

Supporting Information

Cyclotides from Brazilian *Palicourea sessilis* and Their Effects on Human Lymphocytes

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Table S1. Obtained masses of cyclotides from *Palicourea sessilis*.

| Cyclotide | Leaves | | Stem | |
|--------------|------------------|--------|------------------|---------|
| | Obtained mass | mg/g* | Obtained mass | mg/g* |
| pase A (1) | 5.4 | (0.21) | 8.2 | (0.07) |
| pase B (2) | 6.7 | (0.26) | 1.0 | (0.001) |
| pase C (3) | 3.6 | (0.14) | 3.1 | (0.03) |
| pase D (4) | - | - | 2.5 | (0.02) |
| pase E (5) | - | - | 2.9 | (0.02) |
| kalata S (6) | 1.1 | (0.04) | - | - |

*Concentrations based on dried leaves (26.15 g, 198 mg 80%-C₁₈ leave extract) and dried stems (111.35 g, 103 mg 80%-C₁₈ stem extract).

Table S2. Sequence fragments of pase (A–E) and kalata S cyclotides, generated through enzymatic digestion and characterization using MALDI-TOF/TOF-MS/MS.

| Cyclotide (Da) | Sequences identified in the precursor ion | Precursor Mass (Da) | | Enzyme(s) |
|---------------------|---|------------------------|---------|-----------|
| | | obs. | calc. | |
| pase A 2889.01 | NGLPVCGETCVGGTCNTPGCVCSWPVCTR | 3255.07 | 3255.23 | T |
| | VCSWPVCTR | 3255.35 | 3255.23 | E |
| pase B 2903.30 | NGLPVCGETCVGGTCNTPGCVCSWPICTR | 3269.04 | 3269.24 | T |
| | TPGCVCSWPICTRNGLPV | 3269.34 | 3269.24 | E |
| pase C 2905.04 | NGLPTCGETCVGGTCNTPGCVCSWPICTR | 3271.12 | 3271.22 | T |
| | PGCVCSWPICTRNGLT | 3271.19 | 3271.22 | E |
| pase D 2887.00 | NGLPVCGETCVGGTCNTPGCVCAWPICTR | 3253.10 | 3253.24 | T |
| | GGTCNTPGCVCAWPICTRNGLPV | 3253.30 | 3253.24 | E |
| pase E 2983.08 | RNGLPVCGE | 1001.49 | 1001.46 | E; T |
| | TCVTGSCYTPGCSCSWPVCK | 2366.84 | 2366.82 | E; T |
| kalata S 2977.00 | NGLPVCGETCVGGTCNTPGCSCSWPVCTR | 3242.89 | 3243.19 | T |
| | SCSWPVCTRNGLPVCGE | 3242.85 | 3243.19 | E |

obs. observed, calc. calculated, T: Trypsin and E: Endoproteinase GluC

Table S3. ¹H Chemical shifts (ppm) of pase A at pH 4.5 and 298K (BMRB code 50464).

| Residue | NH | H _α | H _{βa} | H _{βb} | H _{γa} | H _{γb} | H _{δa} | H _{δb} | H _ε |
|---------|-----|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 1 | Gly | 8.98 | 3.6; 4.24 | | | | | | |
| 2 | Leu | 7.74 | 5.08 | 1.70 | 1.93 | 1.50 | 0.92 | 0.99 | |
| 3 | Pro | | 5.10 | 1.75 | 2.47 | 2.18 | 2.06 | 3.80 | |
| 4 | Val | 8.16 | 4.67 | 2.59 | | 0.87 | 0.87 | | |
| 5 | Cys | 8.05 | 4.44 | 3.03 | 3.37 | | | | |
| 6 | Gly | 8.53 | 3.74; 3.84 | | | | | | |
| 7 | Glu | 7.17 | 4.80 | 1.96 | 1.88 | 2.51 | 2.41 | | |
| 8 | Thr | 8.47 | 4.56 | 4.44 | | 1.16 | 1.16 | | |
| 9 | Cys | 8.33 | 4.96 | 3.19 | 2.92 | | | | |
| 10 | Val | 8.54 | 3.87 | 2.05 | | 0.98 | 1.03 | | |
| 11 | Gly | 8.72 | 3.85; 4.25 | | | | | | |
| 12 | Gly | 8.27 | 4.06; 4.42 | | | | | | |
| 13 | Thr | 7.87 | 4.71 | 4.10 | | 1.15 | 1.15 | | |
| 14 | Cys | 8.61 | 4.71 | 2.70 | 3.07 | | | | |
| 15 | Asn | 10.42 | 4.71 | 2.78 | | | | | |
| 16 | Thr | 9.06 | 4.41 | 4.26 | | 1.33 | 1.33 | | |
| 17 | Pro | | 4.26 | 1.90 | 2.32 | 2.15 | 2.01 | 3.71 | 4.71 |
| 18 | Gly | 8.78 | 3.67; 4.19 | | | | | | |
| 19 | Cys | 7.69 | 5.35 | 2.61 | 3.83 | | | | |
| 20 | Val | 9.40 | 4.44 | 2.05 | | 0.86 | 0.86 | | |
| 21 | Cys | 8.97 | 4.59 | 2.80 | 3.08 | | | | |
| 22 | Ser | 8.99 | 4.75 | 3.85 | 3.85 | | | | |
| 23 | Trp | 7.34 | 4.09 | | | | | | 10.41 |
| 24 | Pro | | 3.45 | -0.17 | 1.73 | 1.32 | 1.42 | 3.26 | 3.20 |
| 25 | Val | 8.24 | 4.22 | 1.94 | | 0.85 | 0.85 | | |
| 26 | Cys | 7.70 | 5.07 | 2.75 | 3.22 | | | | |
| 27 | Thr | 9.92 | 5.07 | | | | | | |
| 28 | Arg | 8.76 | 4.75 | 1.69 | 1.61 | 1.41 | 1.41 | 3.18 | 6.96 |
| 29 | Asn | 9.6 | 4.40 | 2.85 | 3.09 | | | | |

Table S4. ¹H Chemical shifts (ppm) of pase B at pH 3.5 and 298K.

| Residue | NH | H _α | H _{βa} | H _{βb} | H _{γa} | H _{γb} | H _{δa} | H _{δb} | H _ε |
|---------------|------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 1 Gly | 8.99 | 3.60; 4.23 | | | | | | | |
| 2 Leu | 7.76 | 5.07 | 1.70 | 1.94 | 1.49 | 0.92 | 0.99 | | |
| 3 Pro | | 5.06 | 1.78 | 2.48 | 2.18 | 2.05 | 3.79 | | |
| 4 Val | 8.12 | 4.68 | 2.60 | | 0.87 | 0.87 | | | |
| 5 Cys | 8.09 | 4.44 | 3.05 | 3.38 | | | | | |
| 6 Gly | 8.50 | 3.73; 3.82 | | | | | | | |
| 7 Glu | 7.13 | 4.74 | 2.33 | 2.48 | 1.86 | | | | |
| 8 Thr | 8.48 | 4.57 | 4.45 | | 1.15 | 1.15 | | | |
| 9 Cys | 8.34 | 5.01 | 2.85 | 3.20 | | | | | |
| 10 Val | 8.57 | 3.83 | 2.06 | | 0.98 | 1.04 | | | |
| 11 Gly | 8.67 | 3.85; 4.28 | | | | | | | |
| 12 Gly | 8.27 | 4.06; 4.45 | | | | | | | |
| 13 Thr | 7.87 | 4.71 | 4.09 | | 1.14 | 1.14 | | | |
| 14 Cys | 8.55 | 4.69 | 2.66 | 3.09 | | | | | |
| 15 Asn | | | | | | | | | |
| 16 Thr | | | | | | | | | |
| 17 Pro | | 4.22 | 1.91 | 2.32 | 2.15 | 2.01 | 3.70 | 4.22 | |
| 18 Gly | 8.78 | 3.68; 4.18 | | | | | | | |
| 19 Cys | 7.70 | 5.35 | 2.61 | 3.84 | | | | | |
| 20 Val | 9.46 | 4.35 | 2.01 | | 0.87 | 0.87 | | | |
| 21 Cys | 8.94 | 4.61 | 2.78 | 3.07 | | | | | |
| 22 Ser | 9.06 | 4.76 | 3.85 | 3.85 | | | | | |
| 23 Trp | | | | | | | | | 10.41 |
| 24 Pro | | 3.46 | -0.26 | 1.73 | 1.28 | 1.40 | 3.2 | | |
| 25 Ile | 8.23 | 4.26 | 1.80 | | 1.12, 1.34 | 0.86 | 0.73 | | |
| 26 Cys | 7.63 | 5.18 | 2.74 | 3.22 | | | | | |
| 27 Thr | 9.90 | 5.05 | | | | | | | |
| 28 Arg | 8.77 | 4.76 | 1.62 | 1.70 | 1.40 | | 3.18 | 3.18 | 6.94 |
| 29 Asn | 9.62 | 4.40 | 2.86 | 3.09 | | | | | |

Table S5. ¹H Chemical shifts (ppm) of pase C at pH 4.7 and 298K.

| Residue | NH | H _α | H _{βa} | H _{βb} | H _{γa} | H _{γb} | H _{δa} | H _{δb} | H _ε |
|---------------|-------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 1 Gly | | 3.71; 4.25 | | | | | | | |
| 2 Leu | 7.81 | 5.06 | 1.69 | 2.02 | 1.50 | 0.92 | 0.99 | | |
| 3 Pro | | 5.10 | 1.77 | 2.49 | 2.18 | 2.03 | 3.78 | | |
| 4 Thr | 8.40 | 4.60 | | | | | | | |
| 5 Cys | 7.92 | 4.44 | 3.02 | 3.39 | | | | | |
| 6 Gly | | 3.73; 3.83 | | | | | | | |
| 7 Glu | 7.15 | 4.73 | 1.83 | 1.83 | 2.46 | 2.31 | | | |
| 8 Thr | 8.50 | 4.56 | 4.44 | | 1.14 | 1.15 | | | |
| 9 Cys | 8.34 | 5.03 | 3.20 | 2.83 | | | | | |
| 10 Val | 8.59 | 3.82 | 2.07 | | 0.99 | 1.05 | | | |
| 11 Gly | | | | | | | | | |
| 12 Gly | 8.29 | 4.06; 4.46 | | | | | | | |
| 13 Thr | 7.86 | 4.71 | 4.08 | | 1.14 | 1.14 | | | |
| 14 Cys | 8.54 | 4.69 | 2.67 | 3.09 | | | | | |
| 15 Asn | 10.42 | 4.71 | 2.78 | | | | | | |
| 16 Thr | 9.06 | 4.41 | 4.26 | | 1.33 | 1.33 | | | |
| 17 Pro | | 4.24 | 1.91 | 2.32 | 2.15 | 2.00 | 3.66 | 4.71 | |
| 18 Gly | 8.96 | 3.59; 4.25 | | | | | | | |
| 19 Cys | 7.70 | 5.36 | 2.62 | 3.83 | | | | | |
| 20 Val | 9.38 | 4.42 | 2.04 | | 0.86 | 0.86 | | | |
| 21 Cys | 8.94 | 4.61 | 2.78 | 3.07 | | | | | |
| 22 Ser | 9.07 | 4.75 | 3.85 | 3.85 | | | | | |
| 23 Trp | | 4.09 | 3.28 | 3.28 | | | | | 10.41 |
| 24 Pro | | 3.47 | -0.26 | 1.73 | 1.28 | 1.40 | 3.20 | 3.20 | |
| 25 Ile | 8.23 | 4.27 | 1.81 | | 1.12, 1.34 | 0.86 | | | |
| 26 Cys | 7.64 | 5.16 | 2.76 | 3.23 | | | | | |
| 27 Thr | 9.90 | 5.04 | | | | | | | |
| 28 Arg | 9.3 | 4.75 | 1.77 | 1.59 | 1.37 | 1.37 | 3.09 | 3.24 | 6.96 |
| 29 Asn | | | | | | | | | |

Table S6. ¹H Chemical shifts (ppm) of pase D at pH 3.5 and 298K.

| Residue | NH | H _α | H _{βa} | H _{βb} | H _{γa} | H _{γb} | H _{δa} | H _{δb} | H _ε |
|---------|-----|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 1 | Gly | 8.96 | 3.68, 4.22 | | | | | | |
| 2 | Leu | 7.77 | 5.08 | 1.69 | 1.93 | 1.49 | 0.92 | 0.98 | |
| 3 | Pro | | 5.08 | 1.77 | 2.47 | 2.18 | 2.05 | 3.79 | |
| 4 | Val | 8.14 | 4.68 | 2.59 | | 0.87 | 0.87 | | |
| 5 | Cys | 8.12 | 4.42 | 3.09 | 3.39 | | | | |
| 6 | Gly | 8.52 | 3.73, 3.82 | | | | | | |
| 7 | Glu | 7.14 | 4.73 | 1.88 | 1.88 | 2.40 | 2.28 | | |
| 8 | Thr | 8.44 | 4.58 | 4.44 | 1.15 | 1.15 | | | |
| 9 | Cys | 8.29 | 4.99 | 3.16 | 2.86 | | | | |
| 10 | Val | 8.54 | 3.86 | 2.07 | | 1.01 | 1.01 | | |
| 11 | Gly | 8.72 | 3.85, 4.26 | | | | | | |
| 12 | Gly | 8.28 | 4.03; 4.45 | | | | | | |
| 13 | Thr | 7.84 | 4.70 | 4.08 | | 1.14 | 1.14 | | |
| 14 | Cys | 8.52 | 4.68 | 2.66 | 3.16 | | | | |
| 15 | Asn | 10.42 | 4.71 | 2.78 | | | | | |
| 16 | Thr | 9.87 | 4.32 | | | 1.32 | 1.32 | | |
| 17 | Pro | | 4.21 | 1.91 | 2.32 | 2.15 | 2.01 | 3.71 | |
| 18 | Gly | 8.77 | 3.67; 4.18 | | | | | | |
| 19 | Cys | 7.70 | 5.36 | 2.61 | 3.85 | | | | |
| 20 | Val | 9.43 | 4.39 | 2.01 | | 0.87 | 0.87 | | |
| 21 | Cys | 8.93 | 4.57 | 2.81 | 3.06 | | | | |
| 22 | Ala | 9.12 | 4.72 | 1.27 | 1.27 | | | | |
| 23 | Trp | 7.33 | 4.10 | 3.27 | 3.27 | | | | 10.39 |
| 24 | Pro | | 3.50 | -0.17 | 1.74 | 1.30 | 1.41 | 3.20 | 3.20 |
| 25 | Ile | 8.26 | 4.30 | 1.85 | | 1.15, 1.35 | 0.86 | 0.74 | |
| 26 | Cys | 7.58 | 5.18 | 2.75 | 3.20 | | | | |
| 27 | Thr | 9.68 | 5.07 | | | 0.73 | | | |
| 28 | Arg | 8.86 | 4.81 | 1.77 | 1.61 | 1.40 | 1.40 | 3.18 | 3.18 |
| 29 | Asn | 9.58 | 4.40 | 2.86 | 3.09 | | | | 6.96 |

Table S7 ^1H Chemical shifts (ppm) of pase E at pH 4.5 and 298K.

| Residue | NH | H $_{\alpha}$ | H $_{\beta a}$ | H $_{\beta b}$ | H $_{\gamma a}$ | H $_{\gamma b}$ | H $_{\delta a}$ | H $_{\delta b}$ | H $_{\epsilon}$ |
|---------------|-------|---------------|----------------|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1 Gly | 8.69 | 3.58; 4.24 | | | | | | | |
| 2 Leu | 7.88 | 5.16 | 1.70 | 1.95 | 1.51 | 0.95 | 0.99 | | |
| 3 Pro | | 5.17 | 1.65 | 2.55 | 2.12 | 2.22 | 3.84 | 3.84 | |
| 4 Val | 8.04 | 4.68 | 2.61 | | 0.88 | 0.88 | | | |
| 5 Cys | 8.19 | 4.42 | 3.35 | 3.11 | | | | | |
| 6 Gly | 8.61 | 3.74; 3.85 | | | | | | | |
| 7 Glu | 7.32 | 4.75 | 2.25 | 1.89 | 2.44 | 2.44 | | | |
| 8 Thr | 8.59 | 4.59 | 4.49 | | 1.19 | 1.19 | | | |
| 9 Cys | 8.20 | 5.19 | 3.31 | 2.86 | | | | | |
| 10 Val | 8.30 | 3.73 | 2.15 | | 1.05 | 1.13 | | | |
| 11 Thr | 7.91 | 4.63 | | | | | | | |
| 12 Gly | 8.19 | 4.06; 4.42 | | | | | | | |
| 13 Ser | 7.96 | 4.71 | 3.59 | 3.59 | | | | | |
| 14 Cys | 8.27 | 4.55 | 2.62 | 3.07 | | | | | |
| 15 Tyr | 9.02 | 4.80 | 3.69 | 3.89 | | | | | |
| 16 Thr | 10.01 | 4.36 | 4.36 | | 1.35 | 1.35 | | | |
| 17 Pro | | 4.24 | 1.92 | 2.32 | 2.16 | 2.04 | 3.73 | 4.17 | |
| 18 Gly | 8.78 | 3.71; 4.16 | | | | | | | |
| 19 Cys | 7.81 | 5.14 | 2.51 | 3.90 | | | | | |
| 20 Ser | 9.35 | 4.68 | 3.80 | 3.80 | | | | | |
| 21 Cys | 9.11 | 4.81 | 3.13 | 4.54 | | | | | |
| 22 Ser | | | | | | | | | |
| 23 Trp | | | | | | | | | 10.41 |
| 24 Pro | | 3.55 | -0.32 | 1.77 | 1.30 | 1.38 | 3.22 | 3.18 | |
| 25 Val | 8.43 | 4.19 | 1.93 | | 0.88 | 0.88 | | | |
| 26 Cys | 7.87 | 4.90 | 2.69 | 3.15 | | | | | |
| 27 Lys | 9.25 | 5.05 | 1.81 | 1.81 | 1.53 | 1.37 | 0.77 | 0.77 | 2.80 |
| 28 Arg | 8.78 | 4.75 | 1.63 | 1.72 | 1.39 | 1.39 | 3.20 | | 6.92 |
| 29 Asn | 9.65 | 4.40 | 2.83 | 3.11 | | | | | |

Table S8. Statistical analysis of pase A structures.

| Energies (kcal/mol) | Pase A^a |
|---|---------------------------|
| Overall | -847.01 ± 29.45 |
| Bonds | 10.64 ± 1.13 |
| Angles | 29.09 ± 4.00 |
| Improper | 10.75 ± 1.67 |
| Dihedral | 116.67 ± 1.92 |
| van der Waals | -92.98 ± 8.75 |
| NOE | 0.011 ± 0.01 |
| cDih | 0.59 ± 0.47 |
| Stereochemical quality^b | |
| Clashes (all atoms) | 10.23 ± 5.46 |
| Poor rotamers | 0.83 ± 1.73 |
| Ramachandran outliers (%) | 2.71 ± 1.69 |
| Ramachandran favored (%) | 86.42 ± 5.17 |
| Overall Molprobity score | 2.17 ± 1.69 |
| RMSD from mean structure (Å)^c | |
| Mean global backbone (residues 4-8, 19-27) | 0.81 ± 0.25 |
| Mean global heavy (residues 4-8, 19-27) | 1.73 ± 0.41 |
| Distance restraints | |
| Intraresidue (i-j =0) | 95 |
| Sequential (i-j =1) | 84 |
| Medium range (i-j <5) | 4 |
| Long range (i-j ≥5) | 2 |
| Hydrogen bonds | 16 |
| Disulfide bonds | 3 |
| Total | 204 |
| Dihedral angle restraints | |
| φ | 21 |
| ψ | 21 |
| χ ¹ | 8 |
| Total | 50 |
| Violations from experimental restraints | |
| Total NOE violations exceeding 0.2 Å | 0 |
| Total dihedral violations exceeding 2.0° | 2 (highest 0.84) |

^aAll statistics are given as mean ± SD.^bAccording to MolProbity.^cMean RMSD was calculated using MOLMOL.

Figure S1. Multiple sequence alignment of reported Möbius cyclotides extracted from

Cybase.¹⁰

| | | |
|-------------------|-------------------------------------|----|
| Cter_4 | CGETCFGG-TCYTPGCVCD-PWPICTKNGDPLA- | 31 |
| Cter_37 | CGETCFGG-TCYTPGCVCD-PWPICTKNGSPT-- | 30 |
| Cter_1 | CGETCFGG-TCNTPNCVCD-PWPICTNNGLPV-- | 30 |
| varv_peptide_B | CGETCFGG-TCNTPGCS-CD-PWPMCSRNGLPV-- | 30 |
| varv_peptide_G | CGETCFGG-TCNTPGCS-CD-PWPVCSRNGVPV-- | 30 |
| varv_peptide_H | CGETCFGG-TCNTPGCS-CE-TWPVCSRNGLPV-- | 30 |
| cycloviolacin_O23 | CGETCFGG-TCNTPGCTCDSSWPICTHNGLPV-- | 31 |
| kalata_B6 | CGETCFGG-TCNTPGCS-CD-SWPICTRNGLPV-- | 30 |
| kalata_B10 | CGETCFGG-TCNTPGCS-CD-SWPICTRDGLPT-- | 30 |
| kalata_B10_linear | CGETCFGG-TCNTPGCS-CD-SWPICTRDGLPT-- | 30 |
| kalata_B3 | CGETCFGG-TCNTPGCTCD-PWPICTRDGLPT-- | 30 |
| vhl-2 | CGETCFTG-TCYTNCGCTCD-PWPVCTRNGLPV-- | 30 |
| cycloviolacin_O32 | CGETCFGG-TCNTPGCTCD-PWPVCTNDGAPV-- | 30 |
| cycloviolacin_O36 | CGETCFGG-TCNTPGCTCD-PFPVCTHDGLPT-- | 30 |
| cycloviolacin_O24 | CGETCFGG-TCNTPGCTCD-PWPVCTHNGLPV-- | 30 |
| Oak6_cyclotide_2 | CGETCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| kalata_B14 | CGESCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| kalata_B13 | CGETCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| cycloviolacin_H3 | CGETCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| vaby_D | CGETCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| vaby_E | CGETCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| Oak6_cyclotide_1 | CGETCFGG-TCNTPGCTCD-PWPVCTRNGLPV-- | 30 |
| vitri_peptide_23 | CGETCTLG-TCYTPGCTCS--WPICTKNGLPV-- | 29 |
| psybra_1 | CGETCTLG-TCNTPGCTCS--WPICTKNGLPV-- | 29 |
| Mobo_A | CGETCTLG-TCNTPGCTCS--WPICTRNGFPT-- | 29 |
| Mden_A | CGETCTLG-TCNTPGCTCS--WPICTKNGIPT-- | 29 |
| kalata_B7 | CGETCTLG-TCYTPGCTCS--WPICKRNGLPV-- | 29 |
| viphi_B | CGETCTIG-TCYTAGCTCS--WPICTRNGLPV-- | 29 |
| vodo_N | CGETCTLG-KCYTAGCTCS--WPVCTRNGLPV-- | 29 |
| Viba_16 | CGETCTLG-TCYTVGCTCS--WPVCTRNGLPV-- | 29 |
| varv_peptide_F | CGETCTLG-TCYTAGCTCS--WPVCTRNGVPI-- | 29 |
| Vinc_A | CGETCTLG-TCYTAGCTCS--WPVCTRNGIPV-- | 29 |
| vila_D | CGETCAFG-TCYTPGCTCS--WPVCTRNGIPV-- | 29 |
| vibi_C | CGETCAFG-TCYTPGCTCS--WPVCTRNGLPV-- | 29 |
| vitri_D | CGETCFTG-TCYTPGCTCS--WPVCTRNGLPV-- | 29 |
| pase_E | CGETCVTG-TCYTPGCTCS--WPVCKRNGLPV-- | 29 |
| cycloviolacin_O21 | CGETCVTG-TCYTPGCTCS--WPVCTRNGLPV-- | 29 |
| vitri_peptide_18a | CGETCFQG-TCNTPGCTCK--WPICTKNGVPI-- | 29 |
| psyleio_E | CGETCFGG-TCNTPGCTCS--WPICTKSVTPIV-- | 30 |
| psyleio_B | CGETCFGG-TCNTPGCTCS--WPVCKRNGDLPI-- | 29 |
| psyleio_C | CGETCFGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| kalata_B15 | CGESCFGG-TCYTPGCTCS--WPICTRNGLPV-- | 29 |
| psyleio_A | CGETCFTG-TCNTPGCTCS--YPICTRNGLPV-- | 29 |
| psyleio_D | CGESCFGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| kalata_B2 | CGETCFGG-TCNTPGCTCS--WPICTRNGLPV-- | 29 |
| kalata_B11 | CGETCFGG-TCNTPGCTCS--DPICTRNGLPV-- | 29 |
| paltet_1 | CGETCFTG-TCNTPGCTCS--YPVCTRNGLPV-- | 29 |
| vibi_A | CGETCFGG-TCNTPGCTCS--YPICTRNGLPV-- | 29 |
| vibi_D | CGETCFGG-RCNTPGCTCS--YPICTRNGLPV-- | 29 |
| vibi_B | CGETCFGG-TCNTPGCTCS--YPICTRNGLPV-- | 29 |
| vaby_C | CGETCAGG-RCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| vaby_A | CGETCAGG-TCNTPGCTCS--WPICTRNGLPV-- | 29 |
| vaby_B | CGETCAGG-TCNTPGCTCS--WPICTRNGLPV-- | 29 |
| cycloviolacin_O22 | CGETCVGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| vigno_2 | CGETCAGG-TCNTPGCTCS--WPVCRDGS SPL- | 30 |
| mech_7 | CGETCTIG-TCNTPGCTCS--WPVCTRNGIPV-- | 29 |
| Psysol_2 | CGESCVGG-TCNTPGCTCT--WPVCTRNGLPV-- | 29 |
| vitri_C | CGETCVGG-TCNTPGCTCT--WPVCTRNGLPV-- | 29 |
| kalata_B4 | CGETCVGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| cycloviolacin_O34 | CGETCVGG-TCNTEYCTCS--WPVCTRNGLPV-- | 29 |
| cycloviolacin_O35 | CGETCVGG-TCNTPYCFCS--WPVCTRNGLPV-- | 29 |
| cycloviolacin_O33 | CGETCVGG-TCNTPYCTCS--WPVCTRNGLPV-- | 29 |
| chacur_1 | CGETCVGG-TCNTPGCTCS--WPICTRNGLPV-- | 29 |
| riden_A | CGETCVGG-TCNTPGCTCT--WPVCTRNGLPV-- | 29 |
| kalata_B1 | CGETCVGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| Viba_15 | CGETCVGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| Viba_17 | CGETCVGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| pase_A | CGETCVGG-TCNTPGCTCS--WPVCTRNGLPV-- | 29 |
| pase_D | CGETCVGG-TCNTPGCTCS--WPICTRNGLPV-- | 29 |
| pase_C | CGETCVGG-TCNTPGCTCS--WPICTRNGLPV-- | 29 |

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| pase_B | CGETCVGG-TCNTPGCVCS--WPICTRNLPLV-- | 29 |
| vigno_5 | CGETCVGG-TCNTPGCSG--WPVAVRNLPL-- | 29 |
| vigno_1 | CGETCAGG-TCNTPGCS--WPVAVRNLPL-- | 29 |
| vitri_B | CGESCVGG-TCNTPGCS--WPVCTTNGYPI-- | 29 |
| vigno_4 | CGETCVGG-TCNTPGCS--WPVCTRNLPL-- | 29 |
| vigno_3 | CGETCVGG-TCNTPGCS--WPVCTRNLPL-- | 29 |
| varv_peptide_C | CGETCVGG-TCNTPGCS--WPVCTRNGVPI-- | 29 |
| varv_peptide_D | CGETCVGG-TCNTPGCS--WPVCTRNLPL-- | 29 |
| cycloviolacin_O12 | CGETCVGG-TCNTPGCS--WPVCTRNLPL-- | 29 |
| vocC | CGETCVGG-TCNTPGCS--WPVCTRNLPL-- | 29 |
| cycloviolacin_O28 | CGETCVGG-TCNTPGCS--WPVCFRDGLPV-- | 29 |
| vitri_E | CGETCVGG-TCNTPGCS--WPVCFRNLPLV-- | 29 |
| viba_30_linear | CGETCVGG-TCNTPGCS--WPVCTRNGPPV-- | 29 |
| cycloviolacin_T1 | CGETCVGG-TCNTPGCS--WPVCTRNGIPV-- | 29 |
| cycloviolacin_O31 | CGETCVGG-TCNTPGCS--IPVCTRNLPLV-- | 29 |
| viba_32 | CGEACVGG-TCNTPGCS--WPVCTRNLPLV-- | 29 |
| kalata_S | CGETCVGG-TCNTPGCS--WPVCTRNLPLV-- | 29 |
| vitri_peptide_24/28 | CGDSCVFF-GCDDEGCTCG-PWSLCYRNGEFV-- | 30 |
| Cter_36 | CGETCFGG-TCYTPNCVCD--PWPICTKNGSPT-- | 30 |
| vitri_peptide_21 | CGETCTLSDRCYTKGCTCN--WPICTKNGGGLD- | 31 |
| Cter_M | CGETCTL-GTCYVPCSCS--WPICTKNGLPT-- | 29 |
| Mden_F | CGETCFE-GKNTPKCTCI--NPICTKNGLPI-- | 29 |
| Mden_H | CGETCFE-GKNTPKCTCN--KPICTKNGLPI-- | 29 |
| Mobo_B | CGETCAK-GKYTPKCTCN--WPICTKNGKPI-- | 29 |
| mech_2 | CGETCTL-GKNTPKCTCN--WPICTKNGLPT-- | 29 |
| mech_3 | CGETCTL-GKNTPKCTCN--WPICTKNGLPT-- | 29 |
| Mra25 | CGESCTL-GECYTPGCTCS--WPICTKNGSAIL- | 30 |
| cliotide_T19 | CGESCLL-GKYTPGCTCS--RPICTKNGSVIK- | 30 |
| cliotide_T20 | CGESCLL-GKYTPGCTCD--RPICTKNGSAIR- | 30 |
| cT31 | CGESCFA-GKYTPGCTCD--RPICTKNGDPLK- | 30 |
| Cter_2 | CGESCFA-GKYTPGCTCE--YPICTMNGDPLK- | 30 |
| Cter_7 | CGESCFA-GKYTPGCTCE--YPICTMNGDPFK- | 30 |
| vitri_peptide_94b | CGETCTL-GTCYTPGCS--WPICTKNGVAV-- | 29 |
| cliotide_T32 | CGETCFG-GTCYTPGCS--YPICTKNGDLFK- | 30 |
| cliotide_T2 | CGESCQV-GECYTPGCS--WPICTKNGEFLK- | 30 |
| Cter_5 | CGESCQV-GECYTPGCS--YPICTKNGEFLK- | 30 |
| vitri_peptide_29 | CLETCFGG-KCNAHRTCS--QWPLCAKNGVPSSD | 32 |
| cycloviolacin_O27 | CGESCFCG-KCYTPGCS--KYPLCAKNGSIPA- | 31 |
| cycloviolacin_O26 | CGESCFCG-KCYTPGCS--KYPLCAKNGSIPA- | 31 |
| cycloviolacin_O14 | CGESCFCG-KCYTPGCS--KYPLCAKNGSIPA- | 31 |
| Vinc_B | CGESCFCG-KCYTPGCS--KYPLCAKNGSIPA- | 31 |
| Cter_35 | CGETCVLG-TCYTPGCSA-P-VICLNNGAF--- | 28 |
| Panitide_L8 | CGETCVLG-TCYTPGCS--AYPLCVQD----- | 26 |
| Panitide_L2 | CGETCVLG-RCYTPNCR--QYPICVRQLPI--- | 28 |
| Panitide_L1 | CGETCVLG-TCYTPGCR--QYPICVRQLPI--- | 28 |
| Panitide_L6 | CGETCVLG-TCYTPGCS--AYPICVRQLPI--- | 28 |
| Panitide_L5 | CGETCVLG-TCYTPGCS--AYPICARQLPI--- | 28 |
| Glopa_C | CGETCFEGGNCRIPGCTCV--WPFCKNGDIPL- | 31 |
| chassatide_C4 | CGETCFTG-ICFTAGCS--PWPTCTRNGAS--- | 29 |
| chassatide_C1 | CGETCFTG-ICFTAGCS--PWPTCTRNGDA--- | 29 |
| kalata_B12 | CGDTCFVL-GCNDSSCS--YPICVKDGSL--- | 28 |
| vitri_peptide_38 | CYETCFTG-FCFIGGCKD--FPVCKNGDGT--- | 28 |
| vitri_peptide_22a | CGETCFTG-LCYSSGCSI--YPVCKNRNGAPV-- | 29 |
| vodo_M | CGESCFTG-KCYTPGCS--WPVCTRNGAPI-- | 29 |
| vitri_peptide_39 | CGESCFTG-TCYTPGCS--WPVCTRNGAPI-- | 29 |
| vitri_peptide_39_linear | CGESCFTG-TCYTPGCS--WPVCTRNGAPI-- | 29 |
| Mra26 | CGETCVGN-KCYTPGCTCT--WPVCYRNGHPI-- | 29 |
| Globa_E | CGETCVKG-KCNTPGCVCS--WPVCKKNGSAFG- | 30 |
| Mra24 | CGETCLLG-TCYTPGCTCK--RPVCKKNGHPT-- | 29 |
| violacin_A | CGETCFKF-KCYTPRCSCS--YPVCKSAIS---- | 27 |
| cliotide_T15 | CGETCFKT-KCYTKGCS--YPVCKRNLPL-- | 29 |
| Cter_30 | CGETCFKT-KCYTPGCS--YPVCKKNGFPI-- | 29 |
| mela_5 | CGESCFCF-KCYTPGCS--YPICKKDGSAIA- | 30 |
| cycloviolacin_O16 | CGETCFTG-KCYTPGCS--YPICKKINGLPL-- | 29 |
| mela_6 | CGETCFKG-KCYTPGCS--YPICKKDGIPV-- | 29 |
| mela_7 | CGETCFKG-KCYTPGCS--YPICKKNGLPT-- | 29 |
| cycloviolacin_O15 | CGETCFTG-KCYTPGCS--YPICKKNGLPL-- | 29 |
| cliotide_T18 | CGETCFTG-TCYTPGCTCS--YPVCKKNGLPI-- | 29 |
| mela_2 | CGETCFKG-KCYTPGCTCS--YPLCKKDGKPT-- | 29 |
| mela_1 | CGETCFKG-KCYTPGCTCS--YPICKKDGKPT-- | 29 |
| Mden_B | CGETCFTG-KCYTPGCTCS--YPICKKNGLPI-- | 29 |
| mela_3 | CGETCFKG-KCYTPGCTCS--YPICKKDGKPI-- | 29 |
| Mden_C | CGETCFKG-KCYTPGCTCS--YPVCKKNGKPI-- | 29 |
| mela_4 | CGETCFKG-KCYTPGCTCS--YPICKKNGKPI-- | 29 |

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