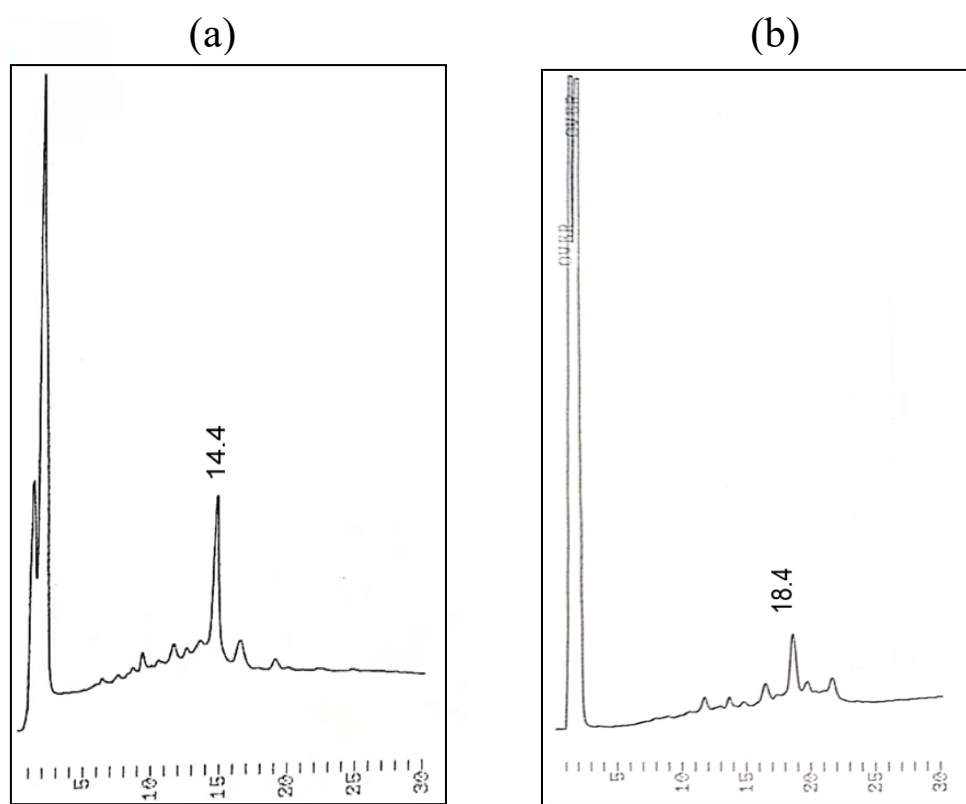
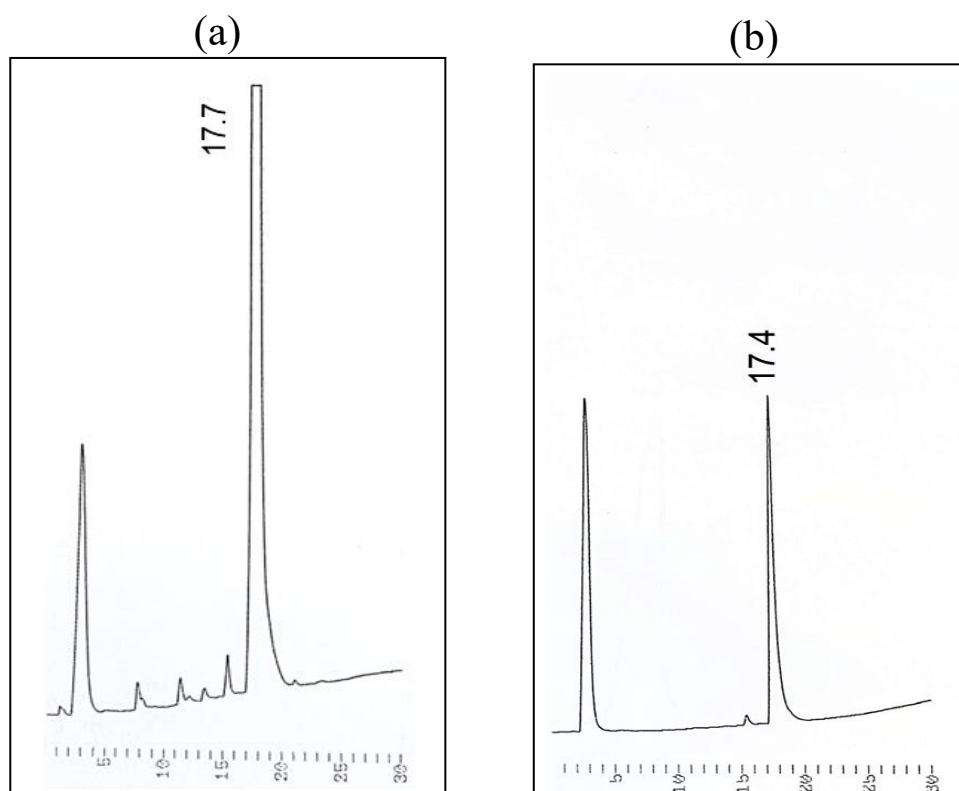


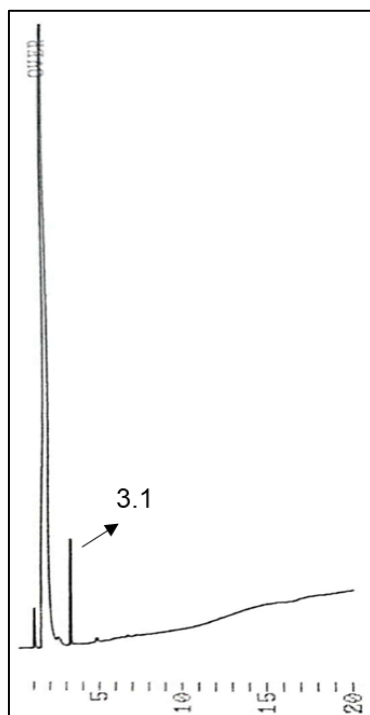
## Supporting information



**Figure S1 HPLC chart of the protected sidechain [LW2] and [CW2]. Column: Chromolith® performance, RP-18e (4.6 × 100 mm), Flow Rate: 1.300 mL/min, Eluent: 50– 100 % B in 30 min, Solvent A: 0.1% TFA in H<sub>2</sub>O Solvent B: 0.1% TFA in CH<sub>3</sub>CN, Detect: UV 220 nm. (a) protected sidechain linear [LW2] a retention time, RT= 14.4 min; (b) protected sidechain cyclic [CW2] a retention time, RT=18.4 min.**

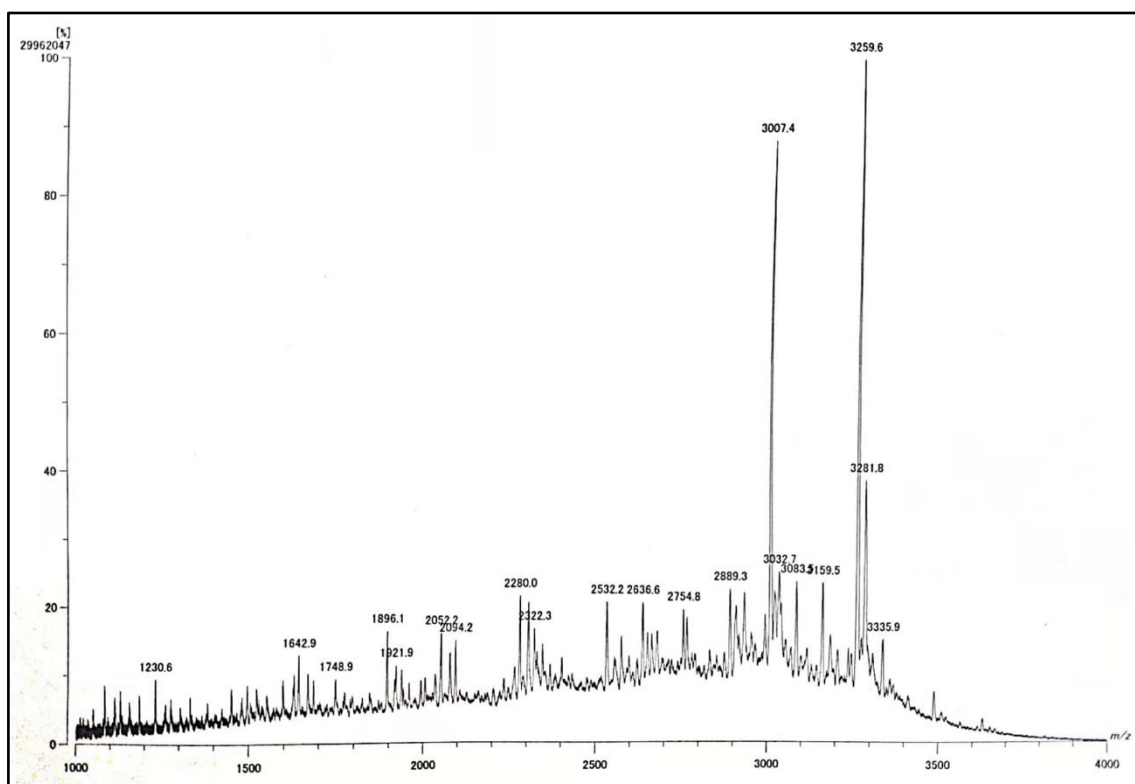


**Figure S2 HPLC trace analysis of the deprotected sidechain [LW2] and [CW2]. Column: Chromolith® performance, RP-18e (4.6 × 100 mm), Flow Rate: 1.300 mL/min, Eluent: 0 – 100 % B in 30 min, Solvent A: 0.1% TFA in H<sub>2</sub>O Solvent B: 0.1% TFA in CH<sub>3</sub>CN, Detect: UV 220 nm. (a) HPLC trace analysis of [LW2] a retention time, RT= 17.7min; (b) HPLC trace analysis of [CW2] a retention time, RT= 17.4min.**

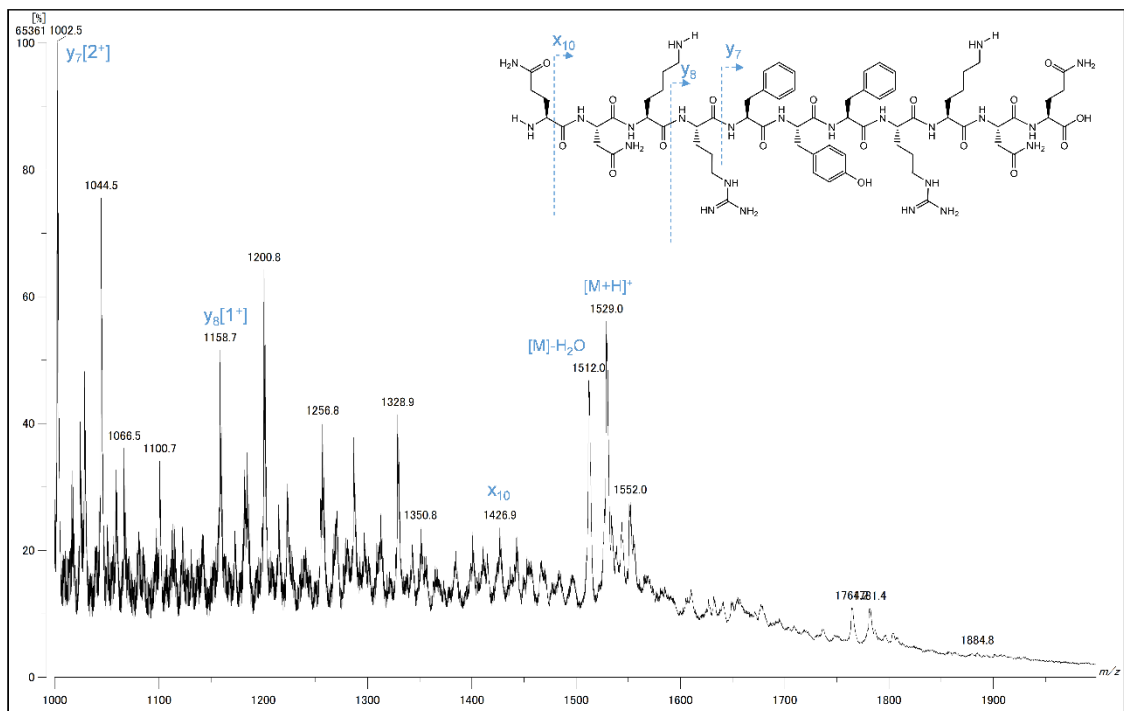


**Figure S3 HPLC trace analysis of the pure cyclic deprotected CEG using solvent B gradient of 0-100%. RT= 3.1 min. Column: Chromolith performance, RP-18e (4.6 × 100 mm), Flow Rate: 2.000 mL/min, Eluent: 0 – 100 % B in 15 min, Solvent A: 0.1% TFA in H<sub>2</sub>O Solvent B: 0.1% TFA in CH<sub>3</sub>CN, Detect: UV 220 nm**

**Figure S4 Mass spectra of thesis peptides. Identification of the synthesized compound was done by Fast Atom Bombardment (FAB) + mass spectroscopy (a, b, c) and Electrospray Ionization Time-of-Flight (ESI-TOF) mass spectrometry (d) for the determination of the molecular weight of the compound.**



(a) FAB<sup>+</sup> Mass spectrum of protected LW2 [M+3H]<sup>+</sup>

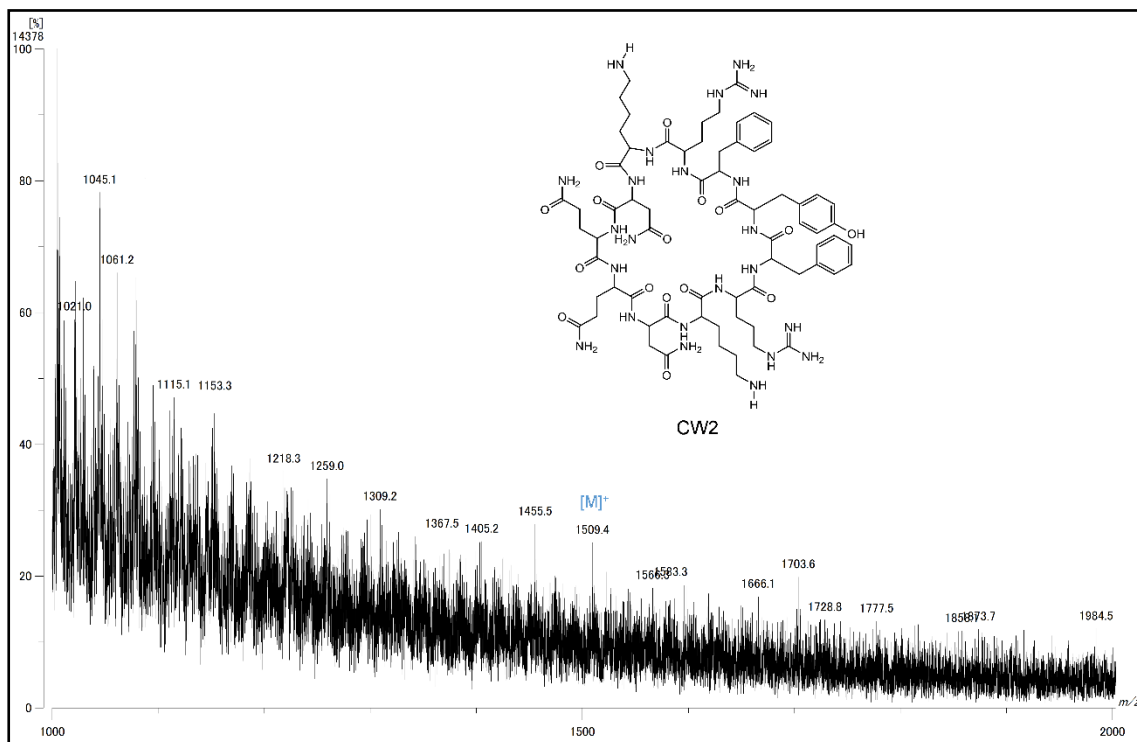


(i)

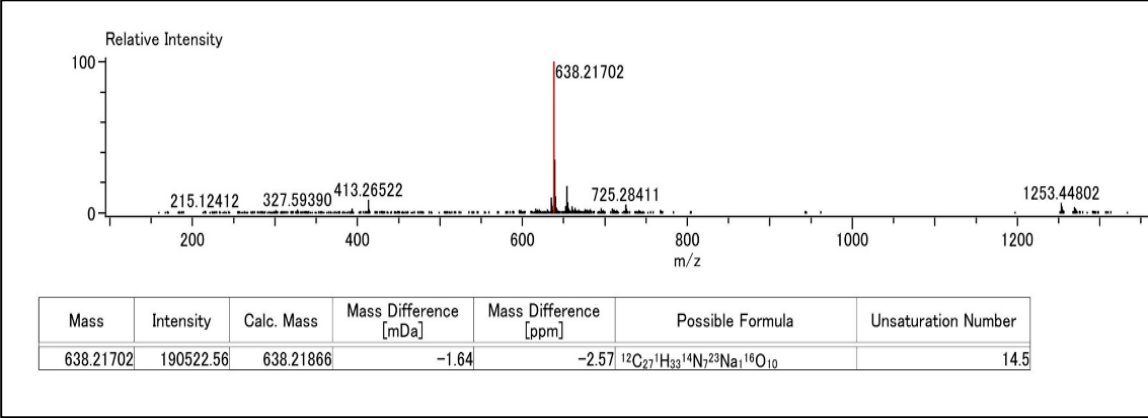
Inlet: Direct		Ion Mode: FAB+	
RT: 3.26 min		Scan#: 27	
Elements: 12C 69/0, 13C 0/0, H 106/106, N 23/23, O 17/17			
Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50			
Unsaturation (U.S.): -0.5 - 50.0			
Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1 1528.8122	100.00	-1.0 / -1.5	28.5 12C69 H106 N23 O17

(ii)

(b) FAB<sup>+</sup> Mass spectrum of LW2 [M+H]<sup>+</sup>, (i) FAB<sup>+</sup> Mass fragmentation pattern of LW2, (ii) FAB<sup>+</sup> Mass data of LW2.



(c)FAB<sup>+</sup> Mass spectrum of CW2 [M]<sup>+</sup>



(d)ESI-TOF Mass spectrum of CEG  $[M+Na]^+$

**Table S1 The score of molecule docking between BSA/CW2 and FA.**

Name	S-Score	Rmsd-Refine	E-Refine
BSA	-8.3599	1.6010	-24.5977
CW2	-4.2035	1.9949	-16.4607



**Table S2 Yield and purity for synthesized compounds.**

Peptide Name	Yield (%)	Chromatographic Purity (%)
LW2	97.02	97.4
CW2	50.24	98.3
CEG	45.86	>99.0