h7-18,33-34H,1-6H3,(H,39,47)(H,40,48)/b43-41+,44-42+	-9.292
InChI=1S/C7H14N2O2/c1-3-5(4-2)6(10)9-7(8)11/h5H,3-4H2,1-2H3,(H3,8,9,10,11)	-1.133
InChI=1S/C4H5N3O2/c1-2-3(4(5)8)7-9-6-2/h1H3,(H2,5,8)	-1.704
InChI=1S/C10H13Br2NO/c11-5-7-13(8-6-12)9-1-3-10(14)4-2-9/h1-4,14H,5-8H2	-4.125
InChI=1S/C12H20N2O3S/c1-3-4-8(2)7-12(5-6-15)9(16)13-11(18)14-10(12)17/h8,15H,3-7H2,1-2H3,(H2,13,14,16,17,18)	-3.09
InChI=1S/C13H16N2O6/c1-7-9(14(17)18)6-10(15(19)20)12(21-8(2)16)11(7)13(3,4)5/h6H,1-5H3	-4.472
InChI=1S/C6H10N6/c7-4-10-5(8)12-6(11-4)9-3-1-2-3/h3H,1-2H2,(H5,7,8,9,10,11,12)	-1.179
InChI=1S/C4H7Cl3O2/c1-2-9-3(8)4(5,6)7/h3,8H,2H2,1H3	-0.612
InChI=1S/C9H7ClO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,(H,11,12)/b6-5+	-2.457
InChI=1S/C20H28O2/c1-3-20-11-10-16-15-7-5-14(22-2)12-13(15)4-6-17(16)18(20)8-9-19(2h5,7,12,16-19,21H,3-4,6,8-11H2,1-2H3	-4.876
InChI=1S/C12H14O4/c1-4-5-8-6-9(13-2)11-12(10(8)14-3)16-7-15-11/h4,6H,1,5,7H2,2-3H3	-3.512
InChI=1S/C20H23ClN4OS/c21-15-6-7-19-17(14-15)25(16-4-1-2-5-18(16)27-19)9-3-8-23-10-12-2h1-2,4-7,14H,3,8-13H2,(H2,22,26)	-6.556
InChI=1S/C12H4Cl6O/c13-5-1-9(17)11(3-7(5)15)19-12-4-8(16)6(14)2-10(12)18/h1-4H	-8.36
InChI=1S/C10H10Cl2N2OS/c11-8-2-1-7(3-9(8)12)16-5-6-4-14-10(13)15-6/h1-3,6H,4-5H2,(H2,13,14)	-3.766
InChI=1S/C12H13N3O4/c16-12(9-13-14-5-7-19-8-6-14)10-1-3-11(4-2-10)15(17)18/h1-4,9H,5-8H2/b13-9+	-1.664
InChI=1S/C17H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h18H,2-17H2,1H3	-7.506

"InChi"	"logS(M)"
InChI=1S/C9H19N/c1-8(10-2)7-9-5-3-4-6-9/h8-10H,3-7H2,1-2H3	-1.791
InChI=1S/C14H22O/c1-13(2,3)10-14(4,5)11-6-8-12(15)9-7-11/h6-9,15H,10H2,1-5H3	-4.469
InChI=1S/C14H12ClN3O/c1-2-18-12-8-9(15)5-6-11(12)17-14(19)10-4-3-7-16-13(10)18/h3-8H,2H2,1H3,(H,17,19)	-5.36
InChI=1S/C15H18ClN3O/c1-11(12-2-3-12)15(20,8-19-10-17-9-18-19)13-4-6-14(16)7-5-13/h4-7,9-12,20H,2-3,8H2,1H3	-3.319
InChI=1S/C15H23NO3/c1-2-3-4-5-6-7-13-8-10-16(14(17)12-13)11-9-15(18)19/h8,10,12H,2-7,9,11H2,1H3,(H,18,19)	-4.4
InChI=1S/C4H11NO4S2/c1-3-10(6,7)5-11(8,9)4-2/h5H,3-4H2,1-2H3	0.541
InChI=1S/C3H9NO2/c4-3(1-5)2-6/h3,5-6H,1-2,4H2	0.974
InChI=1S/C10H19N/c1-9(2)5-4-6-10(3)7-8-11/h9-10H,4-7H2,1-3H3	-3.588
InChI=1S/C9H7NO4/c11-9(12)6-5-7-3-1-2-4-8(7)10(13)14/h1-6H,(H,11,12)/b6-5+	-2.218
InChI=1S/C17H27NO2/c1-18(2)13-16(17(19)11-5-4-6-12-17)14-7-9-15(20-3)10-8-14/h7-10,16,19H,4-6,11-13H2,1-3H3	0.257
InChI=1S/C6H4N4O3/c11-2-1-7-4-3(8-2)5(12)10-6(13)9-4/h1H,(H,8,11)(H2,7,9,10,12,13)	-3.13
InChI=1S/C3H8O/c1-2-3-4/h4H,2-3H2,1H3	0.62
InChI=1S/C5H6N2O/c6-5-4(8)2-1-3-7-5/h1-3,8H,(H2,6,7)	-0.346
InChI=1S/C33H27ClN4O6/c1-42-27-14-13-20(32(40)35-21-10-5-4-6-11-21)16-26(27)37-38-30-2 h4-18,37H,1-3H3,(H,35,40)(H,36,41)/b38-30-	-7.847
InChI=1S/C15H26O/c1-10-5-8-15(16)13(2,3)11-6-7-14(15,4)12(10)9-11/h10-12,16H,5-9H2,1-4H3	-3.726
InChI=1S/C8H15N5O/c1-4-9-6-11-7(10-5-2)13-8(12-6)14-3/h4-5H2,1-3H3,(H2,9,10,11,12,13)	-1.79
InChI=1S/C15H22O9/c16-4-6-3-8(18)7-1-2-22-14(10(6)7)24-15-13(21)12(20)11(19)9(5-17) h1-3,7-21H,4-5H2	0.012
InChI=1S/C11H13NO2S/c15-11-12-7-6-10(14-11)8-13-9-4-2-1-3-5-9/h1-5,10H,6-8H2,(H,12,15)	-3.02
InChI=1S/C6H7NO2S2/c1-3-4(2-5(8)9)11-6(10)7-3/h2H2,1H3,(H,7,10)(H,8,9)	-0.57
InChI=1S/C12H14N2O/c15-12(11-6-2-1-3-7-11)10-13-14-8-4-5-9-14/h1-3,6-7,10H,4-5,8-9H2/b13-10+	-2.058
InChI=1S/C7H16O5S2/c1-4-13(9,10)7(3,6-8)14(11,12)5-2/h8H,4-6H2,1-3H3	-0.165
InChI=1S/C21H30O2/c1-16(9-7-10-17(2)15-20(22)23-6)12-13-19-18(3)11-8-14-21(19,4)5/h7,9-10,12-13,15H,8,11,14H2,1-6H3/b10-7+,13-12+,16-9+,17-15+	-8.444
InChI=1S/C10H21NO/c1-5-9(6-2)10(12)11(7-3)8-4/h9H,5-8H2,1-4H3	-1.088

"InChi"	"logS(M)"
InChI=1S/C10H16N2O3S/c1-2-3-4-10(5-6-13)7(14)11-9(16)12-8(10)15/h13H,2-6H2,1H3,(H2,11,12,14,15,16)	-2.17
InChI=1S/C15H16N4O/c1-19(11-12-5-3-2-4-6-12)18-17-14-9-7-13(8-10-14)15(16)20/h2-10H,11H2,1H3,(H2,16,20)/b18-17+	-3.514
InChI=1S/C9H17NO2/c1-10(12)9(11)8-6-4-2-3-5-7-8/h8,12H,2-7H2,1H3	-1.45
InChI=1S/C15H24O2/c1-11-7-9-14(3)12(2)6-5-8-15(14,4)13(11)17-10-16/h6,10-11,13H,5,7-9H2,1-4H3	-5.031
InChI=1S/C13H21N2O4PS/c1-5-11(4)14-20(21,18-6-2)19-13-9-10(3)7-8-12(13)15(16)17/h7-9,11H,5-6H2,1-4H3,(H,14,21)	-4.814
InChI=1S/C16H23N5O5/c1-5-20(6-2)11(22)7-8-12(23)26-10-21-9-17-14-13(21)15(24)19(4)16(h9H,5-8,10H2,1-4H3	-1.14
InChI=1S/C16H9NO2/c18-17(19)14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16(12)15(10)11/h1-9H	-7.321
InChI=1S/C11H15Cl2O3PS2/c1-4-14-17(18,15-5-2)16-8-6-9(12)11(13)10(7-8)19-3/h6-7H,4-5H2,1-3H3	-6.081
InChI=1S/C10H12N2O5S/c11-18(16,17)8-3-1-7(2-4-8)12-9(13)5-6-10(14)15/h1-4H,5-6H2,(H,12,13)(H,14,15)(H2,11,16,17)	-2.03
InChI=1S/C8H17N/c1-7(2)5-6-8(3,4)9-7/h9H,5-6H2,1-4H3	-0.821
InChI=1S/C5H5N5O2/c6-2-1-3(9-4(11)7-1)10-5(12)8-2/h(H5,6,7,8,9,10,11,12)	-3.46
InChI=1S/C7H7N3O/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3H,8H2,(H2,9,10)	-0.719
InChI=1S/C8H10N4O2/c1-11(2)10-9-7-4-3-5-8(6-7)12(13)14/h3-6H,1-2H3/b10-9+	-2.966
InChI=1S/C20H12N2O6/c23-13-8-6-11(21-10-4-2-1-3-5-10)15-17(13)20(26)18-14(24)9-7-12(2h1-9,21,23-24H	-8.646
InChI=1S/C15H16O4S/c1-11(2)19-13-5-9-15(10-6-13)20(17,18)14-7-3-12(16)4-8-14/h3-11,16H,1-2H3	-4.171
InChI=1S/C12H11N/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H,13H2	-2.861
InChI=1S/C16H15NO2/c1-2-19-16(18)14-8-10-15(11-9-14)17-12-13-6-4-3-5-7-13/h3-12H,2H2,1H3/b17-12+	-4.061
InChI=1S/C10H21N/c1-9(2)7-6-8-10(3,4)11(9)5/h6-8H2,1-5H3	-1.541
InChI=1S/C12H24N2O4/c1-3-5-6-7-12(4-2,8-17-10(13)15)9-18-11(14)16/h3-9H2,1-2H3,(H2,13,15)(H2,14,16)	-3.195
InChI=1S/C12H12N2O2S/c13-9-3-1-5-11(7-9)17(15,16)12-6-2-4-10(14)8-12/h1-8H,13-14H2	-3.512
InChI=1S/C10H22O/c1-3-5-7-9-11-10-8-6-4-2/h3-10H2,1-2H3	-3.769
InChI=1S/C4H5Cl/c1-3-4(2)5/h3H,1-2H2	-2.551

"InChi"	"logS(M)"
InChI=1S/C9H16O4/c1-4-5-6-12-9(11)7(2)13-8(3)10/h7H, 4-6H2,1-3H3	-0.754
InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,7H,1,4,6,8H2,2-3H3	-4.386
InChI=1S/C13H19NO/c1-4-14(5-2)11(3)13(15)12-9-7-6-8-10-12/ h6-11H,4-5H2,1-3H3	-2.287
InChI=1S/C4H7NO5/c1-2-9-4(6)3-10-5(7)8/h2-3H2,1H3	-1.711
InChI=1S/C15H10Cl2N2O2/ c16-9-5-6-13-11(7-9)15(19(21)8-14(20)18-13)10-3-1-2-4-12(10)17/ h1-7,21H,8H2	-4.465
InChI=1S/C9H10O3/c1-5-3-2-4-6-7(5)9(11)12-8(6)10/h2-3,5-7H, 4H2,1H3	-0.736
InChI=1S/C20H10Cl2F5N3O3/ c21-11-5-4-10(29-19(32)30-17(31)16-13(23)2-1-3-14(16)24)7-15(11)3 h1-8H,(H2,29,30,31,32)	-7.403
InChI=1S/C16H26O7/ c1-13(2)15(17)22-11-9-20-7-5-19-6-8-21-10-12-23-16(18)14(3)4/ h1,3,5-12H2,2,4H3	-1.419
InChI=1S/C11H16N4O3/ c1-14-9-8(10(17)15(2)11(14)18)12-7(13-9)5-3-4-6-16/h16H, 3-6H2,1-2H3,(H,12,13)	-2.491
InChI=1S/C20H32N2O3S/ c1-6-8-13-22(14-9-7-2)26-21(5)19(23)24-17-12-10-11-16-15-20(3,4)2 h10-12H,6-9,13-15H2,1-5H3	-6.103
InChI=1S/C9H20O3/c1-3-5-11-7-9(10)8-12-6-4-2/h9-10H, 3-8H2,1-2H3	-0.343
InChI=1S/C24H29ClO4/ c1-12(26)24(29-13(2)27)8-6-16-14-10-20(25)19-11-21(28)15-9-18(15) h10-11,14-18H,5-9H2,1-4H3	-7.026
InChI=1S/C10H18O/c1-3-8(2)9-6-4-5-7-10(9)11/h8-9H,3-7H2,1-2H3	-2.427
InChI=1S/C21H28N2O/ c1-2-11-21(18-4-3-5-20(24)15-18)12-14-23(16-21)13-10-17-6-8-19(22 h3-9,15,24H,2,10-14,16,22H2,1H3	-3.68
InChI=1S/C13H17IO3/ c1-2-3-4-5-8-17-13(16)10-6-7-12(15)11(14)9-10/h6-7,9,15H, 2-5,8H2,1H3	-4.43
InChI=1S/C9H11NO3/c1-13-8-4-2-7(3-5-8)9(12)10-6-11/h2-5,11H, 6H2,1H3,(H,10,12)	-1.22
InChI=1S/C15H23NO/ c1-4-8-15(9-10-16(2)12-15)13-6-5-7-14(11-13)17-3/h5-7,11H, 4,8-10,12H2,1-3H3	-3.172
InChI=1S/C13H18O3/c1-2-3-4-7-10-16-13(15)11-8-5-6-9-12(11)14/ h5-6,8-9,14H,2-4,7,10H2,1H3	-5.046
InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/ h6-8,12H,5,9H2,1-4H3/b8-7+	-3.259
InChI=1S/C14H16ClNO3/ c1-9-4-3-5-10(2)13(9)16(12(17)8-15)11-6-7-19-14(11)18/h3-5,11H, 6-8H2,1-2H3	-3.285
InChI=1S/C6H5FN2O3/c1-3(10)9-5(11)4(7)2-8-6(9)12/h2H,1H3,(H, 8,12)	-0.6
InChI=1S/C4H10O2/c1-2-6-4-3-5/h5H,2-4H2,1H3	1.045

"InChi"	"logS(M)"
InChI=1S/C15H26O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h12-13,16H,1,5-10H2,2-4H3	-4.484
InChI=1S/C23H23F2NO2/c1-2-23(17-9-13-19(24)14-10-17,18-11-15-20(25)16-12-18)28-22(27)21-h1,9-16,21H,3-8H2,(H,26,27)	-7.659
InChI=1S/C13H13ClN2O2S/c1-9-2-3-10(14)8-13(9)16-19(17,18)12-6-4-11(15)5-7-12/h2-8,16H,15H2,1H3	-3.98
InChI=1S/C6H8N2O3/c1-2-3-4(9)7-6(11)8-5(3)10/h3H,2H2,1H3,(H2,7,8,9,10,11)	-0.92
InChI=1S/C8H5IO2/c9-6-2-1-5-4-11-8(10)7(5)3-6/h1-3H,4H2	-3.211
InChI=1S/CHF3/c2-1(3)4/h1H	-1.233
InChI=1S/C9H9N5O6S3/c1-13-8(21-9(11-13)22(10,17)18)12-23(19,20)7-4-2-3-6(5-7)14(15)16/h2-5H,1H3,(H2,10,17,18)/b12-8+	-2.67
InChI=1S/C7H9N5/c1-12(2)7-5-6(9-3-8-5)10-4-11-7/h3-4H,1-2H3,(H,8,9,10,11)	-1.3
InChI=1S/C15H12O4/c1-11(16)18-14-10-6-5-9-13(14)15(17)19-12-7-3-2-4-8-12/h2-10H,1H3	-4.108
InChI=1S/C18H17NO2S/c1-11(2)13-4-6-14(7-5-13)18-19-15-9-12(10-17(20)21)3-8-16(15)22-1h3-9,11H,10H2,1-2H3,(H,20,21)	-5.197
InChI=1S/C20H22Cl3NO2/c1-24-9-8-13-10-17(25-2)18(26-3)11-14(13)16(24)7-5-12-4-6-15(21)2h4,6,10-11,16H,5,7-9H2,1-3H3	-6.472
InChI=1S/C11H14FNO2/c1-8(2)13(11(15)7-14)10-5-3-9(12)4-6-10/h3-6,8,14H,7H2,1-2H3	-1.179
InChI=1S/C12H11NO5/c14-9-6-12(18,7-10(15)16)11(17)13(9)8-4-2-1-3-5-8/h1-5,18H,6-7H2,(H,15,16)	-0.68
InChI=1S/C8H7NO3/c10-7(8(11)12)9-6-4-2-1-3-5-6/h1-5H,(H,9,10)(H,11,12)	-1.302
InChI=1S/C13H18O/c1-13(2,3)12-8-6-11(7-9-12)5-4-10-14/h6-10H,4-5H2,1-3H3	-3.159
InChI=1S/C14H12N2O2/c17-15-13(11-7-3-1-4-8-11)14(16-18)12-9-5-2-6-10-12/h1-10,15,17H/b14-13+	-5.413
InChI=1S/C15H16Cl3N3O2/c1-2-4-20(15(22)21-5-3-19-10-21)6-7-23-14-12(17)8-11(16)9-13(14)1h3,5,8-10H,2,4,6-7H2,1H3	-4.045
InChI=1S/C16H10F5N5O4S2/c17-10-11(18)13(20)15(14(21)12(10)19)32(29,30)26-16-23-6-5-9(25-1h1-6H,(H2,22,27,28)(H2,23,24,25,26)	-1.57
InChI=1S/C10H11N3O2S/c11-8-3-5-9(6-4-8)16(14,15)13-10-2-1-7-12-10/h1,3-7H,2,11H2,(H,12,13)	-1.69
InChI=1S/C9H10O2/c1-6-3-4-7(2)8(5-6)9(10)11/h3-5H,1-2H3,(H,10,11)	-2.92
InChI=1S/C8H11N3O2/c9-3-1-5-11(6-2-4-10)7-8(12)13/h1-2,5-7H2,(H,12,13)	0.458
InChI=1S/C4H6O5/c5-2(4(8)9)1-3(6)7/h2,5H,1H2,(H,6,7)(H,8,9)	0.64

"InChi"	"logS(M)"
InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H2,2H3	-0.068
InChI=1S/C12H7NO3/c14-7-1-3-9-11(5-7)16-12-6-8(15)2-4-10(12)13-9/h1-6,14H	-1.028
InChI=1S/C2H5BrO/c3-1-2-4/h4H,1-2H2	0.903
InChI=1S/C9H6Cl6O3S/c10-5-6(11)8(13)4-2-18-19(16)17-1-3(4)7(5,12)9(8,14)15/h3-4H,1-2H2/p+1	-5.956
InChI=1S/C21H31N5O2/c27-18-16-21(6-1-2-7-21)17-19(28)26(18)11-4-3-10-24-12-14-25(15-1h5,8-9H,1-4,6-7,10-17H2	-4.257
InChI=1S/C14H9Cl2NO/c15-10-5-3-6-11(16)14(10)17-12-7-2-1-4-9(12)8-13(17)18/h1-7H,8H2	-3.882
InChI=1S/C7H7NO4S/c8-13(11,12)6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)(H2,8,11,12)	-1.096
InChI=1S/C7H16N2/c8-6-7(9)4-2-1-3-5-7/h1-6,8-9H2	0.347
InChI=1S/C8H4F2O3/c9-8(10)12-6-3-1-2-5(4-11)7(6)13-8/h1-4H	-2.156
InChI=1S/C14H23N3O2/c1-10-12(15(2)3)13(18)16(4)14(19)17(10)11-8-6-5-7-9-11/h11H,5-9H2,1-4H3	-3.171
InChI=1S/C20H24O4/c1-13(20(22)24-19-6-4-3-5-18(19)21)14-7-8-16-12-17(23-2)10-9-15(1h7-13,18-19,21H,3-6H2,1-2H3	-5.07
InChI=1S/C22H33N3O/c1-21(2)15-19(18-9-7-6-8-10-18)16-22(3,4)25(21)20(26)17-24-13-11-h6-10,15H,11-14,16-17H2,1-5H3	-4.66
InChI=1S/C12H6Cl4O2S/c13-7-1-3-8(4-2-7)19(17,18)12-6-10(15)9(14)5-11(12)16/h1-6H	-6.659
InChI=1S/C6H4N4O/c11-5-2-8-6-4(10-5)1-7-3-9-6/h1-3H,(H,10,11)	-2.71
InChI=1S/C23H28N2O5/c1-12-16-10-25-6-5-13-15-8-20(27-2)21(28-3)9-18(15)24-22(13)19(25h8-9,11-12,14,16,19,24H,5-7,10H2,1-4H3	-2.803
InChI=1S/C7H15NOS/c1-4-7(5-2,10-3)6(8)9/h4-5H2,1-3H3,(H2,8,9)	-1.597
InChI=1S/C10H18O2/c1-7(2)8-4-5-10(3,12)9(11)6-8/h8-9,11-12H,1,4-6H2,2-3H3	-0.231
InChI=1S/C9H8N4O2/c14-7-4-2-1-3-6(7)8(15)12-9-10-5-11-13-9/h1-5,14H,(H2,10,11,12,13,15)	-0.875
InChI=1S/C12H7Cl3/c13-8-5-6-10(12(15)7-8)9-3-1-2-4-11(9)14/h1-7H	-6.49
InChI=1S/C7H4FN/c8-7-3-1-6(5-9)2-4-7/h1-4H	-1.81
InChI=1S/C12H9N3O/c1-8-11(9-2-4-14-5-3-9)6-10(7-13)12(16)15-8/h2-6H,1H3,(H,15,16)	-3.989
InChI=1S/C18H26N2O4S2/c1-15-14-18(20-17-9-5-4-8-16(15)17)24-12-7-3-2-6-10-19-11-13-25-2h4-5,8-9,14,19H,2-3,6-7,10-13H2,1H3,(H,21,22,23)	-3.961
InChI=1S/C4H8O2/c1-3(5)4(2)6/h3,5H,1-2H3	1.055
InChI=1S/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3	1.045
InChI=1S/C22H14/c1-2-8-16-14-22-20-12-6-4-10-18(20)17-9-3-5-11-19(17)21(22)13-15(h1-14H	-8.241

"InChi"	"logS(M)"
InChI=1S/C13H11N3/c14-16-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1-8H,14H2,(H,15,16)	-3.648
InChI=1S/C18H16N2O4/c1-11-6-15(21)19(17(11)23)9-13-4-3-5-14(8-13)10-20-16(22)7-12(2)18(20)24/h3-8H,9-10H2,1-2H3	-3.9
InChI=1S/C21H32O3/c1-13(22)24-19-7-6-17-16-5-4-14-12-15(23)8-10-20(14,2)18(16)9-11-21(17,3)20(19)25/h14,16-19H,4-12H2,1-3H3	-5.35
InChI=1S/C22H42O6/c1-5-9-11-19(7-3)21(23)27-17-15-25-13-14-26-16-18-28-22(24)20(8-4)12-10-6-2/h19-20H,5-18H2,1-4H3	-5.42
InChI=1S/C18H42N6/c1-19(2)10-7-13-22-16-23(14-8-11-20(3)4)18-24(17-22)15-9-12-21(5)6/h7-18H2,1-6H3	0.164
InChI=1S/C5H13O4P/c1-4-5-9-10(6,7-2)8-3/h4-5H2,1-3H3	0.473
InChI=1S/C8H17NO2/c1-3-4-5-6-9-8(11)7(2)10/h7,10H,3-6H2,1-2H3,(H,9,11)	-0.383
InChI=1S/C9H13NO2/c1-10-6-9(12)7-3-2-4-8(11)5-7/h2-5,9-12H,6H2,1H3	0.777
InChI=1S/C41H76O6/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-39(44)46-37-41(35-47-40(45)34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2)38-42-43(36-41)3/h17-20,42-43H,3-16,21-38H2,1-2H3/b19-17+,20-18+	-7.124
InChI=1S/C12H11NO3/c1-2-16-12(15)13-10-6-4-3-5-9(10)7-8-11(13)14/h3-8H,2H2,1H3	-1.659
InChI=1S/C18H30N2O/c1-2-3-4-5-6-7-8-9-10-11-15-20-18(21)17-13-12-14-19-16-17/h12-14,16H,2-11,15H2,1H3,(H,20,21)	-3.208
InChI=1S/C20H34N4O4/c25-17-11-5-3-9-15-23(17)19(27)21-13-7-1-2-8-14-22-20(28)24-16-10-4-6-12-18(24)26/h1-16H2,(H,21,27)(H,22,28)	-3.906
InChI=1S/C6H9N3/c1-4-3-5(2)9-6(7)8-4/h3H,1-2H3,(H2,7,8,9)	-0.488
InChI=1S/C7H9NO5S3/c8-16(12,13)7-2-6-5(14-7)1-4(9)3-15(6,10)11/h2,4,9H,1,3H2,(H2,8,12,13)	-1.59
InChI=1S/C12H18N4O2/c1-8(2)5-6-16-11(17)9-10(13-7-14(9)3)15(4)12(16)18/h7-8H,5-6H2,1-4H3	-2.774
InChI=1S/C12H18N2O3/c1-2-9-10(15)13-12(17)14(11(9)16)8-6-4-3-5-7-8/h8-9H,2-7H2,1H3,(H,13,15,17)	-2.766
InChI=1S/C3H6ClNO2/c1-3(2-4)5(6)7/h3H,2H2,1H3	-1.189
InChI=1S/C5H9NO2/c6-5(4(7)8)2-1-3-5/h1-3,6H2,(H,7,8)	-0.269
InChI=1S/C5H12O/c1-5(2)4-6-3/h5H,4H2,1-3H3	-0.901
InChI=1S/C13H14N2O3/c1-4-15-7-10(13(17)18-3)11(16)9-6-5-8(2)14-12(9)15/h5-7H,4H2,1-3H3	-2.7
InChI=1S/C17H28O6/c1-5-15(18)22-11-7-9-20-13-17(3,4)14-21-10-8-12-23-16(19)6-2/h5-6H,1-2,7-14H2,3-4H3	-3.05
InChI=1S/C10H16N2O3/c1-5-10(6-2)7(13)11(3)9(15)12(4)8(10)14/h5-6H2,1-4H3	-1.626

"InChi"	"logS(M)"
InChI=1S/C11H14N2O2/c1-13(2)12-8-11(14)9-4-6-10(15-3)7-5-9/h4-8H,1-3H3/b12-8+	-1.414
InChI=1S/C13H12N2O3S/c14-11-6-8-12(9-7-11)19(17,18)15-13(16)10-4-2-1-3-5-10/h1-9H,14H2,(H,15,16)	-2.95
InChI=1S/C15H13N3O3/c1-2-21-10-4-6-13-12(8-10)15(16)11-5-3-9(18(19)20)7-14(11)17-13/h3-8H,2H2,1H3,(H2,16,17)	-5.149
InChI=1S/C10H18O4/c1-2-3-4-5-6-7-8(9(11)12)10(13)14/h8H,2-7H2,1H3,(H,11,12)(H,13,14)	-2.041
InChI=1S/C7H6ClFN2O4/c8-1-2-15-7(14)11-3-4(9)5(12)10-6(11)13/h3H,1-2H2,(H,10,12,13)	-1.91
InChI=1S/C12H17N5O3/c1-3-16(4-2)6-10(18)20-8-17-11-9(5-15-17)12(19)14-7-13-11/h5,7H,3-4,6,8H2,1-2H3,(H,13,14,19)	-1.79
InChI=1S/C13H15N3/c1-2-4-12-11(3-1)5-6-13(15-12)16-9-7-14-8-10-16/h1-6,14H,7-10H2	-1.491
InChI=1S/C9H6O3/c10-7-5-6-3-1-2-4-8(6)12-9(7)11/h1-5,10H	-0.92
InChI=1S/C9H8N4O6/c14-5-11-7(15)4-12(9(11)16)10-3-6-1-2-8(19-6)13(17)18/h1-3,14H,4-5H2/b10-3+	-2.91
InChI=1S/C10H16N2O3S/c1-6(2)5-10(3-4-13)7(14)11-9(16)12-8(10)15/h6,13H,3-5H2,1-2H3,(H2,11,12,14,15,16)	-2.62
InChI=1S/C8H10O3S/c1-2-11-12(9,10)8-6-4-3-5-7-8/h3-7H,2H2,1H3	-2.131
InChI=1S/C19H18O4/c1-2-23-19(22)16(13-17(20)21)18(14-9-5-3-6-10-14)15-11-7-4-8-12-1h3-12H,2,13H2,1H3,(H,20,21)	-2.191
InChI=1S/C13H22NO3PS/c1-6-16-18(15,14-10(2)3)17-12-7-8-13(19-5)11(4)9-12/h7-10H,6H2,1-5H3,(H,14,15)	-2.965
InChI=1S/C9H8ClN3/c10-6-1-2-7-8(13-11)3-4-12-9(7)5-6/h1-5H,11H2,(H,12,13)	-1.971
InChI=1S/C18H22ClNO3/c1-3-4-5-7-13(2)23-17(21)12-22-16-10-9-15(19)14-8-6-11-20-18(14)1h6,8-11,13H,3-5,7,12H2,1-2H3	-5.748
InChI=1S/C7H4Cl4/c8-6-4-2-1-3-5(6)7(9,10)11/h1-4H	-5.044
InChI=1S/C18H12/c1-3-7-16-13(5-1)9-11-15-12-10-14-6-2-4-8-17(14)18(15)16/h1-12H	-7.821
InChI=1S/C6H14O3/c1-3-7-5-9-6-8-4-2/h3-6H2,1-2H3	-0.128
InChI=1S/C12H22FN/c13-11-9-7-5-3-1-2-4-6-8-10-12-14/h1-11H2	-4.94
InChI=1S/C8H19O4PS3/c1-4-11-13(14,12-5-2)15-7-8-16(9,10)6-3/h4-8H2,1-3H3	-2.54
InChI=1S/C6H12O3/c1-6(2)8-4-5(3-7)9-6/h5,7H,3-4H2,1-2H3	-0.571
InChI=1S/C24H26O2/c1-17(21-6-10-23(25)11-7-21)14-19-4-3-5-20(16-19)15-18(2)22-8-12-h3-13,16-18,25-26H,14-15H2,1-2H3	-6.239
InChI=1S/C8H9FN2O4/c1-2-6(12)15-4-11-7(13)5(9)3-10-8(11)14/h3H,2,4H2,1H3,(H,10,14)	-0.77

"InChi"	"logS(M)"
InChI=1S/C10H12ClN5O4/ c11-10-14-7(12)4-8(15-10)16(2-13-4)9-6(19)5(18)3(1-17)20-9/ h2-3,5-6,9,17-19H,1H2,(H2,12,14,15)	-2.393
InChI=1S/C21H26N2O3/ c1-17(24)18-7-9-21(10-8-18)26-16-20(25)15-22-11-13-23(14-12-22)1 h2-10,20,25H,11-16H2,1H3	-2.588
InChI=1S/C13H20O3/c1-2-3-5-11-6-4-7-13(8-11)16-10-12(15)9-14/ h4,6-8,12,14-15H,2-3,5,9-10H2,1H3	-3.298
InChI=1S/C17H16Cl3NO2/ c18-8-10-21(11-9-19)15-4-6-16(7-5-15)23-17(22)13-2-1-3-14(20)12-1 h1-7,12H,8-11H2	-6.492
InChI=1S/C11H14O5/c12-8-6-15-11(10(14)9(8)13)16-7-4-2-1-3-5-7/ h1-5,8-14H,6H2	-1.66
InChI=1S/C11H13NO2/c1-8-5-3-4-6-10(8)12-11(14)7-9(2)13/h3-6H, 7H2,1-2H3,(H,12,14)	-1.85
InChI=1S/C25H19N3O4/ c1-13-4-9-19-18(12-13)26-22-14-5-6-15-21-16(7-8-17(20(14)21)25(31 h4-9,12H,3,10-11H2,1-2H3	-6.772
InChI=1S/C21H21ClN2O8/ c1-24(2)14-7-5-6-10(16(27)12-9(25)4-3-8(22)11(12)15(6)26)18(29)21 h3-4,6-7,14-15,25-26,28-29,32H,5H2,1-2H3,(H2,23,31)	-2.52
InChI=1S/C20H32N4O2S2/ c1-19(2,17(25)23(5)6)11-9-13-21-15-16(27-13)22-14(28-15)10-12-20(h9-12H2,1-8H3	-5.144
InChI=1S/C3H8NO6P/c4-2(3(5)6)1-10-11(7,8)9/h2H,1,4H2,(H,5,6) (H2,7,8,9)	-0.815
InChI=1S/C8H5Cl3O3/c9-5-1-4(14-3-7(12)13)2-6(10)8(5)11/h1-2H, 3H2,(H,12,13)	-2.94
InChI=1S/C11H20N2O5/ c1-6(2)5-7(12)10(16)13-8(11(17)18)3-4-9(14)15/h6-8H, 3-5,12H2,1-2H3,(H,13,16)(H,14,15)(H,17,18)	-0.897
InChI=1S/C7H8N4S/c8-7(12)11-10-5-6-3-1-2-4-9-6/h1-5H, (H3,8,11,12)/b10-5+	0.106
InChI=1S/C15H19N3O/ c1-4-17-9-10(2)18-14(11(17)3)16-13-8-6-5-7-12(13)15(18)19/ h5-8,10-11H,4,9H2,1-3H3	-2.46
InChI=1S/C9H9N5O6S3/ c1-13-8(21-9(11-13)22(10,17)18)12-23(19,20)7-5-3-2-4-6(7)14(15)16/ h2-5H,1H3,(H2,10,17,18)/b12-8-	-2.79
InChI=1S/C19H21ClO6/ c1-5-6-25-11-7-10(2)19(14(21)8-11)18(22)15-12(23-3)9-13(24-4)16(2 h8-10H,5-7H2,1-4H3	-5.22
InChI=1S/C15H20N2O4S3/ c1-11(2)8-17-9-12-3-5-13(6-4-12)23(18,19)14-7-15(22-10-14)24(16,2(h3-7,10-11,17H,8-9H2,1-2H3,(H2,16,20,21)	-1.16
InChI=1S/C5H9NO2/c1-4(6)3-5(7)8-2/h3H,6H2,1-2H3/b4-3-	-0.806
InChI=1S/C12H17NO2/c1-12(2,3)10-6-4-9(5-7-10)8-11(14)13-15/ h4-7,15H,8H2,1-3H3,(H,13,14)	-2.704
InChI=1S/C15H12Cl2O4/ c1-9(15(18)19)20-11-3-5-12(6-4-11)21-14-7-2-10(16)8-13(14)17/ h2-9H,1H3,(H,18,19)	-5.04
InChI=1S/C5H5Cl3N2OS/c1-2-11-4-9-3(10-12-4)5(6,7)8/h2H2,1H3	-3.325

"InChi"	"logS(M)"
InChI=1S/C17H14O2/c1-11(17(18)19)13-8-9-16-14(10-13)7-6-12-4-2-3-5-15(12)16/h2-11H,1H3,(H,18,19)	-5.327
InChI=1S/C5H5NS/c7-5-3-1-2-4-6-5/h1-4H,(H,6,7)	0.098
InChI=1S/C7H5I2NO2/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2H,10H2,(H,11,12)	-4.846
InChI=1S/C8H10O4/c1-11-6-3-5(9)4-7(12-2)8(6)10/h3-4,9-10H,1-2H3	-0.382
InChI=1S/C24H44O4/c1-21(2)15-11-7-5-9-13-19-27-23(25)17-18-24(26)28-20-14-10-6-8-12h17-18,21-22H,5-16,19-20H2,1-4H3/b18-17+	-6.422
InChI=1S/C17H20N4O/c1-5-21-14-10-12(20(3)4)9-11(2)15(14)19-17(22)13-7-6-8-18-16(13)2h6-10H,5H2,1-4H3,(H,19,22)	-4.871
InChI=1S/C21H21N/c1-22-14-12-18(13-15-22)21-19-8-4-2-6-16(19)10-11-17-7-3-5-9-20(1h2-11H,12-15H2,1H3	-3.09
InChI=1S/C7H4ClNO4/c8-5-3-1-2-4(7(10)11)6(5)9(12)13/h1-3H,(H,10,11)/p-1	-2.632
InChI=1S/C8H6N6O3/c15-7(9-8-10-12-13-11-8)5-1-3-6(4-2-5)14(16)17/h1-4H,(H2,9,10,11,12,13,15)	-2.185
InChI=1S/C18H24N2O4/c1-6-18(3,7-2)14-11-15(24-20-14)19-17(21)16-12(22-4)9-8-10-13(16)h8-11H,6-7H2,1-5H3,(H,19,21)	-5.369
InChI=1S/C57H110O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-54(h54H,4-53H2,1-3H3	-5.473
InChI=1S/C17H18ClN3O/c1-20(2)9-10-21-16-8-7-12(18)11-15(16)19-14-6-4-3-5-13(14)17(21)2h3-8,11,19H,9-10H2,1-2H3	-5.798
InChI=1S/C23H24O4/c1-16(24)26-21-12-8-19(9-13-21)23(18-6-4-3-5-7-18)20-10-14-22(15-h8-15H,3-7H2,1-2H3	-6.624
InChI=1S/C7H8N2O2S/c1-2-11-6(10)5-3-8-7(12)9-4-5/h3-4H,2H2,1H3,(H,8,9,12)	-1.74
InChI=1S/C29H40O2/c1-20-15-22(26(30)24(17-20)28(3)11-7-5-8-12-28)19-23-16-21(2)18-2h15-18,30-31H,5-14,19H2,1-4H3	-8.147
InChI=1S/C3HClF6/c4-1(2(5,6)7)3(8,9)10/h1H	-3.718
InChI=1S/C19H29NO5/c1-13(2)15-9-8-14(3)17(19(22)23-6)18(15)25-12-16(21)24-11-7-10-20(h8-9,13H,7,10-12H2,1-6H3	-3.864
InChI=1S/C42H22Cl4F6N6O4/c43-27-11-9-21(41(47,48)49)15-33(27)55-57-35-23-7-3-1-5-19(23)13-h1-18,55-56H,(H,53,61)(H,54,62)/b57-35-,58-36+	-7.692
InChI=1S/C12H17BrO/c13-7-11(14)12-4-8-1-9(5-12)3-10(2-8)6-12/h8-10H,1-7H2	-3.788
InChI=1S/C23H24N2O2/c1-18(17-19-11-5-2-6-12-19)24-25-22(26)23(27,20-13-7-3-8-14-20)21h2-16,18,24,27H,17H2,1H3,(H,25,26)	-4.54

"InChi"	"logS(M)"
InChI=1S/C20H28N2O/c1-5-15(2)20(19(21)23,13-14-22(3)4)18-12-8-10-16-9-6-7-11-17(16)18-12,15H,5,13-14H2,1-4H3,(H2,21,23)	-4.63
InChI=1S/C6H11BrO3/c1-2-6(7)10-4-5(9)3-8/h2,5-6,8-9H,1,3-4H2	-0.714
InChI=1S/C19H26N2S2/c1-3-9-15(10-4-1)21(16-11-5-2-6-12-16)23-19-20-17-13-7-8-14-18(17)7-8,13-16H,1-6,9-12H2	-6.789
InChI=1S/C6H15NO2/c1-2-7(3-5-8)4-6-9/h8-9H,2-6H2,1H3/p+1	0.875
InChI=1S/C8H14O/c1-2-8(9)6-4-3-5-7-8/h2,9H,1,3-7H2	-1.701
InChI=1S/C2H5N5O4/c1-5(7(10)11)2(3)4-6(8)9/h1H3,(H2,3,4)	-0.61
InChI=1S/C14H18N2O5/c1-7-10(9(3)17)8(2)13(16(20)21)11(14(4,5)6)12(7)15(18)19/h1-6H3	-5.19
InChI=1S/C12H11NO3S2/c1-8-2-4-9(5-3-8)12(14)10-6-11(17-7-10)18(13,15)16/h2-7H,1H3,(H2,13,15,16)	-4.449
InChI=1S/C7H12O3/c1-5(2)7(9)10-4-6(3)8/h6,8H,1,4H2,2-3H3	-0.572
InChI=1S/C13H16O7/c14-5-7-3-1-2-4-8(7)19-13-12(18)11(17)10(16)9(6-15)20-13/h1-5,9-13,15-18H,6H2	-1.198
InChI=1S/C17H26N2O2/c1-4-10-19-11-6-9-15(12-19)21-17(20)18-16-13(2)7-5-8-14(16)3/h5,7-8,15H,4,6,9-12H2,1-3H3,(H,18,20)	-4.459
InChI=1S/C18H22FN3O3/c1-18(2,3)22-10-12(17(24)25)16(23)11-8-13(19)15(9-14(11)22)21-6-4-8-10,20H,4-7H2,1-3H3,(H,24,25)	-3.43
InChI=1S/C4H8N2O2/c1-3(5-7)4(2)6-8/h7-8H,1-2H3/b5-3-,6-4+	-2.16
InChI=1S/C19H24O4/c1-19(2,15-3-7-17(8-4-15)22-13-11-20)16-5-9-18(10-6-16)23-14-12-21-3-10,20-21H,11-14H2,1-2H3	-3.452
InChI=1S/C11H16O2/c12-10(13)11-4-7-1-8(5-11)3-9(2-7)6-11/h7-9H,1-6H2,(H,12,13)	-2.815
InChI=1S/C11H16N2O4S2/c12-11(9-18-19(14,15)16)13-6-7-17-8-10-4-2-1-3-5-10/h1-5H,6-9H2,(H2,12,13)(H,14,15,16)	-1.846
InChI=1S/C12H8O/c1-2-3-5-10-12(13)11-8-6-4-7-9-11/h4,6-9H,1H3	-2.769
InChI=1S/C6H10O6/c7-5(8)3-11-1-2-12-4-6(9)10/h1-4H2,(H,7,8)(H,9,10)	0.671
InChI=1S/C12H6Cl4/c13-8-4-2-5-9(14)11(8)7-3-1-6-10(15)12(7)16/h1-6H	-6.3
InChI=1S/C17H25NO3/c1-15-8-5-6-11-18(15)12-7-13-20-17(19)14-21-16-9-3-2-4-10-16/h2-4,9-10,15H,5-8,11-14H2,1H3	-3.375
InChI=1S/C5H8O/c1-3-5(6)4-2/h1,5-6H,4H2,2H3	0.278
InChI=1S/C12H20N2O2/c1-3-11(15)13-7-9-5-6-10(8-13)14(9)12(16)4-2/h9-10H,3-8H2,1-2H3	-2.387
InChI=1S/C7H3F12N3/c8-4(9,10)2(5(11,12)13)1(20)21-3(22-2,6(14,15)16)7(17,18)19/h22H,(H2,20,21)	-4.665
InChI=1S/C3H4N2O3S/c6-9(7,8)3-1-4-2-5-3/h1-2H,(H,4,5)(H,6,7,8)	0.13
InChI=1S/C14H14/c1-11-3-7-13(8-4-11)14-9-5-12(2)6-10-14/h3-10H,1-2H3	-6.018

"InChi"	"logS(M)"
InChI=1S/C7H14N2O2/c1-3-7(4-2,5(8)10)6(9)11/h3-4H2,1-2H3,(H2,8,10)(H2,9,11)	-1.199
InChI=1S/C12H18ClNO2S/c1-8-7-17-10(3)12(8)14(11(15)5-13)9(2)6-16-4/h7,9H,5-6H2,1-4H3	-2.361
InChI=1S/C17H20N2O5S/c1-9-4-6-10(7-5-9)24-8-11(20)18-12-14(21)19-13(16(22)23)17(2,3)25h4-7,12-13,15H,8H2,1-3H3,(H,18,20)(H,22,23)	-3.15
InChI=1S/C10H16O2/c1-9(2)6-4-5-10(9,3)8(12)7(6)11/h6-7,11H,4-5H2,1-3H3	-0.925
InChI=1S/C20H25N3O3S/c1-5-27(25,26)15-10-11-18-19(14-15)23(13-12-21(2)3)20(24)16-8-6-7h6-11,14H,5,12-13H2,1-4H3	-5.285
InChI=1S/C15H17N3O2/c1-19-13-7-3-11(4-8-13)17-15(16)18-12-5-9-14(20-2)10-6-12/h3-10H,1-2H3,(H3,16,17,18)	-2.735
InChI=1S/C18H18N8/c19-11-4-6-17(15(21)8-11)25-23-13-2-1-3-14(10-13)24-26-18-7-5-12(h1-10H,19-22H2/b25-23+,26-24+	-4.197
InChI=1S/C6H5NOS/c8-6(9)5-2-1-3-7-4-5/h1-4H,(H,8,9)	-1.38
InChI=1S/C19H20N2O/c1-2-13-12-21-10-8-14(13)11-18(21)19(22)16-7-9-20-17-6-4-3-5-15(1h2-7,9,13-14,18H,1,8,10-12H2	-3.19
InChI=1S/C16H25NO6/c1-19-8-6-17(7-9-20-2)16(18)12-10-13(21-3)15(23-5)14(11-12)22-4/h10-11H,6-9H2,1-5H3	-1.322
InChI=1S/C8H5BrO2/c9-6-2-1-5-4-11-8(10)7(5)3-6/h1-3H,4H2	-2.647
InChI=1S/C8H9ClO/c1-5-3-7(9)4-6(2)8(5)10/h3-4,10H,1-2H3	-1.676
InChI=1S/C24H44N4O4/c29-21-13-5-1-9-17-25-22(30)14-6-2-11-19-27-24(32)16-8-4-12-20-28h1-20H2,(H,25,30)(H,26,29)(H,27,32)(H,28,31)	-2.813
InChI=1S/C10H12N2O2/c1-7(13)6-12-9-5-3-2-4-8(9)10(11)14/h2-5,12H,6H2,1H3,(H2,11,14)	-1.124
InChI=1S/C7H6N2S/c8-5-1-2-6-7(3-5)10-4-9-6/h1-4H,8H2	-1.551
InChI=1S/C11H12ClNO2/c1-2-11(14)13-6-9-5-10(12)4-3-8(9)7-15-13/h3-5H,2,6-7H2,1H3	-3.013
InChI=1S/C9H12N4O2/c1-3-4-13-7-6(10-5-11-7)8(14)12(2)9(13)15/h5H,3-4H2,1-2H3,(H,10,11)	-1.591
InChI=1S/C9H9Cl2NO3/c10-5-1-4(2-6(11)8(5)13)3-7(12)9(14)15/h1-2,7,13H,3,12H2,(H,14,15)	-0.796
InChI=1S/C14H16N2O3/c1-4-14(10-8-6-5-7-9-10)11(17)15(2)13(19)16(3)12(14)18/h5-9H,4H2,1-3H3	-2.595
InChI=1S/C19H37N5O7/c1-19(27)7-28-18(13(26)16(19)24-2)31-15-11(23)5-10(22)14(12(15)25h3,9-18,24-27H,4-7,20-23H2,1-2H3	0.349
InChI=1S/C12H26O/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-12H2,1-2H3	-4.27
InChI=1S/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h2,5,7-8,10-11H,1H2	0.277
InChI=1S/C8H8N4O4S3/c9-18(13,14)8-11-10-7(17-8)12-19(15,16)6-4-2-1-3-5-6/h1-5H,(H,10,12)(H2,9,13,14)	-2.9

"InChi"	"logS(M)"
InChI=1S/C12H20N2O/c1-3-7-13-8-10-5-6-11(9-13)14(10)12(15)4-2/h3,10-11H,1,4-9H2,2H3	-1.71
InChI=1S/C9H8O2/c1-7(10)9(11)8-5-3-2-4-6-8/h2-6H,1H3	-1.756
InChI=1S/C14H16N2O4S2/c1-16(2)7-10-5-9(3-4-12(10)17)14(18)11-6-13(21-8-11)22(15,19)20/h3-6,8,17H,7H2,1-2H3,(H2,15,19,20)	-1.54
InChI=1S/C4H6Br2O2/c1-2-4(5,6)3(7)8/h2H2,1H3,(H,7,8)	-0.872
InChI=1S/C15H19N3O2/c1-10(2)16-13-11(3)18(12-8-6-5-7-9-12)15(20)17(4)14(13)19/h5-10,16H,1-4H3	-2.575
InChI=1S/C10H12N2O3/c11-9(13)6-12-10(14)15-7-8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,11,13)(H,12,14)	-1.88
InChI=1S/C13H11NO2/c1-16-11-7-5-10(6-8-11)13(15)12-4-2-3-9-14-12/h2-9H,1H3	-2.498
InChI=1S/C19H17NO3/c1-2-23-18-10-6-5-9-16(18)20-19(22)15-11-13-7-3-4-8-14(13)12-17(1h3-12,21H,2H2,1H3,(H,20,22)	-5.187
InChI=1S/C23H27NO8/c1-24(2)9-8-13-10-18-22(32-12-31-18)20(29-4)15(13)11-16(25)14-6-7h6-7,10H,8-9,11-12H2,1-5H3,(H,26,27)	-2.535
InChI=1S/C4H10N2O3/c7-3-1-6(5-9)2-4-8/h7-8H,1-4H2	0.872
InChI=1S/C12H9N3O5/c16-10-4-1-8(2-5-10)13-11-6-3-9(14(17)18)7-12(11)15(19)20/h1-7,13,16H	-5.444
InChI=1S/C13H13O3P/c1-17(14,15-12-8-4-2-5-9-12)16-13-10-6-3-7-11-13/h2-11H,1H3	-2.202
InChI=1S/C9H18O2/c1-4-6-7-8(5-2)9(10)11-3/h8H,4-7H2,1-3H3	-2.99
InChI=1S/C9H5NO2/c10-4-6-1-2-7-5-12-9(11)8(7)3-6/h1-3H,5H2	-2.702
InChI=1S/C2H2F4/c3-1-2(4,5)6/h1H2	-2.009
InChI=1S/C9H8O/c10-8-4-7-9-5-2-1-3-6-9/h1-8H/b7-4+	-1.969
InChI=1S/C21H28N2O/c1-17-10-8-11-18(2)21(17)23(15-9-14-22(3)4)20(24)16-19-12-6-5-7-1h5-8,10-13H,9,14-16H2,1-4H3	-4.911
InChI=1S/C12H10O/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10H	-3.96
InChI=1S/C10H8O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6H,1H3	-1.32
InChI=1S/C6H5ClS/c7-5-3-1-2-4-6(5)8/h1-4,8H	-1.78
InChI=1S/C6H12ClNO/c7-1-2-8-3-5-9-6-4-8/h1-6H2	0.376
InChI=1S/C15H18N2O3/c1-3-20-15(19)14(17(2)10-18)8-11-9-16-13-7-5-4-6-12(11)13/h4-7,9-10,14,16H,3,8H2,1-2H3	-2.271
InChI=1S/C6H6N2O3/c1-4-2-7-5(6(9)10)3-8(4)11/h2-3H,1H3,(H,9,10)	0.196
InChI=1S/C10H6Cl2/c11-9-3-1-7-2-4-10(12)6-8(7)5-9/h1-6H	-5.922
InChI=1S/C16H22Cl2N2O2/c1-13-2-3-14(16(21)20-8-10-22-11-9-20)12-15(13)19(6-4-17)7-5-18/h2-3,12H,4-11H2,1H3	-3.901
InChI=1S/C31H52O3/c1-21(2)13-10-14-22(3)15-11-16-23(4)17-12-19-31(9)20-18-28-26(7)2h21-23H,10-20H2,1-9H3	-5.772

"InChi"	"logS(M)"
InChI=1S/C15H15N3/c1-18(2)13-5-3-10-7-11-8-12(16)4-6-14(11)17-15(10)9-13/h3-9H,16H2,1-2H3	-4.245
InChI=1S/C6H15N/c1-4-5-6-7(2)3/h4-6H2,1-3H3/p+1	-0.667
InChI=1S/C10H14N4O2/c1-4-5-14-6-11-8-7(14)9(15)13(3)10(16)12(8)2/h6H,4-5H2,1-3H3	0.02
InChI=1S/C5H10N6O4/c12-10(13)8-2-6-1-7(4-8)5-9(3-6)11(14)15/h1-5H2	0.661
InChI=1S/C6H8ClN3O2/c1-5-4-8-6(10(11)12)9(5)3-2-7/h4H,2-3H2,1H3	-2.44
InChI=1S/C6H10ClN5/c1-3(2)9-6-11-4(7)10-5(8)12-6/h3H,1-2H3,(H3,8,9,10,11,12)	-2.706
InChI=1S/C34H26N6S2/c1-5-15-25(16-6-1)29-31(27-19-9-3-10-20-27)37-39-33(35-29)41-23-1h1-22H,23-24H2/b14-13+	-7.025
InChI=1S/C15H18N6O6S/c1-21(2)13(22)9-6-5-7-16-12(9)28(24,25)20-15(23)19-14-17-10(26-3)h5-8H,1-4H3,(H2,17,18,19,20,23)	-3.97
InChI=1S/C7H5Cl3O2/c1-12-7-4(11)2-3(8)5(9)6(7)10/h2,11H,1H3	-2.871
InChI=1S/C4H10O3/c1-5-4(6-2)7-3/h4H,1-3H3	-1.026
InChI=1S/C12H10ClN3O/c13-11-8-10(6-7-14-11)16-12(17)15-9-4-2-1-3-5-9/h1-8H,(H2,14,15,16,17)	-3.803
InChI=1S/C9H20O4S2/c1-5-9(6-2,14(10,11)7-3)15(12,13)8-4/h5-8H2,1-4H3	-2.062
InChI=1S/C14H17N3O4S2/c1-3-21-13(18)8-12-9(2)16-14(22-12)17-23(19,20)11-6-4-10(15)5-7-1h4-7H,3,8,15H2,1-2H3,(H,16,17)	-2.88
InChI=1S/C11H14O2/c1-8-5-4-6-9(2)11(8)13-7-10(3)12/h4-6H,7H2,1-3H3	-1.919
InChI=1S/C6H12O2/c1-5(2)6-7-3-4-8-6/h5-6H,3-4H2,1-2H3	-0.065
InChI=1S/C19H15ClO4/c1-11(21)10-15(12-6-8-13(20)9-7-12)17-18(22)14-4-2-3-5-16(14)24-1h2-9,15,23H,10H2,1H3	-5.836
InChI=1S/C15H10Cl2N2O/c16-9-5-6-13-11(7-9)15(18-8-14(20)19-13)10-3-1-2-4-12(10)17/h1-7H,8H2,(H,19,20)	-4.116
InChI=1S/C11H15ClO2/c1-2-11(7-13,8-14)9-3-5-10(12)6-4-9/h3-6,13-14H,2,7-8H2,1H3	-2.915
InChI=1S/C6H4BrNO2/c7-5-1-4(6(9)10)2-8-3-5/h1-3H,(H,9,10)	-2.02
InChI=1S/C14H15N3O2/c1-19-12-5-9-3-2-4-10-7-17(14(15)16-18)8-11(6-12)13(9)10/h2-6,18H,7-8H2,1H3,(H2,15,16)	-1.21
InChI=1S/C8H18O2/c1-5-9-6-7-10-8(2,3)4/h5-7H2,1-4H3	-0.688
InChI=1S/C17H25NO3/c1-3-5-12-18(13-6-4-2)16(19)14-21-17(20)15-10-8-7-9-11-15/h7-11H,3-6,12-14H2,1-2H3	-3.561
InChI=1S/C19H20Cl2N2OS/c20-14-3-6-16(7-4-14)25-18-13-15(21)5-8-17(18)22-19(24)9-12-23-1h3-8,13H,1-2,9-12H2,(H,22,24)	-5.853

"InChi"	"logS(M)"
InChI=1S/C22H22O8/c1-25-14-5-10(6-15(26-2)20(14)27-3)17-12-7-16-21(30-9-29-16)19(23h5-7,11,17-18,23H,4,8-9H2,1-3H3	-4.503
InChI=1S/C15H12N4/c16-15-17-13(11-7-3-1-4-8-11)14(18-19-15)12-9-5-2-6-10-12/h1-10H,(H2,16,17,19)	-3.045
InChI=1S/C14H7ClF2N4/c15-9-5-2-1-4-8(9)13-18-20-14(21-19-13)12-10(16)6-3-7-11(12)17/h1-7H	-6.12
InChI=1S/C10H18N4O4S3/c1-7(19-5)11-17-9(15)13(3)21-14(4)10(16)18-12-8(2)20-6/h1-6H3/b11-7-,12-8+	-4.005
InChI=1S/C6H14O/c1-3-5-6-7-4-2/h3-6H2,1-2H3	-1.55
InChI=1S/C9H9NO2/c1-2-10-7-5-3-4-6-8(7)12-9(10)11/h3-6H,2H2,1H3	-2.256
InChI=1S/C6H13NO2/c1-4(2)3-5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)	-1.046
InChI=1S/C10H22O2/c1-3-5-7-11-9-10-12-8-6-4-2/h3-10H2,1-2H3	-1.94
InChI=1S/C2H8NO2PS/c1-5-6(3,4)7-2/h1-2H3,(H2,3,4)	0.85
InChI=1S/C16H11F3O3/c17-16(18,19)12-6-3-5-11(8-12)14(20)9-10-4-1-2-7-13(10)15(21)22/h1-8H,9H2,(H,21,22)	-4.765
InChI=1S/C17H36O2/c1-5-9-11-16(7-3)13-18-15-19-14-17(8-4)12-10-6-2/h16-17H,5-15H2,1-4H3	-5.435
InChI=1S/C14H13NO3/c1-9-2-5-11(6-3-9)18-14(17)12-7-4-10(15)8-13(12)16/h2-8,16H,15H2,1H3	-3.861
InChI=1S/C16H16/c1-2-14-4-3-13(1)9-10-15-5-7-16(8-6-15)12-11-14/h1-8H,9-12H2	-5.169
InChI=1S/C21H31NO4/c1-2-25-20(23)21(18-7-4-3-5-8-18)10-12-22(13-11-21)14-16-24-17-19h3-5,7-8,19H,2,6,9-17H2,1H3	-2.705
InChI=1S/C12H8N2O4S2/c15-11(16)7-1-3-9(13-5-7)19-20-10-4-2-8(6-14-10)12(17)18/h1-6H,(H,15,16)(H,17,18)	-2.894
InChI=1S/C17H34N2O/c1-17(2)11-7-5-3-4-6-8-15-20-16-10-14-19-13-9-12-18/h17,19H,3-11,13-16H2,1-2H3	-3.618
InChI=1S/C16H24N2O2/c1-2-16(15(17)19,14-6-4-3-5-7-14)8-9-18-10-12-20-13-11-18/h3-7H,2,8-13H2,1H3,(H2,17,19)	-2.257
InChI=1S/C15H21N4O2P/c1-12-3-4-14(13(2)11-12)17-15(20)16-5-10-22(21,18-6-7-18)19-8-9-1h3-5,10-11H,6-9H2,1-2H3,(H2,16,17,20)/b10-5+	-2.522
InChI=1S/C10H11N3OS/c1-11-9(14)13(2)10-12-7-5-3-4-6-8(7)15-10/h3-6H,1-2H3,(H,11,14)	-3.574
InChI=1S/C10H14N4O11P2/c15-6-4(1-23-27(21,22)25-26(18,19)20)24-10(7(6)16)14-3-13-5-8(14)h2-4,6-7,10,15-16H,1H2,(H,21,22)(H,11,12,17)(H2,18,19,20)	-1.524
InChI=1S/C7H10ClN3/c1-5-6(11(2)3)4-9-7(8)10-5/h4H,1-3H3	-1.26

"InChi"	"logS(M)"
InChI=1S/C10H10O2/c1-2-9-7-5-3-4-6-8(7)10(11)12-9/h3-6,9H,2H2,1H3	-1.747
InChI=1S/C17H13N3O4/c1-24-12-7-8-14(15(10-12)20(22)23)18-19-17-13-5-3-2-4-11(13)6-9-16-10,18H,1H3/b19-17-	-7.991
InChI=1S/C9H8Cl2O3/c1-13-9(12)5-14-8-3-2-6(10)4-7(8)11/h2-4H,5H2,1H3	-2.96
InChI=1S/C12H18N2O/c13-8-10-14-9-4-7-12(15)11-5-2-1-3-6-11/h1-3,5-6,14H,4,7-10,13H2	-0.147
InChI=1S/C7H3Br2NO2/c8-3-1-4(9)6-5(2-3)10-7(11)12-6/h1-2H,(H,10,11)	-3.664
InChI=1S/C25H32ClN5O2/c1-2-24-27-31(25(32)30(24)18-19-33-23-10-4-3-5-11-23)13-7-12-28-14-16-6,8-11,20H,2,7,12-19H2,1H3	-6.117
InChI=1S/C15H20N2O2/c18-14-16-12-15(19-14)7-10-17(11-8-15)9-6-13-4-2-1-3-5-13/h1-5H,6-12H2,(H,16,18)	-2.035
InChI=1S/C11H18N2O2/c1-7(2)6-8-11(15)13-5-3-4-9(13)10(14)12-8/h7-9H,3-6H2,1-2H3,(H,12,14)	-2.042
InChI=1S/C10H12O6/c1-15-9(13)5-3-8(12)6(4-7(5)11)10(14)16-2/h5-6H,3-4H2,1-2H3	-4.154
InChI=1S/C5H9N/c1-4-5(2,3)6/h1H,6H2,2-3H3	1.032
InChI=1S/C8H18O3/c1-7(9)3-5-11-6-4-8(2)10/h7-10H,3-6H2,1-2H3	0.79
InChI=1S/C13H15N3O2/c1-9-11(15(2)3)12(17)14-13(18)16(9)10-7-5-4-6-8-10/h4-8H,1-3H3,(H,14,17,18)	-2.185
InChI=1S/C15H22N2O2/c1-15(14(16)18,13-5-3-2-4-6-13)7-8-17-9-11-19-12-10-17/h2-6H,7-12H2,1H3,(H2,16,18)	-1.735
InChI=1S/C13H11ClN2O2/c1-8-10(14)5-2-6-11(8)16-12-9(13(17)18)4-3-7-15-12/h2-7H,1H3,(H,15,16)(H,17,18)	-6.451
InChI=1S/C8H5NO6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)(H,12,13)	-2.178
InChI=1S/C10H13N3O4/c11-3-1-5-13(6-2-4-12)8(10(16)17)7-9(14)15/h8H,1-2,5-7H2,(H,14,15)(H,16,17)	-1.534
InChI=1S/C12H16O3/c1-2-5-10-6-3-4-7-12(10)15-9-11(14)8-13/h2-4,6-7,11,13-14H,1,5,8-9H2	-2.644
InChI=1S/C14H19NO3/c1-9(2)12-13(16)15-11(14(17)18-12)8-10-6-4-3-5-7-10/h3-7,9,11-12,14,17H,8H2,1-2H3,(H,15,16)	-2.28
InChI=1S/C16H19NO/c1-13(17(2)3)14-9-11-16(12-10-14)18-15-7-5-4-6-8-15/h4-13H,1-3H3	-3.557
InChI=1S/C9H14O2S/c10-9(11)8(12)6-7-4-2-1-3-5-7/h6-7,12H,1-5H2,(H,10,11)/b8-6-	-2.67
InChI=1S/C14H15NO5/c16-12(15-8-4-7-11(15)13(17)18)9-20-14(19)10-5-2-1-3-6-10/h1-3,5-6,11H,4,7-9H2,(H,17,18)	-1.592
InChI=1S/C19H20N2O4/c1-20(2)17(22)12-25-19(24)14-10-11-21-15(14)8-9-16(21)18(23)13-6-3-9,14H,10-12H2,1-2H3	-3.03

"InChi"	"logS(M)"
InChI=1S/C8H7NO4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3	-2.186
InChI=1S/C12H5Cl5/c13-6-1-2-8(14)7(5-6)11-9(15)3-4-10(16)12(11)17/h1-5H	-7.189
InChI=1S/C7H8O2/c8-5-6-2-1-3-7(9)4-6/h1-4,8-9H,5H2	-0.268
InChI=1S/C12H9N3O4/c16-14(17)10-6-7-11(12(8-10)15(18)19)13-9-4-2-1-3-5-9/h1-8,13H	-3.834
InChI=1S/C9H16O/c1-8(2)5-4-6-9(3)7-10/h5,7,9H,4,6H2,1-3H3	-2.448
InChI=1S/C21H28O3/c1-4-5-6-7-8-13-24-21(22)16(2)17-9-10-19-15-20(23-3)12-11-18(19)1h9-12,14-16H,4-8,13H2,1-3H3	-7.12
InChI=1S/C6H8ClN3O3/c7-3-5(11)4-9-2-1-8-6(9)10(12)13/h1-2,5,11H,3-4H2	-1.219
InChI=1S/C10H16O/c1-9(2)6-4-7(9)10(3)8(5-6)11-10/h6-8H,4-5H2,1-3H3	-2.594
InChI=1S/C6H11ClN2O2/c1-3(2)4(7)5(10)9-6(8)11/h3-4H,1-2H3,(H3,8,9,10,11)	-1.358
InChI=1S/C34H58O4/c1-29(2)23-17-13-9-5-7-11-15-21-27-37-33(35)31-25-19-20-26-32(31)h19-20,25-26,29-30H,5-18,21-24,27-28H2,1-4H3	-5.725
InChI=1S/C6H6INO/c1-8-4-5(7)2-3-6(8)9/h2-4H,1H3	-0.009
InChI=1S/C8H5Cl3O2S/c9-4-1-6(11)7(2-5(4)10)13-3-8(12)14/h1-2H,3H2,(H,12,14)	-2.96
InChI=1S/C10H9NO3S/c11-10-3-1-2-7-6-8(15(12,13)14)4-5-9(7)10/h1-6H,11H2,(H,12,13,14)	-2.24
InChI=1S/C10H9NO6/c1-16-9(12)6-3-4-7(10(13)17-2)8(5-6)11(14)15/h3-5H,1-2H3	-2.836
InChI=1S/C12H5Cl3O2/c13-6-5-7(14)11-12(10(6)15)17-9-4-2-1-3-8(9)16-11/h1-5H	-7.58
InChI=1S/C20H23ClN2/c1-22-18-11-12-19(22)14-23(13-18)20(15-5-3-2-4-6-15)16-7-9-17(21)h2-10,18-20H,11-14H2,1H3	-4.387
InChI=1S/C14H10N2O/c17-14-15-12-9-5-4-8-11(12)13(16-14)10-6-2-1-3-7-10/h1-9H,(H,15,16,17)	-2.453
InChI=1S/C7H20N2O7P2S2/c10-7(5-8-1-3-19-17(11,12)13)6-9-2-4-20-18(14,15)16/h7-10H,1-6H2,(H2,11,12,13)(H2,14,15,16)	0.431
InChI=1S/C8H14O2/c1-3-9-7-5-6-8-10-4-2/h3-4H,1-2,5-8H2	-2.648
InChI=1S/C12H15NO3/c1-9(7-8-11(14)15)13-12(16)10-5-3-2-4-6-10/h2-6,9H,7-8H2,1H3,(H,13,16)(H,14,15)	-1.692
InChI=1S/C24H50O12/c25-7-1-13-31-19-21(33-15-3-9-27)23(35-17-5-11-29)24(36-18-6-12-3h21-30H,1-20H2	0.053
InChI=1S/C11H11N3O2S/c12-9-4-6-10(7-5-9)17(15,16)14-11-3-1-2-8-13-11/h1-8H,12H2,(H,13,14)	-2.7
InChI=1S/C12H24N2O4/c1-4-7-14-11(16)18-9-12(5-2,6-3)8-17-10(13)15/h4-9H2,1-3H3,(H2,13,15)(H,14,16)	-3.175
InChI=1S/C10H12O2/c1-6-4-8(3)9(10(11)12)5-7(6)2/h4-5H,1-3H3,(H,11,12)	-3.108

"InChi"	"logS(M)"
InChI=1S/C11H14O2/c1-2-13-11(12)9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3	-2.909
InChI=1S/C2H2F3NO/c3-2(4,5)1(6)7/h(H2,6,7)	-1.485
InChI=1S/C8H7Cl3O3/c1-13-7-4(10)3(9)5(11)8(14-2)6(7)12/h12H,1-2H3	-3.41
InChI=1S/C18H15O4P/c19-23(20-16-10-4-1-5-11-16,21-17-12-6-2-7-13-17)22-18-14-8-3-9-15-18/h1-15H	-5.66
InChI=1S/C16H28O/c1-11-6-7-12-14(2,3)13-10-16(11,12)9-8-15(13,4)17-5/h11-13H,6-10H2,1-5H3	-4.74
InChI=1S/C10H8O2/c11-9-3-1-7-2-4-10(12)6-8(7)5-9/h1-6,11-12H	-2.219
InChI=1S/C20H20O7/c1-22-12-8-6-11(7-9-12)14-10-13(21)15-16(23-2)18(24-3)20(26-5)19(h6-10H,1-5H3	-4.631
InChI=1S/C15H20N4/c1-18(2)11-12-19(15-16-9-6-10-17-15)13-14-7-4-3-5-8-14/h3-10H,11-13H2,1-2H3	-1.838
InChI=1S/C28H35FO7/c1-16(30)34-15-22(33)28-23(35-26(36-28)9-4-5-10-26)13-20-19-7-6-18-8,11-12,19-21,23,32H,4-7,9-10,13-15H2,1-3H3	-5.578
InChI=1S/C13H10O4/c1-7-5-9(14)12-11(17-7)6-10-8(3-4-16-10)13(12)15-2/h3-6H,1-2H3	-3.931
InChI=1S/C7H16O3/c1-6(4-8)10-5-7(2)9-3/h6-8H,4-5H2,1-3H3	0.829
InChI=1S/C7H11N3O3/c1-5(11)4-9-6(2)8-3-7(9)10(12)13/h3,5,11H,4H2,1-2H3	-0.74
InChI=1S/C9H19NO3/c1-7(2)4-9(3,5-11)6-13-8(10)12/h7,11H,4-6H2,1-3H3,(H2,10,12)	-1.673
InChI=1S/C26H50O4/c1-5-9-17-23(7-3)21-29-25(27)19-15-13-11-12-14-16-20-26(28)30-22-h23-24H,5-22H2,1-4H3	-3.329
InChI=1S/C4H5N3O5S/c8-3-2(7-13(10,11)12)1-5-4(9)6-3/h1,7H,(H,10,11,12)(H2,5,6,8,9)	-1.77
InChI=1S/C14H18O/c1-2-3-5-10-14(12-15)11-13-8-6-4-7-9-13/h4,6-9,11-12H,2-3,5,10H2,1H3/b14-11-	-3.047
InChI=1S/C2H4I2/c3-1-2-4/h1-2H2	-3.22
InChI=1S/C21H24FNO2/c22-19-10-8-18(9-11-19)21(25)12-15-23(16-13-21)14-4-7-20(24)17-5-h1-3,5-6,8-11,25H,4,7,12-16H2	-2.97
InChI=1S/C14H26N2O2/c1-13(2,3)9-14(4,5)10-6-7-11(15-17)12(8-10)16-18/h10,17-18H,6-9H2,1-5H3/b15-11+,16-12+	-6.41
InChI=1S/C16H26N2O2/c1-5-18(6-2)11-16(3,4)12-20-15(19)13-7-9-14(17)10-8-13/h7-10H,5-6,11-12,17H2,1-4H3	-3.082
InChI=1S/C11H22N2O4/c1-4-8(3)11(5-2,6-16-9(12)14)7-17-10(13)15/h8H,4-7H2,1-3H3,(H2,12,14)(H2,13,15)	-2.613
InChI=1S/C10H15NO4S2/c12-17(13,14)16-9-7-11-6-8-15-10-4-2-1-3-5-10/h1-5,11H,6-9H2,(H,12,13,14)	-0.418

"InChi"	"logS(M)"
InChI=1S/C2H4N2O6/c5-3(6)9-1-2-10-4(7)8/h1-2H2	-1.349
InChI=1S/C12H9Cl2NO4S2/c13-9-1-5-11(6-2-9)20(16,17)15-21(18,19)12-7-3-10(14)4-8-12/h1-8,15H	-2.48
InChI=1S/C3H4Cl4/c4-1-3(6,7)2-5/h1-2H2	-2.579
InChI=1S/C8H11N/c1-6-4-5-7(2)9-8(6)3/h4-5H,1-3H3	-0.589
InChI=1S/C11H14N2O/c1-8-7-10(12)11(14)13(8)9-5-3-2-4-6-9/h2-6,8,10H,7,12H2,1H3	-1.083
InChI=1S/C10H16N2O3S/c13-8(14)4-2-1-3-7-9-6(5-16-7)11-10(15)12-9/h6-7,9H,1-5H2,(H,13,14)(H2,11,12,15)	-3.046
InChI=1S/C7H16O4S2/c1-5-12(8,9)7(3,4)13(10,11)6-2/h5-6H2,1-4H3	-1.927
InChI=1S/C10H8O3/c11-9(6-7-10(12)13)8-4-2-1-3-5-8/h1-7H,(H,12,13)/b7-6+	-1.398
InChI=1S/C15H14O2/c1-17-15(13-10-6-3-7-11-13)14(16)12-8-4-2-5-9-12/h2-11,15H,1H3	-2.684
InChI=1S/C6H6N4O/c1-11-6-7-2-4-5(10-6)9-3-8-4/h2-3H,1H3,(H,7,8,9,10)	-1.48
InChI=1S/C11H11Cl2NO2/c1-7-6-16-9-5-3-2-4-8(9)14(7)11(15)10(12)13/h2-5,7,10H,6H2,1H3	-3.835
InChI=1S/C9H18N2O4/c1-9(2,3)6(4-14-7(10)12)5-15-8(11)13/h6H,4-5H2,1-3H3,(H2,10,12)(H2,11,13)	-1.57
InChI=1S/C8H10NO5P/c1-6(10)9-7-2-4-8(5-3-7)14-15(11,12)13/h2-5H,1H3,(H,9,10)(H2,11,12,13)	0.13
InChI=1S/C10H20O3/c1-7(2)10(8(3)4)12-6-9(5-11)13-10/h7-9,11H,5-6H2,1-4H3	-2.531
InChI=1S/C15H10ClFN2O/c16-9-5-6-13-11(7-9)15(18-8-14(20)19-13)10-3-1-2-4-12(10)17/h1-7H,8H2,(H,19,20)	-3.612
InChI=1S/C16H14N4O2/c1-20(11-13-4-2-12(10-17)3-5-13)19-18-15-8-6-14(7-9-15)16(21)22/h2-9H,11H2,1H3,(H,21,22)/b19-18+	-4.686
InChI=1S/C18H29NO3/c1-14(2)19-11-17(20)13-22-18-7-5-15(6-8-18)9-10-21-12-16-3-4-16/h5-8,14,16-17,19-20H,3-4,9-13H2,1-2H3	-2.834
InChI=1S/C12H24O/c13-12-10-8-6-4-2-1-3-5-7-9-11-12/h12-13H,1-11H2	-3.989
InChI=1S/C20H34O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h5-6,8-9,11-12H,3-4,7,10,13-19H2,1-2H3/b6-5+,9-8+,12-11+	-8.334
InChI=1S/C11H20O/c1-2-3-4-5-6-7-8-9-10-11-12/h2,11H,1,3-10H2	-3.893
InChI=1S/C12H10O4S/c13-9-5-1-3-7-11(9)17(15,16)12-8-4-2-6-10(12)14/h1-8,13-14H	-3.319
InChI=1S/C15H23NO/c1-12(2)16(14(17)15(3,4)5)11-13-9-7-6-8-10-13/h6-10,12H,11H2,1-5H3	-2.47
InChI=1S/C15H15BrFN3O3/c1-8-13(18-12-5-4-9(16)6-11(12)17)10(14(21)19-23-3)7-20(2)15(8)22h4-7,18H,1-3H3,(H,19,21)	-3.28

"InChi"	"logS(M)"
InChI=1S/C16H13NO2S/c18-15(19)9-7-11-6-8-14-13(10-11)17-16(20-14)12-4-2-1-3-5-12/h1-6,8,10H,7,9H2,(H,18,19)	-4.481
InChI=1S/C12H10O/c1-9(13)11-7-6-10-4-2-3-5-12(10)8-11/h2-8H,1H3	-2.796
InChI=1S/C20H27N3/c1-3-22(4-2)14-9-15-23-19-12-7-5-10-17(19)16-21-18-11-6-8-13-20(18)h5-8,10-13,21H,3-4,9,14-16H2,1-2H3	-5.216
InChI=1S/C20H12N2O2/c23-19-11-5-1-3-7-15(11)21-17-10-14-18(9-13(17)19)22-16-8-4-2-6-1h1-10H,(H,21,23)(H,22,24)	-7.482
InChI=1S/C9H21O3PS3/c1-6-16(10)7-15-13(14,11-8(2)3)12-9(4)5/h8-9H,6-7H2,1-5H3/p+1	-2.307
InChI=1S/C14H18Cl2O4/c1-2-3-6-18-7-8-19-14(17)10-20-13-5-4-11(15)9-12(13)16/h4-5,9H,2-3,6-8,10H2,1H3	-4.428
InChI=1S/C12H3Cl7/c13-4-1-5(10(17)7(15)2-4)9-6(14)3-8(16)11(18)12(9)19/h1-3H	-8.68
InChI=1S/C20H31NO3/c1-4-17(3)24-19-11-9-18(10-12-19)20(22)23-15-7-14-21-13-6-5-8-16(h9-12,16-17H,4-8,13-15H2,1-3H3	-5.129
InChI=1S/C25H34N2O6/c1-5-16-25(4,17-32-23(28)26-19-8-12-21(13-9-19)30-6-2)18-33-24(29h8-15H,5-7,16-18H2,1-4H3,(H,26,28)(H,27,29)	-1.956
InChI=1S/C14H15N3O/c1-9-3-8-13(16-10(9)2)17-14(18)11-4-6-12(15)7-5-11/h3-8H,15H2,1-2H3,(H,16,17,18)	-2.881
InChI=1S/C16H12O6/c1-21-13-3-2-8(4-10(13)18)14-7-12(20)16-11(19)5-9(17)6-15(16)22-1h2-7,17-19H,1H3	-6.199
InChI=1S/C14H31O5P/c1-4-7-12-17-20(15,18-13-8-5-2)19-14-10-9-11-16-6-3/h4-14H2,1-3H3	-2.647
InChI=1S/C12H13NO2/c1-12(9-6-4-3-5-7-9)8-10(14)13(2)11(12)15/h3-7H,8H2,1-2H3	-1.593
InChI=1S/C10H9NO4/c1-10(2)8-4-3-6(11(13)14)5-7(8)9(12)15-10/h3-5H,1-2H3	-3.052
InChI=1S/C22H27NO2/c1-2-21(24)22(19-9-5-3-6-10-19,20-11-7-4-8-12-20)13-14-23-15-17-2h3-12H,2,13-18H2,1H3	-3.524
InChI=1S/C16H22N2O/c1-2-16(19)18-14-8-9-15(18)12-17(11-14)10-13-6-4-3-5-7-13/h3-7,14-15H,2,8-12H2,1H3	-2.811
InChI=1S/C17H19NO2/c1-12(2)20-15-9-6-8-14(11-15)18-17(19)16-10-5-4-7-13(16)3/h4-12H,1-3H3,(H,18,19)	-4.327
InChI=1S/C10H16N2O2/c1-9(2)6-4-5-10(9,3)8(12-14)7(6)11-13/h6,13-14H,4-5H2,1-3H3/b11-7+,12-8-	-2.52
InChI=1S/C16H18N4/c1-11(2)18-19-16(17)20-9-13-7-3-5-12-6-4-8-14(10-20)15(12)13/h3-8H,9-10H2,1-2H3,(H2,17,19)	-2.48

"InChi"	"logS(M)"
InChI=1S/C16H20N2O3S2/c1-2-3-8-18-10-12-4-6-13(7-5-12)16(19)14-9-15(22-11-14)23(17,20)2h4-7,9,11,18H,2-3,8,10H2,1H3,(H2,17,20,21)	-2.21
InChI=1S/C16H16N2O3/c1-17-15(20)12-8-9-13(16(17)21)18(12)14(19)10-7-11-5-3-2-4-6-11/h2-7,10,12-13H,8-9H2,1H3/b10-7+	-2.553
InChI=1S/C24H51N/c1-7-13-16-22(10-4)19-25(20-23(11-5)17-14-8-2)21-24(12-6)18-15-9-h22-24H,7-21H2,1-6H3	-8.248
InChI=1S/C12H19O2PS3/c1-4-10-18-15(16,13-5-2)14-11-6-8-12(17-3)9-7-11/h6-9H,4-5,10H2,1-3H3	-6.017
InChI=1S/C3H7NO2/c1-3(6)4-2-5/h5H,2H2,1H3,(H,4,6)	1.05
InChI=1S/C22H28N4O3/c1-4-24(5-2)13-14-25-21-12-9-18(26(27)28)16-20(21)23-22(25)15-17-h7-12,16H,4-6,13-15H2,1-3H3	-5.833
InChI=1S/C12H14ClN3O/c13-8-1-2-11-10(7-8)15-12(17)16(11)9-3-5-14-6-4-9/h1-2,7,9,14H,3-6H2,(H,15,17)/p+1	-2.663
InChI=1S/C16H20O5/c1-9-3-2-4-12(20-9)8-13-6-10-5-11(17)7-14(18)15(10)16(19)21-13/h5,7,9,12-13,17-18H,2-4,6,8H2,1H3	-3.612
InChI=1S/C9H8N2O2/c10-5-6-11-8-4-2-1-3-7(8)9(12)13/h1-4,11H,6H2,(H,12,13)	-2.289
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)	-2.067
InChI=1S/C10H16N2O5S/c11-8-1-3-9(4-2-8)18(16,17)12-10(5-13,6-14)7-15/h1-4,12-15H,5-7,11H2	-1.4
InChI=1S/C12H18O4/c1-2-16-12-5-3-10(4-6-12)8-15-9-11(14)7-13/h3-6,11,13-14H,2,7-9H2,1H3	-1.818
InChI=1S/C10H12O4/c11-5-8-3-1-2-4-10(8)14-7-9(13)6-12/h1-5,9,12-13H,6-7H2	-0.784
InChI=1S/C6H4O5/c7-5(8)3-1-2-4(11-3)6(9)10/h1-2H,(H,7,8)(H,9,10)	-2.24
InChI=1S/C16H12O2/c1-2-10-7-8-13-14(9-10)16(18)12-6-4-3-5-11(12)15(13)17/h3-9H,2H2,1H3	-5.984
InChI=1S/C5H11NS/c1-5(2)6-3-4-7-5/h6H,3-4H2,1-2H3	-0.226
InChI=1S/C3H3BrF4/c4-1-3(7,8)2(5)6/h2H,1H2	-3.208
InChI=1S/C11H20O2/c1-3-4-5-6-8-11(2)9-7-10(12)13-11/h3-9H2,1-2H3	-2.643
InChI=1S/C18H17Cl2N3O3/c1-23(17(25)10-22-16(24)9-21)15-7-6-11(19)8-13(15)18(26)12-4-2-3-h2-8H,9-10,21H2,1H3,(H,22,24)	-2.33
InChI=1S/C6H13N/c1-7-5-3-2-4-6-7/h2-6H2,1H3	0.23
InChI=1S/C8H7NO2/c10-8(6-9-11)7-4-2-1-3-5-7/h1-6,11H/b9-6+	-2.886
InChI=1S/C14H13NO/c15-14(16)10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-9H,10H2,(H2,15,16)	-3.33
InChI=1S/C10H11ClN4/c1-8(14-7-12)15(2)6-9-3-4-10(11)13-5-9/h3-5H,6H2,1-2H3/b14-8+	-1.724

"InChi"	"logS(M)"
InChI=1S/C13H20FN3O3/c1-2-3-4-5-6-7-8-15-12(19)17-9-10(14)11(18)16-13(17)20/h9H,2-8H2,1H3,(H,15,19)(H,16,18,20)	-4.18
InChI=1S/C7H5Cl3O/c1-11-7-5(9)2-4(8)3-6(7)10/h2-3H,1H3	-4.2
InChI=1S/C14H15O2PS2/c1-11-7-3-5-9-13(11)15-17(18,19)16-14-10-6-4-8-12(14)2/h3-10H,1-2H3,(H,18,19)	-1.061
InChI=1S/C9H9NO4/c11-7-4-2-1-3-6(7)9(14)10-5-8(12)13/h1-4,11H,5H2,(H,10,14)(H,12,13)	-0.856
InChI=1S/C11H13N3/c1-8-9(2)13-14(11(8)12)10-6-4-3-5-7-10/h3-7H,12H2,1-2H3	-1.67
InChI=1S/C14H11Cl2NO3/c15-9-5-6-11(18)13(16)14(9)17-10-4-2-1-3-8(10)7-12(19)20/h1-6,17-18H,7H2,(H,19,20)	-3.801
InChI=1S/C9H16O4/c1-3-12-8(10)6-5-7-9(11)13-4-2/h3-7H2,1-2H3	-1.33
InChI=1S/C9H9ClO/c1-2-9(11)7-4-3-5-8(10)6-7/h3-6H,2H2,1H3	-1.847
InChI=1S/C17H26O3/c1-2-3-4-5-6-7-8-9-15-10-12-16(13-11-15)20-14-17(18)19/h10-13H,2-9,14H2,1H3,(H,18,19)	-3.843
InChI=1S/C17H25N/c1-4-10-16(11-5-1)17(12-6-2-7-13-17)18-14-8-3-9-15-18/h1,4-5,10-11H,2-3,6-9,12-15H2	-3.933
InChI=1S/C8H6Cl2O3/c9-5-2-1-3-6(8(5)10)13-4-7(11)12/h1-3H,4H2,(H,11,12)	-2.81
InChI=1S/C6H4Cl3N/c7-3-1-4(8)6(10)5(9)2-3/h1-2H,10H2	-3.691
InChI=1S/C10H12O2S/c1-2-13-9(10(11)12)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H,11,12)	-1.569
InChI=1S/C11H8O2S/c1-14-10-6-9(12)7-4-2-3-5-8(7)11(10)13/h2-6H,1H3	-4.465
InChI=1S/C9H8N2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-7H,(H,10,11)	-1.889
InChI=1S/C9H8N2O/c1-11-6-10-8-5-3-2-4-7(8)9(11)12/h2-6H,1H3	-0.959
InChI=1S/C4H14N3PS/c1-2-3-4-7-8(5,6)9/h2-4H2,1H3,(H5,5,6,7,9)	-0.773
InChI=1S/C31H20O10/c1-39-17-9-20(34)29-23(37)12-26(40-27(29)10-17)15-4-7-19(33)18(8-h2-13,32-36H,1H3	-7.788
InChI=1S/C9H9ClO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2	-1.907
InChI=1S/C12H15N3O3/c1-3-14(4-2)13-9-12(16)10-5-7-11(8-6-10)15(17)18/h5-9H,3-4H2,1-2H3/b13-9+	-2.731
InChI=1S/C7H10N2/c1-6-2-4-7(9-8)5-3-6/h2-5,9H,8H2,1H3	-1.239
InChI=1S/C7H8N4O/c1-2-12-7-5-6(9-3-8-5)10-4-11-7/h3-4H,2H2,1H3,(H,8,9,10,11)	-1.887
InChI=1S/C51H98O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-49(52)55-46-48(57-51(5h48H,4-47H2,1-3H3	-5.374
InChI=1S/C19H26O2/c1-2-19-10-9-15-14-6-4-13(20)11-12(14)3-5-16(15)17(19)7-8-18(19)2h11,14-17H,2-10H2,1H3	-3.733
InChI=1S/C10H13Cl2O3PS/c1-3-13-16(17,14-4-2)15-10-6-5-8(11)7-9(10)12/h5-7H,3-4H2,1-2H3	-6.109

"InChi"	"logS(M)"
InChI=1S/C34H16O2/c35-33-25-7-3-1-5-17(25)19-9-11-21-22-12-10-20-18-6-2-4-8-26(18)3h1-16H	-5.513
InChI=1S/C2H2Br3NO/c3-2(4,5)1(6)7/h(H2,6,7)	-1.267
InChI=1S/C7H7NO3/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3	-2.384
InChI=1S/C14H14ClN3O4S2/c15-10-7-11-13(8-12(10)23(16,19)20)24(21,22)18-14(17-11)6-9-4-2-1h1-5,7-8,14,17-18H,6H2,(H2,16,19,20)	-3.873
InChI=1S/C13H20O/c1-2-3-4-5-6-7-12-8-10-13(14)11-9-12/h8-11,14H,2-7H2,1H3	-3.66
InChI=1S/C10H16Br2N2O2/c11-3-1-9(15)13-5-7-14(8-6-13)10(16)2-4-12/h1-8H2	-2.155
InChI=1S/C15H13ClN2O/c16-11-6-7-13-12(8-11)15(17-9-14(19)18-13)10-4-2-1-3-5-10/h1-8,15,17H,9H2,(H,18,19)	-3.51
InChI=1S/C12H10ClNO2S/c13-11-8-4-5-9-12(11)14-17(15,16)10-6-2-1-3-7-10/h1-9,14H	-4.32
InChI=1S/C20H29NO/c1-5-20-9-11-21(10-8-14(2)3)19(15(20)4)12-16-6-7-17(22)13-18(16)2h6-8,13,15,19,22H,5,9-12H2,1-4H3	-4.508
InChI=1S/C9H17N/c1-9(10-2)6-7-3-4-8(9)5-7/h7-8,10H,3-6H2,1-2H3	-1.294
InChI=1S/C20H32N2O4/c1-14(2)17-7-6-15(3)18(20(24)25-5)19(17)26-13-16(23)12-22-10-8-21h6-7,14,16,23H,8-13H2,1-5H3	-2.984
InChI=1S/C28H42O2/c1-25(2,3)17-13-19(23(29)21(15-17)27(7,8)9)20-14-18(26(4,5)6)16-2h13-16,29-30H,1-12H3	-6.889
InChI=1S/C32H38N2O8/c1-37-24-12-17(13-25(38-2)29(24)39-3)31(35)42-26-14-18-16-34-11-h6-9,12-13,18,21,23,26-27,30,33H,10-11,14-16H2,1-5H3	-5.289
InChI=1S/C7H12O3/c1-5(2)7(9)10-6(3)4-8/h6,8H,1,4H2,2-3H3	-0.045
InChI=1S/C28H28N2O2/c29-22-28(24-12-6-2-7-13-24,25-14-8-3-9-15-25)18-21-30-19-16-27(1h1-15H,16-21H2,(H,31,32)	-6.332
InChI=1S/C5H8N2O2/c1-5(2)3(8)6-4(9)7-5/h1-2H3,(H2,6,7,8,9)	0.038
InChI=1S/C8H10O3S2/c9-13(10,11)7-6-12-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,9,10,11)	-1.53
InChI=1S/C12H7Cl3O/c13-9-6-5-8(7-11(9)15)16-12-4-2-1-3-10(12)14/h1-7H	-5.199
InChI=1S/C8H6Cl2O2/c9-6-2-1-5(3-8(11)12)7(10)4-6/h1-2,4H,3H2,(H,11,12)	-2.919
InChI=1S/C3H7NO3/c4-2(1-5)3(6)7/h2,5H,1,4H2,(H,6,7)	-0.386
InChI=1S/C6H12NO3PS2/c1-3-9-11(8,10-4-2)7-6-12-5-13-6/h3-5H2,1-2H3	-0.683
InChI=1S/C11H25NO3S2/c1-2-3-4-5-6-7-8-9-12-10-11-16-17(13,14)15/h12H,2-11H2,1H3,(H,13,14,15)	-2.339
InChI=1S/C10H12O3/c1-8(11)13-7-9-3-5-10(12-2)6-4-9/h3-6H,7H2,1-2H3	-2.474
InChI=1S/C3H6O2S2/c4-3(5)2(7)1-6/h2,6-7H,1H2,(H,4,5)	-0.237

"InChi"	"logS(M)"
InChI=1S/C7H9NO3S/c1-5-2-3-6(8)7(4-5)12(9,10)11/h2-4H,8H2,1H3,(H,9,10,11)	-1.494
InChI=1S/C15H12ClN3O/c16-10-6-7-12-13(8-10)19(11-4-2-1-3-5-11)15(20)9-14(17)18-12/h1-8H,9H2,(H2,17,18)	-2.226
InChI=1S/C6H14N2O/c1-3-5-6-8(4-2)7-9/h3-6H2,1-2H3	-1.035
InChI=1S/C20H15O5P/c21-19(22)14-6-10-17(11-7-14)26(25,16-4-2-1-3-5-16)18-12-8-15(9-1h1-13H,(H,21,22)(H,23,24)	-6.01
InChI=1S/C9H14O5/c1-4-5-13-9(12)7(3)14-8(11)6(2)10/h4,6-7,10H,1,5H2,2-3H3	-0.683
InChI=1S/C15H18ClN3O/c1-15(2,3)14(20)13(19-10-17-9-18-19)8-11-4-6-12(16)7-5-11/h4-10,14,20H,1-3H3/b13-8-	-4.54
InChI=1S/C11H12N4O3S/c1-18-11-6-10(13-7-14-11)15-19(16,17)9-4-2-8(12)3-5-9/h2-7H,12H2,1H3,(H,13,14,15)	-1.842
InChI=1S/C10H20/c1-8(2)10-6-4-9(3)5-7-10/h8-10H,4-7H2,1-3H3	-5.355
InChI=1S/C19H26O4S/c1-5-14-21-24(20)23-18-9-7-6-8-17(18)22-16-12-10-15(11-13-16)19(2h1,10-13,17-18H,6-9,14H2,2-4H3/p+1	-5.846
InChI=1S/C43H58N4O12/c1-21-12-11-13-22(2)42(55)45-33-28(20-44-47-17-15-46(9)16-18-47)h11-14,19-21,23-25,29,34-35,39,44,49-51,53H,15-18H2,1-10H3,(H,45,55)/b12-11-,19-14-,22-13-,28-20-	-2.769
InChI=1S/C20H23NO/c22-20(18-12-6-2-7-13-18)19(17-10-4-1-5-11-17)16-21-14-8-3-9-15-2h1-2,4-7,10-13,19H,3,8-9,14-16H2	-4.061
InChI=1S/C8H18O3/c1-4-10-8(11-5-2)6-7(3)9/h7-9H,4-6H2,1-3H3	0.091
InChI=1S/C10H9NO4S/c11-7-1-2-9-6(3-7)4-8(5-10(9)12)16(13,14)15/h1-5,12H,11H2,(H,13,14,15)	-2.68
InChI=1S/C10H10Cl3O4P/c1-15-18(14,16-2)17-10(6-11)8-4-3-7(12)5-9(8)13/h3-6H,1-2H3/b10-6-	-3.407
InChI=1S/C22H26N2O/c1-2-21(25)24-19-13-14-20(24)16-23(15-19)22(17-9-5-3-6-10-17)18-1h3-12,19-20,22H,2,13-16H2,1H3	-4.761
InChI=1S/C8H9NO2/c1-9-8(11)6-4-2-3-5-7(6)10/h2-5,10H,1H3,(H,9,11)	-1.006
InChI=1S/C18H17NO3S/c1-3-22-17(20)11-12-4-9-16-15(10-12)19-18(23-16)13-5-7-14(21-2)8-h4-10H,3,11H2,1-2H3	-5.511
InChI=1S/C18H21ClN2/c1-20-11-13-21(14-12-20)18(15-5-3-2-4-6-15)16-7-9-17(19)10-8-16/h2-10,18H,11-14H2,1H3	-2.879
InChI=1S/C12H18O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h6,11H,1-5,7-9H2	-2.774
InChI=1S/C15H20O5/c1-12(2)4-6-7(9(12)17)13(3)14(5-19-14)10(18)11-15(13,20-11)8(6)16h6-9,11,16-17H,4-5H2,1-3H3	-2.103

"InChi"	"logS(M)"
InChI=1S/C15H12O5/c1-7-6-19-13-8(2)12-9(4-10(7)13)5-11(14(16)18-3)15(17)20-12/h4-6H,1-3H3	-4.9
InChI=1S/C12H14N2O2/c1-3-12(9-7-5-4-6-8-9)10(15)13-11(16)14(12)2/h4-8H,3H2,1-2H3,(H,13,15,16)	-6.282
InChI=1S/C5H13N/c1-4-6(3)5-2/h4-5H2,1-3H3/p+1	0.713
InChI=1S/C28H46O4/c1-23(2)17-11-7-5-9-15-21-31-27(29)25-19-13-14-20-26(25)28(30)32-h13-14,19-20,23-24H,5-12,15-18,21-22H2,1-4H3	-9.42
InChI=1S/C3H5N5S/c4-1-6-2(5)8-3(9)7-1/h(H5,4,5,6,7,8,9)	-0.631
InChI=1S/C4H4O/c1-2-4-5-3-1/h1-4H	-0.82
InChI=1S/C9H10F3N/c10-9(11,12)8-3-1-2-7(6-8)4-5-13/h1-3,6H,4-5,13H2	-1.538
InChI=1S/C7H10O4/c1-2-3-5(7(10)11)4-6(8)9/h4H,2-3H2,1H3,(H,8,9)(H,10,11)/b5-4-	-1.154
InChI=1S/C18H25N/c1-19-14-13-16-9-5-6-10-17(16)18(19)12-11-15-7-3-2-4-8-15/h2-4,7-8,18H,5-6,9-14H2,1H3	-4.66
InChI=1S/C23H25ClN6O10/c1-13(31)25-18-11-20(28(5-7-39-14(2)32)6-8-40-15(3)33)22(38-4)12-h9-12H,5-8H2,1-4H3,(H,25,31)/b27-26+	-5.463
InChI=1S/C4H7ClO2/c1-3(2)7-4(5)6/h3H,1-2H3	-0.988
InChI=1S/C13H17NO4/c1-9(15)17-12-6-4-5-11(7-12)13(8-14-3)18-10(2)16/h4-7,13-14H,8H2,1-3H3	-0.956
InChI=1S/C30H24O8P2/c31-39(33-25-14-5-1-6-15-25,34-26-16-7-2-8-17-26)37-29-22-13-23-3h1-24H	-5.738
InChI=1S/C7H10N2O3/c1-4-5(10)8(2)7(12)9(3)6(4)11/h4H,1-3H3	-0.094
InChI=1S/C12H6Cl4O/c13-7-3-1-2-4-11(7)17-12-6-9(15)8(14)5-10(12)16/h1-6H	-7
InChI=1S/C9H12N4O2/c1-4-13-5-10-7-6(13)8(14)12(3)9(15)11(7)2/h5H,4H2,1-3H3	-0.754
InChI=1S/C13H26N2O4/c1-6-8-13(3,9-18-11(16)14-7-2)10-19-12(17)15(4)5/h6-10H2,1-5H3,(H,14,16)	-3.605
InChI=1S/C24H20N6O3/c1-2-33-24-25-20-9-5-8-19(23(31)32)21(20)30(24)14-15-10-12-16(13-h3-13H,2,14H2,1H3,(H,31,32)(H,26,27,28,29)	-6.498
InChI=1S/C15H18N2O3/c1-4-15(11-8-6-5-7-9-11)12(18)16-14(19)17-13(15)20-10(2)3/h5-10H,4H2,1-3H3,(H,16,18,19)	-3.097
InChI=1S/C34H47NO11/c1-7-35-15-31(16-41-3)20(37)13-21(42-4)33-19-14-32(40)28(45-30(3h8-12,19-29,37-38,40H,7,13-16H2,1-6H3	-3.319
InChI=1S/C8H14ClN3O4S/c9-3-4-12(11-14)8(13)10-7-1-5-17(15,16)6-2-7/h7H,1-6H2,(H,10,13)	-2.742
InChI=1S/C6H4N4O3/c11-4-2-3(7-1-8-4)10-6(13)5(12)9-2/h1H,(H,9,12)(H2,7,8,10,11,13)	-3.69

"InChi"	"logS(M)"
InChI=1S/C8H5Cl3O3/c9-4-1-2-5(10)8(7(4)11)14-3-6(12)13/h1-2H,3H2,(H,12,13)	-2.62
InChI=1S/C6H6ClO3P/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H2,8,9,10)	-1.6
InChI=1S/C9H6Cl6O4S/c10-5-6(11)8(13)4-2-19-20(16,17)18-1-3(4)7(5,12)9(8,14)15/h3-4H,1-2H2	-5.945
InChI=1S/C13H19ClN2O2/c1-3-16(4-2)7-8-18-13(17)11-6-5-10(15)9-12(11)14/h5-6,9H,3-4,7-8,15H2,1-2H3	-2.61
InChI=1S/C12H17NO3/c1-2-3-8-16-11-6-4-10(5-7-11)9-12(14)13-15/h4-7,15H,2-3,8-9H2,1H3,(H,13,14)	-2.606
InChI=1S/C11H13NO3/c13-10-4-2-1-3-9(10)11(14)12-5-7-15-8-6-12/h1-4,13H,5-8H2	-1.704
InChI=1S/C10H13N3O5S/c1-8-7-19(16,17)5-4-12(8)11-6-9-2-3-10(18-9)13(14)15/h2-3,6,8H,4-5,7H2,1H3/b11-6+	-1.824
InChI=1S/C12H12O2/c13-11-9-5-1-2-6-10(9)12(14-11)7-3-4-8-12/h1-2,5-6H,3-4,7-8H2	-2.761
InChI=1S/C8H16O2/c1-3-5-6-7(4-2)8(9)10/h7H,3-6H2,1-2H3,(H,9,10)	-1.858
InChI=1S/C16H23N3O2/c1-18-10-14-6-7-15(11-18)19(14)8-9-21-16(20)12-2-4-13(17)5-3-12/h2-5,14-15H,6-11,17H2,1H3	-1.424
InChI=1S/C3H4ClN5/c4-1-7-2(5)9-3(6)8-1/h(H4,5,6,7,8,9)	-2.385
InChI=1S/C14H11NO5/c1-8-2-4-9(5-3-8)13(17)10-6-11(15(19)20)14(18)12(16)7-10/h2-7,16,18H,1H3	-4.17
InChI=1S/C17H34O2/c1-4-5-6-7-8-9-10-11-12-13-17(18)19-15-14-16(2)3/h16H,4-15H2,1-3H3	-6.733
InChI=1S/C3H8N2OS/c1-4-7-3-5-2-6/h4-6H,2H2,1H3	-0.08
InChI=1S/C12H4Cl6O/c13-5-1-9(17)12(18)11(2-5)19-10-4-7(15)6(14)3-8(10)16/h1-4H	-8.41
InChI=1S/C9H19NO/c1-5-10(6-2)9(11)7-8(3)4/h8H,5-7H2,1-4H3	-0.595
InChI=1S/C3H6N2O2/c1-3(5-7)2-4-6/h2,5,7H,1H3/b3-2-	-0.346
InChI=1S/C6H12N2OS/c1-2-3-7-6(10)8-4-5-9/h2,9H,1,3-5H2,(H2,7,8,10)	-0.942
InChI=1S/C9H14ClN5/c1-5(2)11-8-13-7(10)14-9(15-8)12-6-3-4-6/h5-6H,3-4H2,1-2H3,(H2,11,12,13,14,15)	-3.518
InChI=1S/C10H12O2/c1-9(11)12-8-7-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3	-2.232
InChI=1S/C19H26N2O/c1-14(2)19(18(20)22,12-13-21(3)4)17-11-7-9-15-8-5-6-10-16(15)17/h5-11,14H,12-13H2,1-4H3,(H2,20,22)	-4.107
InChI=1S/C8H9NO2S/c1-2-12(10,11)9-8-6-4-3-5-7-8/h2-7,9H,1H2	-1.5
InChI=1S/C26H40Cl2O5/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-32-26(30)33-24-22(27)19-20H,3-18H2,1-2H3	-7.134
InChI=1S/C27H36O2/c1-18-13-22(26(28)24(15-18)20-9-5-3-6-10-20)17-23-14-19(2)16-25(2-13-16,20-21,28-29H,3-12,17H2,1-2H3	-6.979

"InChi"	"logS(M)"
InChI=1S/C12H16O3/c1-10(2)12(13)15-9-8-14-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3	-3.026
InChI=1S/C18H19ClN2O2/c1-18(2,3)21(17(23)14-7-5-4-6-8-14)20-16(22)13-9-11-15(19)12-10-1h4-12H,1-3H3,(H,20,22)	-4.44
InChI=1S/C44H38Cl4N8O6/c1-21-7-11-29(45)19-35(21)49-41(59)27-9-13-31(47)37(17-27)53-55-h7-20,39-40H,1-6H3,(H,49,59)(H,50,60)(H,51,61)(H,52,62)/b55-53+,56-54+	-7.263
InChI=1S/C16H30O4/c1-10(2)13(20-15(18)12(5)6)16(7,8)9-19-14(17)11(3)4/h10-13H,9H2,1-8H3	-4.333
InChI=1S/C25H32ClFO5/c1-5-21(31)32-25(20(30)13-26)14(2)10-18-17-7-6-15-11-16(28)8-9-22h8-9,11,14,17-19,29H,5-7,10,12-13H2,1-4H3	-5.083
InChI=1S/C6H10N2O5/c7-4(9)1-8(2-5(10)11)3-6(12)13/h1-3H2,(H2,7,9)(H,10,11)(H,12,13)/p-1	-1.764
InChI=1S/C21H25ClN2S/c1-3-23(2)17-10-11-24(14-17)19-12-15-6-4-5-7-20(15)25-21-9-8-16(2h4-9,13,17,19H,3,10-12,14H2,1-2H3	-6.755
InChI=1S/C17H12ClNO2/c18-13-5-7-14(8-6-13)19-17(21)15-9-11-3-1-2-4-12(11)10-16(15)20/h1-10,20H,(H,19,21)	-5.474
InChI=1S/C6H2Cl3NO/c7-4-1-3(10-9)2-5(8)6(4)11/h1-2H	-2.696
InChI=1S/C12H5Cl5/c13-7-4-5-9(15)12(17)10(7)6-2-1-3-8(14)11(6)16/h1-5H	-6.78
InChI=1S/C3H2O3/c4-3-5-1-2-6-3/h1-2H	0.777
InChI=1S/C7H14O3/c1-3-5-10-6-4-7(8)9-2/h3-6H2,1-2H3	-0.633
InChI=1S/C17H19N5O4/c23-16(19-18-12-15-6-7-17(26-15)22(24)25)13-20-8-10-21(11-9-20)1h1-7,12H,8-11,13H2,(H,19,23)/b18-12+	-3.383
InChI=1S/C9H21O3P/c1-4-6-8-11-13(3,10)12-9-7-5-2/h4-9H2,1-3H3	-1.415
InChI=1S/C7H2ClN3O4/c8-7-5(10(12)13)1-4(3-9)2-6(7)11(14)15/h1-2H	-3.069
InChI=1S/C8H7NO3S/c10-8-7-4-2-1-3-6(7)5-13(11,12)9-8/h1-4H,5H2,(H,9,10)	-1.25
InChI=1S/C11H13NO3/c1-8(11(14)15)7-10(13)12-9-5-3-2-4-6-9/h2-6,8H,7H2,1H3,(H,12,13)(H,14,15)	0.39
InChI=1S/C14H16N2O2S/c1-2-11-3-7-13(8-4-11)16-19(17,18)14-9-5-12(15)6-10-14/h3-10,16H,2,15H2,1H3	-4.52
InChI=1S/C9H10O4S/c1-13-9(10)7-14(11,12)8-5-3-2-4-6-8/h2-6H,7H2,1H3	-1.141
InChI=1S/C15H19NO3/c17-14(16-10-6-1-2-7-11-16)12-19-15(18)13-8-4-3-5-9-13/h3-5,8-9H,1-2,6-7,10-12H2	-2.542
InChI=1S/C5H2Cl2O3/c6-2-1-10-4(3(2)7)5(8)9/h1H,(H,8,9)	-1.826
InChI=1S/C4H5NOS2/c1-5-3(6)2-8-4(5)7/h2H2,1H3	0.401
InChI=1S/C9H16O3/c1-3-4-7-12-9(11)6-5-8(2)10/h3-7H2,1-2H3	-1.307

"InChi"	"logS(M)"
InChI=1S/C17H13N3O3/c1-11-6-8-14(15(10-11)20(22)23)18-19-17-13-5-3-2-4-12(13)7-9-16(1h2-10,18H,1H3/b19-17-	-7.969
InChI=1S/C7H6BrNO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,9H2,(H,10,11)	-3.07
InChI=1S/C9H9Cl2NO2/c1-12(9(14)8(10)11)6-2-4-7(13)5-3-6/h2-5,8,13H,1H3	-2.428
InChI=1S/C21H16N2O5S/c24-17-11-13-18(14-12-17)29(27,28)23-20(26)22-19(25)21(23,15-7-3-h1-14,24H,(H,22,25,26)	-4.075
InChI=1S/C3H7NO2/c4-2-1-3(5)6/h1-2,4H2,(H,5,6)	0.787
InChI=1S/C6H10O6S/c7-5(8)1-3-13(11,12)4-2-6(9)10/h1-4H2,(H,7,8)(H,9,10)	-1.967
InChI=1S/C18H35NO/c20-18-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-17-19-18/h1-17H2,(H,19,20)	-2.847
InChI=1S/C12H4Cl6/c13-5-1-2-6(7(14)3-5)10-8(15)4-9(16)11(17)12(10)18/h1-4H	-7.472
InChI=1S/C3H8NO5P/c5-3(6)1-4-2-10(7,8)9/h4H,1-2H2,(H,5,6)(H2,7,8,9)	-1.207
InChI=1S/C12H14O4/c1-12(2,3)11(15)16-9-7-5-4-6-8(9)10(13)14/h4-7H,1-3H3,(H,13,14)	-3.01
InChI=1S/C8H9N3OS/c9-8(13)11-10-7(12)6-4-2-1-3-5-6/h1-5H,(H,10,12)(H3,9,11,13)	-2.078
InChI=1S/C20H32O2/c1-12-10-14(21)11-13-4-5-15-16-6-7-18(22)19(16,2)9-8-17(15)20(12,h12-13,15-18,22H,4-11H2,1-3H3	-5.006
InChI=1S/C17H18F3NO/c1-21-12-11-16(13-5-3-2-4-6-13)22-15-9-7-14(8-10-15)17(18,19)20/h2-10,16,21H,11-12H2,1H3	-1.59
InChI=1S/C17H26N2O2/c1-12(2)19-10-8-15(9-11-19)21-17(20)18-16-13(3)6-5-7-14(16)4/h5-7,12,15H,8-11H2,1-4H3,(H,18,20)	-4.395
InChI=1S/C15H20N2O/c1-12-4-6-13(7-5-12)17-11-8-14(15(17)18)16-9-2-3-10-16/h4-7,14H,2-3,8-11H2,1H3	-2.908
InChI=1S/C12H22O/c1-9(2)7-8-12(5,6)11(13)10(3)4/h7,10H,8H2,1-6H3	-3.489
InChI=1S/C14H10N4O5/c19-13-8-17(14(20)16-13)15-7-11-5-6-12(23-11)9-1-3-10(4-2-9)18(21h1-7H,8H2,(H,16,19,20)/b15-7+	-3.334
InChI=1S/C16H22N2O4S2/c19-24(20,21)23-13-11-17-9-4-1-5-12-22-16-15-7-3-2-6-14(15)8-10-1h2-3,6-8,10,17H,1,4-5,9,11-13H2,(H,19,20,21)	-2.87
InChI=1S/C9H11NO5/c11-5-8(12)6-15-9-3-1-2-7(4-9)10(13)14/h1-4,8,11-12H,5-6H2	-1.725
InChI=1S/C9H10O2/c1-2-3-7-4-5-8(10)9(11)6-7/h2-6,10-11H,1H3/b3-2+	-1.351
InChI=1S/C10H11NO2S/c1-14(12,13)11-8-4-6-9-5-2-3-7-10(9)11/h2-7H,8H2,1H3	-2.817
InChI=1S/C9H8ClN5/c10-6-1-3-7(4-2-6)14-9-13-5-12-8(11)15-9/h1-5H,(H3,11,12,13,14,15)	-2.985

"InChi"	"logS(M)"
InChI=1S/C12H18N2/c1-10-4-6-11(7-5-10)12-13(2)8-9-14(12)3/h4-7,12H,8-9H2,1-3H3	-0.703
InChI=1S/C22H16O8/c1-2-28-20(25)15(16-18(23)11-7-3-5-9-13(11)29-21(16)26)17-19(24)1h3-10,15,26-27H,2H2,1H3	-3.426
InChI=1S/C13H10N2O3S/c16-19(17,18)10-6-7-11-12(8-10)15-13(14-11)9-4-2-1-3-5-9/h1-8H,(H,14,15)(H,16,17,18)	-2.961
InChI=1S/C20H22Cl2N2OS/c21-15-4-7-17(8-5-15)26-19-14-16(22)6-9-18(19)23-20(25)10-13-24-1h4-9,14H,1-3,10-13H2,(H,23,25)	-6.785
InChI=1S/C12H3Cl7/c13-4-1-5(10(17)6(14)2-4)9-11(18)7(15)3-8(16)12(9)19/h1-3H	-8.59
InChI=1S/C3H7IO2S/c1-2-7(5,6)3-4/h2-3H2,1H3	-0.971
InChI=1S/C3H6O/c1-3-4-2/h3H,1H2,2H3	-0.531
InChI=1S/C10H16N2O2S4/c15-9(11-1-5-13-6-2-11)17-18-10(16)12-3-7-14-8-4-12/h1-8H2	-1.353
InChI=1S/C10H18O/c1-7-4-8(2)10(6-11)9(3)5-7/h4,8-11H,5-6H2,1-3H3	-2.371
InChI=1S/C4H9NO3/c1-4(2)3-8-5(6)7/h4H,3H2,1-2H3	-1.952
InChI=1S/C7H14N6/c1-12(2)6-9-5(8)10-7(11-6)13(3)4/h1-4H3,(H2,8,9,10,11)	-1.555
InChI=1S/C12H13N3O6/c16-7(10-8(17)9(18)12(20)21-10)5-14-15-11(19)6-1-3-13-4-2-6/h1-5,7-10,16-18H,(H,15,19)/b14-5+	-0.526
InChI=1S/C15H11ClN2O2/c16-10-6-7-12-13(8-10)18(11-4-2-1-3-5-11)15(20)9-14(19)17-12/h1-8H,9H2,(H,17,19)	-2.997
InChI=1S/C10H9NO3S/c11-9-5-6-10(15(12,13)14)8-4-2-1-3-7(8)9/h1-6H,11H2,(H,12,13,14)	-2.91
InChI=1S/C11H17NO3S2/c12-17(14,15)11-6-4-10(5-7-11)16-9-3-1-2-8-13/h4-7,13H,1-3,8-9H2,(H2,12,14,15)	-2.662
InChI=1S/C12H11NO5S/c1-17-10-4-2-8(3-5-10)12(14)9-6-11(18-7-9)19(13,15)16/h2-7H,1H3,(H2,13,15,16)	-4.148
InChI=1S/C19H31NO3/c1-7-8-12-23-19(21)17-15(4)9-10-16(14(2)3)18(17)22-13-11-20(5)6/h9-10,14H,7-8,11-13H2,1-6H3	-4.877
InChI=1S/C12H6Cl4/c13-8-3-1-7(2-4-8)9-5-6-10(14)12(16)11(9)15/h1-6H	-6.875
InChI=1S/C4H6N2S/c1-6-3-2-5-4(6)7/h2-3H,1H3,(H,5,7)	0.382
InChI=1S/C32H25ClN4O4/c1-19-12-14-22(33)18-26(19)35-32(40)25-16-20-8-6-7-11-24(20)29(3h3-18,36H,1-2H3,(H,34,39)(H,35,40)/b37-29-	-7.752
InChI=1S/C16H16O/c17-16-10-9-12-5-1-2-6-13(12)11-14-7-3-4-8-15(14)16/h1,3-5,7-10,16-17H,2,6,11H2/b10-9-	-5.008
InChI=1S/C8H10N2O2S/c1-13(11,12)7-4-2-6(3-5-7)8(9)10/h2-5H,1H3,(H3,9,10)	-1.38
InChI=1S/C7H10O5/c1-3-11-6(9)5(8)7(10)12-4-2/h3-4H2,1-2H3	0.512

"InChi"	"logS(M)"
InChI=1S/C26H27NO10/c1-9-21(30)13(27)6-16(36-9)37-15-8-26(35,10(2)28)7-12-18(15)25(34h3-5,9,13,15-16,21,29-30,32,34-35H,6-8,27H2,1-2H3	-4.515
InChI=1S/C12H17NO2/c1-4-9(2)10-7-5-6-8-11(10)15-12(14)13-3/h5-9H,4H2,1-3H3,(H,13,14)	-2.53
InChI=1S/C15H18N2/c1-10-7-12(3-5-14(10)16)9-13-4-6-15(17)11(2)8-13/h3-8H,9,16-17H2,1-2H3	-4.151
InChI=1S/C11H24O2/c1-4-7-11(8-12,9-13)10(5-2)6-3/h10,12-13H,4-9H2,1-3H3	-3.168
InChI=1S/C9H10Cl2N2O/c10-7-2-1-3-8(11)6(7)4-5-13-9(12)14/h1-3H,4-5H2,(H3,12,13,14)	-2.949
InChI=1S/C24H27NO2/c1-25-13-12-24-18-8-5-9-21(24)27-23-20(26-15-16-6-3-2-4-7-16)11-1h2-4,6-7,10-11,18-19,21H,5,8-9,12-15H2,1H3	-4.22
InChI=1S/C23H29ClO4/c1-13(25)23(28-14(2)26)10-7-18-16-12-20(24)19-11-15(27)5-8-21(19,h11-12,16-18H,5-10H2,1-4H3	-6.097
InChI=1S/C13H19NO4/c1-5-17-12(15)10-7-11(13(16)18-6-2)9(4)14-8(10)3/h14H,5-7H2,1-4H3	-1.772
InChI=1S/C2H4Cl2O/c3-1-5-2-4/h1-2H2	-0.718
InChI=1S/C19H21NO4/c1-22-15-9-12-11(7-14(15)21)6-13-17-10(4-5-20-13)8-16(23-2)19(24-h7-9,13,20-21H,4-6H2,1-3H3	-3.842
InChI=1S/C18H28N2O4/c1-12(2)14-8-7-13(3)16(18(22)23-6)17(14)24-11-15(21)19-9-10-20(4)h7-8,12H,9-11H2,1-6H3,(H,19,21)	-3.847
InChI=1S/C17H15ClN4O5/c1-10(23)16(17(24)19-13-5-3-4-6-15(13)27-2)21-20-12-8-7-11(18)9-1h3-9,16H,1-2H3,(H,19,24)/b21-20+	-7.306
InChI=1S/C8H12O2/c1-10-8(9)6-7-4-2-3-5-7/h6H,2-5H2,1H3	-1.943
InChI=1S/C5H10O2/c1-4(2)3-5(6)7/h4H,3H2,1-2H3,(H,6,7)	-0.328
InChI=1S/C4H10O2/c1-2-4(6)3-5/h4-6H,2-3H2,1H3	1.045
InChI=1S/C11H20N2O2/c1-3-11(14)15-8-13-9-4-5-10(13)7-12(2)6-9/h9-10H,3-8H2,1-2H3	-0.533
InChI=1S/C18H10O5/c19-15-13(10-6-2-1-3-7-10)17(20)23-16(15)14-11-8-4-5-9-12(11)22-1h1-9,19H/b16-14-	-1.766
InChI=1S/C34H30Cl2N6O6/c1-19(43)31(33(45)37-27-9-5-7-11-29(27)47-3)41-39-25-15-13-21(17-h5-18,31-32H,1-4H3,(H,37,45)(H,38,46)/b41-39+,42-40+	-8.424
InChI=1S/C18H17ClN2O/c1-20-16-7-6-13(19)10-15(16)18-14-5-3-2-4-12(14)8-9-21(18)11-17(2h2-7,10,18H,8-9,11H2,1H3	-4.015
InChI=1S/C25H27ClN2/c1-20-6-5-7-21(18-20)19-27-14-16-28(17-15-27)25(22-8-3-2-4-9-22)2h2-13,18,25H,14-17,19H2,1H3	-4.63
InChI=1S/C15H21NO3/c1-2-3-4-8-11-16-14(17)12-19-15(18)13-9-6-5-7-10-13/h5-7,9-10H,2-4,8,11-12H2,1H3,(H,16,17)	-3.902

"InChi"	"logS(M)"
InChI=1S/C10H12O2/c1-7(2)8-4-3-5-9(11)10(12)6-8/h3-7H,1-2H3,(H,11,12)	-2.136
InChI=1S/C4H8N2O7/c7-5(8)12-3-1-11-2-4-13-6(9)10/h1-4H2	-1.69
InChI=1S/C10H13ClN4O2/c1-13-8-7(9(16)14(2)10(13)17)15(6-12-8)5-3-4-11/h6H,3-5H2,1-2H3	-2.263
InChI=1S/C8H7NO5/c10-8(11)5-14-7-3-1-6(2-4-7)9(12)13/h1-4H,5H2,(H,10,11)	-1.898
InChI=1S/C8H9NO3/c9-7(8(11)12)5-1-3-6(10)4-2-5/h1-4,7,10H,9H2,(H,11,12)	-0.53
InChI=1S/C23H32O2/c1-14-9-16(20(24)18(11-14)22(3,4)5)13-17-10-15(2)12-19(21(17)25)2h9-12,24-25H,13H2,1-8H3	-7.231
InChI=1S/C12H6Cl4/c13-9-4-2-1-3-8(9)7-5-10(14)12(16)11(15)6-7/h1-6H	-6.907
InChI=1S/C6H11N4PS/c7-9-11(12,10-8)6-4-2-1-3-5-6/h1-5H,7-8H2,(H2,9,10,12)	-1.425
InChI=1S/C23H32O6/c1-20-6-3-17-18(4-8-22(27)11-15(25)2-7-21(17,22)13-24)23(20,28)9-h10,13,15-18,25,27-28H,2-9,11-12H2,1H3	-2.695
InChI=1S/C11H10ClNO3/c1-2-5-16-10-4-3-8(6-9(10)12)7-11(14)13-15/h1,3-4,6,15H,5,7H2,(H,13,14)	-2.563
InChI=1S/C5H8O/c1-5(2)3-4-6/h3-4H,1-2H3	0.117
InChI=1S/C23H24N6O4/c1-4-5-8-28(9-10-33-17(3)30)20-6-7-22(16(2)11-20)26-27-23-18(14-2h6-7,11-13H,4-5,8-10H2,1-3H3/b27-26+	-8.881
InChI=1S/C14H28N2O/c1-7-15(8-2)12(17)11-16-13(3,4)9-10-14(16,5)6/h7-11H2,1-6H3	-2.888
InChI=1S/C7H8N2O/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,8H2,(H2,9,10)	-1.226
InChI=1S/C7H7FN2O4/c1-2-14-7(13)10-5(11)4(8)3-9-6(10)12/h3H,2H2,1H3,(H,9,12)	-0.45
InChI=1S/C26H32ClFO5/c1-5-6-22(32)33-26(21(31)14-27)15(2)11-19-18-8-7-16-12-17(29)9-1(h9-10,12,15,18-19H,5-8,11,13-14H2,1-4H3	-5.902
InChI=1S/C8H11N/c1-6-3-7(2)5-8(9)4-6/h3-5H,9H2,1-2H3	-1.402
InChI=1S/C17H34N2O4/c1-7-17(8-2,13-22-15(20)18(9-3)10-4)14-23-16(21)19(11-5)12-6/h7-14H2,1-6H3	-5.622
InChI=1S/C21H32O4/c1-20-8-7-13(23)9-12(20)3-4-14-15-5-6-16(18(25)11-22)21(15,2)10-1h12-16,19,22-23H,3-11H2,1-2H3	-3.866
InChI=1S/C22H35N3O/c23-21(26)22(20-10-4-1-5-11-20,12-18-24-14-6-2-7-15-24)13-19-25-1h1,4-5,10-11H,2-3,6-9,12-19H2,(H2,23,26)	-5.001
InChI=1S/C11H17NO/c1-7-5-12(3)6-10-8(2)11(13)4-9(7)10/h4,7-8,10H,5-6H2,1-3H3	0.168
InChI=1S/C5H7N3/c6-4-2-1-3-8-5(4)7/h1-3H,6H2,(H2,7,8)	-1.75
InChI=1S/C16H20O2/c17-16(18)15-9-7-13-10-12(6-8-14(13)15)11-4-2-1-3-5-11/h6,8,10-11,15H,1-5,7,9H2,(H,17,18)	-4.941

"InChi"	"logS(M)"
InChI=1S/C14H12N2O2/c1-8-13-10(7-12(15-8)14(17)18-2)9-5-3-4-6-11(9)16-13/h3-7,16H,1-2H3	-4.254
InChI=1S/C10H9Cl2NO2/c1-6(14)7-4-2-3-5-8(7)13-10(15)9(11)12/h2-5,9H,1H3,(H,13,15)	-3.259
InChI=1S/C8H14O/c1-7(2)5-4-6-8(3)9/h5H,4,6H2,1-3H3	-1.621
InChI=1S/C6H13O9P/c7-1-2-3(8)4(9)5(10)6(14-2)15-16(11,12)13/h2-10H,1H2,(H2,11,12,13)	0.585
InChI=1S/C12H11FN2O2/c1-8-2-4-9(5-3-8)6-15-7-10(13)11(16)14-12(15)17/h2-5,7H,6H2,1H3,(H,14,16,17)	-2.92
InChI=1S/C8H9N5O4S3/c9-5-2-1-3-6(4-5)20(16,17)13-7-11-12-8(18-7)19(10,14)15/h1-4H,9H2,(H,11,13)(H2,10,14,15)	-1.54
InChI=1S/C18H32O7/c1-4-7-10-23-15(19)13-18(22,17(21)25-12-9-6-3)14-16(20)24-11-8-5-h22H,4-14H2,1-3H3	-3.545
InChI=1S/C12H7N5O9/c18-11-8(3-6(15(20)21)4-9(11)16(22)23)12(19)14-13-5-7-1-2-10(26-7h1-5,18H,(H,14,19)/b13-5+	-3.979
InChI=1S/C10H10O4/c1-14-9-6-7(2-4-8(9)11)3-5-10(12)13/h2-6,11H,1H3,(H,12,13)/b5-3+	-3.05
InChI=1S/C8H6N2OS/c12-8-10-9-7(11-8)6-4-2-1-3-5-6/h1-5H,(H,10,12)	-1.687
InChI=1S/C9H9BrO4S/c1-14-9(11)6-15(12,13)8-4-2-7(10)3-5-8/h2-5H,6H2,1H3	-2.48
InChI=1S/C13H20ClNO/c1-10(16)9-15-13(2,3)8-11-4-6-12(14)7-5-11/h4-7,10,15-16H,8-9H2,1-3H3	-2.315
InChI=1S/C13H15ClO4S/c1-9(2)18-12(15)13(7-8-13)19(16,17)11-5-3-10(14)4-6-11/h3-6,9H,7-8H2,1-2H3	-3.54
InChI=1S/C17H19N5/c1-16(2,9-18)14-5-13(8-22-12-20-11-21-22)6-15(7-14)17(3,4)10-19/h5-7,11-12H,8H2,1-4H3	-2.768
InChI=1S/C9H15N3O6/c13-4-1-10-7(16)11(2-5-14)9(18)12(3-6-15)8(10)17/h13-15H,1-6H2	0.34
InChI=1S/C10H12N4O5S/c1-10(5-13-3-2-11-12-13)8(9(16)17)14-6(15)4-7(14)20(10,18)19/h2-3,7-8H,4-5H2,1H3,(H,16,17)	-1.838
InChI=1S/C9H17NOS/c1-5-6-7-12-9(2,3)8(11)10-4/h5-6H,7H2,1-4H3,(H,10,11)/b6-5+	-2.421
InChI=1S/C17H15ClN6O5S2/c18-11-1-5-14(6-2-11)31(28,29)24-17(25)23-16-20-10-9-15(22-16)21-h1-10H,(H2,19,26,27)(H3,20,21,22,23,24,25)	-4
InChI=1S/C14H16/c1-4-12-7-5-10(2)13-8-6-11(3)14(13)9-12/h5-9H,4H2,1-3H3	-5.62
InChI=1S/C10H20O/c1-2-3-4-5-6-7-8-9-10-11/h10H,2-9H2,1H3	-3.726
InChI=1S/C10H23O3P/c1-4-7-9-12-14(11,6-3)13-10-8-5-2/h4-10H2,1-3H3	-1.569

"InChi"	"logS(M)"
InChI=1S/C16H12FN3O3/c1-19-14-7-6-10(20(22)23)8-12(14)16(18-9-15(19)21)11-4-2-3-5-13(1h2-8H,9H2,1H3	-3.634
InChI=1S/C10H7N5O2/c1-7-4-9(15(16)17)2-3-10(7)14-13-8(5-11)6-12/h2-4,14H,1H3	-4.294
InChI=1S/C12H22O2/c1-3-7-12(13)14-10(2)11-8-5-4-6-9-11/h10-11H,3-9H2,1-2H3	-3.921
InChI=1S/C11H14N4O2/c1-4-5-6-15-10(16)8-9(12-7-13(8)2)14(3)11(15)17/h4-5,7H,6H2,1-3H3/b5-4+	-2.117
InChI=1S/C15H12O4/c16-11-4-1-10(2-5-11)3-8-14(18)13-7-6-12(17)9-15(13)19/h1-9,16-17,19H/b8-3+	-3.047
InChI=1S/C34H28Cl2N8O2/c1-19-5-11-25(12-6-19)43-33(45)31(21(3)41-43)39-37-29-15-9-23(17-h5-18,31-32H,1-4H3/b39-37+,40-38+	-8.27
InChI=1S/C21H29NO2/c23-17-7-6-16-12-19-21(24)9-2-1-8-20(21,18(16)13-17)10-11-22(19)1h6-7,13,15,19,23-24H,1-5,8-12,14H2	-3.829
InChI=1S/C21H27N/c1-20(2,3)22-16-14-21(15-17-22,18-10-6-4-7-11-18)19-12-8-5-9-13-1h4-13H,14-17H2,1-3H3	-4.688
InChI=1S/C6H13NO/c1-2-7-3-5-8-6-4-7/h2-6H2,1H3	0.939
InChI=1S/C11H13NO4/c1-2-3-4-11(13)16-10-7-5-9(6-8-10)12(14)15/h5-8H,2-4H2,1H3	-4.394
InChI=1S/C28H41N3O3/c1-27(2,19-23-13-9-7-10-14-23)29(5)25(33)21-31(17-18-32)22-26(34)h7-16,32H,17-22H2,1-6H3	-4.737
InChI=1S/C11H17N3O2S/c1-17-9-4-10(11(15)16)14(7-2-5-12)8-3-6-13/h10H,2-4,7-9H2,1H3,(H,15,16)	-1.328
InChI=1S/C10H15N/c1-8-4-5-9(6-7-11)10(8,2)3/h4,9H,5-6H2,1-3H3	-2.648
InChI=1S/C5H12N2O4S2/c6-5(7-2-1-3-8)4-12-13(9,10)11/h8H,1-4H2,(H2,6,7)(H,9,10,11)	0.344
InChI=1S/C9H12N4O3/c1-11-7-6(8(15)12(2)9(11)16)13(3-4-14)5-10-7/h5,14H,3-4H2,1-2H3	-0.45
InChI=1S/C25H34N2/c1-16(2)20-11-9-12-21(17(3)4)24(20)26-15-27-25-22(18(5)6)13-10-14h9-14,16-19H,1-8H3	-6.86
InChI=1S/C10H5Cl3/c11-7-2-1-6-3-8(12)5-10(13)9(6)4-7/h1-5H	-6.556
InChI=1S/C18H18O9/c19-16(25-7-11-4-22-11)10-1-2-14(17(20)26-8-12-5-23-12)15(3-10)18h1-3,11-13H,4-9H2	-2.762
InChI=1S/C12H8Cl2O/c13-11-7-6-10(8-12(11)14)15-9-4-2-1-3-5-9/h1-8H	-4.721
InChI=1S/C8H6N2O2/c11-8-7(10-12)5-3-1-2-4-6(5)9-8/h1-4,12H,(H,9,10,11)	-2.546
InChI=1S/C12H10N2O2/c15-10-6-7-11(12(16)8-10)14-13-9-4-2-1-3-5-9/h1-8,15-16H/b14-13+	-3.08
InChI=1S/C19H20F3NO2/c1-14(12-15-6-5-9-17(13-15)19(20,21)22)23-10-11-25-18(24)16-7-3-2h2-9,13-14,23H,10-12H2,1H3	-4.743

"InChi"	"logS(M)"
InChI=1S/C18H19BrN6O5/c1-4-23(5-2)12-6-7-15(16(9-12)20-11(3)26)21-22-18-14(19)8-13(24(2h6-10H,4-5H2,1-3H3,(H,20,26)/b22-21+	-7.38
InChI=1S/C6H10O/c1-3-4-5-6(2)7/h6-7H,3H2,1-2H3	-0.412
InChI=1S/C10H9N5O/c1-2-7(16-3-1)4-11-9-8-10(13-5-12-8)15-6-14-9/h1-3,5-6H,4H2,(H2,11,12,13,14,15)	-3.95
InChI=1S/C6H5N3O5/c7-4-1-3(8(11)12)2-5(6(4)10)9(13)14/h1-2,10H,7H2	-2.486
InChI=1S/C16H16O3S/c17-7-2-1-3-11-4-5-14-13(9-11)15(18)16-12(10-19-14)6-8-20-16/h4-6,8-9,17H,1-3,7,10H2	-3.92
InChI=1S/C4H5N3OS/c1-2-3(8)5-4(9)7-6-2/h1H3,(H2,5,7,8,9)	-1.482
InChI=1S/C14H14N2O/c1-10-5-7-12(8-6-10)14(17)16-13-11(2)4-3-9-15-13/h3-9H,1-2H3,(H,15,16,17)	-3.074
InChI=1S/C17H18N2S2/c20-17-19(12-16-9-5-2-6-10-16)13-18(14-21-17)11-15-7-3-1-4-8-15/h1-10H,11-14H2	-5.176
InChI=1S/C20H16Cl2N2O3/c1-12-18(19(26)15-9-8-14(21)10-16(15)22)20(24(2)23-12)27-11-17(2h3-10H,11H2,1-2H3	-2.651
InChI=1S/C8H13N3O2/c1-2-3-4-9-7(12)11-8-10-5-6-13-8/h5-6H,2-4H2,1H3,(H2,9,10,11,12)	-1.805
InChI=1S/C8H7Cl2NO/c9-7(10)8(12)11-6-4-2-1-3-5-6/h1-5,7H,(H,11,12)	-3.356
InChI=1S/C3H8N2S/c1-4-3(6)5-2/h1-2H3,(H2,4,5,6)	0.982
InChI=1S/C10H20N2O4/c1-3-4-7(2)8(5-15-9(11)13)6-16-10(12)14/h7-8H,3-6H2,1-2H3,(H2,11,13)(H2,12,14)	-2.123
InChI=1S/C17H12Cl2N2O3/c1-9(22)24-17-16(23)20-14-7-6-10(18)8-12(14)15(21-17)11-4-2-3-5-1h2-8,17H,1H3,(H,20,23)	-5.029
InChI=1S/C15H10F6O2/c16-14(17,18)13(15(19,20)21,9-1-5-11(22)6-2-9)10-3-7-12(23)8-4-10/h1-8,22-23H	-3.18
InChI=1S/C8H10N2O3/c9-4-3-6-1-2-8(11)7(5-6)10(12)13/h1-2,5,11H,3-4,9H2	-1.34
InChI=1S/C8H11N3O3/c9-6-1-2-7(10-3-4-12)8(5-6)11(13)14/h1-2,5,10,12H,3-4,9H2	-2.191
InChI=1S/C30H29N3O/c1-29(2,21-13-7-5-8-14-21)23-19-24(30(3,4)22-15-9-6-10-16-22)28(3h5-20,34H,1-4H3	-7.049
InChI=1S/C12H23N5O2S/c1-18-8-4-6-13-10-15-11(14-7-5-9-19-2)17-12(16-10)20-3/h4-9H2,1-3H3,(H2,13,14,15,16,17)	-3.479
InChI=1S/C14H29NO/c1-4-5-6-7-8-9-10-11-12-13-14(16)15(2)3/h4-13H2,1-3H3	-3.909
InChI=1S/C17H22N2/c1-18(2)13-14-19(17-11-7-4-8-12-17)15-16-9-5-3-6-10-16/h3-12H,13-15H2,1-2H3	-2.846
InChI=1S/C6H9BrO/c1-3-6(2,8)4-5-7/h8H,3H2,1-2H3	-1.127

"InChi"	"logS(M)"
InChI=1S/C32H32O13S/c1-37-19-6-13(7-20(38-2)25(19)33)23-14-8-17-18(42-12-41-17)9-15(1h3-9,16,21,23-24,26-29,31-35H,10-12H2,1-2H3	-5.043
InChI=1S/C5H12/c1-5(2,3)4/h1-4H3	-3.337
InChI=1S/C6H10O2S4/c1-3-7-5(9)11-12-6(10)8-4-2/h3-4H2,1-2H3	-4.943
InChI=1S/C16H34/c1-13(10-14(2,3)4)11-16(8,9)12-15(5,6)7/h13H,10-12H2,1-9H3	-3.355
InChI=1S/C14H10N2O2/c15-13-9-3-1-2-4-11(9)16-12-6-5-8(14(17)18)7-10(12)13/h1-7H,(H2,15,16)(H,17,18)	-3.999
InChI=1S/C7H7FN2O4/c1-4(11)14-3-10-2-5(8)6(12)9-7(10)13/h2H,3H2,1H3,(H,9,12,13)	-0.67
InChI=1S/C10H18N2O/c1-3-10(13)12-6-8-4-5-9(7-12)11(8)2/h8-9H,3-7H2,1-2H3	-2.108
InChI=1S/C6H6N2O4/c9-4(10)1-3-2-7-6(12)8-5(3)11/h2H,1H2,(H,9,10)(H2,7,8,11,12)	-1.629
InChI=1S/C32H44O8/c1-17(33)40-27(2,3)13-12-23(36)32(9,39)25-21(35)15-29(6)22-11-10-h10,12-14,19,21-22,25,34-35,39H,11,15-16H2,1-9H3/b13-12+	-6.778
InChI=1S/C9H13NO3S/c10-14(12,13)9-5-3-8(4-6-9)2-1-7-11/h3-6,11H,1-2,7H2,(H2,10,12,13)	-1.032
InChI=1S/C11H12O4S/c1-8(12)15-10-6-4-3-5-9(10)11(13)14-7-16-2/h3-6H,7H2,1-2H3	-2.64
InChI=1S/C9H12N2O2/c1-13-8-5-3-2-4-7(8)11-6-9(10)12/h2-5,11H,6H2,1H3,(H2,10,12)	-1.182
InChI=1S/C7H4ClN3O/c8-6-1-3-7(4-2-6)11(12)10-5-9/h1-4H/b11-10-	-2.948
InChI=1S/C18H16O3/c1-12-8-9-13-5-2-3-7-15(13)17(12)16(18(19)20)11-14-6-4-10-21-14/h2-10,16H,11H2,1H3,(H,19,20)	-4.818
InChI=1S/C10H12BrCl2O3PS/c1-3-14-17(18,15-4-2)16-10-6-8(12)7(11)5-9(10)13/h5-6H,3-4H2,1-2H3	-5.952
InChI=1S/C15H20N2O2/c1-19-13-6-4-12(5-7-13)17-11-8-14(15(17)18)16-9-2-3-10-16/h4-7,14H,2-3,8-11H2,1H3	-2.627
InChI=1S/C11H9NO3S/c1-2-7-12-11(13)8-9-5-3-4-6-10(9)16(12,14)15/h1,3-6H,7-8H2	-1.496
InChI=1S/C11H16O/c1-4-11(2,3)9-5-7-10(12)8-6-9/h5-8,12H,4H2,1-3H3	-2.99
InChI=1S/C9H14N2O2/c1-6(2)8(12)10-5-11-9(13)7(3)4/h1,3,5H2,2,4H3,(H,10,12)(H,11,13)	-1.189
InChI=1S/C6H7NS/c1-7-5-3-2-4-6(7)8/h2-5H,1H3	-0.362
InChI=1S/C7H6N4O2/c1-4(12)11-6-5(2-10-11)7(13)9-3-8-6/h2-3H,1H3,(H,8,9,13)	-2.38
InChI=1S/C15H13N3O/c19-15(14-8-11-16-12-9-14)18-17-10-4-7-13-5-2-1-3-6-13/h1-12H,(H,18,19)/b7-4+,17-10+	-3.048
InChI=1S/C10H14NO5P/c1-3-15-17(14,4-2)16-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3	-3.173

"InChi"	"logS(M)"
InChI=1S/C9H11ClN2O2/c10-6-1-2-8(12-3-4-13)7(5-6)9(11)14/h1-2,5,12-13H,3-4H2,(H2,11,14)	-1.843
InChI=1S/C22H28N2O4/c1-17(25)18-6-5-7-20(14-18)28-16-19(26)15-23-10-12-24(13-11-23)2h3-9,14,19,26H,10-13,15-16H2,1-2H3	-2.876
InChI=1S/C4H6Br2O2S/c5-3-1-9(7,8)2-4(3)6/h3-4H,1-2H2	-1.487
InChI=1S/C11H8O3/c12-10-4-3-7-5-9(11(13)14)2-1-8(7)6-10/h1-6,12H,(H,13,14)	-3.279
InChI=1S/C41H76O4/c1-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-39(42)44-37-41(3,h19-22H,5-18,23-38H2,1-4H3/b21-19+,22-20+	-7.102
InChI=1S/C10H6O3/c11-7-4-5-9(13)10-6(7)2-1-3-8(10)12/h1-5,12H	-1.532
InChI=1S/C9H20O2/c1-3-5-7-10-9-11-8-6-4-2/h3-9H2,1-2H3	-2.807
InChI=1S/C5H2F8/c6-1-3(8,9)2(7)5(12,13)4(1,10)11/h1-2H	-3.634
InChI=1S/C19H30O5/c1-3-5-7-20-8-9-21-10-11-22-14-17-13-19-18(23-15-24-19)12-16(17)6h12-13H,3-11,14-15H2,1-2H3	-4.151
InChI=1S/C12H12N4/c13-9-6-7-12(11(14)8-9)16-15-10-4-2-1-3-5-10/h1-8H,13-14H2/b16-15+	-2.998
InChI=1S/C14H9BrO3/c15-10-7-5-9(6-8-10)13(16)11-3-1-2-4-12(11)14(17)18/h1-8H,(H,17,18)	-3.007
InChI=1S/C10H12ClNO4/c11-7-1-3-9(4-2-7)15-5-8(13)6-16-10(12)14/h1-4,8,13H,5-6H2,(H2,12,14)	-1.463
InChI=1S/C6H18N4/c7-1-3-9-5-6-10-4-2-8/h9-10H,1-8H2	0.835
InChI=1S/C9H7NO4/c1-5-7-3-2-6(10(12)13)4-8(7)9(11)14-5/h2-5H,1H3	-2.616
InChI=1S/C17H30N2O6/c1-3-4-17(2,13-24-15(20)18-5-9-22-10-6-18)14-25-16(21)19-7-11-23-h3-14H2,1-2H3	-3.486
InChI=1S/C13H20O3/c1-2-3-9-15-10-12(14)11-16-13-7-5-4-6-8-13/h4-8,12,14H,2-3,9-11H2,1H3	-1.724
InChI=1S/C12H10O2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8,13-14H	-3.742
InChI=1S/C11H12N2O/c1-12-11(14)13-8-4-6-9-5-2-3-7-10(9)13/h2-7H,8H2,1H3,(H,12,14)	-2.034
InChI=1S/C8H14O2/c9-8(10)6-7-4-2-1-3-5-7/h7H,1-6H2,(H,9,10)	-1.694
InChI=1S/C15H19NO3/c17-14(16-13-9-5-2-6-10-13)11-19-15(18)12-7-3-1-4-8-12/h1,3-4,7-8,13H,2,5-6,9-11H2,(H,16,17)	-3.9
InChI=1S/C3H4Cl3NO2/c4-3(5,6)1-9-2(7)8/h1H2,(H2,7,8)	-1.284
InChI=1S/C20H26N6O5/c1-28-14-4-3-13(9-15(14)29-2)16-30-11-20(10-27,12-31-16)24-17-21-h3-4,9,16,27H,5-8,10-12H2,1-2H3,(H,21,22,23,24)	-4.282
InChI=1S/C10H22O6/c11-1-3-13-5-7-15-9-10-16-8-6-14-4-2-12/h11-12H,1-10H2	0.623
InChI=1S/C12H3Cl7/c13-4-1-5(14)9(6(15)2-4)10-11(18)7(16)3-8(17)12(10)19/h1-3H	-8.49
InChI=1S/C7H16O2/c8-6-4-2-1-3-5-7-9/h8-9H,1-7H2	-0.928

"InChi"	"logS(M)"
InChI=1S/C10H12F6O5/c1-3-20-6(17)5(7(18)21-4-2)8(19,9(11,12)13)10(14,15)16/h5,19H,3-4H2,1-2H3	-2.393
InChI=1S/C15H19NO5/c1-4-16(5-2)14(18)10-20-15(19)12-8-6-7-9-13(12)21-11(3)17/h6-9H,4-5,10H2,1-3H3	-2.11
InChI=1S/C19H14N2/c20-18-15-9-4-5-12-17(15)21-19-14(10-6-11-16(18)19)13-7-2-1-3-8-1h1-12H,(H2,20,21)	-5.84
InChI=1S/C20H21NO/c1-15-16-6-2-4-8-18(16)20(14-21-10-12-22-13-11-21)19-9-5-3-7-17(1h2-9H,10-14H2,1H3	-4.4
InChI=1S/C4H8O3/c1-3(5)4(6)7-2/h3,5H,1-2H3	0.983
InChI=1S/C17H17N5O4S2/c18-28(25,26)15-8-6-14(7-9-15)20-16-10-11-19-17(21-16)22-27(23,24h1-11H,12H2,(H2,18,25,26)(H2,19,20,21,22)	-2.7
InChI=1S/C8H7BrO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2,(H,10,11)	-2.347
InChI=1S/C12H18N2O/c1-2-3-4-5-9-14-12(15)11-7-6-8-13-10-11/h6-8,10H,2-5,9H2,1H3,(H,14,15)	-2.522
InChI=1S/C12H9ClO/c13-10-5-4-8-12(9-10)14-11-6-2-1-3-7-11/h1-9H	-4.211
InChI=1S/C19H32N2/c1-16(2)21(17(3)4)15-9-14-20-13-8-7-11-18-10-5-6-12-19(18)20/h5-6,10,12,16-17H,7-9,11,13-15H2,1-4H3	-5.073
InChI=1S/C12H10O/c1-9(13)11-8-4-6-10-5-2-3-7-12(10)11/h2-8H,1H3	-2.885
InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h5-9H2,1-4H3	-3.655
InChI=1S/C18H36O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18(20)21-17-16-19/h19H,2-17H2,1H3	-6.09
InChI=1S/C9H8O2/c1-2-11-9(10)8-6-4-3-5-7-8/h2-7H,1H2	-2.623
InChI=1S/C16H20N2O5/c1-4-16(12-8-6-5-7-9-12)13(19)17(10-22-2)15(21)18(11-23-3)14(16)2h5-9H,4,10-11H2,1-3H3	-2.427
InChI=1S/C6H7NO/c8-5-6-3-1-2-4-7-6/h1-4,8H,5H2	0.962
InChI=1S/C16H21N5O3/c1-21(2)15(22)13-11(23-3)6-9(7-12(13)24-4)5-10-8-19-16(18)20-14(1h6-8H,5H2,1-4H3,(H4,17,18,19,20)	-2.747
InChI=1S/C8H8O4/c1-12-6-4-2-3-5(7(6)9)8(10)11/h2-4,9H,1H3,(H,10,11)	-2.085
InChI=1S/C9H15N3O2/c1-6-7(10(2)3)8(13)12(5)9(14)11(6)4/h1-5H3	-1.485
InChI=1S/C6H14O/c1-3-6(4-2)5-7/h6-7H,3-5H2,1-2H3	-1.17
InChI=1S/C14H14N2O/c1-15-14(17)16(12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11H,1H3,(H,15,17)	-2.984
InChI=1S/C13H14N2/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1,3,5,7H,2,4,6,8H2,(H2,14,15)	-2.962

"InChi"	"logS(M)"
InChI=1S/C8H11N3/c1-11(2)10-9-8-6-4-3-5-7-8/h3-7H,1-2H3/b10-9+	-2.502
InChI=1S/C6H8N4O4/c1-9-4(3-14-6(7)11)8-2-5(9)10(12)13/h2H,3H2,1H3,(H2,7,11)	-1.843
InChI=1S/C12H27O3P/c1-4-7-10-14-16(13,12-9-6-3)15-11-8-5-2/h4-12H2,1-3H3	-2.7
InChI=1S/C10H14O/c1-3-8-6-5-7-9(4-2)10(8)11/h5-7,11H,3-4H2,1-2H3	-2.305
InChI=1S/C16H23ClN2O2/c1-3-9-19-10-7-13(8-11-19)21-16(20)18-15-12(2)5-4-6-14(15)17/h4-6,13H,3,7-11H2,1-2H3,(H,18,20)	-4.689
InChI=1S/C23H31NO7S/c1-32(29,30)24-23(28)12-8-3-2-7-11-19-20(22(27)15-21(19)26)14-13-h2,4-7,9-10,13-14,17,19-20,22,25,27H,3,8,11-12,15-16H2,1H3,(H,24,28)/b7-2+,14-13+	-3.939
InChI=1S/C9H18N2O/c1-8(2)6-5-7-9(3,4)11(8)10-12/h5-7H2,1-4H3	-2.57
InChI=1S/C14H11Cl2NO2/c1-9-4-2-3-5-13(9)17(19)14(18)11-7-6-10(15)8-12(11)16/h2-8,19H,1H3	-4.17
InChI=1S/C13H19N5/c1-10(13(2,3)4)17-12(16-9-14)18-11-5-7-15-8-6-11/h5-8,10H,1-4H3,(H2,15,16,17,18)	-0.886
InChI=1S/C14H18N2O2/c1-3-5-8-16-14(17)12-10-11(15)6-7-13(12)18-9-4-2/h2,6-7,10H,3,5,8-9,15H2,1H3,(H,16,17)	-2.593
InChI=1S/C20H22O8/c21-10-13-8-4-5-9-14(13)27-20-18(24)17(23)16(22)15(28-20)11-26-1 h1-9,15-18,20-24H,10-11H2	-2.893
InChI=1S/C6H10O2/c1-3-5-4(2)8-6(5)7/h4-5H,3H2,1-2H3	-0.666
InChI=1S/C17H15NO2/c1-20-15-10-8-14(9-11-15)17(19)18-12-4-6-13-5-2-3-7-16(13)18/h2-11H,12H2,1H3	-3.969
InChI=1S/C17H24N2O2/c1-3-19(4-2)13-12-17(14-8-6-5-7-9-14)11-10-15(20)18-16(17)21/h5-9H,3-4,10-13H2,1-2H3,(H,18,20,21)	-2.956
InChI=1S/C10H22O/c1-5-9(2)7-6-8-10(3,4)11/h9,11H,5-8H2,1-4H3	-2.749
InChI=1S/C33H50O6P2/c1-29(2,3)23-13-15-27(25(17-23)31(7,8)9)38-40-34-19-33(20-35-40)2 h13-18H,19-22H2,1-12H3	-6.813
InChI=1S/C10H11F3N2O5/c11-10(12,13)4-2-15(9(19)14-8(4)18)7-1-5(17)6(3-16)20-7/h2,5-7,16-17H,1,3H2,(H,14,18,19)	-0.71
InChI=1S/C5H12O/c1-4-5(2)6-3/h5H,4H2,1-3H3	-0.731
InChI=1S/C9H10O2/c1-8(10)11-7-9-5-3-2-4-6-9/h2-6H,7H2,1H3	-1.685
InChI=1S/C6H12O2/c1-4-8-6(7)5(2)3/h5H,4H2,1-3H3	-1.255
InChI=1S/C28H34O15/c1-10-21(33)23(35)25(37)27(39-10)43-26-24(36)22(34)19(9-29)42-28 h3-7,10,17,19,21-31,33-37H,8-9H2,1-2H3	-5.186
InChI=1S/C14H16ClNO/c1-16(2)9-14(17)12-7-8-13(15)11-6-4-3-5-10(11)12/h3-8,14,17H,9H2,1-2H3	-1.22

"InChi"	"logS(M)"
InChI=1S/C26H36O6/c1-15(27)32-21-13-26(30)20-6-5-17-12-18(28)8-10-24(17,2)19(20)9-11-25(26,29)23(21,3)14-22(31)4/h12,19-21,23,28,30H,5-6,8-13H2,1-3H3	-5.292
InChI=1S/C12H10O2S/c13-15(14,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H	-4.193
InChI=1S/C6H10O4S2/c1-3(5(7)8)11-12-4(2)6(9)10/h3-4H,1-2H3,(H,7,8)(H,9,10)	-0.62
InChI=1S/C18H34O6/c1-2-3-4-5-6-7-8-9-10-11-16(21)23-13-15(20)18-17(22)14(19)12-24-18/h14-15,17-20,22H,2-13H2,1H3	-5.063
InChI=1S/C13H17N3O/c14-13(15-17)16-7-10-5-1-3-9-4-2-6-11(8-16)12(9)10/h1,3,5,11,17H,2,4,6-8H2,(H2,14,15)	-1.35
InChI=1S/C6H13FS/c7-5-3-1-2-4-6-8/h8H,1-6H2	-2.904
InChI=1S/C17H15N3O/c1-13-16(12-18-14-8-4-2-5-9-14)17(21)20(19-13)15-10-6-3-7-11-15/h2-12,18H,1H3/b16-12+	-4.371
InChI=1S/C13H13N3O/c1-9-3-2-8-15-12(9)16-13(17)10-4-6-11(14)7-5-10/h2-8H,14H2,1H3,(H,15,16,17)	-1.831
InChI=1S/C7H10N4O3/c1-3-9-7(13)10-6(12)5(4-8)11-14-2/h3H2,1-2H3,(H2,9,10,12,13)/b11-5+	-2.3
InChI=1S/C7H12O2/c1-6(2)4-3-5-7(8)9/h3-4,6H,5H2,1-2H3,(H,8,9)/b4-3+	-1.149
InChI=1S/C6H10O2/c1-5(2)4-6(7)8-3/h4H,1-3H3	-1.414
InChI=1S/C4H6O2/c5-3-1-2-4-6/h5-6H,3-4H2	1.536
InChI=1S/C3H8O/c1-3(2)4/h3-4H,1-2H3	0.43
InChI=1S/C13H16N2/c1-2-6-11-10(4-1)5-3-7-12(11)13-14-8-9-15-13/h1-2,4,6,12H,3,5,7-9H2,(H,14,15)	-3.809
InChI=1S/C18H15NO4/c1-10(18(21)22)14-7-8-16-15(9-14)19-17(23-16)13-5-3-12(4-6-13)11(h3-10H,1-2H3,(H,21,22)	-3.637
InChI=1S/C9H9N/c1-7-3-4-9(6-10)5-8(7)2/h3-5H,1-2H3	-2.674
InChI=1S/C5H10Cl3O3P/c1-3-10-12(9,11-4-2)5(6,7)8/h3-4H2,1-2H3	-1.754
InChI=1S/C16H33NO4S2/c18-23(19,20)22-15-9-13-17-12-7-4-8-14-21-16-10-5-2-1-3-6-11-16/h16-17H,1-15H2,(H,18,19,20)	-3.815
InChI=1S/C12H17ClO3/c1-2-4-9-5-3-6-11(13)12(9)16-8-10(15)7-14/h3,5-6,10,14-15H,2,4,7-8H2,1H3	-3.576
InChI=1S/C18H18O4/c1-20-14-7-4-13(5-8-14)6-11-17(19)16-10-9-15(21-2)12-18(16)22-3/h4-12H,1-3H3/b11-6+	-4.65
InChI=1S/C11H20N2O4/c1-4-16-10(14)12-6-7-13(9(3)8-12)11(15)17-5-2/h9H,4-8H2,1-3H3	-2.414
InChI=1S/C35H42N2O11/c1-7-46-35(40)48-31-26(42-3)12-18(13-27(31)43-4)33(38)47-28-14-19-8-9,12-13,15,19,23,25,28-29,32,36H,7,10-11,14,16-17H2,1-6H3	-5.727
InChI=1S/C11H25NO3S2/c1-11(2)7-5-3-4-6-8-12-9-10-16-17(13,14)15/h11-12H,3-10H2,1-2H3,(H,13,14,15)	-2.273

"InChi"	"logS(M)"
InChI=1S/C10H6Cl2/c11-9-6-5-7-3-1-2-4-8(7)10(9)12/h1-6H	-6.161
InChI=1S/C10H11I2NO3/ c1-2-3-16-9(14)6-13-4-7(11)10(15)8(12)5-13/h4-5H,2-3,6H2,1H3	-3.504
InChI=1S/C8H18O2/c1-2-3-4-5-8(6-9)7-10/h8-10H,2-7H2,1H3	-1.698
InChI=1S/C16H18N6O7S2/ c1-4-30(24,25)13-14(22-8-6-5-7-10(22)17-13)31(26,27)21-16(23)20-1 h5-9H,4H2,1-3H3,(H2,18,19,20,21,23)	-4.419
InChI=1S/C35H39NO2/ c37-34(24-28-14-5-1-6-15-28,25-29-16-7-2-8-17-29)32-22-13-23-33(3 h1-12,14-21,32-33,36-38H,13,22-27H2	-8.883
InChI=1S/C9H19NO2/c1-3-4-5-6-7-10-9(12)8(2)11/h8,11H, 3-7H2,1-2H3,(H,10,12)	-0.949
InChI=1S/C13H10O/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/ h1-8H,9H2	-5.253
InChI=1S/C11H14O3/c1-8(2)7-14-11(13)9-3-5-10(12)6-4-9/ h3-6,8,12H,7H2,1-2H3	-2.938
InChI=1S/C6H5N5/c7-6-10-3-4-5(11-6)9-2-1-8-4/h1-3H, (H2,7,9,10,11)	-2.298
InChI=1S/C13H10N2O3/ c14-12-7-6-10(15(17)18)8-11(12)13(16)9-4-2-1-3-5-9/h1-8H,14H2	-3.904
InChI=1S/C7H14N2O4S/c1-5(6(2)14(4,11)12)9-13-7(10)8-3/h6H, 1-4H3,(H,8,10)/b9-5-	-0.027
InChI=1S/C3H3NO/c1-2-4-5-3-1/h1-3H	0.383
InChI=1S/C20H36O4/ c1-5-9-11-17(7-3)15-23-19(21)13-14-20(22)24-16-18(8-4)12-10-6-2/ h13-14,17-18H,5-12,15-16H2,1-4H3/b14-13+	-5.457
InChI=1S/C20H10Cl2N2O2/ c21-12-5-6-14-17(18(12)22)20(26)11-8-15-10(7-16(11)24-14)19(25)9- h1-8H,(H,23,25)(H,24,26)	-7.067
InChI=1S/C8H19NO/c1-7(2)9(5-6-10)8(3)4/h7-8,10H,5-6H2,1-4H3	-1.083
InChI=1S/C9H14N2O/c1-2-3-6-12-9-5-4-8(10)7-11-9/h4-5,7H, 2-3,6,10H2,1H3	-2.033
InChI=1S/C18H17ClN2O2/ c1-12-10-21-11-17(22)20-16-8-7-14(19)9-15(16)18(21,23-12)13-5-3-2 h2-9,12H,10-11H2,1H3,(H,20,22)	-4.745
InChI=1S/C7H12ClN3O4/c1-7(2,5(12)13)9-6(14)11(10-15)4-3-8/ h3-4H2,1-2H3,(H,9,14)(H,12,13)	-2.42
InChI=1S/C8H11N/c1-7-4-3-5-8(6-7)9-2/h3-6,9H,1-2H3	-2.05
InChI=1S/C22H24FN3O2/ c23-17-9-7-16(8-10-17)21(27)6-3-13-25-14-11-18(12-15-25)26-20-5-2 h1-2,4-5,7-10,18H,3,6,11-15H2,(H,24,28)	-5.32
InChI=1S/C19H20N2/ c1-2-7-15(8-3-1)14-21-12-6-11-19(21)17-13-20-18-10-5-4-9-16(17)18 h1-5,7-10,13,19-20H,6,11-12,14H2	-3.587
InChI=1S/C18H27NO2/ c1-15(2)17-11-6-7-12-19(17)13-8-14-21-18(20)16-9-4-3-5-10-16/ h3-5,9-10,15,17H,6-8,11-14H2,1-2H3	-4.319
InChI=1S/C18H10BrNO3/ c19-14-11-7-3-4-8-12(11)20-15(18(14)23)13-16(21)9-5-1-2-6-10(9)17 h1-8,13,23H	-4.867

"InChi"	"logS(M)"
InChI=1S/C9H14N2O4/c1-4-15-8-7(11(13)14)5-10(6(2)3)9(8)12/h6H,4-5H2,1-3H3	-4.33
InChI=1S/C19H21NO2/c1-20(2)18(21)13-22-19-16-9-5-3-7-14(16)11-12-15-8-4-6-10-17(15)1h3-10,19H,11-13H2,1-2H3	-5.506
InChI=1S/C25H44OS2/c1-4-6-8-10-12-14-16-27-20-23-18-22(3)25(26)24(19-23)21-28-17-15-h18-19,26H,4-17,20-21H2,1-3H3	-7.327
InChI=1S/C9H14N2O3S/c1-6-4-7(10)8(14-3)5-9(6)15(12,13)11-2/h4-5,11H,10H2,1-3H3	-2.577
InChI=1S/C8H14ClN3O2S/c9-3-4-12(11-14)8(13)10-7-1-5-15-6-2-7/h7H,1-6H2,(H,10,13)	-2.804
InChI=1S/C10H10O3/c1-6-5-7-3-2-4-8(11)9(7)10(12)13-6/h2-4,6,11H,5H2,1H3	-1.97
InChI=1S/C14H11NO/c1-16-12-6-7-14-11(9-12)8-10-4-2-3-5-13(10)15-14/h2-9H,1H3	-4.741
InChI=1S/C6H8N2O2/c1-2-4-3-7-6(10)8-5(4)9/h3H,2H2,1H3,(H2,7,8,9,10)	-1.942
InChI=1S/C22H30N2O3/c1-2-22(26)18-8-10-21(11-9-18)27-17-20(25)16-23-12-14-24(15-13-2h3-11,20,22,25-26H,2,12-17H2,1H3	-3.316
InChI=1S/C11H15FN2O4/c1-2-3-4-5-9(15)18-7-14-10(16)8(12)6-13-11(14)17/h6H,2-5,7H2,1H3,(H,13,17)	-2.11
InChI=1S/C18H21NO4/c1-19(21)8-7-18-11-4-5-13(20)17(18)23-16-14(22-2)6-3-10(15(16)18)h3-6,11-13,17,20H,7-9H2,1-2H3	-2.899
InChI=1S/C13H13N3O/c1-9-6-7-15-12(8-9)16-13(17)10-2-4-11(14)5-3-10/h2-8H,14H2,1H3,(H,15,16,17)	-2.311
InChI=1S/C12H19NO3S2/c14-18(15,16)17-11-10-13-9-5-4-8-12-6-2-1-3-7-12/h1-3,6-7,13H,4-5,8-11H2,(H,14,15,16)	-1.742
InChI=1S/C24H40O5/c1-13(4-7-22(28)29)16-5-6-17-15-11-20(26)19-10-14(25)8-9-23(19,2)h13-21,25-27H,4-12H2,1-3H3,(H,28,29)	-4.35
InChI=1S/C13H8Cl2O3/c14-10(15)6-5-9-11(16)7-3-1-2-4-8(7)12(17)13(9)18/h1-4,6,16H,5H2	-3.912
InChI=1S/C17H18F2N2/c18-15-5-1-13(2-6-15)17(21-11-9-20-10-12-21)14-3-7-16(19)8-4-14/h1-8,17,20H,9-12H2/p+2	-2.879
InChI=1S/C4H9N3O2S/c5-4(6)7-2(1-10)3(8)9/h2,10H,1H2,(H,8,9)(H4,5,6,7)	0.588
InChI=1S/C12H6Cl2O2/c13-7-1-3-9-11(5-7)16-10-4-2-8(14)6-12(10)15-9/h1-6H	-7.829
InChI=1S/C24H16Cl3N3O2/c1-13-6-2-5-9-20(13)28-24(32)16-10-14-7-3-4-8-15(14)22(23(16)31)3h2-12,29H,1H3,(H,28,32)/b30-22-	-7.694
InChI=1S/C5H10O/c1-5(2)3-6-4-5/h3-4H2,1-2H3	-0.956
InChI=1S/C12H6Cl4O/c13-8-6-9(14)12(11(16)10(8)15)17-7-4-2-1-3-5-7/h1-6H	-7.06
InChI=1S/C8H16O2/c1-6(2)5-7(3)10-8(4)9/h6-7H,5H2,1-4H3	-2.045

"InChi"	"logS(M)"
InChI=1S/C11H18O/c1-7-8(6-12)4-9-5-10(7)11(9,2)3/h6-10H,4-5H2,1-3H3	-3.558
InChI=1S/C2H5NO/c1-3-2-4/h2H,1H3,(H,3,4)	1.229
InChI=1S/C12H20N4O2/c1-14(2)10-13-11(17)16(12(18)15(10)3)9-7-5-4-6-8-9/h9H,4-8H2,1-3H3	-0.883
InChI=1S/C22H18N2O3S/c25-28(26,27)21-13-7-8-16-14-19(23-17-9-3-1-4-10-17)15-20(22(16)21)24-18-11-5-2-6-12-18/h1-15,23-24H,(H,25,26,27)	-4.673
InChI=1S/C8H8O3/c1-5-3-2-4-6(7(5)9)8(10)11/h2-4,9H,1H3,(H,10,11)	-2.04
InChI=1S/C12H5Cl5/c13-8-2-1-6(3-9(8)14)7-4-10(15)12(17)11(16)5-7/h1-5H	-8.39
InChI=1S/C11H21N/c1-8-9-5-6-10(7-9)11(8,2)12(3)4/h8-10H,5-7H2,1-4H3	-2.036
InChI=1S/C13H12N4O2S/c1-19-11-5-8(20(2)18)3-4-9(11)12-16-10-6-14-7-15-13(10)17-12/h3-7H,1-2H3,(H,14,15,16,17)/p+1	-1.756
InChI=1S/C16H14O3/c1-19-13-8-10-16(18)14(11-13)15(17)9-7-12-5-3-2-4-6-12/h2-11,18H,1H3/b9-7+	-6
InChI=1S/C8H7ClN2O/c1-11-6-4-5(9)2-3-7(6)12-8(11)10/h2-4,10H,1H3/b10-8+	-2.902
InChI=1S/C8H16O3/c1-3-8(4-2)10-6-7(5-9)11-8/h7,9H,3-6H2,1-2H3	-1.614
InChI=1S/C16H30O/c1-15-12-10-8-6-4-2-3-5-7-9-11-13-16(17)14-15/h15H,2-14H2,1H3	-5.744
InChI=1S/C12H5Cl5O/c13-6-3-7(14)5-8(4-6)18-10-2-1-9(15)11(16)12(10)17/h1-5H	-7.86
InChI=1S/C10H10ClN5/c11-9-2-1-8(5-14-9)6-16-4-3-13-10(16)15-7-12/h1-2,5H,3-4,6H2,(H,13,15)	-2.63
InChI=1S/CH3ClO6S2/c2-1(9(3,4)5)10(6,7)8/h1H,(H,3,4,5)(H,6,7,8)	0.676
InChI=1S/C12H26O3/c1-3-5-7-13-9-11-15-12-10-14-8-6-4-2/h3-12H2,1-2H3	-1.862
InChI=1S/C18H19NO3/c1-19-8-5-11-9-14(22-2)17(21)16-15(11)13(19)10-18(16)6-3-12(20)4-h3-4,6-7,9,13,21H,5,8,10H2,1-2H3	-2.976
InChI=1S/C6H15N3/c7-1-4-9-5-2-8-3-6-9/h8H,1-7H2	-0.111
InChI=1S/C4H8S2/c1-4-5-2-3-6-4/h4H,2-3H2,1H3	-1.876
InChI=1S/C12H16N2O2/c1-13(2)11(15)9-6-5-7-10(8-9)12(16)14(3)4/h5-8H,1-4H3	0.487
InChI=1S/C10H23NO3S2/c1-3-5-6-10(4-2)9-11-7-8-15-16(12,13)14/h10-11H,3-9H2,1-2H3,(H,12,13,14)	-1.753
InChI=1S/C10H9NO9S3/c11-10-7-3-5(21(12,13)14)1-2-6(7)8(22(15,16)17)4-9(10)23(18,19)20/h1-4H,11H2,(H,12,13,14)(H,15,16,17)(H,18,19,20)	-0.319
InChI=1S/C20H23FN2O/c21-18-10-8-17(9-11-18)20(24)7-4-12-22-13-15-23(16-14-22)19-5-2-1-3-6,8-11H,4,7,12-16H2	-4.623

"InChi"	"logS(M)"
InChI=1S/C12H11N3O4S/c13-9-1-7-12(8-2-9)20(18,19)14-10-3-5-11(6-4-10)15(16)17/h1-8,14H,13H2	-3.94
InChI=1S/C13H20N2O/c1-4-9-14-11(3)13(16)15-12-8-6-5-7-10(12)2/h5-8,11,14H,4,9H2,1-3H3,(H,15,16)	-2.61
InChI=1S/C11H22O/c1-5-12-10-6-9(2)7-11(3,4)8-10/h9-10H,5-8H2,1-4H3	-4.134
InChI=1S/C10H19N/c1-8-6-9(2,3)11-10(4,5)7-8/h6,11H,7H2,1-5H3	-1.714
InChI=1S/C12H23NO/c14-12-10-8-6-4-2-1-3-5-7-9-11-13-12/h1-11H2,(H,13,14)	-2.82
InChI=1S/C12H2Cl8/c13-3-1-2-4(14)7(15)5(3)6-8(16)10(18)12(20)11(19)9(6)17/h1-2H	-9.1
InChI=1S/C14H10N2O2S/c17-13(18)8-9-4-5-12-11(7-9)16-14(19-12)10-3-1-2-6-15-10/h1-7H,8H2,(H,17,18)	-2.639
InChI=1S/C9H11BrN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)	-2.895
InChI=1S/C10H13N/c1-10(7-11-8-10)9-5-3-2-4-6-9/h2-6,11H,7-8H2,1H3	-1.227
InChI=1S/C23H26N2O/c1-24(2)21-14-10-19(11-15-21)23(26,18-8-6-5-7-9-18)20-12-16-22(17h5-17,26H,1-4H3	-3.063
InChI=1S/C7H19N3/c8-4-1-2-6-10-7-3-5-9/h10H,1-9H2	0.838
InChI=1S/C4H8BrF/c5-3-1-2-4-6/h1-4H2	-2.544
InChI=1S/C9H12N4O2/c1-4-5-10-6-7(11-5)12(2)9(15)13(3)8(6)14/h4H2,1-3H3,(H,10,11)	-1.273
InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h3-7H,2H2,1H3	-2.77
InChI=1S/C16H13N3/c17-15-11-10-12-6-4-5-9-14(12)16(15)19-18-13-7-2-1-3-8-13/h1-11H,17H2/b19-18+	-5.916
InChI=1S/C4H5N/c1-2-3-4-5/h2-3H,1H3/b3-2+	-0.429
InChI=1S/C14H14N2/c1-12(15-13-8-4-2-5-9-13)16-14-10-6-3-7-11-14/h2-11H,1H3,(H,15,16)	-4.529
InChI=1S/C15H19N3O5/c1-8-11(17-3-4-17)14(20)10(9(22-2)7-23-15(16)21)12(13(8)19)18-5-6h9H,3-7H2,1-2H3,(H2,16,21)	-1.717
InChI=1S/C7H6O4/c8-3-4-1-2-5(9)7(11)6(4)10/h1-3,9-11H	-1
InChI=1S/C12H16O/c13-12(9-5-2-6-10-12)11-7-3-1-4-8-11/h1,3-4,7-8,13H,2,5-6,9-10H2	-2.966
InChI=1S/C7H9ClN2O4S2/c1-4-2-5(8)7(16(10,13)14)3-6(4)15(9,11)12/h2-3H,1H3,(H2,9,11,12)(H2,10,13,14)	-4.148
InChI=1S/C15H12F3NO4S/c1-24(21,22)12-6-9(15(16,17)18)4-5-10(12)13(20)11-7-19-23-14(11)8h4-8H,2-3H2,1H3	-4.763
InChI=1S/C6H13NO5/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6,8-12H,7H2	-1.41
InChI=1S/C17H16I2O4/c1-9(2)12-8-11(3-4-15(12)20)23-17-13(18)5-10(6-14(17)19)7-16(21)2h3-6,8-9,20H,7H2,1-2H3,(H,21,22)	-7.233

"InChi"	"logS(M)"
InChI=1S/C13H19N/c1-3-7-13(8-4-1)9-12-14-10-5-2-6-11-14/h1,3-4,7-8H,2,5-6,9-12H2	-2.457
InChI=1S/C11H11Cl2NO3S/c1-6(15)14-9(11(16)17)5-18-10-7(12)3-2-4-8(10)13/h2-4,9H,5H2,1H3,(H,14,15)(H,16,17)	-2.31
InChI=1S/C5H9NO3/c1-2-4(5(8)9)6-3-7/h3-4H,2H2,1H3,(H,6,7)(H,8,9)	-0.592
InChI=1S/C8H6Cl2O3/c9-5-1-2-6(10)7(3-5)13-4-8(11)12/h1-3H,4H2,(H,11,12)	-2.62
InChI=1S/C14H19NO5/c1-17-11-8-10(9-12(18-2)13(11)19-3)14(16)15-4-6-20-7-5-15/h8-9H,4-7H2,1-3H3	-0.932
InChI=1S/C7H7NO/c8-6-4-2-1-3-5-7(6)9/h1-5H,(H2,8,9)	0.404
InChI=1S/C10H9NO/c1-7-5-6-8-3-2-4-9(12)10(8)11-7/h2-6,12H,1H3	-1.731
InChI=1S/C16H31NO/c1-2-3-4-5-6-7-8-9-10-11-14-17-15-12-13-16(17)18/h2-15H2,1H3	-4.67
InChI=1S/C19H24N2O2/c1-2-13-12-21-9-7-14(13)11-17(21)19-18(22,8-10-23-19)15-5-3-4-6-16h2-6,13-14,17,20,22H,1,7-12H2	-2.671
InChI=1S/C6H10N4O/c1-3-11-6-9-4(2)8-5(7)10-6/h3H2,1-2H3,(H2,7,8,9,10)	-1.824
InChI=1S/C7H17NO3S2/c1-7(2,3)6-8-4-5-12-13(9,10)11/h8H,4-6H2,1-3H3,(H,9,10,11)	-0.155
InChI=1S/C19H21NO3/c21-18(23-17-12-7-13-20-14-17)19(22,15-8-3-1-4-9-15)16-10-5-2-6-11h1-6,8-11,17,20,22H,7,12-14H2	-2.593
InChI=1S/C17H21NO4S4/c1-18(2)15(13-23-25(19,20)16-9-5-3-6-10-16)14-24-26(21,22)17-11-7h3-12,15H,13-14H2,1-2H3	-5.76
InChI=1S/C12H12N2O4/c15-10(16)7-14-9(11(17)13-12(14)18)6-8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,15,16)(H,13,17,18)	-1.79
InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3	1.045
InChI=1S/C10H10O4/c1-13-9(11)7-4-3-5-8(6-7)10(12)14-2/h3-6H,1-2H3	-2.826
InChI=1S/C18H19N5O8S/c1-12(24)30-9-7-21(8-10-31-13(2)25)15-5-3-14(4-6-15)19-20-18-16(2h3-6,11H,7-10H2,1-2H3/b20-19+	-7.547
InChI=1S/C19H17ClN2O4/c1-3-24-19(23)12(2)25-14-5-7-15(8-6-14)26-18-11-21-17-10-13(20)4-h4-12H,3H2,1-2H3	-5.969
InChI=1S/C7H9NO/c1-6-2-4-7(8-9)5-3-6/h2-5,8-9H,1H3	-0.789
InChI=1S/C19H22F2N4O3/c1-8-5-24(6-9(2)23-8)17-13(20)15(22)12-16(14(17)21)25(10-3-4-10)7h7-10,23H,3-6,22H2,1-2H3,(H,27,28)	-3.37
InChI=1S/C9H8N2O/c1-6-10-8-5-3-2-4-7(8)9(12)11-6/h2-5H,1H3,(H,10,11,12)	-1.845
InChI=1S/C10H16O4S/c1-9(2)7-3-4-10(9,8(11)5-7)6-15(12,13)14/h7H,3-6H2,1-2H3,(H,12,13,14)	-0.3
InChI=1S/C4H8N2O3/c1-2(3(7)8)6-4(5)9/h2H,1H3,(H,7,8)(H3,5,6,9)/p-1	-0.966

"InChi"	"logS(M)"
InChI=1S/C5H10N2/c1-2-5-6-3-4-7-5/h2-4H2,1H3,(H,6,7)	-0.878
InChI=1S/C24H16N2/c25-17-23-7-3-1-5-21(23)15-13-19-9-11-20(12-10-19)14-16-22-6-2-4-h1-16H/b15-13+,16-14+	-4.221
InChI=1S/C22H30N4O2S2/c1-23(2)30(27,28)18-9-10-22-20(17-18)26(19-7-4-5-8-21(19)29-22)12h4-5,7-10,17H,6,11-16H2,1-3H3	-4.538
InChI=1S/C12H7ClO2/c13-8-4-3-7-11-12(8)15-10-6-2-1-5-9(10)14-11/h1-7H	-5.72
InChI=1S/C6H5N5/c7-5-2-9-4-1-8-3-10-6(4)11-5/h1-3H,(H2,7,8,10,11)	-2.31
InChI=1S/C27H39N3O2/c1-8-27(6,13-9-10-17(2)3)21-11-12-22-23-19(15-28-24(21)23)14-20(1h8,10-12,15,18,20,25,28,31H,1,9,13-14,16H2,2-7H3,(H,29,32)	-8.947
InChI=1S/C13H11N3/c14-10-5-4-8-6-9-2-1-3-11(15)13(9)16-12(8)7-10/h1-7H,14-15H2	-3.106
InChI=1S/C5H6O4/c1-3(5(8)9)2-4(6)7/h1-2H2,(H,6,7)(H,8,9)	-0.225
InChI=1S/C10H6O8/c11-7(12)3-1-4(8(13)14)6(10(17)18)2-5(3)9(15)16/h1-2H,(H,11,12)(H,13,14)(H,15,16)(H,17,18)	-1.259
InChI=1S/C7H5N3O7/c1-3-4(8(12)13)2-5(9(14)15)7(11)6(3)10(16)17/h2,11H,1H3	-2.043
InChI=1S/C15H20N2O4S3/c1-2-3-8-17-10-12-4-6-13(7-5-12)23(18,19)14-9-15(22-11-14)24(16,2h4-7,9,11,17H,2-3,8,10H2,1H3,(H2,16,20,21)	-1.68
InChI=1S/C2H3Br3O/c3-2(4,5)1-6/h6H,1H2	-0.92
InChI=1S/C16H35N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17(2)3/h4-16H2,1-3H3	-3.936
InChI=1S/C8H7BrO3/c1-12-8(11)5-2-3-7(10)6(9)4-5/h2-4,10H,1H3	-3.17
InChI=1S/C14H15N3/c1-10-3-6-12(7-4-10)16-17-14-9-11(2)5-8-13(14)15/h3-9H,15H2,1-2H3/b17-16+	-3.903
InChI=1S/C16H26O/c1-7-15(3,4)12-9-10-14(17)13(11-12)16(5,6)8-2/h9-11,17H,7-8H2,1-6H3	-4.893
InChI=1S/C16H8Cl2FN5O/c17-9-1-4-14(12(18)5-9)24-15(25)11-6-10(19)2-3-13(11)22-16(24)23-h1-8H	-5.575
InChI=1S/C12H2Cl8/c13-4-2-1-3(6(14)7(4)15)5-8(16)10(18)12(20)11(19)9(5)17/h1-2H	-9.29
InChI=1S/C13H20O2/c1-3-13(4-2,10-14)12(15)11-8-6-5-7-9-11/h5-9,12,14-15H,3-4,10H2,1-2H3	-3.093
InChI=1S/C8H11N/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7,9H2	-0.282
InChI=1S/C12H27OP/c1-4-7-10-14(13,11-8-5-2)12-9-6-3/h4-12H2,1-3H3	-0.593
InChI=1S/C14H17N3O3/c1-15-8-10-6-7-11(9-15)16(10)14(18)12-4-2-3-5-13(12)17(19)20/h2-5,10-11H,6-9H2,1H3	-2.326
InChI=1S/C19H19N3O/c1-3-7-15(8-4-1)17-18(16-9-5-2-6-10-16)23-19(21-17)22-13-11-20-12h1-10,20H,11-14H2	-3.759

"InChi"	"logS(M)"
InChI=1S/C20H43O3P/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24(21,22-2)23-3/h4-20H2,1-3H3	-5.53
InChI=1S/C12H20O2/c1-3-9-13-11-5-7-12(8-6-11)14-10-4-2/h3-4,9-12H,5-8H2,1-2H3/b9-3+,10-4+	-3.904
InChI=1S/C17H28N2O/c1-2-3-4-5-6-7-8-9-10-14-19-17(20)16-12-11-13-18-15-16/h11-13,15H,2-10,14H2,1H3,(H,19,20)	-3.027
InChI=1S/C19H26I3N3O9/c1-8(29)25(4-11(32)7-28)17-15(21)12(18(33)23-2-9(30)5-26)14(20)13h9-11,26-28,30-32H,2-7H2,1H3,(H,23,33)(H,24,34)	-3.887
InChI=1S/C13H14O3/c14-8-12(15)9-16-13-6-5-10-3-1-2-4-11(10)7-13/h1-7,12,14-15H,8-9H2	-2.531
InChI=1S/C17H16N4O3S/c18-14-6-8-15(9-7-14)25(23,24)20-16-10-11-21(17(22)19-16)12-13-4-h1-11H,12,18H2,(H,19,20,22)	-4.8
InChI=1S/C13H14O3/c14-8-11(15)9-16-13-7-3-5-10-4-1-2-6-12(10)13/h1-7,11,14-15H,8-9H2	-2.531
InChI=1S/C17H23N7O8/c18-11(16(29)30)3-6-14(27)23-12(4-1-9(25)7-21-19)15(28)24-13(17(3h7-8,11-13H,1-6,18H2,(H4-2,23,24,25,26,27,28,29,30,31,32)/b9-7-,10-8-	-2.553
InChI=1S/C13H22N2O4S2/c1-12-5-6-13(15-11-12)19-9-4-2-3-7-14-8-10-20-21(16,17)18/h5-6,11,14H,2-4,7-10H2,1H3,(H,16,17,18)	-1.932
InChI=1S/C16H12FNO3/c1-9(16(19)20)10-5-6-14-13(8-10)18-15(21-14)11-3-2-4-12(17)7-11/h2-9H,1H3,(H,19,20)	-3.905
InChI=1S/C11H12O5S/c1-8(12)16-10-6-4-3-5-9(10)11(13)15-7-17(2)14/h3-6H,7H2,1-2H3/p+1	-1.782
InChI=1S/C4H6O2/c1-3-4(5)6-2/h3H,1H2,2H3	-0.22
InChI=1S/C7H6N2O2S/c10-12(11)7-4-2-1-3-6(7)8-5-9-12/h1-5H,(H,8,9)	-0.667
InChI=1S/C4H6O4S4/c5-3(6)1-9-11-12-10-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)	-1.452
InChI=1S/C10H20O4/c1-3-4-5-12-6-7-13-8-9-14-10(2)11/h3-9H2,1-2H3	-0.819
InChI=1S/C18H18N3O3PS/c19-13-1-7-16(8-2-13)22-25(26,23-17-9-3-14(20)4-10-17)24-18-11-5-h1-12H,19-21H2	-5.309
InChI=1S/C14H17NO/c1-4-10-15-14(16)12(3)11(2)13-8-6-5-7-9-13/h4-9H,1,10H2,2-3H3,(H,15,16)/b12-11-	-3.528
InChI=1S/C9H6O4/c10-6-3-1-5-2-4-7(11)13-9(5)8(6)12/h1-4,10,12H	-1.616
InChI=1S/C12H22O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h3-10H2,1-2H3	-3.001
InChI=1S/C16H19NO7/c1-4-22-15(20)9-17(3)14(19)10-23-16(21)12-7-5-6-8-13(12)24-11(2)1h5-8H,4,9-10H2,1-3H3	-2.55

"InChi"	"logS(M)"
InChI=1S/C12H16ClNO3/ c1-2-3-6-17-11-5-4-9(7-10(11)13)8-12(15)14-16/h4-5,7,16H, 2-3,6,8H2,1H3,(H,14,15)	-3.782
InChI=1S/C17H17F2N3O3/ c1-7-12(20)6-21(7)15-11(18)4-9-14(13(15)19)22(8-2-3-8)5-10(16(9)2 h4-5,7-8,12H,2-3,6,20H2,1H3,(H,24,25)	-4.17
InChI=1S/C10H18Cl2N6O4/ c11-3-7-17(15-21)9(19)13-5-1-2-6-14-10(20)18(16-22)8-4-12/ h1-8H2,(H,13,19)(H,14,20)	-2.573
InChI=1S/C19H19NO4/ c1-20-6-5-11-8-14-19(24-9-23-14)17-15(11)12(20)7-10-3-4-13(22-2)1 h3-4,8,12,21H,5-7,9H2,1-2H3	-4.119
InChI=1S/C4H8Cl2F2NOP/c5-11(6,10)9(3-1-7)4-2-8/h1-4H2	-1.572
InChI=1S/C10H11NO3/c1-7(12)11(2)9-6-4-3-5-8(9)10(13)14/h3-6H, 1-2H3,(H,13,14)	-2.19
InChI=1S/C10H15N/c1-9(11-2)8-10-6-4-3-5-7-10/h3-7,9,11H, 8H2,1-2H3	-1.05
InChI=1S/C15H23NO3/ c1-4-9-18-14-7-5-6-8-15(14)19-11-13(17)10-16-12(2)3/ h4-8,12-13,16-17H,1,9-11H2,2-3H3	-0.32
InChI=1S/C14H18Cl3N5O2/ c1-14(2)21-12(18)20-13(19)22(14)24-5-3-4-23-11-7-9(16)8(15)6-10(1 h6-7H,3-5H2,1-2H3,(H4,18,19,20,21)	-4.278
InChI=1S/C14H19NO3/ c1-2-3-4-11-18-13-8-5-12(6-9-13)7-10-14(16)15-17/h5-10,17H, 2-4,11H2,1H3,(H,15,16)/b10-7+	-3.816
InChI=1S/C11H22/c1-3-5-7-9-11-10-8-6-4-2/h5,7H, 3-4,6,8-11H2,1-2H3/b7-5+	-5.188
InChI=1S/C9H16O4/c1-4-11-8(10)5-9(3)12-6-7(2)13-9/h7H, 4-6H2,1-3H3	-2.18
InChI=1S/C10H10O5/c11-5-6-15-10(14)8-4-2-1-3-7(8)9(12)13/ h1-4,11H,5-6H2,(H,12,13)	-1.482
InChI=1S/C10H12O/c1-9(7-8-11)10-5-3-2-4-6-10/h2-6,8-9H, 7H2,1H3	-1.87
InChI=1S/C7H7NO3/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3	-2.486
InChI=1S/C7H8ClNO3S/c1-4-2-6(9)7(3-5(4)8)13(10,11)12/h2-3H, 9H2,1H3,(H,10,11,12)	-2.346
InChI=1S/C6H5NO3/c8-6(9)5-1-3-7(10)4-2-5/h1-4H,(H,8,9)	-1.102
InChI=1S/C8H9NO/c1-7(9-10)8-5-3-2-4-6-8/h2-6,10H,1H3/b9-7+	-2.376
InChI=1S/C13H13Cl2N3O3/ c14-9-1-2-11(12(15)3-9)13(6-18-8-16-7-17-18)20-5-10(4-19)21-13/ h1-3,7-8,10,19H,4-6H2	-2.906
InChI=1S/C14H16N2O4/ c15-13(18)11-7-4-8-16(11)12(17)9-20-14(19)10-5-2-1-3-6-10/ h1-3,5-6,11H,4,7-9H2,(H2,15,18)	-2.27
InChI=1S/C24H36N2O9S/ c1-13(33-3)17(25-22(31)15-8-6-10-26(15)2)21-19(29)18(28)20(30)24(h4-5,7,9,13,15,17-21,24,27-30H,6,8,10-12H2,1-3H3,(H,25,31)	-4.565
InChI=1S/C6H12N2O4S/c7-3(5(9)10)1-13-2-4(8)6(11)12/h3-4H, 1-2,7-8H2,(H,9,10)(H,11,12)	-2.56

"InChi"	"logS(M)"
InChI=1S/C21H25N/c1-21(2)19-13-7-5-10-17(19)16(12-9-15-22(3)4)18-11-6-8-14-20(18)2h5-8,10-14H,9,15H2,1-4H3	-5.538
InChI=1S/C6H8Cl2O5/c7-5(9)12-3-1-11-2-4-13-6(8)10/h1-4H2	-4.887
InChI=1S/C14H9Cl2N3O2/c15-8-4-2-1-3-7(8)11-12-9(5-6-10(16)18-12)17-13(20)14(21)19-11/h1-6,14,21H,(H,17,20)	-3.07
InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3	-0.46
InChI=1S/C11H16N2O3/c14-8-11(9(15)13-10(16)12-8)6-4-2-1-3-5-7-11/h1-7H2,(H2,12,13,14,15,16)	-2.98
InChI=1S/C15H9BrO2/c16-10-7-5-9(6-8-10)13-14(17)11-3-1-2-4-12(11)15(13)18/h1-8,13H	-4.607
InChI=1S/C17H24O10/c1-6-3-8(19)11-7(15(23)24-2)5-25-16(10(6)11)27-17-14(22)13(21)12(h5-6,9-14,16-18,20-22H,3-4H2,1-2H3	-0.265
InChI=1S/C25H31NO4/c1-4-13-25(22-6-5-7-24(17-22)30-20(3)28)14-16-26(18-25)15-12-21-8h5-11,17H,4,12-16,18H2,1-3H3	-5.384
InChI=1S/C9H7N/c10-8-4-7-9-5-2-1-3-6-9/h1-7H/b7-4+	-2.083
InChI=1S/C16H24O11/c1-8(17)23-7-13(24-9(2)18)14(25-10(3)19)15(26-11(4)20)16(22-6)27-h13-16H,7H2,1-6H3	-1.82
InChI=1S/C5H10N2O2S/c1-3(8)7-4(2-10)5(6)9/h4,10H,2H2,1H3,(H2,6,9)(H,7,8)	-1.447
InChI=1S/C6H8ClN3O2/c1-5-8-6(10(11)12)4-9(5)3-2-7/h4H,2-3H2,1H3	-2.44
InChI=1S/C9H17N/c1-7-9-4-3-8(5-9)6-10(7)2/h7-9H,3-6H2,1-2H3	-1.087
InChI=1S/C2H7N3/c1-5-2(3)4/h1H3,(H4,3,4,5)	-1.613
InChI=1S/C9H9Cl2NO2/c1-12-9(13)14-5-6-2-3-7(10)8(11)4-6/h2-4H,5H2,1H3,(H,12,13)	-3.139
InChI=1S/C13H11NO3/c15-10-7-5-9(6-8-10)14-13(17)11-3-1-2-4-12(11)16/h1-8,15-16H,(H,14,17)	-2.849
InChI=1S/C19H24N4O7/c1-4-5-29-18(27)23-10-6-22-13-11(15(25)12(20)8(2)14(13)24)9(7-30-h9-10,16H,4-7,20H2,1-3H3,(H2,21,26)	-3.48
InChI=1S/C4H4N2O2/c7-4(8)3-1-5-2-6-3/h1-2H,(H,5,6)(H,7,8)	0.03
InChI=1S/C8H6ClNO/c9-6-2-1-5-3-8(11)10-7(5)4-6/h1-2,4H,3H2,(H,10,11)	-2.969
InChI=1S/C27H48O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4)h18-25,28H,6-17H2,1-5H3	-10.051
InChI=1S/C12H8O2P/c13-15-12-8-4-2-6-10(12)9-5-1-3-7-11(9)14-15/h1-8H/q+1	-1.78
InChI=1S/C6H10O4/c1-4(6(9)10)2-3-5(7)8/h4H,2-3H2,1H3,(H,7,8)(H,9,10)	0.835
InChI=1S/C14H28N2/c1-3-7-13(8-4-1)15-11-12-16-14-9-5-2-6-10-14/h13-16H,1-12H2	-0.98

"InChi"	"logS(M)"
InChI=1S/C14H13N3/c1-3-7-13-10-11(2)15-14(17-13)16-12-8-5-4-6-9-12/h4-6,8-10H,1-2H3,(H,15,16,17)	-4.6
InChI=1S/C7H8ClN/c1-5-6(8)3-2-4-7(5)9/h2-4H,9H2,1H3	-2.151
InChI=1S/C7H5FO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H,9,10)	-1.39
InChI=1S/C11H11N5O5/c17-6-15(7-18)11-12-5-8(13-14-11)1-2-9-3-4-10(21-9)16(19)20/h1-5,17-18H,6-7H2/b2-1+	-0.997
InChI=1S/C8H10N2O/c1-2-11-10-7-8-3-5-9-6-4-8/h3-7H,2H2,1H3/b10-7+	-0.354
InChI=1S/C26H26F2N2/c27-24-12-8-22(9-13-24)26(23-10-14-25(28)15-11-23)30-19-17-29(18h1-15,26H,16-20H2/b7-4+	-6.077
InChI=1S/C13H20O/c1-3-10-9-7-12(11(10)4-1)13(8-9)5-2-6-14-13/h9-12H,1-8H2	-5.942
InChI=1S/C15H22O3/c1-4-15(5-2,14(17)18-6-3)13(16)12-10-8-7-9-11-12/h7-11,13,16H,4-6H2,1-3H3	-3.401
InChI=1S/C16H18N2O3/c1-16(2)15(20)14(18-7-3-4-13(18)19)11-8-10(9-17)5-6-12(11)21-16/h5-6,8,14-15,20H,3-4,7H2,1-2H3	-3.019
InChI=1S/C14H30N2O4/c1-15(2,3)9-11-19-13(17)7-8-14(18)20-12-10-16(4,5)6/h7-12H2,1-6H3/q+2	0.537
InChI=1S/C19H21NO2/c1-20-9-8-13-11-16(21-2)19(22-3)18-14-7-5-4-6-12(14)10-15(20)17(1h4-7,11,15H,8-10H2,1-3H3	-4.35
InChI=1S/C8H14N2O2S2/c1-6-4-13-8(2,14-6)5-10-12-7(11)9-3/h5-6H,4H2,1-3H3,(H,9,11)/b10-5+	-2.37
InChI=1S/C10H11ClO3/c11-8-3-5-9(6-4-8)14-7-1-2-10(12)13/h3-6H,1-2,7H2,(H,12,13)	-3.29
InChI=1S/C7H7NO3/c9-5-6-2-1-3-7(4-6)8(10)11/h1-4,9H,5H2	-2.414
InChI=1S/C11H14N2S2/c1-11(2,3)13-15-10-12-8-6-4-5-7-9(8)14-10/h4-7,13H,1-3H3	-5.137
InChI=1S/C23H34O5/c1-22-9-7-16(26)11-15(22)3-4-17-18-5-6-20(23(18,2)10-8-19(17)22)2h11,14,17-20,24-25H,3-10,12-13H2,1-2H3	-4.25
InChI=1S/C9H5Cl3N4/c10-5-3-1-2-4-6(5)13-9-15-7(11)14-8(12)16-9/h1-4H,(H,13,14,15,16)	-4.537
InChI=1S/C9H8O6/c1-15-7-3-5(9(13)14)4(8(11)12)2-6(7)10/h2-3,10H,1H3,(H,11,12)(H,13,14)	-1.21
InChI=1S/C6H12Cl3O4P/c7-1-4-11-14(10,12-5-2-8)13-6-3-9/h1-6H2	-1.611
InChI=1S/C8H24N4O3P2/c1-9(2)16(13,10(3)4)15-17(14,11(5)6)12(7)8/h1-8H3	0.543
InChI=1S/C8H7NO/c10-8-5-6-3-1-2-4-7(6)9-8/h1-4H,5H2,(H,9,10)	-1.164
InChI=1S/C21H19N3O3S/c1-27-20-13-14(24-28(25)26)11-12-19(20)23-21-15-7-3-5-9-17(15)2h3-13,24H,1-2H3,(H,22,23)	-6.503
InChI=1S/C16H31N3O/c1-15(2)7-6-8-16(3,4)19(15)14(20)13-18-11-9-17(5)10-12-18/h6-13H2,1-5H3	-2.798

"InChi"	"logS(M)"
InChI=1S/C27H33NO2/c29-22-13-12-21-18-25-23-10-4-6-14-27(23,24(21)19-22)15-17-28(25)h1-3,8-9,12-13,19,23,25,29H,4-7,10-11,14-18H2	-4.849
InChI=1S/C12H6Cl4/c13-9-1-7(2-10(14)5-9)8-3-11(15)6-12(16)4-8/h1-6H	-8.375
InChI=1S/C45H74O11/c1-12-34-17-15-13-14-16-27(4)42(51)44(11,53)43(52)32(9)40(50)31(8)h13-15,17-18,21,25-36,38,40-42,46,48,50-51,53H,12,16,19-20,22-24H2,1-11H3/b14-13-,17-15-,21-18-	-10.921
InChI=1S/C3H6O3/c1-6-2-3(4)5/h2H2,1H3,(H,4,5)	1.045
InChI=1S/C10H7NO2/c12-11(13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H	-3.82
InChI=1S/C9H8N2O3/c12-6-3-1-5(2-4-6)7-8(13)11-9(14)10-7/h1-4,7,12H,(H2,10,11,13,14)	-2.173
InChI=1S/C9H18N2O2/c1-3-5-7(6-4-2)8(12)11-9(10)13/h7H,3-6H2,1-2H3,(H3,10,11,12,13)	-2.156
InChI=1S/C12H12N2/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9,14H,13H2	-2.563
InChI=1S/C18H34O4/c1-15(2,3)11-9-10-12-18(21-22-18)14(19)20-17(7,8)13-16(4,5)6/h9-13H2,1-8H3	-6.971
InChI=1S/C17H20FN3O3/c1-2-5-21-10-12(17(23)24)16(22)11-8-13(18)15(9-14(11)21)20-6-3-19h8-10,19H,2-7H2,1H3,(H,23,24)	-3.57
InChI=1S/C21H32O9/c1-5-18(22)28-12-9-25-15-21(8-4,16-26-10-13-29-19(23)6-2)17-27-11h5-7H,1-3,8-17H2,4H3	-2.687
InChI=1S/C22H40O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20(22(25)26)19-21(2h16-17,20H,2-15,18-19H2,1H3,(H,23,24)(H,25,26)/b17-16+	-6.964
InChI=1S/C8H8O2/c1-10-8-6-4-2-3-5-7(8)9/h2-6H,1H3	-1.093
InChI=1S/C8H10O3S/c1-6-4-3-5-8(7(6)2)12(9,10)11/h3-5H,1-2H3,(H,9,10,11)	0.778
InChI=1S/C14H21NO3/c1-3-4-5-6-9-18-12-7-8-13(11(2)15-17)14(16)10-12/h7-8,10,16-17H,3-6,9H2,1-2H3/b15-11+	-4.15
InChI=1S/C10H14O2/c1-11-10(12-2)8-9-6-4-3-5-7-9/h3-7,10H,8H2,1-2H3	-1.63
InChI=1S/C12H22N2O4/c1-3-6-12(2,7-17-10(13)15)8-18-11(16)14-9-4-5-9/h9H,3-8H2,1-2H3,(H2,13,15)(H,14,16)	-3.002
InChI=1S/C18H26N2O4/c1-12(2)9-14-5-7-15(8-6-14)13(3)18(23)24-11-17(22)20(4)10-16(19)2h5-8,12-13H,9-11H2,1-4H3,(H2,19,21)	-3.41
InChI=1S/C12H5Cl5O/c13-7-8(14)10(16)12(11(17)9(7)15)18-6-4-2-1-3-5-6/h1-5H	-7.94
InChI=1S/C20H27NO2/c22-16-6-5-15-11-18-20(23)8-2-1-7-19(20,17(15)12-16)9-10-21(18)13h5-6,12,14,18,22-23H,1-4,7-11,13H2	-2.624
InChI=1S/C8H9NO2/c1-6-4-3-5-8(7(6)2)9(10)11/h3-5H,1-2H3	-3.003
InChI=1S/C10H22O2/c1-2-3-4-5-6-7-8-10(12)9-11/h10-12H,2-9H2,1H3	-2.479

"InChi"	"logS(M)"
InChI=1S/C3H4N2/c1-2-5-3-4-1/h1-3H,(H,4,5)	0.968
InChI=1S/C7H6N4O/c1-11-6-5(4-10-7(11)12)8-2-3-9-6/h2-4H,1H3	-1.371
InChI=1S/C14H17N3O/c18-14-7-3-5-11-4-1-2-6-12(11)17(14)10-13-15-8-9-16-13/h1-2,4,6H,3,5,7-10H2,(H,15,16)	-2.353
InChI=1S/C8H11NO3S/c1-6-3-4-7(12-2)8(5-6)13(9,10)11/h3-5H,1-2H3,(H2,9,10,11)	-1.53
InChI=1S/C6H9NO3/c1-7-3-4(6(9)10)2-5(7)8/h4H,2-3H2,1H3,(H,9,10)	-0.954
InChI=1S/C12H14O3/c1-9(13)7-11(8-12(14)15)10-5-3-2-4-6-10/h2-6,11H,7-8H2,1H3,(H,14,15)	-1.446
InChI=1S/C2H5ClO/c3-1-2-4/h4H,1-2H2	1.094
InChI=1S/C3H7NO2/c1-2(5)3(4)6/h2,5H,1H3,(H2,4,6)	0.944
InChI=1S/C4H8O/c1-5-4-2-3-4/h4H,2-3H2,1H3	-0.118
InChI=1S/C8H2Cl4O2/c9-4-2-1-14-8(13)3(2)5(10)7(12)6(4)11/h1H2	-5.037
InChI=1S/C16H25NOS/c1-5-13(3)17(14(4)6-2)16(18)19-12-15-10-8-7-9-11-15/h7-11,13-14H,5-6,12H2,1-4H3	-5.048
InChI=1S/C35H36N2O3/c1-4-6-19-37(20-7-5-2)26-17-18-29-33(22-26)39-32-21-24(3)31(36-25h8-18,21-23,36H,4-7,19-20H2,1-3H3	-7.404
InChI=1S/C13H12F2N6O/c14-10-1-2-11(12(15)3-10)13(22,4-20-8-16-6-18-20)5-21-9-17-7-19-2h1-3,6-9,22H,4-5H2	-1.8
InChI=1S/C13H17Cl2NO2/c1-10-3-4-11(13(17)18-2)9-12(10)16(7-5-14)8-6-15/h3-4,9H,5-8H2,1-2H3	-5.107
InChI=1S/C7H7IO/c1-5-2-3-7(9)6(8)4-5/h2-4,9H,1H3	-2.466
InChI=1S/C11H15NO2/c1-3-12(4-2)11(14)9-7-5-6-8-10(9)13/h5-8,13H,3-4H2,1-2H3	-1.745
InChI=1S/C20H24O2/c1-3-20-11-10-16-15-7-5-14(22-2)12-13(15)4-6-17(16)18(20)8-9-19(2h5,7,12,18H,3-4,6,8-11H2,1-2H3	-4.773
InChI=1S/C3H9O3PS/c1-5-7(4,6-2)8-3/h1-3H3	-0.376
InChI=1S/C15H24N2O/c1-2-3-4-5-6-7-8-12-17-15(18)14-10-9-11-16-13-14/h9-11,13H,2-8,12H2,1H3,(H,17,18)	-3.14
InChI=1S/C18H28N2O/c1-14(2)19(15(3)4)12-13-20-17-10-6-5-8-16(17)9-7-11-18(20)21/h5-6,8,10,14-15H,7,9,11-13H2,1-4H3	-4.179
InChI=1S/C6H12N2O3S2/c1-6(8-4-2-3-7)5-12-13(9,10)11/h6,8H,2,4-5H2,1H3,(H,9,10,11)	0.649
InChI=1S/C12H5Cl5/c13-7-1-6(2-8(14)3-7)9-4-11(16)12(17)5-10(9)15/h1-5H	-7.47
InChI=1S/C16H19ClO2/c17-15-9-13-11(6-7-12(13)16(18)19)8-14(15)10-4-2-1-3-5-10/h8-10,12H,1-7H2,(H,18,19)	-5.743
InChI=1S/C18H15NO2/c20-16-11-18(17(21)19-16)14-7-3-1-5-12(14)9-10-13-6-2-4-8-15(13)1h1-8H,9-11H2,(H,19,20,21)	-5.267

"InChi"	"logS(M)"
InChI=1S/C10H15NO/c12-11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-9,12H,1-5H2/b11-10-	-1.836
InChI=1S/C2H4FI/c3-1-2-4/h1-2H2	-2.199
InChI=1S/C9H9N3OS/c1-10-8(13)12-9-11-6-4-2-3-5-7(6)14-9/h2-5H,1H3,(H2,10,11,12,13)	-4.237
InChI=1S/C9H8N2O3S/c10-9-6-2-1-5-11-7(6)3-4-8(9)15(12,13)14/h1-5H,10H2,(H,12,13,14)	-2.5
InChI=1S/C5H4N4O2S/c10-4-6-1-2(7-4)8-5(11)9-3(1)12/h(H4,6,7,8,9,10,11,12)	-4.04
InChI=1S/C5H10O2/c1-5(2,3)4(6)7/h1-3H3,(H,6,7)	-0.564
InChI=1S/C21H34O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-10-h14-18,23-24H,4-12H2,1-3H3	-4.881
InChI=1S/C20H25N3O/c1-3-22(4-2)14-9-15-23-19-13-8-7-12-18(19)21-17-11-6-5-10-16(17)2h5-8,10-13,21H,3-4,9,14-15H2,1-2H3	-5.684
InChI=1S/C30H31N/c1-29(2,23-11-7-5-8-12-23)25-15-19-27(20-16-25)31-28-21-17-26(18-h5-22,31H,1-4H3	-7.782
InChI=1S/C19H20N4O2/c1-24-17-10-14(9-15-11-22-19(21)23-18(15)20)7-8-16(17)25-12-13-5-h2-8,10-11H,9,12H2,1H3,(H4,20,21,22,23)	-3.925
InChI=1S/C19H26N2OS/c1-15-6-7-18-17(12-15)16(2)13-19(20-18)22-10-5-3-4-8-21-9-11-23-1h6-7,12-13H,3-5,8-11,14H2,1-2H3	-4.801
InChI=1S/C12H10S/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10H	-4.361
InChI=1S/C13H13OP/c1-15(14,12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11H,1H3	-2.384
InChI=1S/C10H13NO4/c1-11-7(10(14)15)4-6-2-3-8(12)9(13)5-6/h2-3,5,7,11-13H,4H2,1H3,(H,14,15)	-1.02
InChI=1S/C14H22/c1-2-3-4-5-6-8-11-14-12-9-7-10-13-14/h7,9-10,12-13H,2-6,8,11H2,1H3	-6.46
InChI=1S/C12H11N3S/c13-12(16)11(9-4-2-1-3-5-9)10-8-14-6-7-15-10/h1-8,11H,(H2,13,16)	-1.267
InChI=1S/C17H16O/c1-12(11-18)14-8-9-17-15(10-14)7-6-13-4-2-3-5-16(13)17/h2-10,12,18H,11H2,1H3	-5.227
InChI=1S/C16H17NO4/c1-2-20-10-6-4-3-5-9(10)17-15(18)13-11-7-8-12(21-11)14(13)16(17)1h3-6,11-14H,2,7-8H2,1H3	-1.215
InChI=1S/C3H4N2O/c4-2-1-3(5)6/h1H2,(H2,5,6)	0.189
InChI=1S/C8H19NO4S2/c1-3-5-7-14(10,11)9-15(12,13)8-6-4-2/h9H,3-8H2,1-2H3	-0.76
InChI=1S/C8H7Cl2NO/c1-5(12)11-8-3-2-6(9)4-7(8)10/h2-4H,1H3,(H,11,12)	-2.551
InChI=1S/C10H13N5O4/c11-10-6-4(12-2-13-10)5(14-15-6)9-8(18)7(17)3(1-16)19-9/h2-3,7-9,16-18H,1H2,(H,14,15)(H2,11,12,13)	-0.067
InChI=1S/C3H7N3O5/c1-4(5(7)8)2-3-11-6(9)10/h2-3H2,1H3	-0.317
InChI=1S/C12H19NO/c1-10(2)13-9-12(14)8-11-6-4-3-5-7-11/h3-7,10,12-14H,8-9H2,1-2H3	-1.214

"InChi"	"logS(M)"
InChI=1S/C17H24N2O2/c1-17(12-20,13-6-4-3-5-7-13)16(21)19-10-14-8-9-15(11-19)18(14)2/h3-7,14-15,20H,8-12H2,1-2H3	-2.104
InChI=1S/C16H18O2/c1-17-11-13-3-7-15(8-4-13)16-9-5-14(6-10-16)12-18-2/h3-10H,11-12H2,1-2H3	-4.002
InChI=1S/C9H13NO3/c1-10-5-9(13)6-2-3-7(11)8(12)4-6/h2-4,9-13H,5H2,1H3	-3.008
InChI=1S/C12H20O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h7-8H,3-6,9-10H2,1-2H3/b8-7+	-4.314
InChI=1S/C19H21N3O/c1-22(2)14-13-20-19-21-17(15-9-5-3-6-10-15)18(23-19)16-11-7-4-8-12-16/h3-12H,13-14H2,1-2H3,(H,20,21)	-3.583
InChI=1S/C3H4O/c1-2-3-4/h1,4H,3H2	1.251
InChI=1S/C28H27N/c1-21(23-9-5-3-6-10-23)25-13-17-27(18-14-25)29-28-19-15-26(16-20-28)22-29H,1-2H3	-5.964
InChI=1S/C9H9IO3/c1-2-13-9(12)6-3-4-8(11)7(10)5-6/h3-5,11H,2H2,1H3	-3.492
InChI=1S/C18H14ClNO2/c1-11-6-7-14(19)10-16(11)20-18(22)15-8-12-4-2-3-5-13(12)9-17(15)21/h2-10,21H,1H3,(H,20,22)	-5.239
InChI=1S/C9H7NO4S/c11-7-3-4-8(15(12,13)14)6-2-1-5-10-9(6)7/h1-5,11H,(H,12,13,14)	-0.354
InChI=1S/C16H19ClO6/c1-7-4-8(18)5-11(19)16(7)15(20)12-9(21-2)6-10(22-3)13(17)14(12)23/h6-8,11,18-19H,4-5H2,1-3H3	-2.34
InChI=1S/C14H21NO2S/c1-12-6-2-3-8-15(12)9-5-10-17-14(16)13-7-4-11-18-13/h4,7,11-12H,2-3,5-6,8-10H2,1H3	-3.729
InChI=1S/C14H15N3O/c1-10-4-3-9-16-13(10)17(2)14(18)11-5-7-12(15)8-6-11/h3-9H,15H2,1-2H3	-2.884
InChI=1S/C9H13NO8/c11-6(12)2-1-5(9(17)18)10(3-7(13)14)4-8(15)16/h5H,1-4H2,(H,11,12)(H,13,14)(H,15,16)(H,17,18)	0.044
InChI=1S/C28H37N3O5S/c1-27(2,3)30-25(34)23-28(4,5)37-17-31(23)26(35)22(32)21(16-18-10-7-15,21-23,32H,16-17H2,1-6H3,(H,29,33)(H,30,34)	-4.11
InChI=1S/C25H35ClN2/c1-19(2)28(20(3)4)17-7-16-27-18-23(21-12-14-24(26)15-13-21)11-10-5-6,8-9,12-15,19-20,23H,7,10-11,16-18H2,1-4H3	-7.568
InChI=1S/C21H19N5O7/c1-10(27)17(18(28)22-12-5-7-14-16(9-12)24-21(31)23-14)26-25-15-8-4-9,17H,1-3H3,(H,22,28)(H2,23,24,31)/b26-25+	-6.314
InChI=1S/C10H16N2O3/c1-5(2)10(6(3)4)7(13)11-9(15)12-8(10)14/h5-6H,1-4H3,(H2,11,12,13,14,15)	-2.77
InChI=1S/C18H21N3O/c1-19(2)12-13-21-17-11-7-6-10-16(17)20(3)15-9-5-4-8-14(15)18(21)2h4-11H,12-13H2,1-3H3	-4.599
InChI=1S/C4H3N5O2/c10-3-1-2(8-9-7-1)5-4(11)6-3/h(H3,5,6,7,8,9,10,11)	-0.589

"InChi"	"logS(M)"
InChI=1S/C10H9NO3S/c11-9-5-1-4-8-7(9)3-2-6-10(8)15(12,13)14/h1-6H,11H2,(H,12,13,14)	-2.35
InChI=1S/C15H10Cl2N2O5/c1-24-15(21)10-4-2-8(6-13(10)19(22)23)14(20)18-12-7-9(16)3-5-11(12)17-7H,1H3,(H,18,20)	-5.965
InChI=1S/C8H9NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-4H2,(H,9,10,11)	-1.975
InChI=1S/C15H15NO3/c17-10-9-16-15(19)13-8-4-7-12(14(13)18)11-5-2-1-3-6-11/h1-8,17-18H,9-10H2,(H,16,19)	-2.454
InChI=1S/C10H14N2O2/c1-12(2)6-7-14-10(13)9-4-3-5-11-8-9/h3-5,8H,6-7H2,1-2H3	0.103
InChI=1S/C6H12O3/c1-5(4-8-3)9-6(2)7/h5H,4H2,1-3H3	0.083
InChI=1S/C14H11NO/c1-15-12-8-4-2-6-10(12)14(16)11-7-3-5-9-13(11)15/h2-9H,1H3	-4.46
InChI=1S/C23H29NO3/c1-2-27-22(25)23(21-11-7-4-8-12-21)13-15-24(16-14-23)17-18-26-19-h3-12H,2,13-19H2,1H3	-4.681
InChI=1S/C18H23NO2/c1-12(20)19-9-8-18-7-3-2-4-15(18)17(19)10-13-5-6-14(21)11-16(13)1h5-6,11,15,17,21H,2-4,7-10H2,1H3	-3.355
InChI=1S/C23H20N2O5/c26-19-12-6-15(7-13-19)14-20(25-21(27)16-4-2-1-3-5-16)22(28)24-18h1-13,20,26H,14H2,(H,24,28)(H,25,27)(H,29,30)	-4.481
InChI=1S/C15H32/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h13-15H,6-12H2,1-5H3	-6.615
InChI=1S/C9H14N2O3/c1-7(2)8(12)14-6-5-11-4-3-10-9(11)13/h1,3-6H2,2H3,(H,10,13)	0.703
InChI=1S/C22H16N2O2/c1-11-3-5-17-13(7-11)21(25)15-9-20-16(10-19(15)23-17)22(26)14-8-1h3-10H,1-2H3,(H,23,25)(H,24,26)	-7.784
InChI=1S/C25H22N4O8/c1-9-14(10-6-8-13(35-2)23(36-3)20(10)30)15(26)19(29-17(9)25(33)34h5-8,29H,26-27H2,1-4H3,(H,33,34)/b14-10-	-1.036
InChI=1S/C48H66N6O6/c1-7-13-16-34(10-4)31-58-43(55)37-19-25-40(26-20-37)49-46-52-47(5h19-30,34-36H,7-18,31-33H2,1-6H3,(H3,49,50,51,52,53,54)	-8.216
InChI=1S/C23H30N2O2/c1-2-27-22(26)23(20-10-5-3-6-11-20)14-18-25(19-15-23)17-9-16-24-2h3-8,10-13,24H,2,9,14-19H2,1H3	-4.964
InChI=1S/C4H10O4S2/c1-4(9(2,5)6)10(3,7)8/h4H,1-3H3	-1.419
InChI=1S/C9H9N/c1-7-6-8-4-2-3-5-9(8)10-7/h2-6,10H,1H3	-2.32
InChI=1S/C10H14NO5PS/c1-3-15-17(14,16-4-2)18-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3	-3.472
InChI=1S/C7H12O4/c1-4-6(8)11-5(2)7(9)10-3/h5H,4H2,1-3H3	-0.862
InChI=1S/C7H14FO2P/c1-11(8,9)10-7-5-3-2-4-6-7/h7H,2-6H2,1H3	-1.688
InChI=1S/C19H15NO6/c1-11(21)10-15(12-6-8-13(9-7-12)20(24)25)17-18(22)14-4-2-3-5-16(1h2-9,15,22H,10H2,1H3	-3.857

"InChi"	"logS(M)"
InChI=1S/C10H10F9NO4S/c1-3-6(21)24-5-4-20(2)25(22,23)10(18,19)8(13,14)7(11,12)9(15,16)17h3H,1,4-5H2,2H3	-5.309
InChI=1S/C9H8ClN5O6S3/c1-14-8(22-9(12-14)23(11,18)19)13-24(20,21)5-2-3-6(10)7(4-5)15(16)h2-4H,1H3,(H2,11,18,19)/b13-8+	-2.47
InChI=1S/C19H33O4P/c1-9-22-24(21,23-10-2)13-14-11-15(18(3,4)5)17(20)16(12-14)19(6,7)8h11-12,20H,9-10,13H2,1-8H3	-4.473
InChI=1S/C20H25BrN4O/c1-4-25(5-2)20(26)22-12-9-14-13-7-6-8-16-18(13)15(19(21)23-16)10-h6-9,12,17,23H,4-5,10-11H2,1-3H3,(H,22,26)	-4.38
InChI=1S/C14H28O/c1-2-3-4-5-6-7-8-9-10-11-12-14-13-15-14/h14H,2-13H2,1H3	-5.985
InChI=1S/C8H10O4/c1-3-6(2)12-8(11)5-4-7(9)10/h1,6H,4-5H2,2H3,(H,9,10)	0.769
InChI=1S/C17H16N2O3/c1-3-6-15-16(10(2)19-22-15)18-13-9-14(20)17(21)12-8-5-4-7-11(12)1h4-5,7-9,20H,3,6H2,1-2H3/b18-13+	-3.7
InChI=1S/C9H10N2O2/c1-7(10-12)9(11-13)8-5-3-2-4-6-8/h2-6,12-13H,1H3/b10-7+,11-9+	-2.3
InChI=1S/C22H26N2O2/c1-23-19-12-13-20(23)15-24(14-19)21(26)22(16-25,17-8-4-2-5-9-17)1h2-11,19-20,25H,12-16H2,1H3	-3.594
InChI=1S/C12H6Cl4/c13-8-3-1-2-7(4-8)9-5-11(15)12(16)6-10(9)14/h1-6H	-7.13
InChI=1S/C13H11NO3/c1-10-3-2-4-13(9-10)17-12-7-5-11(6-8-12)14(15)16/h2-9H,1H3	-4.661
InChI=1S/C27H36F2O5/c1-5-6-7-23(33)34-14-21(31)24-15(2)10-17-18-12-20(28)19-11-16(30)h8-9,11,15,17-18,20,22,24,32H,5-7,10,12-14H2,1-4H3	-5.265
InChI=1S/C12H20N2O3/c1-8(14-13)5-9-6-10(15-2)12(17-4)11(7-9)16-3/h6-8,14H,5,13H2,1-4H3	-1.725
InChI=1S/C15H15NO3/c16-15(18)13-8-4-7-12(14(13)19-10-9-17)11-5-2-1-3-6-11/h1-8,17H,9-10H2,(H2,16,18)	-1.994
InChI=1S/C22H28N2O4/c1-17(25)18-5-3-8-22(13-18)28-16-20(26)15-23-9-11-24(12-10-23)19h3-8,13-14,20,26H,9-12,15-16H2,1-2H3	-2.876
InChI=1S/C20H31NO/c22-20(18-10-4-1-5-11-18,19-12-6-2-7-13-19)14-17-21-15-8-3-9-16-2h1,4-5,10-11,19,22H,2-3,6-9,12-17H2	-5.2
InChI=1S/C11H12N2O/c1-2-4-9-8-5-3-6-10(14)11(8)13-7-12-9/h3,5-7,14H,2,4H2,1H3	-2.921
InChI=1S/C7H7BrO/c8-7-3-1-6(5-9)2-4-7/h1-4,9H,5H2	-1.929
InChI=1S/C12H14N4O3S/c1-2-16-8-7-11(14-12(16)17)15-20(18,19)10-5-3-9(13)4-6-10/h3-8H,2,13H2,1H3,(H,14,15,17)	-2.23
InChI=1S/C40H34N6O8/c1-5-51-29-17-27-31(19-25(29)45-39(49)23-13-9-7-10-14-23)53-37-3h7-20H,5-6H2,1-4H3,(H,41,47)(H,42,48)(H,45,49)(H,46,50)	-7.861

"InChi"	"logS(M)"
InChI=1S/C12H11N3O4S/c13-9-5-7-10(8-6-9)20(18,19)14-11-3-1-2-4-12(11)15(16)17/h1-8,14H,13H2	-4.49
InChI=1S/C10H11NOS/c11-4-3-7-6-13-10-2-1-8(12)5-9(7)10/h1-2,5-6,12H,3-4,11H2	-0.796
InChI=1S/C38H42N8O6S2/c1-25(45(23-47)21-31-19-41-27(3)43-35(31)39)33(15-17-51-37(49)29-5-14,19-20,23-24H,15-18,21-22H2,1-4H3,(H2,39,41,43)(H2,40,42,44)/b33-25-,34-26+	-7.431
InChI=1S/C11H17O5PS2/c1-4-14-17(18,15-5-2)16-10-6-8-11(9-7-10)19(3,12)13/h6-9H,4-5H2,1-3H3	-3.58
InChI=1S/C8H13NO2/c1-8(2)4-6(10)9(3)7(11)5-8/h4-5H2,1-3H3	-0.54
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)	0.732
InChI=1S/C4H6O4/c1-7-3(5)4(6)8-2/h1-2H3	-0.292
InChI=1S/C12H14N2O4/c1-8(11(13)16)14-10(15)7-18-12(17)9-5-3-2-4-6-9/h2-6,8H,7H2,1H3,(H2,13,16)(H,14,15)	-2.717
InChI=1S/C10H9NO2/c1-2-9(13-10(11)12)8-6-4-3-5-7-8/h1,3-7,9H,(H2,11,12)	-1.837
InChI=1S/C8H10N4O3/c1-10-6-5(12(4-13)3-9-6)7(14)11(2)8(10)15/h3,13H,4H2,1-2H3	-0.41
InChI=1S/C14H26O4/c1-3-5-11-17-13(15)9-7-8-10-14(16)18-12-6-4-2/h3-12H2,1-2H3	-3.868
InChI=1S/C17H15Br2N5O2/c1-2-23(9-3-8-20)13-6-4-12(5-7-13)21-22-17-15(18)10-14(24(25)26)1h4-7,10-11H,2-3,9H2,1H3/b22-21+	-4.381
InChI=1S/C6H5N5O/c7-4-3-5(9-2-1-8-3)11-6(12)10-4/h1-2H,(H3,7,9,10,11,12)	-3.36
InChI=1S/C11H14N4O4/c1-4-5-19-11(18)15-6-12-8-7(15)9(16)14(3)10(17)13(8)2/h6H,4-5H2,1-3H3	-1.45
InChI=1S/C6H5NO2/c8-7(9)6-4-2-1-3-5-6/h1-5H	-1.8
InChI=1S/C2H6OS/c3-1-2-4/h3-4H,1-2H2	1.107
InChI=1S/C16H16N2O3/c1-17-16(19)15(18-20-2)13-10-6-7-11-14(13)21-12-8-4-3-5-9-12/h3-11H,1-2H3,(H,17,19)/b18-15-	-3.347
InChI=1S/C14H19N3O/c1-10(2)15-13-11(3)16(4)17(14(13)18)12-8-6-5-7-9-12/h5-10,15H,1-4H3	-1.833
InChI=1S/C8H14O4/c1-3-11-7(9)5-6-8(10)12-4-2/h3-6H2,1-2H3	-0.96
InChI=1S/C15H28ClN3O2/c16-12-13-19(18-21)15(20)17-14-10-8-6-4-2-1-3-5-7-9-11-14/h14H,1-13H2,(H,17,20)	-6.335
InChI=1S/C20H19N7O3/c1-4-26(5-2)16-6-7-18(19(10-16)23-13(3)28)24-25-20-14(11-21)8-17(h6-10H,4-5H2,1-3H3,(H,23,28)/b25-24+	-8.103
InChI=1S/C21H38N2O/c1-6-7-12-18-15-20(2,3)23(21(4,5)16-18)19(24)17-22-13-10-8-9-11-1h15H,6-14,16-17H2,1-5H3	-6.662

"InChi"	"logS(M)"
InChI=1S/C15H12Cl2F4O2/c1-15(2)7(3-10(16)17)11(15)14(22)23-5-6-12(20)8(18)4-9(19)13(6)21h3-4,7,11H,5H2,1-2H3	-6.814
InChI=1S/C16H13NO2S/c1-10(16(18)19)12-7-8-14-13(9-12)17-15(20-14)11-5-3-2-4-6-11/h2-10H,1H3,(H,18,19)	-4.104
InChI=1S/C31H48O4/c1-26(2)22-9-12-31(7)24(29(22,5)11-10-23(26)33)21(32)17-19-20-18-h17,20,22-24,33H,9-16,18H2,1-8H3	-8.942
InChI=1S/C6H8O3/c1-4(7)5-2-3-9-6(5)8/h5H,2-3H2,1H3	0.398
InChI=1S/C13H10O3/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8,14-15H	-2.82
InChI=1S/C22H24N2O3/c1-26-13-2-3-16-15(8-13)22-5-6-23-11-12-4-7-27-17-10-19(25)24(16)h2-4,8,14,17-18,20-21H,5-7,9-11H2,1H3	-3.437
InChI=1S/C20H22N2O2/c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6-8-21-18-5-4-15(24-2)1h1,4-6,8,11,13-14,19-20,23H,7,9-10,12H2,2H3	-2.12
InChI=1S/C12H21N/c1-13(2)12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11H,3-8H2,1-2H3	-2.153
InChI=1S/C16H22N4O3S/c1-6-19(7-2)16(21)20-10-17-15(18-20)24(22,23)14-12(4)8-11(3)9-13(h8-10H,6-7H2,1-5H3	-5.147
InChI=1S/C10H15N5/c1-4-14(5-2)9-6-8(3)13-10-11-7-12-15(9)10/h6-7H,4-5H2,1-3H3	-2.198
InChI=1S/C6H5BrO/c7-5-2-1-3-6(8)4-5/h1-4,8H	-0.876
InChI=1S/C7H10N2O/c8-7(10)4-3-6-2-1-5-9-6/h3-4H,1-2,5H2,(H2,8,10)/b4-3+	-1.493
InChI=1S/C7H4BrClO2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H,10,11)/p-1	-1.952
InChI=1S/C36H56O13/c1-18-30(24(37)14-27(39)47-18)46-17-25-28(40)31(44-4)29(41)32(49h13,18,20-25,27-32,37,39-43H,5-12,14-17H2,1-4H3	-1.94
InChI=1S/C27H44O2/c1-18(2)8-6-9-19(3)24-13-14-25-21(10-7-15-27(24,25)5)11-12-22-16-h11-12,18-19,23-26,28-29H,4,6-10,13-17H2,1-3,5H3/b21-11+,22-12-	-10.329
InChI=1S/C12H8O4S/c13-17(14,15)8-5-6-12-10(7-8)9-3-1-2-4-11(9)16-12/h1-7H,(H,13,14,15)	-0.47
InChI=1S/C11H11Cl2NO3S/c1-6(15)14-10(11(16)17)5-18-7-2-3-8(12)9(13)4-7/h2-4,10H,5H2,1H3,(H,14,15)(H,16,17)	-2.887
InChI=1S/C19H26O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14)1h7,9,11,14-17,21H,3-6,8,10H2,1-2H3	-3.7
InChI=1S/C11H13ClO2S/c1-3-15-11(13)7-14-10-5-4-9(12)6-8(10)2/h4-6H,3,7H2,1-2H3	-5.027
InChI=1S/C16H25N3O2/c1-3-4-5-6-7-8-13-19(2)18-17-15-11-9-14(10-12-15)16(20)21/h9-12H,3-8,13H2,1-2H3,(H,20,21)/b18-17+	-3.77
InChI=1S/C6H4ClNO/c7-8-5-1-3-6(9)4-2-5/h1-4H	-1.311

"InChi"	"logS(M)"
InChI=1S/C31H54N2O8/c1-7-38-28(34)18-26(30(36)40-9-3)32-24-13-11-22(15-20(24)5)17-23-h20-27,32-33H,7-19H2,1-6H3	-5.067
InChI=1S/C13H11ClO/c14-12-8-6-11(7-9-12)13(15)10-4-2-1-3-5-10/h1-9,13,15H	-3.489
InChI=1S/C14H12N2O2S/c1-19(17,18)12-7-5-11(6-8-12)13-10-16-9-3-2-4-14(16)15-13/h2-10H,1H3	-4.178
InChI=1S/C9H10/c1-8(2)9-6-4-3-5-7-9/h3-7H,1H2,2H3	-3.008
InChI=1S/C18H16BrN3O3/c1-23-8-13-9-24-16-7-15-14(6-17(16)25-13)18(21-10-20-15)22-12-4-2h2-7,10,13H,8-9H2,1H3,(H,20,21,22)	-3.22
InChI=1S/C4H4ClNO2/c5-6-3(7)1-2-4(6)8/h1-2H2	-0.97
InChI=1S/C4H4N6/c5-3-2-4(7-1-6-3)9-10-8-2/h1H,(H3,5,6,7,8,9,10)	-0.685
InChI=1S/C20H19N3O5S/c1-3-23(4-2)13-6-5-12-9-15(20(24)28-18(12)10-13)19-22-16-11-14(29h5-11H,3-4H2,1-2H3,(H2,21,25,26)	-7.831
InChI=1S/C5H11Cl2NO/c1-8(9,4-2-6)5-3-7/h2-5H2,1H3	-1.594
InChI=1S/C4H8O2/c5-3-1-2-4-6/h1-2,5-6H,3-4H2/b2-1+	0.847
InChI=1S/C18H27NO2/c1-15-9-11-19(12-10-15)13-18(2,3)14-21-17(20)16-7-5-4-6-8-16/h4-8,15H,9-14H2,1-3H3	-4.288
InChI=1S/C10H14ClO4P/c1-3-13-16(12,14-4-2)15-10-7-5-9(11)6-8-10/h5-8H,3-4H2,1-2H3	-3.515
InChI=1S/C6H6N6/c7-4-3-5(10-2-1-9-3)12-6(8)11-4/h1-2H,(H4,7,8,10,11,12)	-2.69
InChI=1S/C2H6N2O3S2/c3-2(4)1-8-9(5,6)7/h1H2,(H3,3,4)(H,5,6,7)	0.769
InChI=1S/C8H8N4O2S2/c9-6-1-3-7(4-2-6)16(13,14)12-8-11-10-5-15-8/h1-5H,9H2,(H,11,12)	-2.868
InChI=1S/C28H31FN4O/c1-34-25-12-8-21(9-13-25)14-17-32-18-15-24(16-19-32)30-28-31-26-h2-13,24H,14-20H2,1H3,(H,30,31)	-7.224
InChI=1S/C12H16N4O2S2/c1-12(2,3)10-14-15-11(19-10)16-20(17,18)9-6-4-8(13)5-7-9/h4-7H,13H2,1-3H3,(H,15,16)	-3.74
InChI=1S/C12H18O3/c1-2-10-3-5-11(6-4-10)8-15-9-12(14)7-13/h3-6,12-14H,2,7-9H2,1H3	-2.1
InChI=1S/C9H9N3O2S2/c10-6-1-3-7(4-2-6)16(13,14)8-5-12-9(11)15-8/h1-5H,10H2,(H2,11,12)	-2.805
InChI=1S/C11H25NO3S2/c1-10(9-11(2,3)4)5-6-12-7-8-16-17(13,14)15/h10,12H,5-9H2,1-4H3,(H,13,14,15)	-2.181
InChI=1S/C6H12O4/c1-2-6(3-7,4-8)5(9)10/h7-8H,2-4H2,1H3,(H,9,10)	0.517
InChI=1S/C18H25NO2/c1-16-8-5-6-13-19(16)14-7-15-21-18(20)12-11-17-9-3-2-4-10-17/h2-4,9-12,16H,5-8,13-15H2,1H3/b12-11+	-3.981
InChI=1S/C18H19NO/c1-2-4-8(5-3-1)7-19-18-15-10-6-9-11-12(10)16(18)14(11)17(20-18)13h1-5,9-17,19H,6-7H2	-3.4

"InChi"	"logS(M)"
InChI=1S/C12H21NO3/c1-3-4-5-6-7-13-9-10(8-11(13)14)12(15)16-2/h10H,3-9H2,1-2H3	-1.246
InChI=1S/C6H9N3O2/c1-3-5-4-8(2)6(7-5)9(10)11/h4H,3H2,1-2H3	-1.971
InChI=1S/C14H22O2/c1-9(2)12(15)16-11-8-10-6-7-14(11,5)13(10,3)4/h10-11H,1,6-8H2,2-5H3	-4.544
InChI=1S/C9H19NO3/c1-3-5-9(4-2,6-11)7-13-8(10)12/h11H,3-7H2,1-2H3,(H2,10,12)	-1.735
InChI=1S/C7H4BrNS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H	-4.27
InChI=1S/C14H20N2O/c1-15(2)10-11-16-13-8-4-3-6-12(13)7-5-9-14(16)17/h3-4,6,8H,5,7,9-11H2,1-2H3	-2.22
InChI=1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)	0.268
InChI=1S/C6H10N2O3/c1-6(2)4(10)7-5(11)8(6)3-9/h9H,3H2,1-2H3,(H,7,10,11)	0.801
InChI=1S/C5H5N3O3S/c1-3(9)7-5-6-2-4(12-5)8(10)11/h2H,1H3,(H,6,7,9)	-2.067
InChI=1S/C12H19N3O/c1-9(2)15-12(16)11-6-4-10(5-7-11)8-14-13-3/h4-7,9,13-14H,8H2,1-3H3,(H,15,16)	-2.193
InChI=1S/C16H13NO6S/c1-23-16(18)15(11-12-5-3-2-4-6-12)24(21,22)14-9-7-13(8-10-14)17(1h2-11H,1H3/b15-11+	-4.57
InChI=1S/C16H22O4/c1-11(2)9-19-15(17)13-5-7-14(8-6-13)16(18)20-10-12(3)4/h5-8,11-12H,9-10H2,1-4H3	-4.741
InChI=1S/C12H13N3/c1-3-11(7-13-5-1)9-15-10-12-4-2-6-14-8-12/h1-8,15H,9-10H2	0.701
InChI=1S/C8H18O3/c1-2-3-5-10-7-8-11-6-4-9/h9H,2-8H2,1H3	0.79
InChI=1S/C10H13ClO3/c1-7-3-2-4-9(11)10(7)14-6-8(13)5-12/h2-4,8,12-13H,5-6H2,1H3	-2.533
InChI=1S/C12H5Cl5/c13-6-1-2-10(15)8(3-6)9-4-7(14)5-11(16)12(9)17/h1-5H	-7.82
InChI=1S/C34H38N4O6/c1-15-21(7-9-31(41)42)27-14-28-22(8-10-32(43)44)16(2)24(36-28)12-h11-14,19-20,37-40H,7-10H2,1-6H3,(H,41,42)(H,43,44)/b23-11-,24-12-,25-11-,26-13-,27-14-,28-14-,29-12-,30-13-	-8.083
InChI=1S/C9H8N8O2S/c1-16-3-13-6(17(18)19)8(16)20-7-4-5(12-2-11-4)14-9(10)15-7/h2-3H,1H3,(H3,10,11,12,14,15)	-2.539
InChI=1S/C30H32N2O2/c1-2-34-28(33)29(25-12-6-3-7-13-25)18-21-32(22-19-29)23-20-30(24-h3-17H,2,18-23H2,1H3	-2.753
InChI=1S/C40H76O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-24-26-28-30-32-34-36-38-40(41)h17-20H,3-16,21-39H2,1-2H3/b19-17+,20-18+	-7.071
InChI=1S/C8H7N3/c9-8-6-3-1-2-4-7(6)10-5-11-8/h1-5H,(H2,9,10,11)	-1.354
InChI=1S/C10H16N2O3/c1-11-7-2-3-8(11)6-12(5-7)9(13)4-10(14)15/h7-8H,2-6H2,1H3,(H,14,15)	-1.27
InChI=1S/C30H44O9/c1-17-26(33)23(36-3)13-25(38-17)39-19-4-9-28(16-31)21-5-8-27(2)20h12,16-17,19-23,25-26,33-35H,4-11,13-15H2,1-3H3	-3.745

"InChi"	"logS(M)"
InChI=1S/C7H15NO/c9-6-4-7-3-1-2-5-8-7/h7-9H,1-6H2/p+1	0.643
InChI=1S/C16H24ClN3O10/c1-8(21)27-7-11-13(28-9(2)22)12(18-16(24)20(19-25)6-5-17)14(29-10h11-15H,5-7H2,1-4H3,(H,18,24)	-3.08
InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h5-6H,1-4H3	-3.537
InChI=1S/C18H36O2/c1-14(12-17(3,4)5)9-10-20-16(19)11-15(2)13-18(6,7)8/h14-15H,9-13H2,1-8H3	-8.278
InChI=1S/C13H18O3/c1-3-4-11-7-10(2)5-6-13(11)16-9-12(15)8-14/h3,5-7,12,14-15H,1,4,8-9H2,2H3	-3.213
InChI=1S/C17H25NO2/c1-15-9-5-6-12-18(15)13-7-8-14-20-17(19)16-10-3-2-4-11-16/h2-4,10-11,15H,5-9,12-14H2,1H3	-3.861
InChI=1S/C13H20O/c1-4-5-8-12(14)11-7-6-9-13(2,3)10-11/h4,7H,1,5-6,8-10H2,2-3H3	-3.534
InChI=1S/C13H19NO2/c1-2-3-4-5-6-10-16-13(15)12-8-7-9-14-11-12/h7-9,11H,2-6,10H2,1H3	-2.743
InChI=1S/C14H23N3O3/c1-3-5-7-19-12-9-11(14(18)17-15)10-13(16-12)20-8-6-4-2/h9-10H,3-8,15H2,1-2H3,(H,17,18)	-3.988
InChI=1S/C36H74/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-36-34-32-30-28h3-36H2,1-2H3	-8.475
InChI=1S/C12H8N2O5/c15-13(16)9-6-7-12(11(8-9)14(17)18)19-10-4-2-1-3-5-10/h1-8H	-3.784
InChI=1S/C4H10O/c1-4(2,3)5/h5H,1-3H3	1.13
InChI=1S/C8H6ClNO2/c9-8-3-1-7(2-4-8)5-6-10(11)12/h1-6H/b6-5+	-3.014
InChI=1S/C20H24ClNO/c21-19-11-9-18(10-12-19)20(17-7-3-1-4-8-17)23-16-15-22-13-5-2-6-1h1,3-4,7-12,20H,2,5-6,13-16H2	-4.963
InChI=1S/C9H19NO3S/c11-14(12,13)8-4-7-10-9-5-2-1-3-6-9/h9-10H,1-8H2,(H,11,12,13)	-3.08
InChI=1S/C10H12N2O4S/c1-7(13)11-9-3-5-10(6-4-9)17(15,16)12-8(2)14/h3-6H,1-2H3,(H,11,13)(H,12,14)	-2.78
InChI=1S/C10H8O3/c1-12-8-4-2-7-3-5-10(11)13-9(7)6-8/h2-6H,1H3	-3.122
InChI=1S/C19H21N3O3/c1-19(2,3)13-10-12(8-9-17(23)24)11-16(18(13)25)22-20-14-6-4-5-7-1h4-7,10-11,25H,8-9H2,1-3H3,(H,23,24)	-5.531
InChI=1S/C11H16N2O4S2/c12-11(9-18-19(14,15)16)13-7-4-8-17-10-5-2-1-3-6-10/h1-3,5-6H,4,7-9H2,(H2,12,13)(H,14,15,16)	-2.521
InChI=1S/C18H16N2O/c1-10-15-9-19-7-6-13(15)11(2)18-17(10)14-8-12(21-3)4-5-16(14)20-1h4-9,20H,1-3H3	-6.268
InChI=1S/C12H11NO4S/c14-12(15)8-13-18(16,17)11-6-5-9-3-1-2-4-10(9)7-11/h1-7,13H,8H2,(H,14,15)/p-1	-2.85
InChI=1S/C5H13N3O3S2/c1-3-5(2,8-4(6)7)12-13(9,10)11/h3H2,1-2H3,(H4,6,7,8)(H,9,10,11)	0.419

"InChi"	"logS(M)"
InChI=1S/C17H23NO5/c1-4-10-18(11-5-2)16(20)12-22-17(21)14-8-6-7-9-15(14)23-13(3)19/h6-9H,4-5,10-12H2,1-3H3	-2.65
InChI=1S/C13H16N4O5/c1-3-14(4-2)13(18)9-7-11(15-5-6-15)12(17(21)22)8-10(9)16(19)20/h7-8H,3-6H2,1-2H3	-2.59
InChI=1S/C12H10O4S/c13-9-4-3-5-10(8-9)17(15,16)12-7-2-1-6-11(12)14/h1-8,13-14H	-2.29
InChI=1S/C18H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h3-17H2,1-2H3	-7.397
InChI=1S/C13H15NO6S/c1-9(2)20-12(15)13(7-8-13)21(18,19)11-5-3-10(4-6-11)14(16)17/h3-6,9H,7-8H2,1-2H3	-4.261
InChI=1S/C10H20N2O2/c1-3-5-7-9(13)11-12-10(14)8-6-4-2/h3-8H2,1-2H3,(H,11,13)(H,12,14)	-2.16
InChI=1S/C10H10N6O2/c1-15-8(13-6-9(15)16(17)18)3-2-7-4-5-12-10(11)14-7/h2-6H,1H3,(H2,11,12,14)/b3-2+	-2.112
InChI=1S/C11H23NO2/c1-3-4-5-6-7-8-9-12-11(14)10(2)13/h10,13H,3-9H2,1-2H3,(H,12,14)	-2.283
InChI=1S/C15H14N4O2/c1-18-13-12(14(20)19(2)15(18)21)16-11(17-13)9-8-10-6-4-3-5-7-10/h3-9H,1-2H3,(H,16,17)/b9-8+	-6.66
InChI=1S/C12H26O/c1-3-5-6-9-12(8-4-2)10-7-11-13/h12-13H,3-11H2,1-2H3	-5.156
InChI=1S/C8H11N3O6/c12-2-3-5(14)6(15)7(17-3)11-8(16)10-4(13)1-9-11/h1,3,5-7,12,14-15H,2H2,(H,10,13,16)	-0.471
InChI=1S/C6H12N2O/c9-7-8-5-3-1-2-4-6-8/h1-6H2	-1.001
InChI=1S/C15H12Cl2N2O3/c1-22-15(21)10-4-3-9(7-13(10)18)19-14(20)11-6-8(16)2-5-12(11)17/h2-7H,18H2,1H3,(H,19,20)	-5.79
InChI=1S/C5H13N/c1-4(2)5(3)6/h4-5H,6H2,1-3H3	0.126
InChI=1S/C9H9NO4/c10-9(13)6-3-1-2-4-7(6)14-5-8(11)12/h1-4H,5H2,(H2,10,13)(H,11,12)	-1.28
InChI=1S/C7H4ClNO4/c8-5-3-1-2-4(7(10)11)6(5)9(12)13/h1-3H,(H,10,11)	-2.63
InChI=1S/C17H18N2O5S/c18-25(22,23)15-11-12(17(20)21)10-14(19-8-4-5-9-19)16(15)24-13-6-1-3,6-7,10-11H,4-5,8-9H2,(H,20,21)(H2,18,22,23)	-5.19
InChI=1S/C12H22O5/c1-4-5-6-7-8-16-12(15)10(3)17-11(14)9(2)13/h9-10,13H,4-8H2,1-3H3	-2.488
InChI=1S/C11H8O/c12-8-10-6-3-5-9-4-1-2-7-11(9)10/h1-8H	-2.646
InChI=1S/C11H13NO3/c1-11(2,10(14)15)12-9(13)8-6-4-3-5-7-8/h3-7H,1-2H3,(H,12,13)(H,14,15)	-0.76
InChI=1S/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)	1.045
InChI=1S/C16H11NS/c1-2-6-12-11(5-1)9-10-15-16(12)17-13-7-3-4-8-14(13)18-15/h1-10,17H	-5.896

"InChi"	"logS(M)"
InChI=1S/C12H8Cl2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H	-4.8
InChI=1S/C11H11Cl2NO3S/c1-14-10(15)4-5-18(16,17)11(14)7-2-3-8(12)9(13)6-7/h2-3,6,11H,4-5H2,1H3	-1.779
InChI=1S/C12H23N5/c1-6-7-10-15-11(13-8(2)3)17-12(16-10)14-9(4)5/h8-9H,6-7H2,1-5H3,(H2,13,14,15,16,17)	-4.451
InChI=1S/C10H12N4O2/c1-5-6(2)12-8-7(11-5)9(15)14(4)10(16)13(8)3/h1-4H3	-1.343
InChI=1S/C19H23N3O/c1-3-21(4-2)13-14-22-17-11-7-5-9-15(17)19(23)20-16-10-6-8-12-18(1h5-12H,3-4,13-14H2,1-2H3,(H,20,23)	-5.778
InChI=1S/C15H19N3O4/c1-8(2)15(3)14(21)17-12(18-15)11-10(13(19)20)5-9(6-16-11)7-22-4/h5-6,8H,7H2,1-4H3,(H,19,20)(H,17,18,21)	-1.84
InChI=1S/C23H25NO3S2/c25-29(26,27)28-19-18-24-17-16-23(20-10-4-1-5-11-20,21-12-6-2-7-1h1-15,24H,16-19H2,(H,25,26,27)	-4.71
InChI=1S/C10H14O3/c1-2-3-4-7-13-10(11)9-6-5-8-12-9/h5-6,8H,2-4,7H2,1H3	-3.02
InChI=1S/C11H21N5O/c1-6-16(7-2)10-13-9(12-8(3)4)14-11(15-10)17-5/h8H,6-7H2,1-5H3,(H,12,13,14,15)	-4.889
InChI=1S/C14H12N2/c15-13-7-3-11(4-8-13)1-2-12-5-9-14(16)10-6-12/h3-10H,15-16H2	-2.433
InChI=1S/C6H5N5/c7-5-2-9-6-4(11-5)1-8-3-10-6/h1-3H,(H2,7,11)	-2.34
InChI=1S/C6H6ClNO2S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,(H2,8,9,10)	-1.581
InChI=1S/C7H14O3/c1-6(2)9-4-5-10-7(3)8/h6H,4-5H2,1-3H3	-0.166
InChI=1S/C7H10ClN3O2/c1-2-6-5-9-7(11(12)13)10(6)4-3-8/h5H,2-4H2,1H3	-2.961
InChI=1S/C19H14/c1-13-6-7-15-11-16-9-8-14-4-2-3-5-18(14)19(16)12-17(15)10-13/h2-12H,1H3	-6.644
InChI=1S/C15H10BrClN2O/c16-9-5-6-13-11(7-9)15(18-8-14(20)19-13)10-3-1-2-4-12(10)17/h1-7H,8H2,(H,19,20)	-4.567
InChI=1S/C7H15F2N2O2P/c8-2-5-11(6-3-9)14(12)10-4-1-7-13-14/h1-7H2,(H,10,12)	-1.162
InChI=1S/C4H10N2O2/c1-3-5(4-2)6(7)8/h3-4H2,1-2H3	-0.46
InChI=1S/C14H22N2O3S/c1-5-6-7-14(17)16(4)12-8-10-13(11-9-12)20(18,19)15(2)3/h8-11H,5-7H2,1-4H3	-2.85
InChI=1S/C7H8O4S/c1-5-4-6(8)2-3-7(5)12(9,10)11/h2-4,8H,1H3,(H,9,10,11)	-0.29
InChI=1S/C20H12O5/c21-11-5-7-15-17(9-11)24-18-10-12(22)6-8-16(18)20(15)14-4-2-1-3-1h1-10,21-22H	-3.823
InChI=1S/C11H16O/c1-4-11(2,3)9-7-5-6-8-10(9)12/h5-8,12H,4H2,1-3H3	-2.491

"InChi"	"logS(M)"
InChI=1S/C16H35NO4S2/c1-3-5-7-9-11-13-15-22(18,19)17-23(20,21)16-14-12-10-8-6-4-2/h17H,3-16H2,1-2H3	-3.914
InChI=1S/C12H16ClNO2/c1-2-3-6-16-11-5-4-9(7-10(11)13)8-12(14)15/h4-5,7H,2-3,6,8H2,1H3,(H2,14,15)	-3.78
InChI=1S/C14H17N5O3/c1-21-9-4-7(5-10(22-2)11(9)13(16)20)3-8-6-18-14(17)19-12(8)15/h4-6H,3H2,1-2H3,(H2,16,20)(H4,15,17,18,19)	-1.996
InChI=1S/C3H5NO/c4-2-1-3-5/h5H,1,3H2	1.148
InChI=1S/C12H2Cl8/c13-4-1-3(2-5(14)7(4)15)6-8(16)10(18)12(20)11(19)9(6)17/h1-2H	-9.7
InChI=1S/C19H18O7/c1-10-14-7-12(13-8-18(23)24-9-13)3-4-15(14)26-19(10)11(2)25-17(22h3-4,7-8,11H,5-6,9H2,1-2H3,(H,20,21)	-3.361
InChI=1S/C14H14/c1-12-7-5-6-10-14(12)11-13-8-3-2-4-9-13/h2-10H,11H2,1H3	-4.693
InChI=1S/C7H6O2/c8-6-4-2-1-3-5-7(6)9/h1-5H,(H,8,9)	-0.475
InChI=1S/C12H3Cl7/c13-6-3-8(15)7(14)1-4(6)5-2-9(16)11(18)12(19)10(5)17/h1-3H	-8.011
InChI=1S/C38H32N2/c1-29-11-9-17-37(27-29)39(33-13-5-3-6-14-33)35-23-19-31(20-24-35h3-28H,1-2H3	-6.412
InChI=1S/C7H5BrO2/c8-5-1-3-6(9)7(10)4-2-5/h1-4H,(H,9,10)	-3.563
InChI=1S/C12H19N/c1-2-3-4-5-6-11-7-9-12(13)10-8-11/h7-10H,2-6,13H2,1H3	-3.977
InChI=1S/C8H9NO2/c1-2-7-5-3-4-6-8(7)9(10)11/h3-6H,2H2,1H3	-2.799
InChI=1S/C9H19N/c1-8(2)6-5-7-9(3,4)10-8/h10H,5-7H2,1-4H3	-1.06
InChI=1S/C21H43N5O7/c1-9(25-3)13-6-5-10(22)19(31-13)32-16-11(23)7-12(24)17(14(16)27)3h9-20,25-29H,5-8,22-24H2,1-4H3	0.321
InChI=1S/C24H34N2O5/c1-3-31-24(30)19(14-13-17-9-5-4-6-10-17)25-16(2)22(27)26-20-12-8-h4-6,9-10,16,18-21,25H,3,7-8,11-15H2,1-2H3,(H,28,29)	-5.589
InChI=1S/C20H15F3N4O3/c21-8-1-2-15(13(22)3-8)27-7-12(20(29)30)17(28)9-4-14(23)19(25-18(h1-4,7,10-11,16H,5-6,24H2,(H,29,30)	-4.53
InChI=1S/C21H25NO2/c1-2-22-15-9-14-19(16-22)24-21(23)20(17-10-5-3-6-11-17)18-12-7-4-h3-8,10-13,19-20H,2,9,14-16H2,1H3	-3.996
InChI=1S/C7H6N2O5/c1-4-2-5(8(11)12)7(10)6(3-4)9(13)14/h2-3,10H,1H3	-2.588
InChI=1S/C8H11N5O2/c1-13-4-10-7-5(13)6(9-2-3-14)11-8(15)12-7/h4,14H,2-3H2,1H3,(H2,9,11,12,15)	0.08
InChI=1S/C8H18O/c1-4-5-6-8(9)7(2)3/h7-9H,4-6H2,1-3H3	-1.812
InChI=1S/C28H36N2/c1-3-7-23-21(5-1)9-17-29-25(23)19-27-11-14-28(15-12-27,16-13-27)2h1-8,25-26,29-30H,9-20H2	-9.738
InChI=1S/C6H4N2O4/c9-4-2-1-3(7-11)6(10)5(4)8-12/h1-2,9-10H	-0.508
InChI=1S/C9H7NO2S2/c11-8(12)5-13-9-10-6-3-1-2-4-7(6)14-9/h1-4H,5H2,(H,11,12)	-3.229

"InChi"	"logS(M)"
InChI=1S/C22H20/c1-2-3-6-16-9-10-18-14-19-12-11-17-7-4-5-8-21(17)22(19)15-20(18)1h4-5,7-15H,2-3,6H2,1H3	-7.52
InChI=1S/C14H14OS/c15-16(11-13-7-3-1-4-8-13)12-14-9-5-2-6-10-14/h1-10H,11-12H2/p+1	-2.859
InChI=1S/C15H12O5/c1-7-4-12(16)20-14-8(2)13-9(5-10(7)14)6-11(19-13)15(17)18-3/h4-6H,1-3H3	-5.16
InChI=1S/C10H17NO2S2/c11-9(12)13-6-8-7-14-10(15-8)4-2-1-3-5-10/h8H,1-7H2,(H2,11,12)	-3.52
InChI=1S/C10H22O/c1-10(2)8-6-4-3-5-7-9-11/h10-11H,3-9H2,1-2H3	-3.324
InChI=1S/C18H19Br2NO3/c1-23-16-6-2-14(3-7-16)18(22)24-17-8-4-15(5-9-17)21(12-10-19)13-1h2-9H,10-13H2,1H3	-6.779
InChI=1S/C17H17Cl2NO3/c1-3-22-10-23-17(21)12-6-4-5-7-14(12)20-16-13(18)9-8-11(2)15(16)1h4-9,20H,3,10H2,1-2H3	-6.666
InChI=1S/C24H33FO6/c1-21(2)30-19-9-14-13-8-16(25)15-7-12(27)5-6-22(15,3)20(13)17(28)h7,13-14,16-17,19-20,26,28H,5-6,8-11H2,1-4H3	-5.602
InChI=1S/C11H13NO4/c1-11(2)15-8-6-4-5-7(9(8)16-11)14-10(13)12-3/h4-6H,1-3H3,(H,12,13)	-2.934
InChI=1S/C10H13N5O4/c1-6(17)12-10-13-8-7(9(18)14-10)11-4-15(8)5-19-3-2-16/h4,16H,2-3,5H2,1H3,(H2,12,13,14,17,18)	-1.92
InChI=1S/C6H6N2O/c9-8-5-6-3-1-2-4-7-6/h1-5,7H/b6-5-	-1
InChI=1S/C9H16FN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h8H,1-7H2,(H,11,14)	-3.049
InChI=1S/C14H13ClO5S/c1-21(19,20)8-5-6-9(10(15)7-8)14(18)13-11(16)3-2-4-12(13)17/h5-7,13H,2-4H2,1H3	-3.299
InChI=1S/C7H6N4O/c1-4-2-8-6-5(11-4)7(12)10-3-9-6/h2-3H,1H3,(H,8,9,10,12)	-1.65
InChI=1S/C10H8F2N4O/c11-7-2-1-3-8(12)6(7)4-16-5-9(10(13)17)14-15-16/h1-3,5H,4H2,(H2,13,17)	-3.5
InChI=1S/C19H23NO3/c1-2-3-4-8-13-23-16-11-12-17(18(21)14-16)19(20-22)15-9-6-5-7-10-1h5-7,9-12,14,21-22H,2-4,8,13H2,1H3/b20-19+	-3.47
InChI=1S/C7H7NO5S3/c8-16(12,13)6-3-4-5(9)1-2-15(10,11)7(4)14-6/h3H,1-2H2,(H2,8,12,13)	-3.02
InChI=1S/C19H17N3O4S2/c23-14(9-13-5-4-8-27-13)20-15-17(24)22-16(19(25)26)12(11-28-18(1h1-2,4-8,15,18H,9-11H2,(H,20,23)(H,25,26)	-1.32
InChI=1S/C29H42O10/c1-15-22(32)23(33)24(34)25(38-15)39-17-3-8-27(14-30)19-4-7-26(2)1h11,14-15,17-20,22-25,32-36H,3-10,12-13H2,1-2H3	-3.042
InChI=1S/C10H13NO/c1-8(2)11-10(12)9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)	-2.196

"InChi"	"logS(M)"
InChI=1S/C26H27O3P/c1-16-12-18(3)23(19(4)13-16)25(27)30(29,22-10-8-7-9-11-22)26(28)2h7-15H,1-6H3	-6.622
InChI=1S/C12H8Cl2O/c13-9-4-6-11(7-5-9)15-12-3-1-2-10(14)8-12/h1-8H	-5.387
InChI=1S/C15H15NO3/c1-2-19-12-9-7-11(8-10-12)16-15(18)13-5-3-4-6-14(13)17/h3-10,17H,2H2,1H3,(H,16,18)	-3.801
InChI=1S/C15H11NO3/c17-15(13-4-2-1-3-5-13)11-8-12-6-9-14(10-7-12)16(18)19/h1-11H/b11-8+	-4.406
InChI=1S/C32H64O2/c1-3-5-7-9-11-13-15-17-18-19-20-22-24-26-28-30-32(33)34-31-29-27-h3-31H2,1-2H3	-8.983
InChI=1S/C6H9N3O3/c1-5-4-7-6(9(11)12)8(5)2-3-10/h4,10H,2-3H2,1H3	-0.994
InChI=1S/C17H15ClO4/c1-17(2,16(20)21)22-14-9-5-12(6-10-14)15(19)11-3-7-13(18)8-4-11/h3-10H,1-2H3,(H,20,21)	-4.544
InChI=1S/C6H10O/c1-3-5-6(7)4-2/h2,6-7H,3,5H2,1H3	-0.412
InChI=1S/C8H11NO2S/c1-5-8(11)7(3-10)6(4-12)2-9-5/h2,10-12H,3-4H2,1H3	-1.66
InChI=1S/C10H13BrN2O3/c1-5(2)10(4-6(3)11)7(14)12-9(16)13-8(10)15/h5H,3-4H2,1-2H3,(H2,12,13,14,15,16)	-2.564
InChI=1S/C12H5Cl5O/c13-6-1-2-11(8(15)3-6)18-12-9(16)4-7(14)5-10(12)17/h1-5H	-7.33
InChI=1S/C10H9N3O4S2/c11-6-1-3-7(4-2-6)19(16,17)13-10-12-5-8(18-10)9(14)15/h1-5H,11H2,(H,12,13)(H,14,15)	-2.874
InChI=1S/C8H17Cl/c1-3-5-6-8(4-2)7-9/h8H,3-7H2,1-2H3	-4.681
InChI=1S/C16H20N4S2/c1-15(2,7-5-9-17)13-19-11-12(21-13)20-14(22-11)16(3,4)8-6-10-18/h5-8H2,1-4H3	-5.318
InChI=1S/C10H8O2S/c11-10(12)5-7-6-13-9-4-2-1-3-8(7)9/h1-4,6H,5H2,(H,11,12)	-2.28
InChI=1S/C14H19IO3/c1-2-3-4-5-6-9-18-14(17)11-7-8-13(16)12(15)10-11/h7-8,10,16H,2-6,9H2,1H3	-4.56
InChI=1S/C27H28Br2O5S/c1-13(2)21-18(11-15(5)25(30)23(21)28)27(17-9-7-8-10-20(17)35(32,3h7-14,30-31H,1-6H3	-5.18
InChI=1S/C37H40N2O6/c1-38-14-12-24-19-32(42-4)33-21-27(24)28(38)16-22-6-9-26(10-7-22h6-11,18-21,28-29H,12-17H2,1-5H3,(H-,40,41)/p+1	-8.327
InChI=1S/C6H14O2/c1-6(2-4-7)3-5-8/h6-8H,2-5H2,1H3	0.927
InChI=1S/C8H18N2O/c1-4-8(5-2,6-3)10-7(9)11/h4-6H2,1-3H3,(H3,9,10,11)	-1.819
InChI=1S/C28H40N2O9/c1-6-7-8-9-11-20-25(39-22(32)14-16(2)3)18(5)38-28(36)23(17(4)37-2h10,12-13,15-18,20,23,25,33H,6-9,11,14H2,1-5H3,(H,29,31)(H,30,34)	-9.118

"InChi"	"logS(M)"
InChI=1S/C10H22O2/c1-7-9(3,4)11-12-10(5,6)8-2/h7-8H2,1-6H3	-4.1
InChI=1S/C10H19NO2/c1-8(2)9(12)13-7-6-11-10(3,4)5/h11H,1,6-7H2,2-5H3	-1.358
InChI=1S/C10H6O2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H	-2.374
InChI=1S/C23H34O3/c1-4-5-21(25)26-20-9-8-18-17-7-6-15-14-16(24)10-12-22(15,2)19(17)h14,17-20H,4-13H2,1-3H3	-5.93
InChI=1S/C8H13N3O4S/c1-3-16(14,15)5-4-10-7(2)9-6-8(10)11(12)13/h6H,3-5H2,1-2H3	-1.095
InChI=1S/C12H6Cl4/c13-7-5-9(12(16)11(15)6-7)8-3-1-2-4-10(8)14/h1-6H	-6.23
InChI=1S/C16H17N3O2/c1-4-19-13-9-11(21-3)8-10(2)14(13)18-16(20)12-6-5-7-17-15(12)19/h5-9H,4H2,1-3H3,(H,18,20)	-5.153
InChI=1S/C40H71NO14/c1-15-27-40(11,48)33(44)22(5)30(43)20(3)18-38(9,47)35(55-37-32(53h20-27,29,31-35,37,44-45,47-48H,15-19H2,1-14H3	-5.719
InChI=1S/C14H24O2/c1-4-13(14(15)16)12-7-5-11(6-8-12)9-10(2)3/h7,10-11,13H,4-6,8-9H2,1-3H3,(H,15,16)	-5.128
InChI=1S/C12H12N2O2/c1-9-7-14(12(16)13-11(9)15)8-10-5-3-2-4-6-10/h2-7H,8H2,1H3,(H,13,15,16)	-2.256
InChI=1S/C5H7Cl2NO2S/c6-1-4(7)11-2-3(8)5(9)10/h1,3H,2,8H2,(H,9,10)/b4-1+	-1.49
InChI=1S/C10H17NO/c1-9-4-3-5-10(2,7-6-9)8(9)11-12/h12H,3-7H2,1-2H3	-3.074
InChI=1S/C9H17N5O/c1-4-10-7-11-8(13-9(15)12-7)14(5-2)6-3/h4-6H2,1-3H3,(H2,10,11,12,13,15)	-3.64
InChI=1S/C13H13N3/c14-13(15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H,(H3,14,15,16)	-2.158
InChI=1S/C33H24Cl2N4O6/c1-44-28-10-6-5-9-25(28)36-32(42)23-15-18-7-3-4-8-21(18)29(30(23)h3-17,38H,1-2H3,(H,36,42)(H,37,41)/b39-29-	-8.175
InChI=1S/C6H12N2O/c1-7-4-3-5-8(2)6(7)9/h3-5H2,1-2H3	0.892
InChI=1S/C15H13ClO3/c16-13-8-12(9-15(17)18)6-7-14(13)19-10-11-4-2-1-3-5-11/h1-8H,9-10H2,(H,17,18)	-3.753
InChI=1S/C35H45Cl2NO6/c1-33-14-12-26(39)20-24(33)8-11-27-28-13-15-35(43,34(28,2)21-29(4h6-7,9-10,12,14,20,27-29,32,40,43H,3-5,8,11,13,15-19,21-22H2,1-2H3	-9.468
InChI=1S/C9H19NO/c1-8(2)5-7(11)6-9(3,4)10-8/h7,10-11H,5-6H2,1-4H3	-0.197
InChI=1S/C16H12O4/c1-19-12-5-2-10(3-6-12)15-9-14(18)13-7-4-11(17)8-16(13)20-15/h2-9,17H,1H3	-3.233
InChI=1S/C13H16O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10H2	-4.015
InChI=1S/C6H4N2/c7-5-6-1-3-8-4-2-6/h1-4H	-0.415

"InChi"	"logS(M)"
InChI=1S/C7H5ClN2O/c8-4-2-1-3-5-6(4)10-7(9)11-5/h1-3H,(H2,9,10)	-2.193
InChI=1S/C10H14N2O4/c1-3-4-10(5-6(2)13)7(14)11-9(16)12-8(10)15/h3,6,13H,1,4-5H2,2H3,(H2,11,12,14,15,16)	-0.808
InChI=1S/C18H19Br2NO2/c1-14-4-2-3-5-17(14)18(22)23-16-8-6-15(7-9-16)21(12-10-19)13-11-2h2-9H,10-13H2,1H3	-7.06
InChI=1S/C9H8N2O3S/c10-7-3-4-8(15(12,13)14)9-6(7)2-1-5-11-9/h1-5H,10H2,(H,12,13,14)	-2.71
InChI=1S/C20H20FNO3/c1-12-18(23)15-9-10-17(24-4)16(11-22(2)3)20(15)25-19(12)13-5-7-14h5-10H,11H2,1-4H3	-4.173
InChI=1S/C8H8O4/c1-4-2-5(9)7(8(11)12)6(10)3-4/h2-3,9-10H,1H3,(H,11,12)	-2.05
InChI=1S/C15H13N3O4S/c1-18-13(15(20)17-12-8-4-5-9-16-12)14(19)10-6-2-3-7-11(10)23(18,2h2-9,20H,1H3,(H,16,17)/b15-13+	-4.159
InChI=1S/C22H42N4O8S2/c1-21(2,13-27)17(31)19(33)25-7-5-15(29)23-9-11-35-36-12-10-24-16(h17-18,27-28,31-32H,5-14H2,1-4H3,(H,23,29)(H,24,30)(H,25,33)(H,26,34)	-0.991
InChI=1S/C13H17N3O3S2/c14-13(9-20-21(17,18)19)15-7-3-4-10-8-16-12-6-2-1-5-11(10)12/h1-2,5-6,8,16H,3-4,7,9H2,(H2,14,15)(H,17,18,19)	-3.14
InChI=1S/C12H24O6/c1-7-10(4)13-15-11(5,8-2)17-18-12(6,9-3)16-14-10/h7-9H2,1-6H3	-4.305
InChI=1S/C20H23NO5/c1-2-24-20(23)15-9-21-16-8-18(26-11-13-5-6-13)17(7-14(16)19(15)22h7-9,12-13H,2-6,10-11H2,1H3,(H,21,22)	-8.094
InChI=1S/C13H19N5O/c14-13-16-9-11(19-13)10-17-5-7-18(8-6-17)12-3-1-2-4-15-12/h1-4,11H,5-10H2,(H2,14,16)	-1.516
InChI=1S/C11H17NO/c1-4-9-5-6-11(13)10(7-9)8-12(2)3/h5-7,13H,4,8H2,1-3H3	-0.89
InChI=1S/C13H17NO/c1-4-8-13(15)14(5-2)12-10-7-6-9-11(12)3/h4,6-10H,5H2,1-3H3/b8-4+	-2.568
InChI=1S/C10H16ClN5O2/c1-4-18-7(17)5-12-9-14-8(11)15-10(16-9)13-6(2)3/h6H,4-5H2,1-3H3,(H2,12,13,14,15,16)	-2.562
InChI=1S/C9H12N4O2/c1-5-10-7-6(11(5)2)8(14)13(4)9(15)12(7)3/h1-4H3	-1.449
InChI=1S/C11H24O3/c1-3-5-6-10(4-2)8-14-9-11(13)7-12/h10-13H,3-9H2,1-2H3	-2.055
InChI=1S/C6H14N2O/c1-4-6(2,3)8-5(7)9/h4H2,1-3H3,(H3,7,8,9)	-1.014
InChI=1S/C6H3N5/c7-1-4-5-6(10-2-8-4)11-3-9-5/h2-3H,(H,8,9,10,11)	-0.958
InChI=1S/C10H18N4O/c1-4-6-7-15-10-13-8(3)12-9(14-10)11-5-2/h4-7H2,1-3H3,(H,11,12,13,14)	-3.957
InChI=1S/C8H11N/c1-9-7-8-5-3-2-4-6-8/h2-6,9H,7H2,1H3	0.917

"InChi"	"logS(M)"
InChI=1S/C23H32O4/c1-14(24)23(27-15(2)25)12-9-20-18-6-5-16-13-17(26)7-10-21(16,3)19h13,18-20H,5-12H2,1-4H3	-5.567
InChI=1S/C6H11NO2/c1-6(8)7-2-4-9-5-3-7/h2-5H2,1H3	0.889
InChI=1S/C19H22N2/c1-16-7-9-17(10-8-16)18(19-6-2-3-12-20-19)11-15-21-13-4-5-14-21/h2-3,6-12H,4-5,13-15H2,1H3/b18-11-	-3.57
InChI=1S/C9H8O2S/c1-7-6-12(10,11)9-5-3-2-4-8(7)9/h2-6H,1H3	-2.67
InChI=1S/C14H10N2O2/c15-9-5-6-10(16)12-11(9)13(17)7-3-1-2-4-8(7)14(12)18/h1-6H,15-16H2	-5.859
InChI=1S/C7H4Cl4O2/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h12H,1H3	-4.02
InChI=1S/C15H16N2/c1-16-11-12-7-3-4-8-13(12)17(2)15-10-6-5-9-14(15)16/h3-10H,11H2,1-2H3	-5.729
InChI=1S/C16H17F3N6O6S/c1-8-5-4-6-9(11(26)27)10(8)32(29,30)24-14(28)21-12-20-13(25(2)3)2h4-6H,7H2,1-3H3,(H,26,27)(H2,20,21,22,23,24,28)	-5.68
InChI=1S/C7H17N/c1-4-6(2)5-7(3)8/h6-7H,4-5,8H2,1-3H3	-0.88
InChI=1S/C11H12N2O4/c12-9(14)6-13-10(15)7-17-11(16)8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,12,14)(H,13,15)	-1.498
InChI=1S/C14H14ClNO2/c1-9-7-11(8-14(17)18)10(2)16(9)13-5-3-12(15)4-6-13/h3-7H,8H2,1-2H3,(H,17,18)	-3.989
InChI=1S/C17H22ClN3O/c1-16(2)8-7-14(9-13-3-5-15(18)6-4-13)17(16,22)10-21-12-19-11-20-2h3-6,11-12,14,22H,7-10H2,1-2H3	-4.329
InChI=1S/C19H18N4/c20-16-7-9-17(10-8-16)22-19(21)23-11-14-5-1-3-13-4-2-6-15(12-23)1h1-10H,11-12,20H2,(H2,21,22)	-1.83
InChI=1S/C12H11Cl2N3O2/c13-9-1-2-10(11(14)5-9)12(18-3-4-19-12)6-17-8-15-7-16-17/h1-2,5,7-8H,3-4,6H2	-3.003
InChI=1S/C10H10O3/c1-2-8(11)7-3-4-9-10(5-7)13-6-12-9/h3-5H,2,6H2,1H3	-2.403
InChI=1S/C17H22BrNO3/c1-19-13-6-7-14(19)9-15(8-13)22-17(21)16(10-20)11-2-4-12(18)5-3-1h2-5,13-16,20H,6-10H2,1H3	-3.267
InChI=1S/C8H13Br3O2/c1-3-6(4-2)7(12)13-5-8(9,10)11/h6H,3-5H2,1-2H3	-5.717
InChI=1S/C10H14/c1-8(2)10-6-4-9(3)5-7-10/h4-8H,1-3H3	-3.77
InChI=1S/C17H23N/c1-18-11-10-17-9-5-4-8-15(17)16(18)12-13-6-2-3-7-14(13)17/h2-3,6-7,15-16H,4-5,8-12H2,1H3	-3.272
InChI=1S/C3H6N6/c4-1-7-2(5)9-3(6)8-1/h(H6,4,5,6,7,8,9)	-1.559
InChI=1S/C6H12N2O5/c7-3(1-9)5(11)8-4(2-10)6(12)13/h3-4,9-10H,1-2,7H2,(H,8,11)(H,12,13)	-0.585
InChI=1S/C13H24O3/c1-8(2)11-6-5-9(3)7-12(11)16-13(15)10(4)14/h8-12,14H,5-7H2,1-4H3	-2.98

"InChi"	"logS(M)"
InChI=1S/C18H12O2/c1-20-16-10-9-12-11-5-2-3-6-13(11)18(19)15-8-4-7-14(16)17(12)15/h2-10H,1H3	-6.315
InChI=1S/C10H21NO/c1-9(2)4-8(12)5-10(3,6-9)7-11/h8,12H,4-7,11H2,1-3H3	0.489
InChI=1S/C19H19N3O5S/c1-9-11(12(21-27-9)10-7-5-4-6-8-10)15(23)20-13-16(24)22-14(18(25)h4-8,13-14,17H,1-3H3,(H,20,23)(H,25,26)	-4.159
InChI=1S/C7H12O2/c1-4-6(3)7(8)9-5-2/h4,6H,1,5H2,2-3H3	-1.576
InChI=1S/C16H9N5O6/c22-11-7(12(23)19-15(26)18-11)9-5-3-1-2-4-6(5)10(17-9)8-13(24)20-h1-4,17H,(H2,18,19,22,23,26)(H2,20,21,24,25,27)	-7.565
InChI=1S/C5H9O3P/c1-5-2-6-9(7-3-5)8-4-5/h2-4H2,1H3	0.08
InChI=1S/C12H4Cl4O2/c13-7-8(14)10(16)12-11(9(7)15)17-5-3-1-2-4-6(5)18-12/h1-4H	-8.77
InChI=1S/C16H12FN3O3/c1-23-16(22)20-15-18-12-7-4-10(8-13(12)19-15)14(21)9-2-5-11(17)6-h2-8H,1H3,(H2,18,19,20,22)	-5.244
InChI=1S/C7H9NO4S3/c8-15(11,12)6-4-5-2-1-3-14(9,10)7(5)13-6/h4H,1-3H2,(H2,8,11,12)	-2.68
InChI=1S/C14H18O5/c1-2-3-4-7-10-18-14(17)19-12-9-6-5-8-11(12)13(15)16/h5-6,8-9H,2-4,7,10H2,1H3,(H,15,16)	-3.817
InChI=1S/C12H18N2/c1-2-8-14(9-3-1)10-6-12-5-4-7-13-11-12/h4-5,7,11H,1-3,6,8-10H2	0.301
InChI=1S/C22H46O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h23H,2-22H2,1H3	-5.514
InChI=1S/C6H6O4S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4,7H,(H,8,9,10)	0.759
InChI=1S/C11H14N2O2/c1-2-9(10(14)13-11(12)15)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3,(H3,12,13,14,15)	-2.761
InChI=1S/C14H8O4/c15-7-1-3-9-11(5-7)14(18)10-4-2-8(16)6-12(10)13(9)17/h1-6,15-16H	-5.889
InChI=1S/C8H12ClN3O6/c9-3-4-12(11-18)8(17)10-5(7(15)16)1-2-6(13)14/h5H,1-4H2,(H,10,17)(H,13,14)(H,15,16)	-1.767
InChI=1S/C5H15N2O3PS/c6-2-4-7-3-1-5-12-11(8,9)10/h7H,1-6H2,(H2,8,9,10)	0.669
InChI=1S/C3H7NO3/c4-1-2(5)3(6)7/h2,5H,1,4H2,(H,6,7)	-0.823
InChI=1S/C8H7N5O6S3/c9-21(16,17)8-11-10-7(20-8)12-22(18,19)6-3-1-2-5(4-6)13(14)15/h1-4H,(H,10,12)(H2,9,16,17)	-1.46
InChI=1S/C18H24N2O2/c1-19-13-12-14-6-2-4-8-16(14)18(19)11-10-15-7-3-5-9-17(15)20(21)2h3,5,7,9,18H,2,4,6,8,10-13H2,1H3	-5.222
InChI=1S/C14H14N2O5S/c17-13(15-9-14(18)19)8-16-22(20,21)12-6-5-10-3-1-2-4-11(10)7-12/h1-7,16H,8-9H2,(H,15,17)(H,18,19)	-2.695
InChI=1S/C12H18O/c1-11(9-10-13)7-8-12-5-3-2-4-6-12/h2-6,11,13H,7-10H2,1H3	-2.66

"InChi"	"logS(M)"
InChI=1S/C10H20O2/c1-3-5-6-8-9(7-4-2)10(11)12/h9H,3-8H2,1-2H3,(H,11,12)	-2.796
InChI=1S/C13H18N2O2/c16-13(11-15-6-8-17-9-7-15)14-10-12-4-2-1-3-5-12/h1-5H,6-11H2,(H,14,16)	-1.482
InChI=1S/C13H11N3O2/c17-13(16-18)11-6-1-2-7-12(11)15-9-10-5-3-4-8-14-10/h1-9,18H,(H,16,17)/b15-9+	-3.21
InChI=1S/C11H15NO/c1-12(2)9-8-11(13)10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3	-0.658
InChI=1S/C18H26O2/c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(18)20/h14-17,20H,2-10H2,1H3	-4.947
InChI=1S/C11H13NO2/c1-3-8-14-11-6-4-10(5-7-11)12-9(2)13/h3-7H,1,8H2,2H3,(H,12,13)	-2.327
InChI=1S/C7H9BrN2O2/c1-4-5(8)6(11)10(3)7(12)9(4)2/h1-3H3	-1.322
InChI=1S/C4H5Br3O2/c1-2-9-3(8)4(5,6)7/h2H2,1H3	-3.694
InChI=1S/C15H14N2O/c18-14-15(17-11-16-14,12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10,17H,11H2,(H,16,18)	-2.853
InChI=1S/C7H5Cl3O/c1-11-5-3-2-4(8)6(9)7(5)10/h2-3H,1H3	-4.292
InChI=1S/CH3ClO9S3/c2-1(12(3,4)5,13(6,7)8)14(9,10)11/h(H,3,4,5)(H,6,7,8)(H,9,10,11)	0.537
InChI=1S/C11H15Cl2N/c12-6-8-14(9-7-13)10-11-4-2-1-3-5-11/h1-5H,6-10H2	-2.65
InChI=1S/C7H13O5PS/c1-6(7(8)9-2)5-12-13(14,10-3)11-4/h5H,1-4H3/b6-5+	-2.779
InChI=1S/C5H3BrO2/c6-5-2-1-4(3-7)8-5/h1-3H	-1.544
InChI=1S/C6H12O2/c1-3-5-8-6(7)4-2/h3-5H2,1-2H3	-0.82
InChI=1S/C13H17F3N4O4/c1-3-5-18(6-4-2)11-9(19(21)22)7-8(13(14,15)16)10(17)12(11)20(23)24h7H,3-6,17H2,1-2H3	-7.07
InChI=1S/C9H10O3/c1-11-8-4-3-7(6-10)5-9(8)12-2/h3-6H,1-2H3	-1.42
InChI=1S/C8H10O2/c9-5-7-1-2-8(6-10)4-3-7/h1-4,9-10H,5-6H2	-0.386
InChI=1S/C19H26N2O/c1-3-19(22)21-17-9-10-18(21)14-20(13-17)12-15(2)11-16-7-5-4-6-8-16h4-8,11,17-18H,3,9-10,12-14H2,1-2H3/b15-11+	-4.224
InChI=1S/C13H16O2/c14-12(11-7-3-1-4-8-11)13(15)9-5-2-6-10-13/h1,3-4,7-8,15H,2,5-6,9-10H2	-2.665
InChI=1S/C18H18N2O/c1-12(2)20-16-11-13(3)9-10-15(16)17(19-18(20)21)14-7-5-4-6-8-14/h4-12H,1-3H3	-4.115
InChI=1S/C16H22N2O5S2/c1-12-10-16(18-15-5-4-13(22-2)11-14(12)15)23-8-3-6-17-7-9-24-25(1h4-5,10-11,17H,3,6-9H2,1-2H3,(H,19,20,21)	-2.684
InChI=1S/C11H22O/c1-3-4-5-6-7-8-9-11(2)10-12/h10-11H,3-9H2,1-2H3	-4.027
InChI=1S/C7H13ClN2O2/c1-3-7(8,4-2)5(11)10-6(9)12/h3-4H2,1-2H3,(H3,9,10,11,12)	-1.802
InChI=1S/C6H6N4O/c11-2-5-9-4-1-7-3-8-6(4)10-5/h1,3,11H,2H2,(H,7,8,9,10)	-1.52

"InChi"	"logS(M)"
InChI=1S/C15H24N4O4/c1-3-5-9-18(10-6-4-2)12-14(20)17-16-11-13-7-8-15(23-13)19(21)22/h7-8,11H,3-6,9-10,12H2,1-2H3,(H,17,20)/b16-11+	-4.193
InChI=1S/C6H8N2O3S/c7-8-5-2-1-3-6(4-5)12(9,10)11/h1-4,8H,7H2,(H,9,10,11)	-0.828
InChI=1S/C12H18O/c1-3-6-10-8-5-9-11(7-4-2)12(10)13/h5,8-9,13H,3-4,6-7H2,1-2H3	-3.313
InChI=1S/C17H36O6/c1-3-5-7-18-9-11-20-13-15-22-17-23-16-14-21-12-10-19-8-6-4-2/h3-17H2,1-2H3	-1.302
InChI=1S/C14H12N2/c1-2-6-11(7-3-1)10-14-15-12-8-4-5-9-13(12)16-14/h1-9H,10H2,(H,15,16)	-4.801
InChI=1S/C7H5FN2O/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3H,(H2,9,10)	-1.694
InChI=1S/C14H18N4O3S/c1-2-3-9-18-10-8-13(16-14(18)19)17-22(20,21)12-6-4-11(15)5-7-12/h4-8,10H,2-3,9,15H2,1H3,(H,16,17,19)	-3.09
InChI=1S/C7H16O2/c1-3-4-5-9-6-7(2)8/h7-8H,3-6H2,1-2H3	-0.405
InChI=1S/C16H20N2O3/c1-9(2)16(4)15(20)17-13(18-16)12-8-10(3)6-7-11(12)14(19)21-5/h6-9H,1-5H3,(H,17,18,20)	-2.46
InChI=1S/C30H31ClN4O7S/c1-6-35(7-2)43(38,39)19-12-13-25(40-3)24(15-19)33-34-28-20-11-9-8h8-17,33H,6-7H2,1-5H3,(H,32,37)/b34-28-	-7.905
InChI=1S/C10H13N3O2/c1-6-3-2-4-8-12-5-7(9(11)14)10(15)13(6)8/h5-6H,2-4H2,1H3,(H2,11,14)	-2.057
InChI=1S/C19H30N2O/c1-18(2)12-9-13-19(3,4)21(18)17(22)15-20(5)14-16-10-7-6-8-11-16/h6-8,10-11H,9,12-15H2,1-5H3	-4.764
InChI=1S/C20H34O8/c1-5-8-11-25-17(22)14-20(28-16(4)21,19(24)27-13-10-7-3)15-18(23)2h5-15H2,1-4H3	-4.906
InChI=1S/C7H7NO3/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3,9H,8H2,(H,10,11)	-1.957
InChI=1S/C16H10ClNO2/c17-13-14(18-10-6-2-1-3-7-10)16(20)12-9-5-4-8-11(12)15(13)19/h1-9,18H	-4.873
InChI=1S/C3HBr3O2/c4-1(2(5)6)3(7)8/h(H,7,8)	-1.359
InChI=1S/C16H27N3O3/c1-5-7-9-21-14-11-13(16(20)19(4)17-3)12-15(18-14)22-10-8-6-2/h11-12,17H,5-10H2,1-4H3	-4.426
InChI=1S/C18H17NO3/c1-21-17-12-11-15-9-5-6-10-16(15)19(17)18(20)22-13-14-7-3-2-4-8-1h2-12,17H,13H2,1H3	-5.306
InChI=1S/C20H23NO4/c1-11(22)24-16-7-5-13-14-10-12-4-6-15(23-3)18-17(12)20(13,19(16)2h4-7,13-14,16,19H,8-10H2,1-3H3	-1.3
InChI=1S/C13H15N3O3S/c1-19-13-7-4-10(15)8-12(13)16-20(17,18)11-5-2-9(14)3-6-11/h2-8,16H,14-15H2,1H3	-5.08
InChI=1S/C12H4Cl6/c13-5-1-10(17)12(11(18)2-5)6-3-8(15)9(16)4-7(6)14/h1-4H	-8.12

"InChi"	"logS(M)"
InChI=1S/C14H15NO8/c16-8-5-3-1-4-13(23-2-22-4)9(17)6(3)14(21)15-7(5)10(18)12(20)11(8)h1,5,7-8,10-12,16-20H,2H2,(H,15,21)	-3.8
InChI=1S/C13H9Cl2NO/c14-8-5-6-12(16)10(7-8)13(17)9-3-1-2-4-11(9)15/h1-7H,16H2	-7.425
InChI=1S/C10H7NO2/c12-10-8-4-2-1-3-7(8)5-6-9(10)11-13/h1-6,12H	-2.539
InChI=1S/C13H26O4/c1-4-6-8-15-10-13(17-12(3)14)11-16-9-7-5-2/h13H,4-11H2,1-3H3	-3.302
InChI=1S/C32H62O2/c1-3-5-7-9-11-13-15-17-18-19-20-22-24-26-28-30-32(33)34-31-29-27-h17-18H,3-16,19-31H2,1-2H3/b18-17+	-6.981
InChI=1S/C14H19NO4/c1-3-9-19-12-7-5-11(6-8-14(16)15-17)10-13(12)18-4-2/h5-8,10,17H,3-4,9H2,1-2H3,(H,15,16)/b8-6+	-3.14
InChI=1S/C15H14BrNO4S/c16-12-6-8-13(9-7-12)22(20,21)17-14(15(18)19)10-11-4-2-1-3-5-11/h1-9,14,17H,10H2,(H,18,19)	-4.258
InChI=1S/C13H21N3O/c1-3-16(4-2)10-9-15-13(17)11-5-7-12(14)8-6-11/h5-8H,3-4,9-10,14H2,1-2H3,(H,15,17)	-1.669
InChI=1S/C11H15BrClO3PS/c1-3-7-18-17(14,15-4-2)16-11-6-5-9(12)8-10(11)13/h5-6,8H,3-4,7H2,1-2H3	-4.366
InChI=1S/C3H5ClO/c1-3(5)2-4/h2H2,1H3	-0.012
InChI=1S/C14H13NO2/c1-17-13-11(10-6-3-2-4-7-10)8-5-9-12(13)14(15)16/h2-9H,1H3,(H2,15,16)	-2.608
InChI=1S/C24H25NO3/c1-16(2)13-20-22(24(20,3)4)23(26)28-21(15-25)17-9-8-12-19(14-17)2h5-14,20-22H,1-4H3	-7.575
InChI=1S/C8H4N2O/c9-5-7(6-10)4-8-2-1-3-11-8/h1-4H	-1.714
InChI=1S/C10H13FN6O6S/c11-10(1-22-24(13,20)21)6(19)5(18)9(23-10)17-3-16-4-7(12)14-2-15-h2-3,5-6,9,18-19H,1H2,(H2,12,14,15)(H2,13,20,21)	-1.587
InChI=1S/C18H21NO4/c1-19-8-7-17-14-10-3-4-12(22-2)15(14)23-16(17)11(20)5-6-18(17,21)h3-4,13,16,21H,5-9H2,1-2H3	-1.88
InChI=1S/C27H35NO3/c1-29-21-9-8-20-17-24-22-6-4-5-12-27(22,23(20)18-21)13-15-28(24)1h7-10,16,18,22,24H,4-6,11-15,17H2,1-3H3	-6.038
InChI=1S/C24H34Br4O4/c1-5-9-11-15(7-3)13-31-23(29)17-18(20(26)22(28)21(27)19(17)25)24(h15-16H,5-14H2,1-4H3	-5.949
InChI=1S/C7H5NO4/c9-6(10)4-2-1-3-8-5(4)7(11)12/h1-3H,(H,9,10)(H,11,12)	-1.48
InChI=1S/C20H14O4/c21-19(15-8-3-1-4-9-15)23-17-12-7-13-18(14-17)24-20(22)16-10-5-2-h1-14H	-5.601
InChI=1S/C15H19N3O3/c1-11-13(16(2)3)14(20)17(9-10-19)15(21)18(11)12-7-5-4-6-8-12/h4-8,19H,9-10H2,1-3H3	-2.574

"InChi"	"logS(M)"
InChI=1S/C7H6FNO/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H2,9,10)	-0.994
InChI=1S/C5H11N3O/c6-1-3-8-4-2-7-5(8)9/h1-4,6H2,(H,7,9)	0.634
InChI=1S/C10H9BrO4/c1-13-7-3-6(11)5-4-15-10(12)8(5)9(7)14-2/h3H,4H2,1-2H3	-3.931
InChI=1S/C10H11NO2/c1-8(12)7-10(13)11-9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,11,13)	-1.299
InChI=1S/C42H56N6O6/c1-4-28(2)36-42(54)48-24-14-12-21-34(48)40(52)47-23-13-11-20-33(4h5-10,16-19,28,31-36H,4,11-15,20-27H2,1-3H3,(H,43,50)(H,44,49)	-5.57
InChI=1S/C3H6I2O/c4-1-3(6)2-5/h3,6H,1-2H2	-1.397
InChI=1S/C7H5BrO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)	-2.699
InChI=1S/C12H12ClN5O4S/c1-7-14-10(17-12(15-7)22-2)16-11(19)18-23(20,21)9-6-4-3-5-8(9)13/h3-6H,1-2H3,(H2,14,15,16,17,18,19)	-1.71
InChI=1S/C23H28N2O2S/c1-17(26)18-8-9-23-21(16-18)25(20-6-3-4-7-22(20)28-23)13-5-12-24-h3-4,6-9,16,19H,5,10-15H2,1-2H3	-6.26
InChI=1S/C12H12N2/c1-3-7-13-9-10-14-8-4-2-6-12(14)11(13)5-1/h1-8H,9-10H2/q+2	-3.425
InChI=1S/C9H6N2/c10-6-5-8-3-1-2-4-9(8)7-11/h1-4H,5H2	-1.451
InChI=1S/C26H14N2O4/c1-27-23(29)15-7-3-11-13-5-9-17-22-18(26(32)28(2)25(17)31)10-6-14h3-10H,1-2H3	-7.719
InChI=1S/C21H20Br4O4/c1-21(2,11-3-15(22)19(16(23)4-11)28-9-13-7-26-13)12-5-17(24)20(18h3-6,13-14H,7-10H2,1-2H3	-7.395
InChI=1S/C9H7N5O/c15-8(7-6-10-4-5-11-7)14-9-12-2-1-3-13-9/h1-6H,(H,12,13,14,15)	-0.304
InChI=1S/C15H17Cl2N3O/c1-15(2,3)14(21)13(20-9-18-8-19-20)6-10-4-5-11(16)7-12(10)17/h4-9,14,21H,1-3H3/b13-6-	-4.912
InChI=1S/C6H10O2/c1-3-6(8)4-5(2)7/h3-4H2,1-2H3	-0.499
InChI=1S/C12H11NO4/c14-10-6-9(8-4-2-1-3-5-8)7-11(15)12(10)13(16)17/h1-5,9,12H,6-7H2	-1.669
InChI=1S/C9H15NO2/c1-3-9(4-2)7(11)5-6-10-8(9)12/h3-6H2,1-2H3,(H,10,12)	-1.48
InChI=1S/C10H9NO/c1-7(12)8-2-3-10-9(6-8)4-5-11-10/h2-6,11H,1H3	-1.844
InChI=1S/C13H11N3O3/c1-9-6-7-13(17)11(8-9)15-14-10-4-2-3-5-12(10)16(18)19/h2-8,14H,1H3/b15-11+	-5.748
InChI=1S/C8H7ClN2O3/c1-5(12)10-7-4-6(9)2-3-8(7)11(13)14/h2-4H,1H3,(H,10,12)	-0.99
InChI=1S/C20H31NO3/c1-3-4-15-23-19-11-9-18(10-12-19)20(22)24-16-7-14-21-13-6-5-8-17(h9-12,17H,3-8,13-16H2,1-2H3	-5.193
InChI=1S/C2H2Cl2F2/c3-1-2(4,5)6/h1H2	-2.201
InChI=1S/C12H7Cl3O/c13-10-6-9(7-11(14)12(10)15)16-8-4-2-1-3-5-8/h1-7H	-6.77

"InChi"	"logS(M)"
InChI=1S/C46H56N4O9/c1-8-42-16-12-18-50-20-17-44(37(42)50)30-21-31(34(55-5)22-33(30)4h10-14,16,21-22,27,36-39,47,54H,8-9,15,17-20,23-25H2,1-7H3	-8.029
InChI=1S/C10H16N4O7/c11-7-6(8(19)14-10(12)13-7)21-9-5(18)4(17)3(16)2(1-15)20-9/h2-5,9,15-18H,1H2,(H5,11,12,13,14,19)	-1.483
InChI=1S/C7H5ClN2O/c8-4-1-2-6-5(3-4)10-7(9)11-6/h1-3H,(H2,9,10)	-2.532
InChI=1S/C7H10/c1-2-7-4-3-6(1)5-7/h1-2,6-7H,3-5H2	-2.848
InChI=1S/C21H14N2O4/c24-18-9-10-19(25)22(18)16-5-1-14(2-6-16)13-15-3-7-17(8-4-15)23-2h1-12H,13H2	-5.998
InChI=1S/C6H4I2/c7-5-3-1-2-4-6(5)8/h1-4H	-4.217
InChI=1S/C14H31N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h2-15H2,1H3	-5.19
InChI=1S/C14H20N4O4/c1-4-5-6-7-8-22-14(21)18-9-15-11-10(18)12(19)17(3)13(20)16(11)2/h9H,4-8H2,1-3H3	-3
InChI=1S/C6H4N2O5/c9-6-3-4(7(10)11)1-2-5(6)8(12)13/h1-3,9H	-2.68
InChI=1S/C14H15O2PS2/c1-2-16-17(15,18-13-9-5-3-6-10-13)19-14-11-7-4-8-12-14/h3-12H,2H2,1H3	-3.33
InChI=1S/C18H36O2/c1-4-7-9-11-13-15-17(18(19)20-6-3)16-14-12-10-8-5-2/h17H,4-16H2,1-3H3	-7.822
InChI=1S/C21H17N3O2S2/c22-18-10-12-19(13-11-18)28(25,26)24-21-23-20(14-27-21)17-8-6-16h1-14H,22H2,(H,23,24)	-5.61
InChI=1S/C6H10O4/c1-3(5(7)8)4(2)6(9)10/h3-4H,1-2H3,(H,7,8)(H,9,10)/p-2	-0.688
InChI=1S/C21H26O3/c1-2-3-4-5-6-10-15-24-18-13-14-19(20(22)16-18)21(23)17-11-8-7-9-1h7-9,11-14,16,22H,2-6,10,15H2,1H3	-5.514
InChI=1S/C16H16O3/c17-15-11-5-4-10-14(15)16(18)19-12-6-9-13-7-2-1-3-8-13/h1-5,7-8,10-11,17H,6,9,12H2	-5.011
InChI=1S/C19H12O8/c1-8(20)26-13-5-3-4-11-15(13)18(23)16-12(17(11)22)6-10(19(24)25)7h3-7H,1-2H3,(H,24,25)	-3.659
InChI=1S/C6H14O/c1-5-6(2,3)7-4/h5H2,1-4H3	-0.98
InChI=1S/C15H14N2/c1-9-7-10(2)15-12(8-9)14(16)11-5-3-4-6-13(11)17-15/h3-8H,1-2H3,(H2,16,17)	-4.917
InChI=1S/C9H10N2O3/c1-10-5-8-4-9(11(12)13)3-2-7(8)6-14-10/h2-4H,5-6H2,1H3	-2.497
InChI=1S/C26H34O7/c1-18(2)13-14-20-25(3,33-20)24-23(30-4)19(15-16-26(24)17-31-26)32h5-13,19-20,23-24H,14-17H2,1-4H3,(H,27,28)/b7-5+,8-6+,11-9+,12-10+	-6.254
InChI=1S/C9H17NO2/c10-7-9(6-8(11)12)4-2-1-3-5-9/h1-7,10H2,(H,11,12)	-1.581

"InChi"	"logS(M)"
InChI=1S/C16H21N3O2/c1-5-11(2)17-14-12(3)18(4)16(21)19(15(14)20)13-9-7-6-8-10-13/h6-11,17H,5H2,1-4H3	-2.572
InChI=1S/C21H24O4/c1-20(2,24)18(22)16-9-5-14(6-10-16)13-15-7-11-17(12-8-15)19(23)21h5-12,24-25H,13H2,1-4H3	-4.536
InChI=1S/C12H20O4/c1-2-3-4-5-6-7-8-10(12(15)16)9-11(13)14/h6-7,10H,2-5,8-9H2,1H3,(H,13,14)(H,15,16)/b7-6+	-2.404
InChI=1S/C14H16N2/c1-3-14(2)15-11-8-4-6-10-7-5-9-12(16-14)13(10)11/h4-9,15-16H,3H2,1-2H3	-3.248
InChI=1S/C6H3Cl2NO2/c7-4-1-2-6(9(10)11)5(8)3-4/h1-3H	-3.009
InChI=1S/C9H14N2O3/c1-3-5-9(4-2)6(12)10-8(14)11-7(9)13/h3-5H2,1-2H3,(H2,10,11,12,13,14)	-1.49
InChI=1S/C20H20ClN3O/c21-16-8-5-14(6-9-16)17-10-7-15-3-1-2-4-18(15)24(20(17)25)13-19-2h1-6,8-9,17H,7,10-13H2,(H,22,23)	-5.103
InChI=1S/C10H9Cl2NO/c11-2-1-6-3-7-4-10(14)13-9(7)5-8(6)12/h3,5H,1-2,4H2,(H,13,14)	-4.778
InChI=1S/C4H8O2S2/c5-3-1-7-4(6)2-8-3/h3-6H,1-2H2	-1.469
InChI=1S/C15H21IO3/c1-2-3-4-5-6-7-10-19-15(18)12-8-9-14(17)13(16)11-12/h8-9,11,17H,2-7,10H2,1H3	-4.67
InChI=1S/C16H16N2/c1-9-7-17-15-13(11(9)3)5-6-14-12(4)10(2)8-18-16(14)15/h5-8H,1-4H3	-5.194
InChI=1S/C21H14/c1-13-11-16-7-4-6-14-9-10-18-17-8-3-2-5-15(17)12-19(13)21(18)20(1h2-12H,1H3	-8.522
InChI=1S/C17H18N2O3S/c1-12-3-9-16(10-4-12)23-17(11-19(21)22)14-5-7-15(8-6-14)18-13(2)2h3-10,17H,11H2,1-2H3,(H,18,20)	-4.991
InChI=1S/C19H16O4/c1-19(21)11-14(12-7-3-2-4-8-12)16-17(23-19)13-9-5-6-10-15(13)22-1h2-10,14,21H,11H2,1H3	-4.74
InChI=1S/C16H14ClN3O/c1-18-15-10-20(21)16(11-5-3-2-4-6-11)13-9-12(17)7-8-14(13)19-15/h2-9,21H,10H2,1H3/p+1	-3.39
InChI=1S/C11H9NO2/c1-14-11(13)10(8-12)7-9-5-3-2-4-6-9/h2-7H,1H3/b10-7-	-3.015
InChI=1S/C14H17N3O/c1-3-16-8-9-17-13(10(16)2)15-12-7-5-4-6-11(12)14(17)18/h4-7,10H,3,8-9H2,1-2H3	-2.5
InChI=1S/C8H5Cl3O3/c9-4-1-2-5(8(11)7(4)10)14-3-6(12)13/h1-2H,3H2,(H,12,13)	-3.1
InChI=1S/C13H20O3/c1-9(2)12-5-4-10(3)6-13(12)16-8-11(15)7-14/h4-6,9,11,14-15H,7-8H2,1-3H3	-3.283
InChI=1S/C5H4N4S/c10-5-8-3-1-6-2-7-4(3)9-5/h1-2H,(H2,6,7,8,9,10)	-2.524
InChI=1S/C11H20N2O/c1-3-11(14)13-9-5-6-10(13)8-12(4-2)7-9/h9-10H,3-8H2,1-2H3	-1.32

"InChi"	"logS(M)"
InChI=1S/C21H24O10/c22-9-16-18(27)19(28)20(29)21(31-16)30-15-8-12(24)7-14(26)17(15)h1-2,4-5,7-8,16,18-24,26-29H,3,6,9H2	-2.64
InChI=1S/C11H11NO5/c1-7(13)17-9-5-3-2-4-8(9)11(15)16-6-10(12)14/h2-5H,6H2,1H3,(H2,12,14)	-1.79
InChI=1S/C19H28O2/c1-19-10-9-15-14-6-4-13(21-2)11-12(14)3-5-16(15)17(19)7-8-18(19)2h4,15-18,20H,3,5-11H2,1-2H3	-4.761
InChI=1S/C13H12N2O/c16-12-8-10-4-2-1-3-9(10)7-11(12)13-14-5-6-15-13/h1-4,7-8,16H,5-6H2,(H,14,15)	-3.301
InChI=1S/C9H11FN2O3/c1-2-3-4-7(13)12-8(14)6(10)5-11-9(12)15/h5H,2-4H2,1H3,(H,11,15)	-2.3
InChI=1S/C33H24ClNO8/c1-19-25(26-17-22(41-2)15-16-27(26)35(19)31(37)20-11-13-21(34)14h3-17H,18H2,1-2H3,(H,38,39)	-9.268
InChI=1S/C19H25ClN2OS/c1-18(2,3)14-9-7-13(8-10-14)12-24-15-11-21-22(19(4,5)6)17(23)16(1h7-11H,12H2,1-6H3	-7.483
InChI=1S/C11H16N2/c1-12-8-9-13(2)11(12)10-6-4-3-5-7-10/h3-7,11H,8-9H2,1-2H3	-0.132
InChI=1S/C11H22N3O6P/c1-6(9(15)14-7(2)11(17)18)13-10(16)8(12)4-5-21(3,19)20/h6-8H,4-5,12H2,1-3H3,(H,13,16)(H,14,15)(H,17,18)(H,19,20)	0.49
InChI=1S/C9H16O4/c1-3-9(10)13-8-7-12-6-5-11-4-2/h3H,1,4-8H2,2H3	-0.181
InChI=1S/C6H8N2O2S/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H,7H2,(H2,8,9,10)	-0.133
InChI=1S/C12H13NO5/c1-13(7-11(15)16)10(14)8-18-12(17)9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H,15,16)	-2.254
InChI=1S/C24H27N3O4/c1-17-21(22(27(5)26-17)30-20-9-7-6-8-10-20)15-25-29-16-18-11-13-1h6-15H,16H2,1-5H3/b25-15+	-7.46
InChI=1S/C10H12N4O/c1-3-6-7(4-2)14-9-8(13-6)10(15)12-5-11-9/h5H,3-4H2,1-2H3,(H,11,12,14,15)	-1.912
InChI=1S/C43H56N8O6/c1-4-27(2)37-43(57)50-20-11-10-17-34(50)41(55)51-22-19-44-26-36(5h5-9,13-16,25,27,32-37,44-45H,4,10-12,17-24,26H2,1-3H3,(H,46,53)(H,47,52)	-2.75
InChI=1S/C4H9Br/c1-3-4(2)5/h4H,3H2,1-2H3	-3.111
InChI=1S/C18H21F2N3O3/c1-18(2,10-19)23-9-12(17(25)26)16(24)11-7-13(20)15(8-14(11)23)22-h7-9,21H,3-6,10H2,1-2H3,(H,25,26)	-2.6
InChI=1S/C7H5ClN2O/c8-4-2-1-3-5-6(4)11-7(9)10-5/h1-3H,(H2,9,10)	-2.193
InChI=1S/C18H19ClN4/c1-22-8-10-23(11-9-22)18-14-4-2-3-5-15(14)20-16-7-6-13(19)12-17(1h2-7,12,21H,8-11H2,1H3	-4.444
InChI=1S/C8H10N2O/c1-10(9-11)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3	-1.522

"InChi"	"logS(M)"
InChI=1S/C25H40O4/c1-3-5-7-9-11-13-17-21-29-25(27)23-19-15-14-18-22(23)24(26)28-20-h14-15,18-19H,3-13,16-17,20-21H2,1-2H3	-4.781
InChI=1S/C6H12O2/c1-5(7)4-6(2,3)8/h8H,4H2,1-3H3	0.935
InChI=1S/C14H13N3O2/c18-13(10-11-4-2-1-3-5-11)16-17-14(19)12-6-8-15-9-7-12/h1-9H,10H2,(H,16,18)(H,17,19)	-2.47
InChI=1S/C9H10O2/c1-6-4-3-5-7(2)8(6)9(10)11/h3-5H,1-2H3,(H,10,11)	-2.185
InChI=1S/C11H17Cl3N2O2S/c1-3-5-6-7(4-2)8-9(17)16(10(18)15-8)19-11(12,13)14/h7-8H,3-6H2,1-2H3,(H,15,18)	-4.89
InChI=1S/C8H6N2O/c11-8-7-6(3-5-10-8)2-1-4-9-7/h1-5H,(H,10,11)	-1.143
InChI=1S/C12H5Cl5/c13-7-3-1-6(2-4-7)10-11(16)8(14)5-9(15)12(10)17/h1-5H	-7.88
InChI=1S/C8H18N2O6/c1-2-3-4-5-6-8(16-10(13)14)7-15-9(11)12/h8H,2-7H2,1H3,(H,11,12)(H,13,14)/q+2	-4.33
InChI=1S/C28H28O7P2/c29-36(31-21-25-13-5-1-6-14-25,32-22-26-15-7-2-8-16-26)35-37(30,3h1-20H,21-24H2	-7.254
InChI=1S/C12H15Cl2NO/c1-10-2-3-11(9-16)8-12(10)15(6-4-13)7-5-14/h2-3,8-9H,4-7H2,1H3	-4.45
InChI=1S/C34H32N4O9/c39-28(24-6-1-12-35-16-24)44-20-33(21-45-29(40)25-7-2-13-36-17-2h1-4,6-9,12-19,32,43H,5,10-11,20-23H2	-4.811
InChI=1S/C8H18O/c1-4-8(9)6-5-7(2)3/h7-9H,4-6H2,1-3H3	-1.927
InChI=1S/C18H22/c1-17(2,15-11-7-5-8-12-15)18(3,4)16-13-9-6-10-14-16/h5-14H,1-4H3	-6.474
InChI=1S/C12H15NO3/c1-8-3-9(2)5-10(4-8)15-7-11-6-13-12(14)16-11/h3-5,11H,6-7H2,1-2H3,(H,13,14)	-3.387
InChI=1S/C9H12N2O2/c1-11(9(10)12)7-3-5-8(13-2)6-4-7/h3-6H,1-2H3,(H2,10,12)	-1.16
InChI=1S/C11H14N2O4/c12-10(14)16-6-9(7-17-11(13)15)8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H2,12,14)(H2,13,15)	-1.952
InChI=1S/C18H39NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-17-18-23-24(20,21)22/h19H,2-18H2,1H3,(H,20,21,22)	-5.988
InChI=1S/C10H12N2O/c1-12-9(4-5-10(12)13)8-3-2-6-11-7-8/h2-3,6-7,9H,4-5H2,1H3	0.754
InChI=1S/C2H3Br/c1-2-3/h2H,1H2	-1.275
InChI=1S/C10H11NO3/c1-7(12)11-9-5-3-8(4-6-9)10(13)14-2/h3-6H,1-2H3,(H,11,12)	-1.9
InChI=1S/C14H19N3O/c1-3-17(4-2)11-10-13-15-14(16-18-13)12-8-6-5-7-9-12/h5-9H,3-4,10-11H2,1-2H3	-1.502
InChI=1S/C21H24ClNO5/c1-25-18-13-16(20(24)15-3-5-17(22)6-4-15)14-19(26-2)21(18)28-12-9h3-6,13-14H,7-12H2,1-2H3	-2.864

"InChi"	"logS(M)"
InChI=1S/C20H22N2/c1-15-7-5-10-17-18(13-21-20(15)17)19-11-6-12-22(19)14-16-8-3-2-4-h2-5,7-10,13,19,21H,6,11-12,14H2,1H3	-4.156
InChI=1S/C5H7N/c1-2-3-4-5-6/h2-3H,4H2,1H3/b3-2+	-0.96
InChI=1S/C22H35NO2/c1-21-9-7-16(24)12-15(21)5-6-17-18(21)8-10-22(2)19(17)11-14(20(22h5,14,16-19,24H,6-13H2,1-4H3	-1.49
InChI=1S/C9H16N2O2S2/c14-9(10-1-5-12-6-2-10)15-11-3-7-13-8-4-11/h1-8H2	-3.291
InChI=1S/C15H15ClO/c1-10-8-14(17)13(11(2)15(10)16)9-12-6-4-3-5-7-12/h3-8,17H,9H2,1-2H3	-4.301
InChI=1S/C18H14O4S/c1-23-14-4-2-12(3-5-14)17(21)15-9-11(10-16(19)20)8-13-6-7-22-18(1h2-9H,10H2,1H3,(H,19,20)	-5.51
InChI=1S/C13H9ClN2O4/c14-8-4-6-9(7-5-8)15-13(18)10-2-1-3-11(12(10)17)16(19)20/h1-7,17H,(H,15,18)	-4.545
InChI=1S/C10H12N4O2S/c1-2-3-7(15)16-6-17-10-8-9(12-4-11-8)13-5-14-10/h4-5H,2-3,6H2,1H3,(H,11,12,13,14)	-2.69
InChI=1S/C8H6O5/c9-5-1-4(8(12)13)2-6(10)7(11)3-5/h1-3,10-11H,(H,12,13)	0.543
InChI=1S/C9H18O/c1-7(2)5-9(10)6-8(3)4/h7-8H,5-6H2,1-4H3	-2.454
InChI=1S/C8H20N2O2S/c1-5-9(6-2)13(11,12)10(7-3)8-4/h5-8H2,1-4H3	-1.14
InChI=1S/C16H16/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h7-10H,1-6H2	-5.96
InChI=1S/C12H22O3/c1-3-5-7-9-11(13)15-12(14)10-8-6-4-2/h3-10H2,1-2H3	-4.297
InChI=1S/C29H30N4/c1-4-10-25(11-5-1)29(26-12-6-2-7-13-26,27-14-8-3-9-15-27)16-19-32h1-15,17-18,24H,16,19-23H2	-6.518
InChI=1S/C25H20N4O4/c1-33-21-9-5-4-8-20(21)27-25(32)19-14-16-6-2-3-7-18(16)22(23(19)3h2-14,28H,1H3,(H2,26,31)(H,27,32)/b29-22-	-8.167
InChI=1S/C10H10N2O5/c1-6(10(14)15)11-9(13)7-3-2-4-8(5-7)12(16)17/h2-6H,1H3,(H,11,13)(H,14,15)	-1.8
InChI=1S/C18H22O6/c19-10-14-15(20)16(21)17(22)18(24-14)23-9-8-12-6-3-5-11-4-1-2-7-1h1-7,14-22H,8-10H2	-1.11
InChI=1S/C18H29NO3/c1-5-11-18(3,13-20)14-22-17(21)19(4)15(2)12-16-9-7-6-8-10-16/h6-10,15,20H,5,11-14H2,1-4H3	-0.326
InChI=1S/C25H36O6/c1-4-5-21(30)31-25(20(29)14-26)11-9-18-17-7-6-15-12-16(27)8-10-23h12,17-19,22,26,28H,4-11,13-14H2,1-3H3	-5.069
InChI=1S/C7H7NO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,8H2,(H,9,10)	-1.52
InChI=1S/C8H7N3O4/c12-10(13)6-1-2-7(9-3-4-9)8(5-6)11(14)15/h1-2,5H,3-4H2	-3
InChI=1S/C3H3F3O2/c1-8-2(7)3(4,5)6/h1H3	-0.648

"InChi"	"logS(M)"
InChI=1S/C23H15F2NO2/c1-13-21(23(27)28)18-12-16(24)10-11-20(18)26-22(13)15-8-6-14(7-9-h2-12H,1H3,(H,27,28)	-6.39
InChI=1S/C16H19Cl2NO/c1-12-11-15(19(9-7-17)10-8-18)13-5-3-4-6-14(13)16(12)20-2/h3-6,11H,7-10H2,1-2H3	-6.144
InChI=1S/C7H13BrO3/c1-5(2)7(8)11-4-6(10)3-9/h6-7,9-10H,1,3-4H2,2H3	-1.284
InChI=1S/C11H13N/c1-3-9-12(2)10-11-7-5-4-6-8-11/h1,4-8H,9-10H2,2H3	-1.027
InChI=1S/C16H17ClN2OS/c1-18-7-2-8-19-13-5-4-12(20)10-16(13)21-15-6-3-11(17)9-14(15)19/h3-6,9-10,18,20H,2,7-8H2,1H3	-5.679
InChI=1S/C3H6Cl2/c1-2-3(4)5/h3H,2H2,1H3	-1.622
InChI=1S/C16H18N4O2/c21-15(18-12-13-4-2-1-3-5-13)8-11-19-20-16(22)14-6-9-17-10-7-14/h1-7,9-10,19H,8,11-12H2,(H,18,21)(H,20,22)	-2.119
InChI=1S/C12H17NO5/c1-7(14)11(16)18-12(17)10(13)6-8-3-2-4-9(15)5-8/h2-5,7,10-11,14-16H,6,13H2,1H3	0.593
InChI=1S/C8H6O/c1-2-4-8-7(3-1)5-6-9-8/h1-6H	-2.241
InChI=1S/C19H24N4O6/c1-4-7-8-21-19(26)29-16-11-13(10-15(17(16)24)23(27)28)9-14(12-20h9-11,24H,4-8H2,1-3H3,(H,21,26)/b14-9-	-2.32
InChI=1S/C20H27N/c1-2-21(17-9-15-19-11-5-3-6-12-19)18-10-16-20-13-7-4-8-14-20/h3-8,11-14H,2,9-10,15-18H2,1H3	-5.026
InChI=1S/C15H19N3O2/c1-5-17-14(19)13(16(3)4)11(2)18(15(17)20)12-9-7-6-8-10-12/h6-10H,5H2,1-4H3	-2.399
InChI=1S/C8H10O2/c9-5-7-3-1-2-4-8(7)6-10/h1-4,9-10H,5-6H2	0.057
InChI=1S/C24H28N2O4/c1-2-3-4-5-12-17-21(27)30-18-26-22(28)24(25-23(26)29,19-13-8-6-9-h6-11,13-16H,2-5,12,17-18H2,1H3,(H,25,29)	-6.52
InChI=1S/C22H18N2/c1-3-7-18(8-4-1)19-11-13-21(14-12-19)22(24-16-15-23-17-24)20-9-5-h1-17,22H	-6.453
InChI=1S/C15H14N2O/c16-15(18)17-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)17/h1-8H,9-10H2,(H2,16,18)	-4.152
InChI=1S/C20H40N4/c1-23-11-7-19(8-12-23)21-15-17-3-5-18(6-4-17)16-22-20-9-13-24(2)1h17-22H,3-16H2,1-2H3	-3.197
InChI=1S/C11H14O2/c1-2-11(12)13-9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3	-3.117
InChI=1S/C4H9ClO/c1-4(2,6)3-5/h6H,3H2,1-2H3	0.16
InChI=1S/C5H7N3/c6-4-1-2-8-5(7)3-4/h1-3H,(H4,6,7,8)	0.333
InChI=1S/C16H20N2O3/c1-17-13-6-7-14(17)10-18(9-13)16(21)12-4-2-11(3-5-12)8-15(19)20/h2-5,13-14H,6-10H2,1H3,(H,19,20)	-2.54

"InChi"	"logS(M)"
InChI=1S/C77H140O8/c1-5-9-13-17-21-25-29-33-37-41-45-49-53-57-61-65-73(78)82-69-77(h33-40H,5-32,41-72H2,1-4H3/b37-33+,38-34+,39-35+,40-36+	-7.378
InChI=1S/C25H27NO5/c1-17(19-8-9-21-16-22(29-2)11-10-20(21)15-19)24(27)30-12-13-31-25 h3-11,15-17,23H,12-14,26H2,1-2H3	-3.75
InChI=1S/C20H30N2O2/c1-18-11-17-16(21-24-22-17)10-12(18)4-5-13-14(18)6-8-19(2)15(13)7 h12-15,23H,4-11H2,1-3H3	-5.339
InChI=1S/C12H6Cl4O/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6H	-6.82
InChI=1S/C13H15N3O4S/c1-19-7-8-20-11-9-14-13(15-10-11)16-21(17,18)12-5-3-2-4-6-12/ h2-6,9-10H,7-8H2,1H3,(H,14,15,16)	-1.826
InChI=1S/C6H9N3O3/c1-5-4-8(2-3-10)6(7-5)9(11)12/h4,10H, 2-3H2,1H3	-0.837
InChI=1S/C18H16ClNO4S/c1-3-22-17(21)11(2)23-13-5-7-14(8-6-13)24-18-20-15-9-4-12(19)10-1 h4-11H,3H2,1-2H3	-5.67
InChI=1S/C8H8O2/c9-8(10)6-7-4-2-1-3-5-7/h1-5H,6H2,(H,9,10)	-0.89
InChI=1S/C16H25N3O2/c1-2-3-4-5-6-7-8-9-15(20)18-19-16(21)14-10-12-17-13-11-14/ h10-13H,2-9H2,1H3,(H,18,20)(H,19,21)	-4.17
InChI=1S/C9H9N3S/c10-8-7(13-9(11)12-8)6-4-2-1-3-5-6/h1-5H, 10H2,(H2,11,12)	-2.788
InChI=1S/C12H20N2O2/c1-9(7-11(3)15)13-5-6-14-10(2)8-12(4)16/ h5-8H2,1-4H3/b13-9-,14-10+	-2.83
InChI=1S/C4H8OS/c1-3-6-4(2)5/h3-5H,1H2,2H3	0.005
InChI=1S/C8H9FN2O3/c1-2-3-6(12)11-7(13)5(9)4-10-8(11)14/h4H, 2-3H2,1H3,(H,10,14)	-1.28
InChI=1S/C19H41N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20/h2-20H2,1H3	-5.857
InChI=1S/C21H27NO2/c1-16(21(24)19-7-9-20(23)10-8-19)22-13-11-18(12-14-22)15-17-5-3-2 h2-10,16,18,21,23-24H,11-15H2,1H3	-3.093
InChI=1S/C17H20O3/c1-11(2)20-17(18)12(3)13-5-6-15-10-16(19-4)8-7-14(15)9-13/ h5-12H,1-4H3	-5.48
InChI=1S/C12H26N2O4/c1-5-15-9-10-17-7-3-14-4-8-18-12-11-16-6-2-13-1/h13-14H,1-12H2	0.581
InChI=1S/C14H29NO2/c1-4-5-6-7-8-9-10-11-12-14(2,3)13(16)15-17/ h17H,4-12H2,1-3H3,(H,15,16)	-4.8
InChI=1S/C12H5Cl5O/c13-6-1-7(14)3-8(2-6)18-12-5-10(16)9(15)4-11(12)17/h1-5H	-8.06
InChI=1S/C12H13ClF3N3O4/c1-2-4-17(5-3-13)11-9(18(20)21)6-8(12(14,15)16)7-10(11)19(22)23/ h6-7H,2-5H2,1H3	-5.597
InChI=1S/C12H16N4O4S3/c1-7-5-8(2)10(9(3)6-7)23(19,20)15-11-16(4)14-12(21-11)22(13,17)18/ h5-6H,1-4H3,(H2,13,17,18)/b15-11+	-3

"InChi"	"logS(M)"
InChI=1S/C14H17NO3/c1-10(2)18-14(16)15-12-7-5-4-6-11(12)8-9-13(15)17-3/h4-10,13H,1-3H3	-4.273
InChI=1S/C17H20N2O/c1-3-18(15-11-7-5-8-12-15)17(20)19(4-2)16-13-9-6-10-14-16/h5-14H,3-4H2,1-2H3	-3.526
InChI=1S/C13H12Cl2N2/c14-10-6-8(1-3-12(10)16)5-9-2-4-13(17)11(15)7-9/h1-4,6-7H,5,16-17H2	-4.287
InChI=1S/C10H14O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h5-7,11H,3-4H2,1-2H3	-2.179
InChI=1S/C9H9NO3S/c1-10-9(11)8-5-3-2-4-7(8)6-14(10,12)13/h2-5H,6H2,1H3	-1.531
InChI=1S/C3H8FN/c4-2-1-3-5/h1-3,5H2	1
InChI=1S/C8H7NO4/c10-8(11)5-6-1-3-7(4-2-6)9(12)13/h1-4H,5H2,(H,10,11)	-1.705
InChI=1S/C9H20O3/c1-7(2)11-5-9(10)6-12-8(3)4/h7-10H,5-6H2,1-4H3	0.055
InChI=1S/C10H14NO5PS/c1-7-5-9(16-17(18,14-3)15-4)6-8(2)10(7)11(12)13/h5-6H,1-4H3	-5.036
InChI=1S/C4H12FN2OP/c1-6(2)9(5,8)7(3)4/h1-4H3	0.812
InChI=1S/C24H30N2O2/c1-2-26-19-22(13-14-25-15-17-28-18-16-25)24(23(26)27,20-9-5-3-6-1h3-12,22H,2,13-19H2,1H3	-4.878
InChI=1S/C17H28N2O2/c1-4-6-12-19(13-7-5-2)16(17(18)20)14-8-10-15(21-3)11-9-14/h8-11,16H,4-7,12-13H2,1-3H3,(H2,18,20)	-4.93
InChI=1S/C7H9NO4S3/c8-15(11,12)6-3-5-7(13-6)4(9)1-2-14(5)10/h3-4,9H,1-2H2,(H2,8,11,12)/p+1	-1.57
InChI=1S/C12H6Cl4O/c13-7-1-3-8(4-2-7)17-10-6-5-9(14)11(15)12(10)16/h1-6H	-7.01
InChI=1S/C11H11I3O3/c1-2-5(11(16)17)3-6-7(12)4-8(13)10(15)9(6)14/h4-5,15H,2-3H2,1H3,(H,16,17)	-6.549
InChI=1S/C7H14ClNO/c8-2-1-3-9-4-6-10-7-5-9/h1-7H2	0.786
InChI=1S/C8H11N3S/c1-2-6(8(9)12)7-5-10-3-4-11-7/h3-6H,2H2,1H3,(H2,9,12)	-1.607
InChI=1S/C17H27NO3/c1-3-4-5-6-7-8-9-17(20)18-13-14-10-11-15(19)16(12-14)21-2/h10-12,19H,3-9,13H2,1-2H3,(H,18,20)	-4.58
InChI=1S/C4H6O3/c1-3-2-6-4(5)7-3/h3H,2H2,1H3	0.371
InChI=1S/C17H20N2O2S/c1-2-21-17(20)15-13-8-9-19(11-14(13)22-16(15)18)10-12-6-4-3-5-7-1h3-7H,2,8-11,18H2,1H3	-3.261
InChI=1S/C22H24N6O9/c1-14(29)23-19-12-15(26(10-8-21(30)36-2)11-9-22(31)37-3)4-6-17(19h4-7,12-13H,8-11H2,1-3H3,(H,23,29)/b25-24+	-7.333
InChI=1S/C10H16N2O2S/c1-3-12(4-2)15(13,14)10-7-5-9(11)6-8-10/h5-8H,3-4,11H2,1-2H3	-2.63

"InChi"	"logS(M)"
InChI=1S/C11H16N4O2/c1-4-5-6-7-12-8-9(13-7)14(2)11(17)15(3)10(8)16/h4-6H2,1-3H3,(H,12,13)	-2.317
InChI=1S/C14H29NO2/c1-4-7-10-14(11-8-5-2,12-9-6-3)13(16)15-17/h17H,4-12H2,1-3H3,(H,15,16)	-4.16
InChI=1S/C16H13NO/c1-2-16(18)13-7-4-3-6-12(13)9-10-15-14(16)8-5-11-17-15/h1,3-8,11,18H,9-10H2	-3.802
InChI=1S/C8H5F9O/c1-2-18-4-3(9)5(10,11)7(14,15)8(16,17)6(4,12)13/h2H2,1H3	-3.776
InChI=1S/C22H8Br2O2/c23-15-7-14-19-17-9(15)3-1-5-11(17)21(25)13-8-16(24)10-4-2-6-12(2h1-8H	-7.633
InChI=1S/C6H4F2/c7-5-3-1-2-4-6(5)8/h1-4H	-2
InChI=1S/C13H12N2O2/c14-9-4-3-5-10(8-9)15-12-7-2-1-6-11(12)13(16)17/h1-8,15H,14H2,(H,16,17)	-4.09
InChI=1S/C11H19N/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h7H,1-6,8-10H2	-2.46
InChI=1S/C28H47NO4S/c1-8-26(6)17-22(33-23(31)18-34-16-15-29(9-2)10-3)27(7)19(4)11-13-h8,19-20,22,24-25,32H,1,9-18H2,2-7H3	-5.851
InChI=1S/C7H8O3/c1-2-9-7(8)6-4-3-5-10-6/h3-5H,2H2,1H3	-1.522
InChI=1S/C7H9NO3S3/c8-14(10,11)6-3-4-5(9)1-2-12-7(4)13-6/h3,5,9H,1-2H2,(H2,8,10,11)	-2.59
InChI=1S/C18H38O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h19H,2-18H2,1H3	-5.432
InChI=1S/C16H30O2/c1-13(2)7-9-15(5,17)11-12-16(6,18)10-8-14(3)4/h13-14,17-18H,7-10H2,1-6H3	-3.438
InChI=1S/C7H4BrN/c8-7-4-2-1-3-6(7)5-9/h1-4H	-2.869
InChI=1S/C4H3N5/c1-3-4(6-2-5-1)8-9-7-3/h1-2H,(H,5,6,7,8,9)	-0.232
InChI=1S/C14H17N3O2S/c15-9-10-17-12-3-7-14(8-4-12)20(18,19)13-5-1-11(16)2-6-13/h1-8,17H,9-10,15-16H2	-2.35
InChI=1S/C21H22N2O3/c24-17-9-16-18-13-10-21(25)20(6-7-22(21)11-12(13)5-8-26-16)14-3-1h1-5,13,16,18-19,25H,6-11H2	-3.309
InChI=1S/C18H14F3NO2/c1-22-17-14(12-8-5-9-13(10-12)18(19,20)21)15(23)16(24-17)11-6-3-2h2-10,16,22H,1H3	-3.979
InChI=1S/C20H24N2S2/c1-23-16-8-9-20-18(13-16)22(12-10-15-5-4-11-21-14-15)17-6-2-3-7-1h2-3,6-9,13,15,21H,4-5,10-12,14H2,1H3	-3.759
InChI=1S/C10H8N4O4/c1-7-11-10(14(17)18)6-12(7)8-2-4-9(5-3-8)13(15)16/h2-6H,1H3	-3.998
InChI=1S/C42H18N2O6/c45-37-21-5-1-3-7-23(21)39(47)29-25(37)13-9-17-19-11-15-27-31(35(h1-16,43-44H	-8.811
InChI=1S/C10H22O4/c1-2-3-5-12-7-9-14-10-8-13-6-4-11/h11H,2-10H2,1H3	0.685

"InChi"	"logS(M)"
InChI=1S/C6H6O3S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H,7,8,9)	0.849
InChI=1S/C11H13NO2S2/c1-12(7-10(13)14)11(15)16-8-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H,13,14)	-3.23
InChI=1S/C10H18N2O2/c13-11-9-7-5-3-1-2-4-6-8-10(9)12-14/h13-14H,1-8H2/b11-9-,12-10+	-2.581
InChI=1S/C15H12O3/c16-14(11-6-2-1-3-7-11)10-12-8-4-5-9-13(12)15(17)18/h1-9H,10H2,(H,17,18)	-3.447
InChI=1S/C12H22N4O3S/c1-12(2,3)9-14-15-10(20-9)13-11(17)16(4)7-8(18-5)19-6/h8H,7H2,1-6H3,(H,13,15,17)	-1.868
InChI=1S/C12H16ClN3O/c1-16(2)7-3-6-14-12-15-10-8-9(13)4-5-11(10)17-12/h4-5,8H,3,6-7H2,1-2H3,(H,14,15)	-2.433
InChI=1S/C11H15Cl2NO/c1-7(2)14-6-11(15)8-3-4-9(12)10(13)5-8/h3-5,7,11,14-15H,6H2,1-2H3	-2.838
InChI=1S/C14H19NO/c1-10(2)15-14(16)12(4)11(3)13-8-6-5-7-9-13/h5-10H,1-4H3,(H,15,16)/b12-11-	-3.597
InChI=1S/C13H26O/c1-14-13-11-9-7-5-3-2-4-6-8-10-12-13/h13H,2-12H2,1H3	-4.684
InChI=1S/C10H10O/c1-9(8-11)7-10-5-3-2-4-6-10/h2-8H,1H3/b9-7-	-2.475
InChI=1S/C12H18N2O3/c1-5-12(8(4)6-7(2)3)9(15)13-11(17)14-10(12)16/h6,8H,5H2,1-4H3,(H2,13,14,15,16,17)	-2.523
InChI=1S/C20H38O4/c1-3-5-7-9-11-13-15-17-19(21)23-24-20(22)18-16-14-12-10-8-6-4-2/h3-18H2,1-2H3	-6.45
InChI=1S/C12H18/c1-9(2)11-7-5-6-8-12(11)10(3)4/h5-10H,1-4H3	-6.603
InChI=1S/C14H12N2O/c1-17-9-6-7-13-11(8-9)14(15)10-4-2-3-5-12(10)16-13/h2-8H,1H3,(H2,15,16)	-4.067
InChI=1S/C8H16O2/c1-3-8(4-2)5-9-7-10-6-8/h3-7H2,1-2H3	-1.995
InChI=1S/C15H19N3O2/c1-5-17-11(2)13(16(3)4)14(19)18(15(17)20)12-9-7-6-8-10-12/h6-10H,5H2,1-4H3	-1.874
InChI=1S/C31H36N2O11/c1-14(2)7-8-16-13-17(9-11-19(16)34)27(37)33-21-22(35)18-10-12-20(h7,9-13,23,25-26,29,34-36H,8H2,1-6H3,(H2,32,39)(H,33,37)	-5.18
InChI=1S/C9H7NO6/c1-16-9(13)6-3-2-5(10(14)15)4-7(6)8(11)12/h2-4H,1H3,(H,11,12)/p-1	-2.056
InChI=1S/C8H13N/c1-4-8-6(2)5-9-7(8)3/h5,9H,4H2,1-3H3	-2.585
InChI=1S/C4H10N2O/c1-3(2)4(7)6-5/h3H,5H2,1-2H3,(H,6,7)	-0.72
InChI=1S/C10H11NO3/c12-9(6-7-10(13)14)11-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,12)(H,13,14)	-1.861
InChI=1S/C12H10O4/c1-2-15-12(14)11-7-9(13)8-5-3-4-6-10(8)16-11/h3-7H,2H2,1H3	-2.357
InChI=1S/C6H12Br2O4/c7-1-3(9)5(11)6(12)4(10)2-8/h3-6,9-12H,1-2H2	-1.198
InChI=1S/C12H13NO2/c14-12(15)7-3-4-9-8-13-11-6-2-1-5-10(9)11/h1-2,5-6,8,13H,3-4,7H2,(H,14,15)	-2.91

"InChi"	"logS(M)"
InChI=1S/C11H11NO3/c1-2-7-15-10-5-3-9(4-6-10)8-11(13)12-14/h1,3-6,14H,7-8H2,(H,12,13)	-1.762
InChI=1S/C15H14O4/c1-17-12-6-3-11(4-7-12)5-8-13-9-14(18-2)10-15(16)19-13/h3-10H,1-2H3/b8-5+	-2.915
InChI=1S/C9H12O4/c1-9(8(12)13)5-3-2-4-6(9)7(10)11/h4H,2-3,5H2,1H3,(H,10,11)(H,12,13)	-1.964
InChI=1S/C19H24N2OS/c1-3-20(4-2)15-16-23-19(22)21(17-11-7-5-8-12-17)18-13-9-6-10-14-1h5-14H,3-4,15-16H2,1-2H3	-3.174
InChI=1S/C9H20O/c1-8(5-6-10)7-9(2,3)4/h8,10H,5-7H2,1-4H3	-2.557
InChI=1S/C3HCl3F4/c4-3(5,6)2(9,10)1(7)8/h1H	-4.492
InChI=1S/C6H12Cl2O2S2/c7-1-3-11(9)5-6-12(10)4-2-8/h1-6H2/p+2	-2.04
InChI=1S/C20H20BrClN4O6/c1-31-18(27)7-9-25(10-8-19(28)32-2)14-5-3-13(4-6-14)23-24-20-16(2h3-6,11-12H,7-10H2,1-2H3/b24-23+	-7.1
InChI=1S/C9H8O3/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6,10H,(H,11,12)/b6-3+	-0.953
InChI=1S/C8H6N2O/c11-7-3-1-2-6-4-5-9-10-8(6)7/h1-5,11H	-2.409
InChI=1S/C21H26N6O4/c1-23-18-17(20(30)24(2)21(23)31)27(14-22-18)13-16(28)12-25-8-10-h3-7,14,16,28H,8-13H2,1-2H3	-1.726
InChI=1S/C10H13NO2/c11-7-9(6-10(12)13)8-4-2-1-3-5-8/h1-5,9H,6-7,11H2,(H,12,13)	-0.078
InChI=1S/C3H6ClN3O2/c4-1-2-7(6-9)3(5)8/h1-2H2,(H2,5,8)	-0.794
InChI=1S/C20H29NO3/c1-2-21-14-8-13-18(15-21)24-19(22)20(23,17-11-6-7-12-17)16-9-4-3-h3-5,9-10,17-18,23H,2,6-8,11-15H2,1H3	-3.606
InChI=1S/C13H16NO4PS/c1-3-15-19(20,16-4-2)18-13-10-12(17-14-13)11-8-6-5-7-9-11/h5-10H,3-4H2,1-2H3	-5.217
InChI=1S/C9H7ClN2O2/c10-5-1-2-7-6(3-5)9(14)11-4-8(13)12-7/h1-3H,4H2,(H,11,14)(H,12,13)	-3.05
InChI=1S/C6H8N2O3/c1-3-4(2-9)5(10)8-6(11)7-3/h9H,2H2,1H3,(H2,7,8,10,11)	-0.594
InChI=1S/C10H4Cl4/c11-5-3-6-7(12)1-2-8(13)10(6)9(14)4-5/h1-4H	-7.51
InChI=1S/C7H10O4/c1-7(2)4(6(9)10)3-5(8)11-7/h4H,3H2,1-2H3,(H,9,10)/p-1	-1.245
InChI=1S/C12H19NO3/c1-4-16-12-10(14-2)7-9(5-6-13)8-11(12)15-3/h7-8H,4-6,13H2,1-3H3	-0.784
InChI=1S/C17H24N4O5/c1-16(2,3)14(23)25-9-20-8-18-12-11(13(20)22)7-21(19-12)10-26-15(2h7-8H,9-10H2,1-6H3	-3.91
InChI=1S/C10H12N2O5/c1-10(2,3)7-4-6(11(14)15)5-8(9(7)13)12(16)17/h4-5,13H,1-3H3	-4.727
InChI=1S/C10H22O/c1-5-10(4,11)8-6-7-9(2)3/h9,11H,5-8H2,1-4H3	-2.694
InChI=1S/C4H2N4S6/c9-1-5-7-3(11-1)13-14-4-8-6-2(10)12-4/h(H,5,9)(H,6,10)	-3.252
InChI=1S/C18H27NO5/c1-12(2)14-8-7-13(3)16(18(21)22-6)17(14)24-11-15(20)23-10-9-19(4)h7-8,12H,9-11H2,1-6H3	-3.343

"InChi"	"logS(M)"
InChI=1S/C12H14N4O/c1-17-10-4-2-3-8(6-10)5-9-7-15-12(14)16-11(9)13/h2-4,6-7H,5H2,1H3,(H4,13,14,15,16)	-2.196
InChI=1S/C10H21N/c1-6-11-9(2,3)7-8-10(11,4)5/h6-8H2,1-5H3	-1.625
InChI=1S/C19H18N2O3S2/c20-26(23,24)18-10-17(13-25-18)19(22)16-8-6-15(7-9-16)12-21-11-14 h1-10,13,21H,11-12H2,(H2,20,23,24)	-3.37
InChI=1S/C3H7O5P/c4-3(5)1-2-9(6,7)8/h1-2H2,(H,4,5)(H2,6,7,8)	0.501
InChI=1S/C16H20N4O5/c1-6-10(17)13(22)9-7(5-25-15(18)23)16(24-3)14-8(19(14)2)4-20(16)1 h7-8,14H,4-5,17H2,1-3H3,(H2,18,23)	-1.218
InChI=1S/C14H12O3/c15-13(8-9-14(16)17)12-7-3-5-10-4-1-2-6-11(10)12/h1-7H,8-9H2,(H, 16,17)	-3.483
InChI=1S/C6H10N4O/c1-3-4-8-5(7)10-6(9-4)11-2/h3H2,1-2H3, (H2,7,8,9,10)	-1.824
InChI=1S/C16H17F5N2O2S/c1-7(2)6-8-9(15(24)25-3)11(13(17)18)23-12(16(19,20)21)10(8)14-22- h7,13H,4-6H2,1-3H3	-5.2
InChI=1S/C6H4N2O6/c9-5-2-6(10)4(8(13)14)1-3(5)7(11)12/ h1-2,9-10H	-3.409
InChI=1S/C7H9N/c1-2-7-3-5-8-6-4-7/h3-6H,2H2,1H3	-0.001
InChI=1S/C13H10I2O3/c1-6-3-9(7(2)18-6)12(16)8-4-10(14)13(17)11(15)5-8/h3-5,17H,1-2H3	-6.699
InChI=1S/C11H14O3/c1-11(2,3)14-13-10(12)9-7-5-4-6-8-9/h4-8H, 1-3H3	-2.776
InChI=1S/C21H40O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20(2)3/ h11-12,20H,4-10,13-19H2,1-3H3/b12-11+	-6.335
InChI=1S/C9H9ClN4O4S3/c1-14-8(19-9(12-14)20(11,15)16)13-21(17,18)7-4-2-6(10)3-5-7/ h2-5H,1H3,(H2,11,15,16)/b13-8+	-2.44
InChI=1S/C12H20N2/c1-4-14(11-10-13(2)3)12-8-6-5-7-9-12/h5-9H, 4,10-11H2,1-3H3	-1.61
InChI=1S/C28H37FO7/c1-6-23(33)35-15-22(32)28(36-24(34)7-2)16(3)12-20-19-9-8-17-13-18 h10-11,13,16,19-21,31H,6-9,12,14-15H2,1-5H3	-3.77
InChI=1S/C4H10N2O/c1-3(2)6-4(5)7/h3H,1-2H3,(H3,5,6,7)	-1.103
InChI=1S/C24H44O6/c1-4-7-10-13-16-22(25)28-19-21(30-24(27)18-15-12-9-6-3)20-29-23(2 h21H,4-20H2,1-3H3	-6.933
InChI=1S/C5H13NO3S2/c1-2-3-6-4-5-10-11(7,8)9/h6H,2-5H2,1H3, (H,7,8,9)	0.701
InChI=1S/C6H9N3O2/c1-2-7-5(10)9-6-8-3-4-11-6/h3-4H,2H2,1H3, (H2,7,8,9,10)	-0.763
InChI=1S/C12H11BrN2O2/c1-8-10(13)11(16)15(12(17)14(8)2)9-6-4-3-5-7-9/h3-7H,1-2H3	-1.939
InChI=1S/C18H23NO3/c1-12(13-4-8-16(21-3)9-5-13)18(20)22-17-10-14-6-7-15(11-17)19(14) h4-5,8-9,14-15,17H,1,6-7,10-11H2,2-3H3	-3.333

"InChi"	"logS(M)"
InChI=1S/C4H7NO5/c5-1(3(7)8)2(6)4(9)10/h1-2,6H,5H2,(H,7,8)(H,9,10)	-0.827
InChI=1S/C11H9NO3/c13-11(10-7-4-8-15-10)12(14)9-5-2-1-3-6-9/h1-8,14H	-3.194
InChI=1S/C6H10O2/c7-6-4-2-1-3-5-8-6/h1-5H2	0.943
InChI=1S/C10H4Cl4/c11-7-3-1-2-5-6(7)4-8(12)10(14)9(5)13/h1-4H	-7.857
InChI=1S/C9H16N2O3S2/c10-9(5-14-16(12,13)15)11-8-4-6-1-2-7(8)3-6/h6-8H,1-5H2,(H2,10,11)(H,12,13,15)	-2.174
InChI=1S/C28H47NO8/c1-10-22-28(7,34)12-11-21(30)15(2)13-16(3)25(18(5)23(31)19(6)26(3h11-12,15-20,22,24-25,27,32,34H,10,13-14H2,1-9H3/b12-11-	-4.701
InChI=1S/C24H29NO4/c1-5-26-21-10-9-17(14-22(21)27-6-2)13-20-19-16-24(29-8-4)23(28-7-h9-12,14-16H,5-8,13H2,1-4H3	-6.665
InChI=1S/C12H2Cl8/c13-3-1-4(7(15)5(14)2-3)6-8(16)10(18)12(20)11(19)9(6)17/h1-2H	-9.42
InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3	0.081
InChI=1S/C6H12O/c1-2-3-4-5-6-7/h6H,2-5H2,1H3	-1.3
InChI=1S/C15H24N2O3S/c1-5-6-7-8-15(18)17(4)13-9-11-14(12-10-13)21(19,20)16(2)3/h9-12H,5-8H2,1-4H3	-2.95
InChI=1S/C14H11NO3/c16-13(15-10-6-2-1-3-7-10)11-8-4-5-9-12(11)14(17)18/h1-9H,(H,15,16)(H,17,18)	-4.081
InChI=1S/C6H5NO4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,8-9H	-2.073
InChI=1S/C19H16N2O3/c1-13(22)21(14(2)23)19-20-17(15-9-5-3-6-10-15)18(24-19)16-11-7-4-h3-12H,1-2H3	-3.379
InChI=1S/C10H12N2O3/c11-10(15)12-8(9(13)14)6-7-4-2-1-3-5-7/h1-5,8H,6H2,(H,13,14)(H3,11,12,15)/p-1	-2.096
InChI=1S/C22H14/c1-3-7-17-15(5-1)9-11-21-19(17)13-14-20-18-8-4-2-6-16(18)10-12-22h1-14H	-7.87
InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3	0.885
InChI=1S/C14H20N2O2/c1-10-5-4-6-11(2)13(10)15-14(17)18-12-7-8-16(3)9-12/h4-6,12H,7-9H2,1-3H3,(H,15,17)	-2.893
InChI=1S/C10H16NO3P/c1-3-13-15(12,14-4-2)11-10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3,(H,11,12)	-1.877
InChI=1S/C17H24N2O4S2/c1-14-13-17(19-16-8-4-3-7-15(14)16)23-11-6-2-5-9-18-10-12-24-25(2h3-4,7-8,13,18H,2,5-6,9-12H2,1H3,(H,20,21,22)	-3.439
InChI=1S/C12H6Cl4O/c13-8-5-4-7(6-11(8)16)17-12-9(14)2-1-3-10(12)15/h1-6H	-6.56
InChI=1S/C10H7NO3/c1-6(12)11-8-5-3-2-4-7(8)9(13)10(11)14/h2-5H,1H3	-1.917
InChI=1S/C14H18N2O6/c17-7-11(19)13(21)10(18)6-16-9-4-2-1-3-8(9)14(22)15-5-12(16)20/h1-4,10-11,13,17-19,21H,5-7H2,(H,15,22)	-1.46

"InChi"	"logS(M)"
InChI=1S/C36H68O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-32-h17,19-20,22H,3-16,18,21,23-35H2,1-2H3/b19-17+,22-20+	-7.028
InChI=1S/C15H22N2O4/c1-3-9-17-14(19)21-11-15(2,10-20-13(16)18)12-7-5-4-6-8-12/h4-8H,3,9-11H2,1-2H3,(H2,16,18)(H,17,19)	-3.623
InChI=1S/CH4ClN/c1-3-2/h3H,1H3	0.281
InChI=1S/C12H16ClNOS/c1-3-14(4-2)12(15)16-9-10-5-7-11(13)8-6-10/h5-8H,3-4,9H2,1-2H3	-3.964
InChI=1S/C22H29NO3/c1-16(2)19-12-11-17(3)20(21(19)25-14-13-23(4)5)22(24)26-15-18-9-7-h6-12,16H,13-15H2,1-5H3	-5.326
InChI=1S/C10H15NO2/c12-8-6-10(7-9(13)11-8)4-2-1-3-5-10/h1-7H2,(H,11,12,13)	-1.712
InChI=1S/C4H5IO2/c1-3(5)2-4(6)7/h2H,1H3,(H,6,7)/b3-2-	-1.16
InChI=1S/C7H14O3/c1-3-4-5-10-7(9)6(2)8/h6,8H,3-5H2,1-2H3	-0.563
InChI=1S/C7H16O/c1-3-4-5-6-7-8-2/h3-7H2,1-2H3	-2.245
InChI=1S/C13H22N2O6/c1-5-13(6-2,9(16)14-11(18)20-7-3)10(17)15-12(19)21-8-4/h5-8H2,1-4H3,(H,14,16,18)(H,15,17,19)	-4.304
InChI=1S/C15H24N2O/c1-5-16(6-2)10-11-17(12-18)15-13(3)8-7-9-14(15)4/h7-9,12H,5-6,10-11H2,1-4H3	-2.745
InChI=1S/C18H13ClF3NO7/c1-2-28-16(24)9-29-17(25)12-8-11(4-5-14(12)23(26)27)30-15-6-3-10(h3-8H,2,9H2,1H3	-5.873
InChI=1S/C9H6O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)(H,12,13)(H,14,15)	-1.942
InChI=1S/C12H22O4/c1-5-11(6-2,9(13)14)12(7-3,8-4)10(15)16/h5-8H2,1-4H3,(H,13,14)(H,15,16)	-2.964
InChI=1S/C7H5Cl2FN2O3/c8-3-5(11)4(9)7(12-6(3)10)15-1-2(13)14/h1H2,(H2,11,12)(H,13,14)	-3.447
InChI=1S/C16H20N2O/c1-17-11-14-8-9-15(12-17)18(14)16(19)10-7-13-5-3-2-4-6-13/h2-7,10,14-15H,8-9,11-12H2,1H3/b10-7+	-2.613
InChI=1S/C29H40O9/c1-17-9-11-28-15-35-26(33)25(32)18(2)10-12-34-20(19(3)30)7-5-6-8-h5-8,13,18-23,25,30,32H,9-12,14-16H2,1-4H3/b7-5+,8-6+	-2.767
InChI=1S/C17H17ClFNO4/c1-9(2)15-16(21)20(17(22)24-15)13-8-14(11(18)7-12(13)19)23-10-5-3h7-8,10H,3-6H2,1-2H3	-6.21
InChI=1S/C4H4ClN3O2/c1-7-2-3(8(9)10)6-4(7)5/h2H,1H3	-0.932
InChI=1S/C32H34N4O3/c1-2-39-29-28(30(37)38)24-33-31(34-29)36-22-20-35(21-23-36)19-18h3-17,24H,2,18-23H2,1H3,(H,37,38)	-7.223
InChI=1S/C4H6OS/c5-4-2-1-3-6-4/h1-3H2	-0.461
InChI=1S/C16H22N2O/c19-16-9-5-7-14-6-1-2-8-15(14)18(16)13-12-17-10-3-4-11-17/h1-2,6,8H,3-5,7,9-13H2	-3.152
InChI=1S/C6H12Cl2O4S2/c7-1-3-13(9,10)5-6-14(11,12)4-2-8/h1-6H2	-1.449

"InChi"	"logS(M)"
InChI=1S/C9H9NO2/c1-8(10(11)12)7-9-5-3-2-4-6-9/h2-7H,1H3/b8-7-	-2.934
InChI=1S/C23H32N6O4S/c1-5-8-20-24-16(4)21-23(30)25-22(26-29(20)21)18-15-17(9-10-19(18)h9-10,15H,5-8,11-14H2,1-4H3,(H,25,26,30)	-4.844
InChI=1S/C14H9N3/c15-8-9-5-6-13-11(7-9)14(16)10-3-1-2-4-12(10)17-13/h1-7H,(H2,16,17)	-3.839
InChI=1S/C16H20N2O2S/c1-19-15-11-16(17-14-6-3-2-5-13(14)15)20-9-4-7-18-8-10-21-12-18/h2-3,5-6,11H,4,7-10,12H2,1H3	-2.907
InChI=1S/C13H10N2O3/c16-12-7-5-11(6-8-12)15-14-10-3-1-9(2-4-10)13(17)18/h1-8,16H,(H,17,18)/b15-14+	-4.38
InChI=1S/C13H20N2O3S/c1-5-6-13(16)15(4)11-7-9-12(10-8-11)19(17,18)14(2)3/h7-10H,5-6H2,1-4H3	-2.16
InChI=1S/C14H13ClN4O/c1-3-19-12-9(5-4-8-16-12)14(20)18(2)10-6-7-11(15)17-13(10)19/h4-8H,3H2,1-2H3	-4.114
InChI=1S/C8H7ClO3/c9-6-4-2-1-3-5(6)7(10)8(11)12/h1-4,7,10H,(H,11,12)	-0.439
InChI=1S/C11H15NO2/c1-2-9(12)5-8-3-4-10-11(6-8)14-7-13-10/h3-4,6,9H,2,5,7,12H2,1H3	-1.574
InChI=1S/C6H13NO2/c1-3-4(2)5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)	-0.503
InChI=1S/C12H18N2O3S/c1-5-12(15)14(4)10-6-8-11(9-7-10)18(16,17)13(2)3/h6-9H,5H2,1-4H3	-2.48
InChI=1S/C8H10O2/c1-9-7-4-3-5-8(6-7)10-2/h3-6H,1-2H3	-2.097
InChI=1S/C22H25F3N2O3/c1-16(28)20-7-2-3-8-21(20)30-15-19(29)14-26-9-11-27(12-10-26)18-6h2-8,13,19,29H,9-12,14-15H2,1H3	-3.906
InChI=1S/C13H26N2O4/c1-5-13(6-2,9-18-11(16)14-7-3)10-19-12(17)15-8-4/h5-10H2,1-4H3,(H,14,16)(H,15,17)	-3.675
InChI=1S/C16H16N4O4/c1-8-6-11-12(7-9(8)2)20(4-5-24-10(3)21)14-13(17-11)15(22)19-16(23)h6-7H,4-5H2,1-3H3,(H,19,22,23)	-2.874
InChI=1S/C13H13ClN2O2S/c1-9-8-10(14)2-7-13(9)16-19(17,18)12-5-3-11(15)4-6-12/h2-8,16H,15H2,1H3	-4.35
InChI=1S/C7H6N2O3S2/c8-14(11,12)7-9-5-2-1-4(10)3-6(5)13-7/h1-3,10H,(H2,8,11,12)	-2.5
InChI=1S/C12H5Cl5/c13-7-4-10(16)12(11(17)5-7)6-1-2-8(14)9(15)3-6/h1-5H	-7.91
InChI=1S/C3HBr2ClO2/c4-1(2(5)6)3(7)8/h(H,7,8)/b2-1-	-1.007
InChI=1S/C6H10O3/c1-3-6(7)9-5-4-8-2/h3H,1,4-5H2,2H3	0.044
InChI=1S/C26H33NO6/c1-30-23-20-12-16-32-24(20)26(31-2)25(33-17-15-27-13-4-3-5-14-27)h6-7,9-10,12,16,21,28-29H,3-5,8,11,13-15,17H2,1-2H3	-4.811

"InChi"	"logS(M)"
InChI=1S/C7H10ClN3O3/c1-5-9-3-7(11(13)14)10(5)4-6(12)2-8/h3,6,12H,2,4H2,1H3	-1.705
InChI=1S/C17H25NO5/c1-3-5-7-18(8-6-4-2)10-13-14-11(17(22)23-13)9-12(19)15(20)16(14)2h9,13,19-21H,3-8,10H2,1-2H3	-1.905
InChI=1S/C22H17N3O5/c1-27-13-17(22(26)28-2)16-8-4-6-10-19(16)30-21-11-20(24-14-25-21)h3-11,13-14H,1-2H3/b17-13-	-4.828
InChI=1S/C12H14Cl3O4P/c1-3-17-20(16,18-4-2)19-12(8-13)10-6-5-9(14)7-11(10)15/h5-8H,3-4H2,1-2H3/b12-8-	-3.462
InChI=1S/C13H15N3O3/c14-10(13(19)16-7-12(17)18)5-8-6-15-11-4-2-1-3-9(8)11/h1-4,6,10,15H,5,7,14H2,(H,16,19)(H,17,18)	-0.85
InChI=1S/C18H27NO2/c1-16-8-5-6-13-19(16)14-7-15-21-18(20)12-11-17-9-3-2-4-10-17/h2-4,9-10,16H,5-8,11-15H2,1H3	-4.178
InChI=1S/C6H17N2O3PS/c7-3-1-2-4-8-5-6-13-12(9,10)11/h8H,1-7H2,(H2,9,10,11)	0.64
InChI=1S/C12H8N2O/c15-11-7-3-6-10-12(11)14-9-5-2-1-4-8(9)13-10/h1-7,13H	-1.925
InChI=1S/C10H18O4/c11-9(12)7-5-3-1-2-4-6-8-10(13)14/h1-8H2,(H,11,12)(H,13,14)	-2.306
InChI=1S/C4H5Cl3O2/c5-2-1-4(6,7)3(8)9/h1-2H2,(H,8,9)	-0.583
InChI=1S/C13H11N3O/c1-7-12-9(6-11(15-7)13(14)17)8-4-2-3-5-10(8)16-12/h2-6,16H,1H3,(H2,14,17)	-3.694
InChI=1S/C19H28N2O/c1-14(2)10-15-4-6-16(7-5-15)11-19(22)21-17-8-9-18(21)13-20(3)12-1h4-7,14,17-18H,8-13H2,1-3H3	-4.36
InChI=1S/C10H20N6O/c1-14(2)8-11-9(15(3)4)13-10(12-8)16(5)6-7-17/h17H,6-7H2,1-5H3	-2.627
InChI=1S/C15H16N2O/c1-12(13-8-4-2-5-9-13)16-17-15(18)14-10-6-3-7-11-14/h2-12,16H,1H3,(H,17,18)	-3.539
InChI=1S/C6H6N2O2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H,7H2	-1.96
InChI=1S/C6H5BrN2O2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H,8H2	-3.558
InChI=1S/C17H26N4O3S2/c1-12(16(5-6-22)26-25-10-15-4-3-7-24-15)21(11-23)9-14-8-19-13(2)2h8,11,15,22H,3-7,9-10H2,1-2H3,(H2,18,19,20)/b16-12-	-2.874
InChI=1S/C13H18N2O/c16-13(11-15-8-4-5-9-15)14-10-12-6-2-1-3-7-12/h1-3,6-7H,4-5,8-11H2,(H,14,16)	-2.237
InChI=1S/C15H16N6O/c16-13(17)9-3-1-5-11(7-9)20-15(22)21-12-6-2-4-10(8-12)14(18)19/h1-8H,(H3,16,17)(H3,18,19)(H2,20,21,22)	-1.77
InChI=1S/C27H34N4O/c28-22-26(23-10-4-1-5-11-23,24-12-6-2-7-13-24)14-19-30-20-15-27(1h1-2,4-7,10-13H,3,8-9,14-21H2,(H2,29,32)	-5.943
InChI=1S/C12H15ClO3/c1-2-3-6-16-11-5-4-9(7-10(11)13)8-12(14)15/h4-5,7H,2-3,6,8H2,1H3,(H,14,15)	-3.673

"InChi"	"logS(M)"
InChI=1S/C13H18N2O3/c1-10(16)15-12(9-18-2)13(17)14-8-11-6-4-3-5-7-11/h3-7,12H,8-9H2,1-2H3,(H,14,17)(H,15,16)	-3.398
InChI=1S/C17H11ClF4N2S/c18-10-5-6-14-12(7-10)16(11-3-1-2-4-13(11)19)23-8-15(25)24(14)9-1h1-7H,8-9H2	-5.461
InChI=1S/C28H46O4/c1-5-9-11-17-23(15-7-3)21-31-27(29)25-19-13-14-20-26(25)28(30)32-h13-14,19-20,23-24H,5-12,15-18,21-22H2,1-4H3	-9.65
InChI=1S/C21H26ClNO2/c1-4-23-12-11-16-13-20(24-2)21(25-3)14-18(16)19(23)10-7-15-5-8-17h5-6,8-9,13-14,19H,4,7,10-12H2,1-3H3	-5.389
InChI=1S/C6H10N2O6/c9-5(10)1-3-7(8(13)14)4-2-6(11)12/h1-4H2,(H,9,10)(H,11,12)	0.686
InChI=1S/C7H17N/c1-3-5-7(8)6-4-2/h7H,3-6,8H2,1-2H3	-0.943
InChI=1S/C24H32N2O3/c1-4-24(28)20-6-9-23(10-7-20)29-17-22(27)16-25-11-13-26(14-12-25)h5-10,15,22,27H,4,11-14,16-17H2,1-3H3	-4.248
InChI=1S/C6H12N2O4/c7-5(9)11-3-1-2-4-12-6(8)10/h1-4H2,(H2,7,9)(H2,8,10)	-1.472
InChI=1S/C11H13NO3/c1-3-11(14)15-10-6-4-9(5-7-10)12-8(2)13/h4-7H,3H2,1-2H3,(H,12,13)	-2.72
InChI=1S/C13H16N2O2S/c1-2-8-13(9-6-4-3-5-7-9)10(16)14-12(18)15-11(13)17/h2,4,6,9H,1,3,5,7-8H2,(H2,14,15,16,17,18)	-4.535
InChI=1S/C10H18O/c1-9(2)7-4-5-10(3,6-7)8(9)11/h7-8,11H,4-6H2,1-3H3	-2.27
InChI=1S/C16H18N2O5/c1-9(2)12(19)23-16(10(3)11-7-5-4-6-8-11)13(20)17-15(22)18-14(16)2h4-10H,1-3H3,(H2,17,18,20,21,22)	-4.386
InChI=1S/C16H18O9/c17-9-3-1-8(5-10(9)18)2-4-13(20)25-12-7-16(24,15(22)23)6-11(19)14h1-5,11-12,14,17-19,21,24H,6-7H2,(H,22,23)/b4-2+	-0.947
InChI=1S/C14H11F2NO3S/c15-14(16)21(19,20)17-12-8-4-7-11(9-12)13(18)10-5-2-1-3-6-10/h1-9,14,17H	-3.913
InChI=1S/C10H9Cl3O3/c11-6-4-8(13)9(5-7(6)12)16-3-1-2-10(14)15/h4-5H,1-3H2,(H,14,15)	-3.829
InChI=1S/C15H21NO/c1-4-5-11-16-15(17)13(3)12(2)14-9-7-6-8-10-14/h6-10H,4-5,11H2,1-3H3,(H,16,17)/b13-12-	-4.18
InChI=1S/C3H4N2O3S/c6-9(7,8)3-4-1-2-5-3/h1-2H,(H,4,5)(H,6,7,8)	-0.3
InChI=1S/C10H9NO3S/c11-9-3-1-7-2-4-10(15(12,13)14)6-8(7)5-9/h1-6H,11H2,(H,12,13,14)	-3.05
InChI=1S/C12H5Cl5O/c13-7-2-1-6(5-9(7)15)18-10-4-3-8(14)11(16)12(10)17/h1-5H	-7.67
InChI=1S/C16H17N3O7S2/c1-25-16(18-10(20)5-9-3-2-4-27-9)13(23)19-11(12(21)22)8(6-26-15(1h2-4,14H,5-7H2,1H3,(H2,17,24)(H,18,20)(H,21,22)	-3.609
InChI=1S/C8H16O2/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3,(H,9,10)	-2.3
InChI=1S/C2H3BrCl2O/c3-2(4,5)1-6/h6H,1H2	-0.442

"InChi"	"logS(M)"
InChI=1S/C4H9NOS/c1-4(6)5-2-3-7/h7H,2-3H2,1H3,(H,5,6)	0.152
InChI=1S/C3HBrI2O2/c4-2(6)1(5)3(7)8/h(H,7,8)/b2-1+	-1.289
InChI=1S/C10H16N2O3/c1-3-5-10(6-4-2)7(13)11-9(15)12-8(10)14/h3-6H2,1-2H3,(H2,11,12,13,14,15)	-2.53
InChI=1S/C22H20N2O4/c1-13-3-7-15(8-4-13)23-19-11-18(22(27)28)20(12-17(19)21(25)26)24-h3-12,23-24H,1-2H3,(H,25,26)(H,27,28)	-5.071
InChI=1S/C4H6O3/c1-3(5)7-4(2)6/h1-2H3	0.07
InChI=1S/C11H16O3/c1-9-4-3-5-10(6-9)14-8-11(2,13)7-12/h3-6,12-13H,7-8H2,1-2H3	-1.88
InChI=1S/C20H22Cl3NO2/c1-24-7-6-12-9-19(25-2)20(26-3)10-14(12)18(24)5-4-13-8-16(22)17(2h8-11,18H,4-7H2,1-3H3	-6.472
InChI=1S/C10H9Cl2NO2/c1-5-4-6(11)2-3-7(5)10(9(13)14)8(12)15-10/h2-4,8H,1H3,(H2,13,14)	-3.059
InChI=1S/C7H14O2/c1-2-3-4-8-5-7-6-9-7/h7H,2-6H2,1H3	-0.814
InChI=1S/C18H22N2S/c1-14(12-19(2)3)13-20-15-8-4-6-10-17(15)21-18-11-7-5-9-16(18)20/h4-11,14H,12-13H2,1-3H3	-5.501
InChI=1S/C36H32Cl4N6O8/c1-17(47)33(35(49)41-27-15-29(51-3)23(39)13-31(27)53-5)45-43-25-h7-16,33-34H,1-6H3,(H,41,49)(H,42,50)/b45-43+,46-44+	-8.005
InChI=1S/C13H17NO5/c15-8-6-14(7-9-16)12(17)10-19-13(18)11-4-2-1-3-5-11/h1-5,15-16H,6-10H2	0.43
InChI=1S/C15H14O3/c1-15(2)11-6-4-3-5-10(11)14-12(17)7-9(16)8-13(14)18-15/h3-8,16-17H,1-2H3	-4.651
InChI=1S/C9H14N4O5/c14-5-3-11(4-6-15)8(16)7-12-2-1-10-9(12)13(17)18/h1-2,14-15H,3-7H2	-1.383
InChI=1S/C17H14O2/c1-11(17(18)19)16-10-12-6-2-3-7-13(12)14-8-4-5-9-15(14)16/h2-11H,1H3,(H,18,19)	-5.327
InChI=1S/C12H8N4O2/c17-11-9-6-15-16(10(9)13-7-14-11)12(18)8-4-2-1-3-5-8/h1-7H,(H,13,14,17)	-4.23
InChI=1S/C3H7ClO3S/c1-8(5,6)7-3-2-4/h2-3H2,1H3	-0.433
InChI=1S/C10H13NO2/c1-2-3-4-8-5-6-9(10(12)13)11-7-8/h5-7H,2-4H2,1H3,(H,12,13)	-2.232
InChI=1S/C40H62O6/c1-37(2,3)29-23-27(24-30(35(29)43)38(4,5)6)17-19-33(41)45-21-15-1h23-26,43-44H,13-22H2,1-12H3	-8.106
InChI=1S/C16H26N2S2/c1-7-9-15(3,4)13-17-11-12(19-13)18-14(20-11)16(5,6)10-8-2/h7-10H2,1-6H3	-7.402
InChI=1S/C8H8O/c1-7-2-4-8(6-9)5-3-7/h2-6H,1H3	-1.724
InChI=1S/C16H11BrN4/c17-11-2-1-3-12(7-11)21-16-13-6-10-4-5-18-14(10)8-15(13)19-9-20-1h1-9,18H,(H,19,20,21)	-2.82

"InChi"	"logS(M)"
InChI=1S/C22H20N4O6/c1-3-32-22(28)19-18-12-13-24(14-4-6-16(7-5-14)26(29)30)21(27)20(1h4-11H,3,12-13H2,1-2H3	-6.619
InChI=1S/C10H14O2/c1-3-11-9-7-5-6-8-10(9)12-4-2/h5-8H,3-4H2,1-2H3	-2.41
InChI=1S/C22H26O3/c1-15(2)10-19-20(22(19,3)4)21(23)25-14-17-12-18(24-13-17)11-16-8-h5-10,12-13,19-20H,11,14H2,1-4H3	-6.052
InChI=1S/C6H14O3/c1-2-6(3-7,4-8)5-9/h7-9H,2-5H2,1H3	0.872
InChI=1S/C7H6Cl2/c1-5-2-3-6(8)7(9)4-5/h2-4H,1H3	-3.776
InChI=1S/C18H21NS/c1-19(2)12-5-8-16-15-7-4-3-6-14(15)9-10-18-17(16)11-13-20-18/h3-4,6-8,11,13H,5,9-10,12H2,1-2H3/b16-8+	-5.444
InChI=1S/C16H13NO4S/c18-16-10-14(22(19,20)21)8-11-6-7-13(9-15(11)16)17-12-4-2-1-3-5-1h1-10,17-18H,(H,19,20,21)	-1.976
InChI=1S/C10H5Br5O2/c1-2-5(16)17-3-4-6(11)8(13)10(15)9(14)7(4)12/h2H,1,3H2	-7.806
InChI=1S/C8H12N4O3/c1-3-6-4-10-8(12(14)15)11(6)5-7(13)9-2/h4H,3,5H2,1-2H3,(H,9,13)	-1.612
InChI=1S/C16H35O2P/c1-13(9-15(3,4)5)11-19(17,18)12-14(2)10-16(6,7)8/h13-14H,9-12H2,1-8H3,(H,17,18)	-4.366
InChI=1S/C13H13N3O3S2/c14-21(17,18)12-6-9-5-11(20-13(9)19-12)8-15-7-10-3-1-2-4-16-10/h1-6,15H,7-8H2,(H2,14,17,18)	-1.33
InChI=1S/C8H5NO2S/c9-5-12-7-3-1-2-6(4-7)8(10)11/h1-4H,(H,10,11)	-2.457
InChI=1S/C6H8O4/c1-3-5(7)10-4(2)6(8)9-3/h3-4H,1-2H3	-0.936
InChI=1S/C16H22N2/c1-17-15-9-10-16(17)13-18(12-15)11-5-8-14-6-3-2-4-7-14/h2-8,15-16H,9-13H2,1H3/b8-5+	-2.367
InChI=1S/C7H4ClNO2/c8-4-1-2-5-6(3-4)11-7(10)9-5/h1-3H,(H,9,10)	-1.796
InChI=1S/C6H10O8/c7-1(3(9)5(11)12)2(8)4(10)6(13)14/h1-4,7-10H,(H,11,12)(H,13,14)	-0.323
InChI=1S/C12H24O/c1-3-4-5-6-7-8-9-10-12(2)11-13/h11-12H,3-10H2,1-2H3	-5.152
InChI=1S/C18H24N2O2/c1-2-18(22)20-15-8-9-16(20)13-19(12-15)11-10-17(21)14-6-4-3-5-7-1h3-7,15-16H,2,8-13H2,1H3	-2.796
InChI=1S/C13H16O5/c1-10(14)16-8-13(18-11(2)15)9-17-12-6-4-3-5-7-12/h3-7,13H,8-9H2,1-2H3	-2.803
InChI=1S/C23H32N2O/c1-5-25(6-2)17-16-23(22(24)26,15-14-18(3)4)21-13-9-11-19-10-7-8-1h7-14H,5-6,15-17H2,1-4H3,(H2,24,26)	-6.106
InChI=1S/C15H30O3/c1-3-4-5-6-7-8-9-10-11-12-13-18-15(17)14(2)16/h14,16H,3-13H2,1-2H3	-4.634
InChI=1S/C10H4Cl4/c11-7-1-2-8(12)6-4-10(14)9(13)3-5(6)7/h1-4H	-7.516

"InChi"	"logS(M)"
InChI=1S/C9H14O4/c1-3-12-8(11)6-9(2)5-4-7(10)13-9/h3-6H2,1-2H3	-0.747
InChI=1S/C16H12ClNO/c17-14-9-7-13(8-10-14)16(19)18-11-3-5-12-4-1-2-6-15(12)18/h1-10H,11H2	-4.483
InChI=1S/C20H34O5/c1-2-3-6-9-15(21)12-13-17-16(18(22)14-19(17)23)10-7-4-5-8-11-20(24)25/h4,7,12-13,15-19,21-23H,2-3,5-6,8-11,14H2,1H3,(H,24,25)/b7-4+,13-12+	-2.33
InChI=1S/C15H11NO/c1-3-7-12(8-4-1)14-11-16-15(17-14)13-9-5-2-6-10-13/h1-11H	-5.553
InChI=1S/C11H22O2/c1-9(8-11(3,4)5)6-7-13-10(2)12/h9H,6-8H2,1-5H3	-3.989
InChI=1S/C13H18N4O4/c1-13(2,3)11(19)21-7-17-6-14-9-8(17)10(18)16(5)12(20)15(9)4/h6H,7H2,1-5H3	-2.17
InChI=1S/C8H11N/c1-6-3-4-8(9)7(2)5-6/h3-5H,9H2,1-2H3	-1.335
InChI=1S/C9H7NO5/c11-8(5-9(12)13)6-3-1-2-4-7(6)10(14)15/h1-4H,5H2,(H,12,13)	-1.843
InChI=1S/C18H12N4O4/c1-11-3-5-13(7-15(11)19-9-23)21-17(25)22(18(21)26)14-6-4-12(2)16(h3-8H,1-2H3	-5.037
InChI=1S/C9H5ClN4/c10-8-3-1-2-4-9(8)14-13-7(5-11)6-12/h1-4,14H	-3.358
InChI=1S/C12H19N/c1-2-3-9-12(13)10-11-7-5-4-6-8-11/h4-8,12H,2-3,9-10,13H2,1H3	-2.356
InChI=1S/C18H21N3O/c1-20(2)12-7-13-21-17-11-6-5-10-16(17)19-15-9-4-3-8-14(15)18(21)2h3-6,8-11,19H,7,12-13H2,1-2H3	-4.642
InChI=1S/C9H8N2O3/c10-9(12)6-5-7-3-1-2-4-8(7)11(13)14/h1-6H,(H2,10,12)/b6-5+	-1.284
InChI=1S/C15H23N3O4/c1-12-4-6-13(7-5-12)18(8-2-10-21-14(16)19)9-3-11-22-15(17)20/h4-7H,2-3,8-11H2,1H3,(H2,16,19)(H2,17,20)	-3.162
InChI=1S/C15H15NO4S/c17-15(18)14(11-12-7-3-1-4-8-12)16-21(19,20)13-9-5-2-6-10-13/h1-10,14,16H,11H2,(H,17,18)	-2.924
InChI=1S/C17H31NO3/c1-2-3-4-5-6-7-8-9-10-11-12-18-14-15(17(20)21)13-16(18)19/h15H,2-14H2,1H3,(H,20,21)	-3.223
InChI=1S/C3H5N3S2/c1-7-3-6-5-2(4)8-3/h1H3,(H2,4,5)	-0.516
InChI=1S/C9H6N2S3/c10-5-12-6-13-9-11-7-3-1-2-4-8(7)14-9/h1-4H,6H2	-3.28
InChI=1S/C7H5N3O/c11-7-6-5(9-4-10-7)2-1-3-8-6/h1-4H,(H,9,10,11)	-2.066
InChI=1S/C8H6O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5H,(H,10,11)	-0.37
InChI=1S/C33H56N4OS2/c1-9-11-13-15-17-19-21-39-30-35-29(36-31(37-30)40-22-20-18-16-14h23-24,38H,9-22H2,1-8H3,(H,34,35,36,37)	-7.469
InChI=1S/C4H8N2O/c7-5-6-3-1-2-4-6/h1-4H2	1

"InChi"	"logS(M)"
InChI=1S/C20H25N3S/c1-21-13-15-22(16-14-21)11-6-12-23-17-7-2-4-9-19(17)24-20-10-5-3-h2-5,7-10H,6,11-16H2,1H3	-5.194
InChI=1S/C13H21NO3/c1-4-16-12-9-10(6-7-14)8-11(15-3)13(12)17-5-2/h8-9H,4-7,14H2,1-3H3	-1.502
InChI=1S/C19H15N5O4/c1-28-19-12-15(22-20-13-2-7-16(8-3-13)24(26)27)6-11-18(19)23-21-1h2-12,23H,1H3/b22-20+	-6.964
InChI=1S/C12H7Cl3O/c13-9-6-11(15)12(7-10(9)14)16-8-4-2-1-3-5-8/h1-7H	-6.58
InChI=1S/C22H17ClN2/c23-21-14-8-7-13-20(21)22(25-16-15-24-17-25,18-9-3-1-4-10-18)19-1h1-17H	-7.534
InChI=1S/C12H5Cl5/c13-6-1-2-7(9(14)3-6)8-4-11(16)12(17)5-10(8)15/h1-5H	-7.95
InChI=1S/C16H23NO5/c1-19-13-8-10-6-5-7-11(17-16(18)22-4)9-12(10)14(20-2)15(13)21-3/h8,11H,5-7,9H2,1-4H3,(H,17,18)	-3.326
InChI=1S/C7H8O2/c1-5-4-6(8)2-3-7(5)9/h2-4,8-9H,1H3	-0.207
InChI=1S/C20H36N2/c1-15(2)7-9-17(5)21-19-11-13-20(14-12-19)22-18(6)10-8-16(3)4/h11-18,21-22H,7-10H2,1-6H3	-5.575
InChI=1S/C13H22O/c1-4-5-8-12(14)11-7-6-9-13(2,3)10-11/h4,11H,1,5-10H2,2-3H3	-4.779
InChI=1S/C12H20O2/c1-8(13)14-10-11(2,3)9-5-6-12(10,4)7-9/h9-10H,5-7H2,1-4H3	-3.875
InChI=1S/C11H25NO3S2/c1-3-4-5-6-7-8-11(2)12-9-10-16-17(13,14)15/h11-12H,3-10H2,1-2H3,(H,13,14,15)	-2.273
InChI=1S/C3H5Cl3/c1-2(4)3(5)6/h2-3H,1H3	-1.89
InChI=1S/C6H9NO2S/c1-4(8)7-5-2-3-10-6(5)9/h5H,2-3H2,1H3,(H,7,8)	-0.064
InChI=1S/C10H12O3/c1-10(2,9(11)12)13-8-6-4-3-5-7-8/h3-7H,1-2H3,(H,11,12)	-1.998
InChI=1S/C14H12/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-8H,9-10H2	-4.635
InChI=1S/C20H21NO3/c1-12(19(22)23)14-7-10-17-16(11-14)21-18(24-17)13-5-8-15(9-6-13)2h5-12H,1-4H3,(H,22,23)	-5.642
InChI=1S/C7H14O3/c1-6(9-3)4-5-10-7(2)8/h6H,4-5H2,1-3H3	-0.688
InChI=1S/C12H11N3O2/c1-9(11-3-2-8-17-11)14-15-12(16)10-4-6-13-7-5-10/h2-8H,1H3,(H,15,16)/b14-9-	-3.694
InChI=1S/C6H10O3/c1-3-9-6(8)4-5(2)7/h3-4H2,1-2H3	-0.073
InChI=1S/C6H10O/c1-3-4-6(2)5-7/h4-5H,3H2,1-2H3/b6-4-	-1.057
InChI=1S/C7H6O4/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3,8-9H,(H,10,11)	-0.928
InChI=1S/C4H4ClNO2S2/c5-3-1-2-4(9-3)10(6,7)8/h1-2H,(H2,6,7,8)	-3.296
InChI=1S/C17H33NO7/c1-2-3-4-5-6-7-8-9-10-18-17(23)24-11-12-13(19)14(20)15(21)16(22)2h12-16,19-22H,2-11H2,1H3,(H,18,23)	-3.56

"InChi"	"logS(M)"
InChI=1S/C20H26N2O/c1-4-22(2,3)16-15-20(19(21)23,17-11-7-5-8-12-17)18-13-9-6-10-14-18-h5-14H,4,15-16H2,1-3H3,(H-,21,23)/p+1	-2.655
InChI=1S/C11H19NO2/c1-9(2)7-4-5-10(9,3)11(12,6-7)8(13)14/h7H,4-6,12H2,1-3H3,(H,13,14)	-1.596
InChI=1S/C22H43NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22(26)23(18-20-24)19-21-h9-10,24-25H,2-8,11-21H2,1H3/b10-9+	-5.568
InChI=1S/C10H8O4/c1-13-8-6-4-2-3-5-7(6)14-9(8)10(11)12/h2-5H,1H3,(H,11,12)	-2.886
InChI=1S/C17H16ClN5O3/c18-16-12-15(23(25)26)6-7-17(16)21-20-13-2-4-14(5-3-13)22(10-11-2h2-7,12,24H,1,9-11H2/b21-20+	-6.13
InChI=1S/C16H21NO7/c1-4-23-16(19)24-14-12(20-2)9-11(10-13(14)21-3)15(18)17-5-7-22-8-h9-10H,4-8H2,1-3H3	-2.061
InChI=1S/C23H36N2O2/c1-21(2,3)25-20(27)17-8-7-15-14-6-9-18-23(5,13-11-19(26)24-18)16(h11,13-18H,6-10,12H2,1-5H3,(H,24,26)(H,25,27)	-4.504
InChI=1S/C9H8F8O2/c1-4(2)5(18)19-3-7(12,13)9(16,17)8(14,15)6(10)11/h6H,1,3H2,2H3	-4.046
InChI=1S/C6H8N2O/c1-9-6-3-2-5(7)4-8-6/h2-4H,7H2,1H3	-0.149
InChI=1S/C16H23NO3/c1-13(18)14-6-5-7-16(10-14)20-12-15(19)11-17-8-3-2-4-9-17/h5-7,10,15,19H,2-4,8-9,11-12H2,1H3	-1.723
InChI=1S/C37H29N3O3S/c41-44(42,43)36-14-8-7-13-35(36)40-34-25-19-29(20-26-34)37(27-15h1-26,38-39H,(H,41,42,43)	-8.377
InChI=1S/C7H7N3O3/c8-9-7(11)5-1-3-6(4-2-5)10(12)13/h1-4H,8H2,(H,9,11)	-2.16
InChI=1S/C9H11NO2/c1-10(2)8-5-3-7(4-6-8)9(11)12/h3-6H,1-2H3,(H,11,12)	-3.398
InChI=1S/C10H14O3/c11-6-10(12)8-13-7-9-4-2-1-3-5-9/h1-5,10-12H,6-8H2	-1.008
InChI=1S/C12H19BrN2O4S2/c13-11-5-4-6-12(15-11)19-9-3-1-2-7-14-8-10-20-21(16,17)18/h4-6,14H,1-3,7-10H2,(H,16,17,18)	-2.697
InChI=1S/C8H17Cl/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3	-5.172
InChI=1S/C28H29F2N3O/c29-22-11-7-20(8-12-22)25(21-9-13-23(30)14-10-21)4-3-17-32-18-15-h1-2,5-14,24-25H,3-4,15-19H2,(H,31,34)	-4.664
InChI=1S/C13H28O/c1-13(2)11-9-7-5-3-4-6-8-10-12-14/h13-14H,3-12H2,1-2H3	-5.001
InChI=1S/C10H22O/c1-4-5-6-7-8-9-10(2,3)11/h11H,4-9H2,1-3H3	-2.985
InChI=1S/C3H7BrO2/c4-1-3(6)2-5/h3,5-6H,1-2H2	0.043
InChI=1S/C22H29N3S2/c1-3-26-18-9-10-22-20(17-18)25(19-7-4-5-8-21(19)27-22)12-6-11-24-h4-5,7-10,17H,3,6,11-16H2,1-2H3	-6.835
InChI=1S/C7H9NO2/c9-6-4-2-1-3-5(4)7(10)8-6/h4-5H,1-3H2,(H,8,9,10)	0.155

"InChi"	"logS(M)"
InChI=1S/C14H15NO3/c1-2-18-14(17)13(15-11-16)10-6-9-12-7-4-3-5-8-12/h3-11H,2H2,1H3,(H,15,16)/b9-6+,13-10-	-3.348
InChI=1S/C17H21N3/c1-19(2)15-9-5-13(6-10-15)17(18)14-7-11-16(12-8-14)20(3)4/h5-12,18H,1-4H3	-3.698
InChI=1S/C7H4ClNO/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H	-2.058
InChI=1S/C9H9NO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6H,10H2,(H,11,12)/b6-3+	-0.982
InChI=1S/C8H10O/c1-7-3-2-4-8(5-7)6-9/h2-5,9H,6H2,1H3	-0.388
InChI=1S/C3H4ClNO/c1-2(4)3(5)6/h1H2,(H2,5,6)	-0.21
InChI=1S/C28H20N2O6/c1-33-21-11-3-17(4-12-21)15-23-27(31)35-25(29-23)19-7-9-20(10-8-1h3-16H,1-2H3/b23-15-,24-16-	-6.984
InChI=1S/C20H18O4/c1-20(22-2)12-15(13-8-4-3-5-9-13)17-18(24-20)14-10-6-7-11-16(14)2h3-11,15H,12H2,1-2H3	-1.508
InChI=1S/C12H10Cl2N2O2S/c13-8-1-4-10(5-2-8)16-19(17,18)12-6-3-9(15)7-11(12)14/h1-7,16H,15H2	-4.59
InChI=1S/C7H3I3O2/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2H,(H,11,12)	-7.141
InChI=1S/C14H10O4/c15-10-7-5-9(6-8-10)13(16)11-3-1-2-4-12(11)14(17)18/h1-8,15H,(H,17,18)	-2.73
InChI=1S/C19H20N2O3/c20-14-8-10-15(11-9-14)24-13-5-1-4-12-21-18(22)16-6-2-3-7-17(16)1h2-3,6-11H,1,4-5,12-13,20H2	-4.786
InChI=1S/C9H6ClNO3/c1-5(12)11-7-4-6(10)2-3-8(7)14-9(11)13/h2-4H,1H3	-0.874
InChI=1S/C42H56N4O12/c1-20-11-10-12-21(2)41(54)45-32-27(19-44-46-16-14-43-15-17-46)36h10-13,18-20,22-24,28,33-34,38,43-44,48-50,52H,14-17H2,1-9H3,(H,45,54)/b11-10-,18-13-,21-12-,27-19-	-9.067
InChI=1S/C3H7N/c1-2-3-4/h2H,1,3-4H2	1.243
InChI=1S/C18H34ClN2O8PS/c1-5-6-10-7-11(21(3)8-10)17(24)20-12(9(2)19)15-13(22)14(23)16(18(h9-16,18,22-23H,5-8H2,1-4H3,(H,20,24)(H2,25,26,27)	-3.787
InChI=1S/C36H70O3P/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-40(37)39-36-h17-20H,3-16,21-36H2,1-2H3/q+1/b19-17+,20-18+	-9.534
InChI=1S/C7H4BrNO2/c8-4-1-2-5-6(3-4)11-7(10)9-5/h1-3H,(H,9,10)	-2.33
InChI=1S/C8H19O3PS2/c1-4-9-12(13,10-5-2)11-7-8-14-6-3/h4-8H2,1-3H3	-3.634
InChI=1S/C11H14N4O3/c1-11(2,3)10(17)18-6-15-8-7(4-14-15)9(16)13-5-12-8/h4-5H,6H2,1-3H3,(H,12,13,16)	-2.68
InChI=1S/C13H14N4O6/c18-13(15-3-5-23-6-4-15)9-7-11(14-1-2-14)12(17(21)22)8-10(9)16(19h7-8H,1-6H2	-2.89
InChI=1S/C9H10Cl2O3/c10-6-1-2-9(8(11)3-6)14-5-7(13)4-12/h1-3,7,12-13H,4-5H2	-2.764

"InChi"	"logS(M)"
InChI=1S/C10H12O2/c1-8(11)7-9-3-5-10(12-2)6-4-9/h3-6H,7H2,1-2H3	-1.314
InChI=1S/C21H24N2O3/c1-12-16-10-23-8-7-14-13-5-3-4-6-18(13)22-20(14)19(23)9-15(16)17(h3-6,11-12,15-16,19,22H,7-10H2,1-2H3	-3.863
InChI=1S/C12H4Cl6/c13-5-1-7(11(17)9(15)3-5)8-2-6(14)4-10(16)12(8)18/h1-4H	-8.56
InChI=1S/C17H22N2O/c1-17(20-14-13-19(2)3,15-9-5-4-6-10-15)16-11-7-8-12-18-16/h4-12H,13-14H2,1-3H3	-2.82
InChI=1S/C12H11ClN2O2/c13-7-3-4-9-8(6-7)12(17)15-5-1-2-10(15)11(16)14-9/h3-4,6,10H,1-2,5H2,(H,14,16)	-4.7
InChI=1S/C21H23NO3/c1-4-16-25-21(18-11-7-5-8-12-18,19-13-9-6-10-14-19)20(23)24-17-15h1,5-14H,15-17H2,2-3H3	-3.06
InChI=1S/C10H16N2O4/c1-4-6-10(5-2,8(14)16-3)7(13)12-9(11)15/h4H,1,5-6H2,2-3H3,(H3,11,12,13,15)	-1.92
InChI=1S/C9H10S2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-5,9H,6-7H2	-3.367
InChI=1S/C36H60O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-25-35(37)38-30-28-32(3)23-h20,22-23,26-28H,7-19,21,24-25,29-30H2,1-6H3/b23-20+,27-26+,31-22+,32-28+	-5.72
InChI=1S/C12H16ClNO3/c1-14(2)7-8-16-12(15)9-17-11-5-3-10(13)4-6-11/h3-6H,7-9H2,1-2H3	-1.743
InChI=1S/C15H33NO3S2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-14-15-20-21(17,18)19/h16H,2-15H2,1H3,(H,17,18,19)	-4.424
InChI=1S/C7H10ClN3/c1-5-4-6(11(2)3)10-7(8)9-5/h4H,1-3H3	-1.262
InChI=1S/C20H31NO2S/c22-20(23-14-13-21-11-6-1-2-7-12-21)19(18-10-15-24-16-18)17-8-4-3h10,15-17,19H,1-9,11-14H2	-5.982
InChI=1S/C9H9IN4O4S3/c1-14-8(19-9(12-14)20(11,15)16)13-21(17,18)7-4-2-6(10)3-5-7/h2-5H,1H3,(H2,11,15,16)/b13-8+	-2.77
InChI=1S/C3H9NO/c1-3(5)2-4/h3,5H,2,4H2,1H3	1.124
InChI=1S/C41H50N6O2/c1-38(2,3)24-40(7,8)28-20-26(36(48)34(22-28)46-42-30-15-11-12-16-h11-18,20-23,48-49H,19,24-25H2,1-10H3	-7.974
InChI=1S/C11H13ClO3/c1-8-7-9(12)4-5-10(8)15-6-2-3-11(13)14/h4-5,7H,2-3,6H2,1H3,(H,13,14)	-3.678
InChI=1S/C12H18O/c1-10(13)9-12(2,3)11-7-5-4-6-8-11/h4-8,10,13H,9H2,1-3H3	-2.147
InChI=1S/C29H42O3/c1-26(2,3)19-13-14-23(20(17-19)27(4,5)6)32-25(31)18-15-21(28(7,8)9h13-17,30H,1-12H3	-7.341
InChI=1S/C54H78O3/c1-31-37(22-34-25-40(49(4,5)6)46(55)41(26-34)50(7,8)9)32(2)39(24-h25-30,55-57H,22-24H2,1-21H3	-7.981
InChI=1S/C7H7N3O2S/c1-5-9-7-6(3-2-4-8-7)13(11,12)10-5/h2-4H,1H3,(H,8,9,10)	-0.426

"InChi"	"logS(M)"
InChI=1S/C11H16O5/c1-14-9-4-3-5-10(11(9)15-2)16-7-8(13)6-12/h3-5,8,12-13H,6-7H2,1-2H3	-3
InChI=1S/C17H19NO4/c1-11-7-5-8-12(2)15(11)18(13(3)17(20)21-4)16(19)14-9-6-10-22-14/h5-10,13H,1-4H3	-3.117
InChI=1S/C18H23N3O3/c1-2-18(22)20-16-8-9-17(20)13-19(12-16)10-4-6-14-5-3-7-15(11-14)21h3-7,11,16-17H,2,8-10,12-13H2,1H3/b6-4+	-4.219
InChI=1S/C12H18N2O3/c1-3-17-12(16)9-7-13-10-6-4-5-8(2)14(10)11(9)15/h7-8,10,13H,3-6H2,1-2H3	-2.228
InChI=1S/C15H16N2O5/c1-3-11(18)22-15(9(2)10-7-5-4-6-8-10)12(19)16-14(21)17-13(15)20/h4-9H,3H2,1-2H3,(H2,16,17,19,20,21)	-3.863
InChI=1S/C14H19ClO3/c1-2-3-4-5-6-9-18-14(17)11-7-8-13(16)12(15)10-11/h7-8,10,16H,2-6,9H2,1H3	-4.23
InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,7-8H,5-6H2,1-3H3	-4.196
InChI=1S/C16H21ClN2O4S2/c17-13-4-5-14-15(12-13)19-8-6-16(14)23-10-3-1-2-7-18-9-11-24-25(21h4-6,8,12,18H,1-3,7,9-11H2,(H,20,21,22)	-3.671
InChI=1S/C18H20Cl2/c1-3-13-5-9-15(10-6-13)17(18(19)20)16-11-7-14(4-2)8-12-16/h5-12,17-18H,3-4H2,1-2H3	-7.04
InChI=1S/C13H17NO4/c1-3-18-13(17)12(14-9(2)15)8-10-4-6-11(16)7-5-10/h4-7,12,16H,3,8H2,1-2H3,(H,14,15)	-1.859
InChI=1S/C15H21NO2S/c1-15(2,16-8-10-18-11-9-16)14(17)12-4-6-13(19-3)7-5-12/h4-7H,8-11H2,1-3H3	-4.193
InChI=1S/C19H21N3S/c1-14(12-21(2)3)13-22-16-6-4-5-7-18(16)23-19-9-8-15(11-20)10-17(1h4-10,14H,12-13H2,1-3H3	-5.79
InChI=1S/C12H18O5/c1-16-10-4-2-3-5-11(10)17-9-12(6-13,7-14)8-15/h2-5,13-15H,6-9H2,1H3	-1.398
InChI=1S/C20H23FN2O2/c21-17-8-6-16(7-9-17)20(25)19(24)10-11-22-12-14-23(15-13-22)18-4h1-9,19,24H,10-15H2	-2.603
InChI=1S/C10H18O4S2/c1-3-15-7(9(11)12)5-6-8(10(13)14)16-4-2/h7-8H,3-6H2,1-2H3,(H,11,12)(H,13,14)	-1.36
InChI=1S/C17H17N/c1-2-11-18-12-14-7-3-5-9-16(14)17-10-6-4-8-15(17)13-18/h2-10H,1,11-13H2	-4.691
InChI=1S/C13H12N4O5S/c1-9(18)15-12-6-7-14-8-13(12)16-23(21,22)11-4-2-10(3-5-11)17(19)2h2-8,16H,1H3,(H,14,15,18)	-3.39
InChI=1S/C37H21N5O4/c43-31-21-12-4-6-14-23(21)33(45)29-25(31)16-8-18-27(29)38-36-40-3h1-19H,(H2,38,39,40,41,42)	-7.778
InChI=1S/C15H14O6S/c16-15(20-11-12-7-3-1-4-8-12)14(21-22(17,18)19)13-9-5-2-6-10-13/h1-10,14H,11H2,(H,17,18,19)	-1.5

"InChi"	"logS(M)"
InChI=1S/C16H23FN2O6/c1-15(2,3)12(21)24-8-18-7-10(17)11(20)19(14(18)23)9-25-13(22)16(4h7H,8-9H2,1-6H3	-3.9
InChI=1S/C9H7ClO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6H,(H,11,12)/b6-3+	-2.457
InChI=1S/C16H14N2O3/c1-3-14-15(9(2)18-21-14)17-12-8-13(19)16(20)11-7-5-4-6-10(11)12/h4-8,19H,3H2,1-2H3/b17-12+	-2.72
InChI=1S/C14H22N2O4S/c1-4-5-6-7-8(17)15-9-11(18)16-10(13(19)20)14(2,3)21-12(9)16/h9-10,12H,4-7H2,1-3H3,(H,15,17)(H,19,20)	-3.517
InChI=1S/C14H12N2/c1-15-14-10-6-2-4-8-12(10)16-13-9-5-3-7-11(13)14/h2-9H,1H3,(H,15,16)	-4.349
InChI=1S/C14H20O3/c1-5-8-17-13-11(9(2)3)7-6-10(4)12(13)14(15)16/h6-7,9H,5,8H2,1-4H3,(H,15,16)	-4.203
InChI=1S/C12H6Cl4O/c13-8-6-9(14)11(16)12(10(8)15)17-7-4-2-1-3-5-7/h1-6H	-7.02
InChI=1S/C13H17NO3/c1-3-14(4-2)12(15)10-17-13(16)11-8-6-5-7-9-11/h5-9H,3-4,10H2,1-2H3	-2.071
InChI=1S/C21H26N2O4/c1-26-20-6-3-5-18(13-20)23-10-8-22(9-11-23)14-19(25)16-27-21-7-2-h2-7,12-13,15,19,25H,8-11,14,16H2,1H3	-2.805
InChI=1S/C13H16O3/c14-12(15)11-8-4-5-9-13(11,16)10-6-2-1-3-7-10/h1-3,6-7,11,16H,4-5,8-9H2,(H,14,15)	-2.027
InChI=1S/C8H6Cl2O3/c9-5-1-6(10)3-7(2-5)13-4-8(11)12/h1-3H,4H2,(H,11,12)	-2.362
InChI=1S/C13H12O3/c1-2-16-12-8-7-11(13(14)15)9-5-3-4-6-10(9)12/h3-8H,2H2,1H3,(H,14,15)	-4.112
InChI=1S/C21H42O4/c1-19(2)15-13-11-9-7-5-3-4-6-8-10-12-14-16-21(24)25-20(17-22)18-2h19-20,22-23H,3-18H2,1-2H3	-6.856
InChI=1S/C9H8Cl3NO2S/c10-9(11,12)16-13-7(14)5-3-1-2-4-6(5)8(13)15/h1-2,5-6H,3-4H2	-4.77
InChI=1S/C10H12ClNO2/c1-2-9(14-10(12)13)7-5-3-4-6-8(7)11/h3-6,9H,2H2,1H3,(H2,12,13)	-3.11
InChI=1S/C8H18NO4PS2/c1-9-8(10)4-5-15-6-7-16-14(11,12-2)13-3/h4-7H2,1-3H3,(H,9,10)	0.542
InChI=1S/C15H12N2O3/c18-12-8-6-11(7-9-12)15(10-4-2-1-3-5-10)13(19)16-14(20)17-15/h1-9,18H,(H2,16,17,19,20)	-2.029
InChI=1S/C5H9NOS/c1-8-3-2-5(7)4-6/h5,7H,2-3H2,1H3	-0.077
InChI=1S/C10H12N4O4S/c15-1-4-6(16)7(17)10(18-4)14-3-13-5-8(14)11-2-12-9(5)19/h2-4,6-7,10,15-17H,1H2,(H,11,12,19)	-2.071
InChI=1S/C3H4FNS/c4-1-2-6-3-5/h1-2H2	-0.957

"InChi"	"logS(M)"
InChI=1S/C12H20N2O3S/c1-3-8(4-2)7-12(5-6-15)9(16)13-11(18)14-10(12)17/h8,15H,3-7H2,1-2H3,(H2,13,14,16,17,18)	-3.14
InChI=1S/C12H15N5O2/c1-18-9-4-3-7(11(16-9)19-2)5-8-6-15-12(14)17-10(8)13/h3-4,6H,5H2,1-2H3,(H4,13,14,15,17)	-2.823
InChI=1S/C22H32O3/c1-4-20(24)25-15-9-11-21(2)14(13-15)5-6-16-17-7-8-19(23)22(17,3)11h5,15-18H,4,6-13H2,1-3H3	-4.69
InChI=1S/C7H8N4S/c8-7(12)11-10-5-6-2-1-3-9-4-6/h1-5H,(H3,8,11,12)/b10-5+	0.106
InChI=1S/C16H24N4O4/c1-4-5-6-7-8-9-12(21)24-11-20-10-17-14-13(20)15(22)19(3)16(23)18(h10H,4-9,11H2,1-3H3	-3.45
InChI=1S/C17H13ClN6O5/c1-8(25)15(23-22-12-4-2-9(18)6-14(12)24(28)29)16(26)19-10-3-5-11-h2-7,15H,1H3,(H,19,26)(H2,20,21,27)/b23-22+	-7.474
InChI=1S/C17H14O/c1-2-6-14(7-3-1)13-18-17-11-10-15-8-4-5-9-16(15)12-17/h1-12H,13H2	-6.478
InChI=1S/C10H13NO/c1-2-11-10(12)8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,11,12)	-1.246
InChI=1S/C11H12N2O2/c14-10-7-6-9(13-10)11(15)12-8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H,12,15)(H,13,14)	-1.328
InChI=1S/C16H26O2/c1-3-5-12-16(18,13-6-4-2)15(17)14-10-8-7-9-11-14/h7-11,15,17-18H,3-6,12-13H2,1-2H3	-3.223
InChI=1S/C16H14N2O3S/c1-11-15(12-7-9-14(10-8-12)22(17,19)20)16(18-21-11)13-5-3-2-4-6-1h2-10H,1H3,(H2,17,19,20)	-4.52
InChI=1S/C11H16N2O3S2/c1-8-3-4-10(5-9(8)2)6-13-11(12)7-17-18(14,15)16/h3-5H,6-7H2,1-2H3,(H2,12,13)(H,14,15,16)	-2.899
InChI=1S/C9H10ClNO/c1-11(2)9(12)7-3-5-8(10)6-4-7/h3-6H,1-2H3	-1
InChI=1S/C18H15NO2/c1-2-21-18(20)16(13-19)17(14-9-5-3-6-10-14)15-11-7-4-8-12-15/h3-12H,2H2,1H3	-7.744
InChI=1S/C5H9NO2/c1-3-5(7)4(2)6-8/h8H,3H2,1-2H3/b6-4+	-1.951
InChI=1S/C8H19N/c1-7(2)5-4-6-8(3)9/h7-8H,4-6,9H2,1-3H3	-1.421
InChI=1S/C18H22N2O2/c1-12(2)19-10-13(21)11-22-17-9-5-8-16-18(17)14-6-3-4-7-15(14)20-1h3-9,12-13,19-21H,10-11H2,1-2H3	-4.544
InChI=1S/C11H16O2/c1-11(2,3)9-7-8(13-4)5-6-10(9)12/h5-7,12H,1-4H3	-2.927
InChI=1S/C5H8O/c6-5-3-1-2-4-5/h1-4H2	0.554
InChI=1S/C9H11NO3/c11-6-5-10-9(13)7-3-1-2-4-8(7)12/h1-4,11-12H,5-6H2,(H,10,13)	-0.393
InChI=1S/C11H12O4/c1-2-5-10(12)15-9-7-4-3-6-8(9)11(13)14/h3-4,6-7H,2,5H2,1H3,(H,13,14)	-2.598
InChI=1S/C3H6O2S/c4-3(5)1-2-6/h6H,1-2H2,(H,4,5)	0.755
InChI=1S/C9H9ClO/c1-6-3-7(2)5-8(4-6)9(10)11/h3-5H,1-2H3	-3.329

"InChi"	"logS(M)"
InChI=1S/C14H18N4O3S/c1-10(2)9-18-8-7-13(16-14(18)19)17-22(20,21)12-5-3-11(15)4-6-12/h3-8,10H,9,15H2,1-2H3,(H,16,17,19)	-3.11
InChI=1S/C9H18N2O4/c1-6(2)3-7(4-14-8(10)12)5-15-9(11)13/h6-7H,3-5H2,1-2H3,(H2,10,12)(H2,11,13)	-1.601
InChI=1S/C12H24O2/c1-12(2,3)10-8-6-4-5-7-9-11(13)14/h4-10H2,1-3H3,(H,13,14)	-2.111
InChI=1S/C12H6Cl4/c13-8-5-4-7(6-11(8)16)12-9(14)2-1-3-10(12)15/h1-6H	-7.02
InChI=1S/C16H21NO2/c18-12-5-4-11-9-15-13-3-1-2-6-16(13,14(11)10-12)7-8-17(15)19/h4-5,10,13,15,17-18H,1-3,6-9H2	-2.705
InChI=1S/C17H25NO6/c1-9-7-17(3,24-10(2)19)8-12(16(9)23)13(20)4-11-5-14(21)18-15(22)6h9,11-13,20H,4-8H2,1-3H3,(H,18,21,22)	-1.316
InChI=1S/C11H10O2/c12-11(13)9-5-4-8-10-6-2-1-3-7-10/h1-9H,(H,12,13)/b8-4+,9-5+	-3.64
InChI=1S/C16H15FN2O5/c1-2-6-13(20)24-10-18-9-12(17)15(22)19(16(18)23)14(21)11-7-4-3-5-h3-5,7-9H,2,6,10H2,1H3	-3.73
InChI=1S/C12H7Br4O5P/c13-5-1-7(11(17)9(15)3-5)8-2-6(14)4-10(16)12(8)21-22(18,19)20/h1-4,17H,(H2,18,19,20)	-7.896
InChI=1S/C12H24/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-12H2	-7.022
InChI=1S/C14H18N2/c1-10-5-3-6-11-12(9-15-14(10)11)13-7-4-8-16(13)2/h3,5-6,9,13,15H,4,7-8H2,1-2H3	-2.144
InChI=1S/C13H12N2O/c1-10-2-4-11(5-3-10)13(16)15-12-6-8-14-9-7-12/h2-9H,1H3,(H,14,15,16)	-2.986
InChI=1S/C14H13NO/c15-14(16)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H,(H2,15,16)	-2.604
InChI=1S/C12H11ClF3NO3/c13-9-3-1-8(2-4-9)11(12(14,15)16)17-20-7-10-18-5-6-19-10/h1-4,10H,5-7H2/b17-11-	-4.014
InChI=1S/C12H22O3/c1-4-7-14-10-12(6-3,9-13)11-15-8-5-2/h4-5,13H,1-2,6-11H2,3H3	-1.718
InChI=1S/C16H26O3/c1-10(2)6-11(3)7-12(4)8-13(5)14-9-15(17)19-16(14)18/h8,10-12,14H,6-7,9H2,1-5H3/b13-8+	-4.426
InChI=1S/C24H46O4/c1-21(2)15-9-5-7-13-19-27-23(25)17-11-12-18-24(26)28-20-14-8-6-10h21-22H,5-20H2,1-4H3	-6.601
InChI=1S/C12H14N4O2S/c1-8-7-14-12(15-9(8)2)16-19(17,18)11-5-3-10(13)4-6-11/h3-7H,13H2,1-2H3,(H,14,15,16)	-3.143
InChI=1S/C8H14O4/c1-3-10-7(9)6-8(2)11-4-5-12-8/h3-6H2,1-2H3	-0.145
InChI=1S/C9H11FN2O4/c1-2-3-7(13)16-5-12-8(14)6(10)4-11-9(12)15/h4H,2-3,5H2,1H3,(H,11,15)	-1.13

"InChi"	"logS(M)"
InChI=1S/C15H13Cl2NO2/c1-9-7-8-11(16)14(13(9)17)18-12-6-4-3-5-10(12)15(19)20-2/h3-8,18H,1-2H3	-6.856
InChI=1S/C10H20N2S/c1-3-6-11-8-5-9-12(7-4-2)10(11)13/h3-9H2,1-2H3	-2.071
InChI=1S/C9H10O2/c1-6-4-3-5-8(7(6)2)9(10)11/h3-5H,1-2H3,(H,10,11)	-2.54
InChI=1S/C6H8ClN7O/c7-2-4(9)13-3(8)1(12-2)5(15)14-6(10)11/h(H4,8,9,13)(H4,10,11,14,15)	-2.87
InChI=1S/C18H21ClN2O2S/c1-20(2)7-4-8-21-14-9-12(19)5-6-16(14)24-17-11-13(22)10-15(23-3)1h5-6,9-11,22H,4,7-8H2,1-3H3	-5.766
InChI=1S/C8H8N4O/c1-5-8(13)12(2)7-6(11-5)3-9-4-10-7/h3-4H,1-2H3	-1.489
InChI=1S/C7H12O7/c8-1-2(9)3(10)6-4(11)5(12)7(13)14-6/h2-6,8-12H,1H2	0.335
InChI=1S/C6H15NO3/c8-4-1-7(2-5-9)3-6-10/h8-10H,1-6H2	0.826
InChI=1S/C10H13NO2/c1-2-3-7-13-10(12)9-5-4-6-11-8-9/h4-6,8H,2-3,7H2,1H3	-1.837
InChI=1S/C9H7NO6/c1-16-9(13)7-4-5(10(14)15)2-3-6(7)8(11)12/h2-4H,1H3,(H,11,12)/p-1	-1.721
InChI=1S/C28H16N2O4/c29-19-11-9-13(21-23(19)27(33)17-7-3-1-5-15(17)25(21)31)14-10-12-h1-12H,29-30H2	-6.294
InChI=1S/C22H22F3NO6/c1-29-16-8-6-12-13(10-15(16)27)14(26-21(28)22(23,24)25)7-5-11-9-1h6,8-10,14H,5,7H2,1-4H3,(H,26,28)	-3.973
InChI=1S/C12H3Cl7/c13-4-1-2-5(14)10(17)8(4)9-6(15)3-7(16)11(18)12(9)19/h1-3H	-8.15
InChI=1S/C9H13N3O4/c1-3-7-5-10-9(12(14)15)11(7)6-8(13)16-4-2/h5H,3-4,6H2,1-2H3	-2.524
InChI=1S/C10H20O2/c1-3-5-7-9-12-10(11)8-6-4-2/h3-9H2,1-2H3	-3.624
InChI=1S/C6H11NO/c1-7-5-3-2-4-6(7)8/h2-5H2,1H3	-0.356
InChI=1S/C9H11FO3/c10-8-3-1-2-4-9(8)13-6-7(12)5-11/h1-4,7,11-12H,5-6H2	-1.124
InChI=1S/C15H20N2S/c1-16(2)10-11-17(13-15-9-6-12-18-15)14-7-4-3-5-8-14/h3-9,12H,10-11,13H2,1-2H3	-2.258
InChI=1S/C12H15NO3/c1-2-9-16-11-6-3-10(4-7-11)5-8-12(14)13-15/h3-8,15H,2,9H2,1H3,(H,13,14)/b8-5+	-2.773
InChI=1S/C8H6N2O2/c11-7-8(12)10-6-4-2-1-3-5(6)9-7/h1-4H,(H,9,11)(H,10,12)	-2.812
InChI=1S/C11H14N2O3/c1-4-6-11(7-5-2)8(14)12-10(16)13(3)9(11)15/h4-5H,1-2,6-7H2,3H3,(H,12,14,16)	-2.146
InChI=1S/C17H31NO2/c1-15-8-5-6-11-18(15)12-7-13-20-17(19)14-16-9-3-2-4-10-16/h15-16H,2-14H2,1H3	-4.601
InChI=1S/C14H8O5/c15-8-5-9(16)14(19)11-10(8)12(17)6-3-1-2-4-7(6)13(11)18/h1-5,15-16,19H	-4.602

"InChi"	"logS(M)"
InChI=1S/C43H60N2O12/c1-9-11-13-21-31-42(6,7)38(50)39(51)43(54,57-31)28(10-2)40(52)44-h9,11-22,24,27-28,30-31,34-39,47-51,54H,10,23H2,1-8H3,(H,44,52)(H,45,53)/b11-9+,14-12+,17-16+,20-15+,21-13+,25-18-,26-19-,33-32-	-7.176
InChI=1S/C8H9NO2/c1-5-3-2-4-6(7(5)10)8(9)11/h2-4,10H,1H3,(H2,9,11)	-1.535
InChI=1S/C10H4Cl2FNO2/c11-7-8(12)10(16)14(9(7)15)6-3-1-5(13)2-4-6/h1-4H	-4.644
InChI=1S/C8H12ClNO/c1-3-5-10(6-4-2)8(11)7-9/h3-4H,1-2,5-7H2	-0.945
InChI=1S/C12H20O2/c1-6-12(5,14-11(4)13)9-7-8-10(2)3/h6,8H,1,7,9H2,2-5H3	-3.816
InChI=1S/C4H5N/c1-4(2)3-5/h1H2,2H3	-0.407
InChI=1S/C12H22N2O4/c1-4-7-14-11(16)18-9-12(5-2,6-3)8-17-10(13)15/h4H,1,5-9H2,2-3H3,(H2,13,15)(H,14,16)	-3.043
InChI=1S/C17H14N6O5/c1-9(24)15(22-21-10-2-5-12(6-3-10)23(27)28)16(25)18-11-4-7-13-14(h2-8,15H,1H3,(H,18,25)(H2,19,20,26)/b22-21+	-7.526
InChI=1S/C7H11Cl2NO4/c1-3(11)4(7(13)14-2)10-6(12)5(8)9/h3-5,11H,1-2H3,(H,10,12)	-0.62
InChI=1S/C14H7ClF3NO5/c15-10-5-7(14(16,17)18)1-4-12(10)24-8-2-3-11(19(22)23)9(6-8)13(20h1-6H,(H,20,21)	-3.479
InChI=1S/C12H14N4O4S/c1-19-10-11(14-7-15-12(10)20-2)16-21(17,18)9-5-3-8(13)4-6-9/h3-7H,13H2,1-2H3,(H,14,15,16)	-2.061
InChI=1S/C20H30O2/c1-3-20-11-10-16-15-7-5-14(22-2)12-13(15)4-6-17(16)18(20)8-9-19(2h5,16-19,21H,3-4,6-12H2,1-2H3	-4.703
InChI=1S/C18H19Cl2NO2/c1-14-2-4-15(5-3-14)18(22)23-17-8-6-16(7-9-17)21(12-10-19)13-11-2h2-9H,10-13H2,1H3	-6.261
InChI=1S/C16H24N2O5/c1-6-18(7-2)14(19)10-17-16(20)11-8-12(21-3)15(23-5)13(9-11)22-4/h8-9H,6-7,10H2,1-5H3,(H,17,20)	-1.89
InChI=1S/C19H27NO4/c1-6-10-20-11-15(21)12-24-18-16(13(3)4)9-8-14(5)17(18)19(22)23-7-h1,8-9,13,15,20-21H,7,10-12H2,2-5H3	-3.231
InChI=1S/C5H4BrN/c6-5-3-1-2-4-7-5/h1-4H	-0.881
InChI=1S/C16H17BrN2/c1-19(2)11-9-16(14-4-3-10-18-12-14)13-5-7-15(17)8-6-13/h3-10,12H,11H2,1-2H3/b16-9+	-3.219
InChI=1S/C16H20N2/c1-3-7-15(8-4-1)13-17-11-12-18-14-16-9-5-2-6-10-16/h1-10,17-18H,11-14H2	-1.786
InChI=1S/C12H26S/c1-2-3-4-5-6-7-8-9-10-11-12-13/h13H,2-12H2,1H3	-7.574
InChI=1S/C7H4Br2N2O/c8-3-1-4(9)6-5(2-3)11-7(10)12-6/h1-2H,(H2,10,11)	-4.06
InChI=1S/C18H21N3O2/c1-5-12-20(13-6-2)16-14(3)21(15-10-8-7-9-11-15)18(23)19(4)17(16)2h5-11H,1-2,12-13H2,3-4H3	-3.7

"InChi"	"logS(M)"
InChI=1S/C14H19NO2/c1-17-14(16)13(11-7-3-2-4-8-11)12-9-5-6-10-15-12/h2-4,7-8,12-13,15H,5-6,9-10H2,1H3	-0.065
InChI=1S/C13H14N2O4/c1-2-13(9-6-4-3-5-7-9)10(17)14-12(19)15(8-16)11(13)18/h3-7,16H,2,8H2,1H3,(H,14,17,19)	-1.6
InChI=1S/C7H17O4PS3/c1-4-10-12(13,11-5-2)14-7-15(8,9)6-3/h4-7H2,1-3H3	-2.531
InChI=1S/C13H11N3O3/c1-9-3-2-4-12(14-9)15-13(17)10-5-7-11(8-6-10)16(18)19/h2-8H,1H3,(H,14,15,17)	-3.548
InChI=1S/C12H27NO3S2/c1-11(2)5-4-6-12(3)7-8-13-9-10-17-18(14,15)16/h11-13H,4-10H2,1-3H3,(H,14,15,16)	-2.733
InChI=1S/CH3ClN2O/c2-4-1(3)5/h(H3,3,4,5)	0.326
InChI=1S/C17H15NO3/c1-10-3-5-12(6-4-10)16-18-14-9-13(11(2)17(19)20)7-8-15(14)21-16/h3-9,11H,1-2H3,(H,19,20)	-4.173
InChI=1S/C73H108O12/c1-65(2,3)49-33-45(34-50(61(49)78)66(4,5)6)25-29-57(74)82-41-73(4h33-40,78-81H,25-32,41-44H2,1-24H3	-7.071
InChI=1S/C13H18ClNO3/c1-9(2)5-6-18-12-4-3-10(7-11(12)14)8-13(16)15-17/h3-4,7,9,17H,5-6,8H2,1-2H3,(H,15,16)	-3.777
InChI=1S/C16H15NO2S/c1-17-13-9-11(10-15(18)19)7-8-14(13)20-16(17)12-5-3-2-4-6-12/h2-9,16H,10H2,1H3,(H,18,19)	-4.22
InChI=1S/C8H5NO2S/c10-8(11)6-2-1-3-7(4-6)9-5-12/h1-4H,(H,10,11)	-3.25
InChI=1S/C15H23N/c1-2-8-15(16-11-6-7-12-16)13-14-9-4-3-5-10-14/h3-5,9-10,15H,2,6-8,11-13H2,1H3	-3.437
InChI=1S/C14H17ClN2O/c1-16-12-6-7-13(16)9-17(8-12)14(18)10-2-4-11(15)5-3-10/h2-5,12-13H,6-9H2,1H3	-2.567
InChI=1S/C16H18Cl2N2O4/c1-4-23-14(21)12-9-16(3,15(22)24-5-2)20(19-12)13-7-6-10(17)8-11(1h6-8H,4-5,9H2,1-3H3	-4.271
InChI=1S/C15H19BrN2O5/c1-8-4-9(2)15(10(3)14(8)16)17-11(19)5-18(6-12(20)21)7-13(22)23/h4H,5-7H2,1-3H3,(H,17,19)(H,20,21)(H,22,23)	-5.497
InChI=1S/C18H39N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-19H2,1H3	-3.631
InChI=1S/C8H11NO3S/c1-5-3-6(2)8(9)7(4-5)13(10,11)12/h3-4H,9H2,1-2H3,(H,10,11,12)	-1.82
InChI=1S/C12H6Cl4/c13-8-3-1-7(2-4-8)12-10(15)5-9(14)6-11(12)16/h1-6H	-6.94
InChI=1S/C4H3BrN2O2/c5-2-1-6-4(9)7-3(2)8/h1H,(H2,6,7,8,9)	-2.37
InChI=1S/C13H9NS/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H	-4.38
InChI=1S/C6H7NO3S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,7H2,(H,8,9,10)	-1.141

"InChi"	"logS(M)"
InChI=1S/C8H12N2O2/c11-6-8(10-7(12)9-6)4-2-1-3-5-8/h1-5H2,(H2,9,10,11,12)	-1.358
InChI=1S/C16H21NO3/c1-17-12-7-8-13(17)10-14(9-12)20-16(19)15(18)11-5-3-2-4-6-11/h2-6,12-15,18H,7-10H2,1H3	-1.44
InChI=1S/C9H12BrN3O2/c10-7-6(5-13-3-1-2-4-13)11-9(15)12-8(7)14/h1-5H2,(H2,11,12,14,15)	-1.78
InChI=1S/C24H15Cl2N5O3/c25-13-5-7-17(26)19(10-13)30-31-21-15-4-2-1-3-12(15)9-16(22(21)32)h1-11,30H,(H,27,33)(H2,28,29,34)/b31-21-	-7.462
InChI=1S/C17H20N2/c1-3-7-15(8-4-1)17(16-9-5-2-6-10-16)19-13-11-18-12-14-19/h1-10,17-18H,11-14H2	-2.385
InChI=1S/C11H20O/c1-4-11(2,3)9-5-7-10(12)8-6-9/h9H,4-8H2,1-3H3	-2.657
InChI=1S/C14H15Cl2N/c15-7-9-17(10-8-16)14-6-5-12-3-1-2-4-13(12)11-14/h1-6,11H,7-10H2	-5.287
InChI=1S/C12H18N2O/c1-13-8-9-14(2)12(13)10-4-6-11(15-3)7-5-10/h4-7,12H,8-9H2,1-3H3	-0.421
InChI=1S/C8H8N2S/c1-5-2-3-6-7(4-5)11-8(9)10-6/h2-4H,1H3,(H2,9,10)	-2.662
InChI=1S/C10H14O4/c1-13-9-3-2-4-10(5-9)14-7-8(12)6-11/h2-5,8,11-12H,6-7H2,1H3	-1.45
InChI=1S/C14H22N2O2/c1-2-3-4-9-16-10-11-18-14(17)12-5-7-13(15)8-6-12/h5-8,16H,2-4,9-11,15H2,1H3	-3.27
InChI=1S/C13H20O2/c1-3-10-14-12(2)15-11-9-13-7-5-4-6-8-13/h4-8,12H,3,9-11H2,1-2H3	-3.384
InChI=1S/C20H18O2/c1-13(2)6-5-7-14-10-11-17-18(12-14)20(22)16-9-4-3-8-15(16)19(17)2h3-4,6,8-12H,5,7H2,1-2H3	-7.986
InChI=1S/C9H11N3O2/c1-12(2)11-10-8-5-3-7(4-6-8)9(13)14/h3-6H,1-2H3,(H,13,14)/b11-10+	-0.8
InChI=1S/C8H4N2O3S2/c11-3-5-4-14-8(9-5)6-1-2-7(15-6)10(12)13/h1-4H	-3.148
InChI=1S/C32H58O8/c1-8-14-17-26(11-4)22-37-29(34)20-32(40-25(7)33,31(36)39-24-28(1h26-28H,8-24H2,1-7H3	-7.058
InChI=1S/C5H6O2/c1-4-2-3-5(6)7-4/h2H,3H2,1H3	-0.293
InChI=1S/C9H7NO/c11-6-7-5-10-9-4-2-1-3-8(7)9/h1-6,10H	-1.695
InChI=1S/C16H21Cl2NO2/c1-12-5-2-3-8-19(12)9-4-10-21-16(20)13-6-7-14(17)15(18)11-13/h6-7,11-12H,2-5,8-10H2,1H3	-4.218
InChI=1S/C16H20/c1-11(2)14-10-9-13-7-5-6-8-15(13)16(14)12(3)4/h5-12H,1-4H3	-6.23
InChI=1S/C15H21N5O2/c1-20(2)13-11(21-3)6-9(7-12(13)22-4)5-10-8-18-15(17)19-14(10)16/h6-8H,5H2,1-4H3,(H4,16,17,18,19)	-2.702
InChI=1S/C9H11NO2/c1-2-12-8-6-4-3-5-7(8)9(10)11/h3-6H,2H2,1H3,(H2,10,11)	-1.563

"InChi"	"logS(M)"
InChI=1S/C9H15ClN4OS/c1-9(2,5-10)6-12-13-8(16-6)14(4)7(15)11-3/h5H2,1-4H3,(H,11,15)	-2.47
InChI=1S/C20H29NO5/c1-21-9-8-15-13(12-21)6-5-7-16(15)26-20(22)14-10-17(23-2)19(25-4)h10-11,13,15-16H,5-9,12H2,1-4H3	-3.571
InChI=1S/C6H12N3OP/c10-11(7-1-2-7,8-3-4-8)9-5-6-9/h1-6H2	0.065
InChI=1S/C7H10N2O2/c1-4-5(2)11-7(8-4)9-6(3)10/h1-3H3,(H,8,9,10)	-1.208
InChI=1S/C2HBrF4/c3-1(4)2(5,6)7/h1H	-1.901
InChI=1S/C13H20N2O/c1-13(12(14)16,9-10-15(2)3)11-7-5-4-6-8-11/h4-8H,9-10H2,1-3H3,(H2,14,16)	-1.759
InChI=1S/C6H4N4O3/c11-2-1-7-3-4(8-2)9-6(13)10-5(3)12/h1H,(H3,8,9,10,11,12,13)	-3.34
InChI=1S/C19H28N2O/c1-18(2)12-16(15-10-8-7-9-11-15)13-19(3,4)21(18)17(22)14-20(5)6/h7-12H,13-14H2,1-6H3	-4.613
InChI=1S/C20H23NO4/c1-11(22)24-16-7-5-13-14-10-12-4-6-15(23-3)18-17(12)20(13,19(16)2h4,6-7,13-14,19H,5,8-10H2,1-3H3	-2.85
InChI=1S/C6H13NO3/c1-2-3-4-5-6-10-7(8)9/h2-6H2,1H3	-3.127
InChI=1S/C8H8O2/c1-6-3-2-4-7(9)8(10)5-6/h2-5H,1H3,(H,9,10)	-0.982
InChI=1S/C11H13NO4/c1-12(2)10(14)7-16-11(15)8-5-3-4-6-9(8)13/h3-6,13H,7H2,1-2H3	-1.71
InChI=1S/C10H18O/c1-5-10(11)9(4)7-6-8(2)3/h6,9H,5,7H2,1-4H3	-2.701
InChI=1S/C15H28O2/c16-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-17-15/h1-14H2	-5.904
InChI=1S/C20H24N2O4/c23-17-10-3-1-5-12-21(17)19(25)15-8-7-9-16(14-15)20(26)22-13-6-2-h7-9,14H,1-6,10-13H2	-3.958
InChI=1S/C4H8N8O8/c13-9(14)5-1-6(10(15)16)3-8(12(19)20)4-7(2-5)11(17)18/h1-4H2	-4.825
InChI=1S/C16H13N/c1-2-8-15(9-3-1)17-16-11-10-13-6-4-5-7-14(13)12-16/h1-12,17H	-5.496
InChI=1S/C9H10O3/c1-2-12-9-5-7(6-10)3-4-8(9)11/h3-6,11H,2H2,1H3	-1.764
InChI=1S/C12H10Cl2O6/c1-4-8(13)10(19-5(2)15)7(12(17)18)11(9(4)14)20-6(3)16/h1-3H3,(H,17,18)	-3.585
InChI=1S/C11H16N2O3/c1-4-11(6-5-7(2)3)8(14)12-10(16)13-9(11)15/h5H,4,6H2,1-3H3,(H2,12,13,14,15,16)	-2.25
InChI=1S/C57H104O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-54(h25-30,54H,4-24,31-53H2,1-3H3/b28-25+,29-26+,30-27+	-7.248
InChI=1S/C22H26N2O2/c1-23-14-19-12-13-20(15-23)24(19)21(26)22(16-25,17-8-4-2-5-9-17)1h2-11,19-20,25H,12-16H2,1H3	-3.594
InChI=1S/C4H8Cl2O/c5-1-3-7-4-2-6/h1-4H2	-1.12
InChI=1S/C12H13NO6/c14-9(15)6-12(19,7-10(16)17)11(18)13-8-4-2-1-3-5-8/h1-5,19H,6-7H2,(H,13,18)(H,14,15)(H,16,17)	-0.487

"InChi"	"logS(M)"
InChI=1S/C13H20N4O2/c1-4-5-6-7-8-17-12(18)10-11(14-9-15(10)2)16(3)13(17)19/h9H,4-8H2,1-3H3	-3.359
InChI=1S/C16H16N2O2/c1-12-10-16(19)18(17-12)8-9-20-15-7-6-13-4-2-3-5-14(13)11-15/h2-7,11H,8-10H2,1H3	-3.497
InChI=1S/C15H22ClN3O9/c1-7-12(26-8(2)20)13(27-9(3)21)11(14(25-7)28-10(4)22)17-15(23)19(h7,11-14H,5-6H2,1-4H3,(H,17,23)	-3.417
InChI=1S/C10H13ClN2O3S3/c11-8-1-3-9(4-2-8)17-6-5-13-10(12)7-18-19(14,15)16/h1-4H,5-7H2,(H2,12,13)(H,14,15,16)	-3.362
InChI=1S/C2H5NS/c1-2(3)4/h1H3,(H2,3,4)	0.336
InChI=1S/C6H12O2/c1-2-3-4-5-8-6-7/h6H,2-5H2,1H3	-1.602
InChI=1S/C2H6O2S/c1-5(2,3)4/h1-2H3	0.2
InChI=1S/C10H24NO3PS/c1-5-11(6-2)9-10-16-15(12,13-7-3)14-8-4/h5-10H2,1-4H3	-0.95
InChI=1S/C9H16N2O2/c1-6(2)7-3-4-8(10-12)9(5-7)11-13/h6-7,12-13H,3-5H2,1-2H3/b10-8+,11-9+	-2.39
InChI=1S/C16H24N4O2/c1-3-9-19-14-12(15(21)20(10-4-2)16(19)22)17-13(18-14)11-7-5-6-8-11h11H,3-10H2,1-2H3,(H,17,18)	-4.96
InChI=1S/C8H9NO3S/c1-6(10)7-2-4-8(5-3-7)13(9,11)12/h2-5H,1H3,(H2,9,11,12)	-1.876
InChI=1S/C7H10O5S2/c1-2-12-7(13)14-4(6(10)11)3-5(8)9/h4H,2-3H2,1H3,(H,8,9)(H,10,11)	-1.19
InChI=1S/C13H14Cl2O3/c1-12(2,11(16)17)18-9-5-3-8(4-6-9)10-7-13(10,14)15/h3-6,10H,7H2,1-2H3,(H,16,17)	-4.18
InChI=1S/C8H9FO2S/c1-2-12(10,11)8-5-3-7(9)4-6-8/h3-6H,2H2,1H3	-1.249
InChI=1S/C7H5BrO4/c8-4-1-3(7(11)12)5(9)2-6(4)10/h1-2,9-10H,(H,11,12)	-2.62
InChI=1S/C6H14ClN/c1-3-8(4-2)6-5-7/h3-6H2,1-2H3	-0.691
InChI=1S/C24H52N8O2/c25-17-13-14-20(21(33)15-9-5-1-3-7-11-18-30-23(26)27)32-22(34)16-h20-21,33H,1-19,25H2,(H,32,34)(H4,26,27,30)(H4,28,29,31)	-4.065
InChI=1S/C10H14N2O3/c1-2-3-6-15-10-5-4-8(12(13)14)7-9(10)11/h4-5,7H,2-3,6,11H2,1H3	-3.82
InChI=1S/C16H20N2O3/c1-4-16(12-10-8-7-9-11-12)13(19)17(5-2)15(21)18(6-3)14(16)20/h7-11H,4-6H2,1-3H3	-3.638
InChI=1S/C19H24N4O2/c20-18(21)14-4-8-16(9-5-14)24-12-2-1-3-13-25-17-10-6-15(7-11-17)1h4-11H,1-3,12-13H2,(H3,20,21)(H3,22,23)	-4.067
InChI=1S/C13H18ClNO/c1-4-9-13(2,3)12(16)15-11-7-5-10(14)6-8-11/h5-8H,4,9H2,1-3H3,(H,15,16)	-4.022
InChI=1S/C9H10N4O2/c1-4-5(2)11-7-6(10-4)8(14)12-9(15)13(7)3/h1-3H3,(H,12,14,15)	-2.113

"InChi"	"logS(M)"
InChI=1S/C24H40O3/c1-15(4-9-22(26)27)19-7-8-20-18-6-5-16-14-17(25)10-12-23(16,2)21(h15-21,25H,4-14H2,1-3H3,(H,26,27)	-6
InChI=1S/C8H19N/c1-6-9(7(2)3)8(4)5/h7-8H,6H2,1-5H3	-1.242
InChI=1S/C11H22O3/c1-3-4-5-6-7-8-9-14-11(13)10(2)12/h10,12H,3-9H2,1-2H3	-1.273
InChI=1S/C37H52O3/c1-21(25-18-29(35(5,6)7)32(38)15-22(25)2)14-28(26-19-30(36(8,9)10h15-21,28,38-40H,14H2,1-13H3	-7.134
InChI=1S/C16H15BrO2/c17-12-11-16(15(18)19,13-7-3-1-4-8-13)14-9-5-2-6-10-14/h1-10H,11-12H2,(H,18,19)	-4.069
InChI=1S/C27H28N4O5/c1-3-36-27(34)24-22-15-17-30(19-9-7-18(8-10-19)29-16-5-4-6-23(29)h7-14H,3-6,15-17H2,1-2H3	-4.628
InChI=1S/C14H16ClN3O/c1-11-5-3-6-12(2)14(11)18(13(19)9-15)10-17-8-4-7-16-17/h3-8H,9-10H2,1-2H3	-2.81
InChI=1S/C10H14O3/c1-8(11)10(12)7-13-9-5-3-2-4-6-9/h2-6,8,10-12H,7H2,1H3	-1.28
InChI=1S/C43H53NO14/c1-22-26(55-37(51)32(48)30(24-15-11-9-12-16-24)44-38(52)58-39(3,4h9-18,26-28,30-33,35,46-48,53H,19-21H2,1-8H3,(H,44,52)	-7.509
InChI=1S/C17H26N2O/c1-2-17(16(18)20,15-9-5-3-6-10-15)11-14-19-12-7-4-8-13-19/h3,5-6,9-10H,2,4,7-8,11-14H2,1H3,(H2,18,20)	-3.734
InChI=1S/C9H20N4O4/c1-3-9(4-2,5-16-7(14)12-10)6-17-8(15)13-11/h3-6,10-11H2,1-2H3,(H,12,14)(H,13,15)	-2.54
InChI=1S/C10H7N5O2/c1-7-2-3-9(10(4-7)15(16)17)14-13-8(5-11)6-12/h2-4,14H,1H3	-3.398
InChI=1S/C15H17N3/c1-16-15(17-2)18-9-12-7-3-5-11-6-4-8-13(10-18)14(11)12/h3-8H,9-10H2,1-2H3,(H,16,17)	-1.15
InChI=1S/C9H10O2S/c10-9(11)8(12)6-7-4-2-1-3-5-7/h1-5,8,12H,6H2,(H,10,11)	-1.56
InChI=1S/C15H12O2/c16-14(12-7-3-1-4-8-12)11-15(17)13-9-5-2-6-10-13/h1-10H,11H2	-5.658
InChI=1S/C21H16O2/c22-20-11-9-14-5-1-3-7-16(14)18(20)13-19-17-8-4-2-6-15(17)10-12-2h1-12,22-23H,13H2	-6.538
InChI=1S/C10H10O3S2/c11-9(12)7-15-10(14)13-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,12)	-2.68
InChI=1S/C22H25N3O/c1-24-11-13-25(14-12-24)16-20(17-7-3-2-4-8-17)22(26)19-15-23-21-1h2-10,15,20,23H,11-14,16H2,1H3	-2.989
InChI=1S/C13H24O3/c1-9(2)12-5-4-10(3)6-13(12)15-8-11(7-14)16-13/h9-12,14H,4-8H2,1-3H3	-2.279
InChI=1S/C3H7N3O2/c4-3(5)6-1-2(7)8/h1H2,(H,7,8)(H4,4,5,6)	-1.51
InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2	-1.465

"InChi"	"logS(M)"
InChI=1S/C16H16N2S4/c1-17(13-9-5-3-6-10-13)15(19)21-22-16(20)18(2)14-11-7-4-8-12-14/h3-12H,1-2H3	-6.261
InChI=1S/C10H15NO4S2/c1-15-10-4-2-9(3-5-10)8-11-6-7-16-17(12,13)14/h2-5,11H,6-8H2,1H3,(H,12,13,14)	-0.465
InChI=1S/C21H30O2/c1-5-6-7-8-16-12-17(22)13-20(23)21(16)19-11-15(4)9-10-18(19)14(2)h11-13,18-19,22-23H,2,5-10H2,1,3-4H3	-7.756
InChI=1S/C10H12O3/c1-3-9(11)8-6-7(13-2)4-5-10(8)12/h4-6,12H,3H2,1-2H3	-2.107
InChI=1S/C7H14O6/c1-12-7-6(11)5(10)4(9)3(2-8)13-7/h3-11H,2H2,1H3	0.745
InChI=1S/C18H22N2O/c1-2-18(21)20-16-10-11-17(20)14-19(13-16)12-6-9-15-7-4-3-5-8-15/h3-5,7-8,16-17H,2,10-14H2,1H3	-3.213
InChI=1S/C17H19N3O/c1-13-5-7-14(8-6-13)20(12-17-18-9-10-19-17)15-3-2-4-16(21)11-15/h2-8,11,21H,9-10,12H2,1H3,(H,18,19)	-4.787
InChI=1S/C2HCl3/c3-1-2(4)5/h1H	-1.96
InChI=1S/C15H24N2O/c18-14-7-1-6-13-12-5-3-9-16-8-2-4-11(15(12)16)10-17(13)14/h11-13,15H,1-10H2	-2.201
InChI=1S/C4H6N2/c1-4-5-2-3-6-4/h2-3H,1H3,(H,5,6)	0.512
InChI=1S/C17H25NO2/c1-14-8-11-18(12-9-14)15(2)10-13-20-17(19)16-6-4-3-5-7-16/h3-7,14-15H,8-13H2,1-2H3	-3.798
InChI=1S/C40H56/c1-31(19-13-21-33(3)25-27-37-35(5)23-15-29-39(37,7)8)17-11-12-18-h11-14,17-22,25-28H,15-16,23-24,29-30H2,1-10H3/b12-11+,19-13+,20-14+,27-25+,28-26+,31-17-,32-18+,33-21-,34-22+	-7.554
InChI=1S/C5H10ClF/c6-4-2-1-3-5-7/h1-5H2	-2.666
InChI=1S/C19H29NO2/c1-15(2)17-8-10-18(11-9-17)19(21)22-14-6-13-20-12-5-4-7-16(20)3/h8-11,15-16H,4-7,12-14H2,1-3H3	-4.871
InChI=1S/C7H5N3O/c8-6-9-10(11)7-4-2-1-3-5-7/h1-5H/b10-9-	-2.304
InChI=1S/C10H8O7/c1-17-7-5(9(13)14)2-4(8(11)12)3-6(7)10(15)16/h2-3H,1H3,(H,11,12)(H,13,14)(H,15,16)	-1.535
InChI=1S/C2H3Br2Cl/c3-1-2(4)5/h2H,1H2	-2.555
InChI=1S/C28H52O4/c1-3-5-7-9-11-13-15-17-19-21-25-31-27(29)23-24-28(30)32-26-22-20-h23-24H,3-22,25-26H2,1-2H3/b24-23+	-6.48
InChI=1S/C4H6Cl4O/c5-3(6)1-9-2-4(7)8/h3-4H,1-2H2	-1.12
InChI=1S/C9H10F6O4/c1-3-19-6(17)5(4(2)16)7(18,8(10,11)12)9(13,14)15/h5,18H,3H2,1-2H3	-1.236
InChI=1S/C4H10N2O/c1-3-6(4-2)5-7/h3-4H2,1-2H3	0.016
InChI=1S/C15H14N2O3/c16-15(20)17-11-7-3-1-5-9(11)13(18)14(19)10-6-2-4-8-12(10)17/h1-8,13-14,18-19H,(H2,16,20)	-2.03
InChI=1S/C4H5N3O2/c1-6-3-2-5-4(6)7(8)9/h2-3H,1H3	-0.374

"InChi"	"logS(M)"
InChI=1S/C29H38ClFO8/c1-16(33)37-15-23(35)29-24(38-25(2,3)39-29)12-20-21-10-17(14-32)1h11,14,20-22,24,34H,6-10,12-13,15H2,1-5H3	-5.716
InChI=1S/C5H5NO2/c7-6-4-5-2-1-3-8-5/h1-4,7H/b6-4+	-0.641
InChI=1S/C3H4O3/c4-3-5-1-2-6-3/h1-2H2	0.946
InChI=1S/C12H9NO3/c1-6-5-15-11-4-10-7(2-8(6)11)3-9(13)12(14)16-10/h2-5H,13H2,1H3	-5.08
InChI=1S/C22H20N6O6/c1-26-18-17(19(29)27(2)22(26)32)28(13-25-18)11-16(34-21(31)15-6-4h3-10,13,16H,11-12H2,1-2H3	-4.139
InChI=1S/C8H10O/c1-7-5-3-4-6-8(7)9-2/h3-6H,1-2H3	-2.689
InChI=1S/C11H17NO/c1-8-5-4-6-9(2)11(8)13-7-10(3)12/h4-6,10H,7,12H2,1-3H3	-1.337
InChI=1S/C12H20O4/c1-3-15-11(13)9-5-7-10(8-6-9)12(14)16-4-2/h9-10H,3-8H2,1-2H3	-2.251
InChI=1S/C14H19NO/c1-9-8-12(14(3,4)5)13(16)10(2)11(9)6-7-15/h8,16H,6H2,1-5H3	-4.258
InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-8H,4-5H2,1-3H3	-2.572
InChI=1S/C8H5NO4/c10-8-7-3-6(9(11)12)2-1-5(7)4-13-8/h1-3H,4H2	-2.651
InChI=1S/C12H9I/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H	-5.449
InChI=1S/C10H7NO2/c12-9-6-5-7-3-1-2-4-8(7)10(9)11-13/h1-6,12H	-2.937
InChI=1S/C12H11N5/c1-2-4-9(5-3-1)6-13-11-10-12(15-7-14-10)17-8-16-11/h1-5,7-8H,6H2,(H2,13,14,15,16,17)	-3.6
InChI=1S/C15H10O5S/c1-21(19)9-3-5-13-11(7-9)14(16)10-6-8(15(17)18)2-4-12(10)20-13/h2-7H,1H3,(H,17,18)/p+1	-5.02
InChI=1S/C12H9NO2/c14-11-5-1-9(2-6-11)13-10-3-7-12(15)8-4-10/h1-8,14H	-1.639
InChI=1S/C18H14Cl4N2O/c19-13-2-4-16(21)12(7-13)10-25-18(9-24-6-5-23-11-24)15-3-1-14(20)h1-8,11,18H,9-10H2	-3.54
InChI=1S/C10H8O2/c1-7-2-4-9-8(6-7)3-5-10(11)12-9/h2-6H,1H3	-2.261
InChI=1S/C6H9N2OP/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H4,7,8,9)	-1.148
InChI=1S/C9H12O/c1-2-9(10)8-6-4-3-5-7-8/h3-7,9-10H,2H2,1H3	-2.34
InChI=1S/C12H13ClN2O/c13-11-5-3-10(4-6-11)12(16)9-14-15-7-1-2-8-15/h3-6,9H,1-2,7-8H2/b14-9+	-2.86
InChI=1S/C6H3N3O7/c10-6-4(8(13)14)1-3(7(11)12)2-5(6)9(15)16/h1-2,10H	-1.97
InChI=1S/C3H6N2O7/c6-3(1-11-4(7)8)2-12-5(9)10/h3,6H,1-2H2	-0.366
InChI=1S/C8H18N2O/c1-3-5-7-10(9-11)8-6-4-2/h3-8H2,1-2H3	-2.095
InChI=1S/C6H15O3PS2/c1-4-11-5-6-12-10(7,8-2)9-3/h4-6H2,1-3H3	-1.844
InChI=1S/C14H22O/c1-5-10(3)12-8-7-9-13(14(12)15)11(4)6-2/h7-11,15H,5-6H2,1-4H3	-5.059
InChI=1S/C14H23BrN2O4S2/c15-13-6-7-14(17-12-13)21-10-5-3-1-2-4-8-16-9-11-22-23(18,19)20/h6-7,12,16H,1-5,8-11H2,(H,18,19,20)	-3.74

"InChi"	"logS(M)"
InChI=1S/C14H14N2/c1-2-7-13-11(4-1)5-3-6-12(13)10-14-15-8-9-16-14/h1-7H,8-10H2,(H,15,16)	-4.251
InChI=1S/C13H15F3O2/c1-18-9-3-2-4-12(17)10-5-7-11(8-6-10)13(14,15)16/h5-8H,2-4,9H2,1H3	-3.544
InChI=1S/C7H5Br3O2/c1-2-3(8)5(10)7(12)6(11)4(2)9/h11-12H,1H3	-4.881
InChI=1S/C18H24O4/c1-3-16(19)21-9-11-5-6-14-15-8-12(18(11)14)7-13(15)10-22-17(20)4-h3-4,11-15,18H,1-2,5-10H2	-4.493
InChI=1S/C17H25N3O/c1-2-17(21)20-15-8-9-16(20)13-19(12-15)11-10-18-14-6-4-3-5-7-14/h3-7,15-16,18H,2,8-13H2,1H3	-2.659
InChI=1S/C21H28O6/c1-19-6-5-12(23)7-11(19)3-4-13-14-8-16(25)21(27,17(26)10-22)20(14h5-7,13-16,18,22,24-25,27H,3-4,8-10H2,1-2H3	-2.665
InChI=1S/C17H14F3N5O4S2/c18-17(19,20)11-2-1-3-14(10-11)31(28,29)25-16-22-9-8-15(24-16)23-h1-10H,(H2,21,26,27)(H2,22,23,24,25)	-1.82
InChI=1S/C46H56N4O10/c1-7-42(55)22-28-23-45(40(53)58-5,36-30(14-18-48(24-28)25-42)29-h9-13,15,20-21,26,28,37-39,47,55-56H,7-8,14,16-19,22-25H2,1-6H3	-5.561
InChI=1S/C17H34O4/c1-13-10-16(8,9)12-17(11-13,20-18-14(2,3)4)21-19-15(5,6)7/h13H,10-12H2,1-9H3	-6.481
InChI=1S/C7H14O3/c1-2-7(3-8)4-9-6-10-5-7/h8H,2-6H2,1H3	0.835
InChI=1S/C22H30O2S/c1-13-9-17(23)15(21(3,4)5)11-19(13)25-20-12-16(22(6,7)8)18(24)10-h9-12,23-24H,1-8H3	-7.112
InChI=1S/C21H21N3O4/c25-18-9-16-19-13-8-17-21(4-5-22(17)10-11(13)3-6-28-16)14-7-12(24h1-3,7,13,16-17,19-20H,4-6,8-10H2	-3.731
InChI=1S/C9H18O4/c1-4-9(13-8(2)10)12-7-5-6-11-3/h9H,4-7H2,1-3H3	-0.017
InChI=1S/C23H34O5/c1-21-7-5-15(24)10-14(21)3-4-17-18(21)11-19(25)22(2)16(6-8-23(17,h9,14-19,24-25,27H,3-8,10-12H2,1-2H3	-2.986
InChI=1S/C4H5N3OS/c5-7-3(8)4-6-1-2-9-4/h1-2H,5H2,(H,7,8)	-0.679
InChI=1S/C19H23N3O2/c1-3-20(4-2)13-14-21-16-10-6-5-9-15(16)19(23)22(24)18-12-8-7-11-1h5-12,24H,3-4,13-14H2,1-2H3	-5.243
InChI=1S/C13H28N2S/c1-4-7-10-14-13(16)15(11-8-5-2)12-9-6-3/h4-12H2,1-3H3,(H,14,16)	-4.184
InChI=1S/C20H28N2O/c1-5-22(4)14-13-20(15(2)3,19(21)23)18-12-8-10-16-9-6-7-11-17(16)1h6-12,15H,5,13-14H2,1-4H3,(H2,21,23)	-4.63
InChI=1S/C39H50N10O6/c1-3-23(2)33-39(55)49-32(13-8-15-43-49)38(54)48-16-7-6-12-30(48)3h4-5,10-11,15,20-23,28-33,41H,3,6-9,12-14,16-19H2,1-2H3,(H,40,42)(H,44,51)(H,45,52)(H,46,50)	-2.6

"InChi"	"logS(M)"
InChI=1S/C20H33N3O4/c1-7-23(8-2)19(26)22-15-9-10-18(17(11-15)14(3)24)27-13-16(25)12-2h9-11,16,21,25H,7-8,12-13H2,1-6H3,(H,22,26)	-1.9
InChI=1S/C9H6Cl3NO2/c10-4-1-2-5(6(11)3-4)9(8(13)14)7(12)15-9/h1-3,7H,(H2,13,14)	-3.292
InChI=1S/C17H16BrCl2NO2/c18-14-3-1-13(2-4-14)17(22)23-16-7-5-15(6-8-16)21(11-9-19)12-10-2h1-8H,9-12H2	-7.026
InChI=1S/C6H12N2O2/c1-5-3-8(7-9)4-6(2)10-5/h5-6H,3-4H2,1-2H3	-0.066
InChI=1S/C4H9NO2/c1-4(7)5-2-3-6/h6H,2-3H2,1H3,(H,5,7)	0.987
InChI=1S/C17H20N2O3/c1-3-21-15-9-5-13(6-10-15)18-17(20)19-14-7-11-16(12-8-14)22-4-2/h5-12H,3-4H2,1-2H3,(H2,18,19,20)	-4.44
InChI=1S/C12H14N4O2/c13-11(14)9-5-3-7(17-9)1-2-8-4-6-10(18-8)12(15)16/h3-6H,1-2H2,(H3,13,14)(H3,15,16)	-1.02
InChI=1S/C7H12O4/c1-10-6(8)4-3-5-7(9)11-2/h3-5H2,1-2H3	-0.434
InChI=1S/C8H16BrNO/c1-3-5-8(9,6-4-2)7(10)11/h3-6H2,1-2H3,(H2,10,11)	-1.828
InChI=1S/C22H34O5/c1-6-20(4)11-16(27-17(25)12-23)21(5)13(2)7-9-22(14(3)19(20)26)10-h6,13-14,16,18-19,23,26H,1,7-12H2,2-5H3	-4.647
InChI=1S/C12H14Cl2O3/c1-2-3-6-16-12(15)8-17-11-5-4-9(13)7-10(11)14/h4-5,7H,2-3,6,8H2,1H3	-3.78
InChI=1S/C8H17NO2/c1-4-11-8(10)7(9)5-6(2)3/h6-7H,4-5,9H2,1-3H3	-0.561
InChI=1S/C5H8O4S2/c1-3-10(6,7)5-11(8,9)4-2/h3-4H,1-2,5H2	-3.92
InChI=1S/C6H10O/c1-3-5-7-6-4-2/h3-4H,1-2,5-6H2	-0.021
InChI=1S/C15H12O3/c16-14(17)10-11-5-4-8-13(9-11)15(18)12-6-2-1-3-7-12/h1-9H,10H2,(H,16,17)	-2.764
InChI=1S/C9H11NO4/c11-4-3-10-9(14)7-5-6(12)1-2-8(7)13/h1-2,5,11-13H,3-4H2,(H,10,14)	-0.544
InChI=1S/C20H14N6O6S/c1-2-32-19(29)15(23-22-11-7-9-12(10-8-11)26(30)31)16(27)18-24-25-h3-10,22H,2H2,1H3/b23-15-	-2.222
InChI=1S/C13H11N3O2/c17-13(10-4-2-1-3-5-10)15-14-11-6-8-12(16-18)9-7-11/h1-9,14H,(H,15,17)	-4.684
InChI=1S/C17H26N2O2/c1-4-10-19-11-8-15(9-12-19)21-17(20)18-16-13(2)6-5-7-14(16)3/h5-7,15H,4,8-12H2,1-3H3,(H,18,20)	-4.459
InChI=1S/C19H29NO5/c1-7-23-19(22)17-14(4)8-9-15(13(2)3)18(17)25-12-16(21)24-11-10-20h8-9,13H,7,10-12H2,1-6H3	-3.864
InChI=1S/C16H12ClNO3/c1-9(16(19)20)10-5-6-14-13(8-10)18-15(21-14)11-3-2-4-12(17)7-11/h2-9H,1H3,(H,19,20)	-4.404
InChI=1S/C11H16N2O/c1-7-5-4-6-8(2)10(7)13-11(14)9(3)12/h4-6,9H,12H2,1-3H3,(H,13,14)	-1.253

"InChi"	"logS(M)"
InChI=1S/C12H15ClO3/c1-2-4-9-5-3-6-11(13)12(9)16-8-10(15)7-14/h2-3,5-6,10,14-15H,1,4,7-8H2	-3.445
InChI=1S/C9H11NO3/c10-9(12)7-3-1-2-4-8(7)13-6-5-11/h1-4,11H,5-6H2,(H2,10,12)	0.066
InChI=1S/C9H12N2O4/c10-8(5-12)9(13)6-1-3-7(4-2-6)11(14)15/h1-4,8-9,12-13H,5,10H2	-1.912
InChI=1S/C7H12O2/c1-4-5-9-7(8)6(2)3/h2,4-5H2,1,3H3	-2.065
InChI=1S/C13H11N3/c14-10-3-4-12-9(6-10)5-8-1-2-11(15)7-13(8)16-12/h1-7H,14-15H2	-3.4
InChI=1S/C19H23NO2/c1-20(2)13-7-12-19(21)16-9-4-3-8-15(16)14-22-18-11-6-5-10-17(18)1h3-6,8-11,21H,7,12-14H2,1-2H3	-4.353
InChI=1S/C12H15ClO2/c1-12(2,3)11(14)8-15-10-6-4-9(13)5-7-10/h4-7H,8H2,1-3H3	-3.854
InChI=1S/CHBr2Cl/c2-1(3)4/h1H	-1.9
InChI=1S/C11H14O4/c1-4-15-11(12)8-5-6-9(13-2)10(7-8)14-3/h5-7H,4H2,1-3H3	-2.023
InChI=1S/C12H16O2/c13-10-6-7-11(12(14)8-10)9-4-2-1-3-5-9/h6-9,13-14H,1-5H2	-2.576
InChI=1S/C6H7N3O2/c7-4-1-2-6(9(10)11)5(8)3-4/h1-3H,7-8H2	-2.185
InChI=1S/C16H17NO2/c1-12-7-5-6-10-14(12)11-17-15(16(18)19)13-8-3-2-4-9-13/h2-10,15,17H,11H2,1H3,(H,18,19)	-3.942
InChI=1S/C9H3F5N4O3S2/c10-2-1(3(11)5(13)6(14)4(2)12)7(19)16-8-17-18-9(22-8)23(15,20)21/h(H2,15,20,21)(H,16,17,19)	-1.37
InChI=1S/C14H18ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h4-9,12-13,19H,1-3H3	-3.392
InChI=1S/C18H24N2O3/c1-3-23-17(21)11-13-4-6-15(7-5-13)18(22)20-9-8-14-10-16(20)19(2)1h4-7,14,16H,3,8-12H2,1-2H3	-2.055
InChI=1S/C9H13N3O/c1-7(2)11-12-9(13)8-3-5-10-6-4-8/h3-7,11H,1-2H3,(H,12,13)	-0.825
InChI=1S/C25H37NO3/c1-23(2,3)26-21(27)20-9-8-18-17-7-6-16-14-15(22(28)29)10-12-24(16h6,14,17-20H,7-13H2,1-5H3,(H,26,27)(H,28,29)	-8.76
InChI=1S/C11H11NO/c1-7-6-9-4-3-5-10(13)11(9)12-8(7)2/h3-6,13H,1-2H3	-3.32
InChI=1S/C10H14O/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7,11H,1-3H3	-2.19
InChI=1S/C22H18I6N2O9/c23-9-5-11(25)19(17(27)15(9)21(33)34)29-13(31)7-38-3-1-37-2-4-39-h5-6H,1-4,7-8H2,(H,29,31)(H,30,32)(H,33,34)(H,35,36)	-10.912
InChI=1S/C18H20N2O/c21-18-13-16(14-20(18)15-7-3-1-4-8-15)h1-10,16,19H,11-14H2	-3.126
InChI=1S/C8H8N2O3/c1-3-8(4-2)5(11)9-7(13)10-6(8)12/h3-4H,1-2H2,(H2,9,10,11,12,13)	-2.06
InChI=1S/CH3Cl/c1-2/h1H3	-0.88
InChI=1S/C7H5ClO4/c8-4-1-3(7(11)12)5(9)2-6(4)10/h1-2,9-10H,(H,11,12)	-2.053

"InChi"	"logS(M)"
InChI=1S/C29H44O12/c1-13-22(34)23(35)24(36)25(40-13)41-15-8-19(32)28(12-30)21-17(3- h7,13,15-19,21-25,30-32,34-38H,3-6,8-12H2,1-2H3	-1.752
InChI=1S/C23H32N2O/c1-5-24(6-2)16-11-17-25(23-19(3)12-10-13-20(23)4)22(26)18-21-14-8 h7-10,12-15H,5-6,11,16-18H2,1-4H3	-5.989
InChI=1S/C31H35NO12/c1-14-26(35)17(32-6-8-42-9-7-32)10-21(43-14)44-19-12-31(40,20(34) h3-5,14,17,19,21,26,33,35,37,39-40H,6-13H2,1-2H3	-4.671
InChI=1S/C8H14O3/c1-3-9-5-7-11-8-6-10-4-2/h3-4H,1-2,5-8H2	-1.053
InChI=1S/C15H10BrClN4S/c1-8-19-20-13-7-18-14(9-4-2-3-5-11(9)17)10-6-12(16)22-15(10)21(8) h2-6H,7H2,1H3	-5.563
InChI=1S/C22H28N2O/c1-18-10-8-11-19(2)22(18)24(17-9-16-23(3)4)21(25)15-14-20-12-6-5- h5-8,10-15H,9,16-17H2,1-4H3/b15-14+	-5.235
InChI=1S/C13H13N3O/c1-9-2-7-12(15-8-9)16-13(17)10-3-5-11(14)6-4-10/h2-8H,14H2,1H3, (H,15,16,17)	-2.311
InChI=1S/C8H19O4P/c1-5-10-13(9,11-6-2)12-7-8(3)4/h8H, 5-7H2,1-4H3	-1.177
InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-12-11-13-12/h12H, 2-11H2,1H3	-5.923
InChI=1S/C8H12N4O5/c9-4-1-10-12(8(16)11-4)7-6(15)5(14)3(2-13)17-7/h1,3,5-7,13-15H, 2H2,(H2,9,11,16)	0.154
InChI=1S/C10H20N2O4/c1-7(2)4-10(3,5-15-8(11)13)6-16-9(12)14/ h7H,4-6H2,1-3H3,(H2,11,13)(H2,12,14)	-2.09
InChI=1S/C12H17NO3/c1-3-6-16-11-5-4-10(7-9(11)2)8-12(14)13-15/ h4-5,7,15H,3,6,8H2,1-2H3,(H,13,14)	-2.565
InChI=1S/C24H27O4P/c1-16-7-17(2)11-22(10-16)26-29(25,27-23-12-18(3)8-19(4)13-23)28-2 h7-15H,1-6H3	-7.312
InChI=1S/C8H18O2/c1-6(2)7(10)8(3,4)5-9/h6-7,9-10H,5H2,1-4H3	-0.667
InChI=1S/C14H13BrN2O2/c1-3-9-16-10(2)12(15)13(18)17(14(16)19)11-7-5-4-6-8-11/h3-8H, 1,9H2,2H3	-2.851
InChI=1S/C6H8N2/c7-5-3-1-2-4-6-8/h1-4H2	-0.131
InChI=1S/C11H13ClO4S/c1-8(2)16-11(13)7-17(14,15)10-5-3-9(12)4-6-10/h3-6,8H,7H2,1-2H3	-2.41
InChI=1S/C7H3ClF3NO2/c8-4-1-2-6(12(13)14)5(3-4)7(9,10)11/ h1-3H	-3.353
InChI=1S/C9H14N2OS/c1-3-4-5-7-6(2)10-9(13)11-8(7)12/ h3-5H2,1-2H3,(H2,10,11,12,13)	-2.367
InChI=1S/C12H26S/c1-9(2)10(3,4)11(5,6)12(7,8)13/h9,13H,1-8H3	-7.712
InChI=1S/C13H17NO4/c1-3-4-9-17-13(16)18-12-7-5-11(6-8-12)14-10(2)15/h5-8H, 3-4,9H2,1-2H3,(H,14,15)	-3.37
InChI=1S/C9H11FN2O4/c1-5(2)4-16-9(15)12-3-6(10)7(13)11-8(12)14/h3,5H,4H2,1-2H3,(H, 11,13,14)	-1.89

"InChi"	"logS(M)"
InChI=1S/C12H18O/c1-10-5-4-6-11(7-10)8-12(2,3)9-13/h4-7,13H,8-9H2,1-3H3	-2.827
InChI=1S/C9H8N2O/c10-7-6-9(12)11-8-4-2-1-3-5-8/h1-5H,6H2,(H,11,12)	-2.728
InChI=1S/C13H20O3/c1-3-5-11-7-4-6-10(2)13(11)16-9-12(15)8-14/h4,6-7,12,14-15H,3,5,8-9H2,1-2H3	-3.342
InChI=1S/C10H9N/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,11H2	-2.88
InChI=1S/C9H12FN/c1-7(11)6-8-2-4-9(10)5-3-8/h2-5,7H,6,11H2,1H3	-0.981
InChI=1S/C8H16N2O2/c1-9(2)7(11)5-6-8(12)10(3)4/h5-6H2,1-4H3	0.503
InChI=1S/C16H30O4/c1-13(2)19-15(17)11-9-7-5-6-8-10-12-16(18)20-14(3)4/h13-14H,5-12H2,1-4H3	-5.156
InChI=1S/C14H4N2O2S2/c15-5-9-10(6-16)20-14-12(18)8-4-2-1-3-7(8)11(17)13(14)19-9/h1-4H	-6.33
InChI=1S/C10H8O2/c11-10-7-6-9(12-10)8-4-2-1-3-5-8/h1-7,9H	-1.321
InChI=1S/C8H16O4/c1-3-10-4-5-11-6-7-12-8(2)9/h3-7H2,1-2H3	0.754
InChI=1S/C14H18O6/c1-17-7-9-19-13(15)11-5-3-4-6-12(11)14(16)20-10-8-18-2/h3-6H,7-10H2,1-2H3	-1.521
InChI=1S/C12H17NO2/c1-9(2)7-10-3-5-11(6-4-10)8-12(14)13-15/h3-6,9,15H,7-8H2,1-2H3,(H,13,14)	-2.704
InChI=1S/C19H14/c1-13-6-7-15-12-19-16(11-17(15)10-13)9-8-14-4-2-3-5-18(14)19/h2-12H,1H3	-6.816
InChI=1S/C4H10S/c1-3-4(2)5/h4-5H,3H2,1-2H3	-1.835
InChI=1S/C9H8ClNO2/c1-2-11-7-5-6(10)3-4-8(7)13-9(11)12/h3-5H,2H2,1H3	-3.058
InChI=1S/C10H11ClN2O2/c1-12(2)6-13-8-5-7(11)3-4-9(8)15-10(13)14/h3-5H,6H2,1-2H3	-1.162
InChI=1S/C25H26N2O2/c1-3-7-21(8-4-1)25(22-9-5-2-6-10-22)27-15-13-26(14-16-27)18-20-11-12,17,25H,13-16,18-19H2	-4.943
InChI=1S/C11H16N2O3S3/c1-9-2-4-10(5-3-9)17-7-6-13-11(12)8-18-19(14,15)16/h2-5H,6-8H2,1H3,(H2,12,13)(H,14,15,16)	-3.129
InChI=1S/C16H31NO7/c1-2-3-4-5-6-7-8-9-17-16(22)23-10-11-12(18)13(19)14(20)15(21)24-11h11-15,18-21H,2-10H2,1H3,(H,17,22)	-2.96
InChI=1S/C18H21ClN2O2S/c1-20(2)7-4-8-21-13-9-12(19)5-6-17(13)24-18-11-16(23-3)15(22)10-14h5-6,9-11,22H,4,7-8H2,1-3H3	-5.848
InChI=1S/C9H16N3O5P/c1-3-16-9(14)12(17-8(2)13)18(15,10-4-5-10)11-6-7-11/h3-7H2,1-2H3	-2.239
InChI=1S/C7H6FNO/c8-7-3-1-6(2-4-7)5-9-10/h1-5,10H/b9-5+	-1.951
InChI=1S/C12H16O4/c1-2-7-15-11-5-3-4-6-12(11)16-9-10(14)8-13/h2-6,10,13-14H,1,7-9H2	-1.921
InChI=1S/C10H22O/c1-9(2)5-4-6-10(3)7-8-11/h9-11H,4-8H2,1-3H3	-3.393
InChI=1S/C22H28N2O2/c1-2-26-21(25)22(19-6-4-3-5-7-19)13-16-24(17-14-22)15-12-18-8-10-h3-11H,2,12-17,23H2,1H3	-4.033

"InChi"	"logS(M)"
InChI=1S/C12H11Cl2NO/c1-4-12(2,3)15-11(16)8-5-9(13)7-10(14)6-8/h1,5-7H,2-3H3,(H,15,16)	-4.232
InChI=1S/C13H17BrO3/c1-2-3-4-5-8-17-13(16)10-6-7-12(15)11(14)9-10/h6-7,9,15H,2-5,8H2,1H3	-4.22
InChI=1S/C6H4ClI/c7-5-2-1-3-6(8)4-5/h1-4H	-3.55
InChI=1S/C11H14O/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-8H,1-3H3	-3.131
InChI=1S/C6H7NO4S/c7-5-3-4(12(9,10)11)1-2-6(5)8/h1-3,8H,7H2,(H,9,10,11)	-1.83
InChI=1S/C8H16O2/c1-4-6-7(3)8(9)10-5-2/h7H,4-6H2,1-3H3	-2.49
InChI=1S/C23H34O6/c1-4-13(2)23(27)29-20-11-16(24)9-15-6-5-14(3)19(22(15)20)8-7-18-1h5-6,9,13-14,16-20,22,24-25H,4,7-8,10-12H2,1-3H3	-3.35
InChI=1S/C42H54N8O6/c1-3-26(2)36-42(56)50-19-9-7-14-35(50)41(55)49-18-8-6-13-33(49)3Sh4-5,11-12,16-17,21,24-26,31-36H,3,6-10,13-15,18-20,22-23H2,1-2H3,(H,43,44)(H,45,52)(H,46,53)(H,47,51)	-3.98
InChI=1S/C12H15ClO3/c1-4-15-11(14)12(2,3)16-10-7-5-9(13)6-8-10/h5-8H,4H2,1-3H3	-3.545
InChI=1S/C10H15ClN2O4S2/c11-9-3-1-5-13-10(9)17-7-2-4-12-6-8-18-19(14,15)16/h1,3,5,12H,2,4,6-8H2,(H,14,15,16)	-1.12
InChI=1S/C18H21NO3S/c1-19-11-5-9-15(13-19)22-17(20)18(21,16-10-6-12-23-16)14-7-3-2-4-h2-4,6-8,10,12,15,21H,5,9,11,13H2,1H3	-2.766
InChI=1S/C6H8BrN3O2/c1-5-8-4-6(10(11)12)9(5)3-2-7/h4H,2-3H2,1H3	-2.839
InChI=1S/C23H17NO7/c24-20-17(29-10-11-30-23(28)31-13-6-2-1-3-7-13)12-16(25)18-19(20)h1-9,12,25H,10-11,24H2	-8.054
InChI=1S/C12H14N2O2/c1-12(2)10(15)14(11(16)13-12)8-9-6-4-3-5-7-9/h3-7H,8H2,1-2H3,(H,13,16)	-1.8
InChI=1S/C5H10O/c1-3-5(6)4-2/h3,5-6H,1,4H2,2H3	0.019
InChI=1S/C77H148O8/c1-69(2)57-49-41-33-25-17-9-13-21-29-37-45-53-61-73(78)82-65-77(Ch69-72H,9-68H2,1-8H3	-7.381
InChI=1S/C9H18O/c1-7-4-8(10)6-9(2,3)5-7/h7-8,10H,4-6H2,1-3H3	-1.992
InChI=1S/C7H14N2O/c1-7(2)4-5-8-9(3)6-10/h5-7H,4H2,1-3H3/b8-5+	-1.381
InChI=1S/C17H22N2O2S/c1-13-10-17(21-8-3-6-19-7-9-22-12-19)18-16-5-4-14(20-2)11-15(13)1h4-5,10-11H,3,6-9,12H2,1-2H3	-3.478
InChI=1S/C12H12O2/c13-7-8-14-12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9,13H,7-8H2	-2.714
InChI=1S/C24H40O3/c1-9-11-17(10-2)16-27-21(25)13-12-18-14-19(23(3,4)5)22(26)20(15-1h14-15,17,26H,9-13,16H2,1-8H3	-7.099
InChI=1S/C15H20N4O4S/c1-3-5-11(20)22-9-19-8-18-13-14(19)16-7-17-15(13)24-10-23-12(21)Ch7-8H,3-6,9-10H2,1-2H3	-3.71

"InChi"	"logS(M)"
InChI=1S/C10H11NO4/c1-7(12)11-8-3-5-9(6-4-8)15-10(13)14-2/h3-6H,1-2H3,(H,11,12)	-1.69
InChI=1S/C15H12O3/c16-14(15(17)18)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H,(H,17,18)	-2.335
InChI=1S/C15H21Cl2NO2/c1-11(2)20-15(19)13-5-4-12(3)14(10-13)18(8-6-16)9-7-17/h4-5,10-11H,6-9H2,1-3H3	-6.088
InChI=1S/C14H19N5O5/c1-3-16(4-2)7-8-17-12(20)10-18(14(17)21)15-9-11-5-6-13(24-11)19(2h5-6,9H,3-4,7-8,10H2,1-2H3/b15-9+	-2.667
InChI=1S/C14H19NO/c1-15-11-7-8-12(15)10-14(9-11)16-13-5-3-2-4-6-13/h2-6,11-12,14H,7-10H2,1H3	-2.296
InChI=1S/C10H14N2O3S/c1-11(2)16(14,15)10-6-4-9(5-7-10)12(3)8-13/h4-8H,1-3H3	-2.37
InChI=1S/C8H9NO5/c1-2-5-13-8(10)6-3-4-7(14-6)9(11)12/h3-4H,2,5H2,1H3	-2.539
InChI=1S/C14H13F4N3O2S/c1-8(2)21(10-5-3-9(15)4-6-10)11(22)7-23-13-20-19-12(24-13)14(16,1h3-6,8H,7H2,1-2H3	-3.812
InChI=1S/C14H14O/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10,14-15H,11H2	-2.52
InChI=1S/C23H32N2O/c1-18(2)25(5,19(3)4)17-16-23(22(24)26,20-12-8-6-9-13-20)21-14-10-'h6-15,18-19H,16-17H2,1-5H3,(H-,24,26)/p+1	-2.784
InChI=1S/C6H6N4/c1-4-9-5-2-7-3-8-6(5)10-4/h2-3H,1H3,(H,7,8,9,10)	-0.41
InChI=1S/C11H12N4O3S/c1-15-7-6-10(13-11(15)16)14-19(17,18)9-4-2-8(12)3-5-9/h2-7H,12H2,1H3,(H,13,14,16)	-2.36
InChI=1S/C12H20O10/c13-1-5-7(15)9(17)11(21-5)3-20-12(4-19-11)10(18)8(16)6(2-14)22-12h5-10,13-18H,1-4H2	-0.006
InChI=1S/C4H8O4/c1-7-4(6)2-8-3-5/h5H,2-3H2,1H3	0.92
InChI=1S/C17H17ClFN3O3/c1-7-12(20)6-21(7)15-11(19)4-9-14(13(15)18)22(8-2-3-8)5-10(16(9)2h4-5,7-8,12H,2-3,6,20H2,1H3,(H,24,25)	-4.48
InChI=1S/C7H4ClNO3/c8-3-1-4-6(2-5(3)10)12-7(11)9-4/h1-2,10H,(H,9,11)	-1.204
InChI=1S/C16H25NO2/c1-2-3-4-5-6-7-8-9-13-19-16(18)15-11-10-12-17-14-15/h10-12,14H,2-9,13H2,1H3	-3.19
InChI=1S/C5H10N2O2/c1-3-4-5(8)7(2)6-9/h3-4H2,1-2H3	-1.535
InChI=1S/C13H11O4P/c14-13(15)10-6-8-12(9-7-10)18(16,17)11-4-2-1-3-5-11/h1-9H,(H,14,15)(H,16,17)	-4.07
InChI=1S/C43H58O3/c1-27(34-24-37(41(44)21-28(34)2)31-14-8-5-9-15-31)20-40(35-25-38(h21-27,31-33,40,44-46H,5-20H2,1-4H3	-7.397

"InChi"	"logS(M)"
InChI=1S/C31H31NO2/c33-30(24-14-5-1-6-15-24,25-16-7-2-8-17-25)28-22-13-23-29(32-28)3h1-12,14-21,28-29,32-34H,13,22-23H2	-6.686
InChI=1S/C9H12O/c1-3-8-4-7(2)5-9(10)6-8/h4-6,10H,3H2,1-2H3	-1.77
InChI=1S/C16H18N2O4/c1-10-6-5-7-17-15(10)18-16(19)11-8-12(20-2)14(22-4)13(9-11)21-3/h5-9H,1-4H3,(H,17,18,19)	-2.743
InChI=1S/C6H13N3O5/c7-6(14)9-8-1-3(11)5(13)4(12)2-10/h1,3-5,10-13H,2H2,(H3,7,9,14)/b8-1+	-0.129
InChI=1S/C8H13N3O2/c1-3-8(4-2)5(9)10-7(13)11-6(8)12/h3-4H2,1-2H3,(H3,9,10,11,12,13)	-1.397
InChI=1S/C15H18ClN3O3S/c16-11-1-2-13-12(9-11)19(15(22)23-13)10-14(21)18-5-3-17(4-6-18)7-h1-2,9,20H,3-8,10H2	-2.683
InChI=1S/C13H20N4O2/c1-4-5-6-7-8-9-14-10-11(15-9)16(2)13(19)17(3)12(10)18/h4-8H2,1-3H3,(H,14,15)	-3.358
InChI=1S/C8H16O4/c1-9-7(10-2)5-6-8(11-3)12-4/h5-8H,1-4H3/b6-5+	0.055
InChI=1S/C8H14O4S/c1-3-5(7(9)10)13-6(4-2)8(11)12/h5-6H,3-4H2,1-2H3,(H,9,10)(H,11,12)	-0.71
InChI=1S/C11H10N2S/c12-11(14)13-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H3,12,13,14)	-2.528
InChI=1S/C7H13NO4/c1-3-11-6(9)5-8-7(10)12-4-2/h3-5H2,1-2H3,(H,8,10)	-0.243
InChI=1S/C14H15N3/c1-10-9-13(11-7-8-11)17-14(15-10)16-12-5-3-2-4-6-12/h2-6,9,11H,7-8H2,1H3,(H,15,16,17)	-4.05
InChI=1S/C9H19NO3S2/c11-15(12,13)14-8-7-10-9-5-3-1-2-4-6-9/h9-10H,1-8H2,(H,11,12,13)	-1.12
InChI=1S/C16H17NO3/c1-17-16(19)14-11-13(12-5-3-2-4-6-12)7-8-15(14)20-10-9-18/h2-8,11,18H,9-10H2,1H3,(H,17,19)	-2.952
InChI=1S/C10H14N2O4S2/c11-18(15,16)10-5-3-9(4-6-10)12-7-1-2-8-17(12,13)14/h3-6H,1-2,7-8H2,(H2,11,15,16)	-2.597
InChI=1S/C7H11NO3/c1-4-7(2)5(9)8(3)6(10)11-7/h4H2,1-3H3	-1.272
InChI=1S/C12H9FN2O4/c13-9-6-15(11(17)14-10(9)16)12(18)19-7-8-4-2-1-3-5-8/h1-6H,7H2,(H,14,16,17)	-2.82
InChI=1S/C17H19N5O6S/c1-27-13-9-14(28-2)19-16(18-13)20-17(24)22-29(25,26)21-12-6-4-3-5h3-6,9-10,21H,7-8H2,1-2H3,(H2,18,19,20,22,24)	-6.394
InChI=1S/C9H10O4/c1-12-7-3-6(5-10)4-8(13-2)9(7)11/h3-5,11H,1-2H3	-1.533
InChI=1S/C16H23ClN2O2/c1-11(2)19-9-7-13(8-10-19)21-16(20)18-15-12(3)5-4-6-14(15)17/h4-6,11,13H,7-10H2,1-3H3,(H,18,20)	-4.626
InChI=1S/C7H5NO3/c9-5-6-3-1-2-4-7(6)8(10)11/h1-5H	-1.814
InChI=1S/C21H23ClFNO5/c1-2-3-6-9-28-19(25)12-29-18-11-17(16(23)10-15(18)22)24-20(26)13-h10-11H,2-9,12H2,1H3	-6.351

"InChi"	"logS(M)"
InChI=1S/C7H6O5/c8-4-2-6(10)5(9)1-3(4)7(11)12/h1-2,8-10H,(H,11,12)	-0.959
InChI=1S/C10H22O5/c1-11-3-5-13-7-9-15-10-8-14-6-4-12-2/h3-10H2,1-2H3	0.653
InChI=1S/C12H6Cl4O/c13-7-1-3-8(4-2-7)17-12-10(15)6-5-9(14)11(12)16/h1-6H	-6.64
InChI=1S/C9H12ClN/c1-11(2)7-8-5-3-4-6-9(8)10/h3-6H,7H2,1-2H3	-1.849
InChI=1S/C10H18O2/c1-5-9(3,11)7-8-10(4,12)6-2/h11-12H,5-6H2,1-4H3	-1.973
InChI=1S/C18H22O2/c1-17(2,15-11-7-5-8-12-15)19-20-18(3,4)16-13-9-6-10-14-16/h5-14H,1-4H3	-5.769
InChI=1S/C13H13O4P/c1-15-18(14,16-12-8-4-2-5-9-12)17-13-10-6-3-7-11-13/h2-11H,1H3	-2.121
InChI=1S/C9H13N/c1-3-8-6-4-5-7(2)9(8)10/h4-6H,3,10H2,1-2H3	-1.706
InChI=1S/C16H32O4/c1-7-14(3,4)17-19-16(12-10-9-11-13-16)20-18-15(5,6)8-2/h7-13H2,1-6H3	-5.46
InChI=1S/C7HCl5O2/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h(H,13,14)	-4.866
InChI=1S/C15H18N2O4/c1-4-15(11-8-6-5-7-9-11)12(18)16(2)14(20)17(10-21-3)13(15)19/h5-9H,4,10H2,1-3H3	-2.63
InChI=1S/C10H11NO4/c1-13-7-3-6(11)5-4-15-10(12)8(5)9(7)14-2/h3H,4,11H2,1-2H3	-2.08
InChI=1S/C11H8N4/c1-2-4-8(5-3-1)10-14-9-6-12-7-13-11(9)15-10/h1-7,11H	-3.07
InChI=1S/C12H27N/c1-4-5-6-7-8-9-10-11-12-13(2)3/h4-12H2,1-3H3	-4.045
InChI=1S/C17H28N2O3/c1-4-7-11-21-16-13-14(8-9-15(16)18)17(20)22-12-10-19(5-2)6-3/h8-9,13H,4-7,10-12,18H2,1-3H3	-3.465
InChI=1S/C6H2Cl3NO2/c7-3-1-5(9)6(10(11)12)2-4(3)8/h1-2H	-3.887
InChI=1S/C13H21O4PS/c1-4-10-15-18(14,16-11-5-2)17-12-6-8-13(19-3)9-7-12/h6-9H,4-5,10-11H2,1-3H3	-3.386
InChI=1S/C4H6O4/c5-1-3-2-7-4(6)8-3/h3,5H,1-2H2	0.928
InChI=1S/C16H19N3O5S/c1-4-24-13-7-5-12(6-8-13)17-15-10-9-14(11-16(15)19(20)21)25(22,23)h5-11,17H,4H2,1-3H3	-4.262
InChI=1S/C15H14ClN3O2/c1-19(10-11-2-6-13(16)7-3-11)18-17-14-8-4-12(5-9-14)15(20)21/h2-9H,10H2,1H3,(H,20,21)/b18-17+	-5.557
InChI=1S/C6H14O/c1-4-6(2,3)5-7/h7H,4-5H2,1-3H3	-1.04
InChI=1S/C8H16N2O2/c1-3-5-7(11)9-10-8(12)6-4-2/h3-6H2,1-2H3,(H,9,11)(H,10,12)	-1
InChI=1S/C10H9NO6S2/c11-19(15,16)10-5-9(6-17-10)18(13,14)8-3-1-7(12)2-4-8/h1-6,12H,(H2,11,15,16)	-2.4
InChI=1S/C10H20O5P2S2/c1-9(2)5-11-16(18,12-6-9)15-17(19)13-7-10(3,4)8-14-17/h5-8H2,1-4H3	-5.393

"InChi"	"logS(M)"
InChI=1S/C8H9NO2/c1-6-3-4-8(9(10)11)7(2)5-6/h3-5H,1-2H3	-3.056
InChI=1S/C2H2Br2Cl2/c3-1(5)2(4)6/h1-2H	-2.564
InChI=1S/C7H5NO4/c9-6(10)4-2-1-3-5(8-4)7(11)12/h1-3H,(H,9,10)(H,11,12)	-1.524
InChI=1S/C7H11N3O2/c1-10-4-9-3-5(10)2-6(8)7(11)12/h3-4,6H,2,8H2,1H3,(H,11,12)	0.073
InChI=1S/C22H26N2O2/c1-3-22-11-7-12-23-13-10-16-15-8-5-6-9-17(15)24(19(16)20(22)23)18h5-6,8-9,14,20H,3-4,7,10-13H2,1-2H3	-4.84
InChI=1S/C15H24N2O/c1-6-17(7-2)13(5)15(18)16-14-11(3)9-8-10-12(14)4/h8-10,13H,6-7H2,1-5H3,(H,16,18)	-3.344

External Set I

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C11H12N2O/c1-9-8-11(14)13(12(9)2)10-6-4-3-5-7-10/h3-8H,1-2H3	1	0.45
InChI=1S/C9H11NO2/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6H,2,10H2,1H3	1	-2.19
InChI=1S/C16H13ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)2h2-9H,10H2,1H3	1	-3.81
InChI=1S/C6H6Cl6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-6H	1	-4.54
InChI=1S/C10H19O6PS2/c1-5-15-9(11)7-8(10(12)16-6-2)19-17(18,13-3h8H,5-7H2,1-4H3	1	-3.35
InChI=1S/C8H6N4O5/c13-6-4-11(8(14)10-6)9-3-5-1-2-7(17-5)12(15h1-3H,4H2,(H,10,13,14)/b9-3+	1	-3.33
InChI=1S/C12H12N2O3/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(1h3-7H,2H2,1H3,(H2,13,14,15,16,17)	1	-2.3
InChI=1S/C15H12N2O2/c18-13-15(17-14(19)16-13,11-7-3-1-4-8-11)12h1-10H,(H2,16,17,18,19)	1	-4.07
InChI=1S/C19H28O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(2h11,14-17,21H,3-10H2,1-2H3	1	-4.1
InChI=1S/C7H8N4O2/c1-10-5-4(8-3-9-5)6(12)11(2)7(10)13/h3H,1-2H3,(H,8,9)	1	-1.38
InChI=1S/C18H28N2O4/c1-5-6-18(23)20-14-7-8-17(16(9-14)13(4)21)2h7-9,12,15,19,22H,5-6,10-11H2,1-4H3,(H,20,23)	2	-2.56
InChI=1S/C16H19N3O5S/c1-16(2)11(15(23)24)19-13(22)10(14(19)25-1h3-6,9-11,14,20H,17H2,1-2H3,(H,18,21)(H,23,24)	2	-2.12
InChI=1S/C15H14F3N3O4S2/c16-15(17,18)10-7-11-13(8-12(10)26(19,22)23h1-5,7-8,14,20-21H,6H2,(H2,19,22,23)	2	-4.3
InChI=1S/C9H11NO2/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6H,2,10H2,1H3	2	-2.19
InChI=1S/C15H14ClN3O4S3/c16-11-6-12-14(7-13(11)25(17,20)21)26(22,23h1-7H,8-9H2,(H,18,19)(H2,17,20,21)	2	-4.84
InChI=1S/C18H19ClN4/c1-22-8-10-23(11-9-22)18-14-4-2-3-5-15(14)2h2-7,12,20H,8-11H2,1H3	2	-4.6

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C20H29N3O2/ c1-4-7-14-25-19-15-17(16-10-8-9-11-18(16)22 h8-11,15H,4-7,12-14H2,1-3H3,(H,21,24)	2	-4.04
InChI=1S/C18H20O2/ c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11 h5-12,19-20H,3-4H2,1-2H3/b18-17-	2	-4.39
InChI=1S/C13H8F2O3/ c14-8-2-3-9(11(15)6-8)7-1-4-12(16)10(5-7)13(h1-6,16H,(H,17,18)	2	-4.99
InChI=1S/C24H40N8O4/ c33-15-11-31(12-16-34)23-26-20-19(21(27-23 h33-36H,1-18H2	2	-5.14
InChI=1S/C19H19N7O6/ c20-19-25-15-14(17(30)26-19)23-11(8-22-15)7 h1-4,8,12,21H,5-7H2,(H,24,29)(H,27,28)(H, 31,32)(H3,20,22,25,26,30)	2	-5.96
InChI=1S/C12H11ClN2O5S/ c13-9-5-10(15-6-7-2-1-3-20-7)8(12(16)17)4-11 h1-5,15H,6H2,(H,16,17)(H2,14,18,19)	2	-4.47
InChI=1S/C7H8ClN3O4S2/ c8-4-1-5-7(2-6(4)16(9,12)13)17(14,15)11-3-10 h1-2,10-11H,3H2,(H2,9,12,13)	2	-2.72
InChI=1S/C19H24N2/ c1-20(2)14-7-15-21-18-10-5-3-8-16(18)12-13- h3-6,8-11H,7,12-15H2,1-2H3	2	-4.3
InChI=1S/C19H16ClNO4/ c1-11-15(10-18(22)23)16-9-14(25-2)7-8-17(16 h3-9H,10H2,1-2H3,(H,22,23)	2	-5.48
InChI=1S/C16H14O3/ c1-11(16(18)19)13-8-5-9-14(10-13)15(17)12-6 h2-11H,1H3,(H,18,19)	2	-3.41
InChI=1S/C14H22N2O/ c1-5-16(6-2)10-13(17)15-14-11(3)8-7-9-12(14 h7-9H,5-6,10H2,1-4H3,(H,15,17)	2	-1.82
InChI=1S/C13H19NO4S/ c1-3-9-14(10-4-2)19(17,18)12-7-5-11(6-8-12)1 h5-8H,3-4,9-10H2,1-2H3,(H,15,16)	2	-4.83
InChI=1S/C12H13ClN4/ c1-2-9-10(11(14)17-12(15)16-9)7-3-5-8(13)6-4 h3-6H,2H2,1H3,(H4,14,15,16,17)	2	-4
InChI=1S/C11H12N4O2S/ c1-8-6-7-13-11(14-8)15-18(16,17)10-4-2-9(12 h2-7H,12H2,1H3,(H,13,14,15)	2	-3.11
InChI=1S/C9H10N4O2S2/ c1-6-11-12-9(16-6)13-17(14,15)8-4-2-7(10)3-5 h2-5H,10H2,1H3,(H,12,13)	2	-2.77
InChI=1S/C32H41NO2/ c1-31(2,3)26-18-16-25(17-19-26)30(34)15-10- h4-9,11-14,16-19,29-30,34-35H, 10,15,20-24H2,1-3H3	2	-7.74
InChI=1S/C10H7N3S/ c1-2-4-8-7(3-1)12-10(13-8)9-5-14-6-11-9/ h1-6H,(H,12,13)	2	-3.97

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C12H18N2O3S/ c1-3-4-9-13-12(15)14-18(16,17)11-7-5-10(2)6- h5-8H,3-4,9H2,1-2H3,(H2,13,14,15)	2	-3.54
InChI=1S/C19H22ClN5O/ c20-16-5-3-6-17(15-16)23-13-11-22(12-14-23) h1-3,5-7,9,15H,4,8,10-14H2	2	-3.27
InChI=1S/C4H6N4O3S2/ c1-2(9)6-3-7-8-4(12-3)13(5,10)11/h1H3, (H2,5,10,11)(H,6,7,9)	3	-2.38
InChI=1S/C23H27Cl2N3O2/ c24-19-4-3-5-21(23(19)25)28-13-11-27(12-14- h3-6,8,16H,1-2,7,9-15H2,(H,26,29)	3	-6.64
InChI=1S/C22H19ClO3/ c23-16-11-9-14(10-12-16)13-5-7-15(8-6-13)19 h1-4,9-13,15,26H,5-8H2	3	-6.07
InChI=1S/C10H12ClNO2/ c11-9-3-1-7(2-4-9)8(6-12)5-10(13)14/ h1-4,8H,5-6,12H2,(H,13,14)	3	-1.78
InChI=1S/C15H14ClN3O4S3/ c16-11-6-12-14(7-13(11)25(17,20)21)26(22,23 h1-7H,8-9H2,(H,18,19)(H2,17,20,21)	3	-4.84
InChI=1S/C14H10BrN3O/ c15-9-4-5-11-10(7-9)14(17-8-13(19)18-11)12- h1-7H,8H2,(H,18,19)	3	-3.39
InChI=1S/C15H12N2O/ c16-15(18)17-13-7-3-1-5-11(13)9-10-12-6-2-4 h1-10H,(H2,16,18)	3	-3.22
InChI=1S/C16H17N9O5S3/ c1-24-16(20-22-23-24)33-4-6-3-31-13-9(12(27 h5,9,13H,3-4H2,1-2H3,(H2,17,18)(H,19,26) (H,28,29)/b21-8+	3	-3.27
InChI=1S/C18H19N3O5S/ c1-2-3-10-8-27-17-13(16(24)21(17)14(10)18(2 h2-7,12-13,17,22H,8,19H2,1H3,(H,20,23)(H, 25,26)/b3-2+	3	-1.68
InChI=1S/C17H14F3N3O2S/ c1-11-2-4-12(5-3-11)15-10-16(17(18,19)20)22 h2-10H,1H3,(H2,21,24,25)	3	-5.89
InChI=1S/C10H13ClN2O3S/ c1-2-7-12-10(14)13-17(15,16)9-5-3-8(11)4-6-9 h3-6H,2,7H2,1H3,(H2,12,13,14)	3	-3.17
InChI=1S/C20H27N5O2/ c26-20-12-9-15-14-17(10-11-18(15)21-20)27-1 h10-11,14,16H,1-9,12-13H2,(H,21,26)	3	-4.93
InChI=1S/C10H16N6S/ c1-8-9(16-7-15-8)5-17-4-3-13-10(12-2)14-6-1 h7H,3-5H2,1-2H3,(H,15,16)(H2,12,13,14)	3	-1.52
InChI=1S/C17H18FN3O3/ c18-13-7-11-14(8-15(13)20-5-3-19-4-6-20)21(h7-10,19H,1-6H2,(H,23,24)	3	-3.57

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C23H29ClFN3O4/ c1-30-21-13-19(26)18(24)12-17(21)23(29)27-2 h4-7,12-13,20,22H,3,8-11,14,26H2,1-2H3,(H, 27,29)	3	-6.78
InChI=1S/C18H22N2/ c1-19-13-6-14-20-17-9-4-2-7-15(17)11-12-16- h2-5,7-10,19H,6,11-14H2,1H3	3	-3.83
InChI=1S/C22H29FO5/ c1-12-8-16-15-5-4-13-9-14(25)6-7-19(13,2)21(h6-7,9,12,15-17,24,26,28H, 4-5,8,10-11H2,1-3H3	3	-3.56
InChI=1S/C8H7ClN2O2S/ c1-5-10-7-3-2-6(9)4-8(7)14(12,13)11-5/ h2-4H,1H3,(H,10,11)	3	-3.43
InChI=1S/C14H11Cl2NO2/ c15-10-5-3-6-11(16)14(10)17-12-7-2-1-4-9(12 h1-7,17H,8H2,(H,18,19)	3	-5.34
InChI=1S/C22H26N2O4S/ c1-15(25)28-20-21(16-9-11-17(27-4)12-10-16) h5-12,20-21H,13-14H2,1-4H3	3	-3.02
InChI=1S/C20H28N2O5/ c1-3-27-20(26)16(12-11-15-8-5-4-6-9-15)21-1 h4-6,8-9,14,16-17,21H,3,7,10-13H2,1-2H3, (H,24,25)	3	-1.36
InChI=1S/C18H22O2/ c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(1 h3,5,10,14-16,19H,2,4,6-9H2,1H3	3	-5.38
InChI=1S/C9H10N2O3S2/ c1-2-14-6-3-4-7-8(5-6)15-9(11-7)16(10,12)13/ h3-5H,2H2,1H3,(H2,10,12,13)	3	-3.76
InChI=1S/C29H32O13/ c1-11-36-9-20-27(40-11)24(31)25(32)29(41-2(h4-7,11,15,20-22,24-27,29-32H, 8-10H2,1-3H3	3	-3.6
InChI=1S/C15H13FO2/ c1-10(15(17)18)12-7-8-13(14(16)9-12)11-5-3- h2-10H,1H3,(H,17,18)	3	-4.34
InChI=1S/C19H19N7O6/ c20-19-25-15-14(17(30)26-19)23-11(8-22-15)7 h1-4,8,12,21H,5-7H2,(H,24,29)(H,27,28)(H, 31,32)(H3,20,22,25,26,30)	3	-5.96
InChI=1S/C9H13N5O4/ c10-9-12-7-6(8(17)13-9)11-3-14(7)4-18-5(1-15 h3,5,15-16H,1-2,4H2,(H3,10,12,13,17)	3	-1.78
InChI=1S/C21H27N5O4S/ c1-15-13-24-19(14-23-15)20(27)22-12-11-16-7 h7-10,13-14,17H,2-6,11-12H2,1H3,(H,22,27) (H2,25,26,28)	3	-5.61
InChI=1S/C17H17ClO6/ c1-8-5-9(19)6-12(23-4)17(8)16(20)13-10(21-2 h6-8H,5H2,1-4H3	3	-4.52
InChI=1S/C21H23ClFNO2/ c22-18-7-5-17(6-8-18)21(26)11-14-24(15-12-2 h3-10,26H,1-2,11-15H2	3	-5.71

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C36H47N5O4/ c1-36(2,3)39-35(45)31-24-40(22-26-12-9-15-3 h4-15,21,28-29,31-33,42-43H, 16-20,22-24H2,1-3H3,(H,38,44)(H,39,45)	3	-4.53
InChI=1S/C19H16ClNO4/ c1-11-15(10-18(22)23)16-9-14(25-2)7-8-17(16 h3-9H,10H2,1-2H3,(H,22,23)	3	-5.48
InChI=1S/C26H28Cl2N4O4/ c1-19(33)31-10-12-32(13-11-31)21-3-5-22(6-4 h2-9,14,18,23H,10-13,15-17H2,1H3	3	-5.47
InChI=1S/C20H23N/ c1-21-14-6-12-20-13-11-15(16-7-2-4-9-18(16) h2-5,7-10,15,21H,6,11-14H2,1H3	3	-4.62
InChI=1S/C16H16ClN3O3S/ c1-9-5-3-4-6-14(9)20-10(2)19-13-8-12(17)15(2 h3-8,10,19H,1-2H3,(H2,18,22,23)	3	-3.88
InChI=1S/C15H16O2/ c1-11(16)3-4-12-5-6-14-10-15(17-2)8-7-13(14 h5-10H,3-4H2,1-2H3	3	-4.4
InChI=1S/C14H14O3/ c1-9(14(15)16)10-3-4-12-8-13(17-2)6-5-11(12 h3-9H,1-2H3,(H,15,16)	3	-4.23
InChI=1S/C32H45N3O4S/ c1-21-25(15-10-16-28(21)36)30(38)33-26(20-4 h5-7,10,13-16,22-23,26-27,29,36-37H, 8-9,11-12,17-20H2,1-4H3,(H,33,38)(H,34,39)	3	-6.21
InChI=1S/C15H14N4O/ c1-9-6-8-17-14-12(9)18-15(20)11-3-2-7-16-13 h2-3,6-8,10H,4-5H2,1H3,(H,18,20)	3	-3.41
InChI=1S/C17H18N2O6/ c1-9-13(16(20)24-3)15(14(10(2)18-9)17(21)25 h5-8,15,18H,1-4H3	3	-4.71
InChI=1S/C16H18FN3O3/ c1-2-19-9-11(16(22)23)15(21)10-7-12(17)14(8 h7-9,18H,2-6H2,1H3,(H,22,23)	3	-2.88
InChI=1S/C19H21N/ c1-20-14-6-11-19-17-9-4-2-7-15(17)12-13-16- h2-5,7-11,20H,6,12-14H2,1H3	3	-3.93
InChI=1S/C18H20FN3O4/ c1-10-9-26-17-14-11(16(23)12(18(24)25)8-22(h7-8,10H,3-6,9H2,1-2H3,(H,24,25)	3	-2.03
InChI=1S/C15H11ClN2O2/ c16-10-6-7-12-11(8-10)13(9-4-2-1-3-5-9)18-15 h1-8,15,20H,(H,17,19)	3	-4.03
InChI=1S/C20H21NO4/ c1-22-17-6-5-13(10-18(17)23-2)9-16-15-12-20 h5-8,10-12H,9H2,1-4H3	3	-4.33
InChI=1S/C21H26ClN3OS/ c22-17-6-7-21-19(16-17)25(18-4-1-2-5-20(18) h1-2,4-7,16,26H,3,8-15H2	3	-4.48
InChI=1S/C11H11N5/ c12-10-7-6-9(11(13)14-10)16-15-8-4-2-1-3-5-8 h1-7H,(H4,12,13,14)/b16-15+	3	-4.02

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C14H20N2O2/ c1-10(2)16-8-11(17)9-18-14-5-3-4-13-12(14)6 h3-7,10-11,15-17H,8-9H2,1-2H3	3	-3.75
InChI=1S/C23H36O7/ c1-4-13(2)23(29)30-20-11-17(25)9-15-6-5-14(h5-6,9,13-14,16-20,22,24-26H, 4,7-8,10-12H2,1-3H3,(H,27,28)	3	-4.86
InChI=1S/C12H14N2O2/ c1-2-12(9-6-4-3-5-7-9)10(15)13-8-14-11(12)1(h3-7H,2,8H2,1H3,(H,13,15)(H,14,16)	3	-2.53
InChI=1S/C13H19NO4S/ c1-3-9-14(10-4-2)19(17,18)12-7-5-11(6-8-12)1 h5-8H,3-4,9-10H2,1-2H3,(H,15,16)	3	-4.83
InChI=1S/C17H20N2S/ c1-18(2)12-7-13-19-14-8-3-5-10-16(14)20-17- h3-6,8-11H,7,12-13H2,1-2H3	3	-4.45
InChI=1S/C17H20N2S/ c1-13(18(2)3)12-19-14-8-4-6-10-16(14)20-17- h4-11,13H,12H2,1-3H3	3	-4.38
InChI=1S/C27H36N2O4/ c1-4-33-25-17-20(12-13-22(25)27(31)32)18-2(h6-7,10-13,17,19,23H, 4-5,8-9,14-16,18H2,1-3H3,(H,28,30)(H,31,32)	3	-4.77
InChI=1S/C37H48N6O5S2/ c1-24(2)33(42-36(46)43(5)20-29-22-49-35(40- h6-15,19,22-25,28,31-33,44H, 16-18,20-21H2,1-5H3,(H,39,45)(H,41,47)(H, 42,46)	3	-5.17
InChI=1S/C24H32O4S/ c1-14(25)29-19-13-15-12-16(26)4-8-22(15,2)1 h12,17-19,21H,4-11,13H2,1-3H3	3	-4.21
InChI=1S/C18H14N4O5S/ c23-16-9-6-13(11-15(16)18(24)25)21-20-12-4- h1-11,23H,(H,19,22)(H,24,25)/b21-20+	3	-6.41
InChI=1S/C9H9N3O2S2/ c10-7-1-3-8(4-2-7)16(13,14)12-9-11-5-6-15-9/ h1-6H,10H2,(H,11,12)	3	-2.62
InChI=1S/C11H13N3O3S/ c1-7-8(2)13-17-11(7)14-18(15,16)10-5-3-9(12 h3-6,14H,12H2,1-2H3	3	-3.13
InChI=1S/C20H17FO3S/ c1-12-17(9-13-3-6-15(7-4-13)25(2)24)16-8-5-1 h3-10H,11H2,1-2H3,(H,22,23)/p+1/b17-9+	3	-4.96
InChI=1S/C22H24N2O8/ c1-21(31)8-5-4-6-11(25)12(8)16(26)13-9(21)7 h4-6,9-10,15,25,27-28,31-32H,7H2,1-3H3, (H2,23,30)	3	-3.22
InChI=1S/C21H27FO6/ c1-18-6-5-12(24)7-11(18)3-4-13-14-8-15(25)2 h5-7,13-16,23,25-26,28H,3-4,8-10H2,1-2H3	3	-3.52
InChI=1S/C12H11N7/ c13-9-7(6-4-2-1-3-5-6)16-8-10(14)18-12(15)19 h1-5H,(H6,13,14,15,17,18,19)	3	-4.11

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C19H16O4/ c1-12(20)11-15(13-7-3-2-4-8-13)17-18(21)14- h2-10,15,21H,11H2,1H3	3	-4.78
InChI=1S/C10H17N/ c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H, 1-6,11H2	4	-2.19
InChI=1S/C25H29I2NO3/ c1-4-7-11-22-23(18-10-8-9-12-21(18)31-22)24 h8-10,12,15-16H,4-7,11,13-14H2,1-3H3	4	-10.4
InChI=1S/C20H22ClN3O/ c1-3-24(4-2)13-14-11-16(6-8-20(14)25)23-18- h5-12,25H,3-4,13H2,1-2H3,(H,22,23)	4	-5.49
InChI=1S/C18H31NO4/ c1-14(2)19-11-17(20)13-23-18-7-5-16(6-8-18) h5-8,14-15,17,19-20H,9-13H2,1-4H3	4	-2.09
InChI=1S/C32H40BrN5O5/ c1-16(2)12-24-29(40)37-11-7-10-25(37)32(42) h6,8-9,13,16-18,23-25,34,42H, 7,10-12,14-15H2,1-5H3,(H,35,39)	4	-5.5
InChI=1S/C29H41NO4/ c1-25(2,3)26(4,32)20-15-27-10-11-29(20,33-5) h8-9,17,20-21,24,31-32H,6-7,10-16H2,1-5H3	4	-6.07
InChI=1S/C18H18ClNS/ c1-20(2)11-5-7-14-15-6-3-4-8-17(15)21-18-10 h3-4,6-10,12H,5,11H2,1-2H3/b14-7-	4	-5.99
InChI=1S/C27H22Cl2N4/ c1-17(2)30-24-16-27-25(15-23(24)31-20-11-7- h3-17,31H,1-2H3/b30-24+	4	-9.05
InChI=1S/C22H27NO2/ c1-4-22(24)10-8-18-16-6-5-15-11-19-14(13-23 h1,11,13,16-18,24H,5-10,12H2,2-3H3	4	-6.1
InChI=1S/C10H12N4O3/ c15-3-6-1-2-7(17-6)14-5-13-8-9(14)11-4-12-1(h4-7,15H,1-3H2,(H,11,12,16)	4	-1.24
InChI=1S/C13H8F2O3/ c14-8-2-3-9(11(15)6-8)7-1-4-12(16)10(5-7)13(h1-6,16H,(H,17,18)	4	-4.99
InChI=1S/C17H21NO/ c1-18(2)13-14-19-17(15-9-5-3-6-10-15)16-11- h3-12,17H,13-14H2,1-2H3	4	-3.21
InChI=1S/C24H21F2NO3/ c25-17-5-1-15(2-6-17)22(29)14-13-21-23(16-3 h1-12,21-23,28-29H,13-14H2	4	-4.94
InChI=1S/C35H38Cl2N8O4/ c1-3-25(2)45-34(46)44(24-40-45)29-7-5-27(6- h4-13,18,22-25,31H,3,14-17,19-21H2,1-2H3	4	-8.98
InChI=1S/C18H14Cl4N2O/ c19-13-2-1-12(16(21)7-13)10-25-18(9-24-6-5- h1-8,11,18H,9-10H2	4	-5.82
InChI=1S/C29H35NO2/ c1-5-15-29(32)16-14-26-24-12-8-20-17-22(31) h6-7,9-10,17,24-26,32H, 8,11-14,16,18H2,1-4H3	4	-5.22

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C17H19N3O3S/ c1-10-8-18-15(11(2)16(10)23-4)9-24(21)17-19 h5-8H,9H2,1-4H3,(H,19,20)/p+1	4	-3.7
InChI=1S/C19H20N2O3S/ c1-2-13-3-6-15(20-12-13)9-10-24-16-7-4-14(5 h3-8,12,17H,2,9-11H2,1H3,(H,21,22,23)	4	-6.2
InChI=1S/C13H20N2O2/ c1-3-15(4-2)9-10-17-13(16)11-5-7-12(14)8-6-1 h5-8H,3-4,9-10,14H2,1-2H3	4	-2.3
InChI=1S/C20H24N2O2/ c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6 h3-6,8,11,13-14,19-20,23H, 1,7,9-10,12H2,2H3	4	-3.06
InChI=1S/C28H27NO4S/ c30-21-8-4-20(5-9-21)28-26(24-13-10-22(31)1 h4-13,18,30-31H,1-3,14-17H2	4	-6.82
InChI=1S/C46H62N4O11/ c1-22(2)21-50-18-16-46(17-19-50)48-34-31-32 h12-15,20,22-23,25-27,30,37-38,41,49,52-54H 16-19,21H2,1-11H3,(H,47,57)/b13-12-, 20-15-,24-14-	4	-4.09
InChI=1S/C38H50N6O5/ c1-38(2,3)43-37(49)32-20-26-14-7-8-15-27(26 h4-6,9-13,16-18,26-27,30-33,45H, 7-8,14-15,19-23H2,1-3H3,(H2,39,46)(H, 41,48)(H,42,47)(H,43,49)	4	-5.92
InChI=1S/C12H14N4O4S/ c1-19-11-7-10(14-12(15-11)20-2)16-21(17,18) h3-7H,13H2,1-2H3,(H,14,15,16)	4	-3.74
InChI=1S/C26H29NO/ c1-4-25(21-11-7-5-8-12-21)26(22-13-9-6-10-1 h5-18H,4,19-20H2,1-3H3/b26-25-	4	-7.52
InChI=1S/C33H30N4O2/ c1-4-9-30-35-31-21(2)18-24(32-34-27-12-7-8- h5-8,10-19H,4,9,20H2,1-3H3,(H,38,39)	4	-6.73
InChI=1S/C32H41NO2/ c1-31(2,3)26-18-16-25(17-19-26)30(34)15-10- h4-9,11-14,16-19,29-30,34-35H, 10,15,20-24H2,1-3H3	4	-7.74
InChI=1S/C10H7N3S/ c1-2-4-8-7(3-1)12-10(13-8)9-5-14-6-11-9/ h1-6H,(H,12,13)	4	-3.97
InChI=1S/C8H14ClN5/ c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H, 4H2,1-3H3,(H2,10,11,12,13,14)	1	-3.69
InChI=1S/C11H11ClO3/ c1-2-5-15-10-4-3-8(6-9(10)12)7-11(13)14/ h2-4,6H,1,5,7H2,(H,13,14)	3	-4.4
InChI=1S/C13H18Br2N2O/ c14-9-5-8(13(16)12(15)6-9)7-17-10-1-3-11(18 h5-6,10-11,17-18H,1-4,7,16H2	3	-3.87
InChI=1S/C8H14ClN5/ c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H, 4H2,1-3H3,(H2,10,11,12,13,14)	3	-3.69

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C10H16N2O3/ c1-4-6(3)10(5-2)7(13)11-9(15)12-8(10)14/ h6H,4-5H2,1-3H3,(H2,11,12,13,14,15)	3	-2.22
InChI=1S/C12H9N/ c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/ h1-8,13H	3	-5.19
InChI=1S/C9H9N3O2/ c1-14-9(13)12-8-10-6-4-2-3-5-7(6)11-8/ h2-5H,1H3,(H2,10,11,12,13)	3	-4.56
InChI=1S/C16H19N3O4S/ c1-8-7-24-15-11(14(21)19(15)12(8)16(22)23)1 h2-3,6,10-11,15H,4-5,7,17H2,1H3,(H,18,20) (H,22,23)	3	-1.18
InChI=1S/C21H30O4/ c1-20-8-7-13(23)9-12(20)3-4-14-15-5-6-16(18 h9,14-17,19,22,24H,3-8,10-11H2,1-2H3	3	-3.29
InChI=1S/C15H10O4/ c16-10-3-1-9(2-4-10)13-8-19-14-7-11(17)5-6-1 h1-8,16-17H	3	-5.23
InChI=1S/C21H19F2N3O3/ c1-24-6-8-25(9-7-24)19-11-18-15(10-17(19)23 h2-5,10-12H,6-9H2,1H3,(H,28,29)	3	-3.83
InChI=1S/C12H11N/ c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/ h1-10,13H	3	-3.53
InChI=1S/C9H11NO4/ c10-6(9(13)14)3-5-1-2-7(11)8(12)4-5/ h1-2,4,6,11-12H,3,10H2,(H,13,14)	3	-1.76
InChI=1S/C18H24O2/ c1-18-9-8-14-13-5-3-12(19)10-11(13)2-4-15(1 h3,5,10,14-17,19-20H,2,4,6-9H2,1H3	3	-5
InChI=1S/C10H18O/ c1-9(2)8-4-6-10(3,11-9)7-5-8/h8H, 4-7H2,1-3H3	3	-1.66
InChI=1S/C16H14O3/ c17-15(10-11-16(18)19)14-8-6-13(7-9-14)12-4 h1-9H,10-11H2,(H,18,19)	3	-5.18
InChI=1S/C14H12FNO3/ c1-7-2-3-8-4-9(15)5-10-12(8)16(7)6-11(13(10) h4-7H,2-3H2,1H3,(H,18,19)	3	-3.9
InChI=1S/C25H24N6O2/ c1-2-21(32)30-14-6-7-18(15-30)31-25-22(24(2 h2-5,8-13,16,18H,1,6-7,14-15H2, (H2,26,27,28)	3	-4.85
InChI=1S/C17H15NO3/ c1-11(17(20)21)12-6-8-14(9-7-12)18-10-13-4- h2-9,11H,10H2,1H3,(H,20,21)	3	-4.65
InChI=1S/C13H12N2O5S/ c1-21(18,19)14-12-8-7-10(15(16)17)9-13(12)2 h2-9,14H,1H3	3	-4.74
InChI=1S/C22H23NO7/ c1-23-8-7-11-9-14-20(29-10-28-14)21(27-4)15 h5-6,9,17-18H,7-8,10H2,1-4H3	3	-4.48

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C19H20N2O3/ c1-2-3-9-17-18(23)20(14-7-5-4-6-8-14)21(19(1 h4-8,10-13,17,22H,2-3,9H2,1H3	3	-3.94
InChI=1S/C10H13NO2/ c1-3-13-10-6-4-9(5-7-10)11-8(2)12/h4-7H, 3H2,1-2H3,(H,11,12)	3	-2.3
InChI=1S/C17H14O4S/ c1-22(19,20)14-9-7-12(8-10-14)15-11-21-17(1 h2-10H,11H2,1H3	3	-4.61
InChI=1S/C21H22N2O2/ c24-18-10-16-19-13-9-17-21(6-7-22(17)11-12(h1-5,13,16-17,19-20H,6-11H2	3	-3.38
InChI=1S/C12H14N4O2S/ c1-8-7-12(15-9(2)14-8)16-19(17,18)11-5-3-10(h3-7H,13H2,1-2H3,(H,14,15,16)	3	-2.16
InChI=1S/C15H24N2O2/ c1-4-5-10-16-14-8-6-13(7-9-14)15(18)19-12-1 h6-9,16H,4-5,10-12H2,1-3H3	3	-3.11
InChI=1S/C10H12N4OS/ c1-7(15)13-9-4-2-8(3-5-9)6-12-14-10(11)16/ h2-6H,1H3,(H,13,15)(H3,11,14,16)/b12-6+	3	-3.5
InChI=1S/C5H4N4O2/ c10-4-2-3(7-1-6-2)8-5(11)9-4/h1H, (H3,6,7,8,9,10,11)	3	-3.6
InChI=1S/C9H8O4/ c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H, 1H3,(H,11,12)	1	-1.64
InChI=1S/C10H6Cl8/ c11-3-1-2-4(5(3)12)9(16)7(14)6(13)8(2,15)10(h2-5H,1H2	1	-6.59
InChI=1S/C9H11Cl3NO3PS/ c1-3-14-17(18,15-4-2)16-9-7(11)5-6(10)8(12)1 h5H,3-4H2,1-2H3	1	-5.7
InChI=1S/C14H9Cl5/ c15-11-5-1-9(2-6-11)13(14(17,18)19)10-3-7-1 h1-8,13H	1	-7.9
InChI=1S/C12H21N2O3PS/ c1-6-15-18(19,16-7-2)17-11-8-10(5)13-12(14- h8-9H,6-7H2,1-5H3	1	-3.75
InChI=1S/C9H10Cl2N2O/ c1-13(2)9(14)12-6-3-4-7(10)8(11)5-6/h3-5H, 1-2H3,(H,12,14)	1	-3.84
InChI=1S/C10H14NO5PS/ c1-3-14-17(18,15-4-2)16-10-7-5-9(6-8-10)11(1 h5-8H,3-4H2,1-2H3	1	-4.27
InChI=1S/C12H4Cl6/ c13-7-3-11(17)9(15)1-5(7)6-2-10(16)12(18)4-8 h1-4H	1	-7.4
InChI=1S/C20H14O4/ c21-15-9-5-13(6-10-15)20(14-7-11-16(22)12-8 h1-12,21-22H	1	-5.08

"InChi"	"EXTERNAL SET"	"logS(M)"
InChI=1S/C20H32O5/ c1-2-3-6-9-15(21)12-13-17-16(18(22)14-19(17 h4,7,12-13,15-17,19,21,23H, 2-3,5-6,8-11,14H2,1H3,(H,24,25)/b7-4+, 13-12+	1	-2.4
InChI=1S/C14H11Cl2NO2/ c1-8-6-7-10(15)13(12(8)16)17-11-5-3-2-4-9(1 h2-7,17H,1H3,(H,18,19)	2	-6.72
InChI=1S/C11H8O2/ c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H, (H,12,13)	2	-3.81
InChI=1S/C7H6O3/c8-6-4-2-1-3-5(6)7(9)10/ h1-4,8H,(H,9,10)	2	-1.88
InChI=1S/C9H8O4/ c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H, 1H3,(H,11,12)	3	-1.67
InChI=1S/C33H34N6O6/ c1-3-42-32-34-28-15-9-14-27(31(40)43-21(2)4 h7-9,12-19,21,24H,3-6,10-11,20H2,1-2H3,(H, 35,36,37,38)	3	-6.79
InChI=1S/C24H40O4/ c1-14(4-9-22(27)28)18-7-8-19-17-6-5-15-12-1 h14-21,25-26H,4-13H2,1-3H3,(H,27,28)	3	-4.62
InChI=1S/C23H30O6/ c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14 h10,16-17,20,28H,4-9,11-12H2,1-3H3	3	-4.22
InChI=1S/C62H111N11O12/ c1-25-27-28-40(15)52(75)51-56(79)65-43(26-2 h25,27,34-47,49-52,75H,26,28-33H2,1-24H3, (H,63,77)(H,64,76)(H,65,79)(H,66,78)/ b27-25+	3	-5.03
InChI=1S/C26H32F2O7/ c1-13-8-17-18-10-20(27)19-9-16(31)6-7-23(19 h6-7,9,13,17-18,20-21,32H,8,10-12H2,1-5H3	3	-4.82
InChI=1S/C23H30O7/ c1-21-7-6-13(25)8-12(21)4-5-14-15-9-16(20(2 h6-8,14-17,19,24,26,29H,4-5,9-11H2,1-3H3	3	-3.33
InChI=1S/C14H12O3/ c15-12-5-3-10(4-6-12)1-2-11-7-13(16)9-14(17 h1-9,15-17H/b2-1+	3	-3.75
InChI=1S/C21H20O6/ c1-26-20-11-14(5-9-18(20)24)3-7-16(22)13-17 h3-12,24-25H,13H2,1-2H3/b7-3+,8-4+	4	-5.36
InChI=1S/C16H23NO2/ c1-2-16(13-8-4-3-5-9-13)18-12-15(19-16)14-1 h3-5,8-9,14-15,17H,2,6-7,10-12H2,1H3	4	-1.96
InChI=1S/C17H12ClNO2S/ c18-13-8-6-11(7-9-13)16-14(10-15(20)21)22-1 h1-9H,10H2,(H,20,21)	4	-5.84
InChI=1S/C11H12I3NO2/ c1-2-5(11(16)17)3-6-7(12)4-8(13)10(15)9(6)14 h4-5H,2-3,15H2,1H3,(H,16,17)	4	-5.49

External Set II

"InChi"	"logS(M)"
InChI=1S/C23H25N3O/c27-23(13-11-20-7-5-15-25-18-20)16-22(26-21-8-2-1-3-9-21)12-10-19-4-7,10-18,21,26H,1-3,8-9H2/b12-10+,13-11+,22-16+	-4.947
InChI=1S/C17H16F3N7O/c1-26(8-11-3-5-12(6-4-11)17(18,19)20)14-7-13(21-9-22-14)15(28)24-3-7,9-10H,8H2,1-2H3,(H,24,25,28)	-3.762
InChI=1S/C19H19N3O2/c23-12-11-22-18(7-5-16-3-1-9-20-14-16)13-19(24)8-6-17-4-2-10-21-1-10,13-15,22-23H,11-12H2/b7-5+,8-6+,18-13-	-2.361
InChI=1S/C24H25F3N2O5/c1-28-8-10-29(11-9-28)13-16-17(30)6-5-15-21(31)20(23(24(25,26)27)4-7,12,30H,8-11,13H2,1-3H3	-4.174
InChI=1S/C26H24ClN5O3S/c1-16-7-8-17(26-29-20-5-3-4-6-24(20)36-26)13-21(16)28-25(33)18-14-3-8,13-15H,9-12H2,1-2H3,(H,28,33)	-6.523
InChI=1S/C18H17N5O/c1-23(12-14-6-5-9-19-11-14)17-10-16(20-13-21-17)18(24)22-15-7-3-2-11,13H,12H2,1H3,(H,22,24)	-3.824
InChI=1S/C20H19FN4O2/c1-25(12-14-3-5-15(21)6-4-14)19-11-18(22-13-23-19)20(26)24-16-7-9-3-11,13H,12H2,1-2H3,(H,24,26)	-4.208
InChI=1S/C20H19ClN4O/c1-2-25(13-15-8-10-16(21)11-9-15)19-12-18(22-14-23-19)20(26)24-17-3-12,14H,2,13H2,1H3,(H,24,26)	-5.301
InChI=1S/C17H17FN6O/c1-23(10-12-3-5-13(18)6-4-12)16-9-14(19-11-20-16)17(25)21-15-7-8-3-9,11H,10H2,1-2H3,(H,21,22,25)	-4.046
InChI=1S/C21H23N3O2/c1-26-14-4-13-24-20(9-7-18-5-2-11-22-16-18)15-21(25)10-8-19-6-3-12-2-3,5-12,15-17,24H,4,13-14H2,1H3/b9-7+,10-8+,20-15-	-3.047
InChI=1S/C20H21N3O2/c1-25-13-12-23-19(8-6-17-4-2-10-21-15-17)14-20(24)9-7-18-5-3-11-2-11,14-16,23H,12-13H2,1H3/b8-6+,9-7+,19-14-	-3.048
InChI=1S/C24H27FN6O/c1-29-10-12-31(13-11-29)21-5-3-4-20(14-21)28-24(32)22-15-23(27-17-3-9,14-15,17H,10-13,16H2,1-2H3,(H,28,32)	-4.131
InChI=1S/C20H19FN4O2/c1-25(12-14-4-3-5-15(21)10-14)19-11-18(22-13-23-19)20(26)24-16-6-3-11,13H,12H2,1-2H3,(H,24,26)	-5.301
InChI=1S/C23H24ClN5O2/c1-29(14-15-3-5-16(24)6-4-15)21-13-20(27-23(28-21)26-18-7-8-18)22-3-6,9-13,18H,7-8,14H2,1-2H3,(H,25,30)(H,26,27,28)	-5.301
InChI=1S/C19H17FN4O/c1-24(12-14-7-9-16(20)10-8-14)18-11-17(21-13-22-18)23-19(25)15-5-2-11,13H,12H2,1H3,(H,21,22,23,25)	-5.301
InChI=1S/C20H23F3N4O/c1-27(12-14-7-9-15(10-8-14)20(21,22)23)18-11-17(24-13-25-18)19(28)7-11,13,16H,2-6,12H2,1H3,(H,26,28)	-5.301

"InChi"	"logS(M)"
InChI=1S/C22H23FN4O2/c1-15(2)29-19-10-8-18(9-11-19)26-22(28)20-12-21(25-14-24-20)27(3)h4-12,14-15H,13H2,1-3H3,(H,26,28)	-5.301
InChI=1S/C19H17FN4O/c1-24(13-14-7-9-16(20)10-8-14)18-11-15(12-21-23-18)19(25)22-17-5-h2-12H,13H2,1H3,(H,22,25)	-4.398
InChI=1S/C20H21N3O2/c24-11-3-10-23-18(7-6-16-4-1-8-21-14-16)12-19(25)13-20(23)17-5-2-h1-2,4-9,12,14-15,20,24H,3,10-11,13H2/b7-6+	-2.609
InChI=1S/C15H12F3N7OS/c1-25(6-9-2-3-11(19-5-9)15(16,17)18)12-4-10(20-7-21-12)13(26)23-1h2-5,7-8H,6H2,1H3,(H,23,24,26)	-3.719
InChI=1S/C19H15FN2O2/c20-16-9-6-14(7-10-16)12-22-13-15(8-11-18(22)23)19(24)21-17-4-2-1h1-11,13H,12H2,(H,21,24)	-3.77
InChI=1S/C24H26F3N7O/c1-32-9-11-34(12-10-32)19-6-4-18(5-7-19)31-23(35)20-13-22(30-16-2h3-8,13-14,16H,9-12,15H2,1-2H3,(H,31,35)	-3.783
InChI=1S/C23H26FN5O2/c1-28(2)12-13-31-20-10-8-19(9-11-20)27-23(30)21-14-22(26-16-25-2h4-11,14,16H,12-13,15H2,1-3H3,(H,27,30)	-3.81
InChI=1S/C23H26FN7O/c1-29-9-11-31(12-10-29)21-8-7-19(14-25-21)28-23(32)20-13-22(27-1h3-8,13-14,16H,9-12,15H2,1-2H3,(H,28,32)	-3.824
InChI=1S/C20H21N3O2/c24-13-3-12-23-19(8-6-17-4-1-10-21-15-17)14-20(25)9-7-18-5-2-11-2h1-2,4-11,14-16,23-24H,3,12-13H2/b8-6+,9-7+,19-14-	-2.832
InChI=1S/C17H19F3N4O/c1-11(2)23-16(25)14-8-15(22-10-21-14)24(3)9-12-4-6-13(7-5-12)17(1h4-8,10-11H,9H2,1-3H3,(H,23,25)	-4.886
InChI=1S/C21H23N3O2/c1-26-12-4-11-24-19(8-7-17-5-2-9-22-15-17)13-20(25)14-21(24)18-6-h2-3,5-10,13,15-16,21H,4,11-12,14H2,1H3/b8-7+	-2.892
InChI=1S/C15H13FN6OS/c1-22(7-10-2-4-11(16)5-3-10)13-6-12(17-8-18-13)14(23)20-15-21-19-h2-6,8-9H,7H2,1H3,(H,20,21,23)	-3.893
InChI=1S/C20H20N4O3S/c1-24(13-15-8-10-17(11-9-15)28(2,26)27)19-12-18(21-14-22-19)20(25h3-12,14H,13H2,1-2H3,(H,23,25)	-5
InChI=1S/C21H23N3O/c1-17(2)14-24-20(9-7-18-5-3-11-22-15-18)13-21(25)10-8-19-6-4-12-2h3-13,15-17,24H,14H2,1-2H3/b9-7+,10-8+,20-13-	-3.774

Most important descriptors (recursive variable selection)

Knime report *powered by Birt*

"Descriptors"	"Occurences"
NumRotatableBonds	963.4
TPSA	862
LabuteASA	772
ALOGP (#1)	563.5
SlogP	559
Mi	433
Me	313
Mv	310
NumAromaticRings	286
GD	267.4
RBF	248.5
C%	247
Sv	242.5
BLI	229.75
PW2	227.5
NumSaturatedRings	218.2
N%	206.8
MAXDP	205
MATS2e	197
PW4	193
PW3	186.4
GATS3s	183
GATS3e	179.5
DECC	172
GATS1s	170.8
MATS4e	168.25
HNar	166.75
MATS5m	166
GATS4m	166
MATS4m	163
GATS3m	162
MATS1m	161.2
GATS5m	160
MATS2s	158.5
MATS5e	157
MATS5i	155.5
MATS3e	154.75
SIC2	154
MATS4v	154

"Descriptors"	"Occurences"
GATS4s	151
IC2	149.5
ZM1Mad	149
GATS2e	149
ZM1V	148.75
MATS7e	148
MATS6m	148
ATSC1e	148
SCBO	146.5
MATS8m	146.5
MATS8v	145
MATS3m	143.5
MATS4i	142
MATS2m	142
MATS2i	142
IC3	142
MATS7i	140.5
MATS5v	140.5
IC1	140.5
CIC2	140.5
X1A	139
MATS7v	139
GATS5e	139
DELS	139
MATS1p	135
SIC3	133
MATS5p	133
JGI6	133
GATS5i	133
GATS3v	133
MATS6i	131.5
MATS6e	131.5
MSD	130
MATS3p	130
GATS2i	130
JGI5	128.5
ZM2Kup	127
MATS7s	127
BIC2	127
MCD	124

"Descriptors"	"Occurences"
MATS3v	124
GATS6s	124
GATS4e	124
MATS6v	122.5
MATS2v	121
ATSC5e	121
JGI4	118
JGI3	118
PJI2	117.25
X5A	117
P_VSA_v_3	115
P_VSA_LogP_2	112