

Supplementary Materials: An Smp43-Derived Short-Chain α -Helical Peptide Displays a Unique Sequence and Possesses Antimicrobial Activity against Both Gram-Positive and Gram-Negative Bacteria

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Table S1. Sequence alignments of scorpion venom-derived long-chain noncysteine-containing AMPs.

Name	Sequence	AA ^a	Identity%	Reference
Smp43	G-VWDWIKKTAGKIWNSEPVKALKSQALNAAKNFVAEKIGATPS	43	100	[1]
Opistoporin-2	GKVWDWIKSTAKKLWNSEPVKELKNTALNAAKNFVAEKIGATPS	44	84.1	[2]
Opistoporin-1	GKVWDWIKSTAKKLWNSEPVKELKNTALNAAKNLVAEKIGATPS	44	81.8	[2]
Pandinin-1	GKVWDWIKSAAKKIWSSEPVSQKQVLNAAKNYVAEKIGATPT	44	75.0	[3]
Heterin-1	G-VWDWLKKTAKNVWNSDIVKQLKGKAINAAKNYVAEKIGATPS	43	74.4	[4]
Hadrurin	G-ILDTIKSIASKVWNSKTVQDLKRKGIN----WVANKLGVSPQAA	41	40.0	[5]
Vejovine	G-IWSSIKNLASKAWNSDIGQSLRNKAAGAINKFVADKIGVTPSQAAS	47	35.0	[6]
Im-1	-FSFKRLKGFAKKLWNSKLARKIRTKGLKYVKNFAKDMLSEGEEAPPAAEPPVEAPQ	56	21.4	[7]
Parabutoporin	---FK-LGSFLKKAWKSKLAKKLRAKGKEMLDYAKGLLEGGSSEVPGQ	45	14.6	[2]
BmKbpp	---FR-FGSFLKKVWWSKLAKKLRSKGKQLLDYANKVLNGPEEEAAAPAE	47	14.0	[8]

^aAA, Number of residues.

Table S2. Amino acid sequences and physiochemical properties of Smp43-derived peptides.

	Name	Sequence	z^a	$\langle H \rangle^b$	$\langle \mu H \rangle^c$	MW ^d (Da)
1	Smp43(1-14)	GVWDWIKKTAGKIW-NH ₂	3	0.600	0.590	1687.0
2	Smp43(3-16)	WDWIKKTAGKIWNS-NH ₂	3	0.467	0.572	1732.0
3	Smp43(5-18)	WIKKTAGKIWNSEP-NH ₂	3	0.367	0.363	1656.9
4	Smp43(7-20)	KKTAGKIWNSEPVK-NH ₂	4	0.094	0.206	1584.9
5	Smp43(9-22)	TAGKIWNSEPVKAL-NH ₂	2	0.379	0.259	1512.8
6	Smp43(11-24)	GKIWNSEPVKALKS-NH ₂	3	0.265	0.332	1555.8
7	Smp43(13-26)	IWNSEPVKALKSQA-NH ₂	2	0.342	0.267	1569.8
8	Smp43(15-28)	NSEPVKALKSQALN-NH ₂	2	0.131	0.231	1497.7
9	Smp43(17-30)	EPVKALKSQALNAA-NH ₂	2	0.221	0.302	1438.7
10	Smp43(19-32)	VKALKSQALNAAKN-NH ₂	4	0.102	0.312	1454.7
11	Smp43(21-34)	ALKSQALNAAKNFV-NH ₂	3	0.301	0.327	1473.7
12	Smp43(23-36)	KSQALNAAKNFVAE-NH ₂	2	0.134	0.273	1489.7
13	Smp43(25-38)	QALNAAKNFVAEKI-NH ₂	2	0.265	0.334	1515.7
14	Smp43(27-40)	LNAAKNFVAEKIGA-NH ₂	2	0.281	0.303	1444.7
15	Smp43(29-42)	AAKNFVAEKIGATP-NH ₂	2	0.272	0.189	1415.6

^a z , net charge; ^b $\langle H \rangle$, the mean hydrophobicity value per residue; ^c $\langle \mu H \rangle$, the hydrophobic moments. A value of 0.5 means that the peptide has about 50% of the maximum possible amphipathicity. ^dMW, the molecular weights of the peptides were measured by mass spectrometry.

Table S3. Minimum inhibitory concentrations of Smp43-derived peptides against the tested bacterial strains.

Peptides	Smp43(1-14)	Smp43(3-16)	Smp43(5-18)	Smp43(7-20)	Smp43(9-22)	Smp43(11-24)	Smp43(13-26)	Smp43(15-28)	Smp43(17-30)	Smp43(19-32)	Smp43(21-34)	Smp43(23-36)	Smp43(25-38)	Smp43(27-40)	Smp43(29-42)
Bacterial strains	Minimum inhibitory concentrations (μg/mL)														
Gram-positive bacteria															
<i>Staphylococcus aureus</i> ATCC29213	5	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
<i>Enterococcus faecalis</i> ATCC29212	10	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
Gram-negative bacteria															
<i>Escherichia coli</i> ATCC25922	10	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
<i>Klebsiella pneumoniae</i> ATCC700603	10	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
<i>Pseudomonas aeruginosa</i> ATCC27853	10	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
<i>Acinetobacter baumannii</i> ATCC19606	5	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
HC10 ^a	75	>200	>200	>200	>200	>200	>200	>200	>200	>200	>200	>200	>200	>200	>200

^aHC₁₀, the concentration of the peptide that causes 10% hemolysis of of human red blood cells.

Table S4. Sequence alignments between Smp43(1-14) and other scorpion venom-derived short-chain noncysteine-containing AMPs.

Name	Sequence	AA ^a	Identity%	Reference
Smp43(1-14)	GVWDWIKKTAGKIW-NH ₂	14	100	This study
Uy17	-ILSAIWSGIKGLL-NH ₂	13	23.5	[9]
Uy192	-FLSTIWNGIKGLL-NH ₂	13	23.5	[9]
IsCT	-ILGKIWEGIKSLF-NH ₂	13	23.5	[10]
Spiniferin	-ILGEIWKGIDIL-NH ₂	13	23.5	[4]
BmKn2	-FIGAIARLLSKIF-NH ₂	13	21.4	[11]
VsCT2	-FLKGIIDTVSKLF-NH ₂	13	21.4	[12]
VsCT1	-FLKGIIDTVSNWL-NH ₂	13	20.0	[12]
Um3	GFWGKLWEGVKSAL-NH ₂	14	20.0	[9]
Smp13	-ILQDIWNGIKNLF-NH ₂	13	17.7	[1]
UyCT3	-ILSAIWSGIKSLF-NH ₂	13	17.7	[9]
VmCT1	-FLGALWNVAKSVF-NH ₂	13	17.7	[12]
Pantinin-3	-FLSTIWNGIKSLN-NH ₂	13	17.7	[13]
VmCT2	-FLSTLWNAAKSIF-NH ₂	13	14.3	[12]
Hp1404	GILGKLWEGVKSIF-NH ₂	14	14.3	[14]
UyCT1	GFWGKLWEGVKNAI-NH ₂	14	14.3	[9]
UyCT5	-IWSAIWSGIKGLL-NH ₂	13	14.3	[15]
Hp1035	-IFSAGGFLKSIF-NH ₂	13	14.3	[16]
Meucin-13	-IFGAIAGLLKNIF-NH ₂	13	14.3	[17]
StCT1	GFWGSLWEGVKSIV-NH ₂	14	14.3	[18]
StCT2	GFWGKLWEGVKSAL-NH ₂	14	14.3	[19]
OcyC1	-ILSAIWSGIKSLF-NH ₂	13	14.3	[20]
OcyC2	GILGKIWEGVKSIL-NH ₂	14	14.3	[20]
Pantinin-1	GILGKLWEGFKSIV-NH ₂	14	14.3	[13]
Pantinin-2	-IFGAIWKGISLL-NH ₂	13	14.3	[13]
Lausporin-1	-FLSALWGVAKSLF-NH ₂	13	11.8	[21]
IsCT2	-IFGAIWNGIKSLF-NH ₂	13	7.1	[10]
Um5	-IFKAIWGGIKSLF-NH ₂	13	7.1	[9]
Hp1090	-IFKAIWSGIKSLF-NH ₂	13	7.1	[16]
NDBP-5.5	-IFSAGLLSNLL-NH ₂	13	7.1	[15]
Um4	-FFSALLSGIKSLF	13	0.00	[9]

^aAA, Number of residues.

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