

Table S2. Theoretical transfer energies and biological activities of the peptides.

Minimal inhibitory concentrations(MIC) have been converted into μM . The colony formation unit (CFU, cell/ml) is the bacterial concentration at which bactericidal activity is measured. Hemolytic activity is described as the percentage of erythrocyte (RBC represents Red Blood Cell, hRBC is from human) lysis after treatment of certain concentration of the peptide and certain time (30min-3hr).

A) Peptides from arthropods:

PDB	Name	10% Anionic	30% Anionic	MIC(μM)			CFU	Hemolytic	Ref.
				G-		G+			
				E. Coli	P.A.	S.Aureus			
1f0d	CA(1-8)-MA(1-12) *	-9.3 \pm 2.2	-15.6 \pm 0.3	3.125	1.56	3.125	2x10 ⁶	0%at100 μM 4% hRBC	[1]
1f0f	CA(1-8)-MA(1-12), G ⁹ I ¹⁰ G ¹¹ deletion*	-5.0 \pm 2.8	-9.5 \pm 1.5	6.25	3.125	3.125	2x10 ⁶	0%at100 μM 4% hRBC	
1f0e	CA(1-8)-MA(1-12), G ⁹ I ¹⁰ G ¹¹ \rightarrow P [*]	-5.5 \pm 0.5	-12.1 \pm 2.4	6.25	1.56	3.125	2x10 ⁶	0%at100 μM 4% hRBC	
2jmy	CM15, CecropinA- Melittin hybrid	-10.5 \pm 0.9	-13.2 \pm 0.3	0.5-1	2-4	0.5-2	1x10 ⁵	45%at64 μM 1% hRBC (1hr)	[2,3]
2mlt	Melittin	-16.4 \pm 0.6	-19.7 \pm 2.5	2,3,8	2	0.5	2x10 ⁶	50%at1.7 μM 1x10 ⁹ hRBC(1hr)	[4,5]
	Cecropin A [▲]	-15.5 \pm 1.4	-19.5 \pm 1.9	0.35	2.6	?	2x10 ⁵	13%at 145 μM Sheep RBC	[6,7]
1t51	IsCT	-8.5 \pm 1.1	-10.6 \pm 0.5	4	2	2	2x10 ⁶	72%at50 μM 50%at18 μM 4% hRBC (1hr) 50%at70 μM (sheep RBC 1hr)	[8]
1t52	IsCT E7K	-9.6 \pm 0.5	-11.0 \pm 1.5	2	2	2	2x10 ⁶	30%at50 μM 4% hRBC	
1t54	IsCT W6A	-8.4 \pm 0.9	-9.9 \pm 0.5	64	32	64	2x10 ⁶	5.0%at50 μM 4% hRBC	
1t55	IsCT E7K, G8P, S11K	-9.2 \pm 0.6	-14.0 \pm 1.1	2	2	2	2x10 ⁶	0.0%at50 μM 4% hRBC	
2pco	Latarcin 1	-2.1 \pm 0.5	-11.5 \pm 1.9	0.7,1.0	4.1	?	1x10 ⁵	20%at80 μM 2x10 ⁷ Rabbit RBC 3hr	[9,10]
2g9p	Latarcin 2a	-11.1 \pm 1.4	-17.2 \pm 1.6	0.5,0.7	6.7	?	10 ⁵	50%at6 μM 20%at5 μM hRBC	[11,12]
1zrw	Spinigerin	-9.8 \pm 1.8	-9.6 \pm 2.2	16	16	8	(2-4)x10 ⁶	0%at100 μM 4% hRBC	[13]
1zrx	Stomoxyn	-7.8 \pm 0.4	-12.1 \pm 0.7	0.19- 0.39	0.39- 0.78	?	?	8%at100 μM 4% hRBC	[14]
2l3i	Oxyopinin 4a	-11.1 \pm 0.7	-17.1 \pm 0.6	0.5		10	?prev	50%at 7 μM	[15]
1kv4	Moricin	-16.7 \pm 1.4	-21.3 \pm 3.3	0.31	0.81	0.21	?	?	[16]
2jr8	Manduca Sexta Moricin	-10.8 \pm 0.7	-19.2 \pm 0.6	1.38		1.38- 2.76	5x10 ⁵		[17]
2k38	Cupiennin 1a	-11.0 \pm 0.5	-16.3 \pm 1.1	0.31- 0.63	0.31- 0.63	0.31- 0.63	(1.7- 3.8)x10 ⁵	50%at24.4 μM	[18]
1d7n	Mastoparan M	-10.5 \pm 1.1	-12.0 \pm 1.6	4.22	4.22	2.11	10 ⁵	10% at50 μM 1% sheep RBC 1hr	[19,20]
2czp	Mastoparan X	-5.9 \pm 0.8	-8.5 \pm 0.2					Visible at 9.6 μM	[21]

* CecropinA-Magainin hybrid [▲] Built as ideal alpha-helix ? No data available NE No Effect.

B) Peptides from amphibian skin secretions:

PDB	Name	10% Anionic	30% Anionic	MIC(μ M)			CFU	Hemolytic	Ref.
				G-		G+			
				E. Coli	P.A.	S.Aureus			
1vm2	mutant peptide A2	-8.2 \pm 0.1	-9.4 \pm 0.2	250	?	?	1x10 ⁶	?	[22]
1vm3	mutant peptide A3	-8.8 \pm 0.4	-9.4 \pm 0.1	NE	?	?	1x10 ⁶	?	
1vm4	mutant peptide A4	-8.7 \pm 0.5	-10.3 \pm 0.1	100	?	?	1x10 ⁶	?	
1vm5	Aurein 1.2	-9.1 \pm 0.8	-10.7 \pm 0.1	75	?	8	1x10 ⁶	?	
1o53	Nontoxic membrane anchor E. coli enzyme IIA(Glucose)	-5.3 \pm 0.7	-7.4 \pm 0.9	NE	?	?	1x10 ⁶	?	
2f3a	LLAA(LL-37 derived Aurein 1.2 analog)	-9.6 \pm 0.8	-13.0 \pm 0.3	20	?	?	1.8x10 ⁶	?	[23]
2jpy	Phylloseptin-H2	-13.9 \pm 0.5	-14.9 \pm 0.3	3.7	7.6	1.9	1x10 ⁵	2.05%at64 μ M hRBC(30min)	[24,25]
2jq0	Phylloseptin-H1	-10.3 \pm 0.2	-11.9 \pm 0.2	1.9	7.9	3.9	1x10 ⁵	0.98%at32 μ M hRBC(30min)	
2jq1	Phylloseptin-H3	-10.6 \pm 0.9	-11.7 \pm 0.1	4.1	8.2	4.1	1x10 ⁵	?	
2g9l	Gaegurin -4	-14.7 \pm 0.9	-17.8 \pm 0.8	20.00	26.67		1x10 ⁶	2%at100 μ M 10% hRBC	[26-28]
2k10	Ranatuerin-2CSa	-15.4 \pm 1.3	-18.2 \pm 0.5	5	?	10	1x10 ⁶	50%at150 μ M 1x10 ⁷ hRBC(1hr)	[29,30]
2k9b	Dermadistinctin K	-5.0 \pm 2.2	-8.8 \pm 2.3	?	?	?	?	35%at46.7 μ M Peritoneal cell(4hr)	[31]
	Dermaseptin-S1 [▲]	-7.7 \pm 0.1	-11.2 \pm 1.2	12	>24	6	5x10 ⁵	50%at>100 μ M 10 ⁹ hRBC (30min) 50%at 12 μ M hRBC(3hr)	[32]
1xkm	Distinctin	-6.6 \pm 1.6	-9.5 \pm 0.5	14.5	28,29	28,29	1x10 ⁴	No hemolysis upto 1mM	[33,34]
2mag	Magainin 2	-7.6 \pm 0.6	-10.7 \pm 1.0	38 ⁺	76		(1-5)x10 ⁵	50%at430 μ M 1.8x10 ⁸ hRBC(30min)	[35,36]

[▲] Built as ideal alpha-helix ⁺ Inconsistent values reported by different articles.

C) Peptides from cathelicidin family:

PDB	Name	10% Anionic	30% Anionic	MIC(μ M)			CFU	Hemolytic	Ref.
				G-		G+			
				E. Coli	P.A.	S.Aureus			
1fry	SMAP-29(sheep cathelicidin)	-10.5 \pm 3.3	-17.0 \pm 0.6	0.25	1.25	0.5	(1.0-2.0) \times 10 ⁵	19.4%at20 μ M 10% hRBC	[37]
1hu5	Ovispirin-1	-12.1 \pm 1.2	-16.5 \pm 1.1	?	1.66	1	4 \times 10 ⁵	70.2% at 35 μ M 5% hRBC 50% at 13.5 μ M 3.5% hRBC 30min	[38-41]
1hu6	Novispirin G10	-7.6 \pm 2.5	-13.0 \pm 0.2	3.5	2.97	4.6	4 \times 10 ⁵	2.50%at 36 μ M 5% hRBC 50% at 1470 μ M	
1hu7	Novispirin T7	-6.3 \pm 2.6	-11.4 \pm 0.4	?	4.64	3.3	4 \times 10 ⁵	10%at35 μ M 5% hRBC	
2k6o	LL-37(human cathelicidin) ⁺	-15.7 \pm 0.5	-19.1 \pm 1.9	27.8	27.8	55.6	1 \times 10 ⁵	50%at~75 μ M 5% hRBC(1hr)	[42,43]
2lmf	LL-27(LL-37 N terminus 1-27)	-5.1 \pm 2.0	-8.6 \pm 0.4	160		24			[44]
2f3a	LLAA(LL37 derived Aurein1.2 analog)	-9.6 \pm 0.8	-13.0 \pm 0.3	20	?	?	1.8 \times 10 ⁶	?	[23]
2fbs	FK-13(LL37 core peptide)	-6.7 \pm 0.9	-10.1 \pm 1.0	40	?	?	2 \times 10 ⁶	?	[45]
1lyp	CAP18 (rabbit)	-14.7 \pm 1.6	-25.2 \pm 1.5	2.5	5.0	>5.0(~20?)	5-10 \times 10 ³	0% upto 500 μ M	[46,47]
2amn	Fowlicidin-1(chicken cathelicidin)	-8.8 \pm 1.0	-17.4 \pm 0.6	4.0	?	0.5	5 \times 10 ⁵	50%at6 μ M 0.5% hRBC 2hr	[48]
2gdl	Fowlicidin-2(chicken cathelicidin)	-6.3 \pm 3.0	-10.1 \pm 3.8	4-8	?	1	4 \times 10 ⁵	50%at100 μ M hRBC	[49]
2hfr	Fowlicidin-3(chicken cathelicidin)	-12.6 \pm 2.0	-13.6 \pm 1.6	2	?	1	4 \times 10 ⁵	50%at9 μ M hRBC	[49]

D) Miscellaneous peptides :

PDB	Name	10% Anionic	30% Anionic	MIC(μ M)			CFU	Hemolytic	Ref.
				G-		G+			
				E. Coli	P.A.	S.Aureus			
1z64	Pleurocidin ⁺	-8.2 \pm 0.6	-10.8 \pm 0.7	2.75	35	26.35	2x10 ⁷	29%at50 μ M 4% hRBC	[52-54]
2jos	Piscidin 1	-11.6 \pm 0.7	-13.4 \pm 1.0	3.1	12.5	3.1	1x10 ⁵	50%at12 μ M 5% hRBC 30min	[55,56]
	Warnericin-RK [▲]	-12.7 \pm 0.9	-13.3 \pm 0.3	20.0	20.0	20.0	1x10 ⁶	50%at1.2 μ M 1% hRBC 30min	[57]
2kam	δ -hemolysin	-13.0 \pm 0.6	-14.1 \pm 0.4	NA	NA	NA	NA	50% at8-10 μ M(guinea pig RBC 30min)	[57,58]
1p0g	HP(2-20)	-7.6 \pm 0.8	-11.0 \pm 0.4	3.13,12.5	6.25	12.5	?	50% at ~150 μ M (low salt buffer) 15% at 215 μ M (high salt buffer)	[59,60]
1p0j	HP(2-20) Analog1	-8.6 \pm 0.4	-13.2 \pm 0.6	0.78,6.25	3.13	3.13			
1p0l	HP(2-20) Analog2	-7.4 \pm 0.6	-11.9 \pm 0.2	3.13,6.25	6.25	6.25			
1p0o	HP(2-20) Analog3	-8.2 \pm 1.3	-12.4 \pm 0.3	1.56,3.13	3.13	1.56,3.13		0% at 100uM 8% hRBC	
1amt	Alamethicin	-8.2 \pm 0.2	-8.0 \pm 0.2	7.64	?	?	?	50%at 30 μ M 1.8x10 ⁸ cell/ml hRBC(30min)	[61,62]
1xc0	Pardaxin	-20.3 \pm 2.0	-22.7 \pm 2.8	13	25	?	1x10 ⁶	50%at 50 μ M 5% hRBC 30min	[63,64]

[▲] Built from ideal alpha-helix

⁺ Inconsistent results between different articles.

NA No activity against the target organism.

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