

Table S5. Comparison of calculated and experimental membrane binding free energies of small molecules. Experimental values are obtained from partition coefficients of these molecules between water and phospholipid vesicles¹²⁻¹⁶.

Small molecule	ΔG_{exp} (kcal/mol)	ΔG_{calc} (kcal/mol)
Ibuprofen	-5.26	-5.7
Morphine	-2.57	-3.0
Phenol	-2.68	-3.4
3-Me-phenol	-3.18	-3.8
4-Et-phenol	-3.92	-4.3
Acetylsalicylic acid (Hb)	-3.26	-2.9
Aniline	-2.2	-3.2
3,4-dimethylaniline	-3.06	-3.5
2,4,6-trimethylaniline	-3.76	-3.6
p-xylene	-4.06	-4.9
N,N-dimethylaniline	-3.18	-2.9
2-allylphenol	-4.17	-5.1
2-phenylphenol	-4.72	-5.8
4-amino-3-methylphenol	-2.88	-2.4
9-anthracenomethanol	-4.77	-5.7
benzocaine	-3.09	-2.6
4-biphenylcarboxaldehyde	-4.28	-5.6
cinnamamide	-2.54	-3.8
1,5-dihydroxynaphthalene	-3.70	-2.6
1-naphtaldehyde	-3.82	-4.9
Indole	-3.77	-4.1
3-Me-indole	-4.46	-4.4
N-Me-indole	-3.88	-4.0

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