Sub-Monomer Synthesis of A Hybrid Peptoid-Azapeptoid Library

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Materials and Equipment

All of the chemical reagents and solvents from commercial sources were used without further purification. TentaGel Macrobeads NH_2 (160 μm, 0.48 mmol/g) resin was purchased from Rapp Polymere. Knorr Amide MBHA (0.69 mmol/g) resin was purchased from NovaBiochem. 5 mL and 10 mL Disposable Reaction Columns (Intavis AG) were used as reaction vessels for solid phase synthesis. Syntheses of peptoids under microwave conditions were performed in a 1550 W microwave oven (GE model JE 1860BH04) with 10% power. HPLC was carried out on Waters systems equipped with Waters 1525 binary HPLC pumps and a 2487 dual λ absorbance detector, or a 2998 photodiode array detector. The mobile phase comprised of buffer A (H_2O containing 5% CH_3CN and 0.1% trifluoroacetic acid (TFA)) and buffer B (CH_3CN containing 0.1% TFA). Analytical HPLC was conducted using a Vydac C-18 column (5 μm, 250 x 4.6 mm, Alltech, Deerfield, IL) at a flow rate of 1.0 mL/min with UV detection at 220 nm. MS and MS/MS (MALDI-TOF) were performed on a 4800 Proteomics Analyzer (Applied Biosystems) with α-cyano-4-hydroxycinnamic acid (CHCA) as a matrix.

Synthetic Protocols

(i) **Fmoc-deprotection:** All the compounds were synthesized in Knorr Amide RAM resin. Knorr Amide RAM resin (100 mg) in DMF (2 mL) was swollen at room temperature (~23 °C) for 1 hour in the 5 mL disposable reaction column. Fmoc protecting group was then removed by incubation of the resin with 20 % piperidine in DMF (2 mL) for 30 mins.

(ii) **Bromo acylation:** The resin was thoroughly washed with DMF. After Fmoc group was removed, 2-bromoacetic acid (1 mL, 2 M in DMF) and DIC (1 mL, 3.4 M in

DMF) were added. The reaction vessel containing the resin was shaken for about 10 mins at 37 ºC.

(iii) **Bromide displacement:** The resin was then washed again with DMF. Then a solution of amine/acyl hydrazide/carbazate/semicarbazide (2 mL, 2 M in NMP) was added and shaken at 37 ºC for 1h. The bromoacylation and SN2 displacement reactions were repeated to obtain the desired chain length.

(iv) **Acetyl capping:** The acetyl capping reactions were carried out using acetic acid (2M, 1mL) and (DIC) (3.4 M, 1 mL) for 30 mins at room temperature. The resin was then thoroughly washed with DMF and finally with DCM.

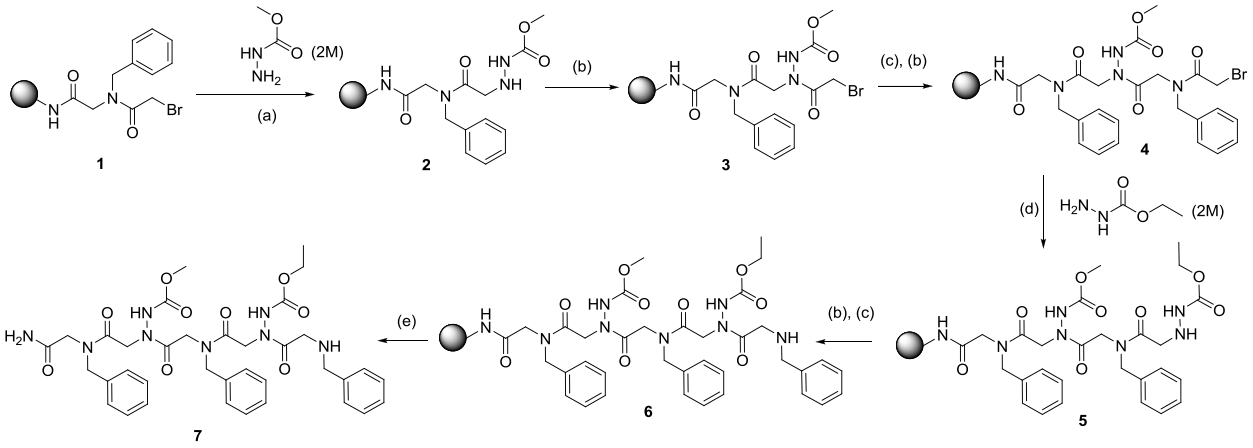
(v) **TFA cleavage:** The resin was treated with the cleavage cocktail of 96% TFA, 2% TIS and 2% water for 1h at room temperature. The cleavage cocktail solution was then dried by flushing argon and cold ether was added to precipitate out the compounds, which were then subjected to reverse phase HPLC to confirm the purity of the products.

Synthesis of the first tetramer peptoid-azapeptoid hybrid library by split and pool strategy: The synthesis of the peptoid-azapeptoid hybrid library was carried out on TentaGel Macrobeads NH_2 (1 g, 160 µm, 0.48 mmol/g) resin. The beads were incubated with anhydrous DMF for 1h and Fmoc-L- methionine (10 equiv.) was coupled using O-Benzotriazole-N,N,N’,N’-tetramethyl-uronium-hexafluoro-phosphate (HBTU) (10 equiv.), hydroxybenzotriazole **(**HOBt) monohydrate (10 equiv.) and N-methylmorpholine (NMM) (20 equiv.) for 2h. The beads were then washed thoroughly with DMF and the Fmoc group was deprotected by using 20 mL of 20% piperidine. After Fmoc deprotection, α-bromoacetic acid (10 mL, 2M) and DIC (10 mL, 3.4 M) was added to the resin, microwave-assisted acylation reaction was carried out (15 seconds, 10% power, 2×). The resin was then washed thoroughly by DMF and reacted with 2M solution of N-Boc-diamminobutane to displace the resin-bound bromide. The acylation and the displacement steps were further repeated two times. After two N-Boc-diamminobutane have been introduced, the beads were reacted with α-bromoacetic acid (10 mL, 2 M) and DIC (10 mL, 3.4 M) and microwave-assisted acylation reaction was carried out (15 seconds, 10% power, 2×). After the acylation reaction was complete, the beads washed with DMF and were treated with isobutyl amine (2M). After the Met-Nlys-Nlys-Nleu linker was synthesized, the beads were reacted with

α-bromoacetic acid (10 mL, 2 M) and DIC (10 mL, 3.4 M) and microwave-assisted acylation reaction was carried out (15 seconds, 10% power, 2×). After the acylation reaction was complete, the beads washed with DMF and splitted into thirteen reaction vessels in roughly equal amount, and each vessel was treated with a monomer (2 mL, 2 M in NMP) and the bromide displacement reactions were carried out for 1h at 37 ºC. The beads were then washed extensively with DMF and pooled in a 25 mL reaction vessel and treated with α-bromoacetic acid (10 mL, 2 M) and DIC (10 mL, 3.4 M) and the acylation reaction was carried out for 10 mins at 37 ºC. The bromide displacement and acylation reactions were repeated until the tetramer aza-peptoid was obtained. 50 mg of each of the resin-bound peptoid library was treated with 1mL TFA cleavage cocktail (96% TFA: 2% TIS: 2%Water) and few beads were picked up for CNBr cleavage. Each bead was isolated into a single well of a 96-well plate and treated with 20 µL of a CNBr solution (30 mg/mL in 0.1 N HCl) and incubated at 60 ºC for 1h. The cleavage mixture was removed by evaporation and the resulting residue was dissolved in CH_3CN/H_2O (50:50) and submitted to tandem MALDI mass spectrometry for sequencing analysis.

Synthesis of the second tetramer peptoid-azapeptoid hybrid library by split and pool strategy:

The second library was synthesized using same protocol as described for first library. However, we used 75 µm TentaGel resin for this library synthesis.



Scheme S1. Synthesis of peptoid-azapeptoid hybrid **7**. (a) 37 ºC, 1h; (b) $BrCH_2COOH$ (2 M in DMF), DIC (2 M in DMF), 37 ºC, 10 mins; (c) Benzyl amine (2 M in DMF), 37 ºC, 1h; (d) 37 ºC,1h ; (e) TFA cocktail, 1h, rt.

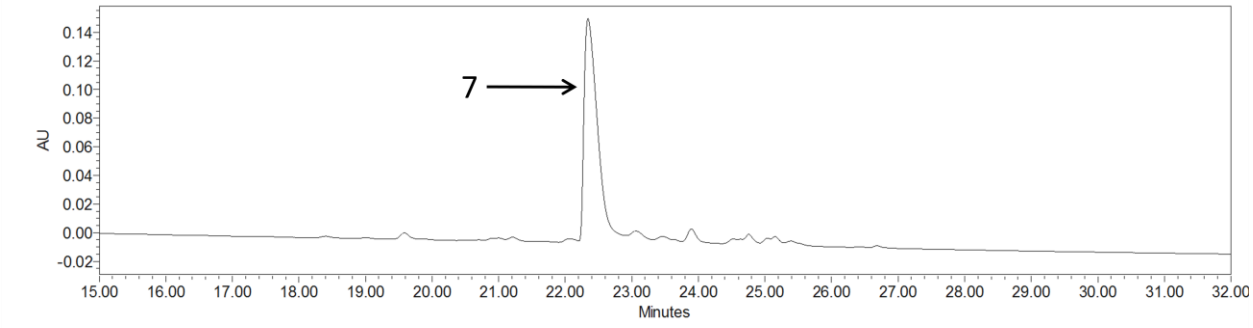


Figure S1. HPLC spectrum of crude reaction mixture of **7** obtained after TFA cleavage.

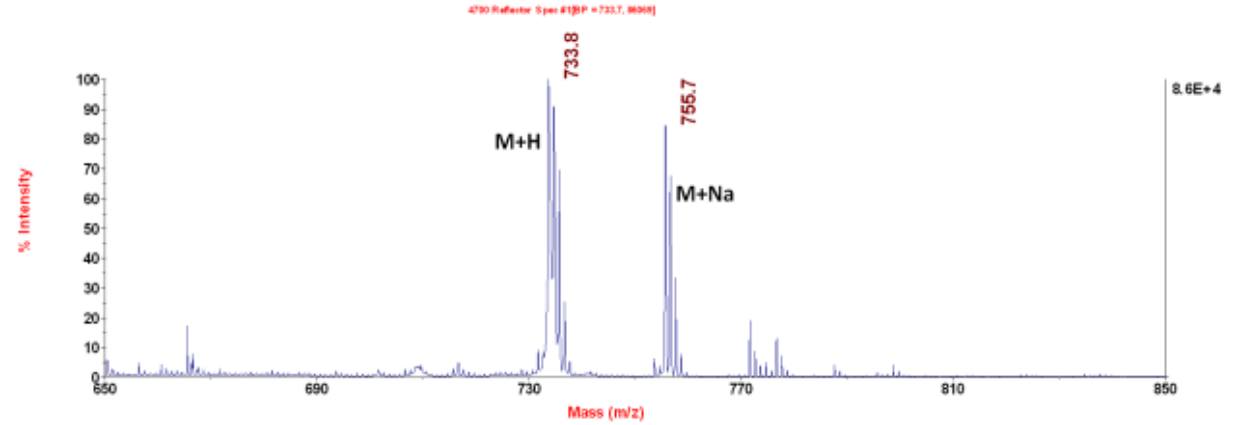


Figure S2. MALDI TOF MS spectra of HPLC purified 7.

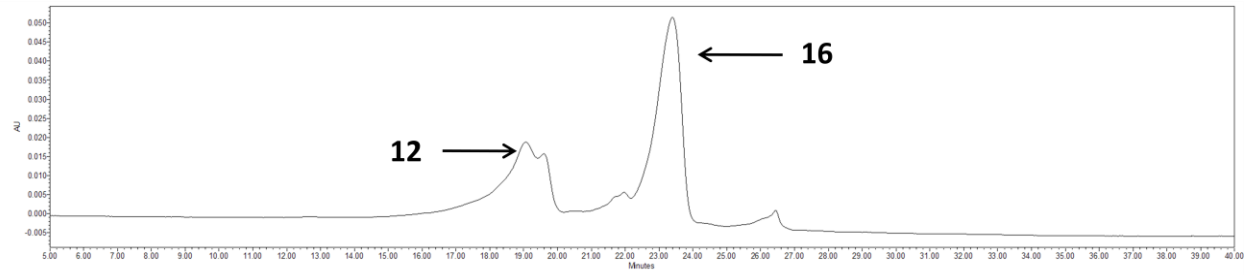


Figure S3. HPLC chromatogram of crude reaction mixture obtained from reaction of **8** with isopropyl amine.

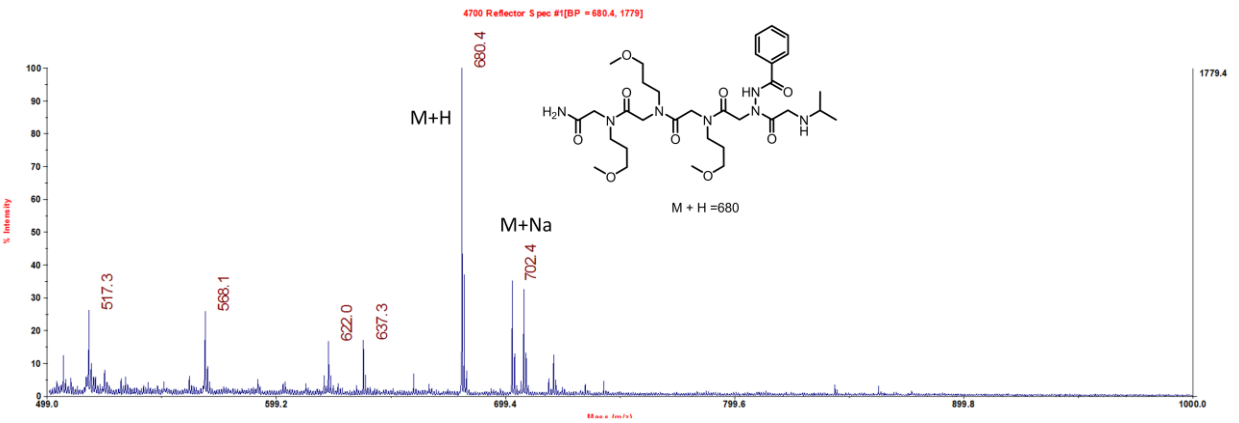


Figure S4. MALDI TOF MS spectrum purified **16** obtained from reaction of **8** with isopropyl amine.

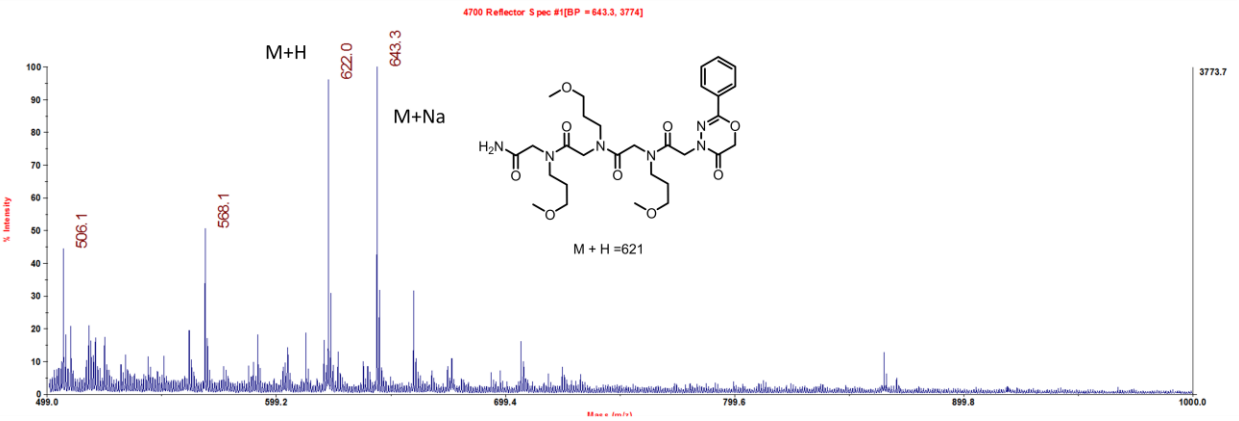


Figure S5. MALDI TOF MS spectrum purified **16** obtained from reaction of **8** with isopropyl amine.

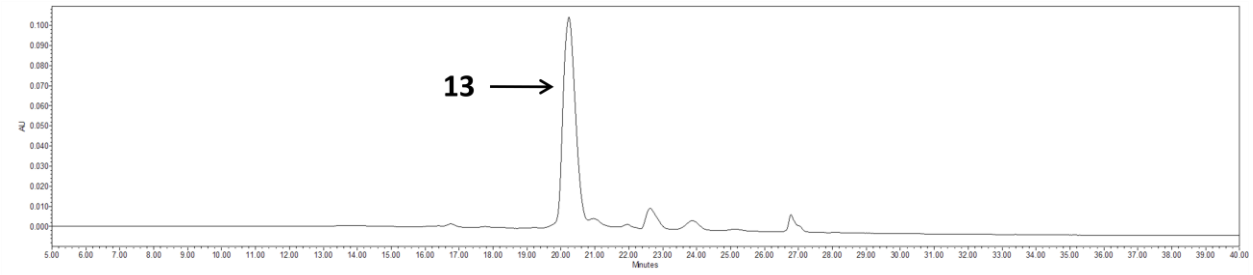


Figure S6. HPLC chromatogram of crude reaction mixture obtained from reaction of **9** with isopropyl amine.

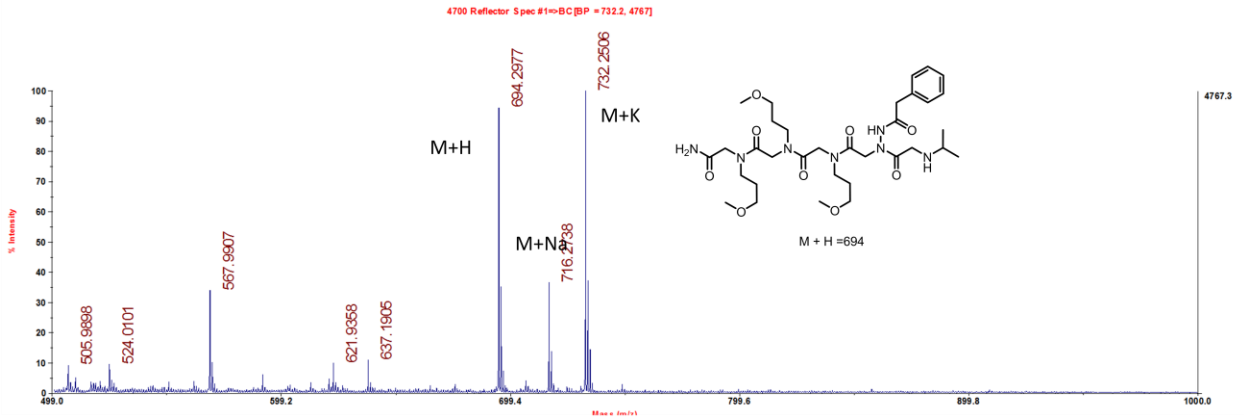


Figure S7. MALDI TOF MS spectrum purified **13** obtained from reaction of **9** with isopropyl amine.

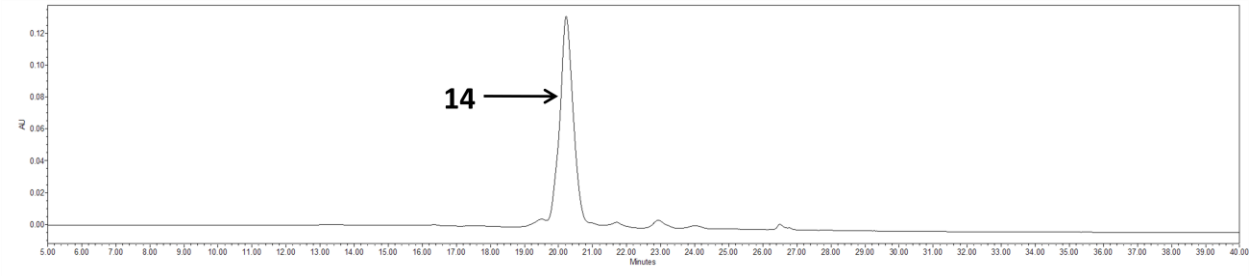


Figure S8. HPLC chromatogram of crude reaction mixture obtained from reaction of **10** with isopropyl amine.

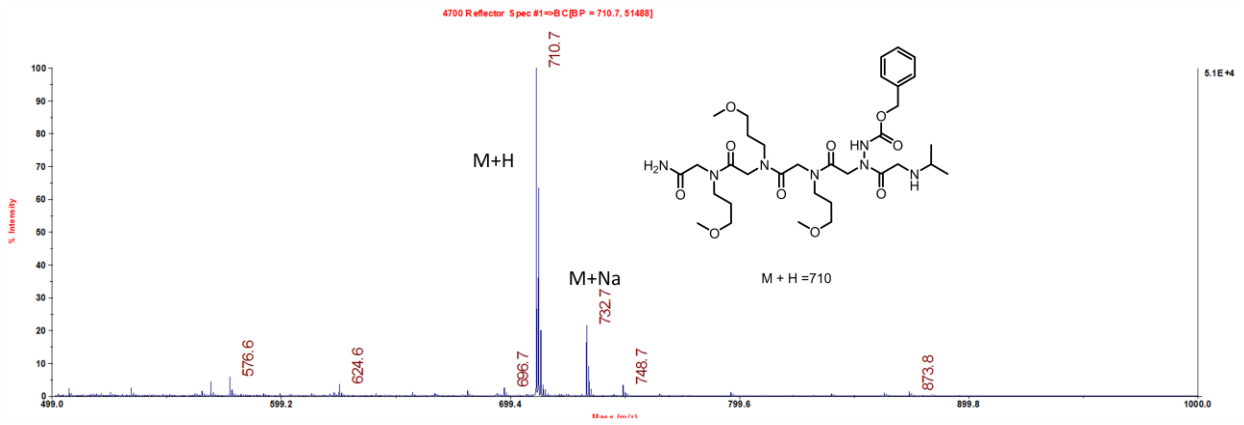


Figure S9. MALDI TOF MS spectrum purified **14** obtained from reaction of **10** with isopropyl amine.

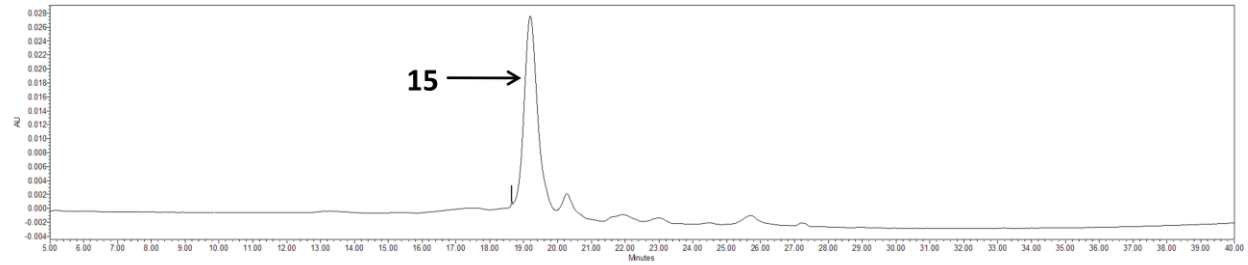


Figure S10. HPLC chromatogram of crude reaction mixture obtained from reaction of **10** with isopropyl amine.

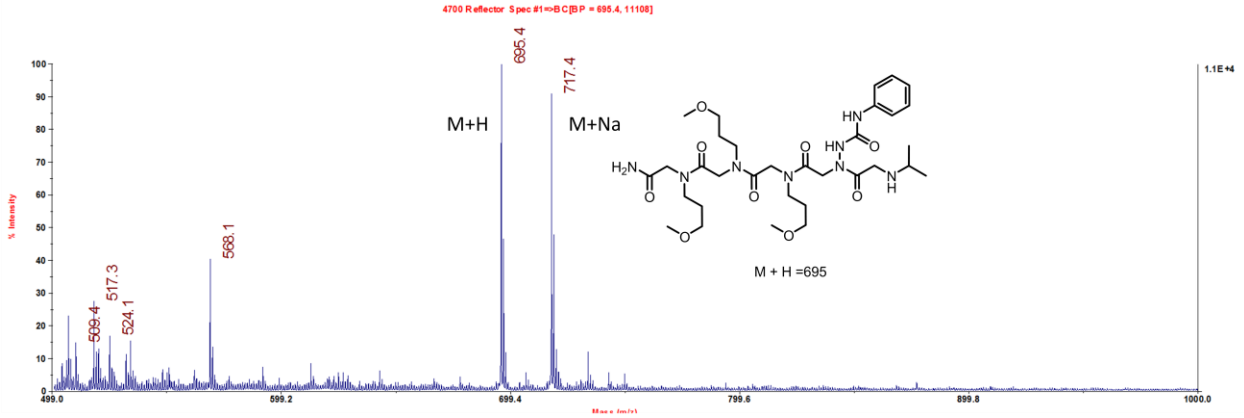


Figure S11. MALDI TOF MS spectrum purified **15** obtained from reaction of **10** with isopropyl amine.

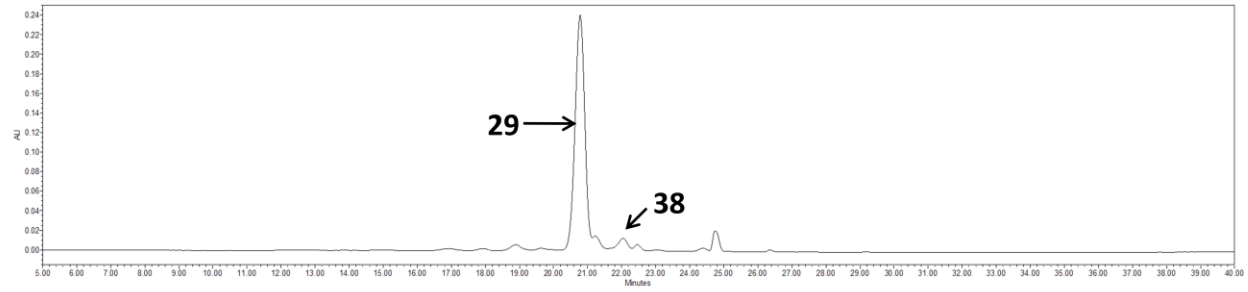


Figure S12. HPLC chromatogram of crude reaction mixture obtained from reaction of **20** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

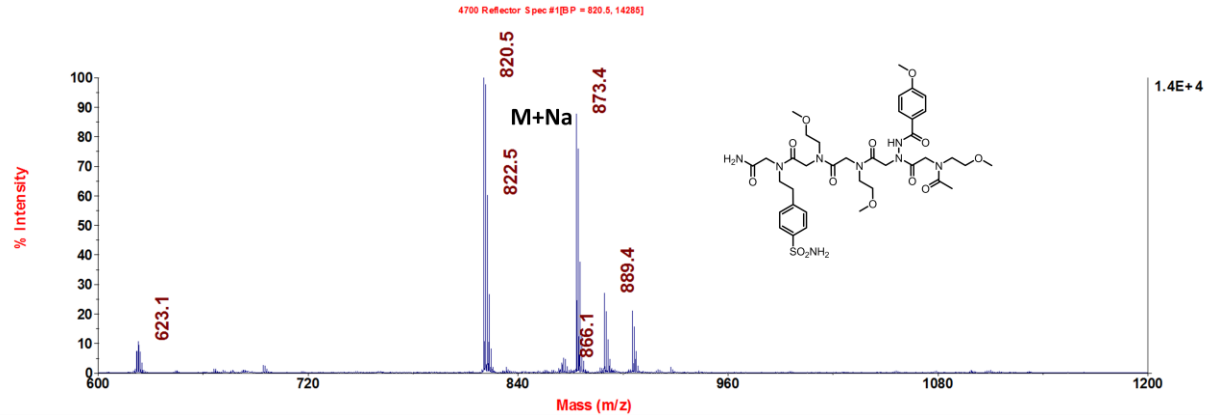


Figure S13. HPLC MALDI TOF MS spectrum purified **29** obtained from reaction of **20** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

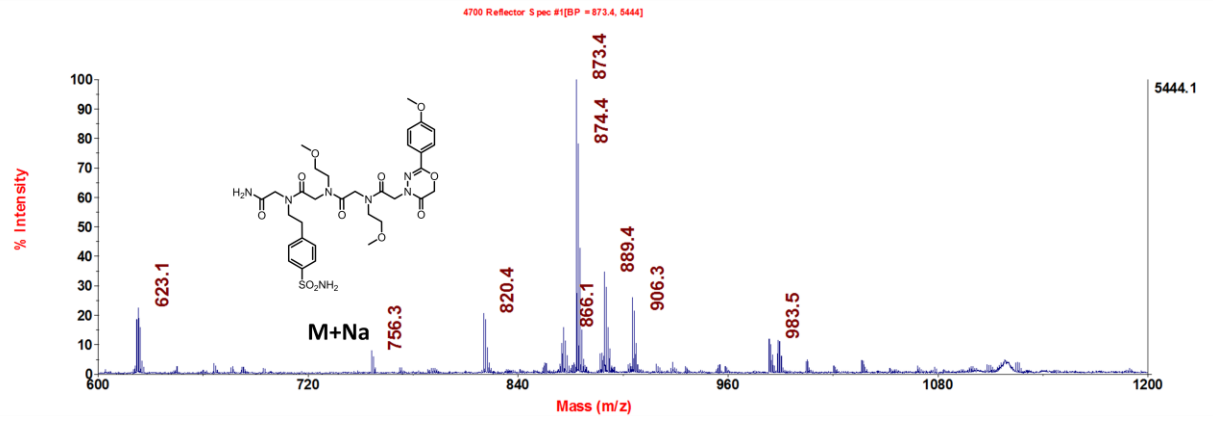


Figure S14. HPLC MALDI TOF MS spectrum purified **38** obtained from reaction of **20** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

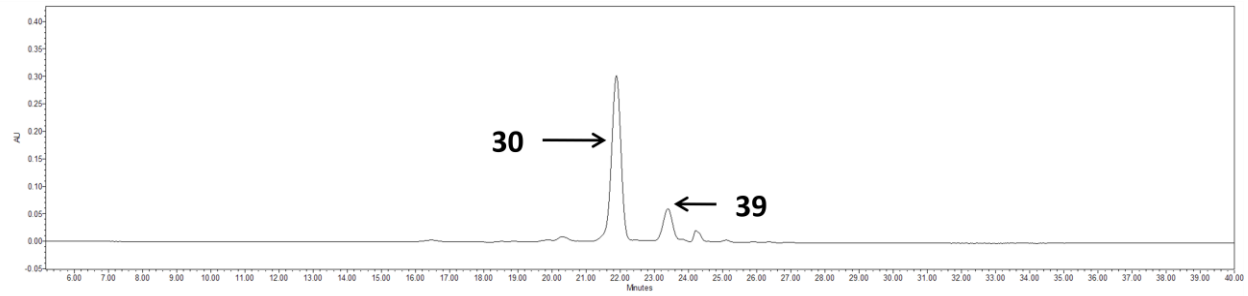


Figure S15. HPLC chromatogram of crude reaction mixture obtained from reaction of **21** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

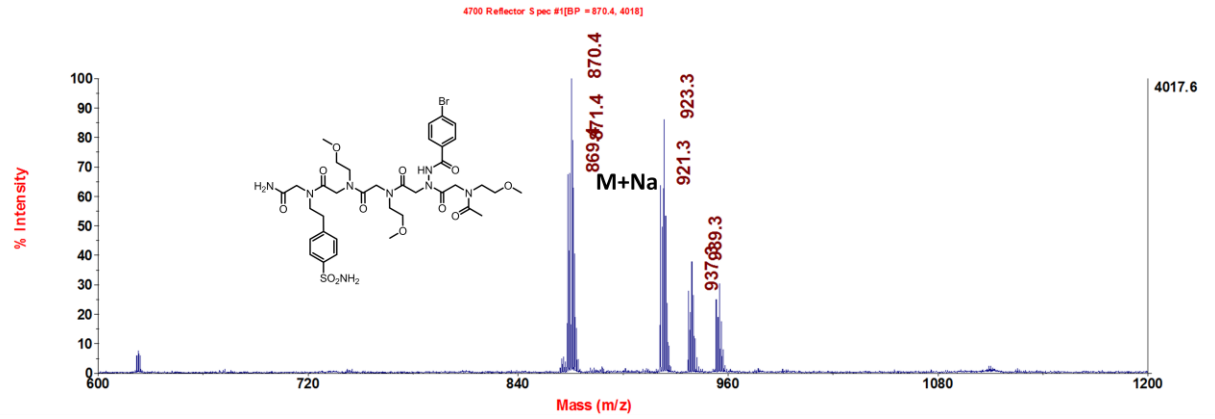


Figure S16. HPLC MALDI TOF MS spectrum purified **30** obtained from reaction of **21** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

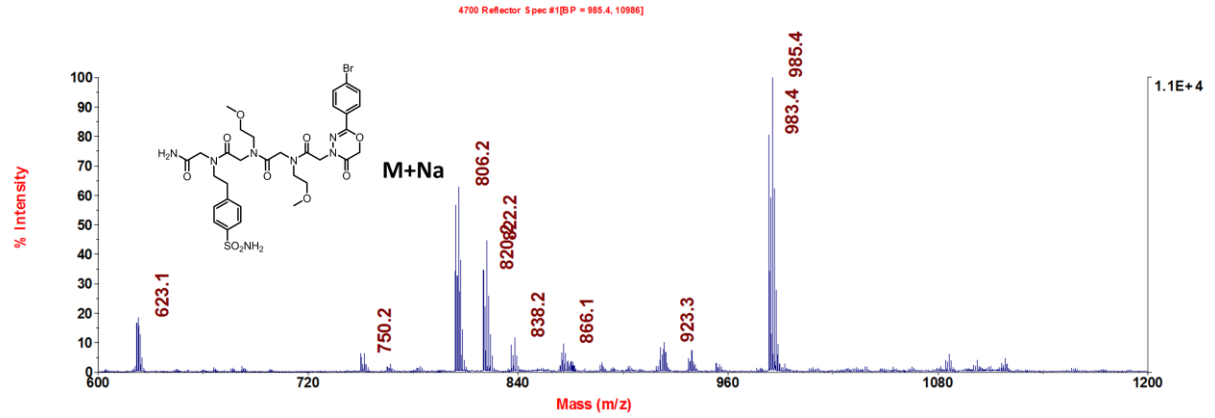


Figure S17. HPLC MALDI TOF MS spectrum purified **39** obtained from reaction of **21** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

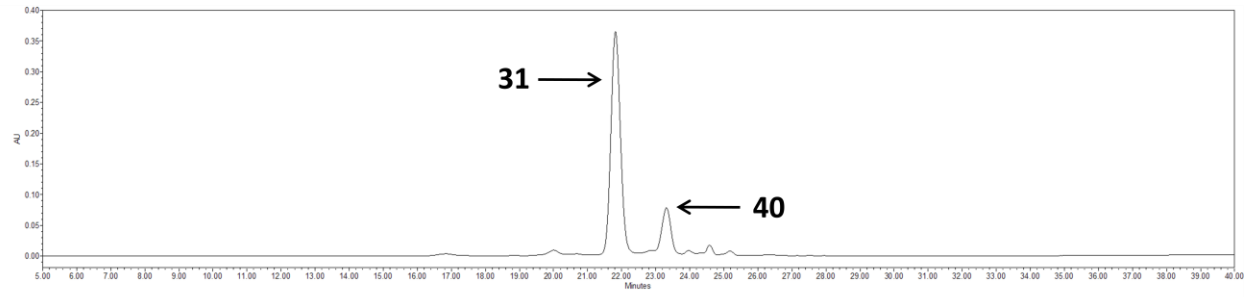


Figure S18. HPLC chromatogram of crude reaction mixture obtained from reaction of **22** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

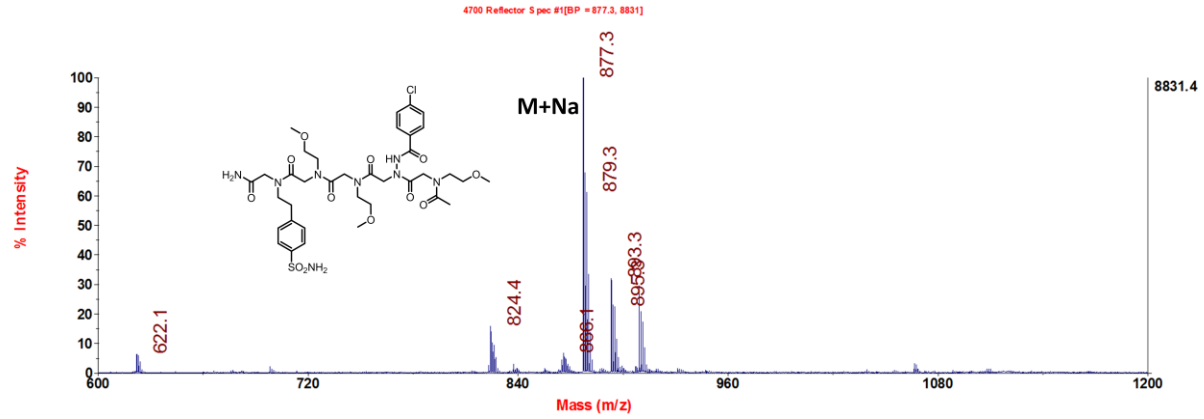


Figure S19. HPLC MALDI TOF MS spectrum purified **31** obtained from reaction of **22** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

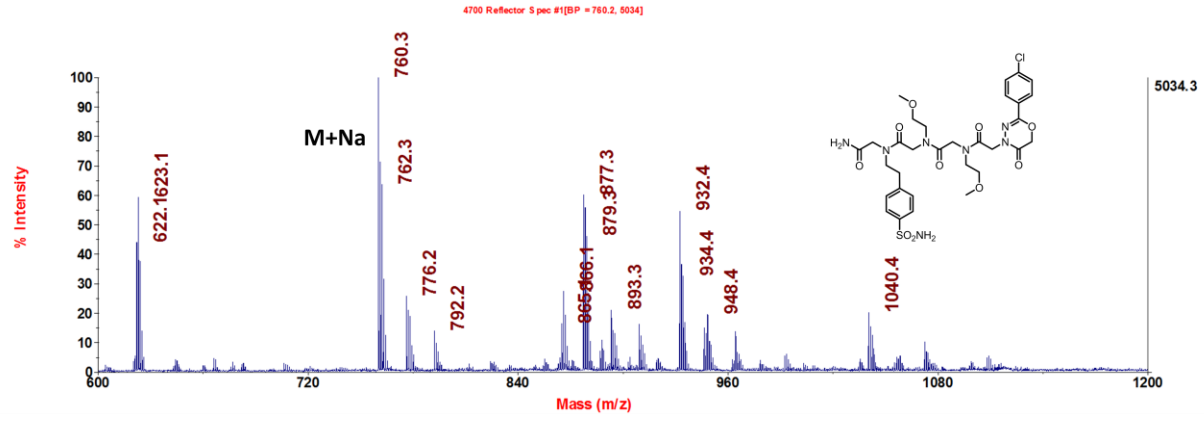


Figure S20. HPLC MALDI TOF MS spectrum purified **40** obtained from reaction of **22** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

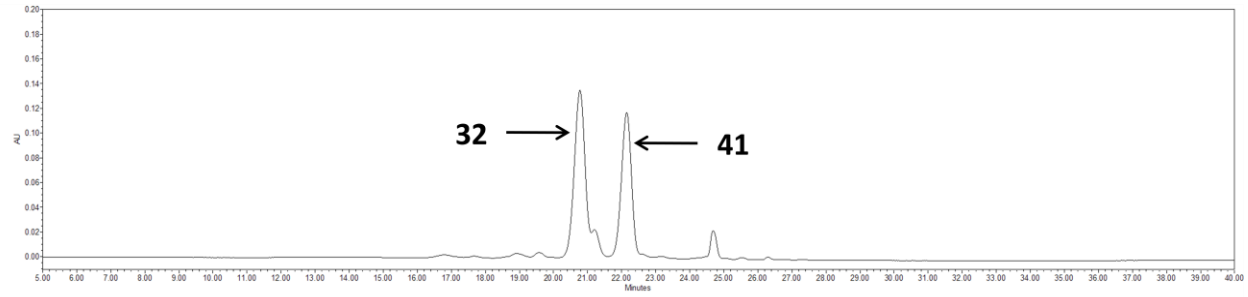


Figure S21. HPLC chromatogram of crude reaction mixture obtained from reaction of **23** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

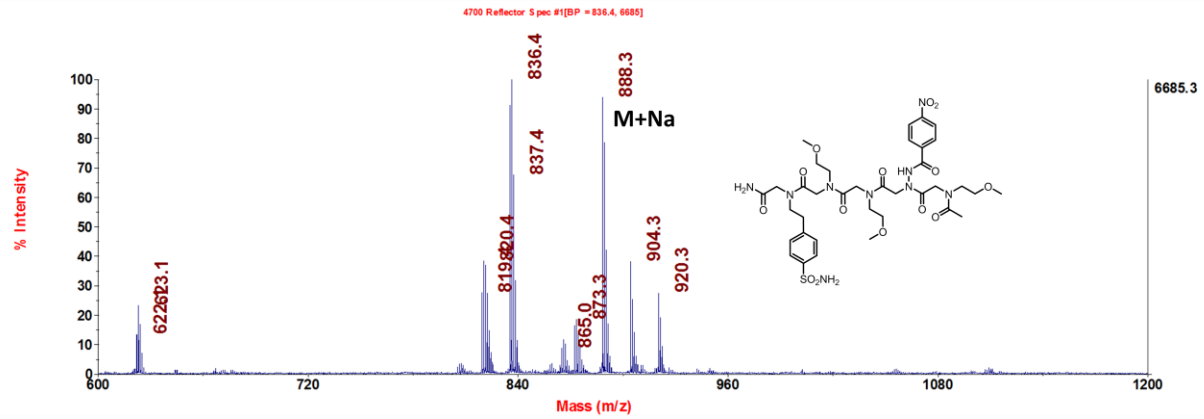


Figure S22. HPLC MALDI TOF MS spectrum purified **32** obtained from reaction of **23** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

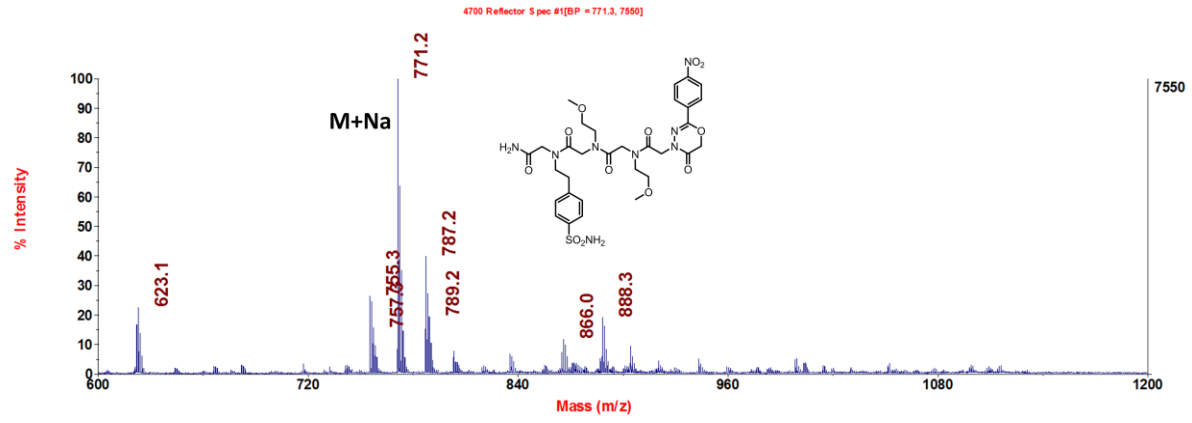


Figure S23. HPLC MALDI TOF MS spectrum purified **41** obtained from reaction of **23** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

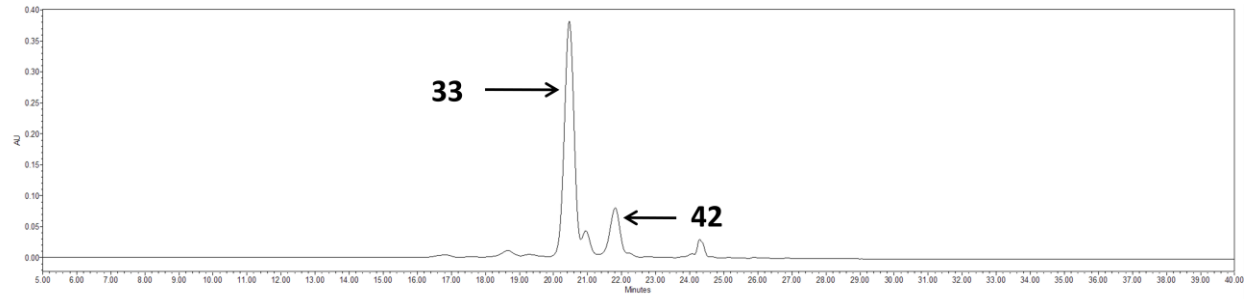


Figure S24. HPLC chromatogram of crude reaction mixture obtained from reaction of **24** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

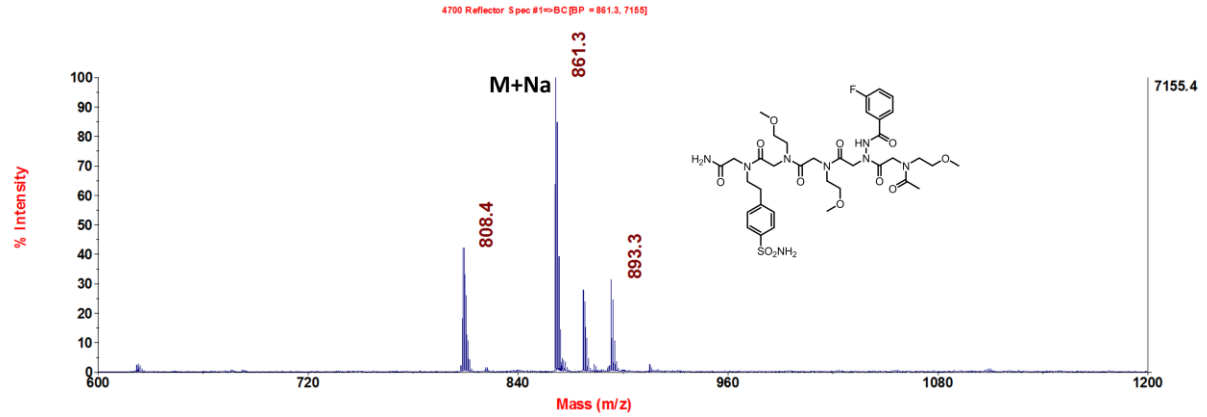


Figure S25. HPLC MALDI TOF MS spectrum purified **33** obtained from reaction of **24** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

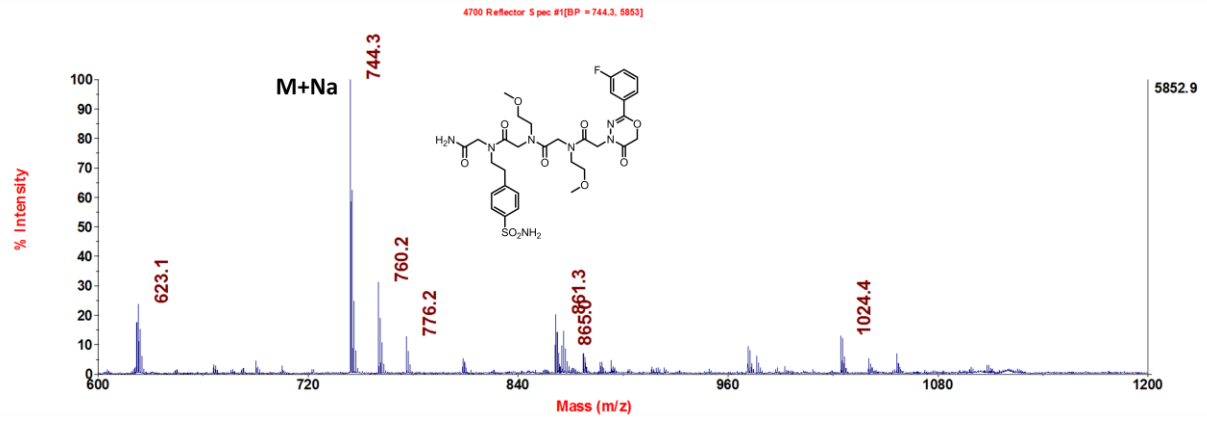


Figure S26. HPLC MALDI TOF MS spectrum purified **42** obtained from reaction of **24** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

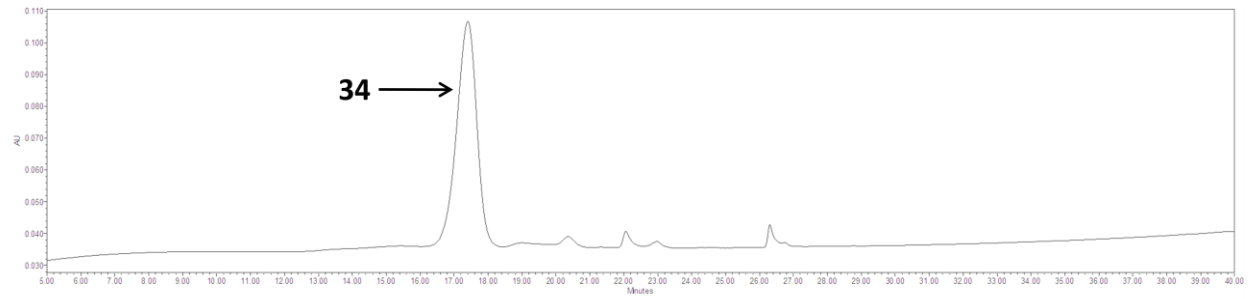


Figure S27. HPLC chromatogram of crude reaction mixture obtained from reaction of **25** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

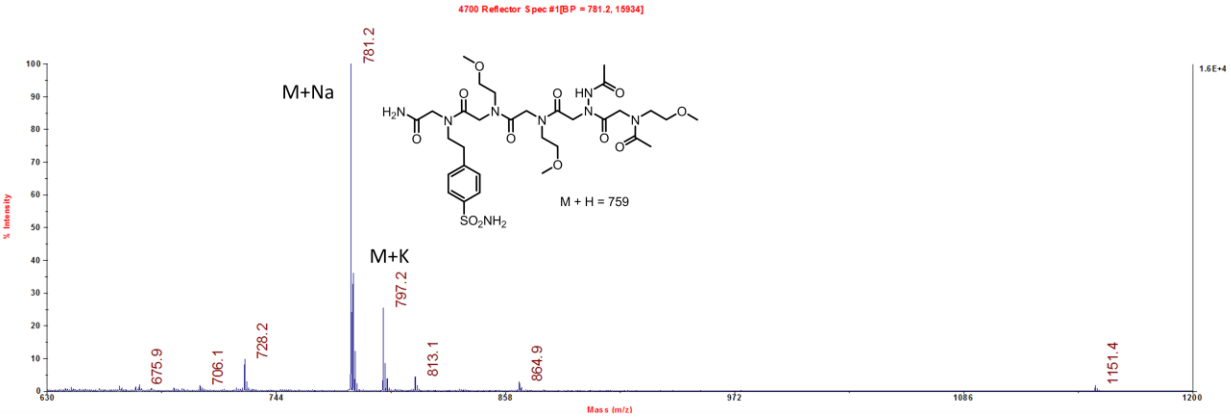


Figure S28. MALDI TOF MS spectrum purified **34** obtained from reaction of **25** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

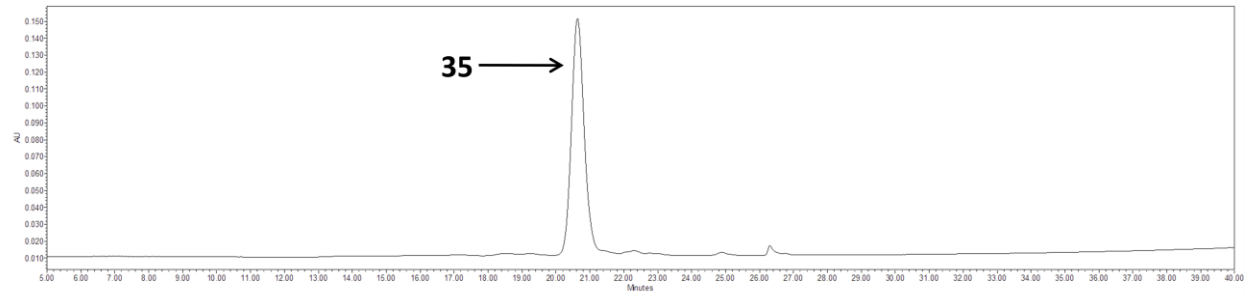


Figure S29. HPLC chromatogram of crude reaction mixture obtained from reaction of **26** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

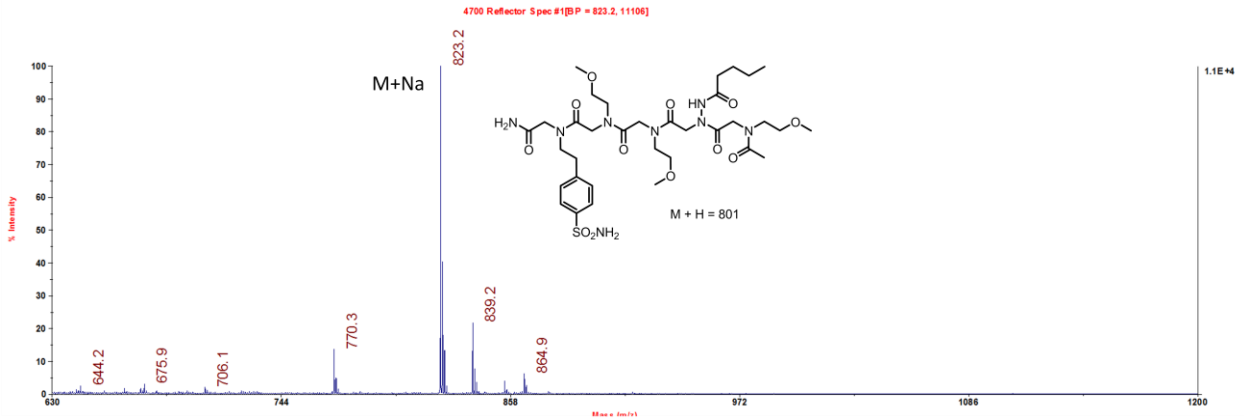


Figure S30. MALDI TOF MS spectrum purified **35** obtained from reaction of **26** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

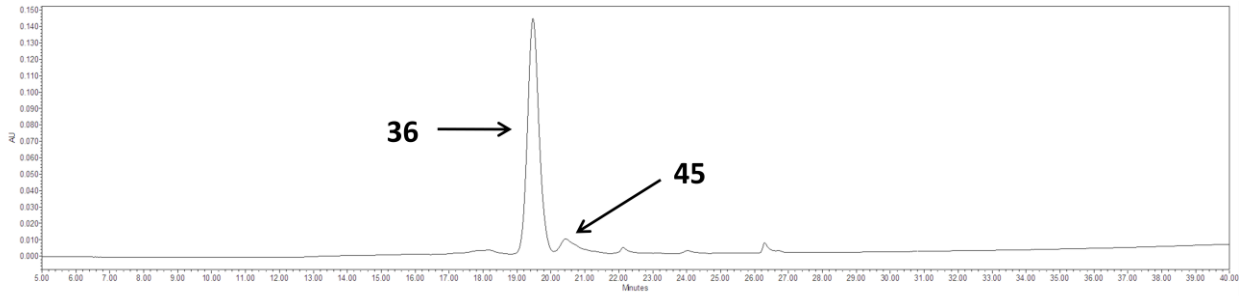


Figure S31. HPLC chromatogram of crude reaction mixture obtained from reaction of **27** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

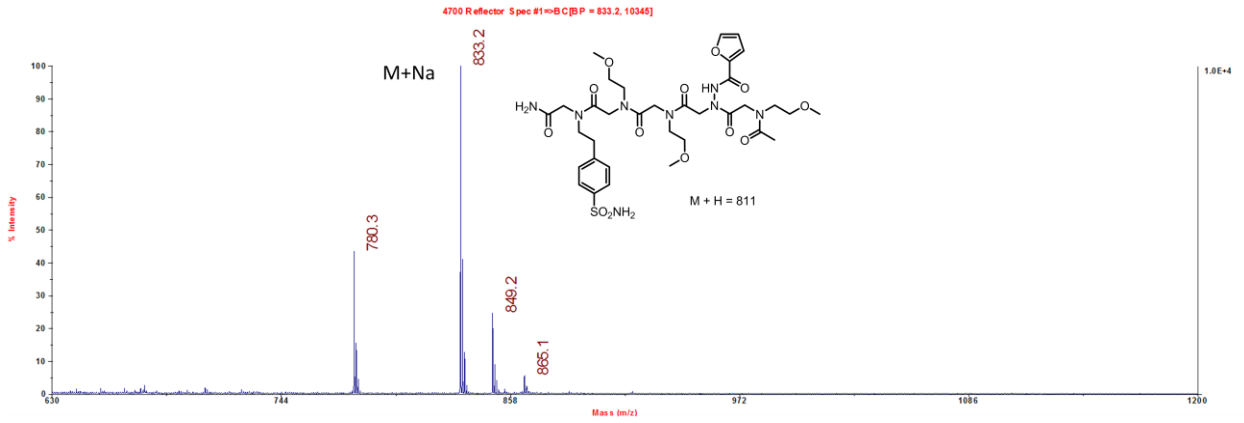


Figure S32. MALDI TOF MS spectrum purified **36** obtained from reaction of **27** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

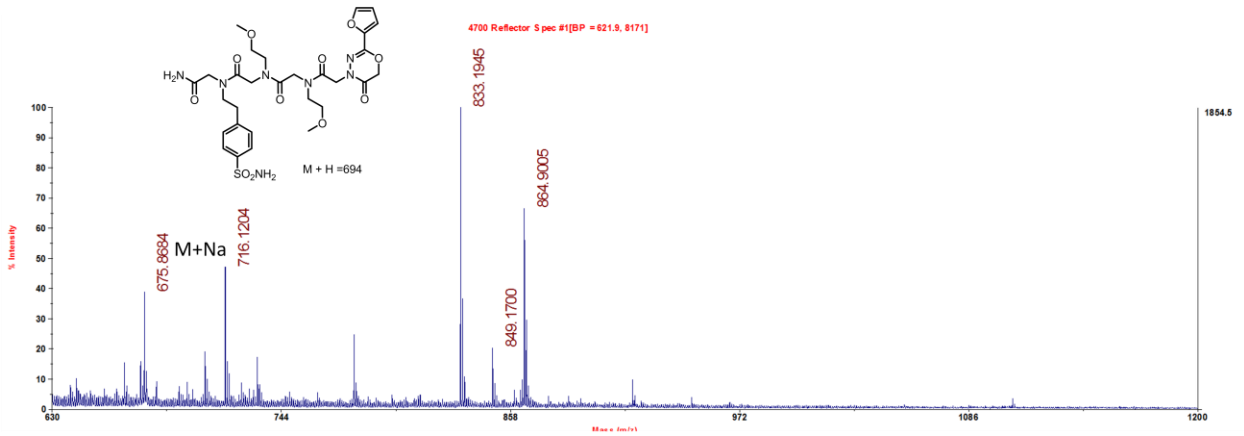


Figure S33. MALDI TOF MS spectrum purified **45** obtained from reaction of **27** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

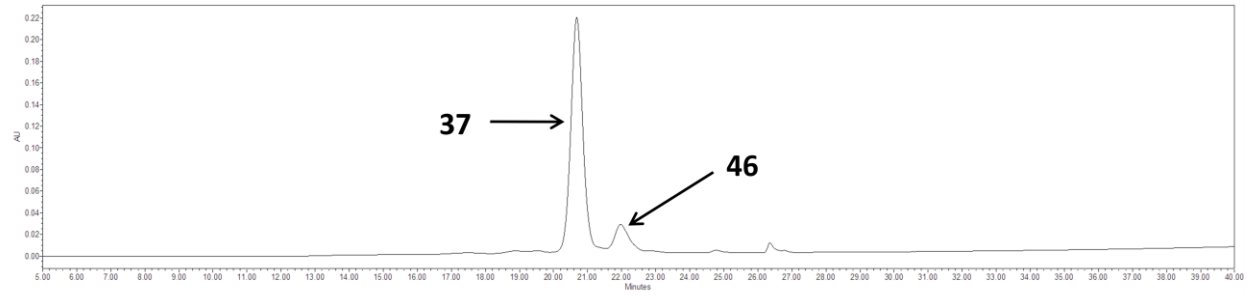


Figure S34. HPLC chromatogram of crude reaction mixture obtained from reaction of **28** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

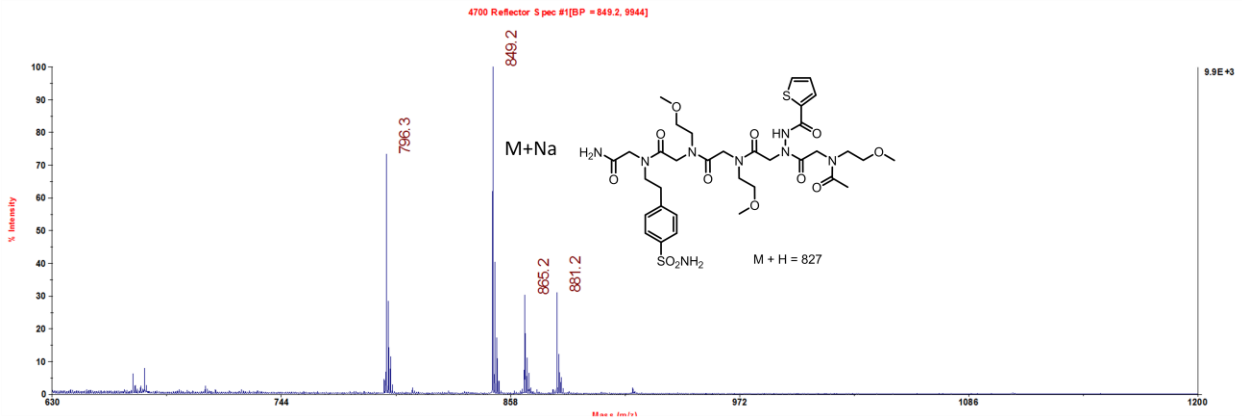


Figure S35. MALDI TOF MS spectrum purified **37** obtained from reaction of **28** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

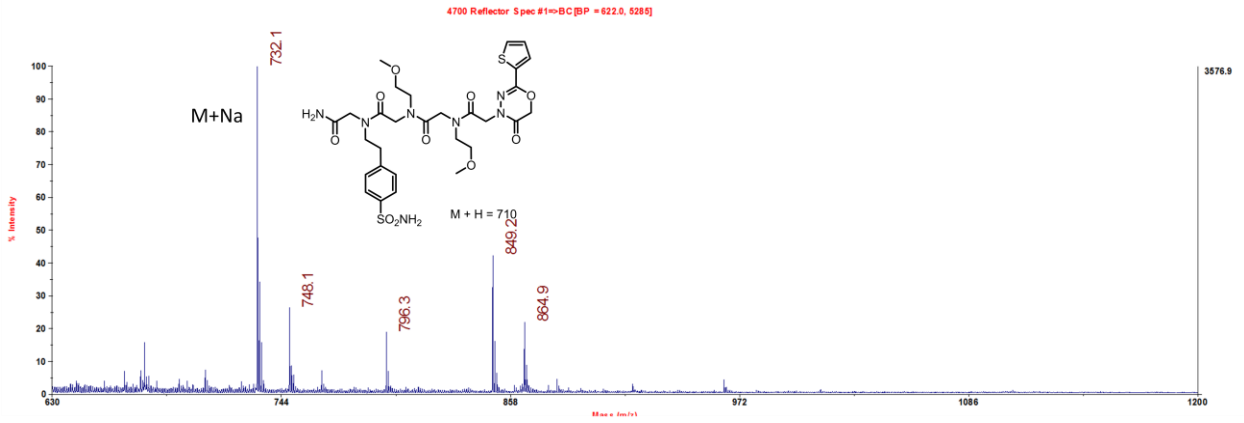


Figure S36. MALDI TOF MS spectrum purified **46** obtained from reaction of **28** with 2-methoxyethyl amine followed by capping with acetic acid and diisopropylcarbodiimide.

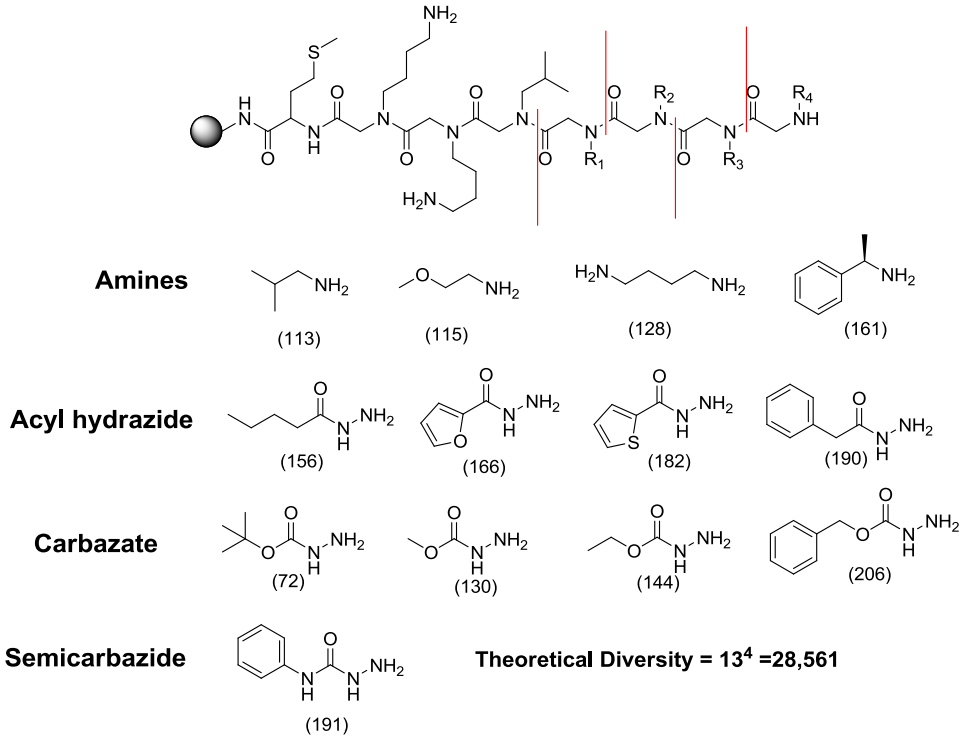
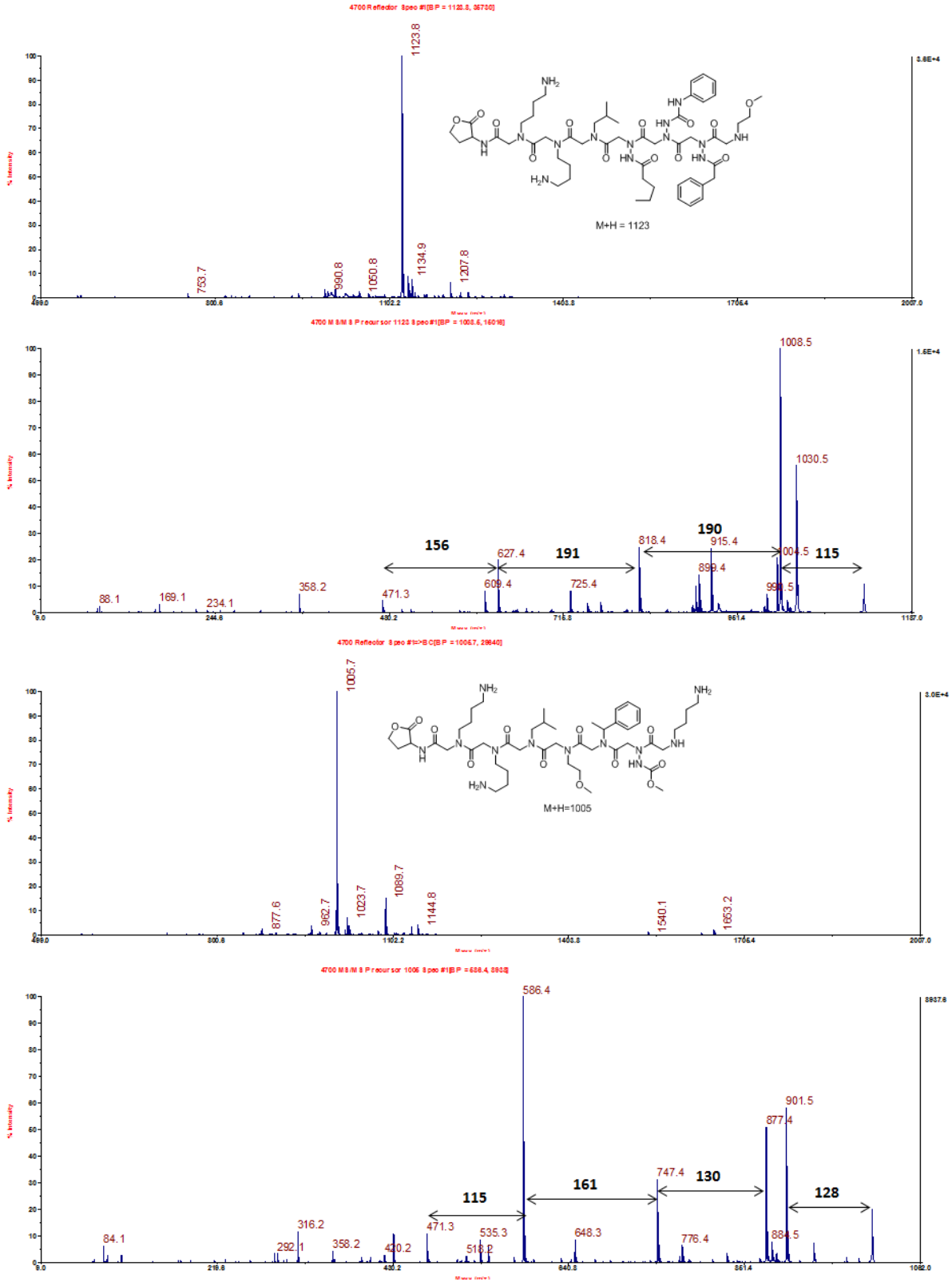
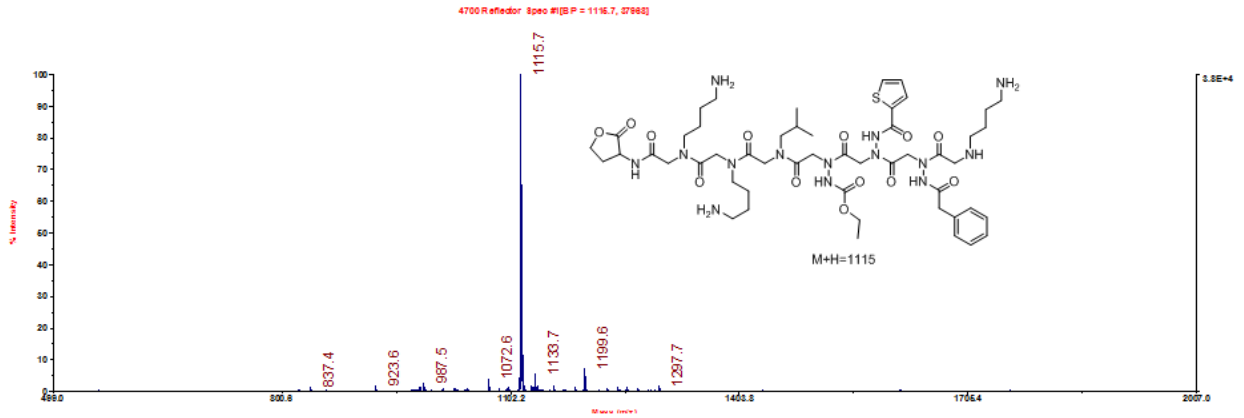
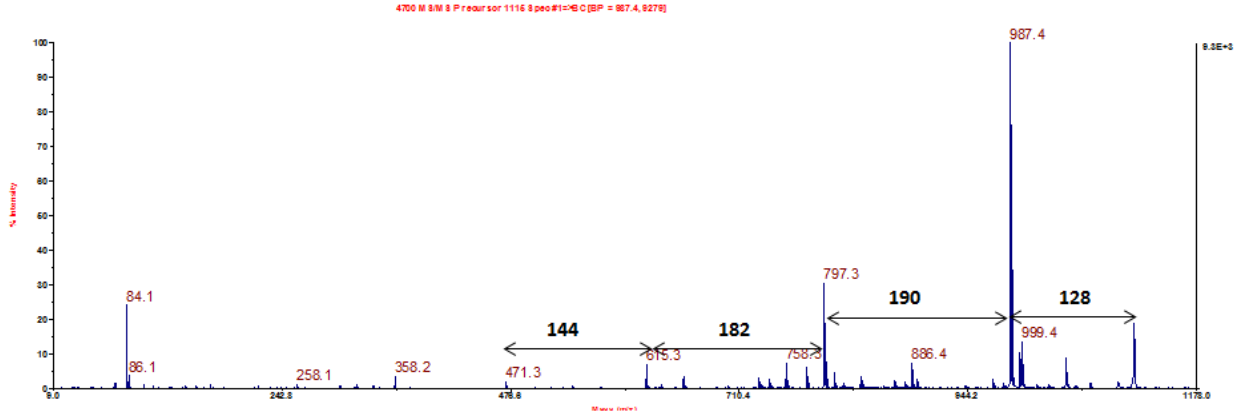


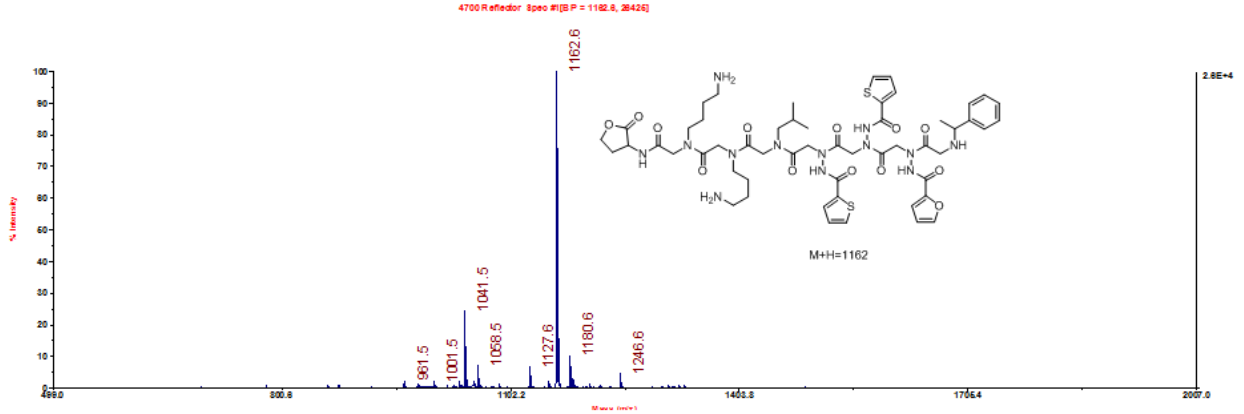
Figure S37. General structure of tetramer hybrid peptoid-azapeptoid library and the chemical structure of the different sub-monomers used in positions R1-R4. The numbers in the parentheses indicates the mass of the fragment that cleaves off the oligomer in MALDI TOF MS MS when that particular monomer is involved. (The numbers below the sub-monomers indicate the mass loss during MALDI TOF MS MS for respective sub-monomers present at particular position).

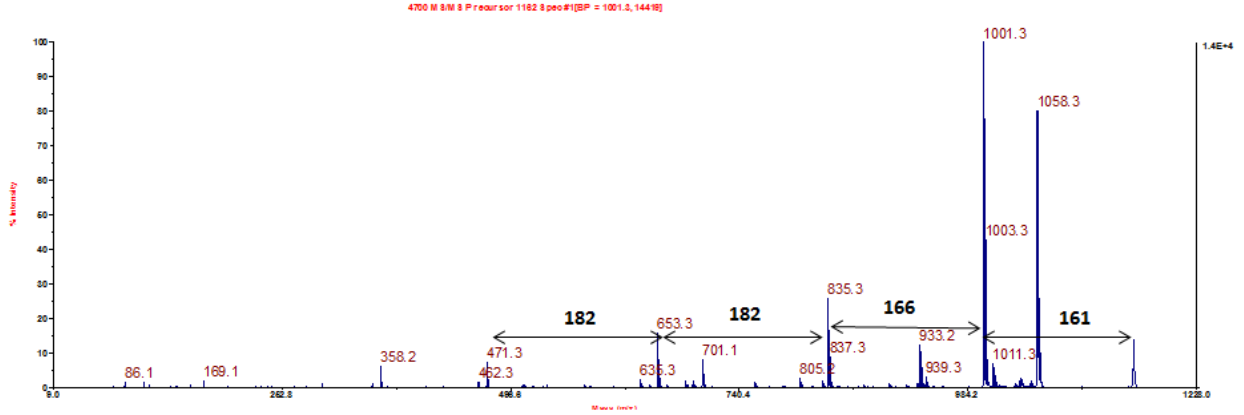
Figure S38. Representative MALDI TOF MS and MSMS spectra of some compounds of the tetramer peptoid-azapeptoid hybrid library obtained after single bead cleavage by using CNBr.

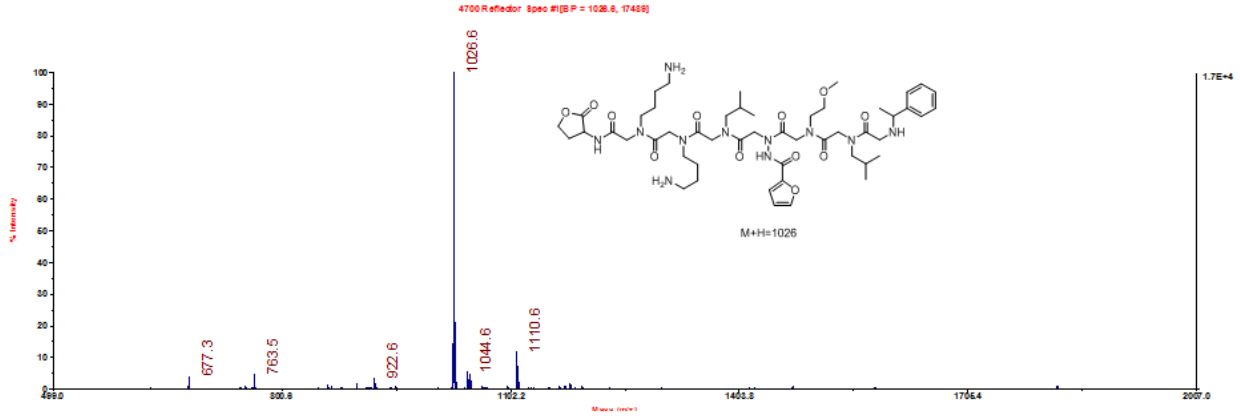


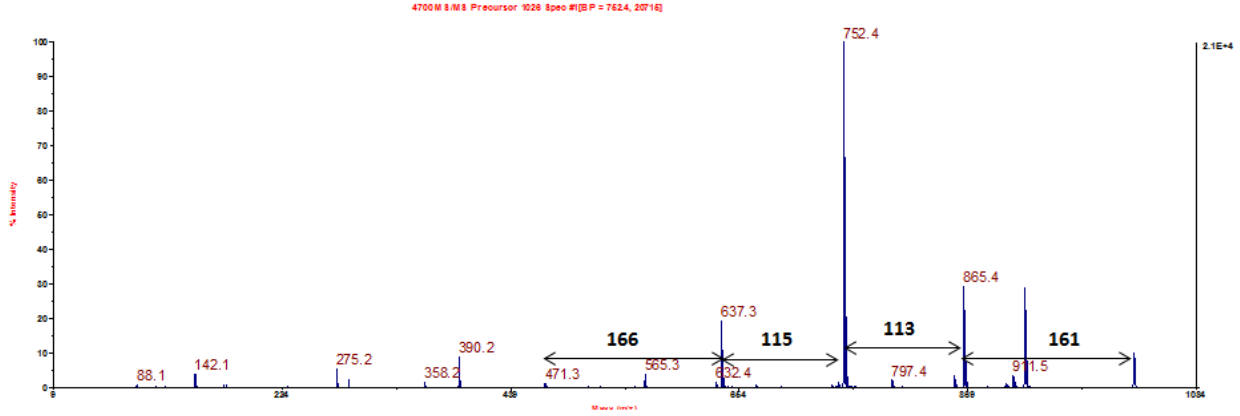

4700 Reflector Spec #1[BP = 1115.7, 37983]
1115.7
837.4
923.6
987.5
1072.6
1133.7
1199.6
1297.7
M+H=1115

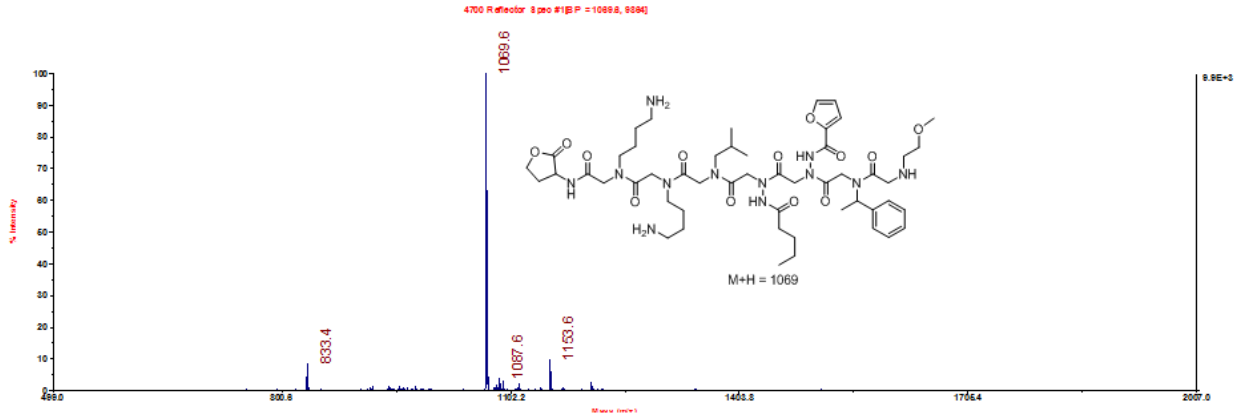

4700 MS/MS Precursor 1115 Spec#1=>BC[BP = 987.4, 9279]
987.4
797.3
84.1
86.1
258.1
358.2
471.3
615.3
758.5
886.4
999.4
144
182
190
128

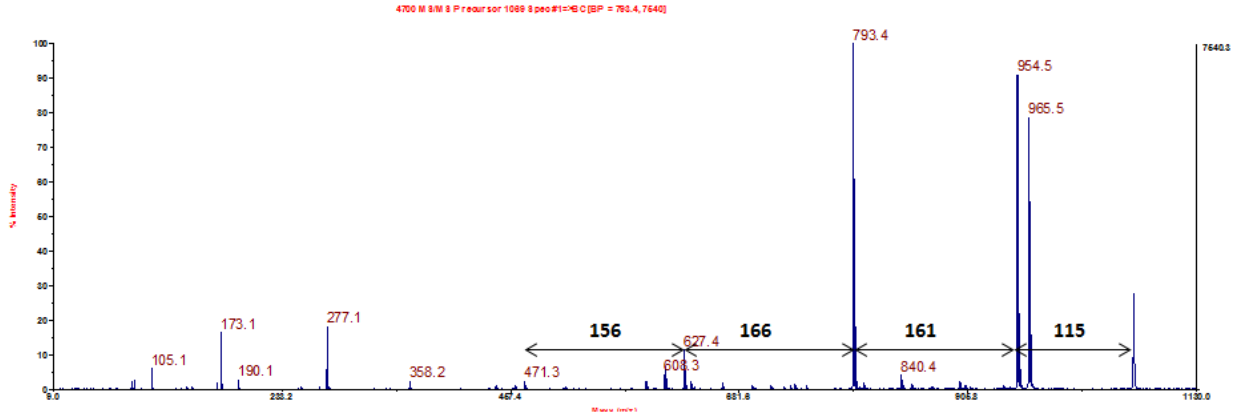

4700 Reflector Spec #1[BP = 1162.6, 28426]
1162.6
961.5
1001.5
1041.5
1068.5
1127.6
1180.6
1246.6
M+H=1162

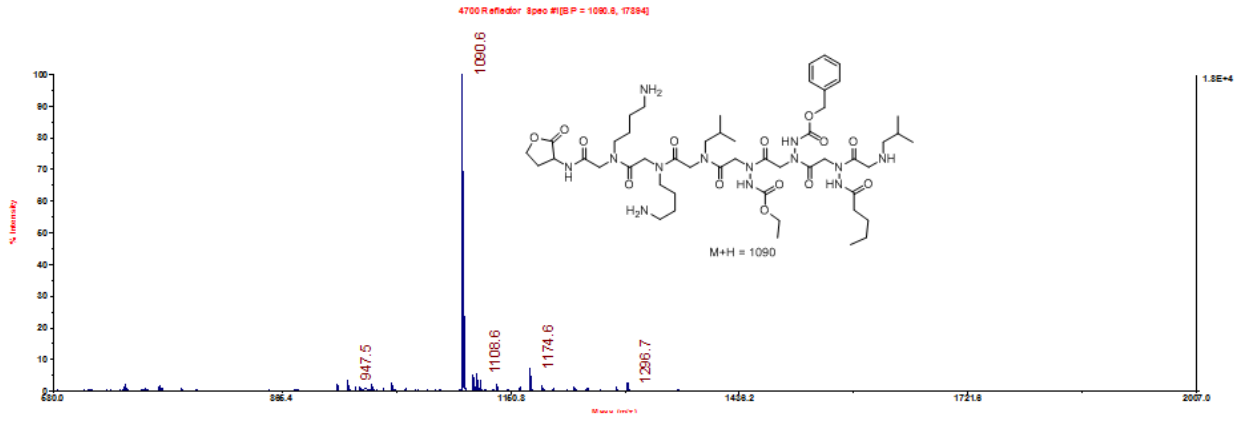

4700 MS/MS Precursor 1162 Spec#1[BP = 1001.3, 14416]
1001.3
1058.3
1003.3
835.3
653.3
471.3
701.1
837.3
933.2
1011.3
939.3
805.2
636.3
462.3
358.2
169.1
86.1
182
182
166
161

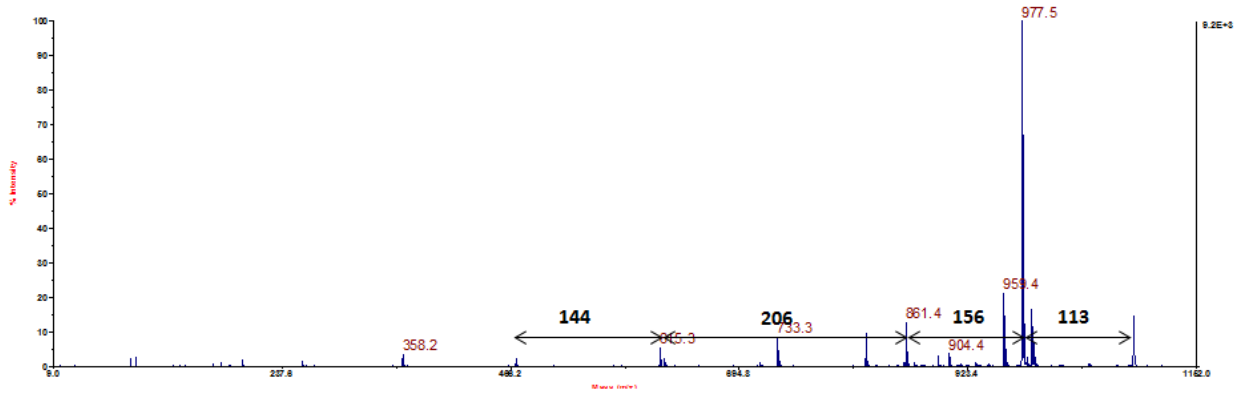

4700 Reflector Spec #1[BP = 1026.6, 17439]
1026.6
677.3
763.5
922.6
1044.6
1110.6
M+H=1026

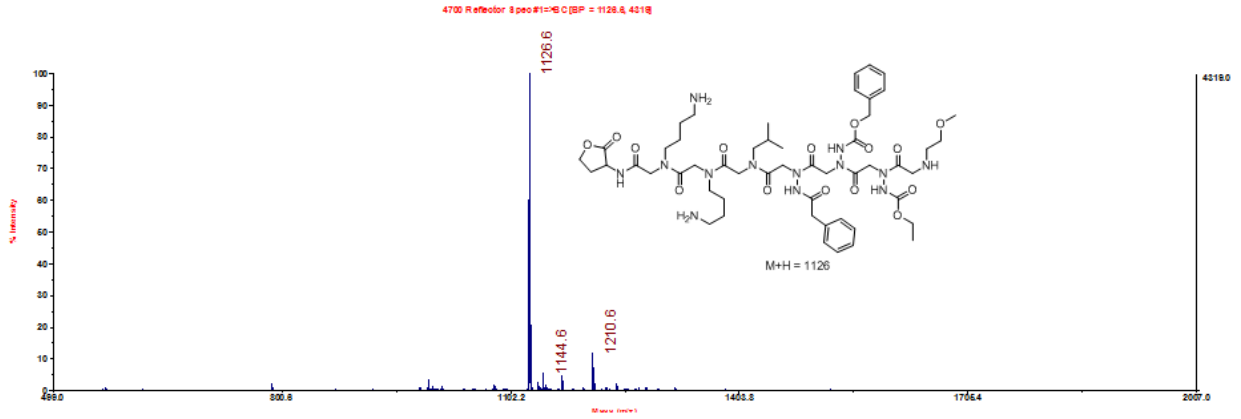

4700 MS/MS Precursor 1026 Spec #1[BP = 752.4, 20716]
752.4
637.3
865.4
166
115
113
161
88.1
142.1
275.2
390.2
358.2
471.3
565.3
632.4
797.4
911.5

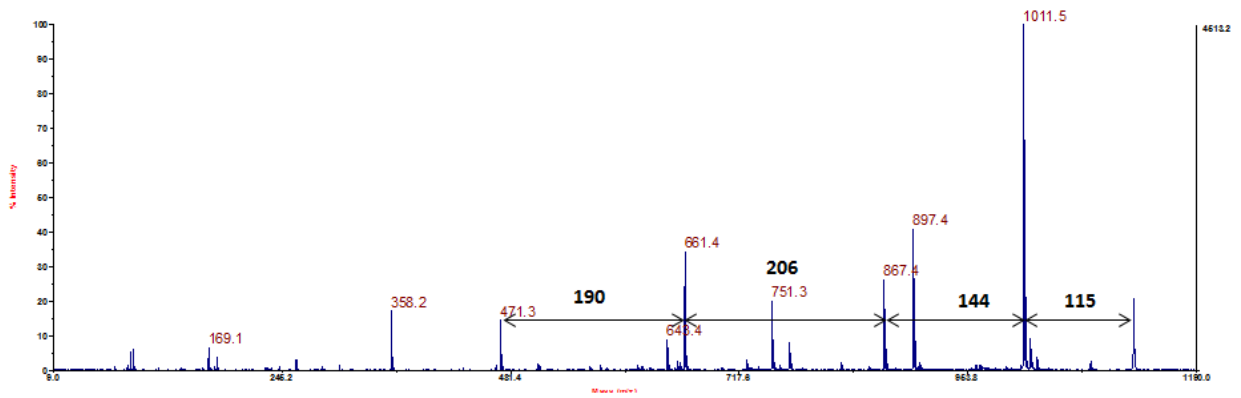

4700 Reflector Spec #1[BP = 1069.6, 9384]
1069.6
833.4
1087.6
1153.6
M+H = 1069

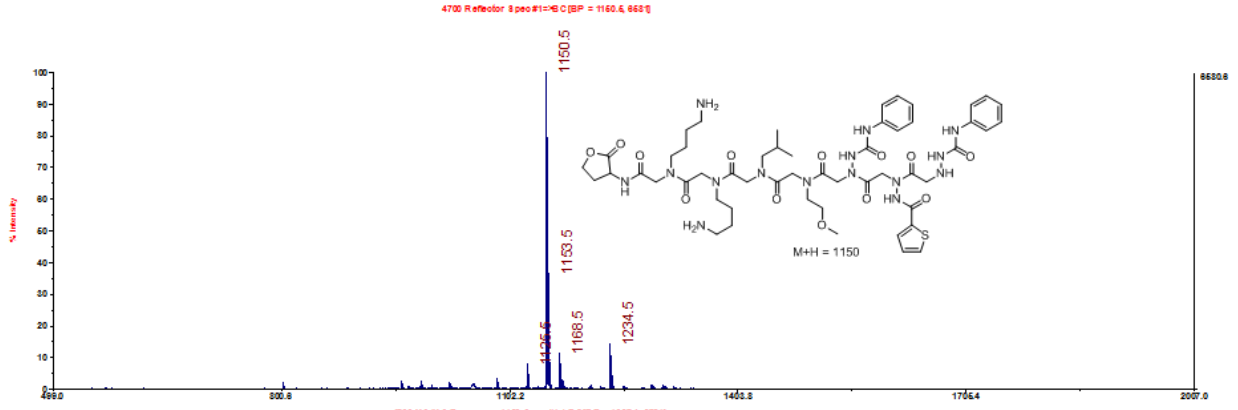

4700 MS/MS Precursor 1069 Spec #1=>BC[BP = 793.4, 7640]
793.4
954.5
965.5
173.1
277.1
105.1
190.1
358.2
471.3
627.4
608.3
840.4
156
166
161
115

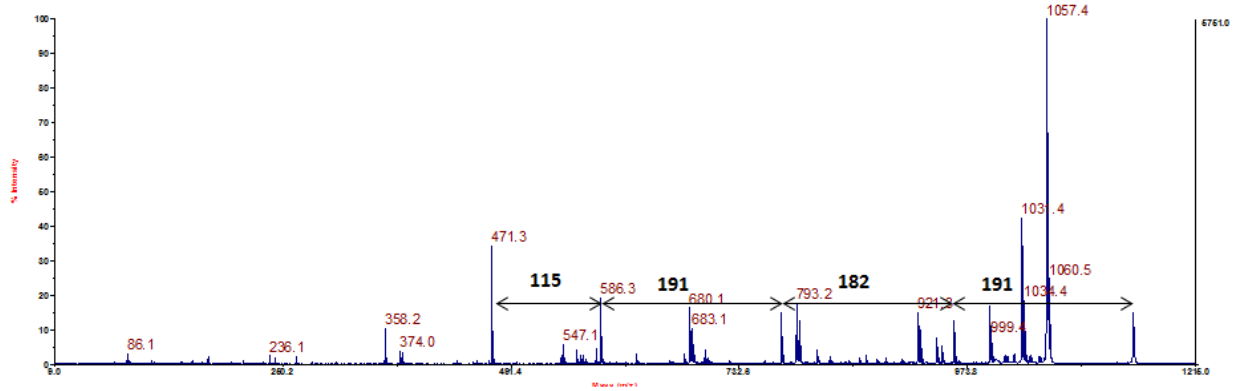

1090.6
947.5
1108.6
1174.6
1296.7
M+H = 1090

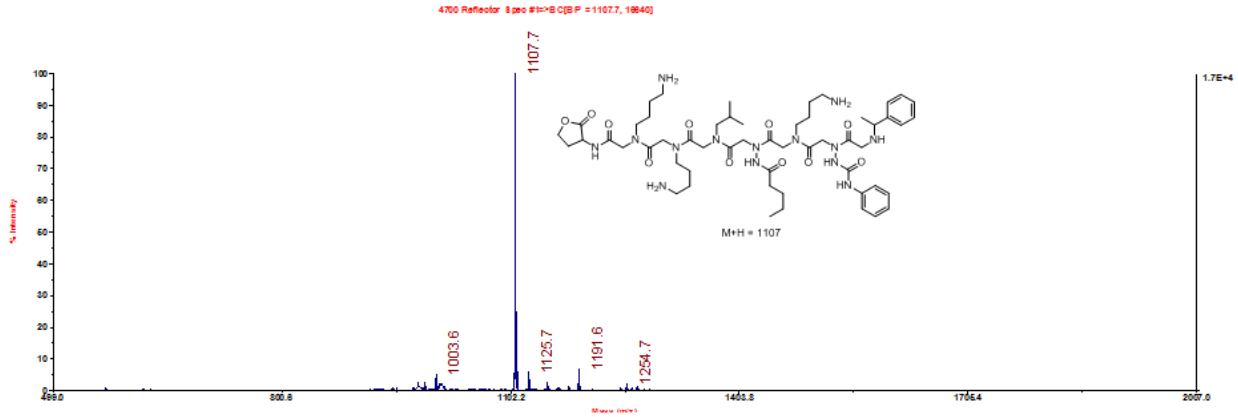

977.5
959.4
144
206
861.4
156
113
733.3
358.2
904.4

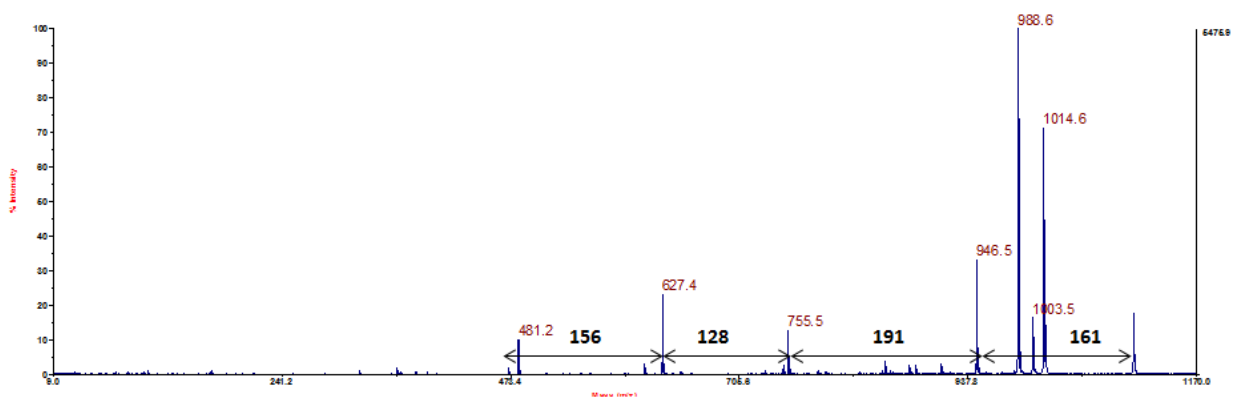

1126.6
1144.6
1210.6
M+H = 1126

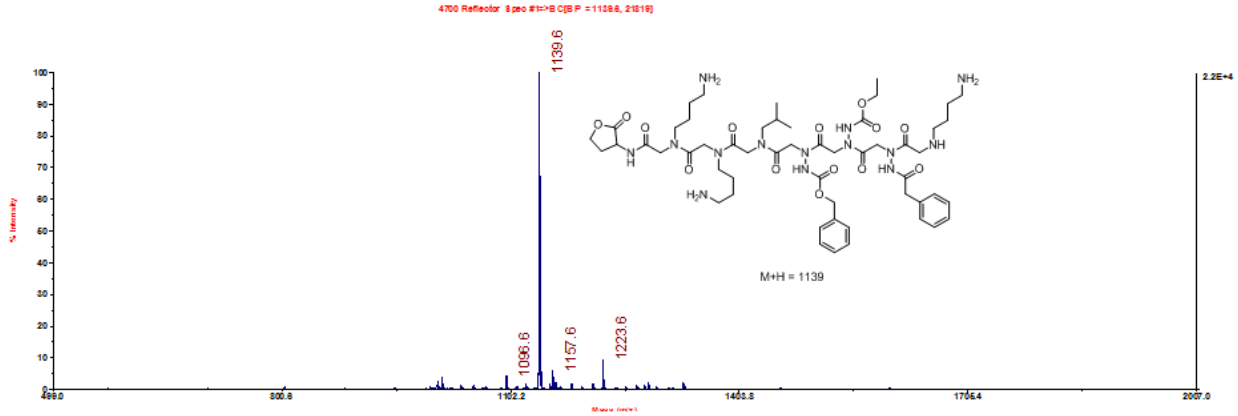

1011.5
897.4
661.4
206
867.4
190
751.3
358.2
471.3
144
115
169.1
645.4

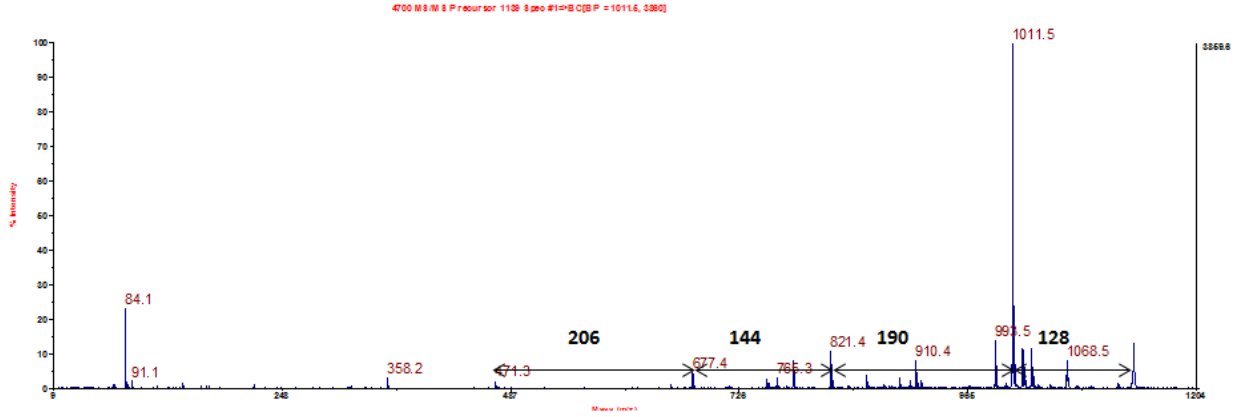

4700 Reflector Spec #1=>BC[BP = 1150.5, 6631]
1150.5
1153.5
1168.5
1234.5
M+H = 1150

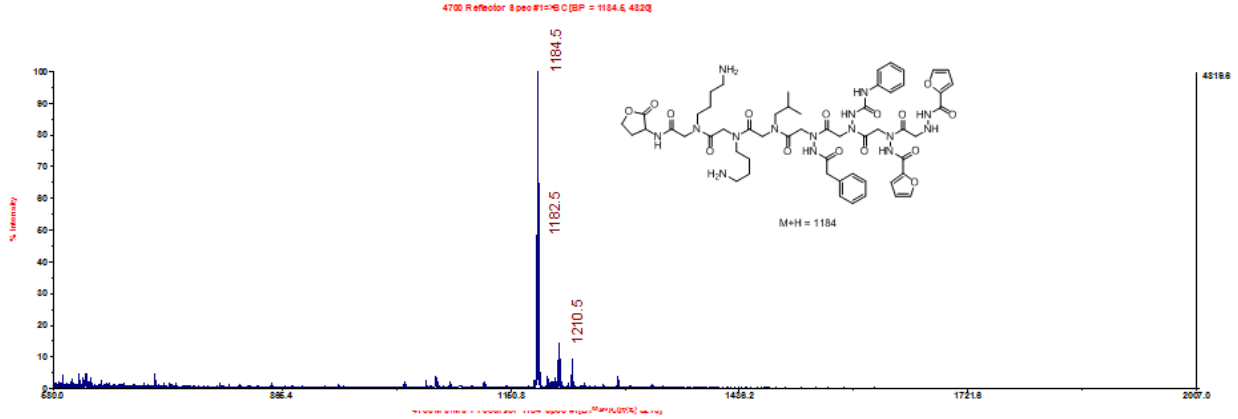

4700 MS/MS Precursor 1150 Spec #1=>BC[BP = 1057.4, 5761]
1057.4
471.3
115
586.3
191
680.1
683.1
793.2
182
191
1060.5
358.2
374.0
86.1
236.1
547.1

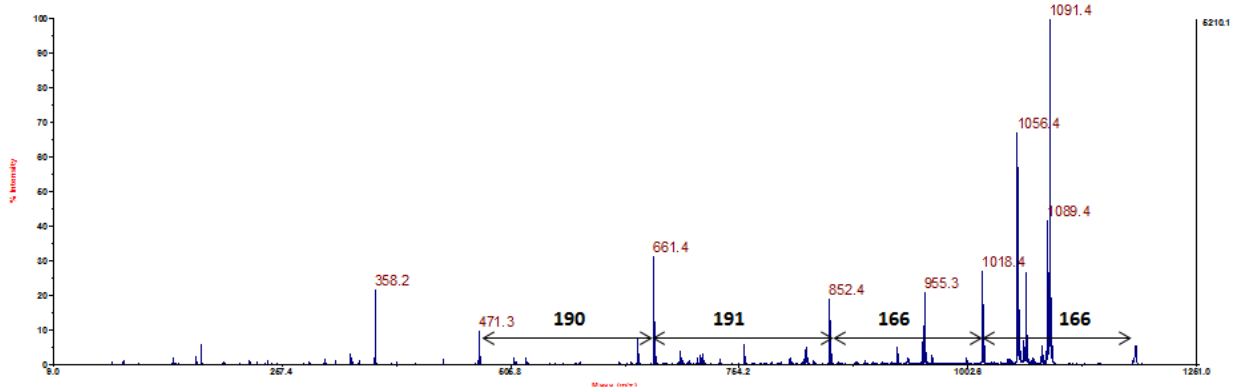

4700 Reflector Spec #1=>BC[BP = 1107.7, 16840]
1107.7
1003.6
1125.7
1191.6
1254.7
M+H = 1107

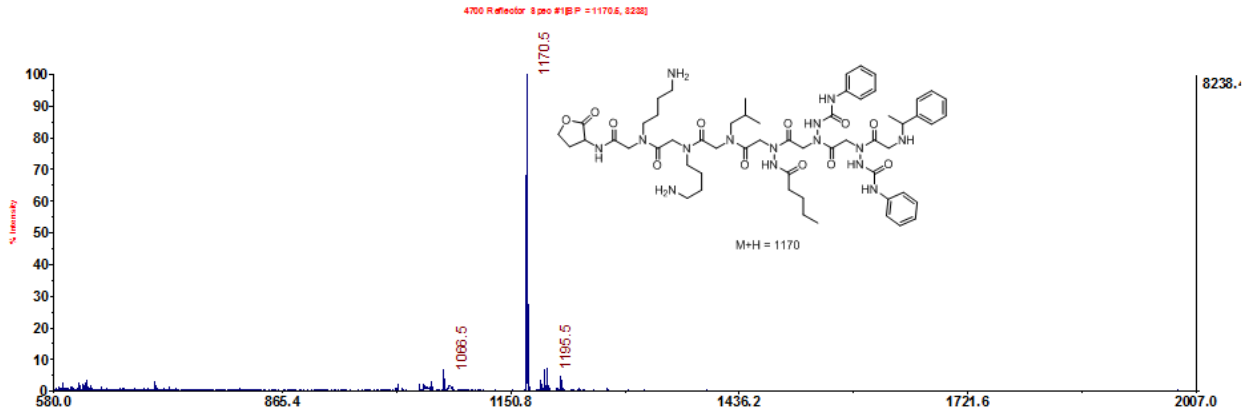

4700 MS/MS Precursor 1107 Spec #1=>BC[BP = 988.6, 6476]
988.6
1014.6
946.5
627.4
1003.5
481.2
156
128
755.5
191
161

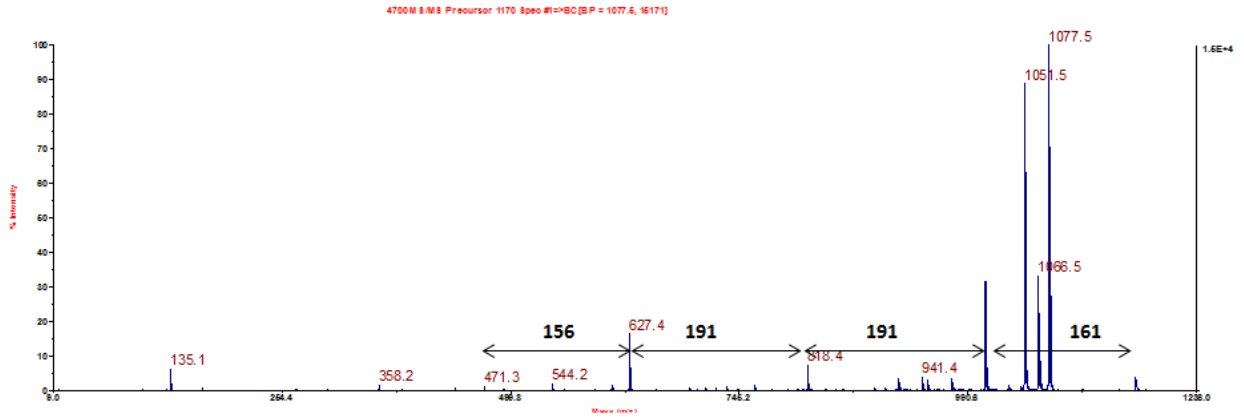

1139.6
1096.6
1157.6
1223.6
M+H = 1139

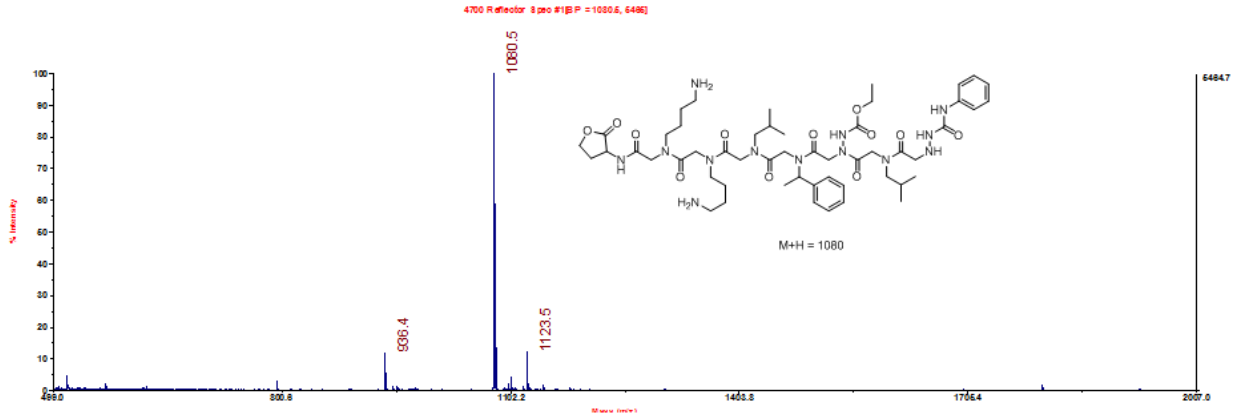

1011.5
84.1
91.1
358.2
206
144
821.4
190
910.4
992.5
128
1068.5

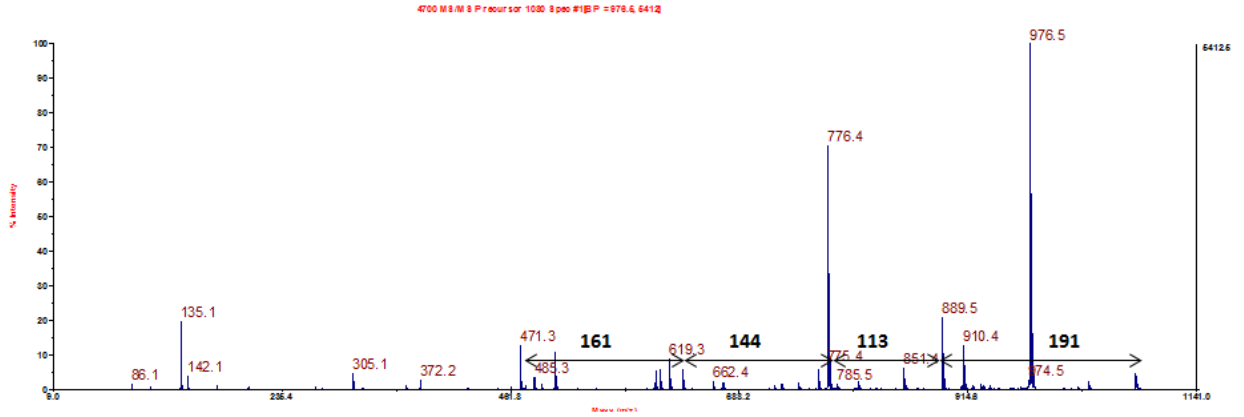

1184.5
1182.5
1210.5
M+H = 1184

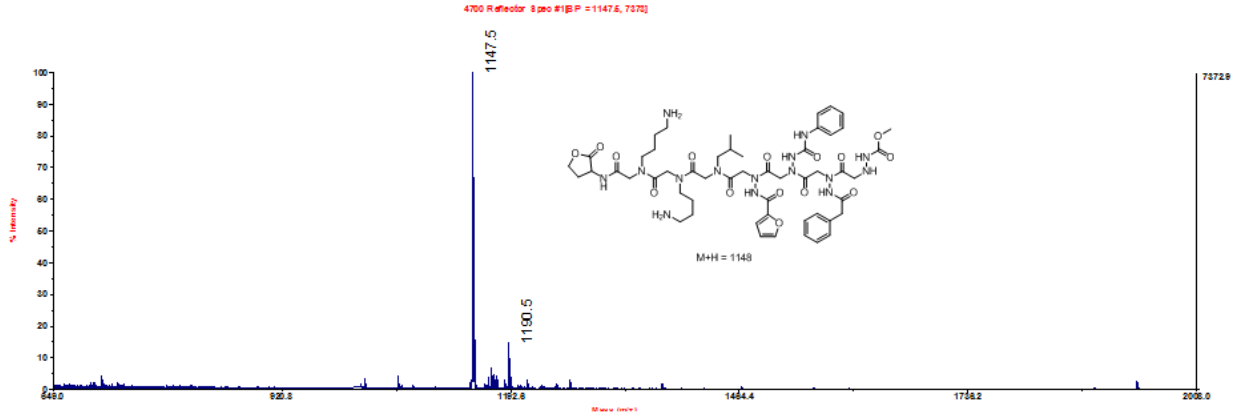

1091.4
1056.4
1089.4
661.4
1018.4
358.2
852.4
955.3
471.3
190
191
166
166

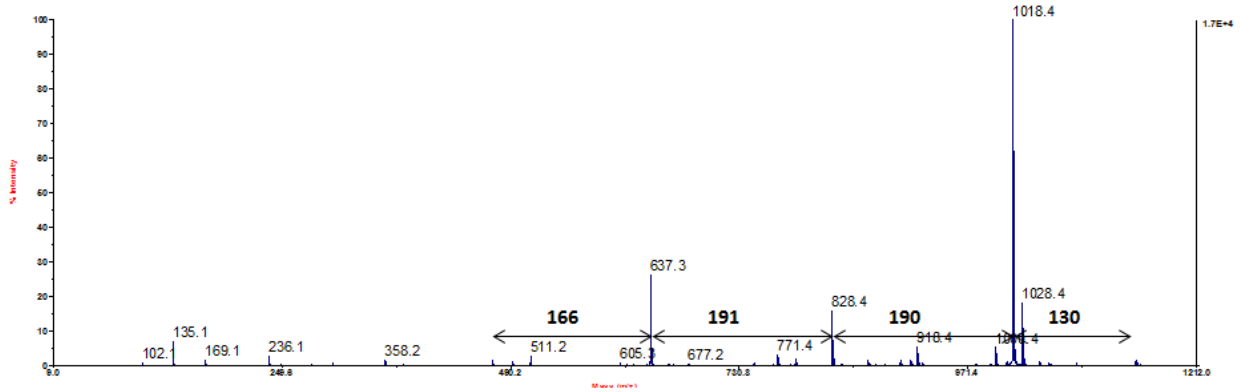

4700 Reflector Spec #1[BP = 1170.5, 8238]
1170.5
1066.5
1195.5
M+H = 1170
% Intensity
580.0
865.4
1150.8
1436.2
1721.6
2007.0

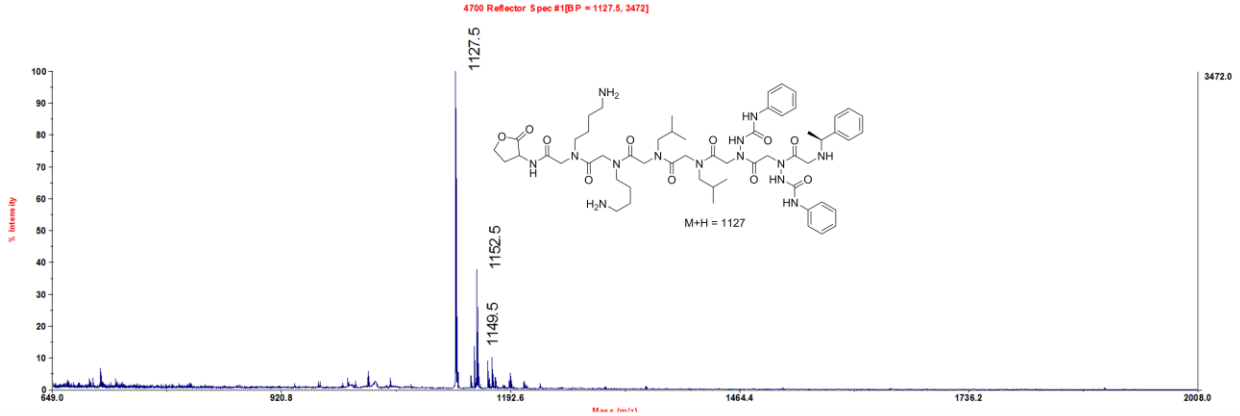

4700 MS/MS Precursor 1170 Spec #1=>BC[BP = 1077.5, 16171]
1077.5
1051.5
1066.5
156
627.4
191
191
161
135.1
358.2
471.3
544.2
818.4
941.4
% Intensity

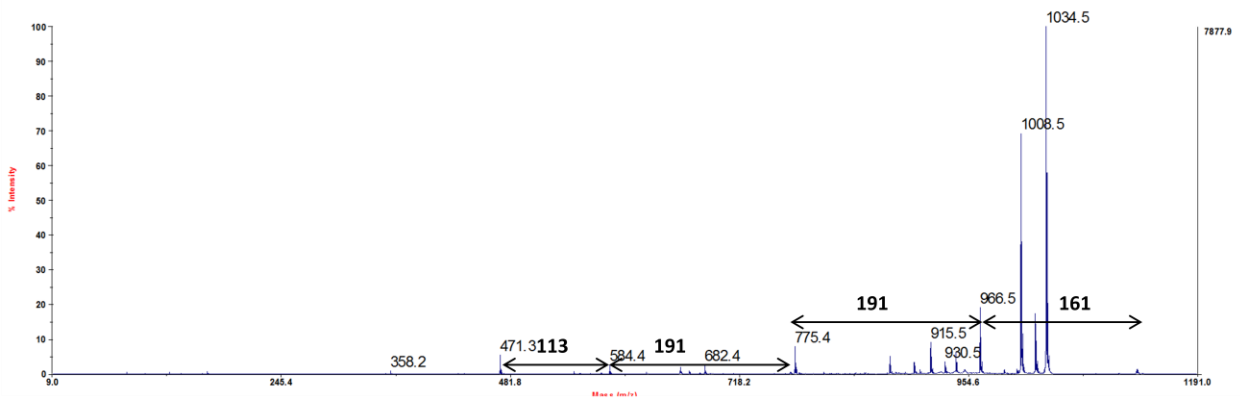

4700 Reflector Spec #1[BP = 1080.5, 6486]
1080.5
996.4
1123.5
M+H = 1080
% Intensity

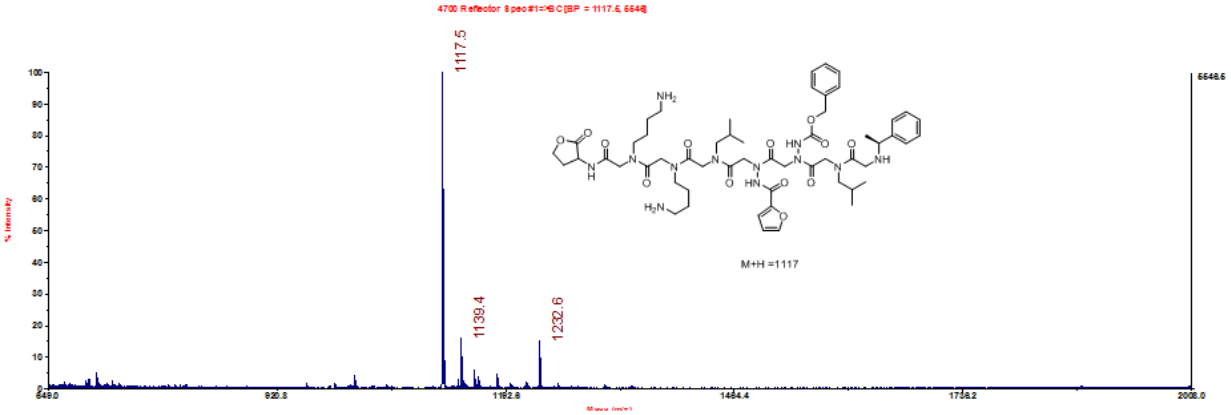

4700 MS/MS Precursor 1080 Spec #1[BP = 976.5, 6412]
976.5
776.4
889.5
910.4
135.1
471.3
161
619.3
144
113
191
86.1
142.1
305.1
372.2
485.3
662.4
725.4
785.5
851.4
974.5
% Intensity

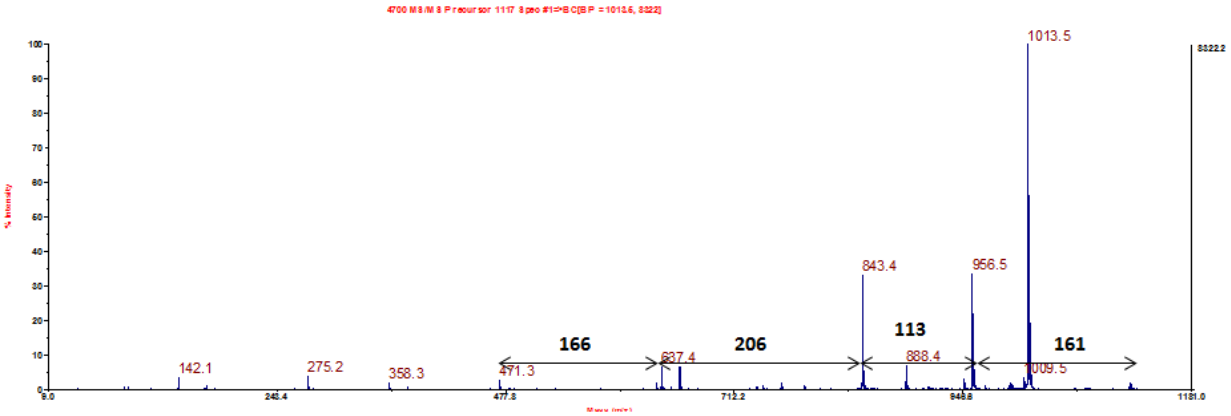

4700 Reflector Spec #1[BP = 1147.5, 7372]
1147.5
1190.5
M+H = 1148
% Intensity

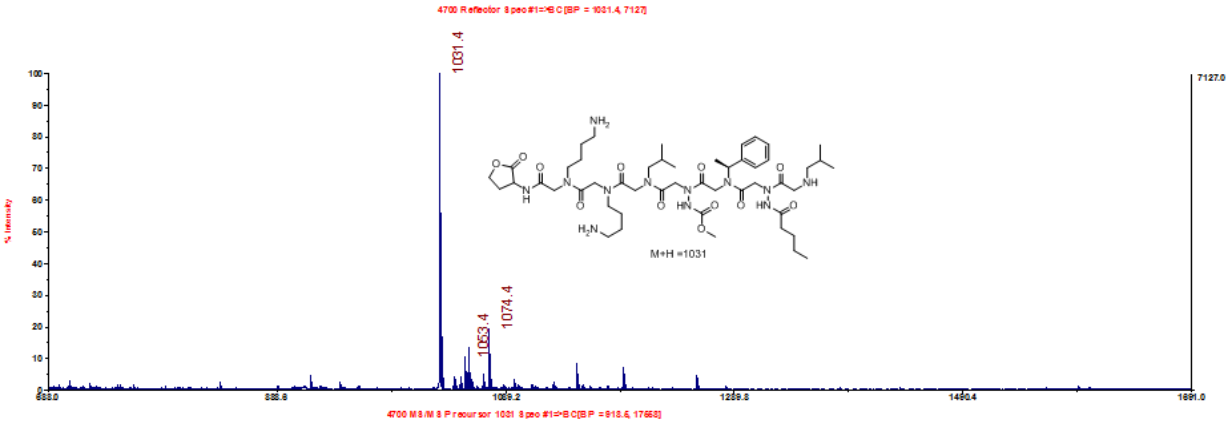

4700 MS/MS Precursor 1147 Spec #1[BP = 1018.4, 18640]
1018.4
637.3
828.4
1028.4
166
191
190
130
135.1
102.1
169.1
236.1
358.2
511.2
605.3
677.2
771.4
918.4
% Intensity

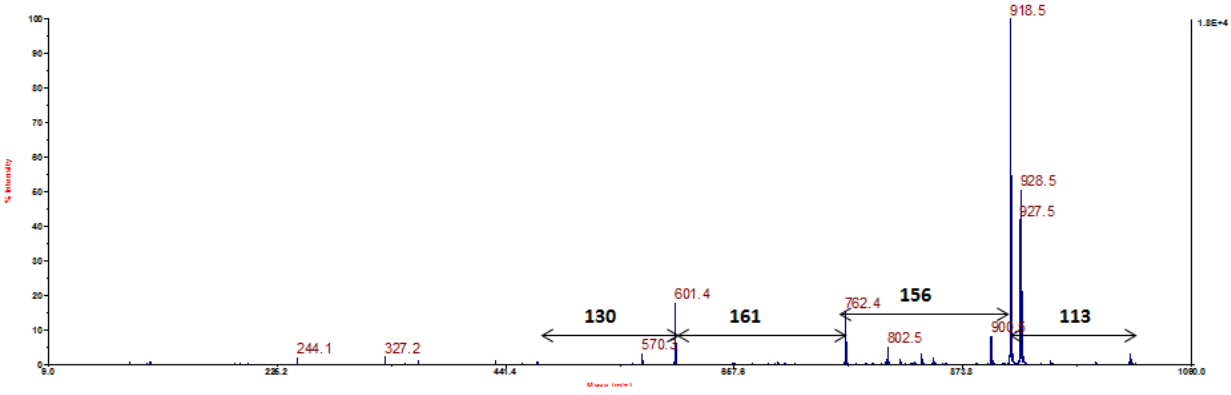

4700 Reflector Spec #1[BP = 1127.5, 3472]
1127.5
1152.5
1149.5
M+H = 1127
% Intensity

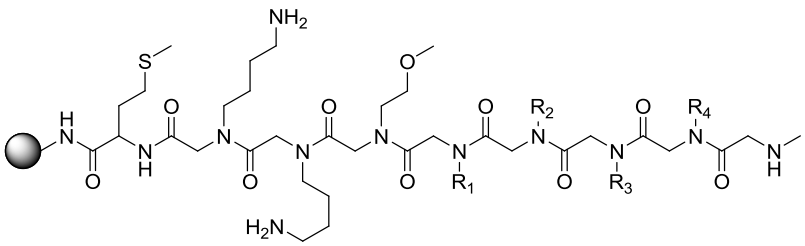

4700 MS/MS Precursor 1127 Spec #1[BP = 1034.5, 7878]
1034.5
1008.5
966.5
191
161
775.4
915.5
930.5
471.3
113
584.4
191
682.4
358.2
% Intensity


4700 Reflector Spec #1=>BC[BP = 1117.5, 6548]
1117.5
1139.4
1232.6
M+H =1117

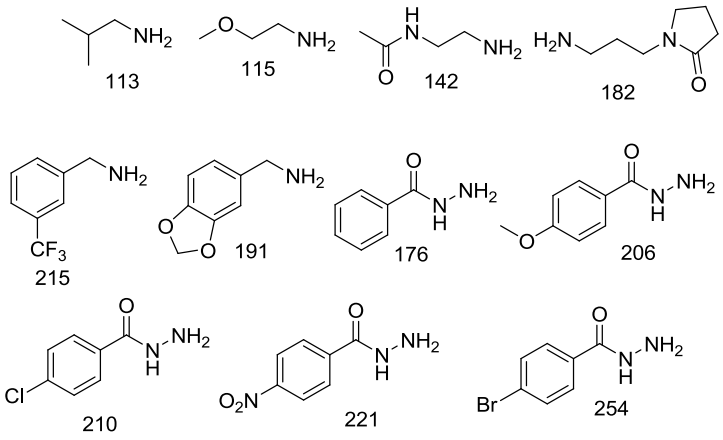

4700 MS/MS Precursor 1117 Spec #1=>BC[BP = 1013.5, 8322]
1013.5
843.4
956.5
166
206
113
161
142.1
275.2
358.3
471.3
637.4
888.4
1009.5


4700 Reflector Spec #1=>BC[BP = 1031.4, 7127]
1031.4
1053.4
1074.4
M+H =1031

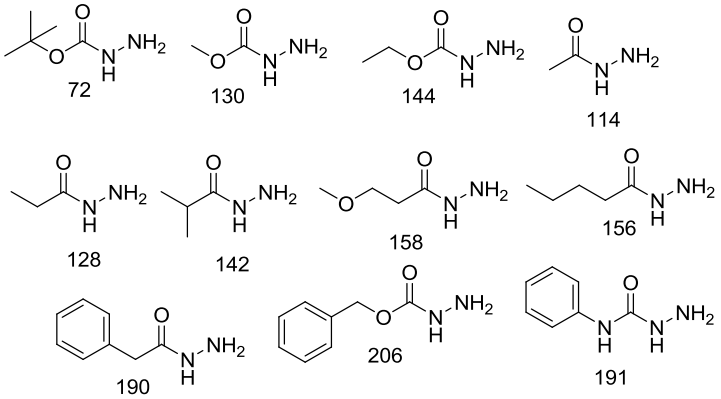

4700 MS/MS Precursor 1031 Spec #1=>BC[BP = 918.5, 17553]
918.5
928.5
927.5
130
161
156
113
244.1
327.2
570.3
601.4
762.4
802.5
900.5



Positions R_1 and R_3



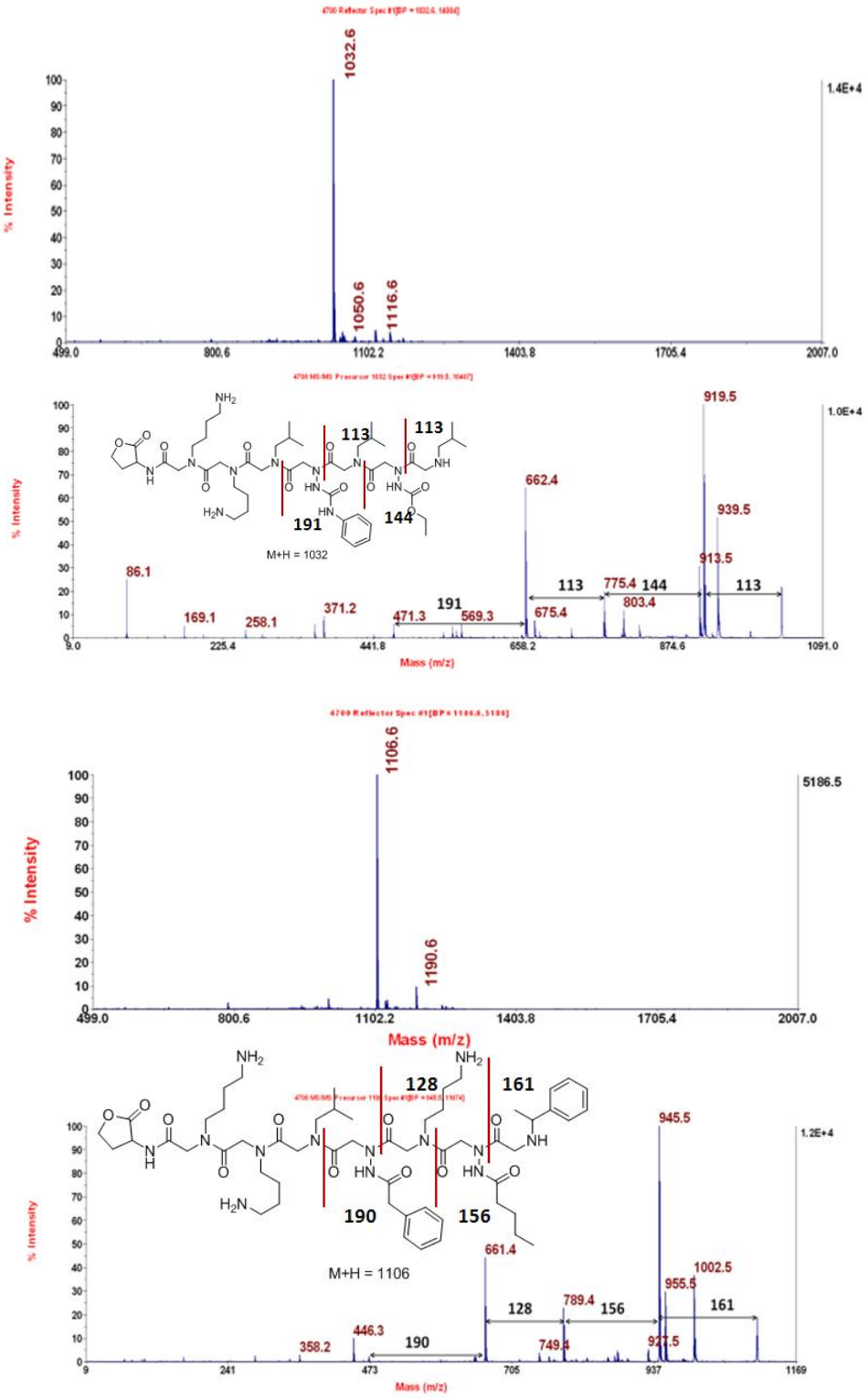
Positions R_2 and R_4

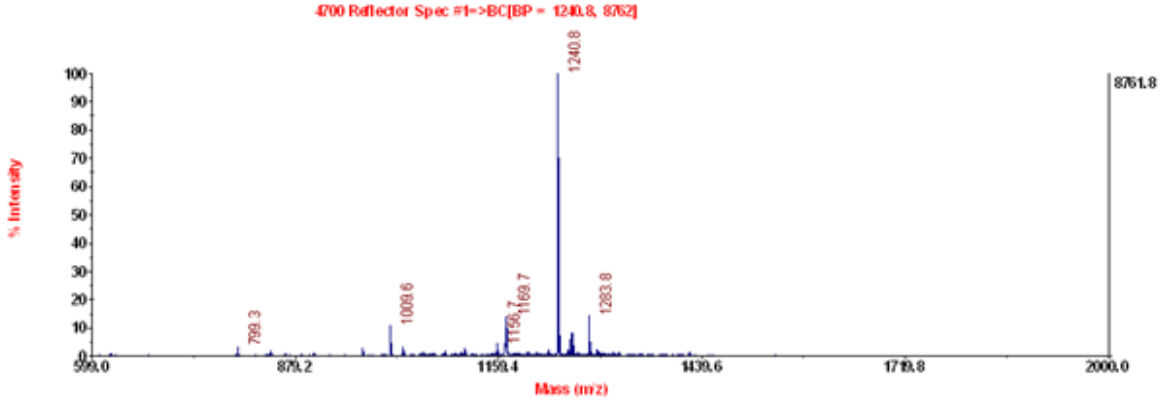


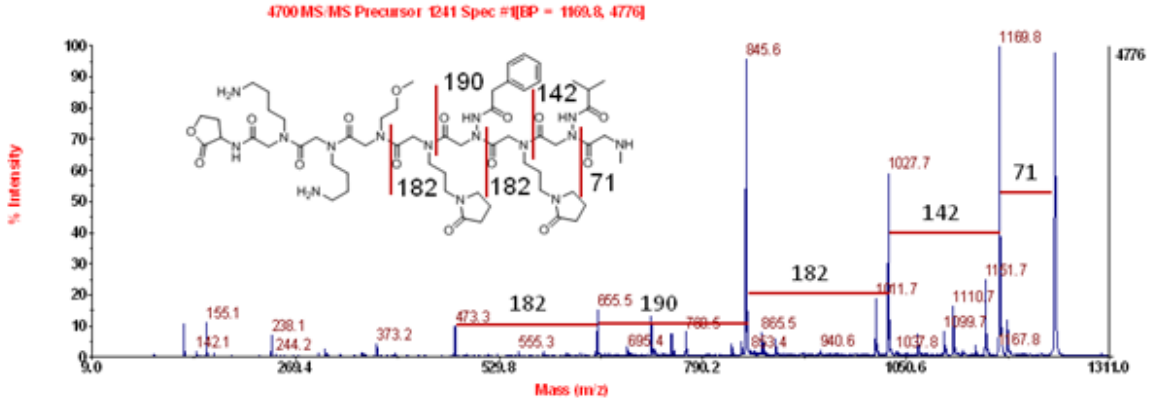
Theoretical Diversity = 11^4 = 14,641

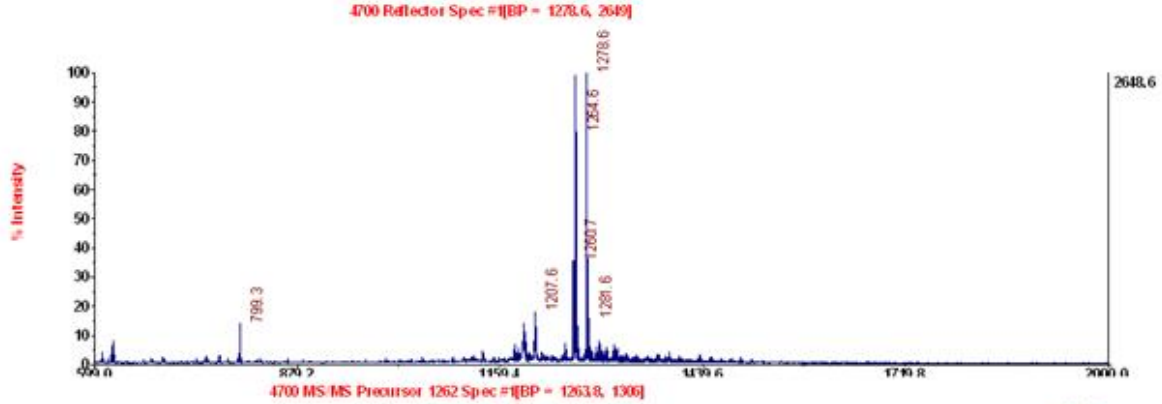
Figure S39. Peptoid-azapeptoid library synthesized by using primary amines and aryl acyl hydrazides at positions 1 and 3. Alkyl or benzyl acyl hydrazides, carbazates and semicarbazides are used at positions 2 and 4 as spacers between aryl acyl hydrazides and amines. (The numbers below the sub-monomers indicate the mass loss during MALDI TOF MS MS for respective sub-monomers present at particular position).

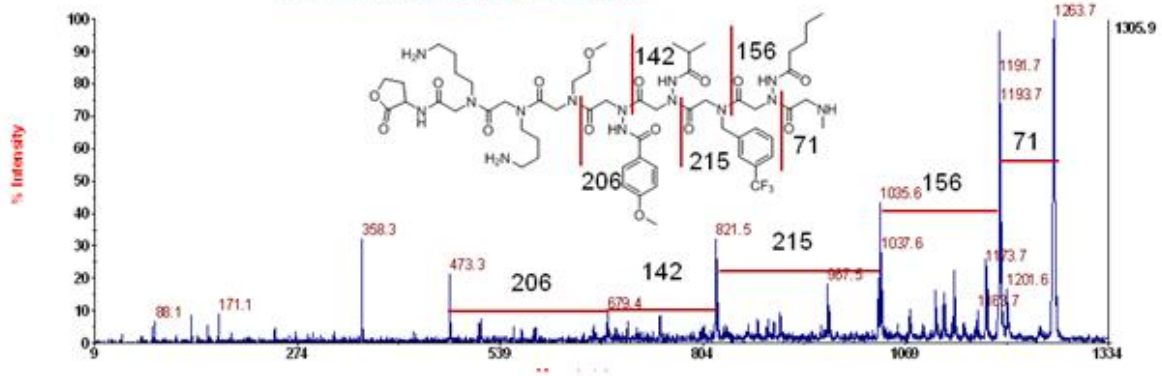
Figure S40. Representative MALDI TOF MS and MSMS spectra of some compounds of the tetramer peptoid-azapeptoid hybrid library obtained after single bead cleavage by using CNBr. (smalll peaks that appear at 799 and 1260 were also present in the MS spectrum of matrix alone).

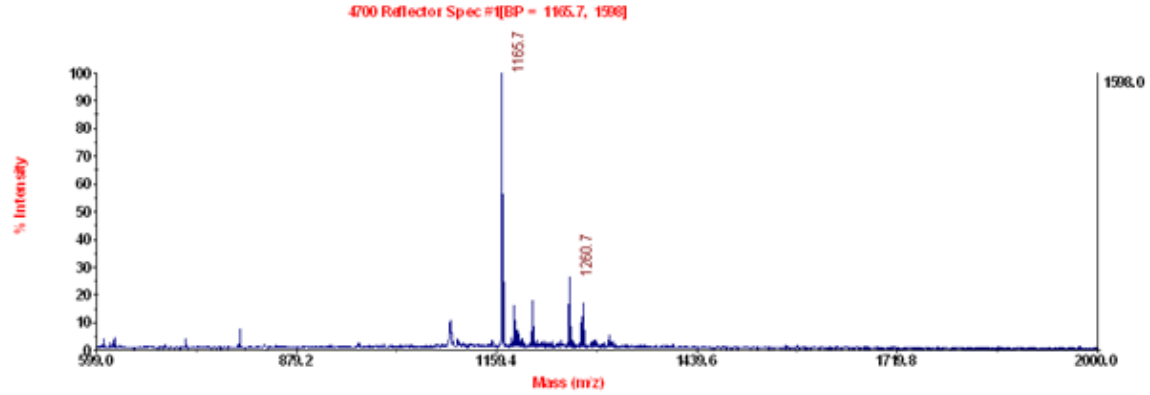


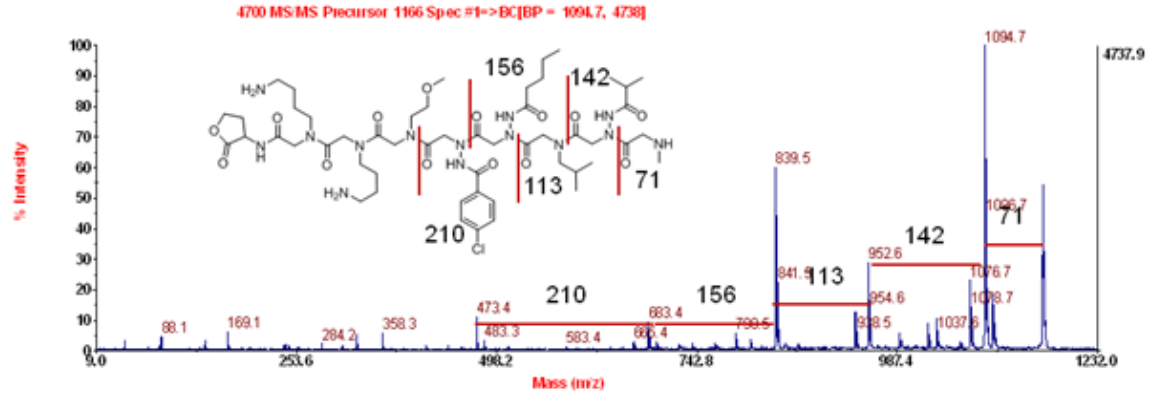

4700 Reflector Spec #1=>BC[BP = 1240.8, 8762]
% Intensity
Mass (m/z)
1240.8
8761.8
1009.6
1169.7
1283.8
799.3

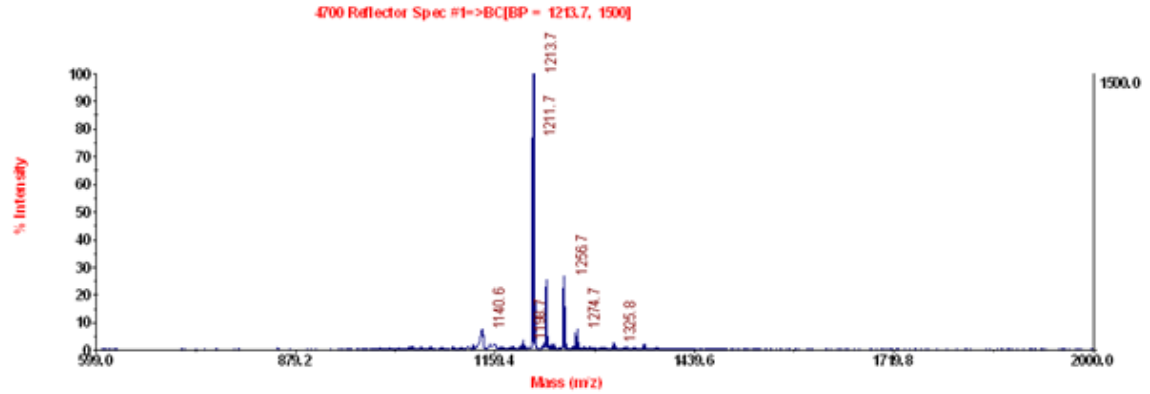

4700 MS/MS Precursor 1241 Spec #1[BP = 1169.8, 4776]
% Intensity
Mass (m/z)
1169.8
4776
845.6
1027.7
190
142
182
182
71
142
182
190
155.1
142.1
238.1
244.2
373.2
473.3
555.3
655.5
695.4
865.5
940.6
1037.8
1099.7
1110.7
1151.7
1167.8

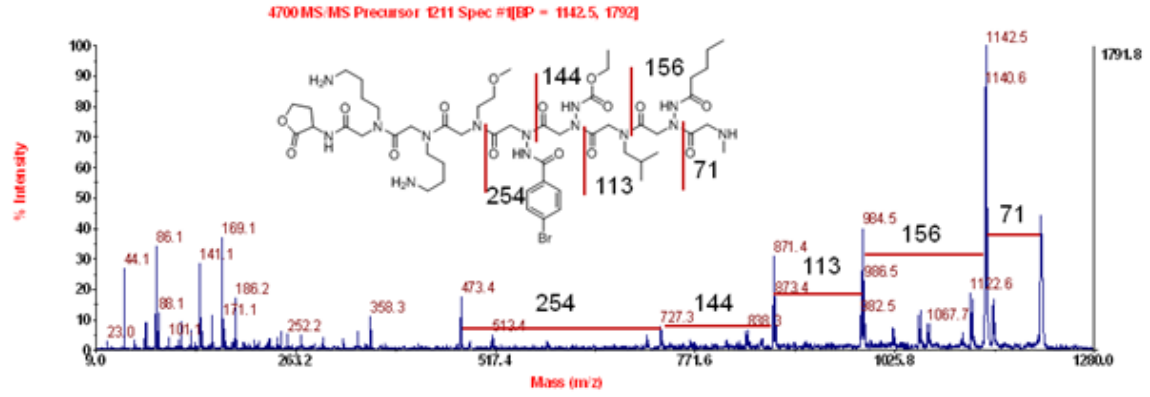

4700 Reflector Spec #1[BP = 1278.6, 2649]
% Intensity
1278.6
2648.6
1254.6
1260.7
1207.6
1281.6
799.3

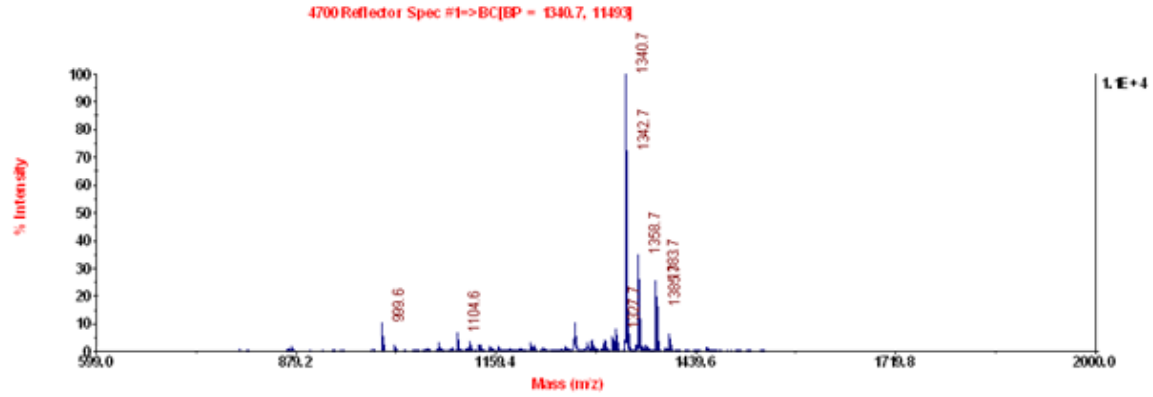

4700 MS/MS Precursor 1262 Spec #1[BP = 1263.8, 1306]
% Intensity
1263.7
1305.9
1191.7
1193.7
71
142
156
215
206
71
1035.6
156
358.3
821.5
215
473.3
206
142
1037.6
1193.7
1201.6
88.1
171.1
679.4

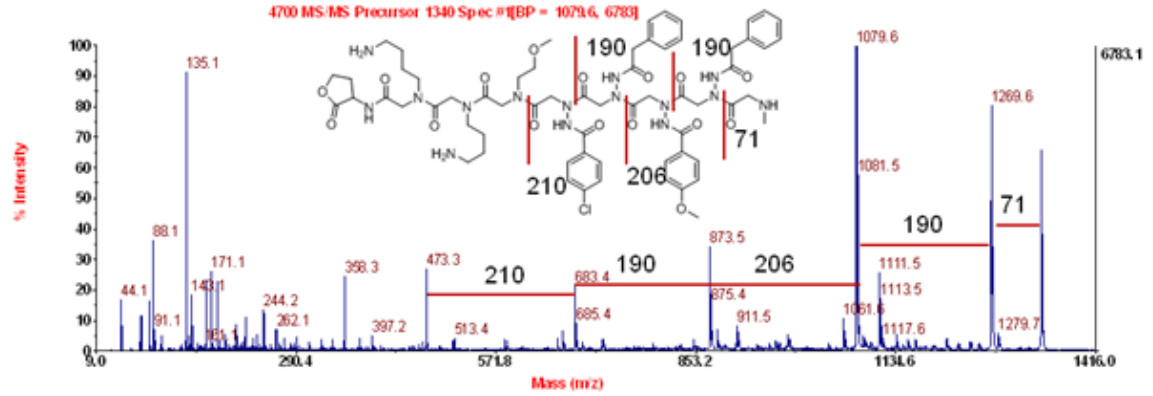

4700 Reflector Spec #1[BP = 1165.7, 1598]
% Intensity
Mass (m/z)
1165.7
1260.7
1598.0
599.0
879.2
1159.4
1439.6
1719.8
2000.0

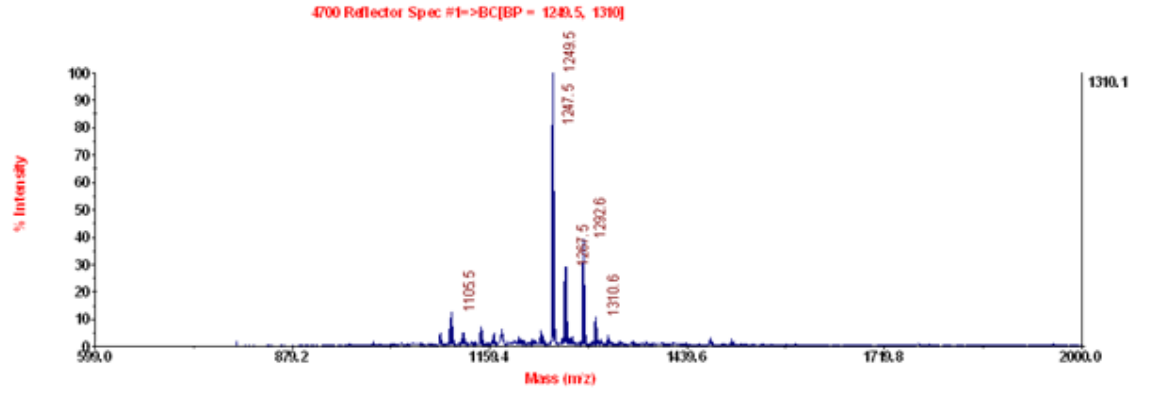

4700 MS/MS Precursor 1166 Spec #1=>BC[BP = 1094.7, 4738]
% Intensity
Mass (m/z)
156
142
113
71
210
1094.7
839.5
952.6
473.4
883.4
799.5
954.6
88.1
169.1
284.2
358.3
483.3
583.4
9.0
253.6
498.2
742.8
987.4
1232.0
4737.9

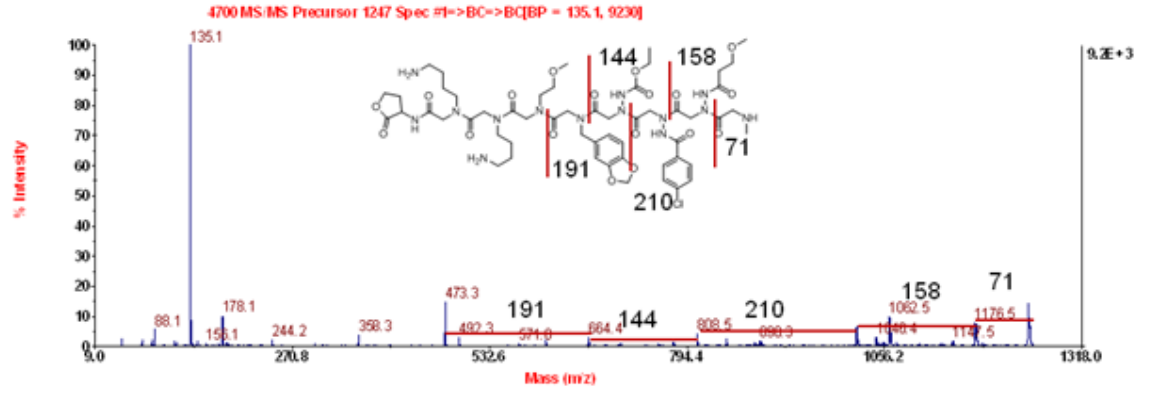

4700 Reflector Spec #1=>BC[BP = 1213.7, 1500]
% Intensity
Mass (m/z)
1213.7
1211.7
1256.7
1140.6
1274.7
1325.8
599.0
879.2
1159.4
1439.6
1719.8
2000.0
1500.0

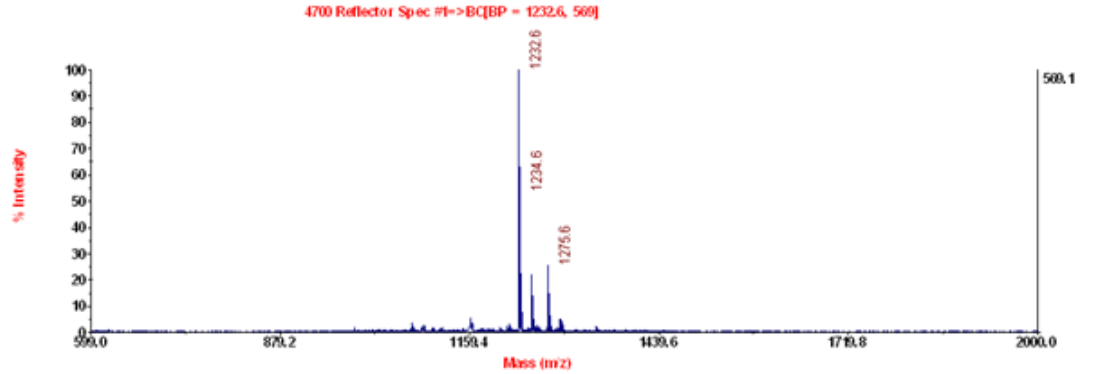

4700 MS/MS Precursor 1211 Spec #1[BP = 1142.5, 1792]
% Intensity
Mass (m/z)
144
156
113
71
254
1142.5
1140.6
984.5
871.4
873.4
886.5
882.5
1122.6
1067.7
727.3
473.4
358.3
252.2
169.1
86.1
44.1
141.1
186.2
171.1
88.1
23.0
9.0
263.2
517.4
771.6
1025.8
1280.0
1791.8

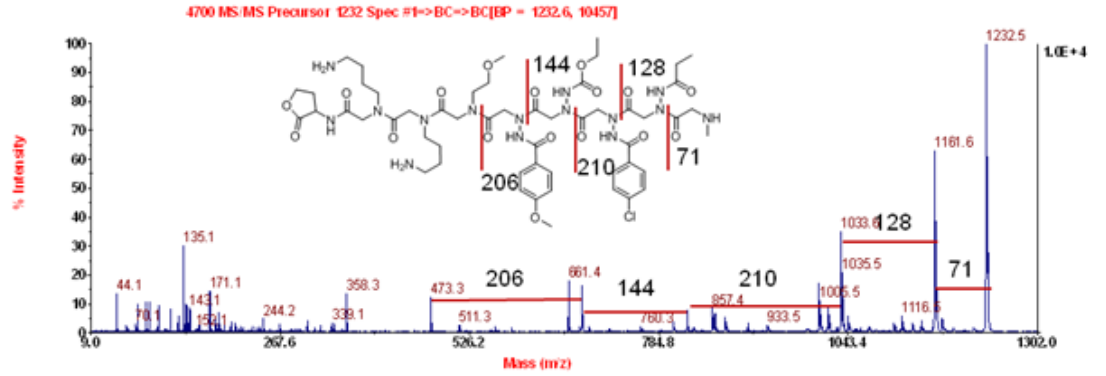

4700 Reflector Spec #1=>BC[BP = 1340.7, 11493]
% Intensity
Mass (m/z)
1340.7
1342.7
1358.7
1383.7
1104.6
999.6
1.1E+4

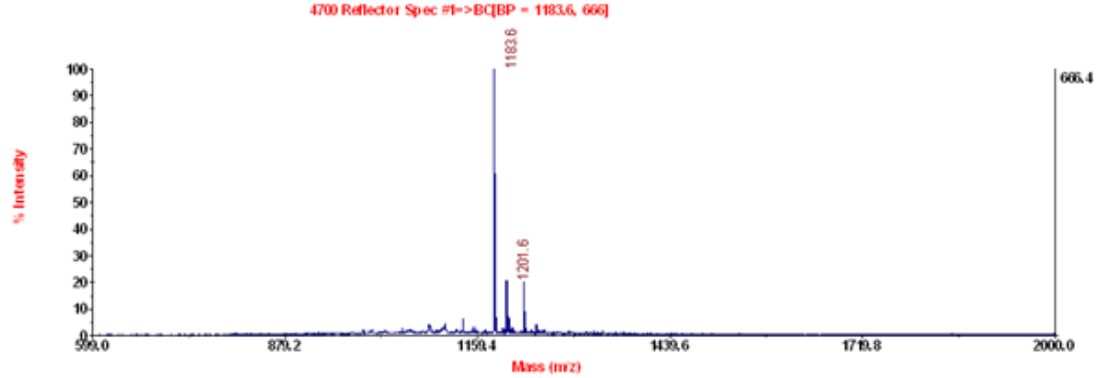

4700 MS/MS Precursor 1340 Spec #1[BP = 1079.6, 6783]
% Intensity
Mass (m/z)
190
190
71
210
206
1079.6
1269.6
1081.5
71
190
873.5
210
190
206
683.4
875.4
685.4
911.5
1111.5
1113.5
1117.6
1279.7
135.1
88.1
171.1
358.3
473.3
244.2
262.1
397.2
513.4
44.1
91.1
6783.1

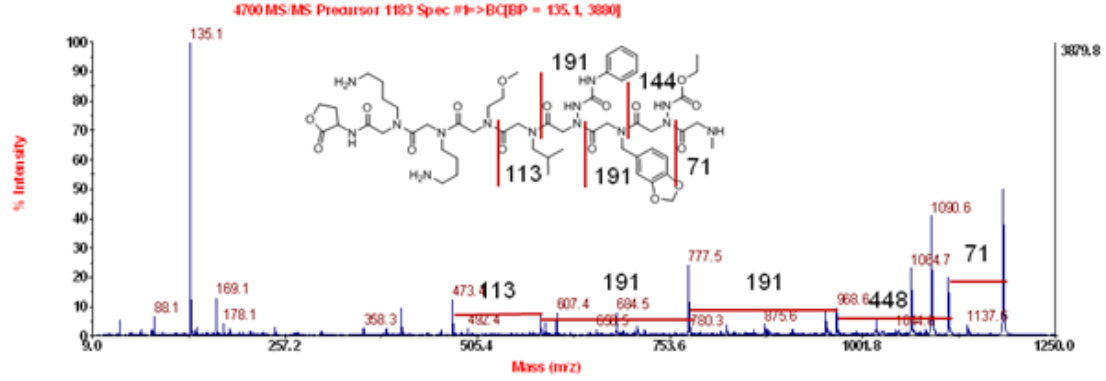

4700 Reflector Spec #1=>BC[BP = 1249.5, 1310]
% Intensity
Mass (m/z)
1249.5
1247.5
1292.6
1267.5
1310.6
1105.5
1310.1

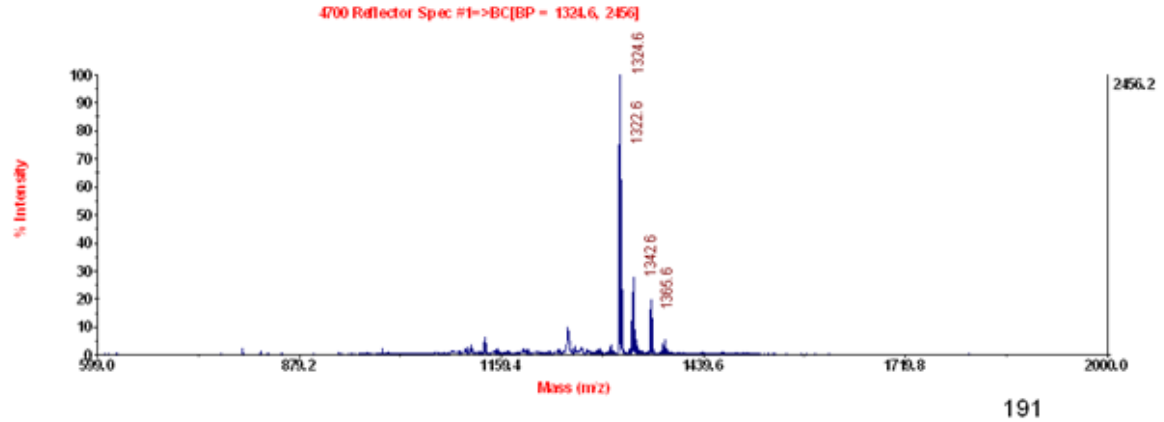

4700 MS/MS Precursor 1247 Spec #1=>BC=>BC[BP = 135.1, 9230]
% Intensity
Mass (m/z)
144
158
191
71
210
135.1
473.3
191
144
210
158
71
178.1
88.1
244.2
358.3
1062.5
1176.5
9.2E+3

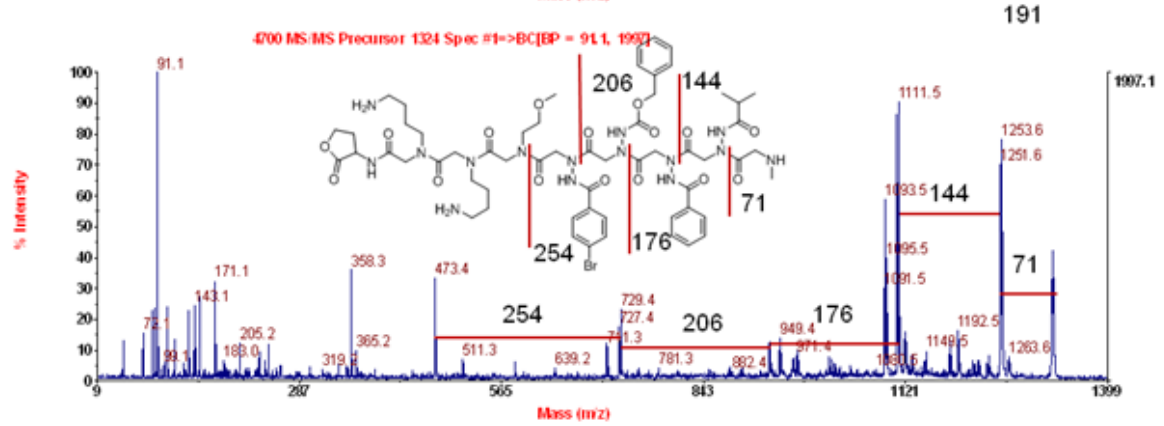

4700 Reflector Spec #1=>BC[BP = 1232.6, 569]
% Intensity
Mass (m/z)
1232.6
1234.6
1275.6
569.1

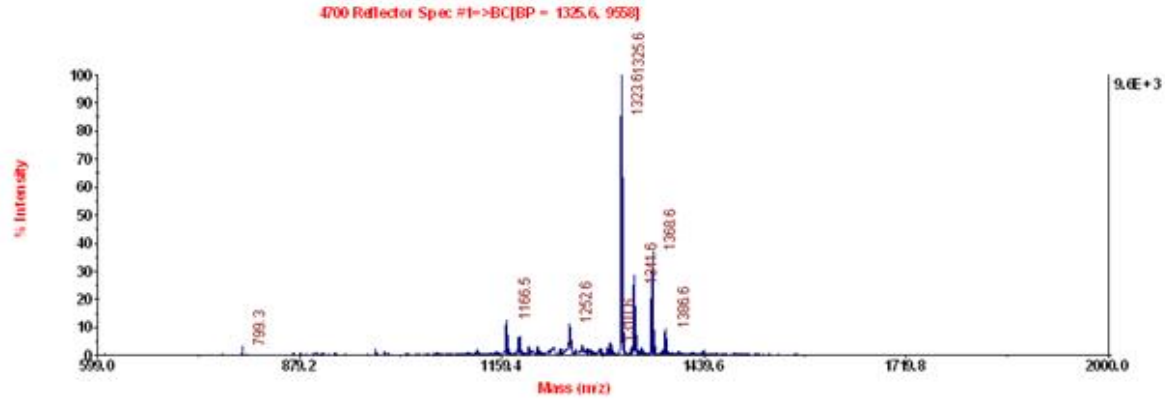

4700 MS/MS Precursor 1232 Spec #1=>BC=>BC[BP = 1232.6, 10457]
% Intensity
Mass (m/z)
144
128
206
210
71
1232.5
1.0E+4
1161.6
135.1
1039.6
1035.5
44.1
171.1
358.3
473.3
206
661.4
144
210
71
511.3
857.4
933.5
1005.5
1116.6
244.2
339.1

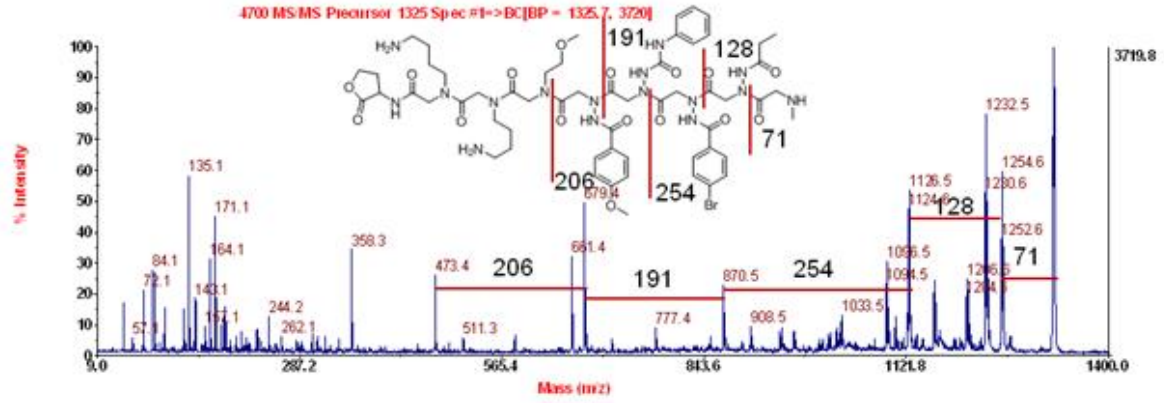

4700 Reflector Spec #1=>BC[BP = 1183.6, 666]
% Intensity
Mass (m/z)
1183.6
1201.6
666.4

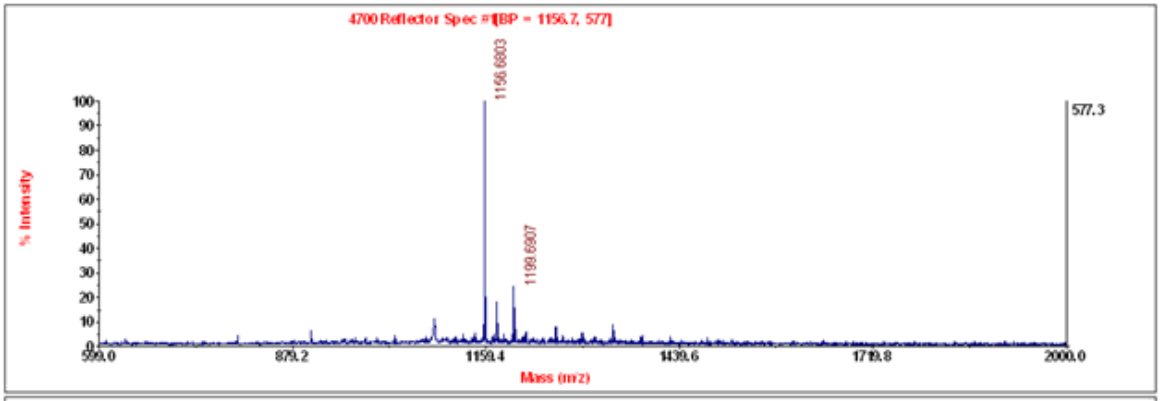

4700 MS/MS Precursor 1183 Spec #1=>BC[BP = 135.1, 3880]
% Intensity
Mass (m/z)
191
144
113
191
71
135.1
3879.8
1090.6
1064.7
71
777.5
191
191
113
448
169.1
88.1
178.1
358.3
473.4
492.4
607.4
684.5
780.3
875.6
968.6
1137.6

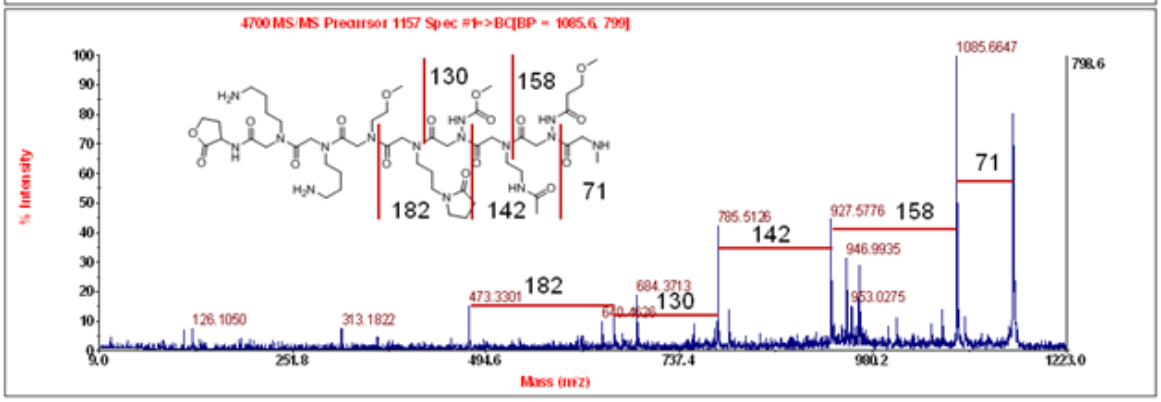

4700 Reflector Spec #1=>BC[BP = 1324.6, 2456]
% Intensity
Mass (m/z)
1324.6
1322.6
1342.6
1365.6
2456.2

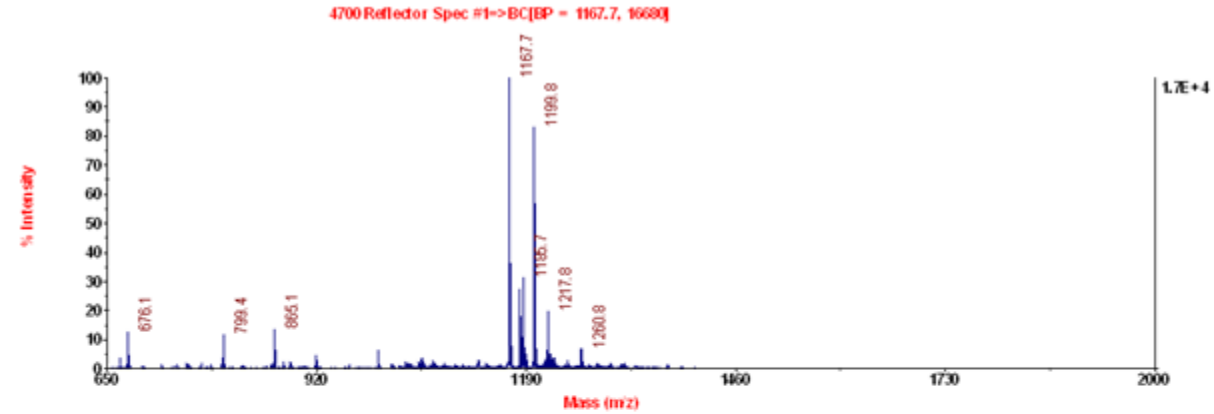

4700 MS/MS Precursor 1324 Spec #1=>BC[BP = 91.1, 1997]
% Intensity
Mass (m/z)
191
206
144
254
176
71
91.1
1997.1

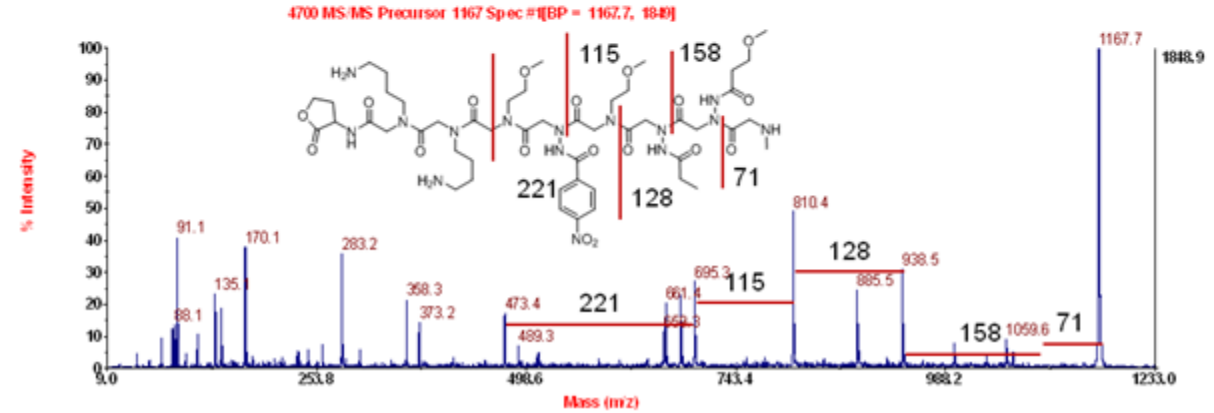

4700 Reflector Spec #1=>BC[BP = 1325.6, 9558]
% Intensity
Mass (m/z)
1325.6
1323.6
1368.6
1252.6
1166.5
799.3
9.6E+3


4700 MS/MS Precursor 1325 Spec #1=>BC[BP = 1325.7, 3720]
% Intensity
Mass (m/z)
191
206
128
254
71
3719.8


4700 Reflector Spec #1[BP = 1156.7, 577]
1156.6803
1199.6907
577.3
% Intensity
Mass (m/z)


4700 MS/MS Precursor 1157 Spec #1=>BC[BP = 1085.6, 799]
130
158
182
142
71
1085.6647
798.6
785.5126
927.5776
946.9935
953.0275
473.3301
684.3713
640.4628
126.1050
313.1822
Mass (m/z)


4700 Reflector Spec #1=>BC[BP = 1167.7, 16680]
1167.7
1199.8
1185.7
1217.8
1260.8
676.1
799.4
865.1
1.7E+4
% Intensity
Mass (m/z)


4700 MS/MS Precursor 1167 Spec #1[BP = 1167.7, 1848]
115
158
221
128
71
1167.7
1848.9
810.4
938.5
885.5
695.3
661.4
473.4
489.3
373.2
358.3
283.2
170.1
135.1
91.1
88.1
1059.6
% Intensity
Mass (m/z)