**Supplementary Information**

**Experimental Methods**

**Peptide synthesis.** The peptides were synthesized by solid state synthesis using Fmoc chemistry and purified by HPLC on C18 column. The identities of the peptides were confirmed by ESI-MS analysis on micrOTOF mass-spectrometer (Bruker), for details see Table S5. The concentrations of stock solutions were determined by amino acid analysis.

**Broth microdilution assay.** The assaywas performed according to the standard protocol [1], except that the 2x stock peptides were prepared and serially diluted in PBS with 0.05% BSA sterilized by filtration through 0.22 μm membrane [2]. Bacteria were grown to mid-logarithmic phase at 37 °C in Mueller-Hinton broth, diluted to approximately 2 x 105 CFU/ml, and 25 µL of the suspensions were mixed with 25 µL of the peptide dilutions. After incubation for 18 h at 37 °C, the minimal inhibitory concentration (MIC) was determined as the lowest peptide concentration resulting in the complete inhibition of visible bacterial growth. The results are medians derived from 3-5 independent experiments which were performed in triplicates.

**Structural analysis.** The peptide and micelle solutions in 10 mM NaH2PO4/Na2HPO4 50 mM NaF pH 7.4 were mixed giving final peptide concentrations 20-30 µM and peptide to lipid ratio from 1:1000 to 1:1500 and incubated at 25 °C for 1 h before data collection. Circular dichroism measurements were performed on Chirascan (Applied Photophysics), spectra were converted to mean-residue Δε units (M-1cm-1) and analyzed using CDSSTR algorithm [3] in DichroWeb [4].

**Table S1**. Sequences of natural α-helical antimicrobial peptides from APD2 used in this study. Most structural data were obtained by nuclear magnetic resonance (NMR) or circular dichroism spectroscopy (CD) in a membrane-mimicking environment modeled by SDS or DPC micelles, or trifluoroethanol solutions (TFE). In a few cases where a peptide was not studied experimentally, but its close homologs had a helical structure, the structure assignment was made based on homology.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| № | Peptide sequence | APD ID | Peptidename | Structureelucidation method | Reference (structural analysis)  | Unique patterns |
| 1. 1
 | GLWSKIKEVGKEAAKAAAKAAGKAALGAVSEAV | AP00001 | Dermaseptin-B2 | NMR in TFE / SDS | Biochemistry 42(34):10311-23. | 38 |
|  | GLFDIIKKIAESI | AP00012 | Aurein 1.1 | *by homology to Aurein 1.2* | Eur Biophys J. 33(2):109-16.  | 1 |
|  | GLFDIIKKIAESF | AP00013 | Aurein 1.2 | NMR in lipid bilayer | Eur Biophys J. 33(2):109-16. | 1 |
|  | GLFDIVKKVVGALGSL | AP00015 | Aurein 2.2 | NMR in lipid bilayer | Biophys J. 92(8):2854-64.  | 0 |
|  | GLFDIVKKVVGAIGSL | AP00016 | Aurein 2.3 | NMR in lipid bilayer | Biophys J. 92(8):2854-64.  | 0 |
|  | KSSAYSLQMGATAIKQVKKLFKKWGW | AP00035 | Plantaricin A | NMR in DPC micelles | J Biol Chem. 280(24):22945-50. | 16 |
| 1. 1
 | GIGASILSAGKSALKGLAKGLAEHFAN | AP00050 | Bombinin-like peptide 1 | CD in TFE | J Biol Chem. 266(34):23103-11. | 19 |
|  | GIGSAILSAGKSALKGLAKGLAEHFAN | AP00051 | Bombinin-like peptide 2 | CD in TFE | J Biol Chem. 266(34):23103-11. | 19 |
|  | GIGAAILSAGKSALKGLAKGLAEHF | AP00052 | Bombinin-like peptide 3 | CD in TFE | J Biol Chem. 266(34):23103-11. | 19 |
|  | GIGAAILSAGKSIIKGLANGLAEHF | AP00053 | Bombinin-like peptide 4 | CD in TFE | J Biol Chem. 266(34):23103-11. | 7 |
|  | LIGPVLGLVGSALGGLLKKI | AP00056 | Bombinin H4 | NMR in DPC micelles | PDB ID: 2AP8 | 4 |
|  | GIGGVLLSAGKAALKGLAKVLAEKYAN | AP00061 | Maximin 4 | NMR in SDS micelles | Eur Biophys J. 40(4):447-62. | 23 |
|  | GIFSKLGRKKIKNLLISGLKNVGKEVGMDVVRTGIDIAGCKIKGEC | AP00080 | Esculentin-1 | CD / NMR in TFE | Biopolymers. 97(11):873-81. | 8 |
|  | GILDTLKQFAKGVGKDLVKGAAQGVLSTVSCKLAKTC | AP00088 | Esculentin-2EM | NMR | Biochem Biophys Res. Commun. 352(3):592-7. | 13 |
|  | FLPLIGRVLSGIL | AP00094 | Temporin A | CD / NMR in SDS / DPC micelles | J Med Chem. 51(8):2354-62. | 0 |
|  | LLPIVGNLLKSLL | AP00095 | Temporin B | NMR in SDS micelles | PDB ID: 6GIL | 3 |
|  | FVQWFSKFLGRIL | AP00101 | Temporin L | CD / NMR in SDS / DPC micelles | J Med Chem. 51(8):2354-62. | 0 |
|  | SWLSKTAKKLENSAKKRISEGIAIAIQGGPR | AP00134 | Cecropin P1 | CD / NMR | Eur J Biochem. 209(1):163-9. | 13 |
|  | GWLKKIGKKIERVGQHTRDATIQTIGVAQQAANVAATLK | AP00135 | Cecropin 2 | CD | FEBS Lett. 137(2):283-7. | 19 |
|  | KWKLFKKIEKVGQNIRDGIIKAGPAVAVVGQATQIAK | AP00139 | Cecropin A | NMR | Biochemistry 27(20), 7620-7629 | 14 |
|  | KKLLKWLKKLL | AP00143 | L5K5W | CD in SDS micelles | J Pept Sci. 15(9):583-8.  | 20 |
|  | GIGKFLHSAKKFGKAFVGEIMNS | AP00144 | Magainin 2 | NMR in DPC micelles | J Biomol NMR. 9(2):127-35. | 6 |
|  | VNYGNGVSCSKTKCSVNWGQAFQERYTAGINSFVSGVASGAGSIGRRP | AP00145 | Carnobacteriocin B2 | NMR | Biochemistry 38(47):15438-47. | 0 |
|  | GIGAVLKVLTTGLPALISWIKRKRQQ | AP00146 | Melittin | X-Ray | PDB ID: 2MLT | 1 |
|  | AKIPIKAIKTVGKAVGKGLRAINIASTANDVFNFLKPKKRKA | AP00147 | BM Moricin | NMR | FEBS Lett. 518(1-3):33-8. | 14 |
|  | RGLRRLGRKIAHGVKKYGPTVLRIIRIAG | AP00155 | SMAP-29 | NMR in SDS / TFA | Eur J Biochem. 269(4):1181-9. | 5 |
|  | ALWKTMLKKLGTMALHAGKAALGAAADTISQGTQ | AP00157 | Dermaseptin-S1 | CD | Biochemistry 30(36):8824-30. | 19 |
|  | ALWFTMLKKLGTMALHAGKAALGAAANTISQGTQ | AP00158 | Dermaseptin-S2 | *by homology to Dermaseptin-S1* | Eur J Biochem. 219(1-2):145-54. | 16 |
|  | ALWKNMLKGIGKLAGKAALGAVKKLVGAES | AP00159 | Dermaseptin-S3 | *by homology to Dermaseptin-S1* | Eur J Biochem. 219(1-2):145-54. | 31 |
|  | ALWMTLLKKVLKAAAKALNAVLVGANA | AP00160 | Dermaseptin-S4 | NMR in DPC micelles | J Biol Chem. 281(14):9432-8.  | 32 |
|  | GLWSKIKTAGKSVAKAAAKAAVKAVTNAV | AP00161 | Dermaseptin-S5 | *by homology to Dermaseptin-S4* | Eur J Biochem. 219(1-2):145-54. | 37 |
|  | GLWNKIKEAASKAAGKAALGFVNEMV | AP00162 | Dermaseptin-B5 | *by homology to Dermaseptin-S4* | J Biol Chem. 273(24):14690-7. | 24 |
|  | ALWKDILKNVGKAAGKAVLNTVTDMVNQ | AP00163 | Dermaseptin-B4 | *by homology to Dermaseptin-S4* | J Biol Chem. 273(24):14690-7. | 21 |
|  | ALWKTIIKGAGKMIGSLAKNLLGSQAQPES | AP00164 | Dermaseptin-B9 | *by homology to Dermaseptin-S4* | J Biol Chem. 273(24):14690-7. | 14 |
|  | GWGSFFKKAAHVGKHVGKAALTHYL | AP00166 | Pleurocidin | NMR in DPC / TFE | Biochemistry 44(19):7282-93. | 10 |
|  | GWMSKIASGIGTFLSGMQQ | AP00167 | Phylloxin-B1 | CD in TFE | Eur J Biochem. 267(2):370-8. | 0 |
|  | RSGRGECRRQCLRRHEGQPWETQECMRRCRRRG | AP00184 | MBP-1 | CD | J Biol Chem. 267(26):18814-20. | 0 |
|  | LKLKSIVSWAKKVL | AP00200 | Mastoparan B | NMR in DPC / SDS micelles | J Biomol Struct Dyn. 18(4):595-606. | 3 |
|  | INLKALAALAKKIL | AP00201 | Mastoparan | NMR in lipid bilayer | Eur J Biochem. 268(2):302-9. | 10 |
|  | GMASKAGAIAGKIAKVALKAL | AP00210 | PGLa | NMR in lipid bilayer | Biophys J. 90(5): 1676–1686. | 19 |
|  | GWLKKIGKKIERVGQHTRDATIQGLGIAQQAANVAATAR | AP00230 | Sarcotoxin IA | NMR | Eur J Biochem. 217(2):639-44. | 19 |
|  | SDEKASPDKHHRFSLSRYAKLANRLANPKLLETFLSKWIGDRGNRSV | AP00234 | Seminalplasmin | CD / NMR in DPC micelles | Eur J Biochem. 220(1):111-6. | 2 |
|  | GLLSVLGSVAKHVLPHVVPVIAEHL | AP00240 | Caerin 1.1 | NMR in TFE  | Eur J Biochem. 247(2):545-57. | 1 |
|  | GLLGVLGSVAKHVLPHVVPVIAEHL | AP00241 | Caerin 1.2 | *by homology to caerin 1.1* | Peptides 25(6):1035-54. | 1 |
|  | GLLSVLGSVAQHVLPHVVPVIAEHL | AP00242 | Caerin 1.3 | NMR | J. Peptide Res. 51**:**121-126 | 0 |
|  | GLLSSLSSVAKHVLPHVVPVIAEHL | AP00243 | Caerin 1.4 | *by homology to caerin 1.1* | Peptides 25(6):1035-54. | 1 |
|  | GLLSVLGSVVKHVIPHVVPVIAEHL | AP00244 | Caerin 1.5 | *by homology to caerin 1.1* | Peptides 25(6):1035-54. | 0 |
|  | GLFSVLGAVAKHVLPHVVPVIAEK | AP00245 | Caerin 1.6 | *by homology to caerin 1.1* | J Pept Sci. 3(3):181-5. | 1 |
|  | GLFKVLGSVAKHLLPHVAPVIAEK | AP00246 | Caerin 1.7 | *by homology to caerin 1.1* | J Pept Sci. 3(3):181-5. | 9 |
|  | GLFKVLGSVAKHLLPHVVPVIAEK | AP00247 | Caerin 1.8 | *by homology to caerin 1.1* | J Pept Res. 51(2):121-6. | 8 |
|  | GLFGVLGSIAKHVLPHVVPVIAEK | AP00248 | Caerin 1.9 | *by homology to caerin 1.1* | J Pept Res. 51(2):121-6. | 1 |
|  | GLWQKIKSAAGDLASGIVEGIKS | AP00257 | Caerin 4.1 | NMR in TFE | Australian J Chem. 53:257-265 | 3 |
|  | GLFVGVLAKVAAHVVPAIAEHF | AP00260 | Maculatin 1.1 | NMR in DPC / TFE | Eur J Biochem. 267(7):1894-908. | 3 |
|  | VFQFLGKIIHHVGNFVHGFSHVF | AP00276 | Clavanin A | CD / NMR in SDS / TFE | Sci Rep. 6:27128.  | 0 |
|  | VFQFLGRIIHHVGNFVHGFSHVF | AP00277 | Clavanin B | CD  | FEBS Lett. 400(2):158-62. | 0 |
|  | VFHLLGKIIHHVGNFVYGFSHVF | AP00278 | Clavanin C | CD | FEBS Lett. 400(2):158-62. | 1 |
|  | AFKLLGRIIHHVGNFVYGFSHVF | AP00279 | Clavanin D | CD | FEBS Lett. 400(2):158-62. | 0 |
|  | LFKLLGKIIHHVGNFVHGFSHVF | AP00280 | Clavanin E | *by homology to clavanins* | FEBS Lett. 410(2-3):490-2. | 6 |
|  | GLLRKGGEKIGEKLKKIGQKIKNFFQKLVPQPEQ | AP00281 | mCRAMP | CD / NMR in SDS / DPC / TFE  | J Pept Res. 60(1):1-9. | 19 |
|  | TRSSRAGLQFPVGRVHRLLRK | AP00308 | Buforin II | NMR in TFE  | FEBS Lett. 398(1):87-90. | 0 |
|  | LLGDFFRKSKEKIGKEFKRIVQRIKDFLRNLVPRTES | AP00310 | LL-37 | NMR in lipid micelles | J Biol Chem. 283(47):32637-43.  | 11 |
|  | SLGSFLKGVGTTLASVGKVVSDQFGKLLQAGQG | AP00315 | Dermatoxin B1 | CD | Eur J Biochem. 267(14):4583-92. | 0 |
|  | GVIDAAKKVVNVLKNLF | AP00325 | Uperin 3.6 | NMR in TFE | J Pept Res. 54(2):137-45. | 4 |
|  | GFGKAFHSVSNFAKKHKTA | AP00328 | Styelin A | *by homology* | Comp Biochem Physiol B Biochem Mol Biol. 118(3):515-21. | 0 |
|  | GFGPAFHSVSNFAKKHKTA | AP00329 | Styelin B | *by homology* | Comp Biochem Physiol B Biochem Mol Biol. 118(3):515-21. | 0 |
|  | GWLRKAAKSVGKFYYKHKYYIKAAWQIGKHAL | AP00330 | Styelin D | CD in TFE | J Biol Chem. 275(49):38417-26. | 17 |
|  | GWLRKAAKSVGKFYYKHKYYIKAAWKIGRHAL | AP00331 | Styelin E | by homology to Styelin D | FEBS Lett. 412:144-148 | 24 |
|  | FFGWLIKGAIHAGKAIHGLIHRRRH | AP00339 | Chrysophsin-1 | CD | Eur J Biochem. 270(4):675-86. | 4 |
|  | FFGWLIRGAIHAGKAIHGLIHRRRH | AP00340 | Chrysophsin-2 | CD | Eur J Biochem. 270(4):675-86. | 1 |
|  | FIGLLISAGKAIHDLIRRRH | AP00341 | Chrysophsin-3 | CD | Eur J Biochem. 270(4):675-86. | 1 |
|  | GLFDVIKKVASVIGGL | AP00351 | Citropin 1.1 | NMR in TFE | Eur J Biochem. 265(2):627-37. | 0 |
|  | GRFKRFRKKFKKLFKKLSPVIPLLHLG | AP00366 | BMAP-27 | NMR in ethanol | PDB ID: 2KET | 20 |
|  | GGLRSLGRKILRAWKKYGPIIVPIIRIG | AP00367 | BMAP-28 | CD | J Biol Chem. 271(45):28375-81. | 4 |
|  | RIIDLLWRVRRPQKPKFVTVWVR | AP00369 | PMAP-23 | NMR in DPC micelles | Biochem Biophys Res Commun. 290(1):204-12. | 0 |
|  | VGRFRRLRKKTRKRLKKIGKVLKWIPPIVGSIPLGCG | AP00370 | PMAP-36 | CD in TFE | FEBS J. 272(17):4398-406. | 28 |
|  | GLLSRLRDFLSDRGRRLGEKIERIGQKIKDLSEFFQS | AP00371 | PMAP-37 | CD in TFE | Eur J Biochem. 228(3):941-6. | 2 |
|  | GKVWDWIKSTAKKLWNSEPVKELKNTALNAAKNLVAEKIGATPS | AP00374 | Opistoporin 1 | CD in TFE | Eur J Biochem. 269(19):4799-810. | 10 |
|  | GKVWDWIKSTAKKLWNSEPVKELKNTALNAAKNFVAEKIGATPS | AP00375 | Opistoporin 2 | CD in TFE | Eur J Biochem. 269(19):4799-810. | 10 |
|  | GWKDWAKKAGGWLKKKGPGMAKAALKAAMQ | AP00376 | Ponericin G1 | CD in TFE | J Biol Chem. 276(21):17823-9.  | 29 |
|  | GLVDVLGKVGGLIKKLLP | AP00381 | Ponericin G6 | CD in TFE | J Biol Chem. 276(21):17823-9. | 5 |
|  | LLKELWTKIKGAGKAVLGKIKGLL | AP00384 | Ponericin L2 | CD in TFE | J Biol Chem. 276(21):17823-9. | 11 |
|  | WLGSALKIGAKLLPSVVGLFKKKKQ | AP00386 | Ponericin W1 | CD in TFE | J Biol Chem. 276(21):17823-9. | 6 |
|  | HVDKKVADKVLLLKQLRIMRLLTRL | AP00399 | Spinigerin | CD / NMR in TFE | Biopolymers 81(2):92-103. | 5 |
|  | SIGSALKKALPVAKKIGKIALPIAKAALP | AP00414 | Ceratotoxin A | CD / NMR in methanol | Biopolymers 39(5):653-64. | 32 |
|  | SIGSAFKKALPVAKKIGKAALPIAKAALP | AP00415 | Ceratotoxin B | CD / NMR in methanol | Biopolymers 39(5):653-64. | 32 |
|  | GLRKRLRKFRNKIKEKLKKIGQKIQGFVPKLAPRTDY | AP00418 | CAP18(106-142) | NMR in TFE | FEBS Lett. 370(1-2):46-52. | 18 |
|  | HSSGYTRPLRKPSRPIFIRPIGCDVCYGIPSSTARLCCFRYGDCCHL | AP00420 | Penaeidin-4d | CD / NMR | J Biol Chem. 280(16):16009-18. | 0 |
|  | GLLGPLLKIAAKVGSNLL | AP00427 | CPF-ST3 | NMR in TFE / micelles | Biochim Biophys Acta. 1804(4):1020-8.  | 8 |
|  | GLICESCRKIIQKLEDMVGPQPNEDTVTQAASQVCDKLKILRGLCKKIMRSFLRRISWDILTGKKPQAICVDIKICKEKTGLI | AP00429 | Porcine NK-Lysin | NMR | Nat Struct Biol. 4(10):793-5. | 8 |
|  | ILGKIWEGIKSLF | AP00430 | IsCT | NMR | Biochem Biophys Res Commun. 323(2):712-9. | 1 |
|  | KKKKPLFGLFFGLF | AP00432 | The K4 peptide | NMR in DPC / SDS micelles | Biochim Biophys Acta. 1808(1):106-16.  | 0 |
|  | GLMSVLGHAVGNVLGGLFKS | AP00434 | Frenatin 3 | NMR in TFE  | Biopolymers 70(3):424-34. | 1 |
|  | GWFGKAFRSVSNFYKKHKTYIHAGLSAATLL | AP00435 | Styelin C | *by homology to Styelin D* | Comp Biochem Physiol B Biochem Mol Biol. 118(3):515-21. | 1 |
|  | GLLKRIKTLL | AP00447 | Anoplin | NMR | Chembiochem. 16(2):242-53. | 0 |
|  | FFHHIFRGIVHVGKTIHRLVTG | AP00473 | Piscidin 1 | NMR in lipid bilayer | J Am Chem Soc. 136(9):3491-504 | 0 |
|  | FIHHIFRGIVHAGRSIGRFLTG | AP00474 | Piscidin 3 | NMR in lipid bilayer | J Am Chem Soc. 136(9):3491-504.  | 0 |
|  | GLNTLKKVFQGLHEAIKLINNHVQ | AP00475 | Pseudin-1 | CD | Biochem Biophys Res Commun. 288(4):1001-5. | 1 |
|  | GLNALKKVFQGIHEAIKLINNHVQ | AP00476 | Pseudin-2 | CD | Biochem Biophys Res Commun. 288(4):1001-5. | 1 |
|  | GINTLKKVIQGLHEVIKLVSNHE | AP00477 | Pseudin-3  | CD | Biochem Biophys Res Commun. 288(4):1001-5. | 1 |
|  | GINTLKKVIQGLHEVIKLVSNHA | AP00478 | Pseudin-4 | CD | Biochem Biophys Res Commun. 288(4):1001-5. | 1 |
|  | FSFKRLKGFAKKLWNSKLARKIRTKGLKYVKNFAKDMLSEGEEAPPAAEPPVEAPQ | AP00482 | Im-1 | CD in TFE | Biosci Biotechnol Biochem. 74(2):364-9.  | 24 |
|  | RGFRKHFNKLVKKVKHTISETAHVAKDTAVIAGSGAAVVAAT | AP00484 | Stomoxyn | CD / NMR in TFE | Biopolymers 81(2):92-103. | 14 |
|  | GFGALFKFLAKKVAKTVAKQAAKQGAKYVVNKQME | AP00485 | Cupiennin 1a | NMR in lipid bilayer | Biochemistry 46(11):3576-85. | 31 |
|  | RQRVEELSKFSKKGAAARRRK | AP00492 | Misgurin | CD in TFE | FEBS Lett. 411(2-3):173-8. | 6 |
|  | NLVSGLIEARKYLEQLHRKLKNCKV | AP00493 | Distinctin | NMR | Proc Natl Acad Sci U S A. 102(18):6309-14. | 0 |
|  | KWKLFKKIPKFLHLAKKF | AP00494 | P-18 | CD in TFE and SDS | Biotechnol Lett. 26(4):337-41. | 17 |
|  | AKKVFKRLEKLFSKIQNDK | AP00496 | HP 2-20 | NMR in SDS micelles | PDB ID: 1P0G | 16 |
|  | GLVRKGGEKFGEKLRKIGQKIKEFFQKLALEIEQ | AP00498 | rCRAMP | CD in TFE | Infect Immun. 68(5):2748-55. | 12 |
|  | VGALAVVVWLWLWLW | AP00499 | Gramicidin A | NMR in lipid bilayer | Journal of Biomolecular NMR 8**:**1-14 | 0 |
|  | FLRFIGSVIHGIGHLVHHIGVAL | AP00502 | Clavaspirin | CD | J Pept Res. 58(6):445-56. | 0 |
|  | LAHQKPFIRKSYKCLHKRCR | AP00504 | human MUC7 20-Mer | CD in TFE | Biochem J. 375(Pt 1): 175–182. | 3 |
|  | DSHAKRHHGYKRKFHEKHHSHRGY | AP00505 | human Histatin 5 | CD / NMR in TFE | Biochem Cell Biol. 76(2-3):247-56. | 0 |
|  | GLLSKVLGVGKKVLCGVSGLC | AP00507 | Nigrocin-2 | CD / NMR in SDS / TFE | FEBS Lett. 507(1):95-100. | 5 |
|  | VAIALKAAHYHTHKE | AP00509 | Human Calcitermin | CD in TFE | FEBS Lett. 504(1-2):5-10. | 5 |
|  | ILQKAVLDCLKAAGSSLSKAAITAIYNKIT | AP00510 | Dicynthaurin | CD in lipid bilayer | Biochim Biophys Acta. 1527(3):141-8. | 7 |
|  | FLGGLIKIVPAMICAVTKKC | AP00513 | Ranalexin | CD / NMR in DPC / TFE | Eur J Biochem. 253(1):221-8. | 1 |
|  | IWLTALKFLGKHAAKHLAKQQLSKL | AP00516 | Lycotoxin I | CD in lipid bilayer | J Pept Sci. 14(4):528-34. | 19 |
|  | KIKWFKTMKSIAKFIAKEQMKKHLGGE | AP00517 | Lycotoxin II | CD in lipid bilayer | J Pept Sci. 14(4):528-34. | 15 |
|  | GVVDILKGAAKDIAGHLASKVMNKL | AP00533 | Ocellatin-F1 | NMR in DPC / TFE | Peptides 103:72-83. | 11 |
|  | GLGSVFGRLARILGRVIPKVAKKLGPKVAKVLPKVMKEAIPMAVEMAKSQEEQQPQ | AP00535 | Pilosulin 1 | CD in TFE / SDS | Biochem J. 390(Pt 1): 177–188. | 25 |
|  | IDWKKLLDAAKQIL | AP00541 | Polybia-MPI | CD in TFE / SDS | Peptides 29(6):963-8.  | 5 |
|  | ILGTILGLLKSL | AP00542 | Polybia-CP | CD in TFE | Toxicology 288(1-3):27-33.  | 2 |
|  | FLSLIPHAINAVSAIAKHN | AP00546 | Phylloseptin-H1 | CD / NMR in lipid bilayers | Peptides 29(10):1633-44. | 0 |
|  | RFGRFLRKIRRFRPKVTITIQGSARFG | AP00548 | Chicken CATH-2 | NMR in TFE | PDB ID: 2GDL | 1 |
|  | GKIPVKAIKKAGAAIGKGLRAINIASTAHDVYSFFKPKHKKK | AP00554 | Sl moricin | NMR | Biochim Biophys Acta. 1752(1):83-92. | 24 |
|  | KGRGKQGGKVRAKAKTRSS | AP00555 | Parasin I | CD / NMR in SDS | Peptides 29(7):1102-8. | 9 |
|  | GFMKYIGPLIPHAVKAISDLI | AP00556 | Kassinatuerin-1 | CD in TFE | Peptides 26(11):2104-10. | 1 |
|  | RVKRVWPLVIRTVIAGYNLYRAIKKK | AP00557 | Chicken CATH-1 | NMR in TFE  | FEBS J. 273(12):2581-93. | 0 |
|  | GKVWDWIKSAAKKIWSSEPVSQLKGQVLNAAKNYVAEKIGATPT | AP00562 | Pandinin 1 | CD / NMR in DPC / TFE | Biochem J. 359(Pt 1):35-45. | 7 |
|  | GILSSFKGVAKGVAKDLAGKLLETLKCKITGC | AP00592 | Ranatuerin-2CSa | NMR in TFE | Biochim Biophys Acta. 1784(6):924-9.  | 13 |
|  | ILPILSLIGGLLGK | AP00605 | Temporin-1CEb | CD in TFE | Biochimie 94(2):434-41.  | 1 |
|  | RVKRFWPLVPVAINTVAAGINLYKAIRRK | AP00613 | Chicken CATH-3 | NMR in TFE | FEBS J. 274(2):418-28. | 1 |
|  | ALLGDFFRKSKEKIGKEFKRIVQRIKDFLRNLVPRTES | AP00624 | ALL-38 | *by homology to LL-37* | J Biol Chem. 278(31):28540-6. | 11 |
|  | KRIVQRIKDFLRNLVPRTES | AP00625 | human KR-20 | *by homology to LL-37* | J Immunol. 172(5):3070-7. | 1 |
|  | KSKEKIGKEFKRIVQRIKDFLRNLVPRTES | AP00626 | human KS-30 | *by homology to LL-37* | J Immunol. 172(5):3070-7. | 10 |
|  | RKSKEKIGKEFKRIVQRIKDFLRNLVPRTES | AP00627 | human RK-31 | *by homology to LL-37* | J Immunol. 172(5):3070-7. | 10 |
|  | LLGDFFRKSKEKIGKEFKRIVQR | AP00628 | LL-23 | NMR in DPC / SDS micelles | Biochemistry 51(2):653-64. | 10 |
|  | LLGDFFRKSKEKIGKEFKRIVQRIKDFLR | AP00629 | human LL-29 | *by homology to LL-37* | FASEB J. 20(12):2068-80. | 11 |
|  | GFFALIPKIISSPLFKTLLSAVGSALSSSGEQE | AP00641 | Pardaxin 1 | CD lipid vesicles | Biophys J. 98(4):576-85 | 3 |
|  | GFFALIPKIISSPLFKTLLSAVGSALSSSGGQE | AP00644 | Pardaxin 4 | NMR in DPC micelles | J Biol Chem. 279(44):45815-23. | 3 |
|  | GFFAFIPKIISSPLFKTLLSAVGSALSSSGDQE | AP00645 | Pardaxin 5 | *by homology to Pardaxin 1* | FEBS Lett. 435(2-3):173-7 | 2 |
|  | FWGALAKGALKLIPSLFSSFSKKD | AP00660 | Pandinin 2 | CD / NMR in DPC / TFE | Biochem J. 359(Pt 1):35-45. | 5 |
|  | RLGNFFRKVKEKIGGGLKKVGQKIKDFLGNLVPRTAS | AP00676 | RL-37 | CD in lipid bilayer | Antimicrob Agents Chemother. 45(10):2695-702. | 15 |
|  | GLRKKFRKTRKRIQKLGRKIGKTGRKVWKAWREYGQIPYPCRI | AP00677 | CAP11 | *by homology to cathelicidins* | Mol Biol Rep. 39(12): 10957–10970 | 17 |
|  | RLKELITTGGQKIGEKIRRIGQRIKDFFKNLQPREEKS | AP00678 | K9CATH | *by homology to cathelicidins* | Dev Comp Immunol. 31(12):1278-96. | 5 |
|  | GLFGRLRDSLQRGGQKILEKAERIWCKIKDIFR | AP00680 | SMAP-34 | *by homology to cathelicidins* | Mol Biol Rep. 39(12): 10957–10970 | 2 |
|  | KRFGRLAKSFLRMRILLPRRKILLAS | AP00686 | eCATH-1 | CD in TFE | Antimicrob Agents Chemother. 45(3):715-22. | 5 |
|  | KRRHWFPLSFQEFLEQLRRFRDQLPFP | AP00687 | eCATH-2 | CD in TFE | Antimicrob Agents Chemother. 45(3):715-22. | 0 |
|  | KRFHSVGSLIQRHQQMIRDKSEATRHGIRIITRPKLLLAS | AP00688 | eCATH-3 | CD in TFE | Antimicrob Agents Chemother. 45(3):715-22. | 0 |
|  | GFFKKAWRKVKHAGRRVLDTAKGVGRHYVNNWLNRYR | AP00691 | HFIAP-1 | *by homology to cathelicidins* | Mol Biol Rep. 39(12): 10957–10970 | 6 |
|  | GWFKKAWRKVKNAGRRVLKGVGIHYGVGLI | AP00692 | HFIAP-3 | *by homology to cathelicidins* | Mol Biol Rep. 39(12): 10957–10970 | 7 |
|  | FKRIVQRIKDFLR | AP00708 | GF-17 | NMR in SDS micelles | Antimicrob Agents Chemother. 56(2):845-56. | 2 |
|  | GLLNGLALRLGKRALKKIIKRLCR | AP00722 | Cryptonin | CD in TFE | Arch Insect Biochem Physiol. 66(4):204-13. | 13 |
|  | SLLSLIRKLIT | AP00723 | Decoralin | CD in TFE / SDS | Peptides 28(12):2320-7.  | 0 |
|  | LLGDFFRKAREKIGEEFKRIVQRIKDFLRNLVPRTES | AP00733 | Organgutan ppyLL-37 | CD in TFE | J Biol Chem. 281(29):19861-71. | 8 |
|  | SLGNFFRKARKKIGEEFKRIVQRIKDFLQHLIPRTEA | AP00734 | Gibbon hmdSL-37 | CD in TFE | J Biol Chem. 281(29):19861-71. | 12 |
|  | RLGNFFRKAKKKIGRGLKKIGQKIKDFLGNLVPRTES | AP00735 | pobRL-37 | CD in TFE | J Biol Chem. 281(29):19861-71. | 19 |
|  | RLGDILQKAREKIEGGLKKLVQKIKDFFGKFAPRTES | AP00736 | cjaRL-37 | CD in TFE  | J Biol Chem. 281(29):19861-71. | 18 |
|  | FLSLIPHAINAVSTLVHHF | AP00757 | Phylloseptin-H2 | NMR in TFE | Peptides 29(10):1633-44.  | 0 |
|  | FLSLIPHAINAVSALANHG | AP00758 | Phylloseptin-H3 | NMR in TFE | Peptides 29(10):1633-44.  | 0 |
|  | GLRSKIWLWVLLMIWQESNKFKKM | AP00764 | Dermaseptin-S9 | NMR in TFE | Biochemistry 45(2):468-80. | 1 |
|  | IYWIADQFGIHLATGTARKLLDAMASGASLGTAFAAILGVTLPAWALAAAGALGATAA | AP00766 | Gassericin A | CD | Appl Environ Microbiol. 70(5): 2906–2911. | 7 |
|  | FRGLAKLLKIGLKSFARVLKKVLPKAAKAGKALAKSMADENAIRQQNQ | AP00772 | Oxyopinin 1 | CD in TFE | J Biol Chem. 277(26):23627-37.  | 35 |
|  | GKFSVFGKILRSIAKVFKGVGKVRKQFKTASDLDKNQ | AP00773 | Oxyopinin 2a | CD in TFE | J Biol Chem. 277(26):23627-37.  | 17 |
|  | GKFSGFAKILKSIAKFFKGVGKVRKGFKEASDLDKNQ | AP00774 | Oxyopinin 2b | CD in TFE | J Biol Chem. 277(26):23627-37.  | 20 |
|  | GKLSGISKVLRAIAKFFKGVGKARKQFKEASDLDKNQ | AP00775 | Oxyopinin 2c | CD in TFE | J Biol Chem. 277(26):23627-37.  | 18 |
|  | GKFSVFSKILRSIAKVFKGVGKVRKGFKTASDLDKNQ | AP00776 | Oxyopinin 2d | CD in TFE | J Biol Chem. 277(26):23627-37.  | 17 |
|  | GRRRRSVQWCAVSQPEATKCFQWQRNMRKVRGPPVSCIKRDSPIQCIQA | AP00780 | Human lactoferricin | NMR in DPC / SDS micelles | Antimicrob Agents Chemother. 49(8):3387-95. | 0 |
|  | IIGPVLGLVGSALGGLLKKI | AP00793 | Bombinin H2 | NMR in DPC / SDS micelles | Toxicon 52(2):246-54. | 4 |
|  | LSPNLLKSLL | AP00859 | Temporin H | CD in TFE | Eur J Biochem. 267(5):1447-54. | 2 |
|  | FLPILASLAAKFGPKLFCLVTKKC | AP00878 | Brevinin-1BYa | CD in TFE | Eur Biophys J. 40(4):555-64. | 5 |
|  | KRFKKFFKKLKNSVKKRAKKFFKKPRVIGVSIPF | AP00895 | OH-CATH | *by homology to OH-CATH* | Peptides 29(10):1685-91. | 29 |
|  | KRFKKFFKKLKKSVKKRAKKFFKKPRVIGVSIPF | AP00896 | BF-CATH | CD in TFE / SDS | Peptides 32(12):2497-503.  | 38 |
|  | KRFKKFFKKLKNSVKKRAKKFFKKPKVIGVTFPF | AP00897 | NA-CATH | NMR in lipid bilayer | Biochim Biophys Acta. 1848(10 Pt A):2394-405. | 29 |
|  | FLSGIVGMLGKLF | AP00898 | Temporin-SHa | CD/ NMR in SDS micelles | Biochemistry 47(40):10513-25. | 1 |
|  | FLPIVTNLLSGLL | AP00899 | Temporin-SHb | CD/ NMR in SDS micelles | Biochemistry 47(40):10513-25. | 0 |
|  | FLSHIAGFLSNLF | AP00900 | Temporin-SHc | CD/ NMR in SDS micelles | Biochemistry 47(40):10513-25. | 0 |
|  | MAKEFGIPAAVAGTVINVVEAGGWVTTIVSILTAVGSGGLSLLAAAGRESIKAYLKKEIKKKGKRAVIAW | AP00929 | Enterocin AS-48 | NMR | Proc Natl Acad Sci U S A. 97(21):11221-6. | 21 |
|  | GLWSKIKAAGKEAAKAAAKAAGKAALNAVSEAV | AP00966 | Dermaseptin-DI1 | CD / NMR in SDS / DPC / TFE  | Biophys J. 96(6):2194-203. | 37 |
|  | KWKLFKKIGAVLKVL | AP01007 | CM15 | NMR in DPC micelles | J Am Chem Soc. 129(16):5228-34. | 17 |
|  | SMWSGMWRRKLKKLRNALKKKLKGEK | AP01010 | Latarcin 1 | NMR in SDS micelles | Biochemistry 47(11):3525-33. | 14 |
|  | GLFGKLIKKFGRKAISYAVKKARGKH | AP01011 | Latarcin 2a | CD / NMR in SDS micelles | Biochemistry 45(35):10759-67. | 17 |
|  | SWKSMAKKLKEYMEKLKQRA | AP01012 | Latarcin 3a | CD in TFE | J Biol Chem. 281(30):20983-92. | 5 |
|  | SWASMAKKLKEYMEKLKQRA | AP01013 | Latarcin 3b  | CD in TFE | J Biol Chem. 281(30):20983-92. | 1 |
|  | GLKDKFKSMGEKLKQYIQTWKAKF | AP01014 | Latarcin 4a | CD in TFE | J Biol Chem. 281(30):20983-92. | 3 |
|  | SLKDKVKSMGEKLKQYIQTWKAKF | AP01015 | Latarcin 4b | CD in TFE | J Biol Chem. 281(30):20983-92. | 2 |
|  | GFFGKMKEYFKKFGASFKRRFANLKKRL | AP01016 | Latarcin 5 | CD in TFE | J Biol Chem. 281(30):20983-92. | 7 |
|  | QAFQTFKPDWNKIRYDAMKMQTSLGQMKKRFNL | AP01018 | Latarcin 6a | CD in TFE | J Biol Chem. 281(30):20983-92. | 1 |
|  | GETFDKLKEKLKTFYQKLVEKAEDLKGDLKAKLS | AP01019 | Latarcin 7 | CD in TFE | J Biol Chem. 281(30):20983-92. | 4 |
|  | MSWLNFLKYIAKYGKKAVSAAWKYKGKVLEWLNVGPTLEWVWQKLKKIAGL | AP01131 | Aureocin A53 | CD / NMR in TFE | Biochemistry 55(4):733-42.  | 28 |
|  | GTWDDIGQGIGRVAYWVGKALGNLSDVNQASRINRKKKH | AP01151 | Lactococcin G-a | NMR in DPC / TFE | Biochim Biophys Acta. 1784(3):543-54.  | 0 |
|  | ALYKKFKKKLLKSLKRL | AP01158 | RP-1 | NMR in DPC / SDS micelles | Biopolymers 91(1):1-13.  | 21 |
|  | KWKIFKKIEHMGQNIRDGLIKAGPAVQVVGQAATIYKG | AP01159 | Hinnavin II | *by homology to cecropins* | Appl Microbiol Biotechnol. 98(13): 5807–5822. | 5 |
|  | GRDYRTCLTIVQKLKKMVDKPTQRSVSNAATRVCRTGRSRWRDVCRNFMRRYQSRVTQGLVAGETAQQICEDLRLCIPSTGPL | AP01161 | Human granulysin | X-Ray | J Mol Biol. 325(2):355-65. | 6 |
|  | LVAYGIAQGTAEKVVSLINAGLTVGSIISILGGVTVGLSGVFTAVKAAIAKQGIKKAIQL | AP01168 | Carnocyclin A | NMR | J Biol Chem. 284(42):28674-81. | 11 |
|  | FNRGGYNFGKSVRHVVDAIGSVAGILKSIR | AP01177 | Plantaricin EF | NMR in DPC micelles | Biochim Biophys Acta. 1784(11):1711-9.  | 0 |
|  | GAWKNFWSSLRKGFYDGEAGRAIRR | AP01178 | Plantaricin JK | NMR in DPC / TFE | Peptides 30(9):1613-21. | 0 |
|  | GFKDLLKGAAKALVKTVLF | AP01223 | Ascaphin-8 | CD in TFE | Chem Biol Drug Des. 72(1):58-64.  | 22 |
|  | VGALAVVVWLFLWLW | AP01224 | Gramicidin B | NMR in SDS micelles | Biochemistry 40(39):11676-86. | 0 |
|  | VGALAVVVWLYLWLW | AP01225 | Gramicidin C | NMR in SDS micelles | Biochemistry 40(39):11676-86. | 0 |
|  | KFFRKLKKSVKKRAKEFFKKPRVIGVSIPF | AP01239 | Cathelicidin-BF | CD / NMR in SDS / TFE | PLoS One 3(9):e3217. | 27 |
|  | ALKAALLAILKIVRVIKK | AP01240 | CM-3 | *predicted* | WO 9628468 (1996) | 14 |
|  | FASLLGKALKALAKQ | AP01241 | MB-21 | CD in lipid bilayer | Biochemistry 39(39):11907-12. | 13 |
|  | GLLSFLPKVIGVIGHLIHPPS | AP01242 | Fallaxidin 4.1 | NMR in DPC / lipid bilayers | Biochemistry 48(50):11892-901. | 0 |
|  | GILDAIKAIAKAAG | AP01249 | Hylaseptin P1 | CD / NMR in TFE | J Biol Chem. 279(13):13018-26.  | 12 |
|  | GFLSILKKVLPKVMAHMK | AP01269 | Melectin | CD in SDS micelles | Chembiochem. 9(17):2815-21.  | 6 |
|  | MRKEFHNVLSSGQLLADKRPARDYNRK | AP01283 | Pep27 | NMR in TFE | Cancer Cell Int. 5:21. | 0 |
|  | AALKGCWTKSIPPKPCFGKR | AP01291 | Odorranain-B1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 0 |
|  | GVLGAVKDLLIGAGKSAAQSVLKTLSCKLSNDC | AP01292 | Odorranain-C1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 5 |
|  | GLGGAKKNFIIAANKTAPQSVKKTFSCKLYNG | AP01294 | Odorranain-E1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 7 |
|  | GFMDTAKNVAKNVAVTLIDNLKCKITKAC | AP01295 | Odorranain-F1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 7 |
|  | FMPILSCSRFKRC | AP01296 | Odorranain-G1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 0 |
|  | GIFGKILGVGKKVLCGLSGWC | AP01297 | Odorranain-H1  | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 5 |
|  | TSRCYIGYRRKVVCS | AP01306 | Odorranain-T1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 0 |
|  | GCSRWIIGIHGQICRD | AP01307 | Odorranain-U1 | CD in SDS micelles | Mol Cell Proteomics. 6(5):882-94. | 0 |
|  | IFGAILPLALGALKNLIK | AP01331 | Hylin a1 | CD/NMR in SDS micelles | Protein Pept Lett. 22(8):719-26. | 4 |
|  | FWGHIWNAVKRVGANALHGAVTGALS | AP01353 | Halocyntin | CD in TFE | J Pept Sci. 15(1):48-55.  | 1 |
|  | GFWKKVGSAAWGGVKAAAKGAAVGGLNALAKHIQ | AP01354 | Papilosin | CD in TFE | J Pept Sci. 15(1):48-55.  | 14 |
|  | FFRHLFRGAKAIFRGARQGWRAHKVVSRYRNRDVPETDNNQEEP | AP01377 | Piscidin 4 | CD in TFE / lipid bilayers | Biochemistry 50(16):3288-99. | 1 |
|  | FFGSVLKLIPKIL | AP01434 | Temporin-PTa | *by homology to temporins* | Toxicon 52(3):465-73. | 5 |
|  | GILSSFKGVAKGVAKNLAGKLLDELKCKITGC | AP01435 | Ranatuerin-2AUa | *by homology to Ranatuerin-2CSa* | Dev Comp Immunol. 29(1):83-90 | 13 |
|  | IIPLPLGYFAKKT | AP01454 | Temporin-1CEc | CD in TFE | Int J Antimicrob Agents. 33(6):538-42. | 1 |
|  | FFPLALLCKVFKKC | AP01455 | Japonicin-1CDYa | CD in TFE | Int J Antimicrob Agents. 33(6):538-42.  | 4 |
|  | VGKTWIKVIRGIGKSKIKWQ | AP01456 | Bactrocerin-1 | CD in TFE | Arch Insect Biochem Physiol. 71(3):117-129 | 1 |
|  | GLKEIFKAGLGSLVKGIAAHVAS | AP01459 | Alyteserin-1c | NMR in DPC / SDS micelles | Biochim Biophys Acta. 1808(8):1975-84. | 8 |
|  | ILGKLLSTAAGLLSNL | AP01461 | Alyteserin-2a | *by homology to bombinin H6* | Peptides 30(6):1069-73. | 2 |
|  | VNWKKVLGKIIKVAK | AP01465 | Lasioglossin LL-I | NMR in TFE | Chembiochem. 10(12):2089-99. | 12 |
|  | VNWKKILGKIIKVAK | AP01466 | Lasioglossin LL-II | NMR in TFE | Chembiochem. 10(12):2089-99. | 14 |
|  | VNWKKILGKIIKVVK | AP01467 | Lasioglossin LL-III | NMR in TFE | Chembiochem. 10(12):2089-99. | 13 |
|  | RPKPQQFFGLM | AP01471 | Substance P | NMR in bicelles | Biochim Biophys Acta. 1808(1):127-39. | 0 |
|  | YPSKPDNPGEDAPAEDMARYYSALRHYINLITRQRY | AP01474 | Neuropeptide Y | NMR | J Biomol NMR. 8(4):379-90. | 0 |
|  | ACDTATCVTHRLAGLLSRSGGVVKNNFVPTNVGSKAF | AP01476 | Calcitonin gene-related peptide | CD in organic solvent | Eur J Biochem. 213(3):927-34. | 0 |
|  | YRQSMNNFQGLRSFGCRFGTCTVQKLAHQIYQFTDKDKDNVAPRSKISPQGY | AP01479 | Adrenomedullin | NMR in SDS micelles | Biopolymers 97(1):45-53.  | 0 |
|  | TITLSTCAILSKPLGNNGYLCTVTKECMPSSCN | AP01511 | Lichenicidin | NMR in methanol | Biochemistry 49(30):6462-72.  | 1 |
|  | LNLKGIFKKVASLLT | AP01516 | Eumenitin | CD in TFE / SDS | Peptides 27(11):2624-31. | 5 |
|  | GAARKSIRLHRLYTWKATIYTR | AP01529 | PP13 | CD in TFE | J Pept Sci. 16(1):58-64. | 0 |
|  | GSCSCSGTISPYGLRTCRATKTKPSHPTTKETHPQTLPT | AP01530 | PP102 | CD in TFE | J Pept Sci. 16(1):58-64. | 0 |
|  | GKWGWIYITILFADVGGFKSSRHPEERRVQERRFKRITRGPD | AP01531 | PP113 | CD in TFE | J Pept Sci. 16(1):58-64. | 0 |
|  | KRRGSVTTRYQFLMIHLLRPKKLFA | AP01533 | EA-CATH1 | CD in TFE | FEBS J. 277(10):2329-39. | 0 |
|  | FFFLSRIF | AP01534 | Temporin-SHf | CD / NMR in SDS / DPC micelles | J Biol Chem. 285(22):16880-92. | 0 |
|  | IFGAIAGLLKNIF | AP01544 | Meucin-13 | CD / NMR in TFE | FASEB J. 23(4):1230-45.  | 0 |
|  | FFGHLFKLATKIIPSLFQ | AP01545 | Meucin-18 | CD / NMR in TFE | FASEB J. 23(4):1230-45.  | 6 |
|  | GMWSKIKNAGKAAKAAAKAAGKAALGAVSEAM | AP01546 | Dermaseptin DA4 | CD in lipid bilayer | FEBS J. 276(22):6773-86. | 37 |
|  | LGAWLAGKVAGTVATYAWNRYV | AP01558 | Hedistin | CD / NMR in DPC micelles | Biochim Biophys Acta. 1788(12):2497-508.  | 6 |
|  | FLLFPLMCKIQGKC | AP01577 | Japonicin-1Npa | CD in TFE / SDS | Biochimie 92(5):475-81. | 2 |
|  | FVLPLVMCKILRKC | AP01579 | Japonicin-1Npb | CD in TFE / SDS | Biochimie 92(5):475-81. | 1 |
|  | GWANTLKNVAGGLCKITGAA | AP01583 | Parkerin | CD in TFE / SDS | Biochimie 92(5):475-81. | 2 |
|  | WRSLGRTLLRLSHALKPLARRSGW | AP01614 | Ci-MAM-A24 | CD in lipid bilayer | Biochem J. 416(1):65-75.  | 1 |
|  | GFKLKGMARISCLPNGQWSNFPPKCIRECAMVSS | AP01623 | Sushi peptide 1 | CD in lipid bilayer | FASEB J. 14(12):1801-13. | 0 |
|  | RRWVRRVRRWVRRVVRVVRRWVRR | AP01633 | WLBU2 | CD in TFE | Antimicrob Agents Chemother. 49(1):316-22. | 0 |
|  | INWKKIFEKVKNLV | AP01634 | Pd\_mastoparan PDD-A | CD in TFE / SDS | Peptides 29(6):992-1003.  | 6 |
|  | INWLKLGKKILGAL | AP01635 | Pd\_mastoparan PDD-B | CD in TFE / SDS | Peptides 29(6):992-1003.  | 7 |
|  | INWLKLGKKMMSAL | AP01636 | Mp\_mastoparan MP | CD in TFE / SDS | Peptides 29(6):992-1003.  | 3 |
|  | INWKKIASIGKEVLKAL | AP01637 | Pm\_mastoparan PMM | CD in TFE / SDS | Peptides 29(6):992-1003.  | 8 |
|  | IDWLKLGKMVIDAL | AP01640 | Polybia-MP-II | CD in TFE / SDS | Peptides 30(8):1387-95. | 0 |
|  | IDWLKLGKMVMDVL | AP01641 | Polybia-MP-III | CD in TFE / SDS | Peptides 30(8):1387-95. | 0 |
|  | FFHHIFRGIVHVGKTIHKLVTG | AP01649 | Piscidin 2 | *by homology to Piscidin 1* | Nature 414(6861):268-9 | 1 |
|  | GIFSKLAGKKIKNLISGLKNIGKEVGMDVVRTGIDIAGCKIKGEC | AP01656 | Esculentin-1c | CD / NMR in SDS / DPC / TFE  | Mol Cells. 17(3):469-76. | 12 |
|  | VIPFVASVAAEMMHHVYCAASKRC | AP01657 | Brevinin-1Ed | CD / NMR in SDS / DPC / TFE  | Mol Cells. 17(3):469-76 | 1 |
|  | RWKIFKKIEKVGRNVRDGIIKAGPAVAVVGQAATVVK | AP01751 | Papiliocin | NMR | PDB ID: 2LA2 | 12 |
|  | GIWSSIKNLASKAWNSDIGQSLRNKAAGAINKFVADKIGVTPSQAASMTLDEIVDAMYYD | AP01753 | Vejovine | CD | Toxicon 57(1):84-92. | 6 |
|  | KPAWCWYTLAMCGAGYDSGTCDYMYSHCFGIKHHSSGSSSYHC | AP01761 | Glycocin F | NMR | Biochemistry 50(14):2748-55.  | 1 |
|  | QLGELIQQGGQKIVEKIQKIGQRIRDFFSNLRPRQEA | AP01768 | FeCath | CD in SDS micelles | PLoS One 6(4):e18756. | 6 |
|  | FLWGLIPGAISAVTSLIKK | AP01791 | Ctriporin | CD / NMR in SDS / DPC micelles | Biopolymers 101(12):1143-53. | 0 |
|  | FVDLKKIANIINSIFGK | AP01794 | Temporin-1CEa | CD in TFE | Biochimie 94(2):434-41. | 2 |
|  | GIRCPKSWKCKAFKQRVLKRLLAMLRQHAF | AP01804 | Oxt 4a | NMR in DPC micelles | FEBS J. 278(22):4382-93.  | 3 |
|  | GMWSKILGHLIR | AP01922 | Halictine 1 | CD / NMR in SDS / TFE | Amino Acids 39(3):763-75.  | 0 |
|  | GKWMSLLKHILK | AP01923 | Halictine 2 | CD / NMR in SDS / TFE | Amino Acids 39(3):763-75.  | 3 |
|  | GLPRKILCAIAKKKGKCKGPLKLVCKC | AP01958 | Lasiocepsin | NMR in SDS micelles | Chembiochem. 15(2):301-8. | 16 |
|  | IFGAIWNGIKSLF | AP01980 | IsCT2 | CD in TFE | Biochem Biophys Res Commun. 293(5):1514-22. | 0 |
|  | GKIPVKAIKQAGKVIGKGLRAINIAGTTHDVVSFFRPKKKKH | AP02016 | MS moricin | CD / NMR in SDS / TFE / methanol | J Pept Sci. 14(7):855-63. | 16 |
|  | GFWGKLWEGVKSAI | AP02026 | StCT2 | CD in TFE | Peptides 36(2):213-20. | 0 |
|  | KPFKKLEKVGRNIRDGIIKAGPAVAVIGQATSIARPTGK | AP02031 | Px-cec1 | CD in TFE / SDS | Protein Expr Purif. 85(2):230-8. | 10 |

**Table S2**. Sequences of natural β-sheet antimicrobial peptides from APD2 used in this study.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| № | Peptide sequence | APD ID | Peptide name | Structure elucidation method | Reference(structural analysis) |
|  | FKCRRWQWRMKKLGAPSITCVRRAF | AP00026 | Lactoferricin B | NMR | Biochemistry 37(12):4288-98 |
|  | GPLSCGRNGGVCIPIRCPVPMRQIGTCFGRPVKCCRSW | AP00047 | Bovine neutrophil beta-defensin 12 | NMR | Biochemistry 34(41):13663-71 |
|  | GSKKPVPIIYCNRRTGKCQRM | AP00102 | Thanatin | NMR | Eur J Biochem. 256(2):404-10 |
|  | MPCSCKKYCDPWEVIDGSCGLFNSKYICCREK | AP00149 | Rabbit kidney defensin 1 | NMR | Biochemistry 39(51):15757-64 |
|  | RCVCTRGFCRCVCRRGVC | AP00151 | Baboon theta-defensin-1 | *by homology to Baboon theta-defensin-2* |  |
|  | RSVCRQIKICRRRGGCYYKCTNRPY | AP00153 | Androctonin | NMR | J Biomol Struct Dyn. 17(2):367-80 |
|  | YSRCQLQGFNCVVRSYGLPTIPCCRGLTCRSYFPGSTYGRCQRY | AP00154 | Tachystatin A2 | NMR | J Biol Chem. 277(26):23651-7 |
|  | RCVCRRGVCRCVCRRGVC | AP00156 | Baboon theta-defensin-2 | NMR | Biochemistry 51(48):9718-26 |
|  | ACYCRIPACIAGERRYGTCIYQGRLWAFCC | AP00176 | Human neutrophil peptide-1 | X-ray | J Biol Chem. 284(42):29180-92 |
|  | CYCRIPACIAGERRYGTCIYQGRLWAFCC | AP00177 | Human neutrophil peptide-2 | X-ray | J Biol Chem. 280(38):32921-9 |
|  | DCYCRIPACIAGERRYGTCIYQGRLWAFCC | AP00178 | Human neutrophil peptide-3 | X-ray | Science 251(5000):1481-5 |
|  | VCSCRLVFCRRTELRVGNCLIGGVSFTYCCTRV | AP00179 | Human neutrophil peptide-3 | X-ray | Protein Sci. 15(12):2749-60 |
|  | ATCYCRTGRCATRESLSGVCEISGRLYRLCCR | AP00180 | Human defensin 5 | X-ray | Protein Sci. 15(12):2749-60  |
|  | ECRRLCYKQRCVTYCRGR | AP00191 | Gomesin | NMR | Eur J Biochem. 269(4):1190-8 |
|  | DTHFPICIFCCGCCHRSKCGMCCKT | AP00193 | Human LEAP-1 | NMR | J Biol Chem. 284(36):24155-67 |
|  | VGECVRGRCPSGMCCSQFGYCGKGPKYCGR | AP00194 | Ac-AMP2 | NMR | J Mol Biol. 258(2):322-33 |
|  | RGGRLCYCRRRFCVCVGR | AP00195 | Protegrin I | NMR | Chem Biol. 3(7):543-50 |
|  | RRWCFRVCYRGFCYRKCR | AP00211 | Polyphemusin I | NMR | Biochim Biophys Acta. 1698(2):239-50 |
|  | KWCFRVCYRGICYRRCR | AP00214 | Tachyplesin I | NMR | PDB ID: 1WO1 |
|  | NPVSCVRNKGICVPIRCPGSMKQIGTCVGRAVKCCRKK | AP00235 | Bovine tracheal antimicrobial peptide |  |  |
|  | GVIPCGESCVFIPCISTLLGCSCKNKVCYRN | AP00275 | Circulin B | NMR | INT.J.PEPT.PROTEIN RES. 11: 99-106 |
|  | GLLCYCRKGHCKRGERVRGTCGIRFLYCCPRR | AP00285 | Cryptdin-4 | NMR | J Biol Chem. 281(38):28068-78 |
|  | LFCKGGSCHFGGCPSHLIKVGSCFGFRSCCKWPWNA | AP00298 | Chicken AvBD2 | NMR | J Biol Chem. 287(10):7746-55 |
|  | GCRFCCNCCPNMSGCGVCCRF | AP00302 | Hepcidin | NMR | J Biol Chem. 280(10):9272-82 |
|  | SAFTVWSGPGCNNRAERYSKCGCSAIHQKGGYDFSYTGQTAALYNQAGCSGVAHTRFGSSARACNPFGWKSIFIQC | AP00428 | MiAMP1 | NMR | J Mol Biol. 293(3):629-38 |
|  | GFCRCLCRRGVCRCICTR | AP00445 | Rhesus theta defensin-1 | NMR | Biochemistry 51(48):9718-26 |
|  | EGTWQHGYGVSSAYSNYHHGSKTHSATVVNNNTGRQGKDTQRAGVWAKATVGRNLTEKASFYYNFW | AP00594 | Lactococcin 972 | NMR | PDB ID: 2LGN |
|  | RWCVYAYVRVRGVLVRYRRCW | AP00727 | Arenicin-1 | NMR | Biochem J. 410(1):113-22 |
|  | RWCVYAYVRIRGVLVRYRRCW | AP00728 | Arenicin-2 | NMR | Biochem Biophys Res Commun. 360(1):156-62 |
|  | RCVCTRGFCRCVCTRGFC | AP00804 | Baboon theta-defensin-3 | *by homology to Baboon theta-defensin-2* |  |
|  | RCVCTRGFCRCICLLGIC | AP00855 | Baboon theta-defensin-4 | *by homology to Baboon theta-defensin-2* |  |
|  | RCVCTRGFCRCFCRRGVC | AP00856 | Baboon theta-defensin-7 | *by homology to Baboon theta-defensin-2* |  |
|  | QWGRRCCGWGPGRRYCVRWC | AP00913 | Ib-AMP1 | NMR | Biochemistry 37(4):983-90 |
|  | YVSCLFRGARCRVYSGRSCCFGYYCRRDFPGSIFGTCSRRNF | AP01005 | Tachystatin B1 | NMR | J Pept Sci. 13(4):269-79 |
|  | YITCLFRGARCRVYSGRSCCFGYYCRRDFPGSIFGTCSRRNF | AP01006 | Tachystatin B2 | NMR | J Pept Sci. 13(4):269-79 |
|  | DYDWSLRGPPKCATYGQKCRTWSPRNCCWNLRCKAFRCRPR | AP01009 | Tachystatin C | *by homology to tachystatins* | J Biol Chem. 274(37):26172-8 |
|  | YLAFRCGRYSPCLDDGPNVNLYSCCSFYNCHKCLARLENCPKGLHYNAYLKVCDWPSKAGCT | AP01153 | Tachycitin | NMR | J Biol Chem. 275(24):17929-32 |
|  | AIKLVQSPNGNFAASFVLDGTKWIFKSKYYDSSKGYWVGIYEVWDRK | AP01154 | LCI | NMR | PDB ID: 2B9K |
|  | FLPKTLRKFFCRIRGGRCAVLNCLGKEEQIGRCSNSGRKCCRKKK | AP01246 | Mouse beta-defensin-14 | *by homology to β-defensins* |  |
|  | RRTCHCRSRCLRRESNSGSCNINGRIFSLCCR | AP01267 | Rhesus macaque oral alpha-defensin-1 | NMR | J Biol Chem. 283(51):35869-77 |
|  | IRNSLTCRFNFGICLPKRCPGRMRQIGTCF | AP01287 | Deer beta-defensin | *by homology to β-defensins* |  |
|  | ARLKKCFNKVTGYCRKKCKVGERYEIGCLSGKLCCAN | AP01315 | Human beta-defensin-28 | *by homology to β-defensins* |  |
|  | DPVTYIRNGGICQYRCIGLRHKIGTCGSPFKCCK | AP01319 | Murine beta-defensin related peptide | *by homology to β-defensins* |  |
|  | LFCRKGTCHFGGCPAHLVKVGSCFGFRACCKWPWDV | AP01320 | Ostrich avian beta defensin 2 | *by homology to β-defensins* |  |
|  | APGNKAECEREKGYCGFLKCSFPFVVSGKCSRFFFCCKNIW | AP01321 | Ostrich avian beta defensin 1 | *by homology to β-defensins* |  |
|  | IPRPLDPCIAQNGRCFTGICRYPYFWIGTCRNGKSCCRRR | AP01322 | Ostrich avian beta defensin 7 | *by homology to β-defensins* |  |
|  | LPVNEAQCRQVGGYCGLRICNFPSRFLGLCTRNHPCCSRVWV | AP01323 | Ostrich avian beta defensin 8 | *by homology to β-defensins* |  |
|  | GPDSCNHDRGLCRVGNCNPGEYLAKYCFEPVILCCKPLSPTPTKT | AP01324 | Chicken avian beta defensin 12 | *by homology to β-defensins* |  |
|  | QPFIPRPIDTCRLRNGICFPGICRRPYYWIGTCNNGIGSCCARGWRS | AP01325 | Chicken avian beta defensin 7 | *by homology to β-defensins* |  |
|  | VTCDLLSFEAKGFAANHSLCAAHCLAIGRRGGSCERGVCICRR | AP01358 | A. dichotoma defensin | *by homology to β-defensins* |  |
|  | AREASKSLIGTASCTCRRAWICRWGERHSGKCIDQKGSTYRLCCRR | AP01378 | Horse defensin alpha 1 | NMR | Biochem Biophys Res Commun. 459(4):668-72 |
|  | YDLSKNCRLRGGICYIGKCPRRFFRSGSCSRGNVCCLRFG | AP01380 | Turtle beta-defensin 1 | *by homology to β-defensins* |  |
|  | EKKCPGRCTLKCGKHERPTLPYNCGKYICCVPVKVK | AP01382 | Ovodefensin | NMR | Proteins 64(2):524-31 |
|  | GFGCPLNQGACHNHCRSIGRRGGYCAGIIKQTCTCYRK | AP01468 | Longicin | *by homology to β-defensins* |  |
|  | AQRCGDQARGAKCPNCLCCGKYGFCGSGDAYCGAGSCQSQCRGC | AP01469 | WAMP-1a | NMR | Biochem Biophys Res Commun. 411(1):14-8 |
|  | AQRCGDQARGAKCPNCLCCGKYGFCGSGDAYCGAGSCQSQCRGCR | AP01470 | WAMP-1b | *by homology to WAMP-1a* |  |
|  | FKVQNQHGQVVKIFHH | AP01718 | Astacidin 1 | CD | J Biol Chem. 278(10):7927-33 |
|  | GTPGFQTPDARVISRFGFN | AP01724 | Capistruin | NMR | J Am Chem Soc. 130(34):11446-54 |
|  | GSQLVYREWVGHSNVIKP | AP01728 | Lariatin A | NMR | J Am Chem Soc. 128(23):7486-91 |
|  | KSLRPRCWIKIKFRCKSLKF | AP01769 | Piceain 1 | CD | J Pept Sci. 17(9):627-31 |
|  | RPRCWIKIKFRCKSLKF | AP01770 | Piceain 2 | CD | J Pept Sci. 17(9):627-31 |
|  | FLGLIFHGLVHAGKLIHGLIHRNRG | AP02038 | HKPLP | CD | J Antibiot (Tokyo) 65(3):117-121 |
|  | VGSEVSDKRTCVSLTTQRLPVSRIKTYTITEGSLRAVIFITKRGLKVCADPQATWVRDVVRSMDRKSNTRNNMIQTKPTGTQQSTNTAVTLTG | AP02084 | XCL1 | NMR | Proc Natl Acad Sci USA 105(13):5057-62 |
|  | SGKSFKAGVCPPKKSAQCLRYKKPECQSDWQCPGKKRCCPDTCGIKCLDPVDTPNPTRRKPGKCPVTYGQCLMLNPPNFCEMDGQCKRDLKCCMGMCGKSCVSPVKA | AP02095 | SLPI  | X-ray | J Synchrotron Radiat. 15(Pt 3):308-11 |

**Table S3**. Patterns with support ≥30 derived from natural α-helical AMPs with Teiresias algorithm (*L=3, W=10, K=3*). Bootstrapping was used to estimate the variation of support for each pattern.

|  |  |  |  |
| --- | --- | --- | --- |
| № | Pattern | Natural α-helical peptides | Bootstrapped sets (n=100) |
| **Support** | **Unique peptides** | **Mean support** | **Std. dev.** | **Mean unique**  | **Std. dev.** |
|  | K...K...K | 82 | 47 | 83.2 | 13.7 | 48.1 | 6.2 |
|  | K...K..K | 64 | 45 | 62.6 | 11.1 | 44.6 | 5.7 |
|  | K..K...K | 55 | 38 | 54.2 | 10.6 | 38.0 | 5.8 |
|  | K..AK | 49 | 37 | 49.0 | 8.3 | 36.7 | 5.2 |
|  | A...A...A | 48 | 29 | 48.7 | 11.5 | 29.0 | 5.1 |
|  | K..GK | 47 | 38 | 48.0 | 7.5 | 38.5 | 5.7 |
|  | K.A.K | 45 | 36 | 46.1 | 8.0 | 36.5 | 5.3 |
|  | K..KK | 45 | 30 | 44.6 | 10.8 | 30.1 | 5.4 |
|  | K...K.L | 45 | 36 | 44.6 | 7.3 | 35.4 | 5.1 |
|  | LK...K | 44 | 42 | 44.0 | 7.0 | 41.9 | 6.3 |
|  | L.K...K | 44 | 38 | 44.0 | 7.5 | 37.9 | 6.0 |
|  | A.K...K | 44 | 33 | 44.4 | 7.5 | 33.1 | 5.4 |
|  | K...K..A | 44 | 30 | 44.3 | 7.2 | 30.2 | 4.6 |
|  | K...KA | 43 | 30 | 44.4 | 9.1 | 30.6 | 5.9 |
|  | A..AA | 42 | 26 | 42.5 | 8.9 | 26.2 | 5.0 |
|  | KAA | 41 | 25 | 41.6 | 9.3 | 24.9 | 4.8 |
|  | K...KI | 41 | 36 | 40.7 | 6.4 | 35.5 | 5.0 |
|  | K...KK | 40 | 27 | 39.5 | 8.8 | 27.0 | 4.7 |
|  | KK..K | 39 | 26 | 37.8 | 9.0 | 25.1 | 4.9 |
|  | AK...K | 39 | 31 | 40.2 | 8.0 | 31.7 | 5.7 |
|  | K...K.A | 39 | 28 | 39.6 | 8.4 | 28.1 | 4.9 |
|  | K......KK | 39 | 28 | 39.4 | 8.4 | 28.7 | 4.8 |
|  | A.KA | 38 | 26 | 39.0 | 7.8 | 26.5 | 4.7 |
|  | K.F.K | 38 | 22 | 36.8 | 10.3 | 21.3 | 4.1 |
|  | K.L....K | 38 | 36 | 37.9 | 6.2 | 36.0 | 5.6 |
|  | A..A...A | 38 | 17 | 38.8 | 11.0 | 17.0 | 3.4 |
|  | KK...K | 37 | 28 | 36.8 | 7.7 | 27.8 | 5.0 |
|  | K.FK | 37 | 26 | 36.3 | 7.7 | 25.6 | 4.6 |
|  | A.K.A | 37 | 27 | 37.7 | 7.9 | 27.4 | 5.0 |
|  | KK......K | 36 | 27 | 36.2 | 7.9 | 27.1 | 5.0 |
|  | K.A.....K | 36 | 32 | 36.6 | 6.9 | 32.4 | 5.6 |
|  | L...AK | 36 | 35 | 36.3 | 6.3 | 35.2 | 6.0 |
|  | K...K....A | 36 | 20 | 37.1 | 9.2 | 20.3 | 4.3 |
|  | KK.....K | 35 | 27 | 34.9 | 7.2 | 27.1 | 5.3 |
|  | FK......K | 35 | 27 | 34.5 | 5.9 | 26.6 | 4.4 |
|  | A...A..A | 35 | 21 | 35.7 | 9.0 | 21.2 | 4.3 |
|  | K...K....L | 35 | 30 | 35.9 | 7.0 | 30.5 | 5.2 |
|  | KKI | 34 | 31 | 33.5 | 6.4 | 30.5 | 5.5 |
|  | AA..A | 34 | 19 | 34.5 | 9.3 | 18.9 | 4.0 |
|  | L.K.L | 34 | 32 | 34.1 | 5.3 | 32.1 | 4.9 |
|  | K....A...A | 34 | 21 | 35.7 | 8.9 | 21.9 | 4.3 |
|  | G....K...K | 34 | 31 | 34.2 | 6.4 | 31.1 | 5.7 |
|  | KI....K | 33 | 31 | 33.8 | 6.1 | 31.6 | 5.5 |
|  | KI.....K | 33 | 30 | 33.6 | 5.5 | 30.6 | 4.5 |
|  | K.V.K | 33 | 29 | 33.6 | 5.2 | 29.3 | 4.4 |
|  | K.L.K | 33 | 29 | 32.7 | 6.0 | 28.8 | 5.1 |
|  | K.A..A | 33 | 20 | 34.0 | 8.8 | 20.5 | 4.6 |
|  | L..KI | 33 | 33 | 33.3 | 5.5 | 33.3 | 5.5 |
|  | K.....A.K | 33 | 28 | 33.5 | 6.6 | 28.5 | 5.2 |
|  | LKK | 32 | 31 | 31.6 | 5.4 | 30.7 | 5.4 |
|  | G.A...A | 32 | 24 | 32.0 | 6.5 | 24.1 | 4.6 |
|  | K..G...K | 32 | 29 | 32.5 | 5.5 | 29.3 | 4.7 |
|  | K..A...A | 32 | 22 | 32.2 | 6.7 | 22.2 | 4.2 |
|  | K.....A..A | 32 | 20 | 32.7 | 8.4 | 20.2 | 4.2 |
|  | K......AK | 32 | 25 | 32.2 | 6.0 | 25.1 | 4.3 |
|  | K......K.F | 32 | 23 | 31.9 | 6.3 | 22.8 | 4.3 |
|  | KIG | 31 | 29 | 30.7 | 5.6 | 28.5 | 4.8 |
|  | LK.L | 31 | 29 | 31.0 | 5.8 | 29.0 | 5.1 |
|  | A.K....A | 31 | 19 | 32.0 | 8.4 | 19.3 | 4.3 |
|  | K.A......A | 31 | 18 | 32.2 | 9.4 | 18.5 | 4.4 |
|  | K....AA | 31 | 22 | 31.4 | 7.3 | 22.0 | 4.8 |
|  | K....V.K | 31 | 27 | 30.7 | 6.1 | 26.8 | 5.1 |
|  | K....I.K | 31 | 30 | 30.2 | 4.7 | 29.5 | 4.5 |
|  | K.....AK | 31 | 26 | 31.7 | 6.3 | 26.5 | 5.1 |
|  | KA..K | 30 | 25 | 30.9 | 5.5 | 25.6 | 3.9 |
|  | KA...A | 30 | 21 | 30.6 | 7.6 | 21.1 | 4.8 |
|  | AA......A | 30 | 16 | 30.8 | 9.9 | 15.9 | 3.9 |
|  | K.I.K | 30 | 29 | 29.6 | 5.5 | 28.5 | 5.2 |
|  | G.L.K | 30 | 28 | 30.2 | 5.2 | 28.4 | 4.9 |
|  | K.A....K | 30 | 26 | 30.6 | 6.2 | 26.5 | 5.0 |
|  | K..K..K | 30 | 27 | 29.5 | 5.5 | 26.7 | 4.8 |
|  | K..A....K | 30 | 23 | 30.8 | 6.6 | 23.5 | 4.5 |
|  | K...K.G | 30 | 29 | 29.6 | 4.9 | 28.8 | 4.7 |
|  | A...A.K | 30 | 23 | 30.3 | 6.4 | 23.1 | 4.5 |
|  | K....L.K | 30 | 30 | 30.5 | 5.3 | 30.5 | 5.3 |
|  | K......K.L | 30 | 27 | 29.6 | 5.8 | 26.5 | 4.8 |

**Figure S1**. Analysis of incidence of patterns with high support (≥30) from Table S3 in natural α-helical AMPs from Table S1 and peptides from Swiss-Prot.





**Figure S2**. Patterns with high support (≥30) from Table S3 mapped to the sequences of three natural
α-helical AMPs, magainin-2, maculatin 1.1, and LL-37, and one synthetic peptide, P1.

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**Table S4**. Analysis of peptides from Swiss-Prot database and *de novo* identification of antimicrobial peptides. From the total of 2454 peptides of length 10–30, 115 which had more than 5 patterns with support ≥30 are presented below. For each of them, we analyzed whether it (or its close homolog) is present in APD3. From 115 candidates, 75 had proven activity, and additional 17 are supposedly antimicrobial based on homology and their identification in skin secretions by mass-spectrometry. From the 75 active peptides, 18 belonged to the α-helical set from which the patterns were derived, 49 sequences from APD3 were identified *de novo*, and 8 peptides were not previously listed in APD3.

Coloring scheme:

|  |  |
| --- | --- |
|  | *de novo* identified peptides from APD3 (49) |
|  | peptides from the initial α-helical set (18) |
|  | *de novo* identified peptides, not listed in APD3 (8) |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **№** | **UniprotID** | **Peptide name** | **Peptidesequence** | **Anti-microbial** | **Belongsto helicalset (273)** | **APD3 ID** | **Reference** |
|  | P81903 | Histone H2B 1 (Fragment)  | MPDPAKTAPKKGSKKAVTKXA | yes |   | AP00338 |   |
|  | C0HL98 | Macropin  | GFGMALKLLKKVL | yes |   | AP01956 |   |
|  | P61507 | M-lycotoxin-Hc1a  | IWLTALKFLGKHAAKHLAKQQLSKL | yes | yes | AP00516 |   |
|  | P0CJ36 | Eumenitin-R  | LNLKGLIKKVASLLN | yes | yes (homolog) | AP01516 (homolog) |   |
|  | P69846 | Grammistin Gs C  | NWRKILGKIAKVAAGLLGSMLAGYQV | yes |   | no | Toxicon **45**: 595–601 |
|  | P0C1M6 | Dominulin-A  | INWKKIAEVGGKILSSL | yes |   | AP01638 |   |
|  | P04205 | Mastoparan-M  | INLKAIAALAKKLL | yes |   | AP00448 |   |
|  | P0C1Q9 | Mastoparan-V2  | INWKKIKSLIKAAMS | yes |   | AP02770 (homolog) |   |
|  | P0C2U9 | U1-lycotoxin-Ls1a  | AGIGKIGDFIKKAIAKYKN | supposedly |  | no | J Mass Spectrom. **39(2)**:193-201 |
|  | C0HK42 | Lasioglossin-1  | VNWKKVLGKIIKVAK | yes | yes | AP01465 |   |
|  | P61508 | M-lycotoxin-Hc2a  | KIKWFKTMKSIAKFIAKEQMKKHLGGE | yes | yes | AP00517 |   |
|  | C0HKN6 | Magainin-R1  | GIGKFLHSAKKFGKAFVGEIMNS | yes | yes | AP00144 |   |
|  | P85371 | Uncharacterized protein IMPP14 | VTAKAVAAAEAASSAR | unknown |  | no |  |
|  | P0C023 | Pilosulin-3b  | LIGLVSKGTCVLVKTVCKKVLKQ | yes |   | AP00891 |   |
|  | P82423 | Ponericin-W1  | WLGSALKIGAKLLPSVVGLFKKKKQ | yes | yes | AP00386 |   |
|  | P85443 | Ocellatin-5  | GLLDFLKAAGKGLVTNL | yes |   | AP01542 (homolog) |   |
|  | C0HKF0 | Ocellatin-F1  | GVVDILKGAAKDIAGHLASKVMNKL | yes | yes | AP00533 |   |
|  | P81474 | Misgurin  | RQRVEELSKFSKKGAAARRRK | yes | yes | AP00492 |   |
|  | P86013 | Lantibiotic paenibacillin  | ASIIKTTIKVSKAVCKTLTCICTGSCSNCK | yes |   | AP01493 |   |
|  | P86170 | Melectin  | GFLSILKKVLPKVMAHMK | yes | yes | AP01269 |   |
|  | P13282 | Histone H2B.2, sperm | MPKSPSKSSPRKGSPRKASPKRGGKGAKRA | unknown |  | no |  |
|  | P83641 | Dermadistinctin-Q1  | ALWKNMLKGIGKLAGQAALGAVKTLVGAES | yes |   | AP00961 |   |
|  | P69845 | Grammistin Gs A  | WWRELLKKLAFTAAGHLGSVLAAKQSGW | yes |   | no | Toxicon **45**: 595–601 |
|  | P62789 | Histone H4 (Fragment)  | MSGRGKGGKGLGKGGAKRHRKVLRD | yes |   | AP02807 |   |
|  | P83837 | Histone H2B (Fragment)  | MPEPAKSAPKKGSTRTAAKGGKKRRKSRK | yes |   | AP02808 (homolog) |   |
|  | P84859 | Guentherin  | VIDDLKKVAKKVRRELLCKKHHKKLN | yes |   | AP00584 |   |
|  | P84469 | Ferric reductase B (Fragment)  | MVKTVAVMVGSLRKDSLAHKLMKVLQK | unknown |  | no |  |
|  | P86641 | Dermaseptin-J9  | GLWKSLLKNVGKAAGKAALNAVTDMVNQS | yes |   | AP00934 |   |
|  | C0HLC3 | Dermaseptin-9TR  | GLWSKIKDAGKAVLKAAGKAALGAVTDAV | supposedly |  | no | Comp Biochem Physiol Part D Genomics Proteomics. **28**:72-79 |
|  | P0C1Q5 | Mastoparan  | INWKALLDAAKKVL | yes |   | AP01638 (homolog) |   |
|  | P69035 | Mastoparan-2  | INWKAIIEAAKQAL | yes |   | AP01638 (homolog) |   |
|  | P0C022 | Eumenine mastoparan-AF  | INLLKIAKGIIKSL | yes |   | AP01517 |   |
|  | P84292 | Hylaseptin-P1  | GILDAIKAIAKAAG | yes | yes | AP01249 |   |
|  | P01516 | Mastoparan-C  | LNLKALLAVAKKIL | yes |   | AP02367 (homolog) |   |
|  | P84921 | Dermaseptin-1  | GLWSKIKETGKEAAKAAGKAALNKIAEAV | yes |   | AP00001 (homolog) |   |
|  | P83637 | Dermaseptin-01  | GLWSTIKQKGKEAAIAAAKAAGQAALGAL | yes |   | AP00947 (homolog) |   |
|  | C0HLC5 | Dermaseptin-3.1TR  | GLFKTLIKGAGKMLGHVAKQFLGSQGQPES | supposedly |  | no | Comp Biochem Physiol Part D Genomics Proteomics. **28**:72-79 |
|  | P84816 | Aggression-stimulating peptide  | GLWDDLKAAAKKVVSSLASAAIEKL | supposedly |  | no | Peptides **26(4)**:597-601. |
|  | P0CJ31 | Ascaphin-7  | GFKDWIKGAAKKLIKTVASAIANQ | yes |   | AP01222 |   |
|  | P0CJ27 | Ascaphin-3  | GFRDVLKGAAKAFVKTVAGHIANI | yes |   | AP01218 |   |
|  | P80008 | Aryl acylamidase (Fragment)  | MDVAEYAAHDATGLAELIREGQVSACEV | unknown |  | no |  |
|  | C0HK47 | Ponericin-Q50  | FWGALFKTVAKVVAPFVPDIVKWVQEKV | yes |   | no | Biochimie **107(B)**:211-215. |
|  | P55791 | Nociceptin  | FGGFTGARKSARKLANQ | unknown |  | no |  |
|  | Q52093 | 30S ribosomal protein S19 | FHGHTKDSKKNIKK | unknown |  | no |  |
|  | O66093 | 30S ribosomal protein S19 | LGEFAPTRTYRGHDKKDNKKDNKKGQKK | unknown |  | no |  |
|  | P59681 | 30S ribosomal protein S20 | MANIKSAIKRAKTSEK | unknown |  | no |  |
|  | P82414 | Ponericin-G1  | GWKDWAKKAGGWLKKKGPGMAKAALKAAMQ | yes | yes | AP00376 |   |
|  | C0HKL7 | Peptide PGLa-BM1  | GMASKAGSVLGKVAKVALKAAL | yes |   | AP01130 |   |
|  | P82415 | Ponericin-G2  | GWKDWLKKGKEWLKAKGPGIVKAALQAATQ | yes |   | AP00377 |   |
|  | P82421 | Ponericin-L1  | LLKELWTKMKGAGKAVLGKIKGLL | yes |   | AP00383 |   |
|  | P82426 | Ponericin-W4  | GIWGTALKWGVKLLPKLVGMAQTKKQ | yes |   | AP00389 |   |
|  | P86914 | Nattererin-2  | GLKDMIKNLAKEAAVKLAGAVINRFSPQPQ | yes |   | no | Rapid Commun. Mass Spectrom. **29:** 2061–2068  |
|  | P83287 | Oncorhyncin-1 (Fragment)  | SKGKKANKDVELARG | yes |   | AP01326 |   |
|  | P82875 | Ranatuerin-1C  | SMLSVLKNLGKVGLGLVACKINKQC | yes |   | AP00122 |   |
|  | Q46490 | 30S ribosomal protein S19 | GHAKKDKKIQKK | unknown |  | no |  |
|  | P29224 | 30S ribosomal protein S19 | GHKLGEFAPTRTFRGHKKEDKKVKR | unknown |  | no |  |
|  | P85058 | Ranatuerin-2SEb  | AIMDTIKDTAKTVAVGLLNKLKCKITGC | yes |   | AP00870 |   |
|  | P84115 | Ranatuerin-2BYb  | GIMDSVKGLAKNLAGKLLDSLKCKITGC | yes |   | AP00888 |   |
|  | P82840 | Ranatuerin-2B  | GLLDTIKGVAKTVAASMLDKLKCKISGC | yes |   | AP00120 |   |
|  | Q9R4P7 | 30S ribosomal protein S20 | ANNAGARKAIRKIEARTEVN | unknown |  | no |  |
|  | C0HKQ5 | Antimicrobial peptide Xac-1  | GFVALLKKLPLILKHLH | yes |   | AP02880 |   |
|  | P84387 | Antimicrobial peptide 1  | GFLGPLLKLAAKGVAKVIPHLIPSRQQ | yes |   | AP00424 |   |
|  | P84382 | Antimicrobial peptide 2  | GVWSTVLGGLKKFAKGGLEAIVNPK | yes |   | AP02290 |   |
|  | P84384 | Antimicrobial peptide 4  | GVFLDALKKFAKGGMNAVLNPK | yes |   | AP00426 |   |
|  | B3EWV3 | Cupiennin-3c  | GFGSLFKFLGKKLAKTVAKQAAKKQME | supposedly |  | no | FEBS J. **279(15)**:2683-94 |
|  | B3EWU9 | Cupiennin-5a  | KFGKVLKFLAKTLAKHLAKKQAQS | supposedly |  | no | FEBS J. **279(15**):2683-94 |
|  | B3EWU1 | Short cationic peptide-1a  | FLAKKVAKTVAKQAAKQGAKYVVNKQME | yes |   | AP00485 |   |
|  | P0CF02 | Dinoponeratoxin Da-3105  | GLKDWWNKHKDKIIAVAKEMGKAGLQAA | supposedly |  | no | Toxicon **55(4)**:702-710. |
|  | B3EWV7 | Cupiennin-4b  | VYGMLFKFLAKKVAKKLISHVAKKQLQ | supposedly |  | no | FEBS J. **279(15**):2683-94 |
|  | Q85BU5 | Uncharacterized 3.0 kDa protein  | MLFKKISKFVGWLSGSSVGSITSKTHE | unknown |  | no |  |
|  | P49832 | Uncharacterized 3.3 kDa protein | MVWLVWKRSTISRKNKKFFKTIFKKN | unknown |  | no |  |
|  | P0CF01 | Dinoponeratoxin Da-2501  | FWGTLAKLALKAVPAVMGMIKKE | supposedly |  | no | Toxicon **55(4)**:702-710. |
|  | P85874 | Mastoparan-like peptide PMM2  | INWKKIASIGKEVLKAL | yes | yes | AP01637 |   |
|  | P84385 | Antimicrobial peptide 5  | GMATKAGTALGKVAKAVIGAAL | yes |   | AP02001 |   |
|  | P82417 | Ponericin-G4  | DFKDWMKTAGEWLKKKGPGILKAAMAAAT | yes |   | AP00379 |   |
|  | P84277 | Palustrin-1d  | ALSILKGLEKLAKMGIALTNCKATKKC | yes |   | AP00617 |   |
|  | C0HK46 | Ponericin-Q49  | FWGALVAGLAPKVAIGIKAINKKG | yes |   | no | Biochimie **107(B)**:211-215. |
|  | P82425 | Ponericin-W3  | GIWGTLAKIGIKAVPRVISMLKKKKQ | yes |   | AP00388 |   |
|  | C0HK88 | Peptide PGLa-B1  | GMASKAGTIAGKIAKTAIKLAL | yes |   | AP02001 (homolog) |   |
|  | C0HL07 | Ranatuerin-2OK  | SFLNFFKGAAKNLLAAGLDKLKCKISGTQC | yes |   | no | Peptides **26(2)**:185-190 |
|  | P0C8D4 | Scolopendra toxin (Fragment)  | XQVVERGLDAKAKAAMLDAHNKARQKVANG | supposedly |  | no | Toxicon **49(6)**:810-826 |
|  | P84826 | Skin secreted peptide 1  | RHHRKRIGHTVKQLAKLVKHIHEY | supposedly |  | no | Gen Comp Endocrinol. **143(2)**:193-199 |
|  | Q46228 | 30S ribosomal protein S19  | FRGHAKGDKKNQKK | unknown |  | no |  |
|  | A0T0S1 | Photosystem I subunit XII  | MITDFQVYIALMAALLASVLAIRLGATLYQ | unknown |  | no |  |
|  | P13193 | Photosystem I subunit III | AIAGLTPPKESKAFAKXEKN | unknown |  | no |  |
|  | C0HKN1 | Caerulein precursor fragment R7  | GLASFLGKALKAGLKIGAHLLGGAPQQ | yes |   | AP01901 (homolog) |   |
|  | C0HK89 | Caerulein precursor fragment B1  | GLGSLLGKAFKIGLKTVGKMMGGAPREQ | yes |   | AP01622 |   |
|  | C0HJB8 | Cyanophlyctin  | FLNALKNFAKTAGKRLKSLLN | yes |   | AP02211 |   |
|  | C0HK91 | Caerulein precursor fragment B4  | GLLTNVLGFLKKAGKGVLSGLLPL | supposedly |  | no | Comp Biochem Physiol C Toxicol Pharmacol. **152(4)**:467-472. |
|  | P83914 | Dermaseptin-like peptide  | DLWNSIKDMAAAAGRAALNAVTGMVNQ | yes |   | no | J Parasitol. **91(6):**1340-1351. |
|  | P82431 | 100 kDa cell wall protein | EPVKKKDLKKATVPL | unknown |  | no |  |
|  | P85028 | Cryptonin  | GLLNGLALRLGKRALKKIIKRLCR | yes | yes | AP00722 |   |
|  | P80084 | ATP synthase subunit | IGTQIVXNXMKSIKNIQKITKAMKMV | unknown |  | no |  |
|  | P81079 | Cytochrome c3 | IGAGVGRDGTIAATKGKAKTLAELIXMYDS | unknown |  | no |  |
|  | A0A193 | Cruzioseptin-3 | KRGFLDVVKHIGKAALGAVTHLINQGEQ | yes |   | AP02715 |   |
|  | P82906 | Brevinin-1Sc  | FFPIVAGVAGQVLKKIYCTISKKC | yes |   | AP00455 |   |
|  | P86152 | Brevinin-2Ej  | GIFLDKLKNFAKGVAQSLLNKASCKLSGQC | supposedly |  | no | Rapid Commun Mass Spectrom. **22(22)**:3517-3525. |
|  | P0C8T3 | Brevinin-2PTa  | GAIKDALKGAAKTVAVELLKKAQCKLEKTC | yes |   | AP01427 |   |
|  | C0HK08 | Cruzioseptin-10  | GFLDVLKGVGKAALGAVTHHINNLVNQQ | supposedly |  | no | J Proteomics. **146**:1-13. |
|  | P0C8T2 | Brevinin-1PTb  | FMGGLIKAATKALPAAFCAITKKC | yes |   | AP01433 |   |
|  | C0HK10 | Cruzioseptin-14  | GFLDIVLHVGLAAGKAALNAVNEAVNQ | supposedly |  | no | J Proteomics. **146**:1-13. |
|  | P29003 | Bombinin-like peptide 2  | GIGSAILSAGKSALKGLAKGLAEHFAN | yes | yes | AP00051 |   |
|  | P82234 | Brevinin-2Tc  | GLWETIKNFGKKFTLNILHKLKCKIGGGC | yes |   | AP00457 |   |
|  | P85833 | Bacteriocin  | KKIDTRTGKTMEKTEKKIELSLKNMKTAT | yes |   | no | World J Microbiol. Biotechnol. **28**:1647–1655  |
|  | P0C007 | Dicynthaurin  | ILQKAVLDCLKAAGSSLSKAAITAIYNKIT | yes | yes | AP00510 |   |
|  | P0DP00 | Conantokin-Oc  | GEEERKAMAELEAKKAQEALKA | unknown |  | no |  |
|  | P80280 | Dermaseptin-4  | ALWMTLLKKVLKAAAKALNAVLVGANA | yes | yes | AP00160 |   |
|  | P84924 | Dermaseptin-4  | ALWKDILKNAGKAALNEINQIVQ | supposedly |  | no |  |
|  | P36191 | Ceratotoxin-B  | SIGSAFKKALPVAKKIGKAALPIAKAALP | yes | yes | AP00415 |   |
|  | P80978 | Cytochrome c | KMLGVVAKKPMSDYE | unknown |  | no |  |
|  | P81487 | Dermaseptin-B5  | GLWNKIKEAASKAAGKAALGFVNEMV | yes | yes | AP00162 |   |
|  | P86692 | Unknown protein 3 | FTAAAEAEAAAA | unknown |  | no |  |
|  | P82034 | Uperin-3.3  | GVLDAFKKIATVVKNLV | yes |   | AP00323 (homolog) |   |
|  | P99503 | Unknown protein | AEAAAAPAPAAAPA | unknown |  | no |  |
|  | P86114 | Venom peptide Ocy8 | GSLGEKYAQKAAEVLTSIIP | supposedly |  | no | Toxicon **51(8)**:1499-1508 |

**Table S5.** Mass-spectrometry analysis results.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Peptide | Sequence | Formula | Calculatedmolecular mass(monoisotopic) | Observed molecular mass |
| P1 | KIGVLKKYFKIGALIKAIIK-NH2 | C111H195N27O21 | 2242.49 | 2242.49 |
| P2 | LKKLKQLLGKLSEFAAAFVA-NH2 | C104H176N26O24 | 2173.32 | 2173.35 |
| P3 | GQLNKFIKKAQRKFHEKFAK-NH2 | C114H185N35O25 | 2444.41 | 2444.42 |
| P4 | KVFKSVVKLLEKTVLKKFSK-NH2 | C113H198N28O25 | 2347.49 | 2347.52 |
| P5 | GALSKHAAELKAKQRTSLEK-NH2 | C93H165N31O28 | 2164.23 | 2164.24 |
| P6 | LKKLVRKAASISASLAARHA-NH2 | C92H168N32O23 | 2089.28 | 2089.29 |
| P7 | KAAKTVFKLFKLQAKRAIEA-NH2 | C106H182N30O24 | 2259.38 | 2259.38 |

**Table S6.** Secondary structure of the peptides in solution and in the model lipid environment estimated by CDSSTR algorithm from circular dichroism experimental data.

|  |  |  |  |
| --- | --- | --- | --- |
| Peptide | No lipids | Anionic micelles (SDS) | Zwitterionic micelles (DPC) |
|  | α-helix | β-sheet +β-turn | Coil | α-helix | β-sheet +β-turn | Coil | α-helix | β-sheet +β-turn | Coil |
| P1 | 1% | 24% | 74 % | 61% | 22% | 16% | 78% | 11% | 10% |
| P2 | 5% | 26% | 68% | 86% | 5% | 8% | 91% | 5% | 4% |
| P3 | 4% | 34% | 61% | 52% | 29% | 19 | 91% | 3% | 5% |
| P4 | 3% | 20% | 77% | 80% | 14% | 5% | 83% | 12% | 4% |
| P5 | 4% | 36% | 58% | 37% | 34% | 28% | 6% | 36% | 58% |
| P6 | 2% | 15% | 82% | 80% | 10% | 10% | 52% | 26% | 23% |
| P7 | 2% | 27% | 70% | 90% | 5% | 5% | 90% | 4% | 5% |

**Table S7.** Calculated physicochemical properties of the designed peptides.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Peptide | Net chargepH 7.4, e | Helicity changewater-DPC, % | AmphiphilicityμH  | HydrophobicityΔGoct, kcal/mol | Membrane bindingΔGif, kcal/mol |
| P1 | 7 | 77 | 3.09 | 13.4 | -6.77 |
| P2 | 4 | 86 | 7.75 | 13.38 | -7.03 |
| P3 | 7 | 87 | 8.25 | 23.69 | -2.82 |
| P4 | 7 | 80 | 4.47 | 19.69 | -3.1 |
| P5 | 4 | 2 | 5.39 | 26.02 | 6.34 |
| P6 | 6 | 50 | 3.79 | 15.48 | -0.36 |
| P7 | 6 | 88 | 5.21 | 19.78 | -3.63 |
| Magainin 2 | 4 | 78 [5] | 5.86 | 16.86 | -7.3 |

**Calculation methodology.** Thermodynamic properties were calculated based on peptide amino acid sequence with the Wimley-White scales [6]. All investigated peptides are amidated on C-terminus, therefore in all calculations we considered protonated N-terminus and neutral histidine residues as these states correspond to pH 7.4. Octanol scale was used for hydrophobicity, and interfacial scale was used for membrane binding free energy calculation [6]. Amphiphilicity was estimated with the value of the hydrophobic moment of a complete helix using interfacial scale [7]. The contribution of the secondary structure change was calculated as 0.4 kcal/mol for each residue that contributes to helix on the membrane [8], free energy correction due to helical content of a peptide in solution was done as described in ref. 9. All calculations were performed in Membrane Protein Explorer (MPEx) software [10].

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