Supporting information

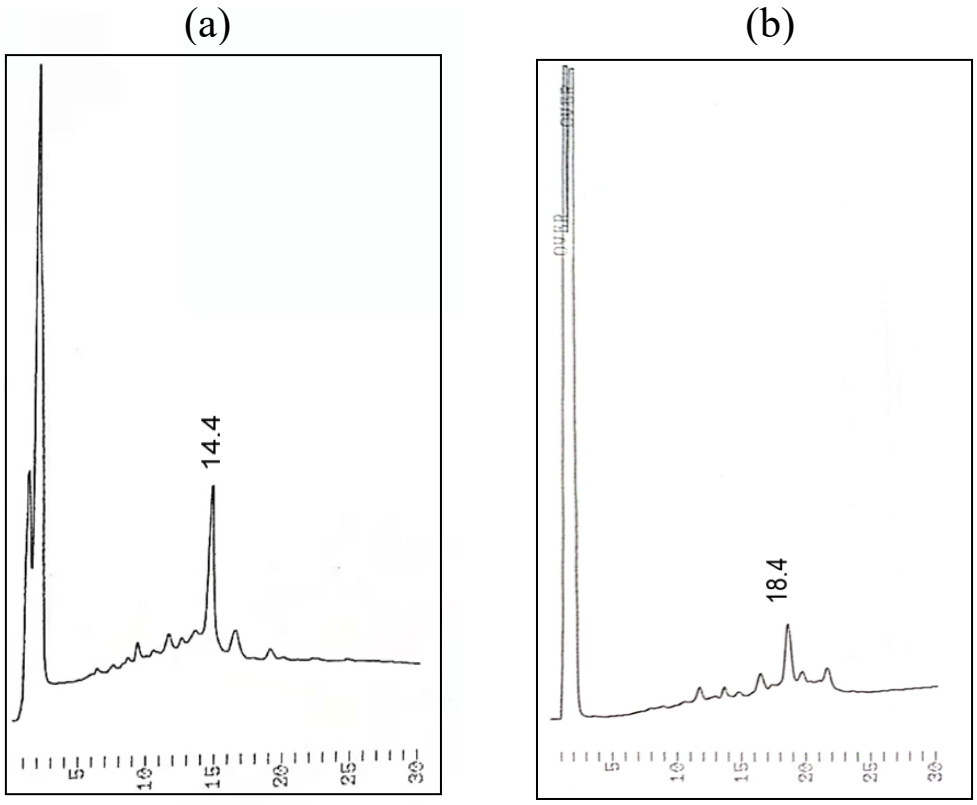


Figure S1 HPLC chart of the protected sidechain [LW2] and [CW2]. Column: Chromolith® performance, RP-18e (4.6 × 100 mm), Flow Rate: 1.300 mL/min, Eluent: 50– 100 % B in 30 min, Solvent A: 0.1% TFA in H_2O Solvent B: 0.1% TFA in CH_3CN, Detect: UV 220 nm. (a) protected sidechain linear [LW2] a retention time, RT= 14.4 min; (b) protected sidechain cyclic [CW2] a retention time, RT=18.4 min.

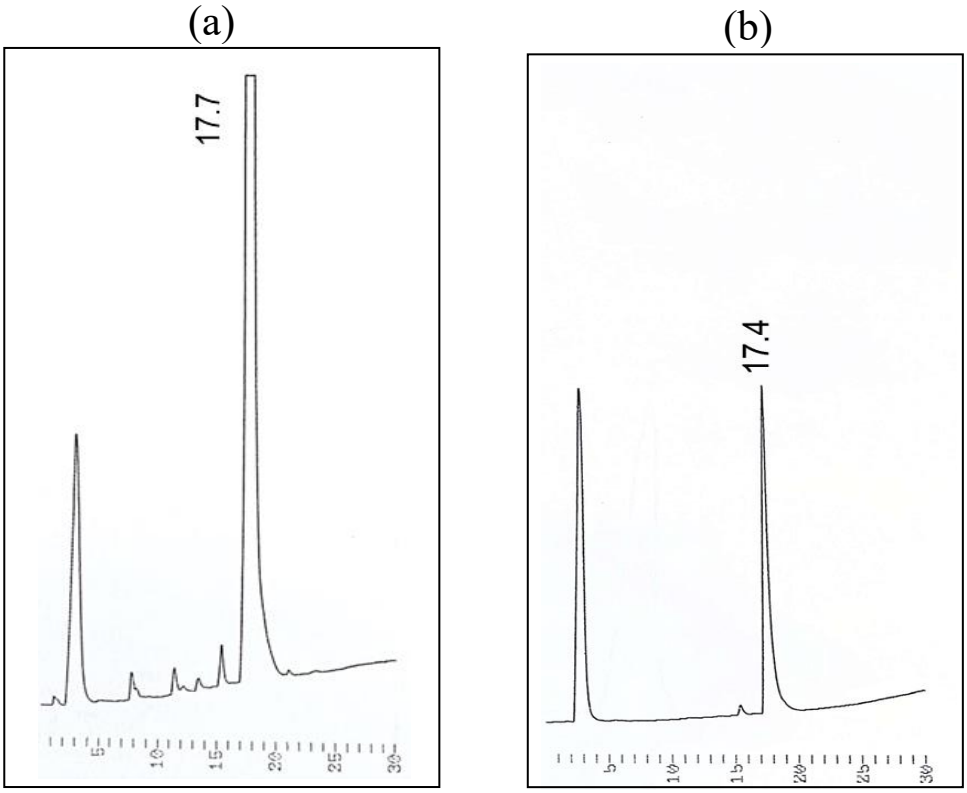


Figure S2 HPLC trace analysis of the deprotected sidechain [LW2] and [CW2]. Column: Chromolith® performance, RP-18e (4.6 × 100 mm), Flow Rate: 1.300 mL/min, Eluent: 0 – 100 % B in 30 min, Solvent A: 0.1% TFA in H_2O Solvent B: 0.1% TFA in CH_3CN, Detect: UV 220 nm. (a) HPLC trace analysis of [LW2] a retention time, RT= 17.7min; (b) HPLC trace analysis of [CW2] a retention time, RT= 17.4min.

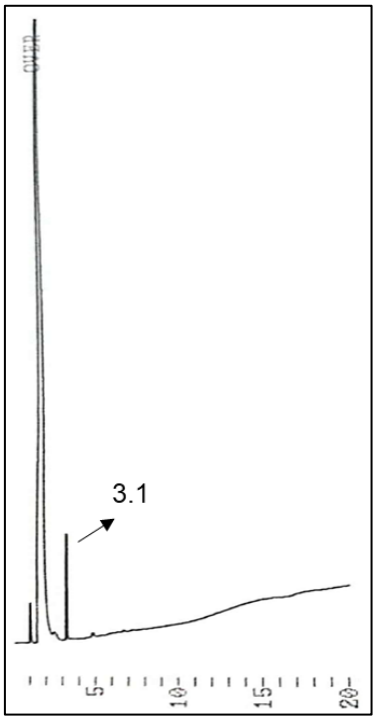
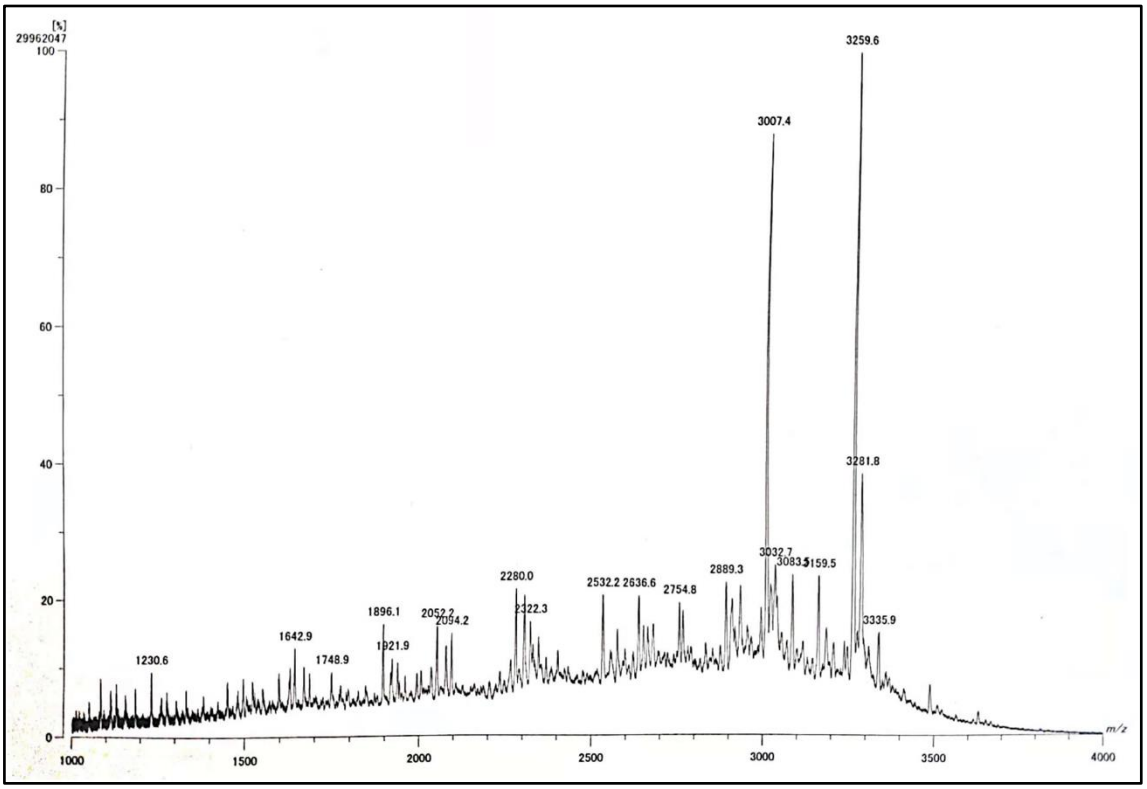
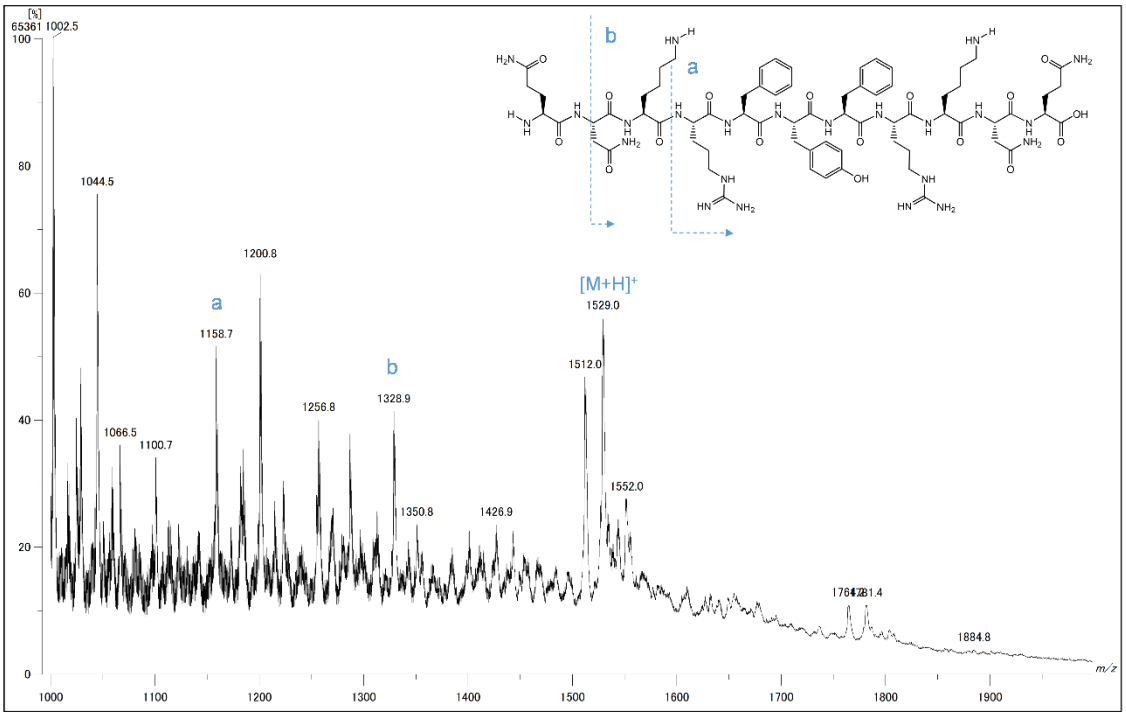


Figure S3 HPLC trace analysis of the pure cyclic deprotected CEG using solvent B gradient of 0-100%. RT= 3.1 min. Column: Chromolith performance, RP-18e (4.6 × 100 mm), Flow Rate: 2.000 mL/min, Eluent: 0 – 100 % B in 15 min, Solvent A: 0.1% TFA in H_2O Solvent B: 0.1% TFA in CH_3CN, Detect: UV 220 nm

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



(a) FAB^{+} Mass spectrum of protected LW2$[M]^{+}$



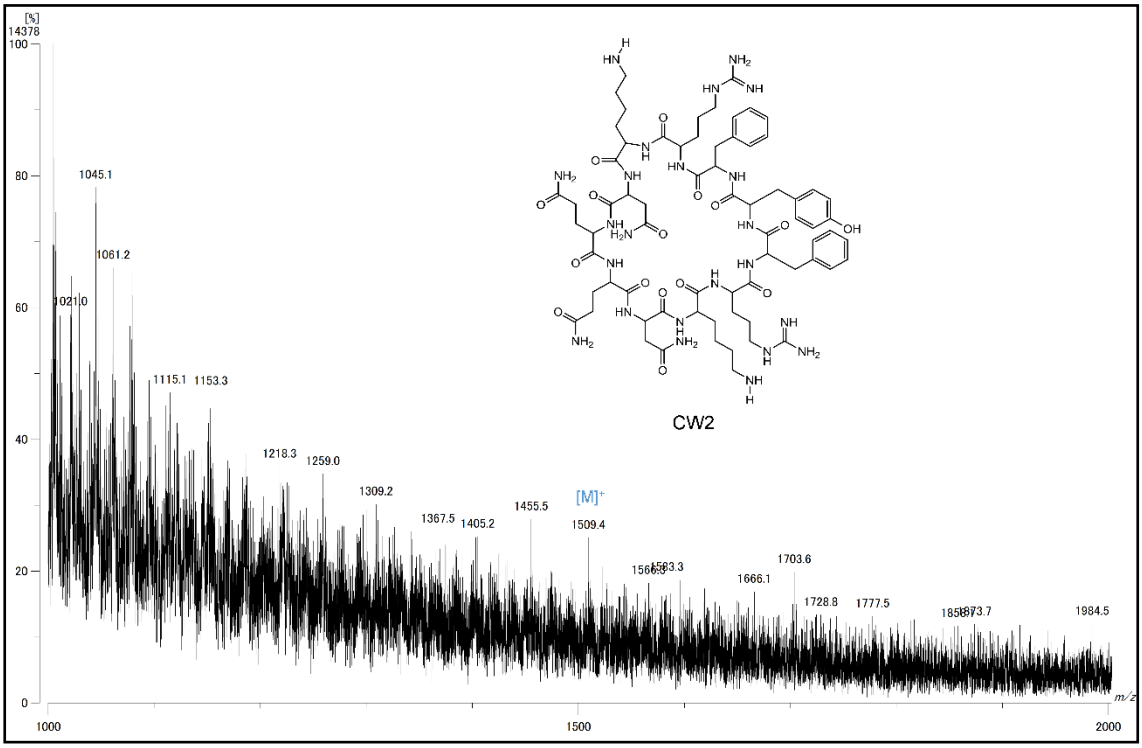
(i)

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

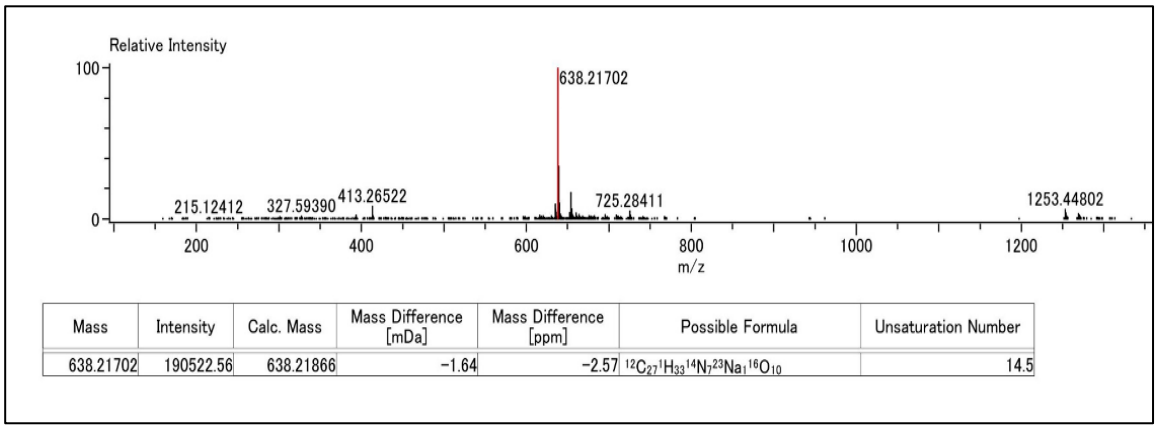
	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	1528.8122	100.00	-1.0 / -1.5	28.5	12C69 H106 N23 O17

(ii)

(b) FAB^+ Mass spectrum of LW2$[M]^+$, (i) FAB^+ Mass fragementation pattern of LW2, (ii) FAB^+ Mass data of LW2.



(c)FAB^{+} Mass spectrum of CW2[M]$^{+}$



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula	Unsaturation Number
638.21702	190522.56	638.21866	-1.64	-2.57	$^{12}C_{27}{}^{1}H_{33}{}^{14}N_{7}{}^{23}Na_{1}{}^{16}O_{10}$	14.5

(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