

Supporting Information

Structure-activity relationship studies of substitutions of cationic amino acid residues on antimicrobial peptides

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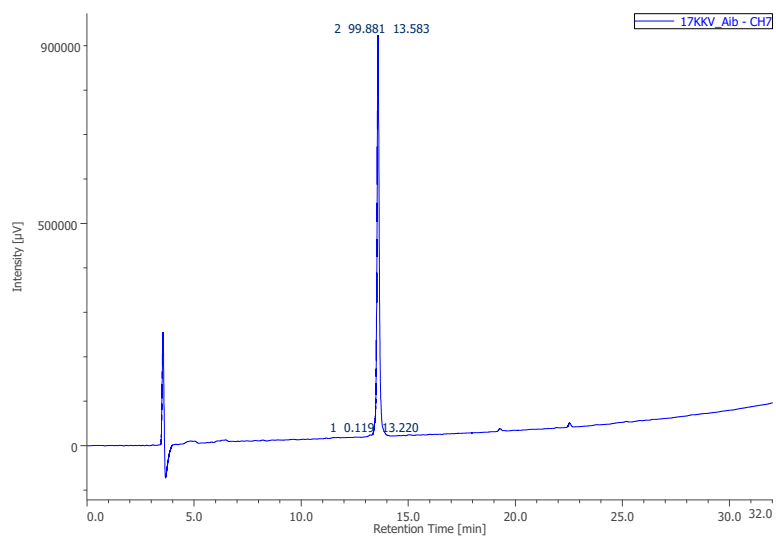
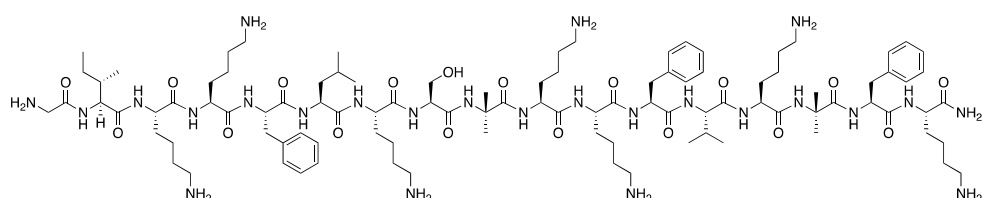
HPLC analytical method

Column	: Preparative column	XBridge BEH C18 OBD Prep Column 5 μ m 19 \times 250 mm (Waters)
	Analysis column	Inertsil WP300 C18 5 μ M 150 \times 3.0 mm (GL Sciences)
Conditions	: solvent A 0.1% TFA/water, solvent B 0.1% TFA/CH ₃ CN	
Flow rate	: preparation	10 mL/min
	Analysis	1.0 mL/min
Gradient	: 10–90% gradient of solvent B	30 min

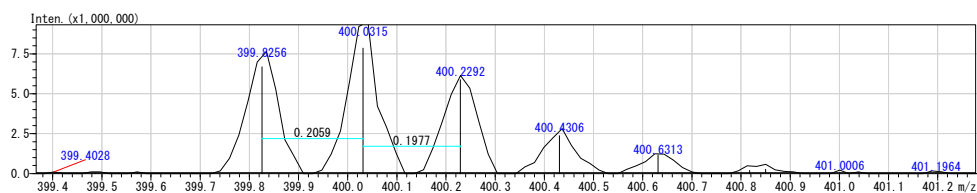
Pep 1

H-Gly-Lys-Lys-Phe-Leu-Lys-Ser-Aib-Lys-Lys-Phe-Val-Lys-Aib-Phe-Lys-NH₂

Purity : 99.9%



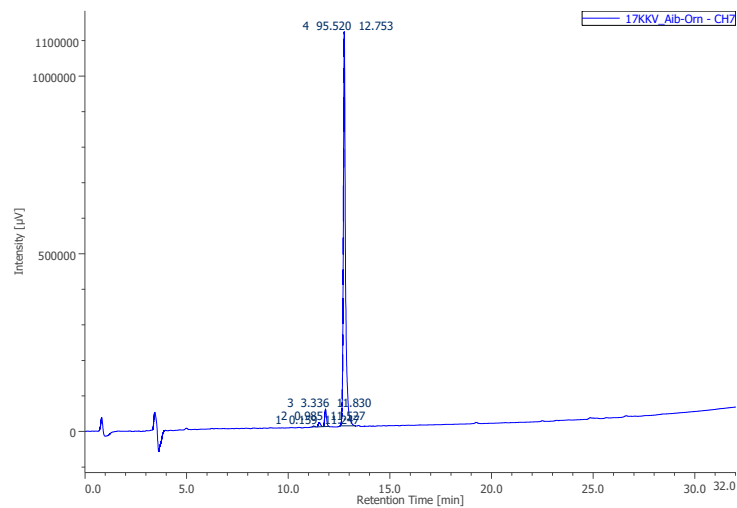
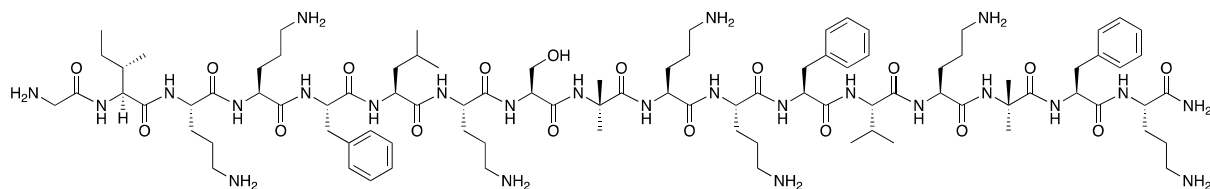
LC-MS (ESI⁺) calcd for C₉₉H₁₆₇N₂₅O₁₈[M+5H]⁵⁺ : 399.85842, found: 399.8256.



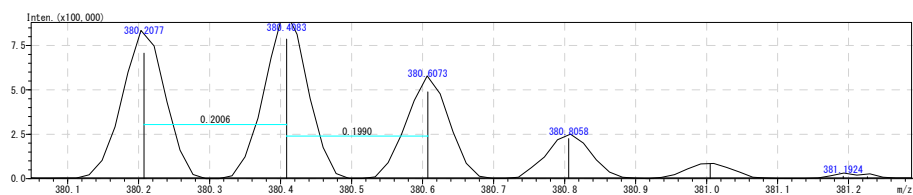
Pep 2

H-Gly-Orn-Orn-Phe-Leu-Orn-Ser-Aib-Orn-Orn-Phe-Val-Orn-Aib-Phe-Orn-NH₂

Purity : 95.5%



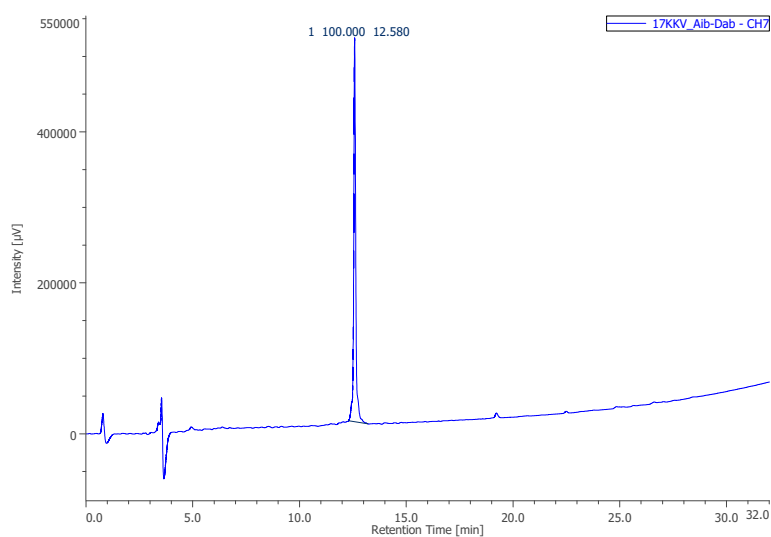
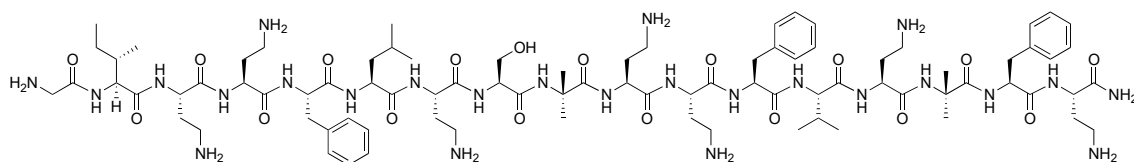
LC-MS (ESI⁺) calcd for C₉₂H₁₅₃N₂₅O₁₈[M+5H]⁵⁺ : 380.2365, found: 380.2077.



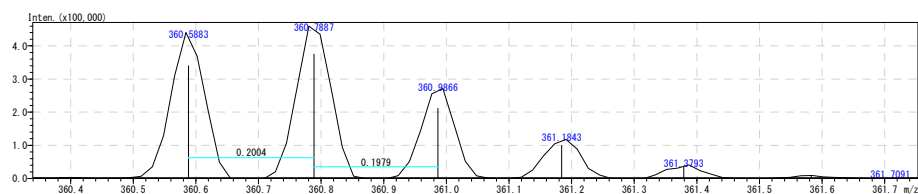
Pep 3

H-Gly-Dab-Dab-Phe-Leu-Dab-Ser-Aib-Dab-Dab-Phe-Val-Dab-Aib-Phe-Dab-NH₂

Purity : 100.0%



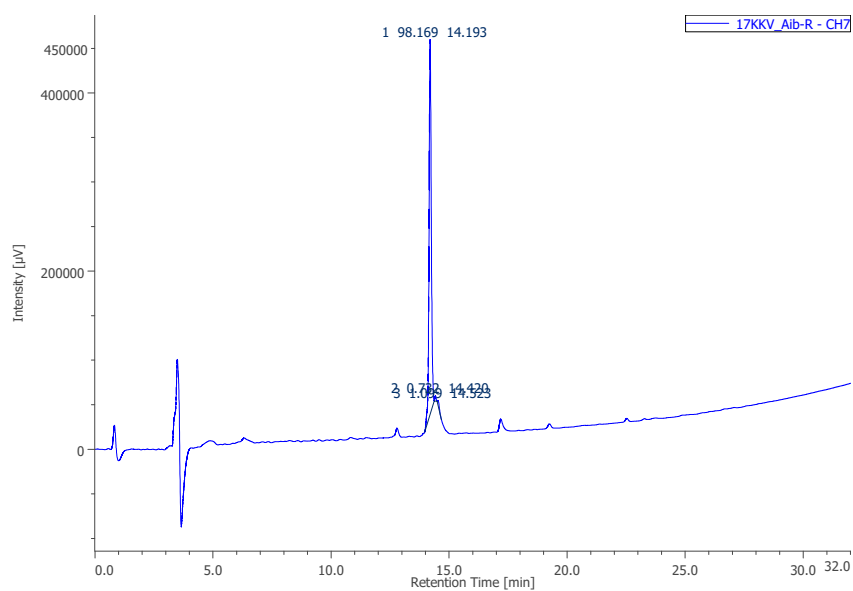
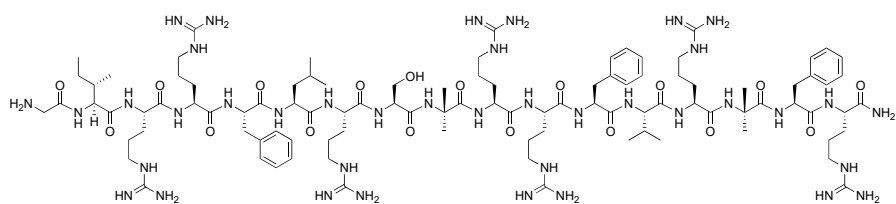
LC-MS (ESI⁺) calcd for C₈₅H₁₃₉N₂₅O₁₈[M+5H]⁵⁺ : 360.6146, found: 360.5883.



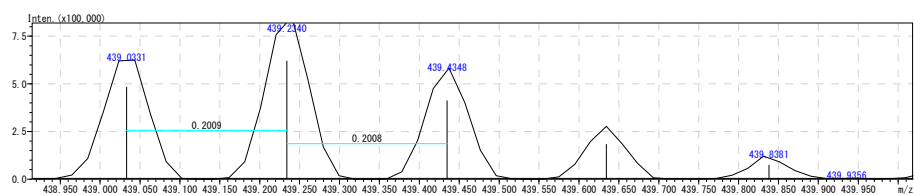
Pep 4

H-Gly-Arg-Arg-Phe-Leu-Arg-Ser-Aib-Arg-Arg-Phe-Val-Arg-Aib-Phe-Arg-NH₂

Purity : 98.2%



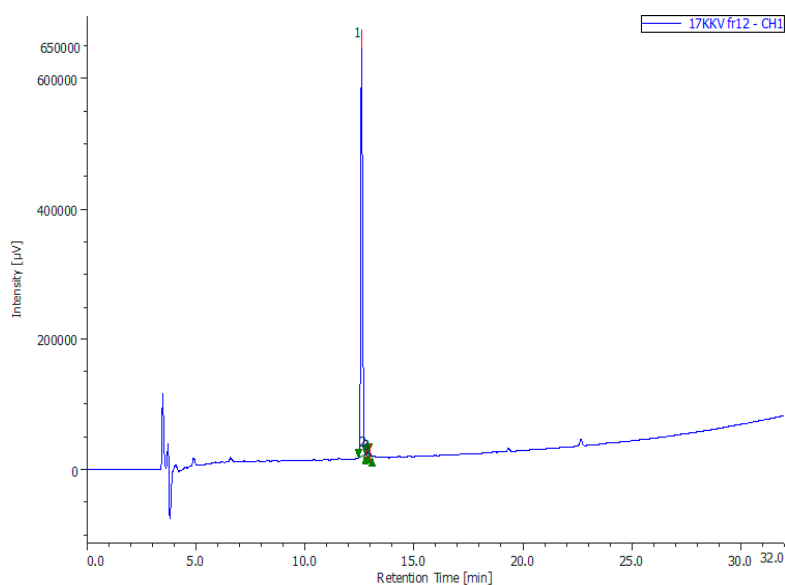
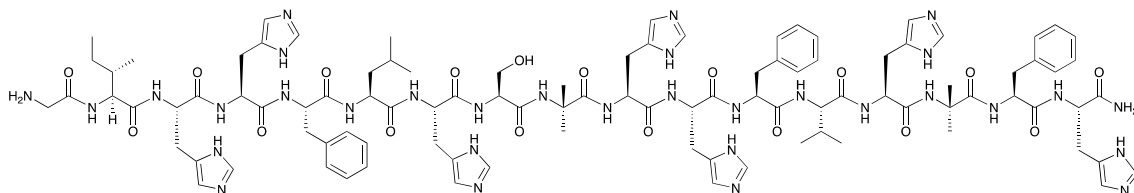
LC-MS (ESI⁺) calcd for C₉₉H₁₆₇N₃₉O₁₈[M+5H]⁵⁺ : 439.06702, found: 439.0331.



Pep 5

H-Gly-His-His-Phe-Leu-His-Ser-Aib-His-His-Phe-Val-His-Aib-Phe-His-NH₂

Purity : 78.2%



LC-MS (ESI⁺) calcd for C₉₉H₁₃₂N₃₂O₁₈[M+5H]⁵⁺ : 412.40794, found: 412.3769.

