

Table S4. Comparison of the free energy from explicit simulations with experimental binding free energy and transfer energy $\langle \Delta W \rangle$ from IMM1.

Peptide	Membrane	$\Delta G_{c, \text{sim}}^0$	ΔG_c^0	$\langle \Delta W \rangle$	Ref.
Lactoferricin	DOPC	-1.05 ± 0.39		-0.9 ± 0.1	[1]
	DOPG	-5.4 ± 1.3	-7.38^+	-7.9 ± 0.7	[2,3]
Protegrin	DMPC/DMPG(7:3)	-2.4 ± 0.8	-7^*	-5.3 ± 1.1	[4,5]
Indolicidin	DOPC	-0.05 ± 0.46	-7.25	-1.1 ± 1.2	[6,7]
	DOPC/DOPG(7:3)	-1.94 ± 0.56	-8.97	-5.5 ± 0.8	
Melittin	DOPC	-10.66 ± 1.35	-5.4	-13.1 ± 0.7	[8,9]

+ The experimental value is obtained for a truncated lactoferricin which has less charge, so the actual value should be more negative.

* The standard state of the experiment is assumed to be ΔG_c^0 .

Reference:

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