

cΔlog k_w^{IAM} : can we afford estimation of small molecules' blood-brain barrier passage based upon *in silico* phospholipophilicity?

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Table S1. Definition of the physico-chemical descriptors reported in the manuscript

Descriptor	Definition
miLogP	octanol-water partition coefficient (log P) calculated by Molinspiration Cheminformatics (1)
Heavy Atoms	Number of heavy atoms
HLB _M	Mean of HLB _{PSA} values, HLB values calculated according to Griffin's method(2) and HLB values calculated according to Davies's method(3)
HLB _{PSA}	hydrophilic-lipophilic balance (HLB) calculated according to the following: $HLB_{PSA} = 20 * \frac{PSA}{Surface}$ in which PSA is the polar surface area and Surface is the total surface
Rotatable bonds	Number of rotatable bonds
TPSA(NO)	topological polar surface area using N,O polar contributions
ALOGPS_logP	octanol-water partition coefficient (log P) calculated by the software ALOGPS 2.1(4)
nO	Number of oxygen atoms
TPSA(Tot)	topological polar surface area using N,O,S,P polar contributions
nROH	number of hydroxyl groups

Table S2. Descriptors employed in the multiple linear regression.

Molecule	nROH	TPSA(Tot)	ALOGPS_logP
1,1,1-trichloroethane	0	0	2.45
1,2-dimethylbenzene	0	0	3.16
1,4-dimethylbenzene	0	0	3.15
1,7-dimethylxanthine	0	72.68	-0.63
1-chloro-2,2,2-trifluoroethane	0	0	1.82
1-Hydroxymidazolam	1	50.41	3.09
2,2-dimethylbutane	0	0	3.74
2-methylpentane	0	0	3.6
3-methylhexane	0	0	4.18
3-methylpentane	0	0	3.98
4-Hydroxymidazolam	1	50.41	3.05
acetaminophen	0	49.33	0.51
acetone	0	17.07	-0.29
aminopyrine	0	30.17	0.94
amobarbital	0	75.27	1.87
antipyrine	0	26.93	1.18
Bretazenil	0	64.43	3.05
cyclohexane	0	0	3.46
cyclopropane	0	0	1.56
desmonomethylpromazine	0	45.2	4.28
didanosine	1	93.03	-1.26
Diethylene glycol divinyl ether	0	27.69	1.26
enflurane	0	9.23	2.24
ethanol	1	20.23	-0.4
ethyl ether	0	9.23	1.12
ethylbenzene	0	0	3.27
flunitrazepam	0	78.49	2.2
Fluroxene	0	9.23	1.7
halothane	0	0	2.5
indinavir	2	118.03	3.26
isobutyl alcohol	1	20.23	0.6
isoflurane	0	9.23	2.3
Isopropyl alcohol	1	20.23	0.04
mesoridazine	0	72.69	3.83
methoxyflurane	0	9.23	2.01
methyl cyclopentane	0	0	3.15
methyl ethyl ketone	0	17.07	0.41
mirtazapine	0	19.37	2.9
m-xylene	0	0	3.15
nevirapine	0	63.57	1.75
N-heptane	0	0	4.33
N-hexane	0	0	4.02
nordazepam	0	41.46	2.79

Northioridazine	0	70.5	5.29
N-pentane	0	0	3.41
Quinidine	1	45.59	2.82
Sulforidazine	0	78.93	4.32
Teflurane	0	0	2.07
thioridazine	0	61.71	5.93
thioxolone	0	78.68	1.97
Tiotidine	0	191.04	0.59
triazolam	0	43.07	2.94
trichloroethylene	0	0	2.45
trifluoperazine	0	39.65	4.87
Valproic acid	1	37.3	2.54
zidovudine	1	133.08	-0.1

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