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Supporting Information

Synthetic Mucin-Like Glycopeptides as Versatile Tools to Measure Effects of Glycan Structure/Density/Position on the Interaction with Adhesion/Growth-Regulatory Galectins in Arrays

Gerard Artigas,^[a] Hiroshi Hinou,^{*,[a, b]} Fayna Garcia-Martin,^[a] Hans-Joachim Gabius,^{*,[c]} and Shin-Ichiro Nishimura^{*,[a, b]}

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Table S1. Sequences of the MUC1-derived (glyco)peptide and glyco amino acid used in this work.

1	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGSTAPPAHGVT-NH ₂
2	5-oxo-hexanoyl-PEG-GVT(GalNAc α 1 $\rightarrow$)SAPDTRPAPGSTAPPAHGVT-NH ₂
3	5-oxo-hexanoyl-PEG-GVTS(GalNAc α 1 $\rightarrow$)APDTRPAPGSTAPPAHGVT-NH ₂
4	5-oxo-hexanoyl-PEG-GVTSAPDT(GalNAc α 1 $\rightarrow$)RPAPGSTAPPAHGVT-NH ₂
5	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGS(GalNAc α 1 $\rightarrow$)TAPPAHGVT-NH ₂
6	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGST(GalNAc α 1 $\rightarrow$)APPAHGVT-NH ₂
7	5-oxo-hexanoyl-PEG-GVT(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)SAPDTRPAPGSTAPPAHGVT-NH ₂
8	5-oxo-hexanoyl-PEG-GVTS(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)APDTRPAPGSTAPPAHGVT-NH ₂
9	5-oxo-hexanoyl-PEG-GVTSAPDT(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)RPAPGSTAPPAHGVT-NH ₂
10	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGS(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)TAPPAHGVT-NH ₂
11	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGST(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)APPAHGVT-NH ₂
12	5-oxo-hexanoyl-PEG-GVT(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)SAPDTRPAPGSTAPPAHGVT-NH ₂
13	5-oxo-hexanoyl-PEG-GVTS(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)APDTRPAPGSTAPPAHGVT-NH ₂
14	5-oxo-hexanoyl-PEG-GVTSAPDT(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)RPAPGSTAPPAHGVT-NH ₂

15	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGS(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)TAPPAHGVN-NH ₂
16	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGST(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)APPAHGVN-NH ₂
17	5-oxo-hexanoyl-PEG-GVT(GalNAc α 1 $\rightarrow$)S(GalNAc α 1 $\rightarrow$)APDTRPAPGSTAPPAHGVN-NH ₂
18	5-oxo-hexanoyl-PEG-GVT(GalNAc α 1 $\rightarrow$)SAPDT(GalNAc α 1 $\rightarrow$)RPAPGSTAPPAHGVN-NH ₂
19	5-oxo-hexanoyl-PEG-GVT(GalNAc α 1 $\rightarrow$)SAPDTRPAPGST(GalNAc α 1 $\rightarrow$)APPAHGVN-NH ₂
20	5-oxo-hexanoyl-PEG-GVTS(GalNAc α 1 $\rightarrow$)APDT(GalNAc α 1 $\rightarrow$)RPAPGSTAPPAHGVN-NH ₂
21	5-oxo-hexanoyl-PEG-GVTS(GalNAc α 1 $\rightarrow$)APDTRPAPGST(GalNAc α 1 $\rightarrow$)APPAHGVN-NH ₂
22	5-oxo-hexanoyl-PEG-GVTSAPDT(GalNAc α 1 $\rightarrow$)RPAPGST(GalNAc α 1 $\rightarrow$)APPAHGVN-NH ₂
23	5-oxo-hexanoyl-PEG-GVTSAPDTRPAPGS(GalNAc α 1 $\rightarrow$)T(GalNAc α 1 $\rightarrow$)APPAHGVN-NH ₂
24	5-oxo-hexanoyl-PEG-GVTS(GalNAc α 1 $\rightarrow$)APDT(GalNAc α 1 $\rightarrow$)RPAPGS(GalNAc α 1 $\rightarrow$)TAPPAHGVN-NH ₂
25	5-oxo-hexanoyl-PEG-GVTS(GalNAc α 1 $\rightarrow$)APDT(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)RPAPGS(GalNAc α 1 $\rightarrow$)TAPPAHGVN-NH ₂
26	5-oxo-hexanoyl-PEG-T(GalNAc α 1 $\rightarrow$)-NH ₂
27	5-oxo-hexanoyl-PEG-S(GalNAc α 1 $\rightarrow$)-NH ₂
28	5-oxo-hexanoyl-PEG-T(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)-NH ₂
29	5-oxo-hexanoyl-PEG-S(Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)-NH ₂
30	5-oxo-hexanoyl-PEG-T(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)-NH ₂

31	5-oxo-hexanoyl-PEG-S(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)]GalNAc α 1 $\rightarrow$)-NH ₂
32	5-oxo-hexanoyl-PPAHGVTSAPDTRPAPGSTA-NH ₂
33	5-oxo-hexanoyl-PPAHGVTSAPDT(Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)RPAPGSTA-NH ₂
34	5-oxo-hexanoyl-PPAHGVT(GalNAc α 1 $\rightarrow$)S(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)[Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)]GalNAc α $\rightarrow$)APDT(Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)RPAPGS(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)[Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)]GalNAc α $\rightarrow$)T(GalNAc α 1 $\rightarrow$)A-NH ₂
35	5-oxo-hexanoyl-PPAHGVTS(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)[Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)]GalNAc α $\rightarrow$)APDT(Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)GalNAc α 1 $\rightarrow$)RPAPGS(Gal β (1 $\rightarrow$ 3)[GlcNAc β (1 $\rightarrow$ 6)[Neu5Ac α (2 $\rightarrow$ 3)Gal β (1 $\rightarrow$ 3)]GalNAc α $\rightarrow$)TA-NH ₂

Synthesis and characterization of compounds **1**, **3**, **4**, **20**, **24**, and **25**;^[1] **2**, **5**, and **6**;^[2] **32**-**35**.^[3]

[1] F. Garcia-Martin, T. Matsushita, H. Hinou and S.-I. Nishimura, *Chemistry-a European Journal* **2014**, 20, 15891-15902.

[2] H. Coelho, T. Matsushita, G. Artigas, H. Hinou, F. J. Canada, R. Lo-Man, C. Leclerc, E. J. Cabrita, J. Jimenez-Barbero, S.-I. Nishimura, F. Garcia-Martin and F. Marcelo, *Journal of the American Chemical Society* **2015**, 137, 12438-12441.

[3] S. Rangappa, G. Artigas, R. Miyoshi, Y. Yokoi, S. Hayakawa, F. Garcia-Martin, H. Hinou and S.-I. Nishimura, *Medchemcomm* **2016**, 7, 1102-1122.

Table S2. Grades of fluorescence intensity* for compound 1~35 after treatment with galectins and galectin related proteins (90 µg/mL) tested in this study.

#	Chimera-type		tandem-repeat-type				Proto-type			GRP
	Gal-3	Gal-3tr	Gal-4	Gal-4N	Gal-4C	Gal-8	Gal-1	GRIFIN	Gal-5	
1				+						+
2										
3										
4										+
5					+			+		+
6				+	+					
7			+	+	+					
8			++++	+	+	+++		+++		
9			+++	+	+			+		+
10			++++++	++	++	++++++		+++	+	
11			++++++	+++	++	+++++		+	+	
12				+		+				
13				+						
14										
15			+++	++	+	++		+		
16				+		+				
17				+						
18										
19				+	+					
20										
21				+++	+					
22					+					
23				+	+					
24										
25			+	+	+					
26										
27										
28			+++++		+					
29			++++	+	+	+		+		
30			+							
31			+++++		+	+		++		
32										
33			+	+		+++++				+
34	+			++		++++++				
35	+++			+++		++++++				

*Each grade are assigned from average value of relative fluorescence intensity (RFU) of the four 100 mM spots for each compound on microarray; + 0.50-1.49 ($\times 10^{-7}$), ++ 1.50-2.49 ($\times 10^{-7}$), +++ 2.50-3.49 ($\times 10^{-7}$), ++++ 3.50-4.49 ($\times 10^{-7}$), +++++ 4.50-5.49 ($\times 10^{-7}$), ++++++ > 5.50 ($\times 10^{-7}$).

Characterization of peptides/glycopeptides

General procedure for the UPLC analyses of purified glycopeptides

All measurements were performed using a Waters Acquity Ultra Performance LC system equipped with binary solvent delivery pump, an auto sampler and a UV detector. Synthetic peptides and glycopeptides purified by semi-preparative RP-HPLC were analyzed on an Acquity UPLC BEN[®]C18 column (1.7 μ m, 2.1 $\times$ 50 mm, Waters) at a flow rate of 0.2 mL/min. All separations were monitored at 220 nm. Column temperature was 40 °C. A gradient of water with 0.1% TFA (eluent A) and acetonitrile with 0.1% TFA (eluent B) were used for the mobile phase. The ratio of B was linearly increased from 2 to 30% in 12.6 min, then the column was washed with 90% B and equilibrium with 2% B. MALDI-TOF MS data were recorded by Ultraflex I (Bruker Daltonics) using DHB [10 mg in 1 mL of 50% acetonitrile with 0.1% TFA (1:1 mixture of eluent A and B for RP-HPLC)].

Compound 7. Analytical UPLC: t_R = 7.269 min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2765.3403, found (m/z) 2765.1069. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 1.9, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.4.

Compound 8. Analytical UPLC: t_R = 7.624 min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2765.3403, found (m/z) 2765.0138. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.3.

Compound 9. Analytical UPLC: t_R = 7.504 min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2765.3403, found (m/z) 2764.9759. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.0, Val (2) 1.9, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.4.

Compound 10. Analytical UPLC: t_R = 7.616 min, peak area ratio 100%. MALDI-TOF-HRMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2765.3403, found (m/z) 2765.1383. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 1.9, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.4.

Compound 11. Analytical UPLC: t_R = 7.538 min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2765.3403, found (m/z) 2765.2273. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 1.9, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.4.

Compound 12. Analytical UPLC: t_R = 7.088 min, peak area ratio 98.4%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2968.4197, found (m/z) 2967.9384. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.2.

Compound 13. Analytical UPLC: t_R = 7.431 min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2968.4197, found (m/z) 2968.4793. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.2, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.2.

Compound 14. Analytical UPLC: t_R = 7.229 min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2968.4197, found (m/z) 2967.9460. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.1, Ala (4) 4.1, Val (2) 2.0, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.2.

Compound 15. Analytical UPLC: t_R = 7.441 min, peak area ratio 98.5%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2968.4197, found (m/z) 2968.0959. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2)

1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.2.

Compound 16. Analytical UPLC: $t_R = 7.341$ min, peak area ratio 100%. MALDI-TOFMS: $C_{117}H_{189}N_{31}O_{46}$ $[M+H]^+$ calcd (m/z) 2968.4197, found (m/z) 2968.3110. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.3.

Compound 17. Analytical UPLC: $t_R = 7.305$ min, peak area ratio 100%. MALDI-TOFMS: $C_{119}H_{192}N_{32}O_{46}$ $[M+H]^+$ calcd (m/z) 2806.3668, found (m/z) 2806.0823 Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.3.

Compound 18. Analytical UPLC: $t_R = 7.363$ min, peak area ratio 100%. MALDI-TOFMS: $C_{119}H_{192}N_{32}O_{46}$ $[M+H]^+$ calcd (m/z) 2806.3668, found (m/z) 2805.9321. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.4.

Compound 19. Analytical UPLC: $t_R = 7.355$ min, peak area ratio 100%. MALDI-TOFMS: $C_{119}H_{192}N_{32}O_{46}$ $[M+H]^+$ calcd (m/z) 2806.3668, found (m/z) 2806.1062. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 1.9, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.4.

Compound 21. Analytical UPLC: $t_R = 7.591$ min, peak area ratio 100%. MALDI-TOFMS: $C_{119}H_{192}N_{32}O_{46}$ $[M+H]^+$ calcd (m/z) 2806.3668, found (m/z) 2806.1647. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.4.

Compound 22. Analytical UPLC: $t_R = 7.718$ min, peak area ratio 99.6%. MALDI-TOFMS: $C_{119}H_{192}N_{32}O_{46}$ $[M+H]^+$ calcd (m/z) 2806.3668, found (m/z) 2806.4264. Amino

acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.8, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 1.9, His (1) 1.1, Arg (1) 1.0, Pro (5) 5.4.

Compound 23. Analytical UPLC: $t_R = 7.484$ min, peak area ratio 100%. MALDI-TOFMS: $C_{119}H_{192}N_{32}O_{46}$ $[M+H]^+$ calcd (m/z) 2806.3668, found (m/z) 2806.0616. Amino acid ratios (numbers in parenthesis are theoretical values): Asp (1) 1.0, Thr (4) 3.7, Ser (2) 1.8, Gly (3) 3.0, Ala (4) 4.1, Val (2) 2.0, His (1) 1.0, Arg (1) 1.0, Pro (5) 5.4.

Compound 26. Analytical UPLC: $t_R = 4.014$ min, peak area ratio 100%. MALDI-TOFMS: $C_{24}H_{42}N_4O_{12}$ $[M+H]^+$ calcd (m/z) 578.2799, $[M+Na]^+$ found (m/z) 601.8256. Amino acid ratios (numbers in parenthesis are theoretical values): Thr (1) 1.0.

Compound 27. Analytical UPLC: $t_R = 3.654$ min, peak area ratio 100%. MALDI-TOFMS: $C_{23}H_{40}N_4O_{12}$ $[M+H]^+$ calcd (m/z) 564.2643, $[M+Na]^+$ found (m/z) 587.7875. Amino acid ratios (numbers in parenthesis are theoretical values): Ser (1) 1.0.

Compound 28. Analytical UPLC: $t_R = 3.748$ min, peak area ratio 100%. MALDI-TOFMS: $C_{30}H_{52}N_4O_{17}$ $[M+H]^+$ calcd (m/z) 740.3327, $[M+Na]^+$ found (m/z) 763.1747. Amino acid ratios (numbers in parenthesis are theoretical values): Thr (1) 1.0.

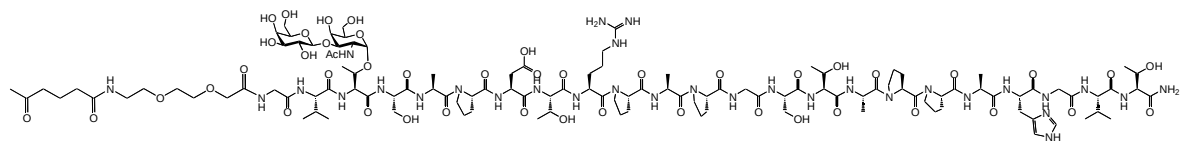
Compound 29. Analytical UPLC: $t_R = 3.$ min, peak area ratio 100%. MALDI-TOFMS: $C_{29}H_{50}N_4O_{17}$ $[M+H]^+$ calcd (m/z) 726.3171, $[M+Na]^+$ found (m/z) 749.1237. Amino acid ratios (numbers in parenthesis are theoretical values): Ser (1) 1.0.

Compound 30. Analytical UPLC: $t_R = 3.382$ min, peak area ratio 95.5%. MALDI-TOFMS: $C_{38}H_{65}N_5O_{22}$ $[M+H]^+$ calcd (m/z) 943.4121, $[M+Na]^+$ found (m/z) 966.5864. Amino acid ratios (numbers in parenthesis are theoretical values): Thr (1) 1.0.

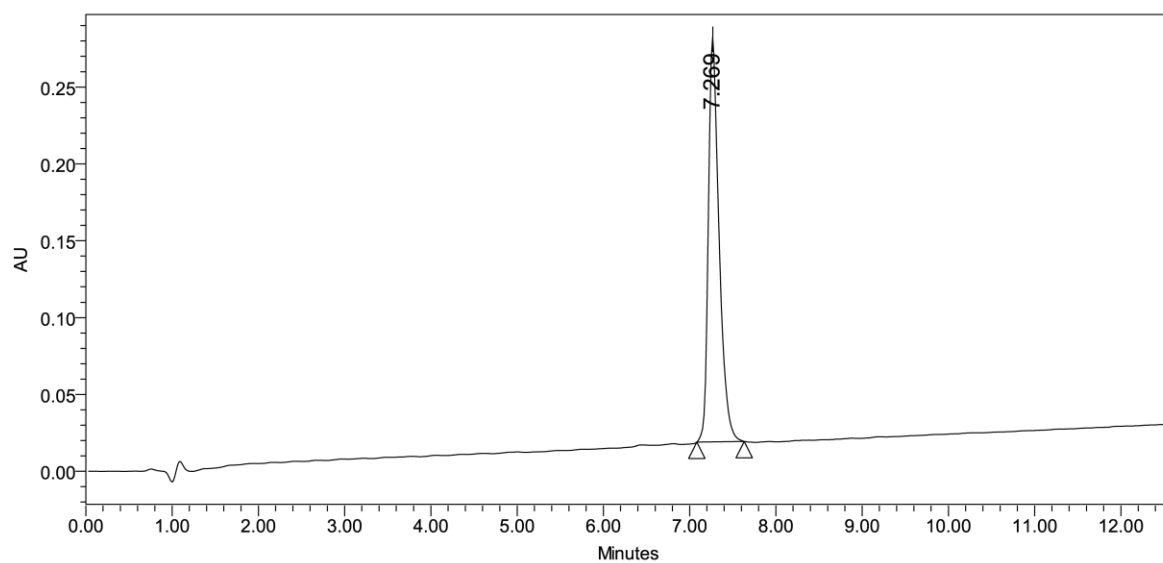
Compound 31. Analytical UPLC: $t_R = 3.464$ min, peak area ratio 100%. MALDI-TOFMS:

$C_{37}H_{63}N_5O_{22}$ $[M+H]^+$ calcd (m/z) 929.3965, $[M+Na]^+$ found (m/z) 952.2437. Amino acid ratios (numbers in parenthesis are theoretical values): Ser (1) 1.0.

Figure S1. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 7**.



(a) UPLC profile



(b) MALDI-TOF MS

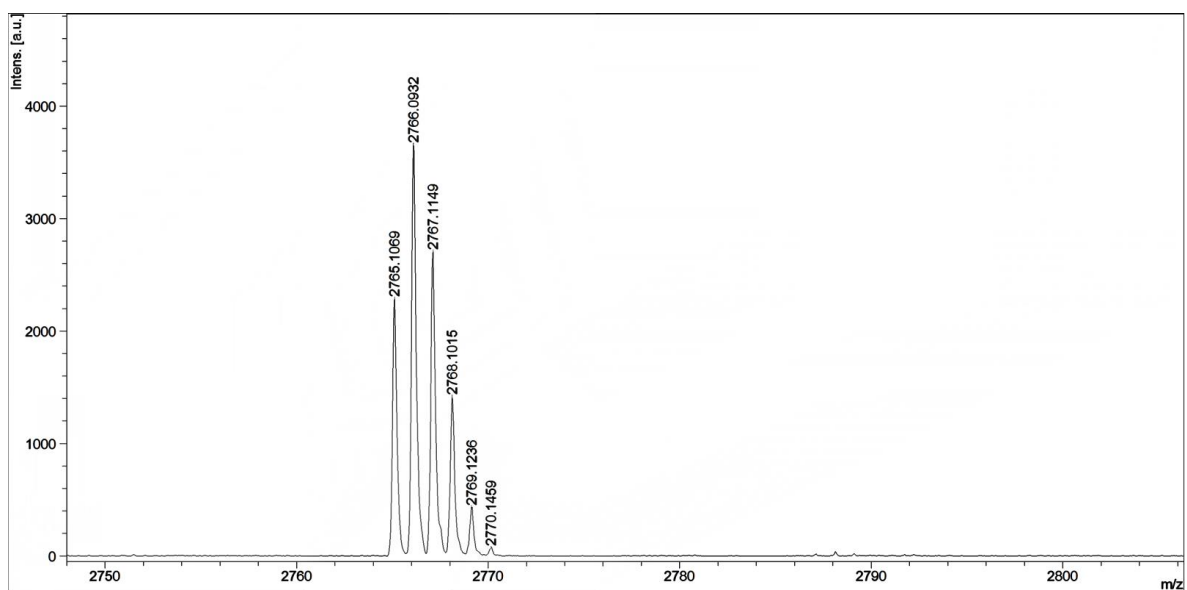
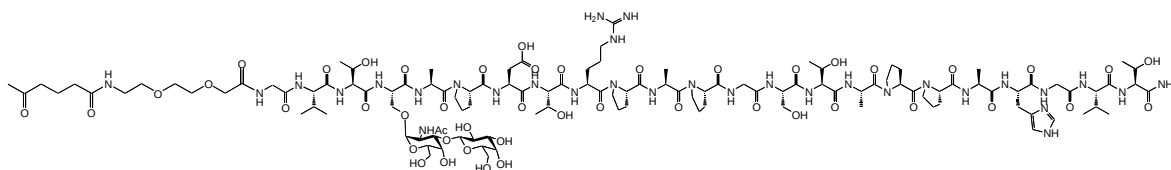
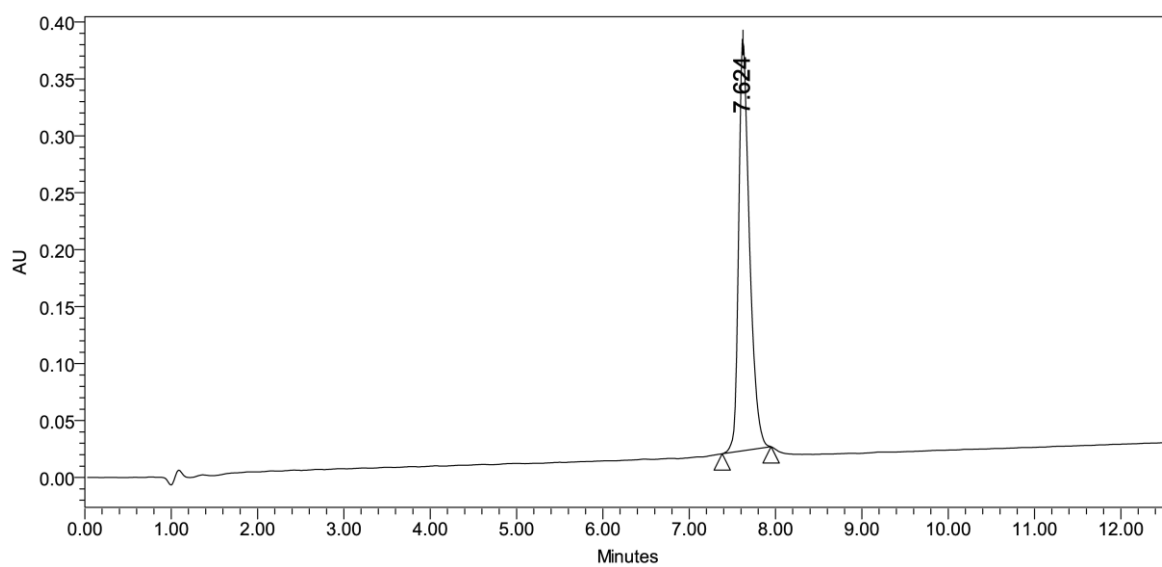


Figure S2. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 8**.



(a) UPLC profile



(b) MALDI-TOF MS

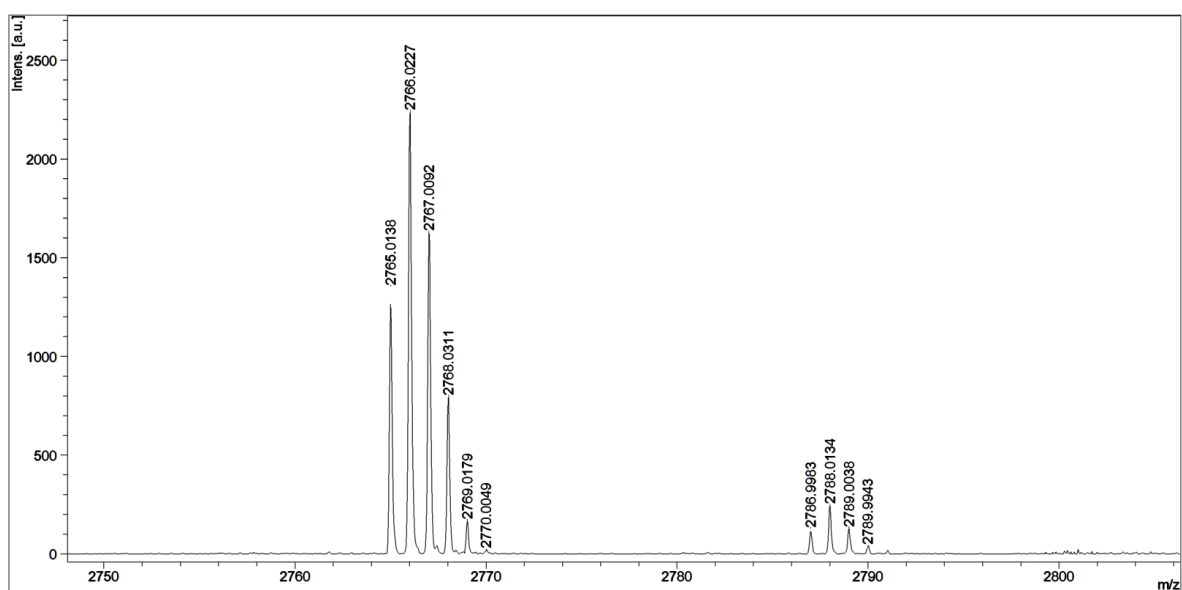
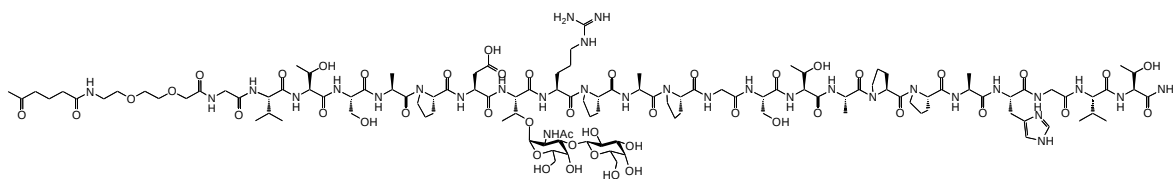
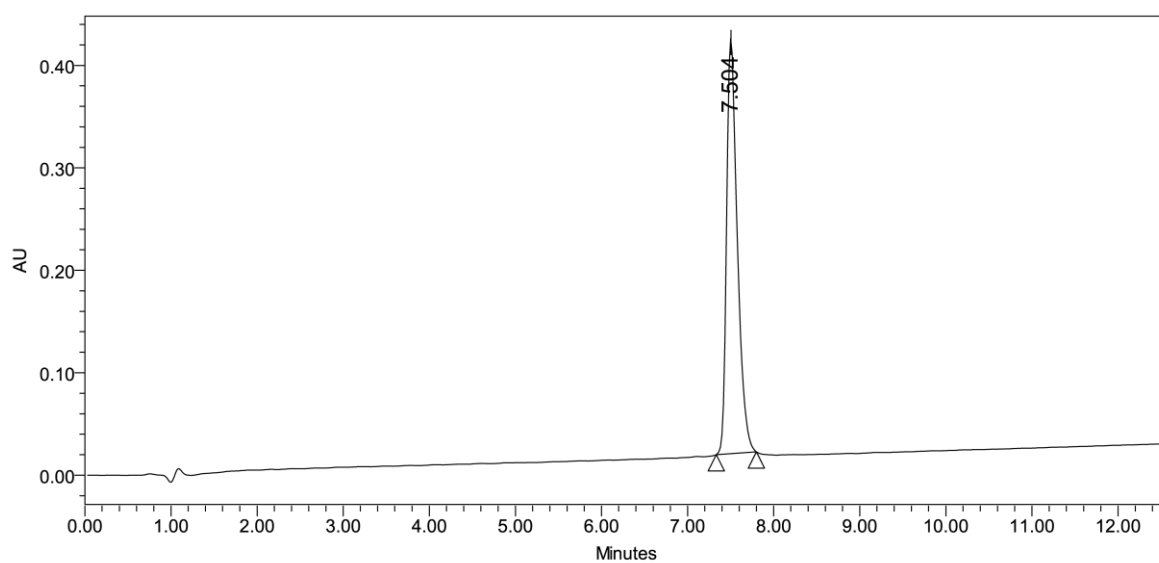


Figure S3. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 9**.



(a) UPLC profile



(b) MALDI-TOF MS

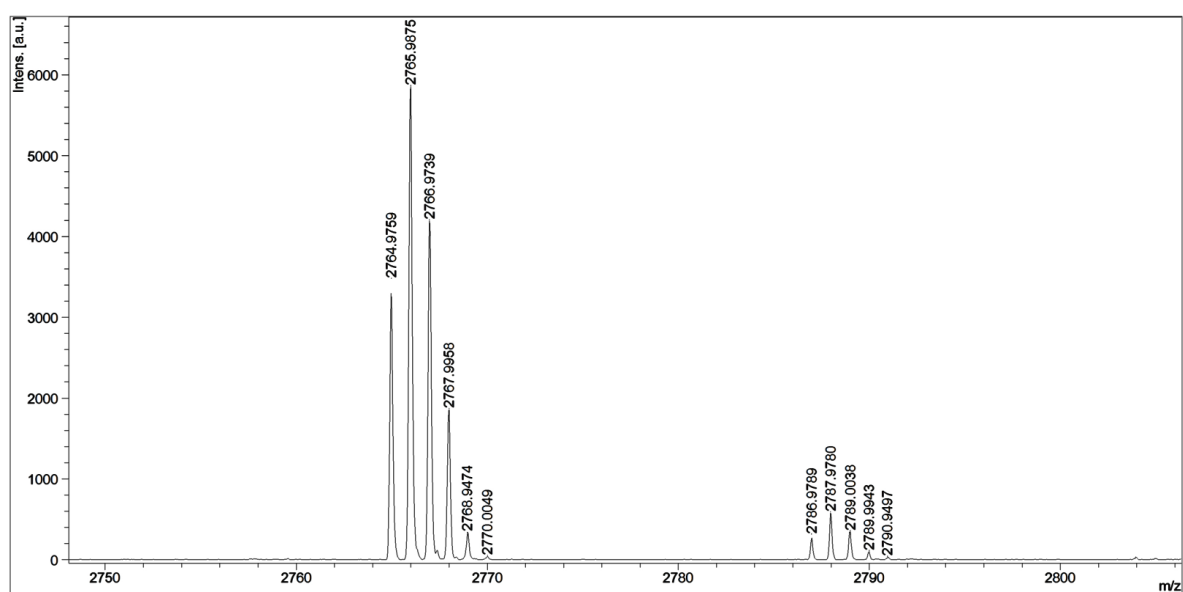
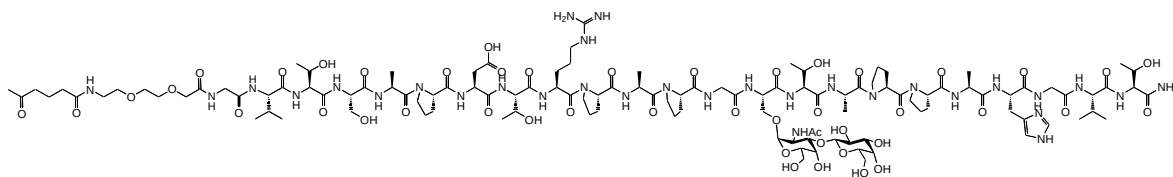
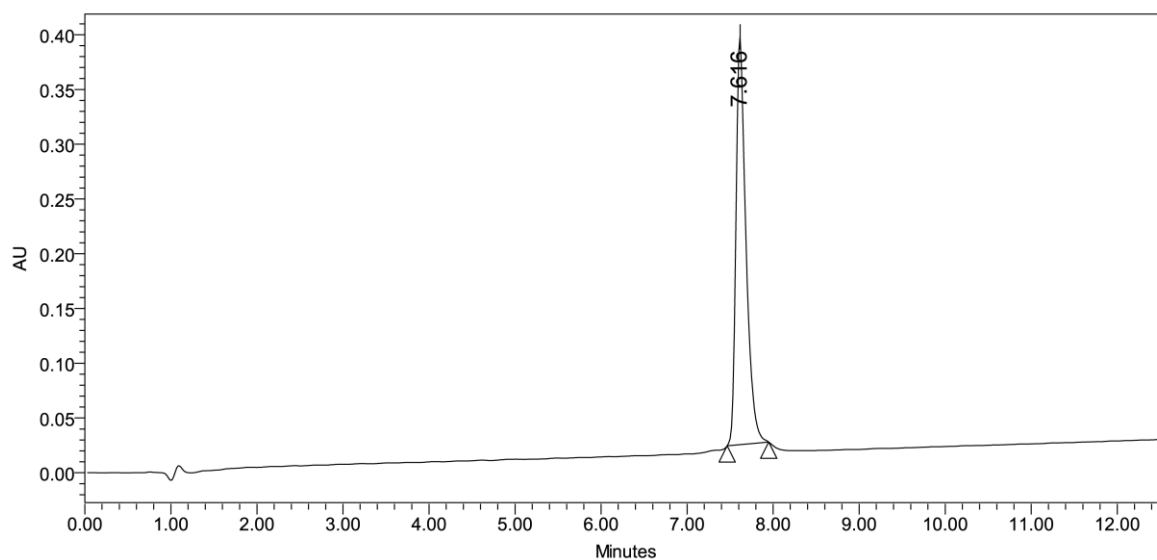


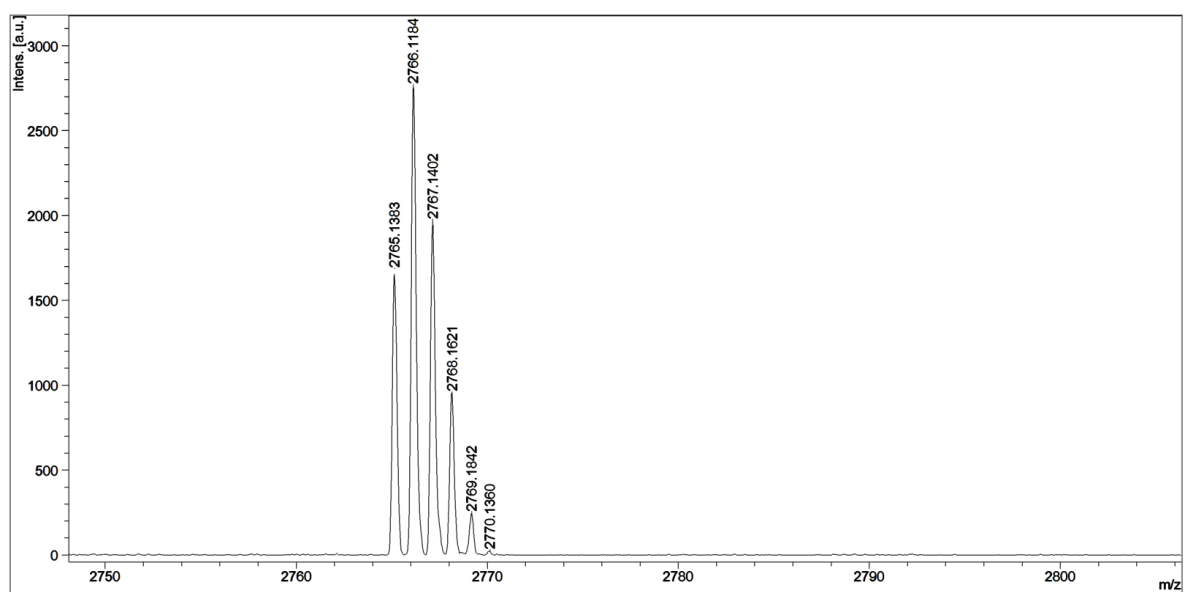
Figure S4. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 10**.



(a) UPLC profile



(b) MALDI-TOF MS



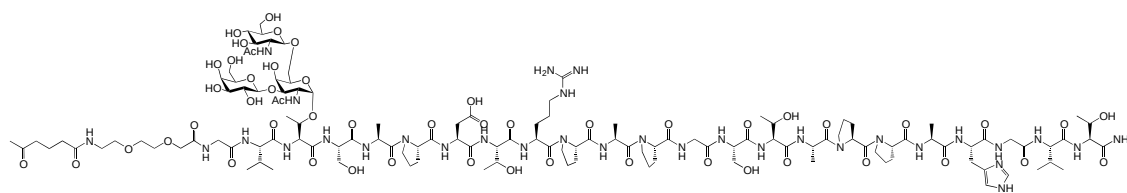
[illegible]

The chromatogram displays a single prominent peak at a retention time of 7.538 minutes. The y-axis represents Absorbance Units (AU) from 0.00 to 0.35, and the x-axis represents time in minutes from 0.00 to 12.00. Two small peaks are visible around 1.0 minute. The baseline is relatively flat with a slight upward trend after 7.5 minutes.

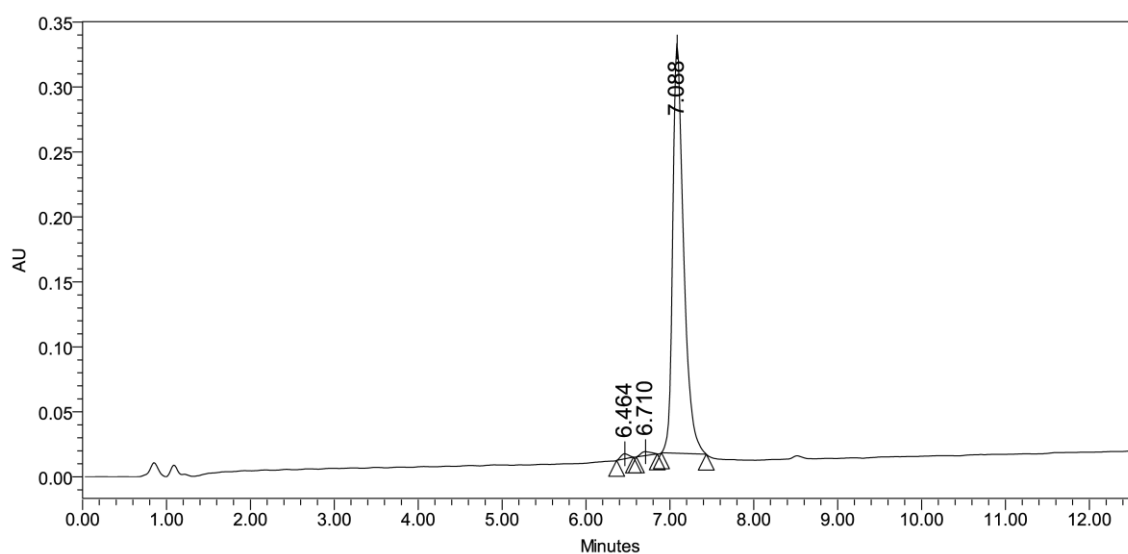
Retention Time (min)	AU
7.538	~0.34

Mass spectrum showing relative intensity (0 to 4000) versus m/z (2750 to 2800). The base peak is at m/z 2766.2241. Other labeled peaks include 2765.2273, 2767.2459, 2768.2326, 2769.2547, and 2770.2066.

Figure S6. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 12**.



(a) UPLC profile



(b) MALDI-TOF MS

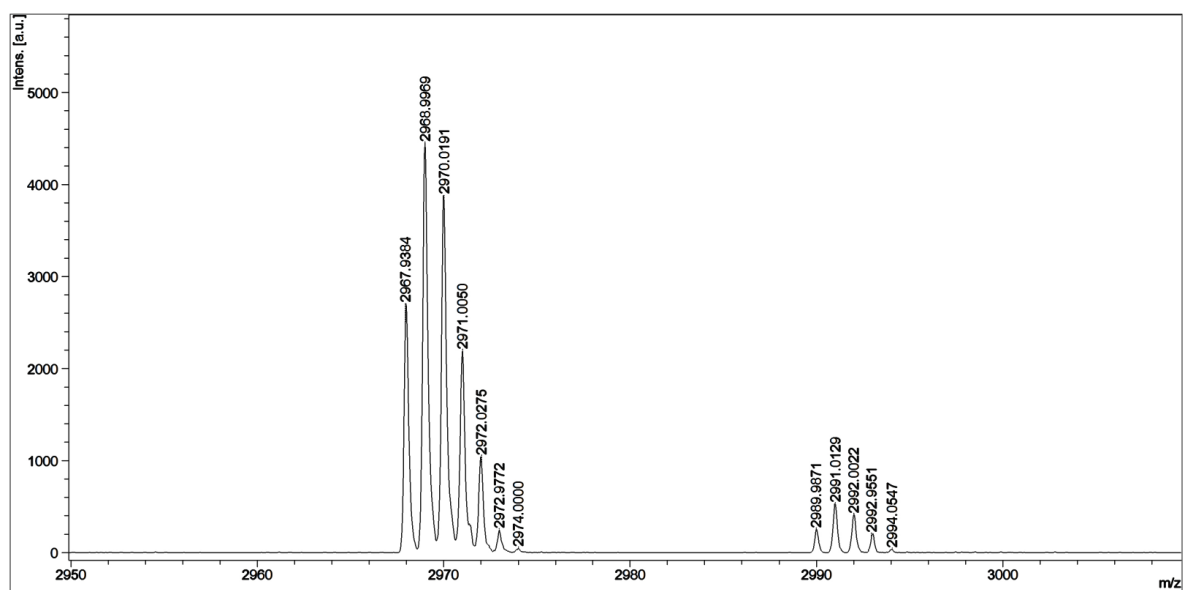
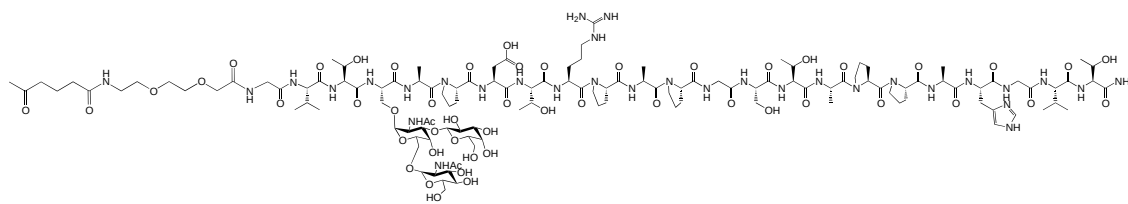
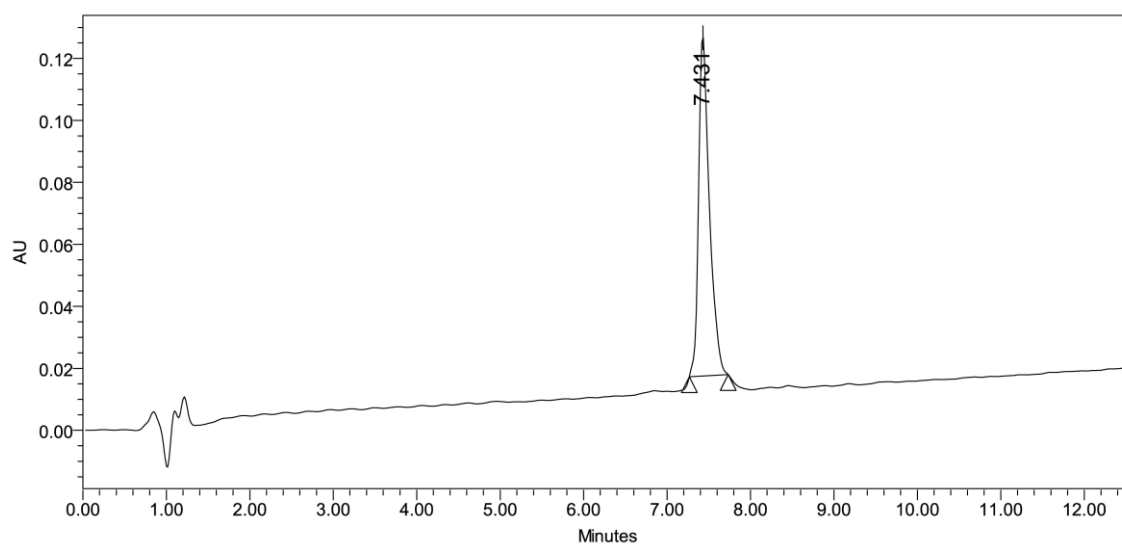


Figure S7. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 13**.



(a) UPLC profile



(b) MALDI-TOF MS

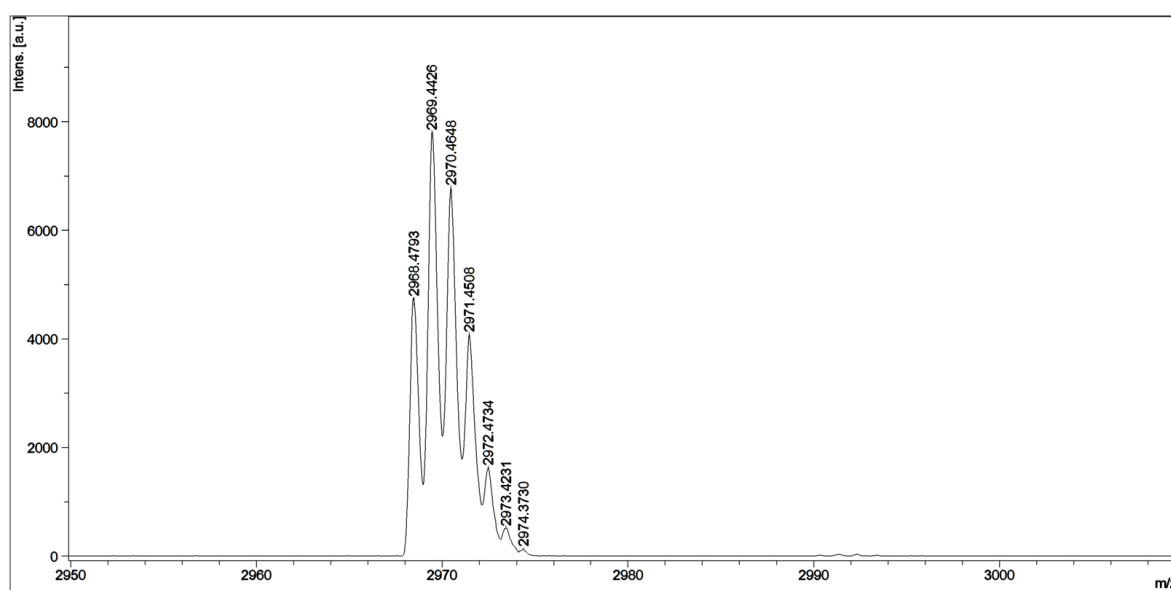
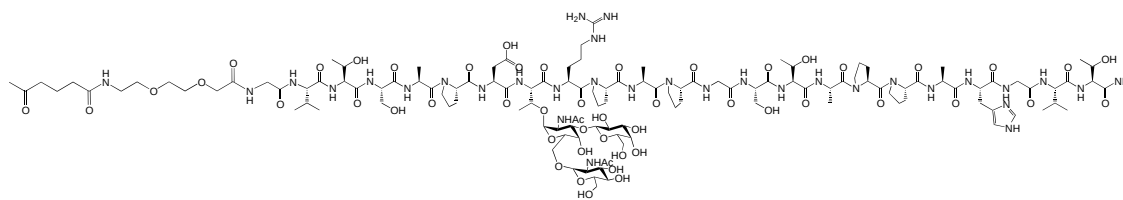
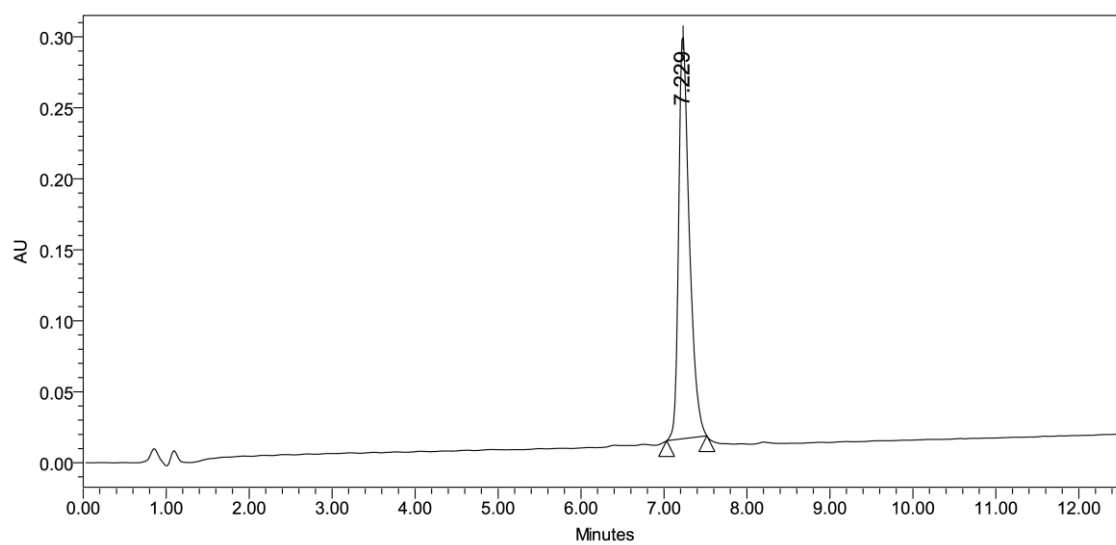


Figure 8. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 14**.



(a) UPLC profile



(b) MALDI-TOF MS

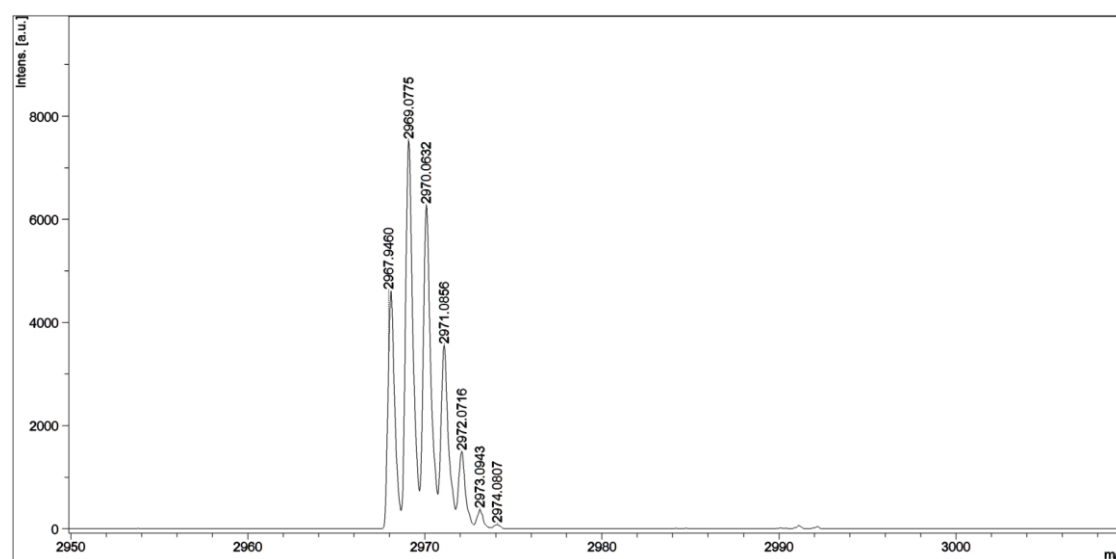
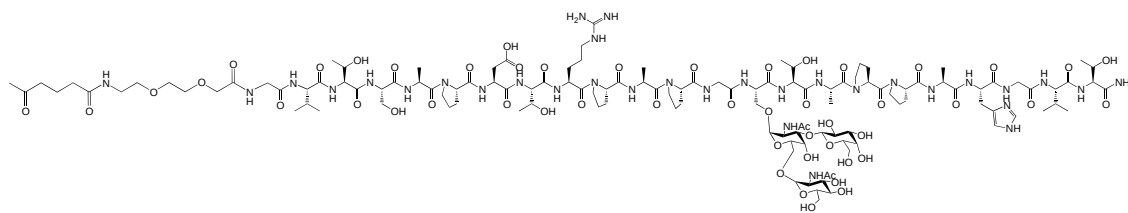
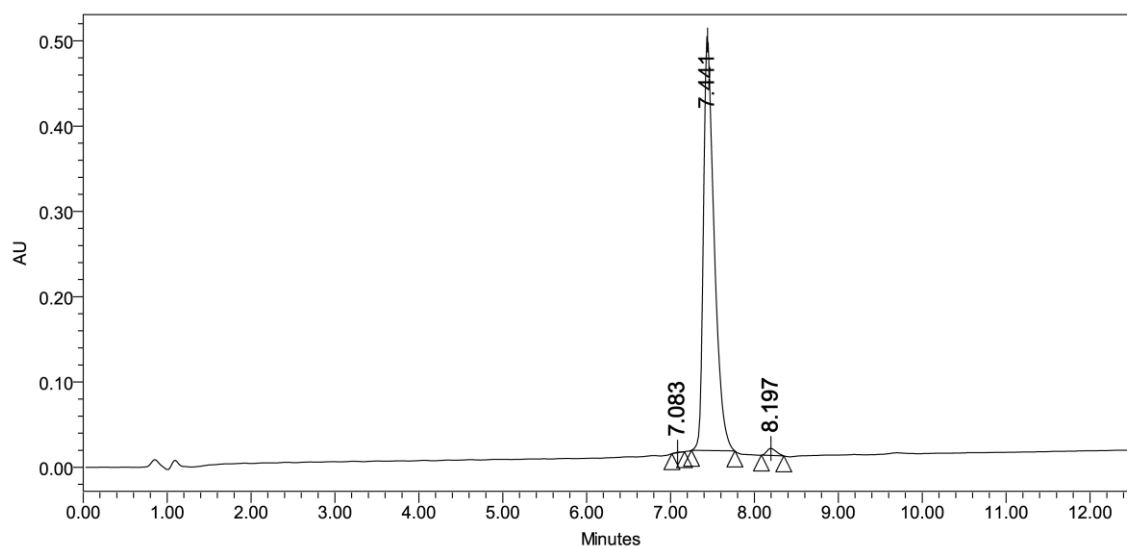


Figure S9. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 15**.



(a) UPLC profile



(b) MALDI-TOF MS

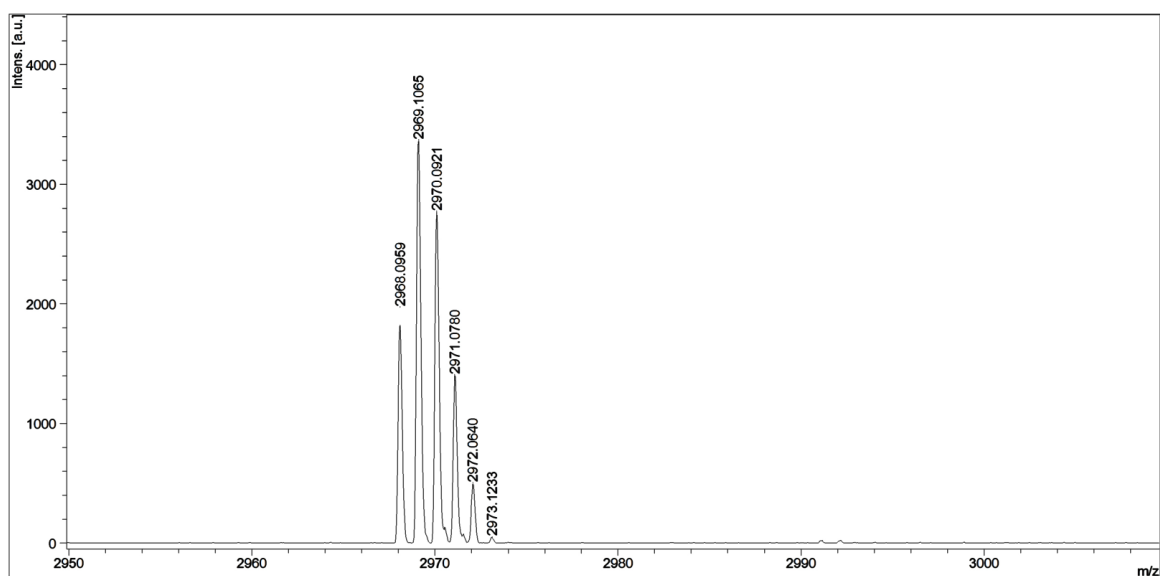
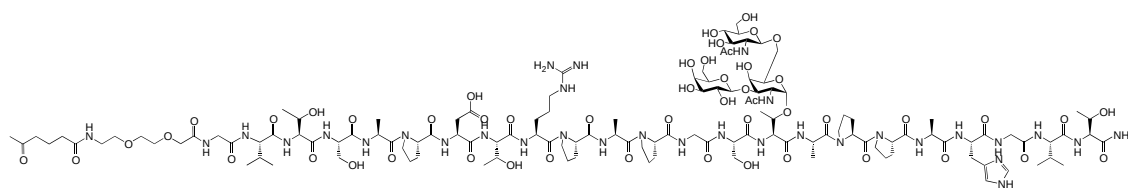
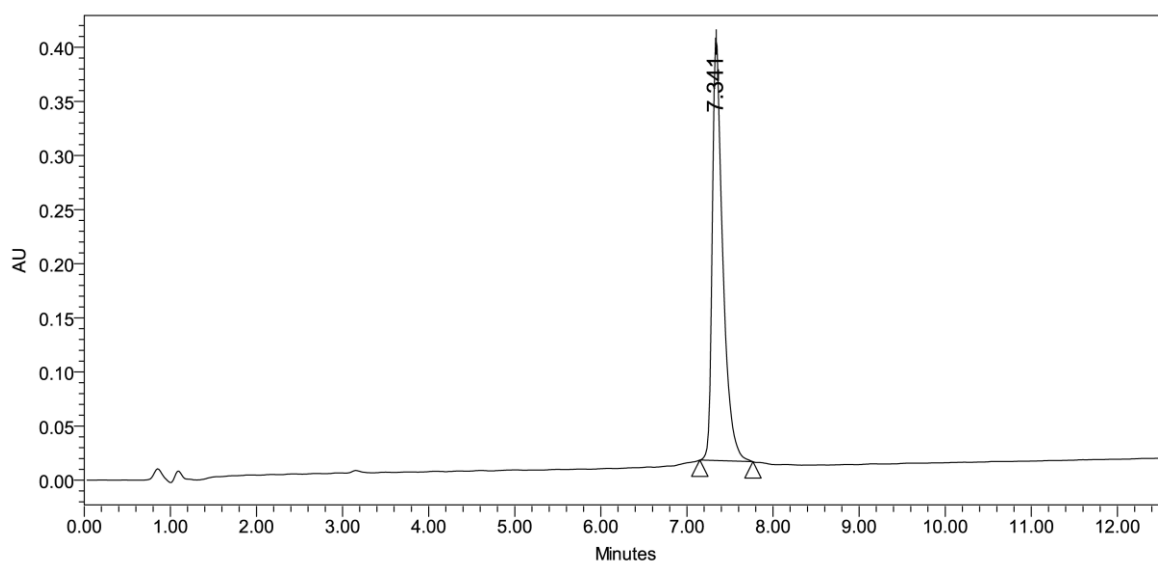


Figure S10. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 16**.



(a) UPLC profile



(b) MALDI-TOF MS

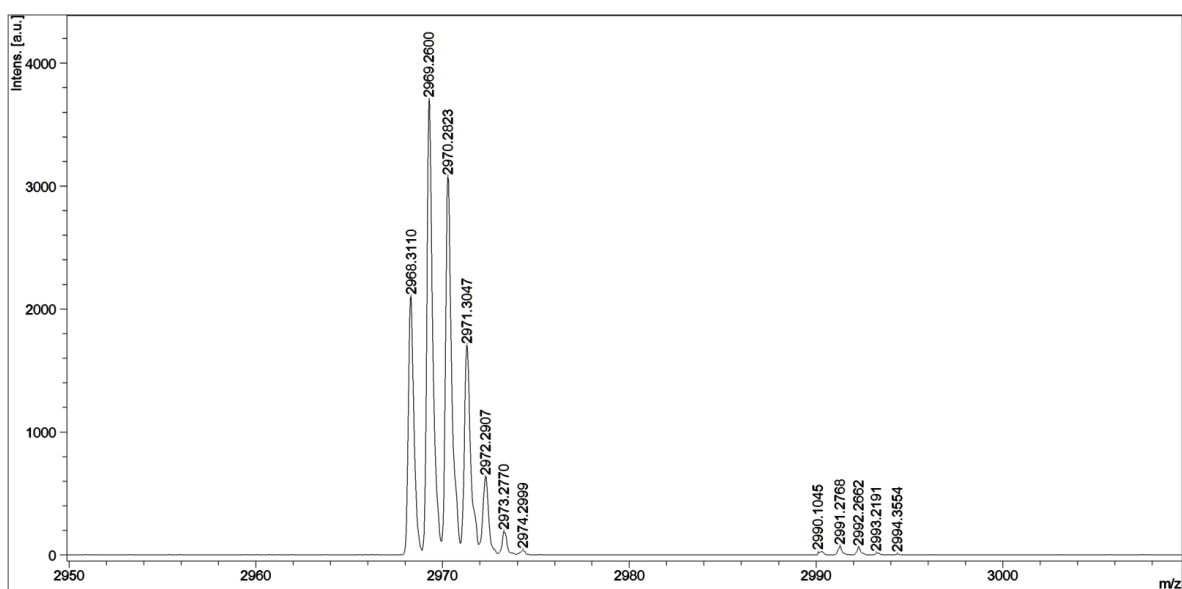
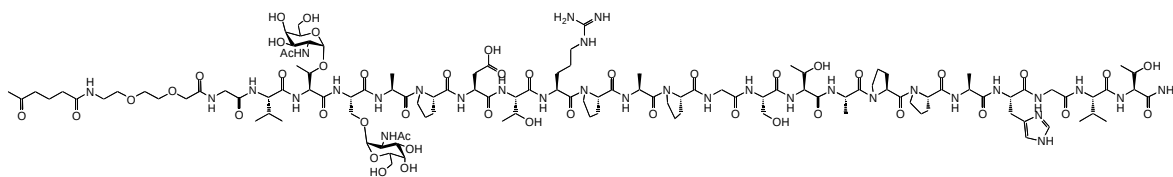
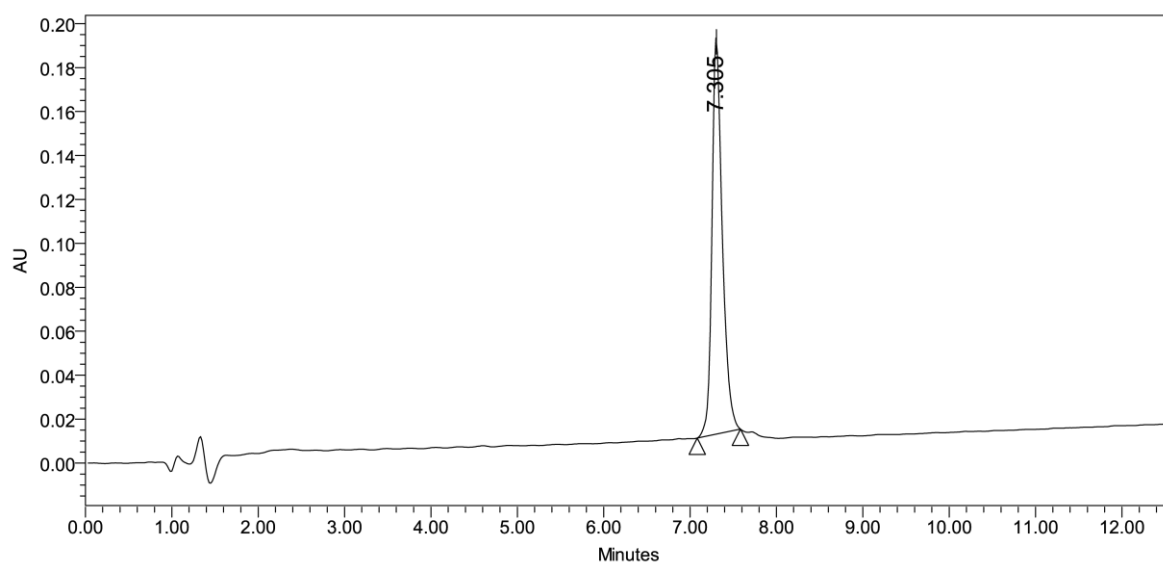


Figure S11. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 17**.



(a) UPLC profile



(b) MALDI-TOF MS

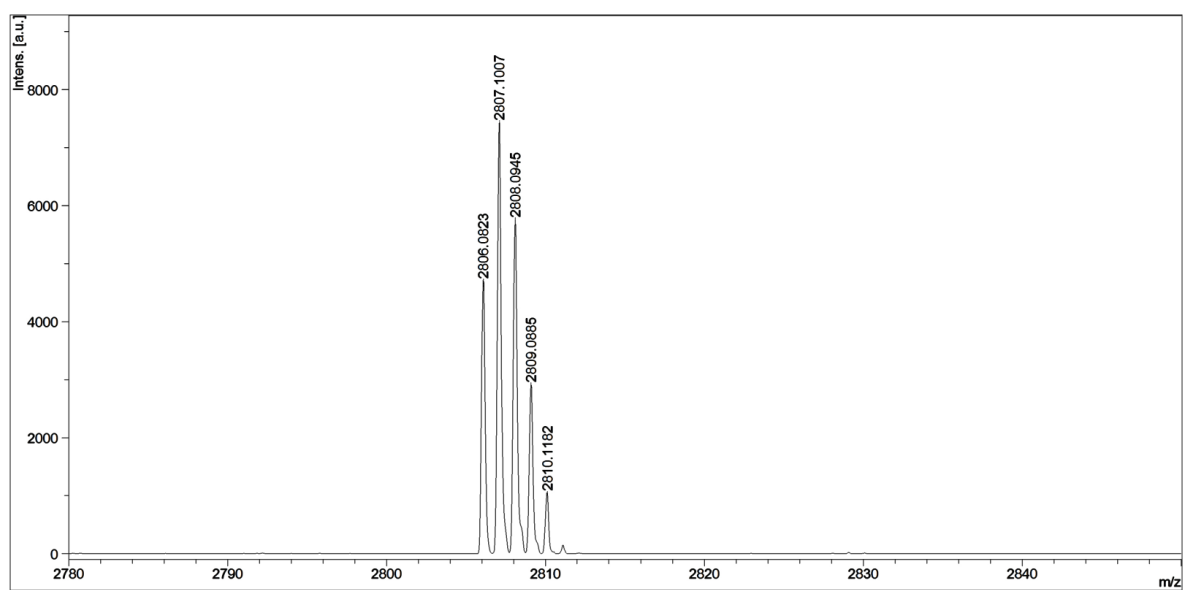
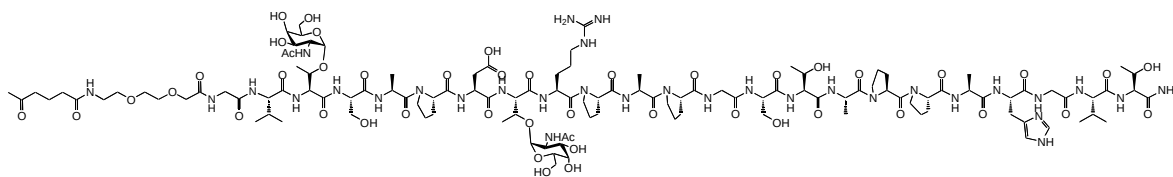
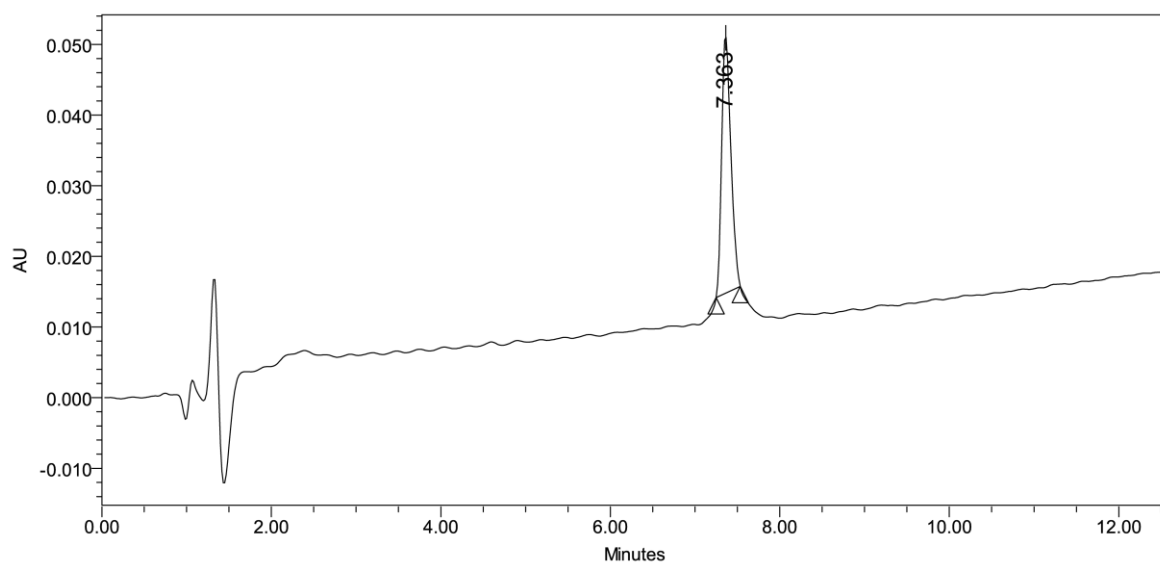


Figure S12. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 18**.



(a) UPLC profile



(b) MALDI-TOF MS

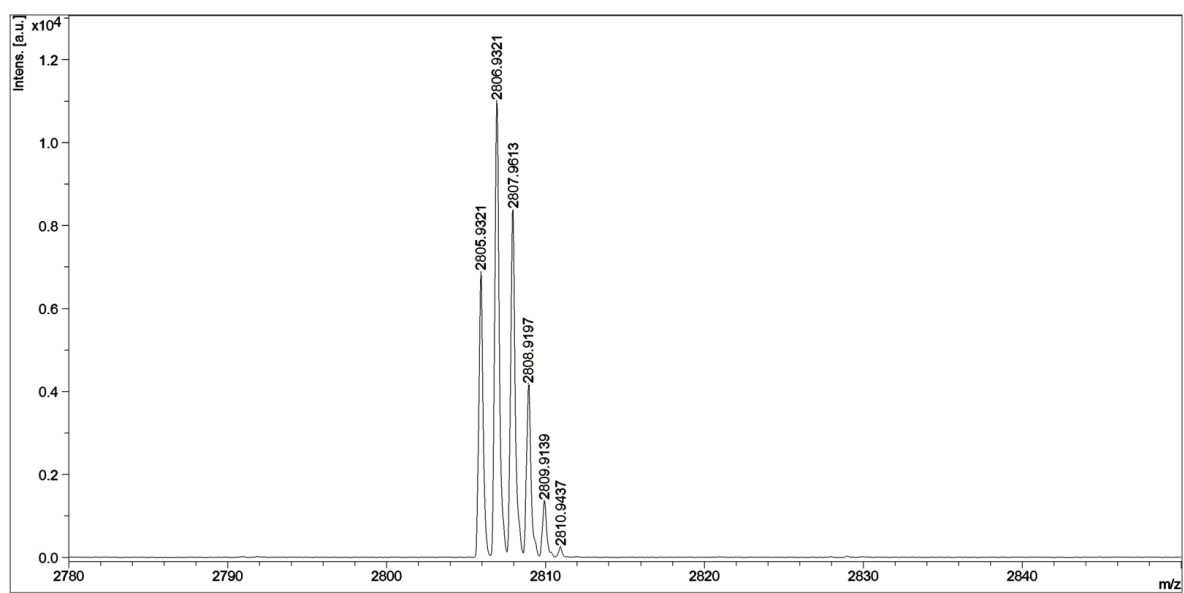
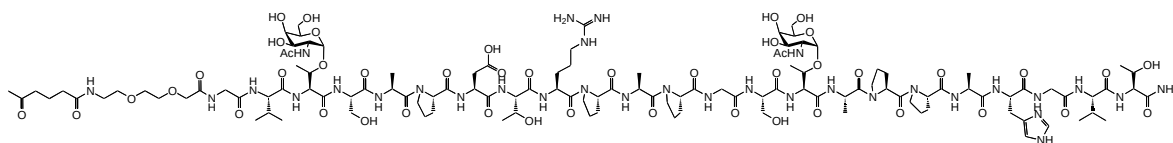
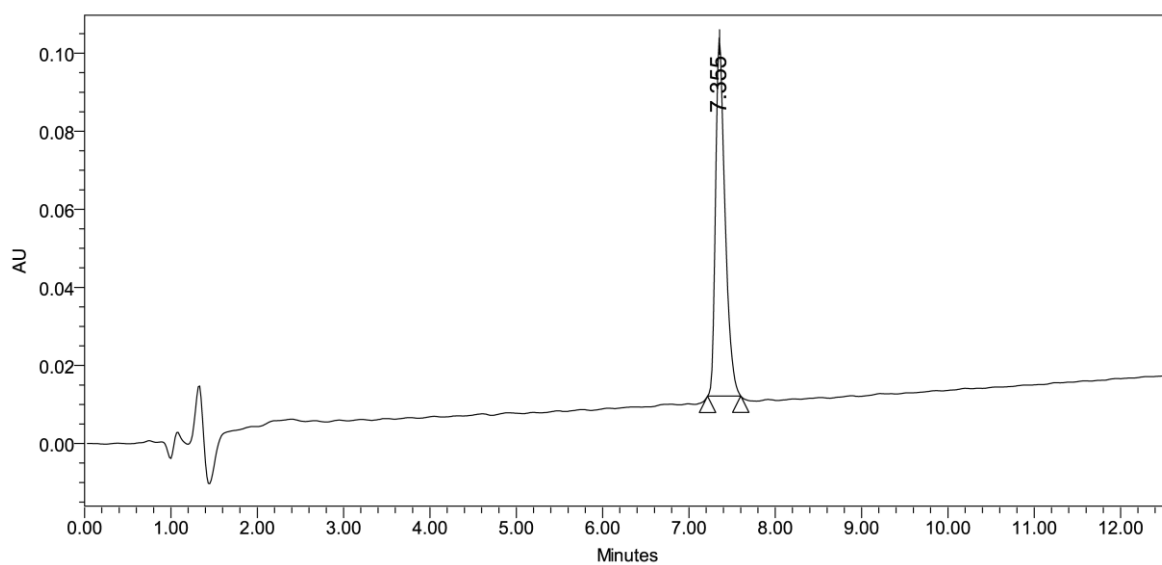


Figure S13. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 19**.



(a) UPLC profile



(b) MALDI-TOF MS

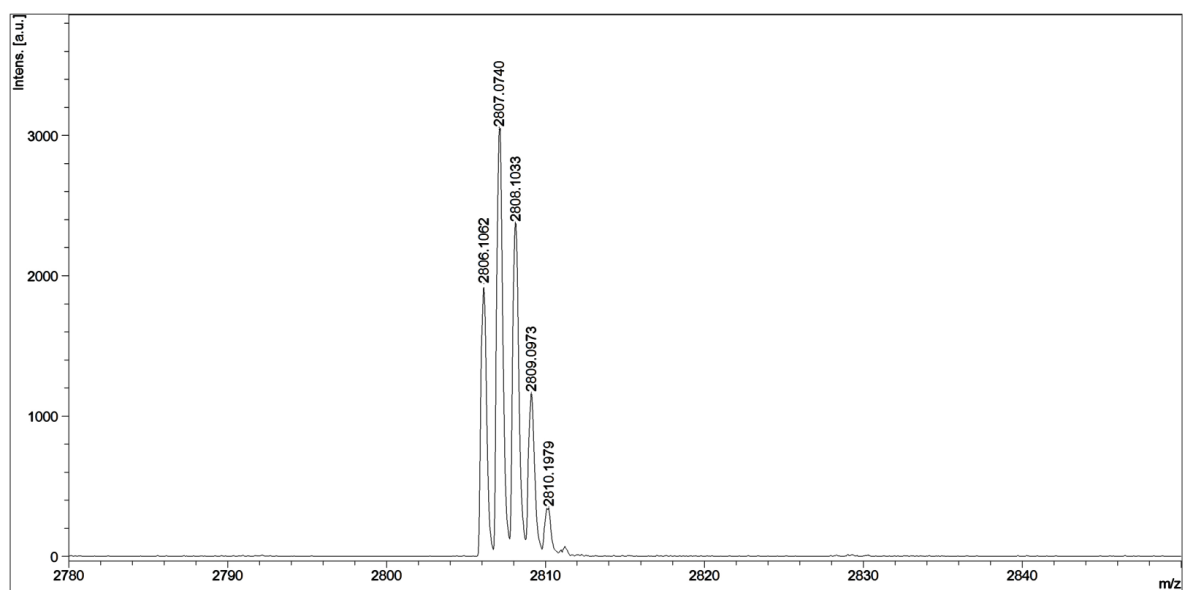
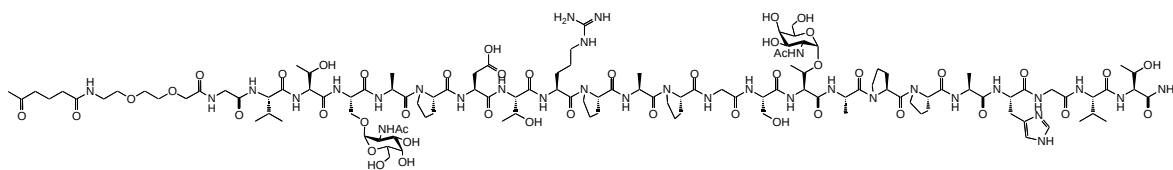
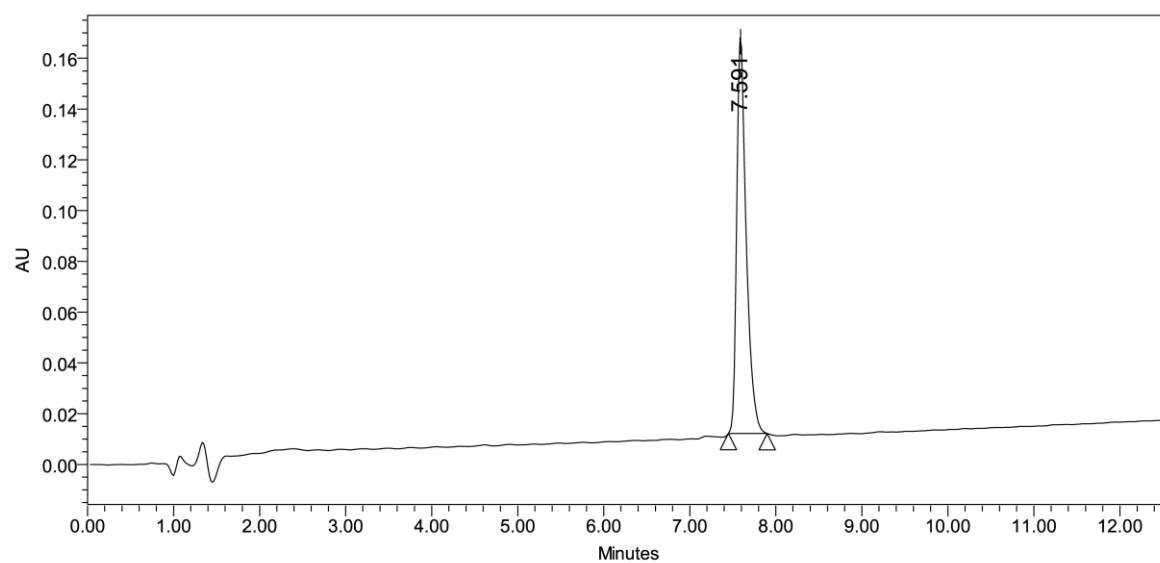


Figure S14. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 21**.



(a) UPLC profile



(b) MALDI-TOF MS

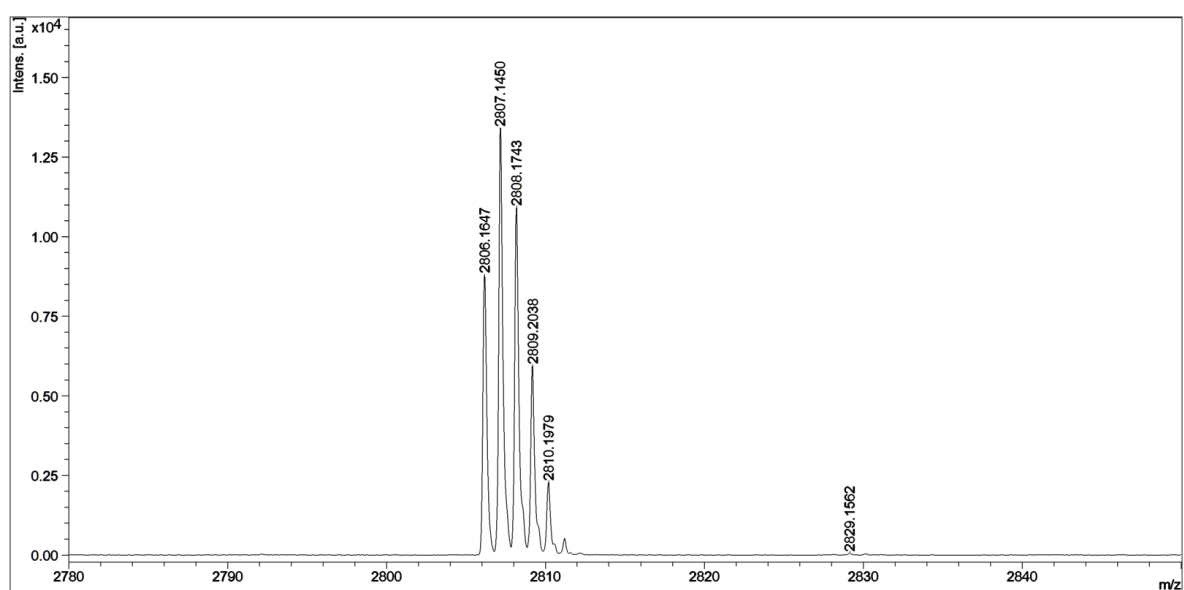
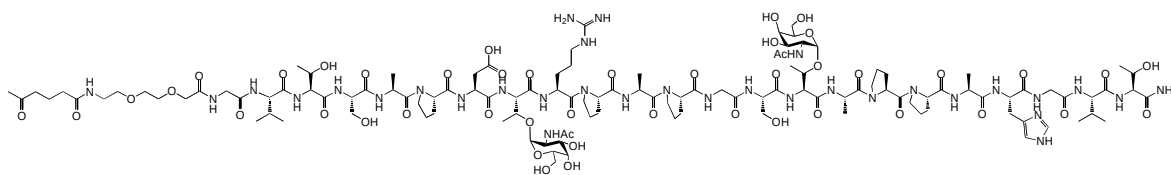
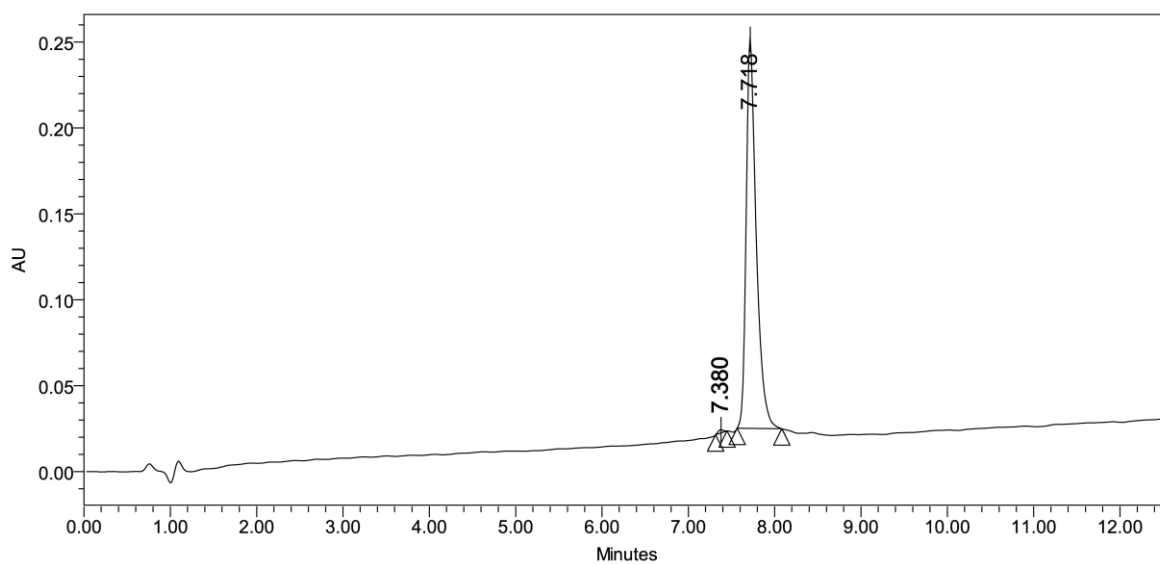


Figure S15. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 22**.



(a) UPLC profile



(b) MALDI-TOF MS

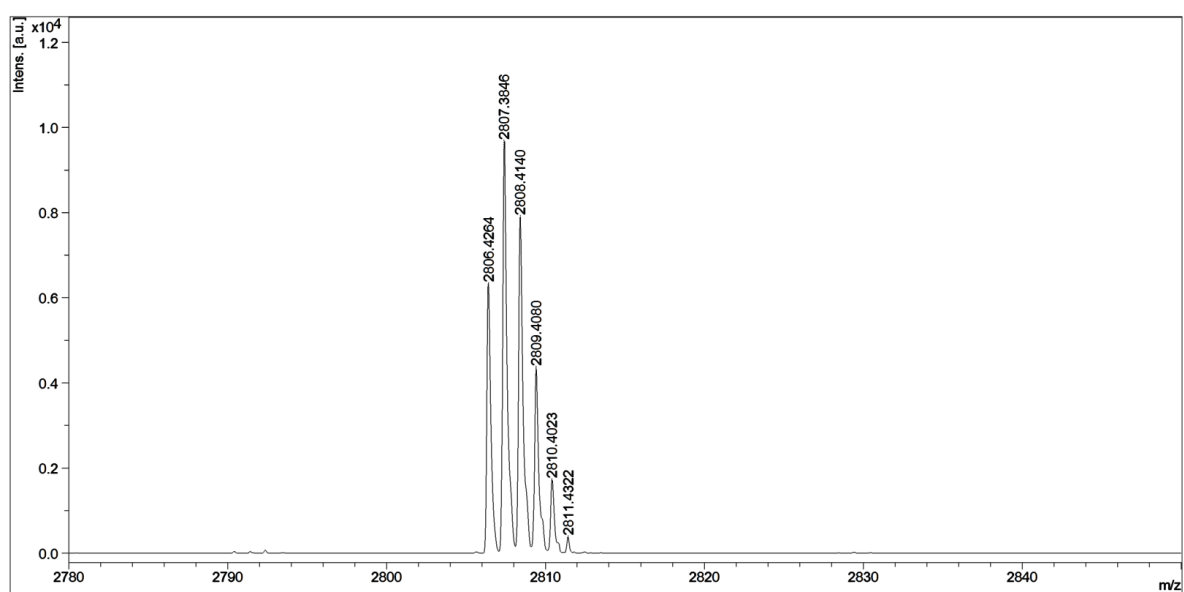
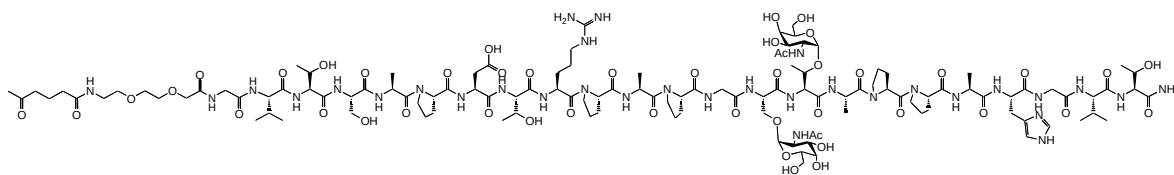
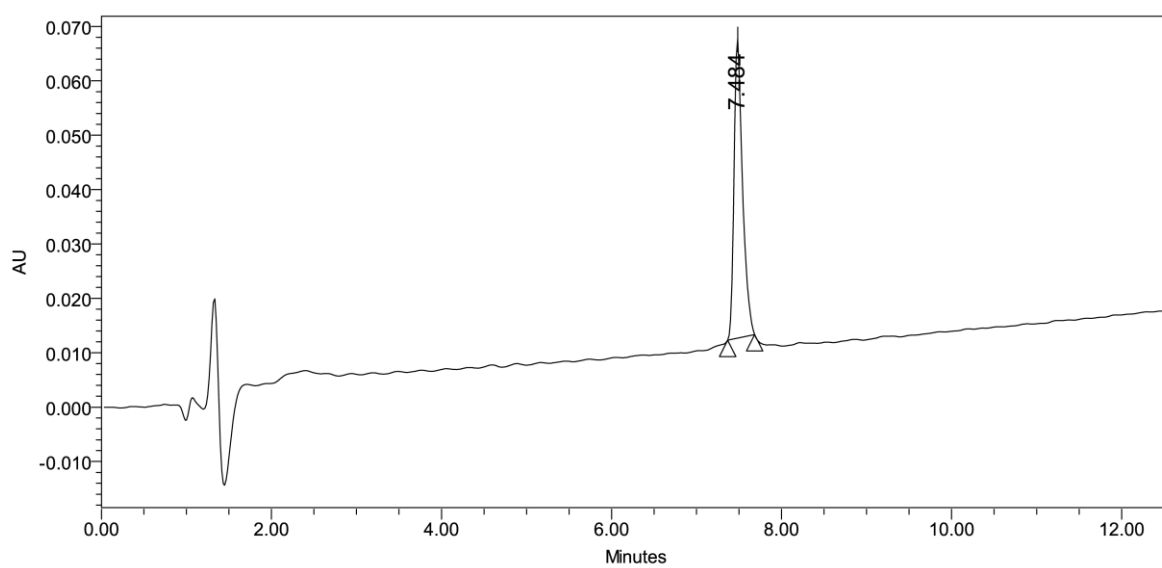


Figure S16. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 23**.



(a) UPLC profile



(b) MALDI-TOF MS

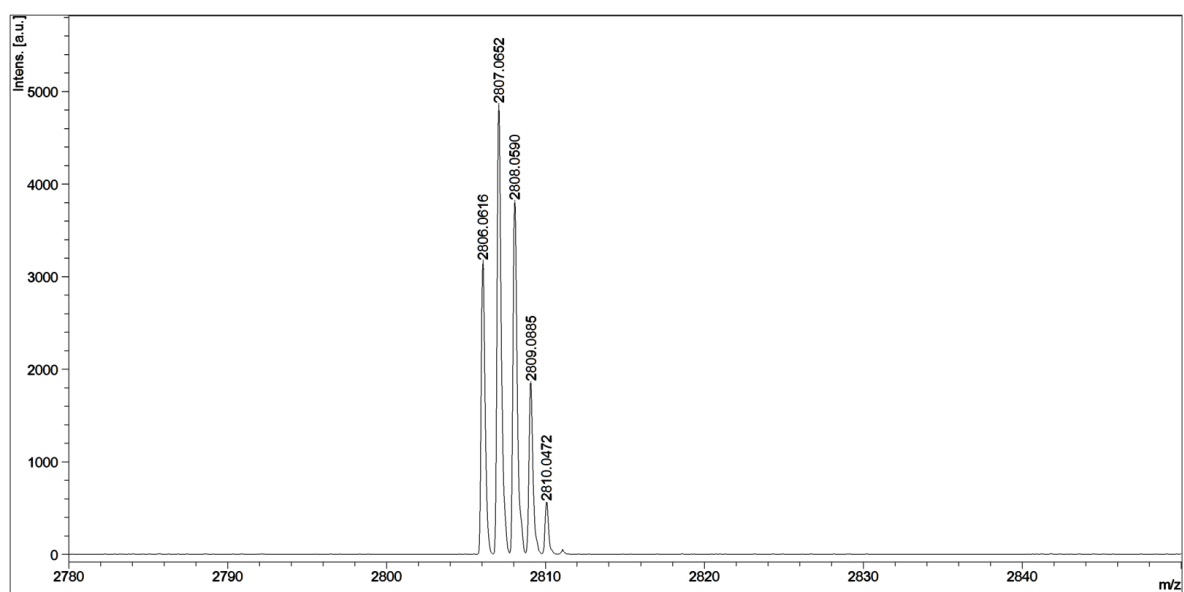
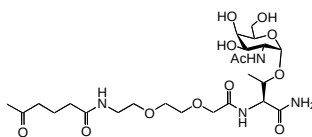
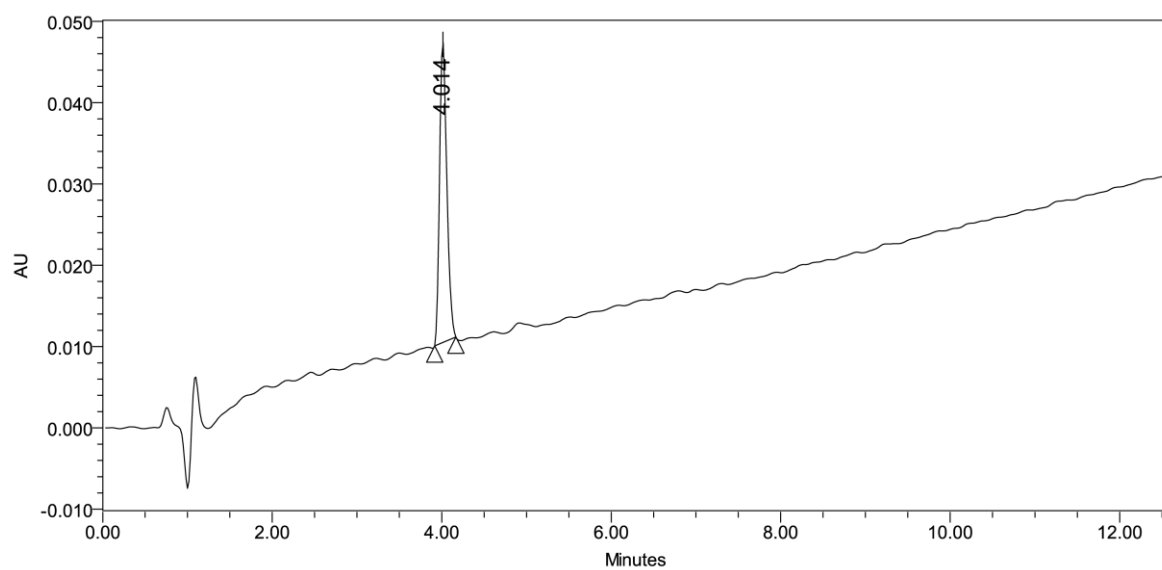


Figure S17. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 26**.



(a) UPLC profile



(b) MALDI-TOF MS

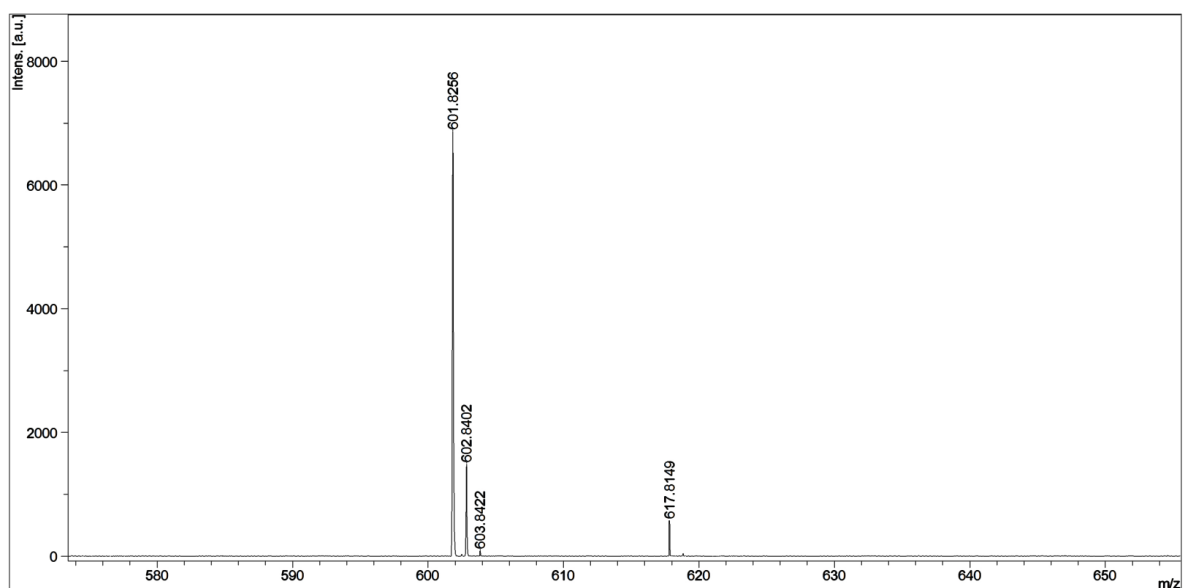
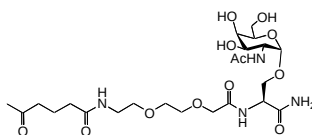
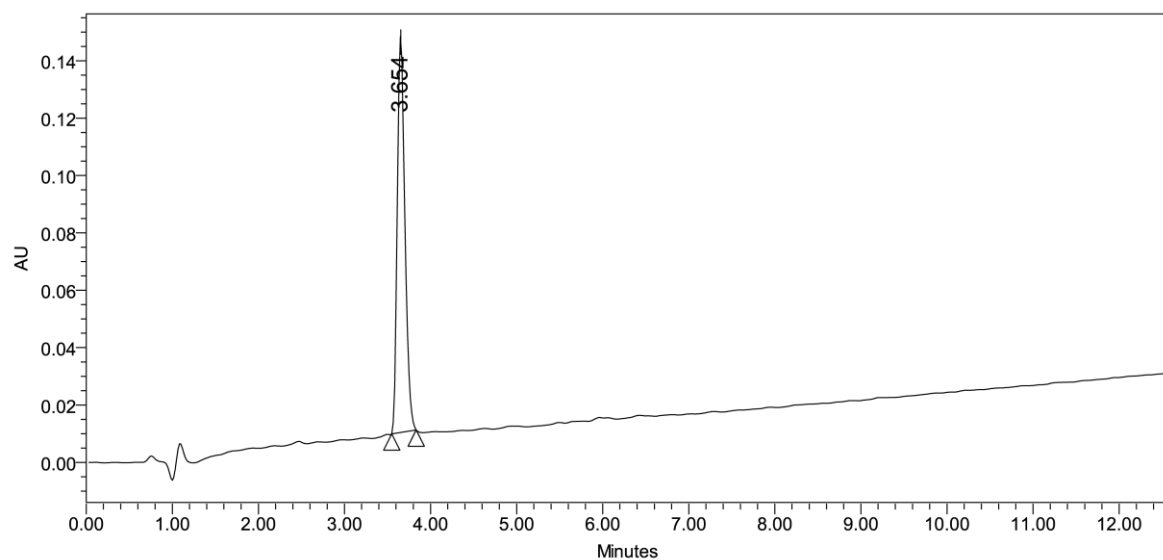


Figure S18. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 27**.



(a) UPLC profile



(b) MALDI-TOF MS

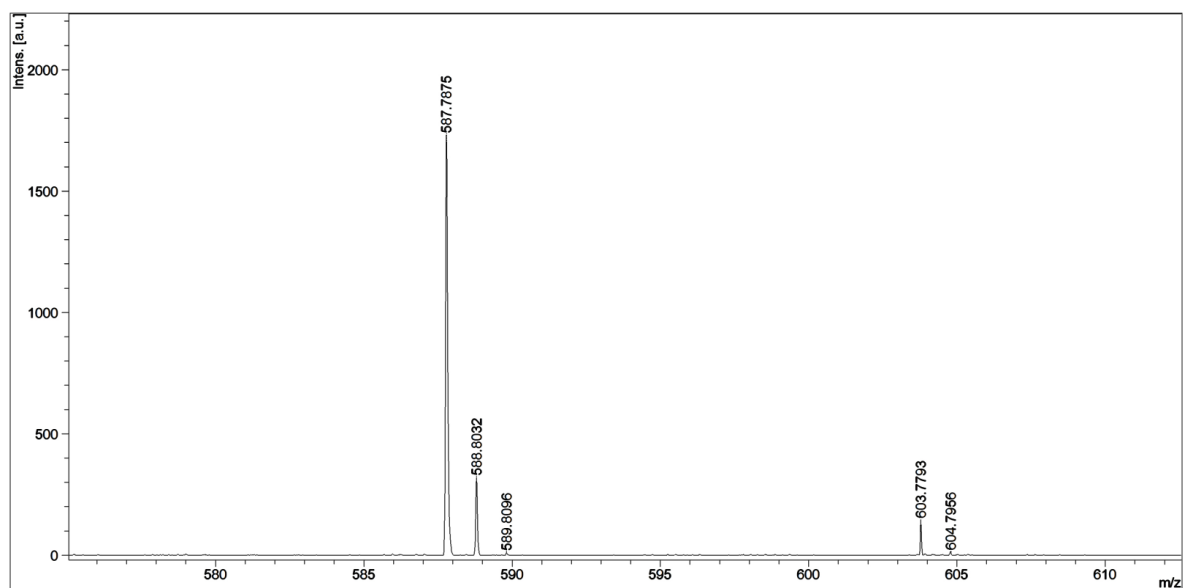
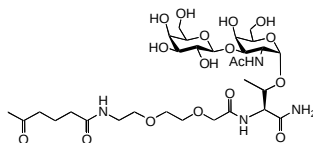
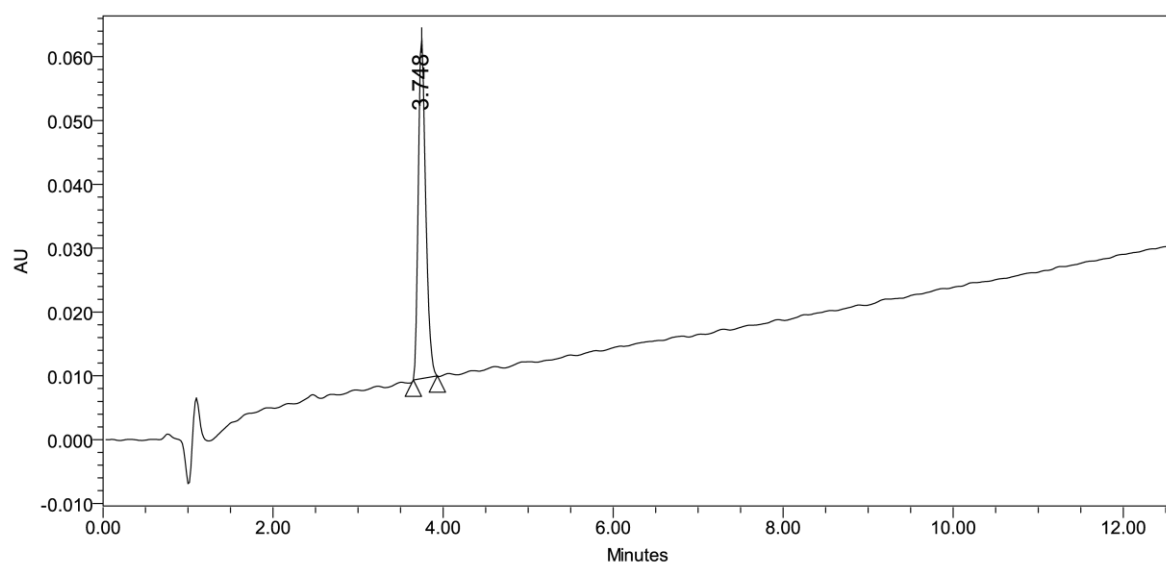


Figure S19. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 28**.



(a) UPLC profile



(b) MALDI-TOF MS

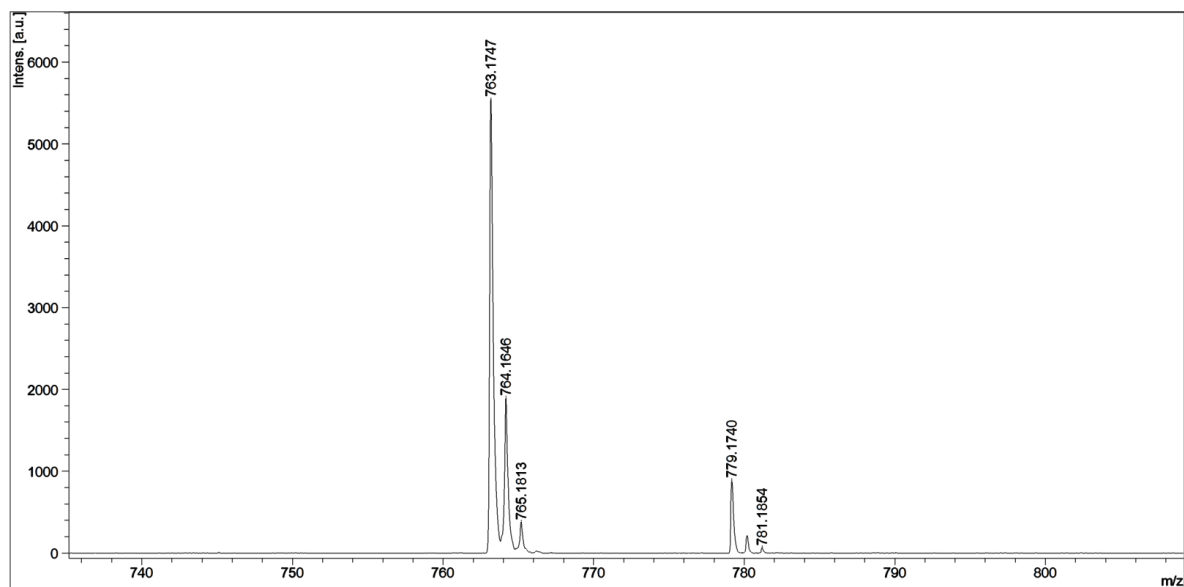
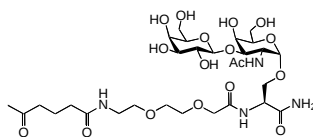
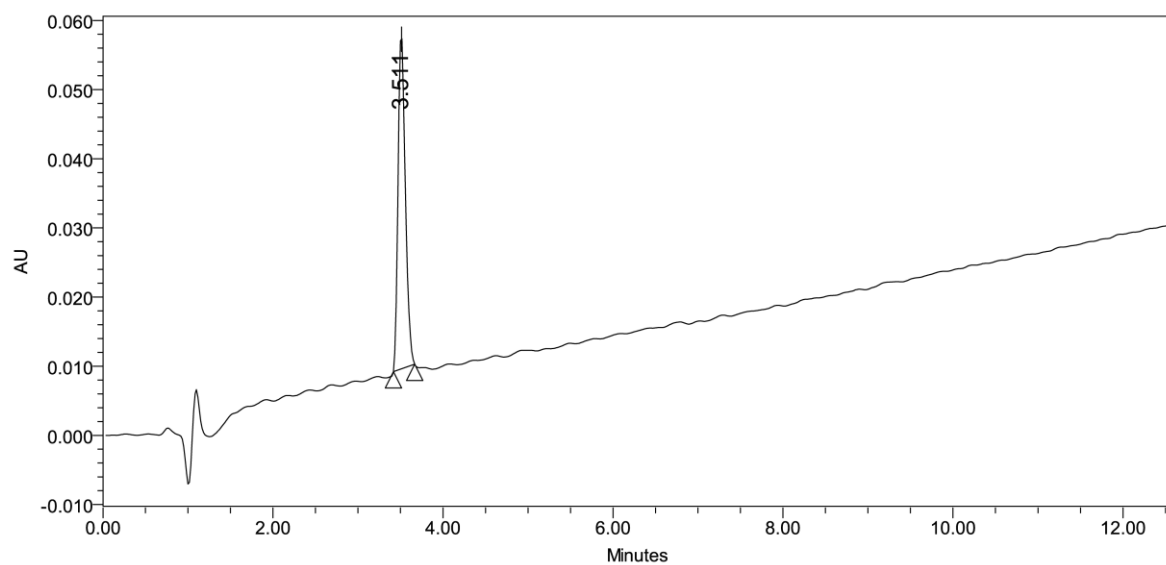


Figure S20. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 29**.



(a) UPLC profile



(b) MALDI-TOF MS

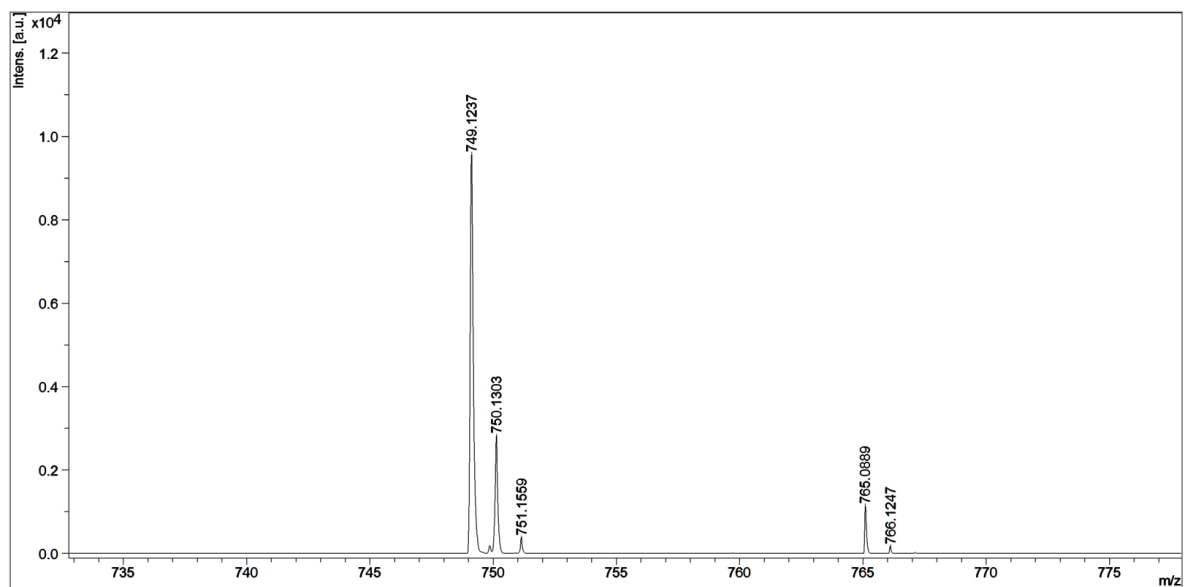
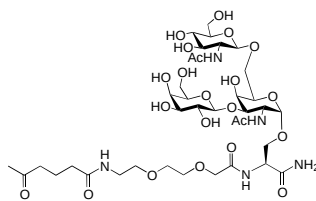
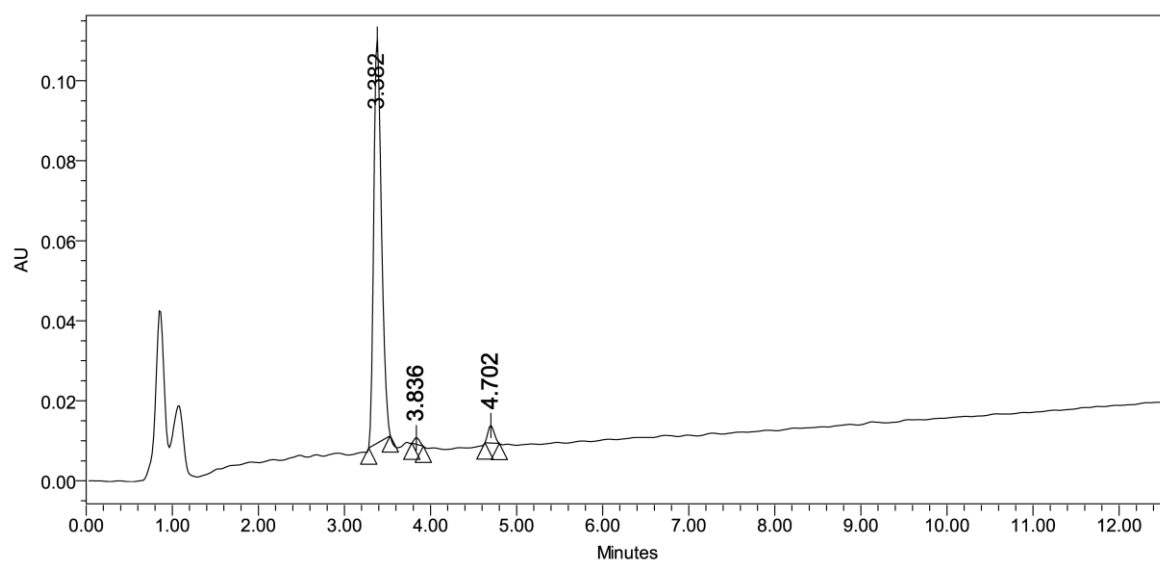


Figure S21. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 30**.



(a) UPLC profile



(b) MALDI-TOF MS

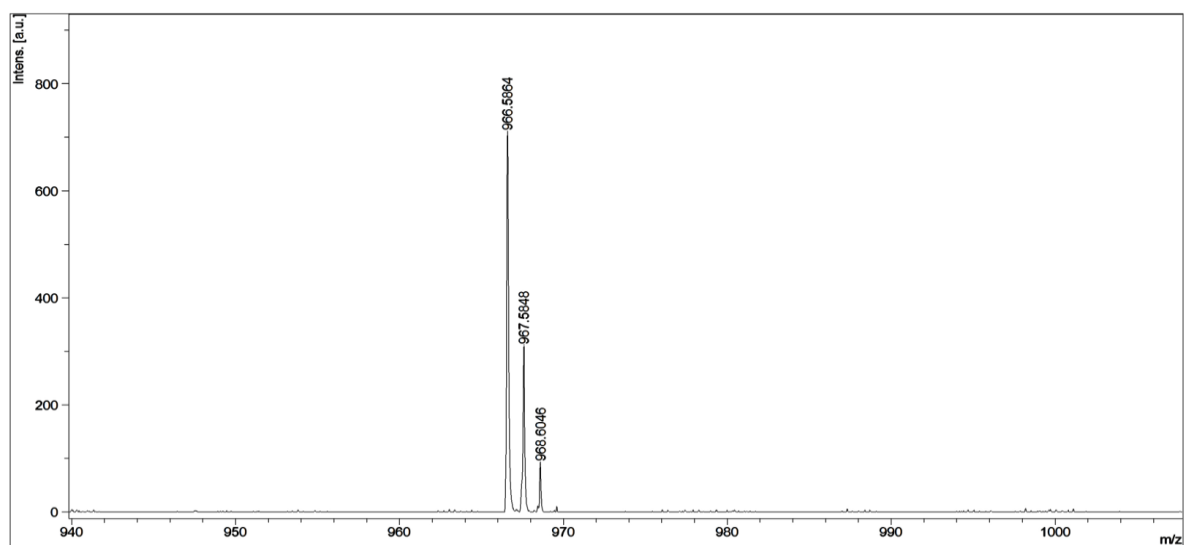
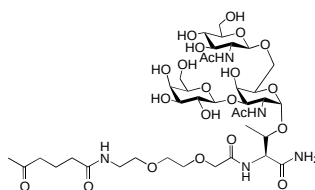
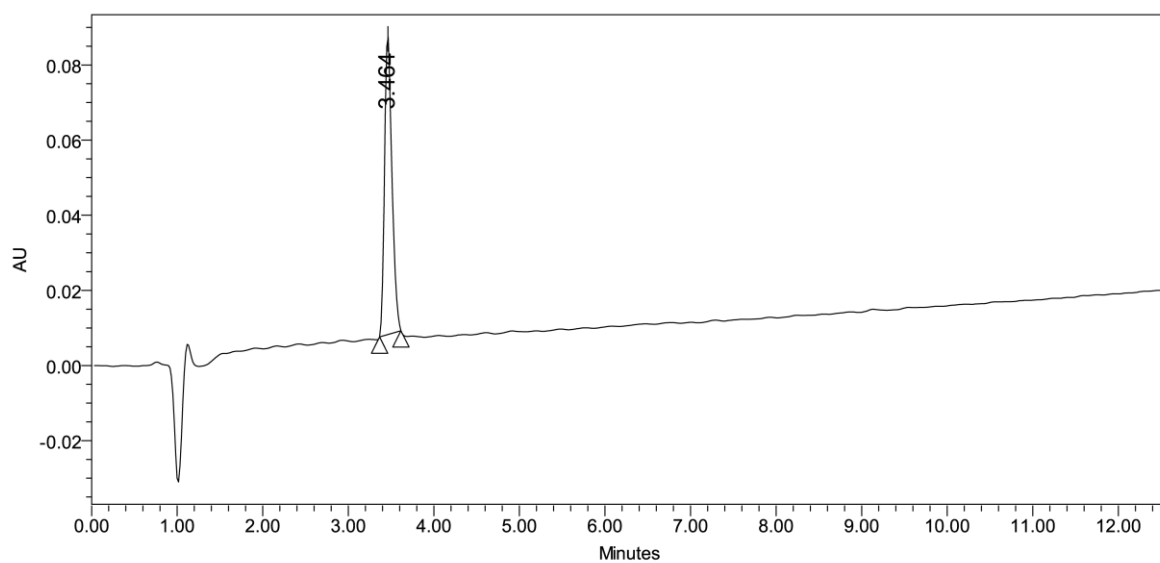


Figure S22. (a) UPLC profile and (b) MALDI-TOF MS of **Compound 31**.



(a) UPLC profile



(b) MALDI-TOF MS

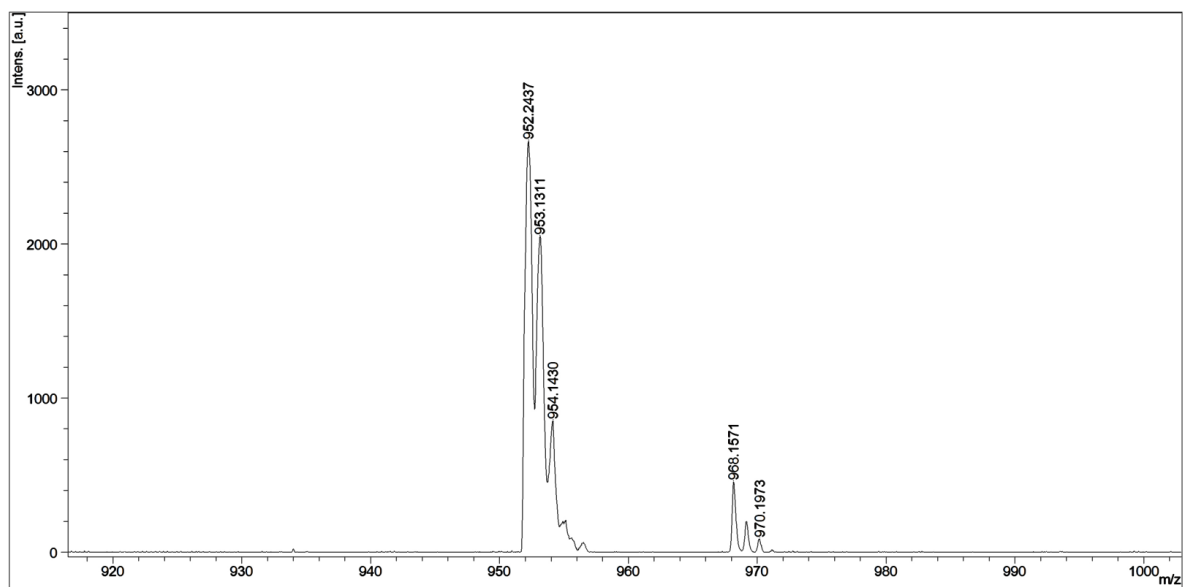


Figure S23. Relative fluorescence units (RFU) with its standard deviation for compound **1~35** after treatment with Gal-3CRD, galectin-1, and C-GRP.

