**Supporting Information**

# Water Solubility and Secondary Structure Stability of Hydrophobic Peptoids via a Minor Backbone Modification

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## X-ray crystallographic measurements:

The single-crystal material was immersed in Paratone–N oil and mounted on a Kappa CCD diffractometer at 293K. Data collection was performed using monochromated Mo Kα radiation, λ = 0.71073 Å, using φ and ω scans to cover the Ewald sphere.[1] Accurate cell parameters were obtained with the amount of indicated reflections.[2] The structure was solved by direct methods (SHELXS-97)[3] and refined by full-matrix least-squares methods against $F^2$ (SHELXL-97).[4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their $U_{iso}$ values constrained to 1.5 times the $U_{eq}$ of their pivot atoms for terminal $sp^3$ carbon atoms and 1.2 times for all other carbon atoms. Software used for molecular graphics: Mercury 3.5.[5]

The X-ray crystallographic coordinates for the structure of **PD'** have been deposited at the Cambridge Crystallographic Data Centre (CCDC) under deposition number CCDC 1497855. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

References:

1. Kappa CCD Server Software, Nonius BV, Delft, The Netherlands, **1997**.

2. Z. Otwinowski and W. Minor, Methods Enzymol. **1997**, *276*, 307.

3. G. M. Sheldrick, Acta Crystallogr., Sect. A: Fundam. Crystallogr. **1990**, *46*, 467.

4. ORTEP, TEXSAN Structure Analysis Package, Molecular Structure Corp., The Woodlands, TX, **1999**.

5. Mercury Software from CCDC: http://www.ccdc.cam.ac.uk/ Solutions/CSDSystem/Pages/Mercury.aspx.

**General method for water solubility test:**

1 mg peptoid was taken in the Eppendorf and water was added gradually (e.g. 5 ul per addition) until a clear solution was obtained. The solubility test was repeated for three times and average values are presented.

**Circular Dichroism (CD):**

CD measurements were performed using a circular dichroism spectrometer Model Jasco 810 Spectropolarimeter and Applied Photophysics Chirascan. The concentration of each measured sample was 100 μM in acetonitrile or water with 0.1cm path length fused quartz cell. Eight scans were taken for each sample at the scan rate of 1 nm/s at 1 nm increments. Data are expressed in per-residue molar ellipticity (deg $cm^2$ $dmol^{-1}$) calculated per mol of amide groups present.

**Procedure for UV-Vis experiments:**

UV-Vis measurements were performed using an Agilent Cary 60 UV-Vis spectrophotometer, Czerny-Turner monochromator. In a typical UV-Vis experiment, 10μL of a peptoid solution (5 mM) were diluted in 3 ml $H_2O$ (to get 17 μM concentration) and the UV- Vis spectrum was measured. Afterwards 1 equivalent of $Cu^{2+}$ (10 μL 5mM) or solution containing mixtures of metal ions (1 equiv. $Cu^{2+}$, $Co^{2+}$, $Zn^{2+}$, $Mn^{2+}$, $Ni^{2+}$ and $Fe^{3+}$, 5mM 10μL) was added and the spectrum was measured again.

**Characterization of the peptoid oligomers:**

All peptoid oligomers were characterized by analytical HPLC using a C18 column. Analysis with analytical C18 column was done using a solvent gradient conducted from 5% to 95% solvent B (0.1% TFA in HPLC grade acetonitrile) over solvent A (0.1% TFA in HPLC grade water) in 10 minutes with a flow rate of 0.7 mL $min^{-1}$. Analysis with preparative C18 column was done using a solvent gradient conducted from 5% to 95% solvent B (0.1% TFA in HPLC grade acetonitrile) over solvent A (0.1% TFA in HPLC grade water) in 50 minutes with a flow rate of 5 mL $min^{-1}$. Additional characterization was conducted by ESI MS. The peptoids were further purified to >95% by RP-HPLC and lyophilized overnight. HPLC traces of the pure peptoid oligomers are depicted in Figures **S6-S37.** All peptoids were subjected again to ESI MS characterization. MS spectra of the pure peptoid oligomers are depicted in Figures **S38-S74**. **PD'** was characterized in solution by ESI MS and $^{1}H$ NMR (**S75-S76**).

**Table S1**. Peptoid oligomer sequences and their corresponding molecular weights.

| Peptoid | Monomer sequence | Mw cal:found | Crude purity |
|---|---|---|---|
| **P1** | (*N*spe)$_6$ | 984.26 : 984.80 | 99 |
| **SP1** | (*N*pm)$_6$-Nea | 1000.19 :1000.32 | 80 |
| **SP2** | (*N*pm)$_6$-Neh | 1001.18 :1002.04 | 76 |
| **SP3** | (*N*spe)$_6$-Nabs | 1211.47:1211.56 | 73 |
| **SP4** | (*N*spe)$_6$-Naa | 1099.32:1099.96 | 71 |
| **P2** | (*N*spe)$_6$- piperazine | 1110.41 : 1110.8 | 85 |
| **P3** | Piperazine- (*N*spe)$_6$ | 1110.41 : 1110.8 | 71 |
| **P-linear** | *N*pl-(*N*spe)$_6$- piperazine | 1243.94:1243.45 | 62 |
| **P4** | *N*pl-(*N*spe)$_6$- piperazine | 1207.50:1207.12 | 40 |
| **P5** | (*N*spe)$_6$- (piperazine)$_2$ | 1236.57 : 1236.96 | 72 |
| **P6** | (*N*spe)$_6$- (piperazine)$_3$ | 1362.73 : 1362.66 | 60 |
| **P7** | (*N*spe)$_6$-homopiperazine | 1224.64 : 1124.69 | 85 |
| **P8** | (*N*spe)$_6$-( homopiperazine)$_2$ | 1264.63 :1264.74 | 82 |
| **P9** | (*N*s1npe)$_4$ | 861.07: 861.89 | 90 |
| **P11** | (*N*Pm)$_2$-*N*sch-*N*cpe-*N*sch-*N*fpm | 1020.77:1020.55 | 82 |
| **P12** | (*N*s1npe)$_4$-piperazine | 988.22:988.83 | 81 |
| **P13** | Piperazine -(*N*s1npe)$_4$ | 988.22:988.52 | 76 |
| **P14** | (*N*s1npe)$_4$-homopiperazine | 1002.25:1003.00 | 80 |
| **P15** | (*N*sch)$_5$-piperazine | 979.43:979.20 | 75 |
| **P16** | (*N*sch)$_5$-homopiperazine | 993.45:993.74 | 76 |
| **P17** | Piperazine -(*N*pm)$_2$-*N*sch-*N*cpe-*N*sch-*N*fpm | 1146.89:1145.49 | 70 |
| **P18** | (*N*s1npe)$_4$- (piperazine)$_2$ | 1114.38:1114.67 | 73 |
| **P19** | (*N*s1npe)$_4$- (piperazine)$_3$ | 1240.54:1240.26 | 68 |
| **P20** | (*N*sch)$_5$- (piperazine)$_2$ | 1105.58:1105.86 | 72 |
| **P21** | (*N*sch)$_5$- (piperazine)$_3$ | 1231.74:1231.87 | 67 |
| **P22** | (Piperazine)$_2$-(*N*pm)$_2$-*N*sch-*N*cpe-*N*sch-*N*fpm | 1146.89:1145.49 | 58 |
| **P23** | (Piperazine)$_3$-(*N*pm)2-*N*sch-*N*cpe-*N*sch-*N*fpm | 1273.02:1272.33 | 47 |
| **P24** | β-peptoids-(*N*spe)$_6$ | 1068.30:1068.49 | 42 |
| **P25** | β-peptoids-(*N*spe)$_6$- piperazine | 1194.55:1194.60 | 35 |
| **P26** | β-peptoids- (*N*spe)$_6$- (piperazine)$_2$ | 1320.71:1320.80 | 31 |
| **P27** | β-peptoids- (*N*spe)$_6$- (piperazine)$_3$ | 1446.86:1446.48 | 25 |
| **P28** | *N*spe-*N*Ecz- *N*spe-*N*Ecz- *N*spe-*N*Ecz | 93.02:933.60 | 90 |
| **P29** | *N*spe-*N*Ecz- *N*spe-*N*Ecz- Nspe-*N*Ecz piperazine | 1059.17:1059.43 | 87 |
| **P30** | *N*spe-*N*Ecz- *N*spe-*N*Ecz- *N*spe-*N*Ecz (piperazine)$_2$ | 1185.33:1185.68 | 82 |
| **P31** | *N*spe-*N*Ecz- *N*spe-*N*Ecz- *N*spe-*N*Ecz (piperazine)$_3$ | 1322.49:1311.96 | 79 |

## Figures

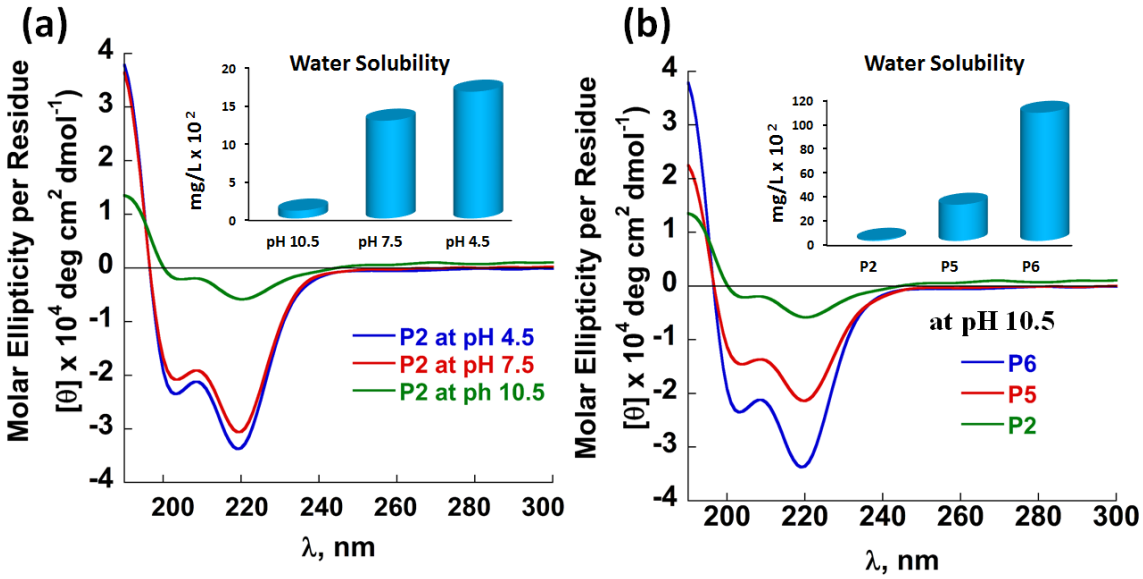



**Figure S1.** (a) CD spectra of **P2** at different pH conditions. Inset: water solubility data for **P2** at the different pH conditions. (b) CD spectra of **P2**, **P5** and **P6** at pH = 10.5. Inset: water solubility data for **P2**, **P5** and **P6** at pH = 10.5.

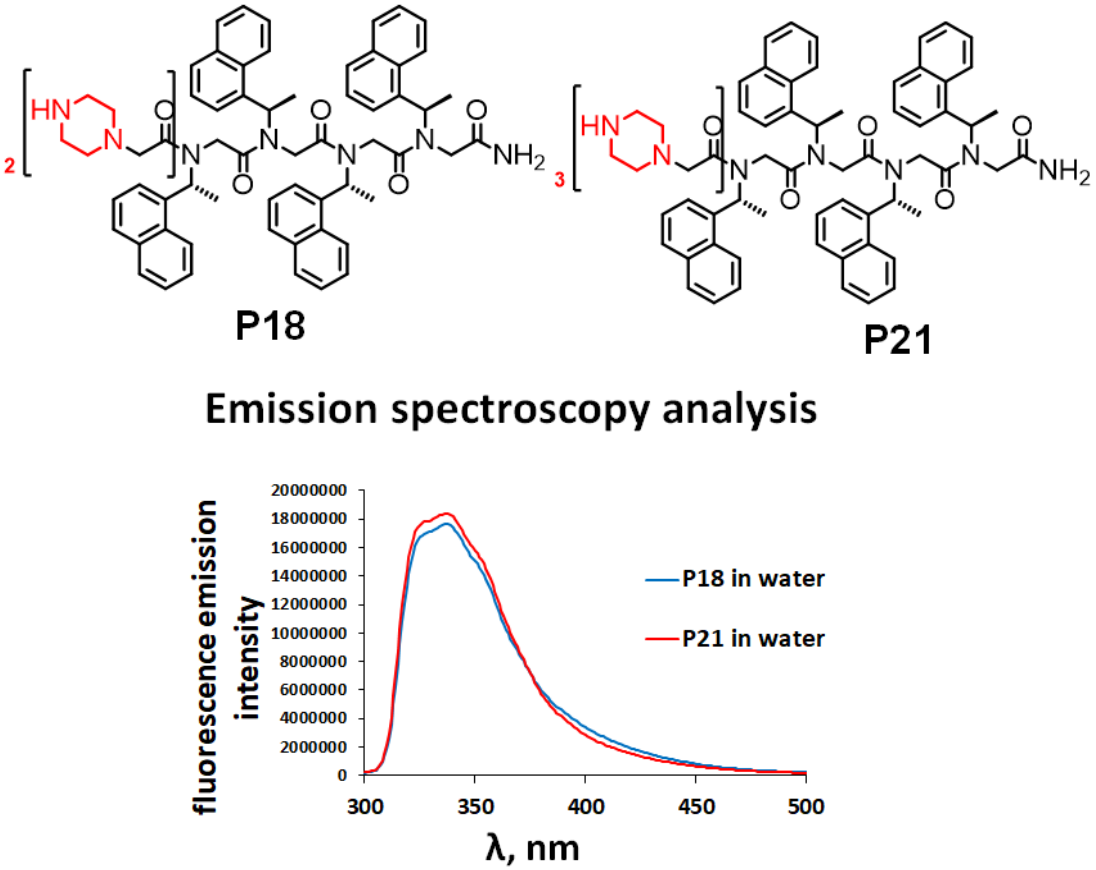



**Figure S2.** Fluorescence emission spectra of 40 μM of **P18** and **P21** in water.

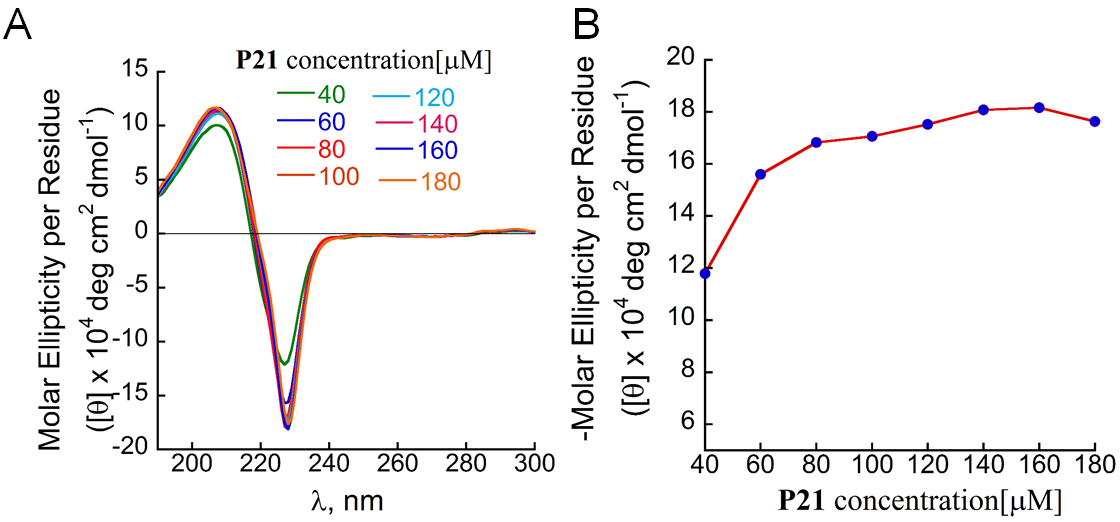



Fig. **S3a**. (A) The CD spectra of **P21** peptides in different concentrations (40-180 μM). (B) Plots of molar ellipticity ([θ]) at 228 nm vs. peptide concentration (40-180 μM).

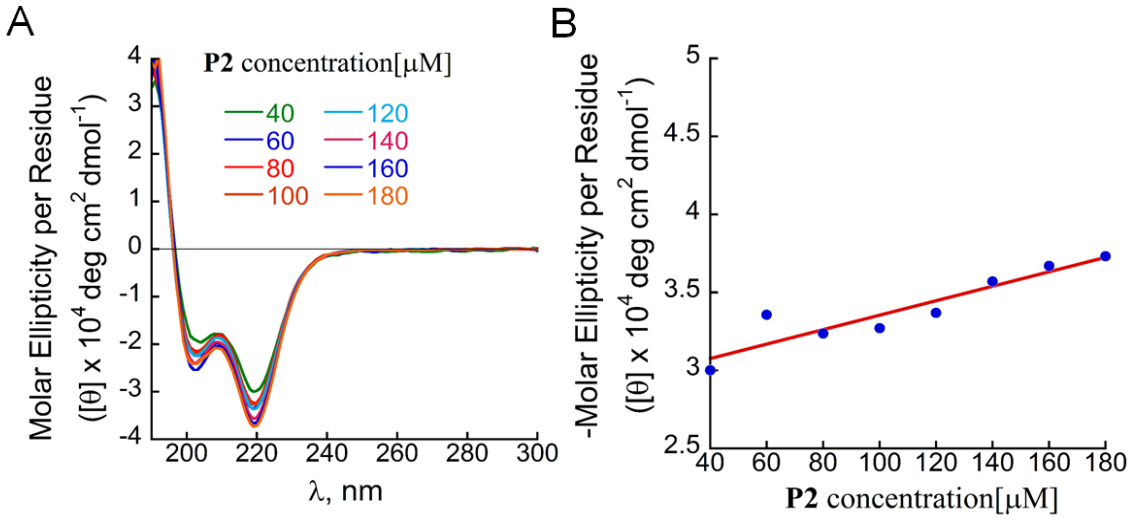



Fig. **S3b**. (A) The CD spectra of **P2** peptides in different concentrations (40-180 μM). (B) Plots of molar ellipticity ([θ]) at 219 nm vs. peptide concentration (40-180 μM).

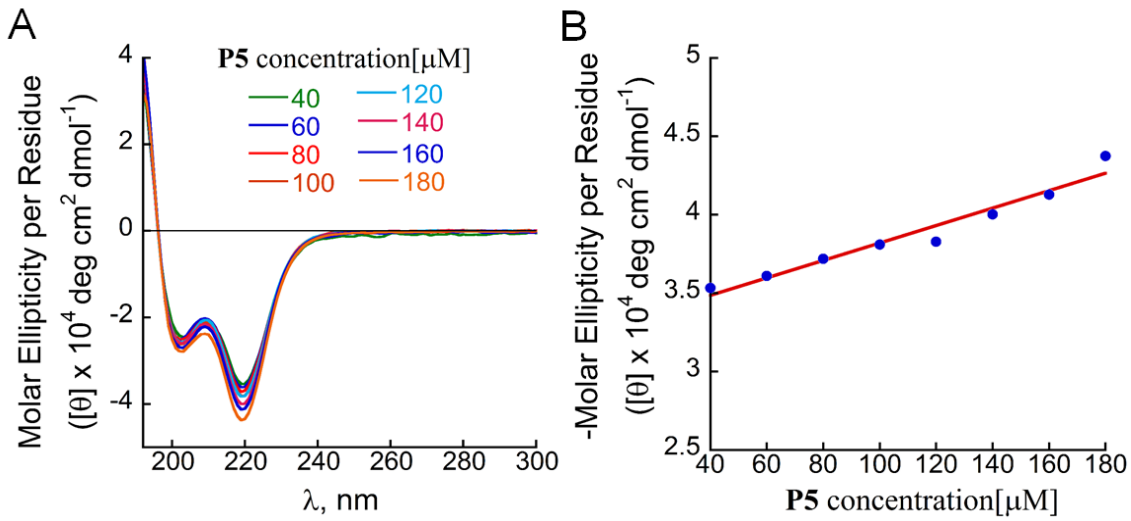



Fig. **S3c**. (A) The CD spectra of **P5** peptides in different concentrations (40-180 μM). (B) Plots of molar ellipticity ([θ]) at 219 nm vs. peptide concentration (40-180 μM).

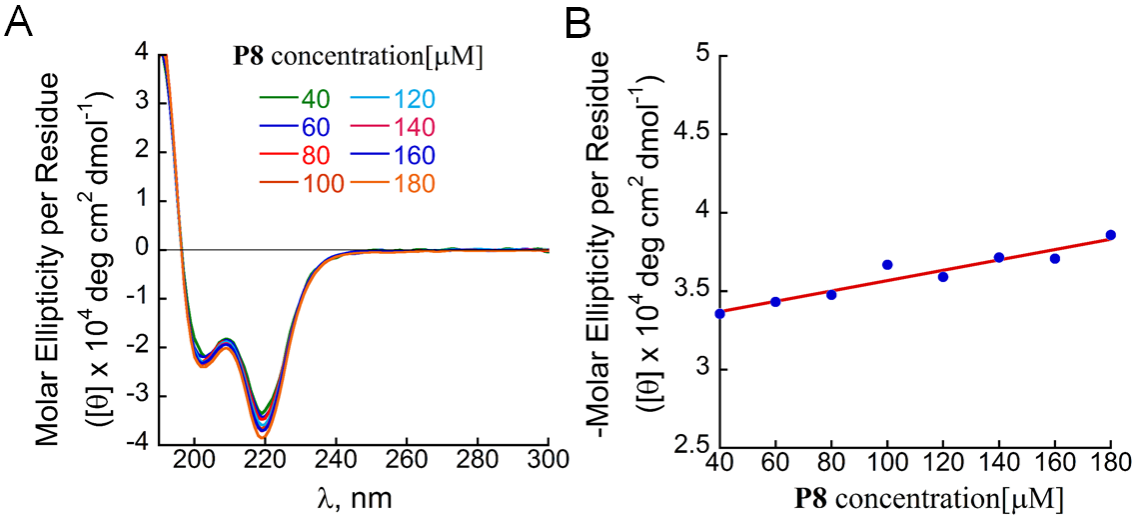
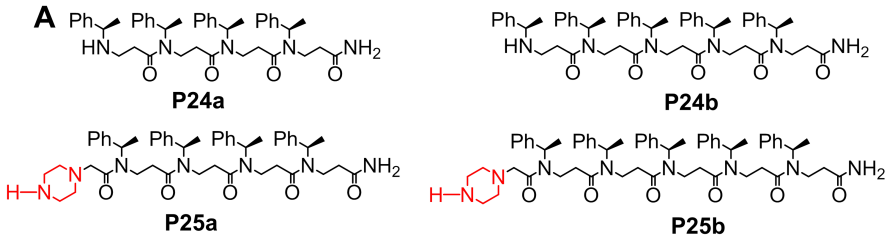



Fig. **S3d**. (A) The CD spectra of **P8** peptides in different concentrations (40-180 μM). (B) Plots of molar ellipticity ([θ]) at 219 nm vs. peptide concentration (40-180 μM).

A




B

| β-Peptoid | Water Solubility (mg/L) |
|---|---|
| **P24a** | <2.0x10$^2$ |
| **P24b** | <2.0x10$^2$ |
| **P25a** | (1.06±0.11)x10$^4$ |
| **P25b** | (2.65±0.18)x10$^3$ |

**Figure S4.** Water solubility data for different length **β-peptoid P24a-P25b.** The above experiments shows clear idea about that the increase of chain length the solubility of the β- peptoid were decrease,

## HPLC

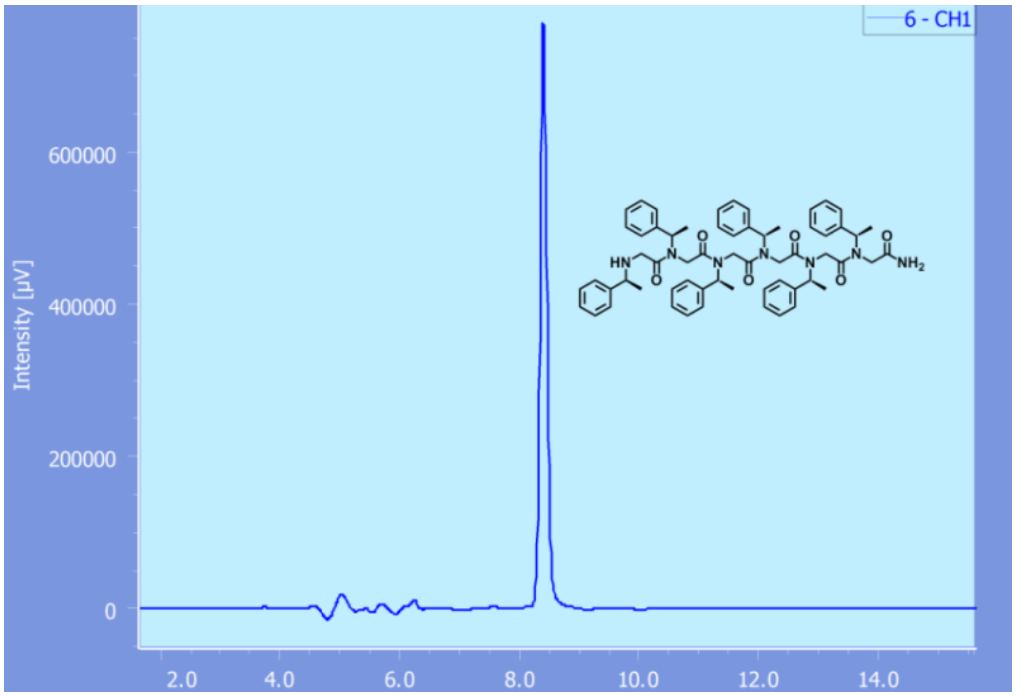



**Figure S6**. HPLC trace of peptoid **P1**

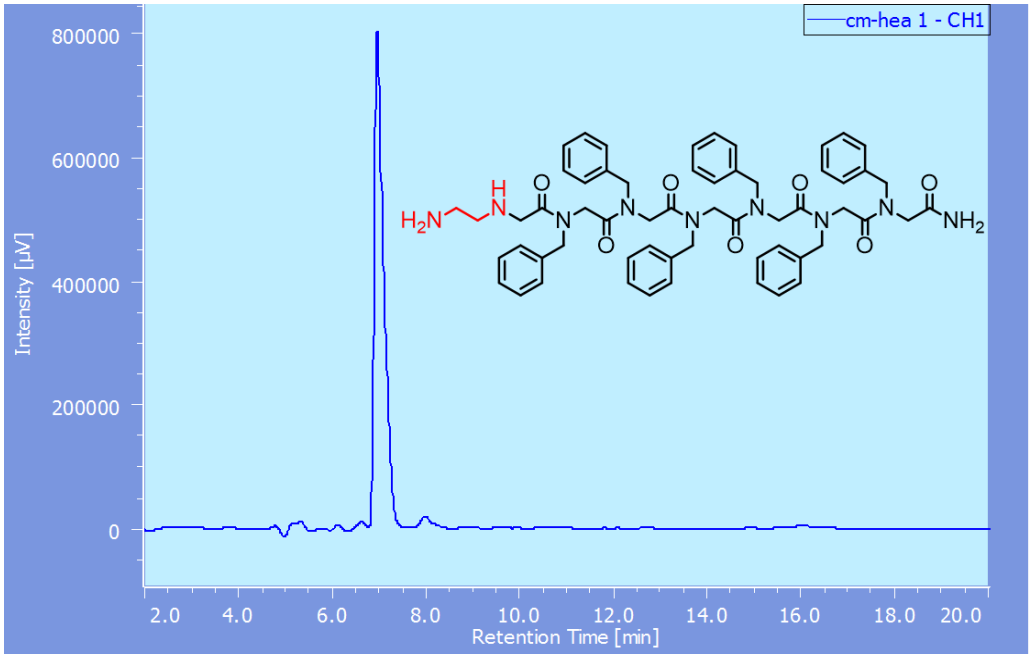



**Figure S7**. HPLC trace of peptoid **SP1**

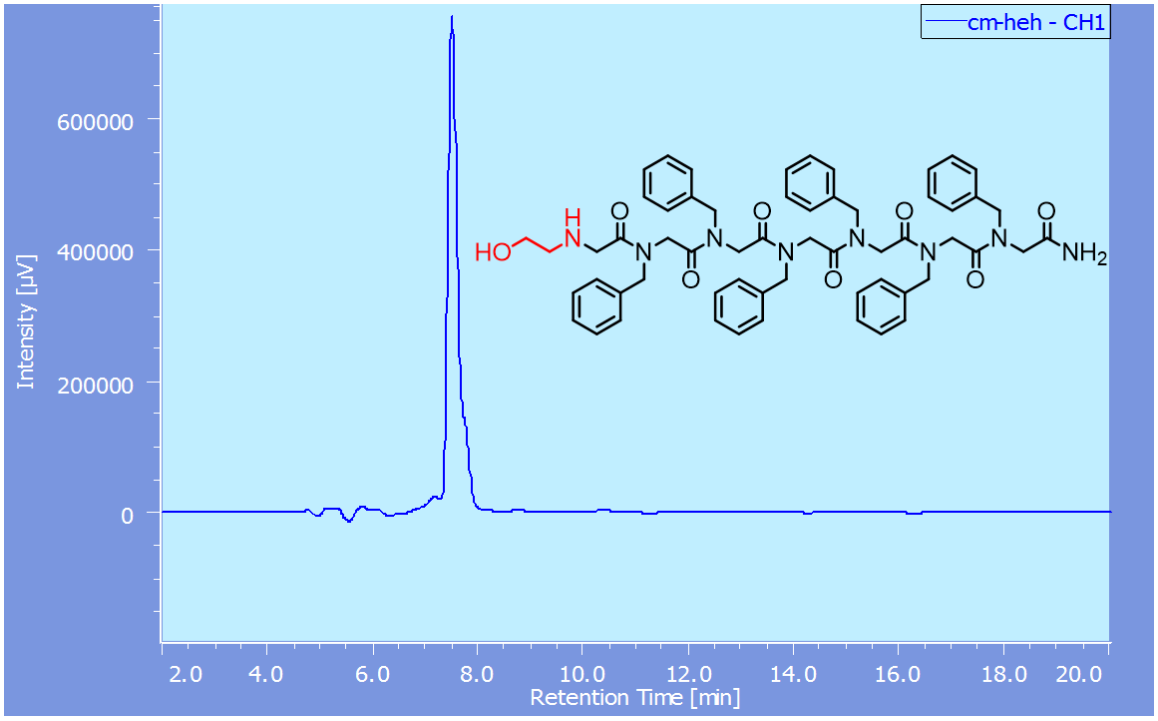



**Figure S8**. HPLC trace of peptoid **SP2**

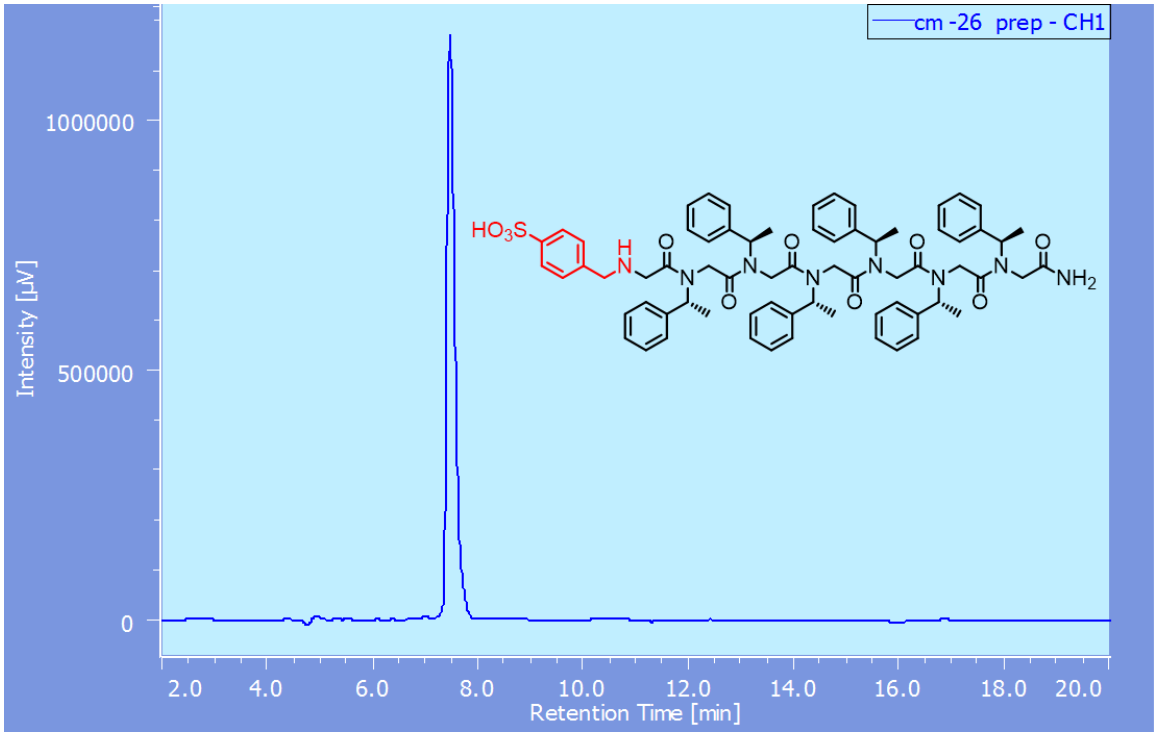



**Figure S9**. HPLC trace of peptoid **SP3**

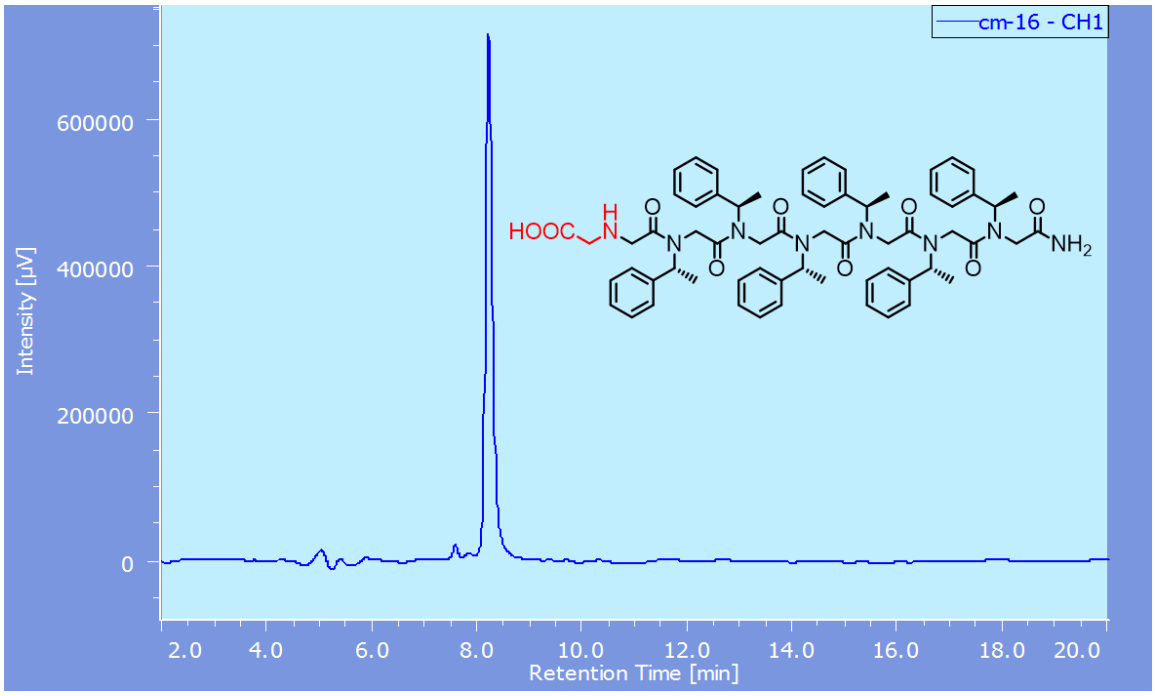



**Figure S10**. HPLC trace of peptoid **SP4**

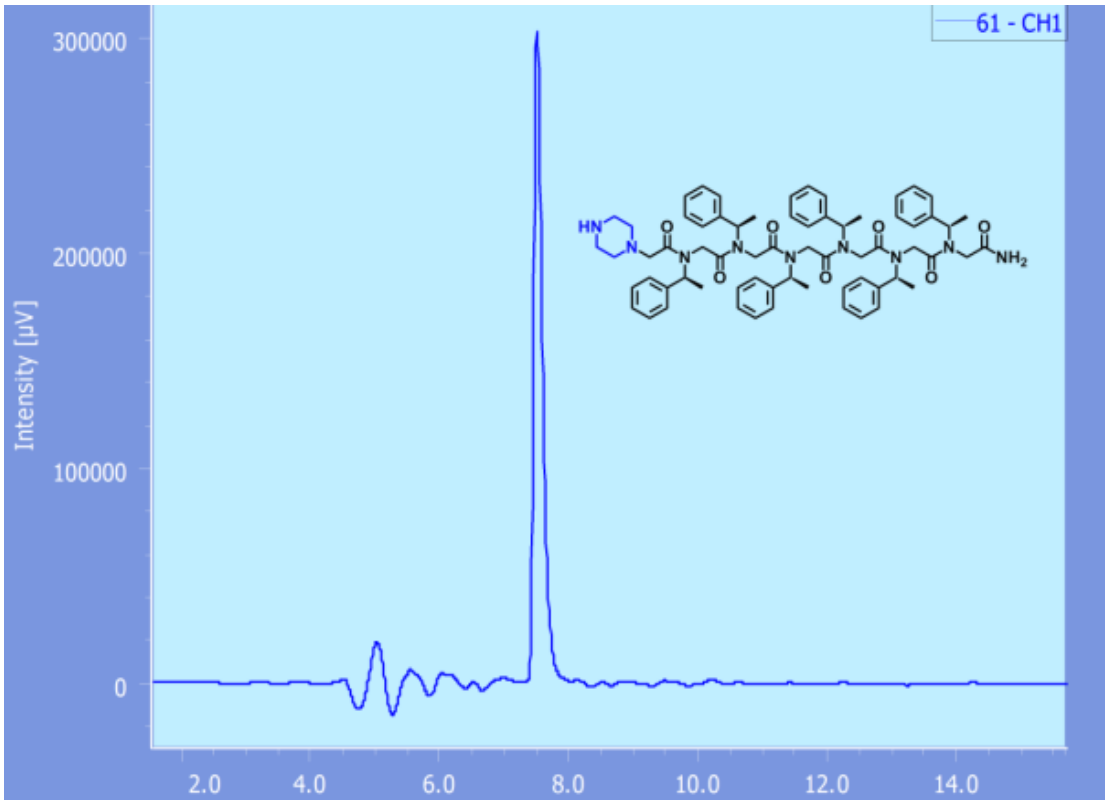



**Figure S11**. HPLC trace of peptoid **P2**

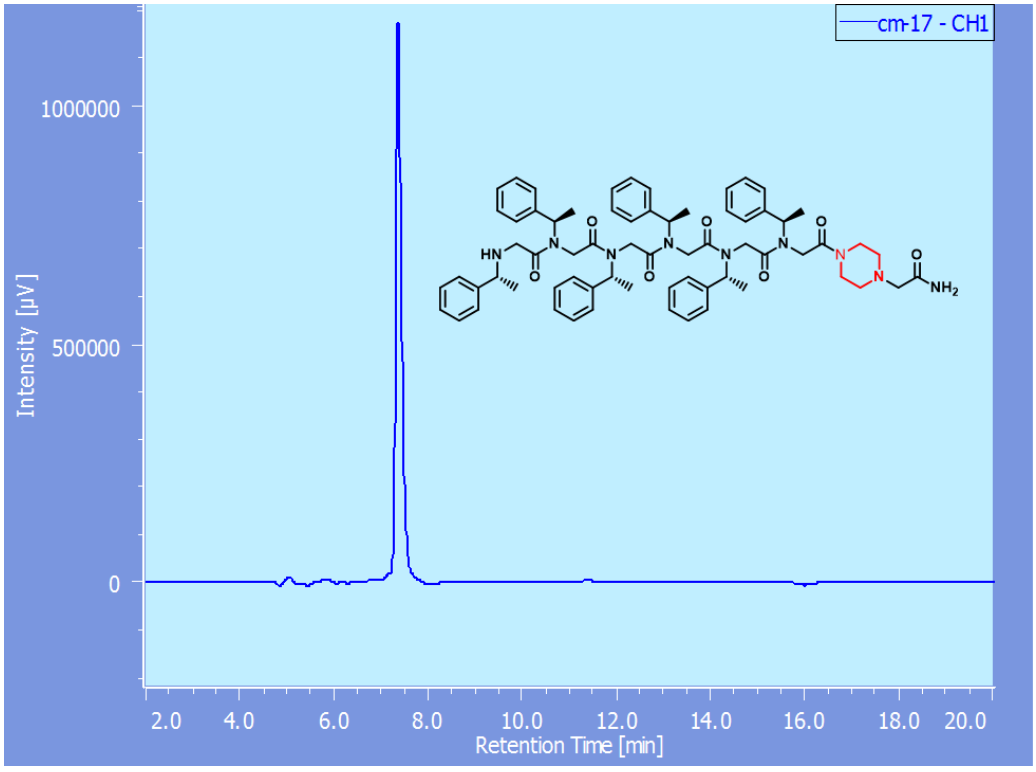



**Figure S12**. HPLC trace of peptoid **P3**

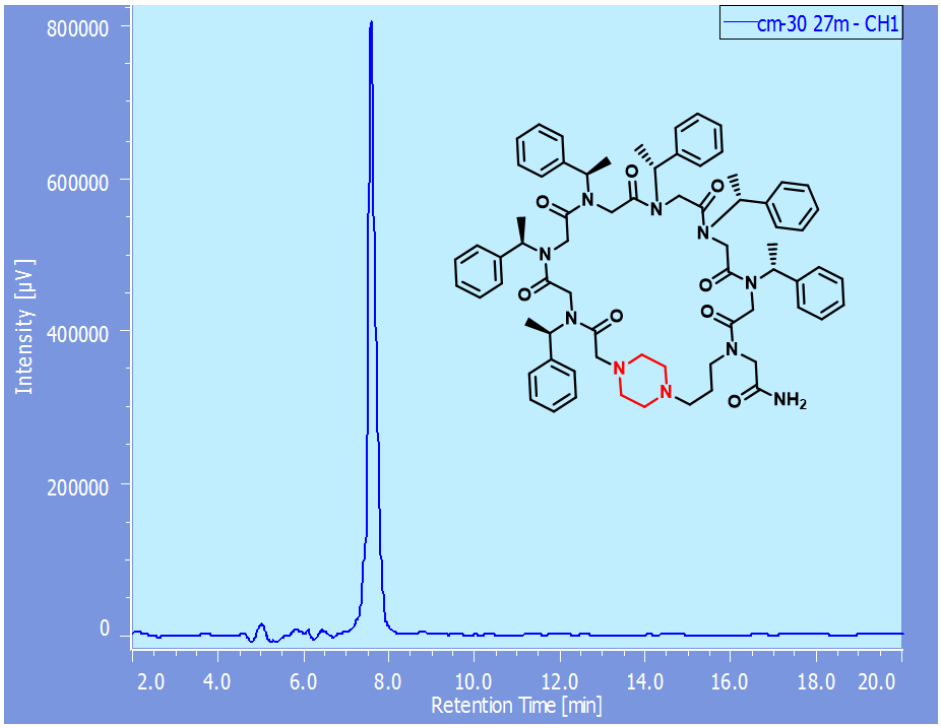



**Figure S13**. HPLC trace of peptoid **P4**

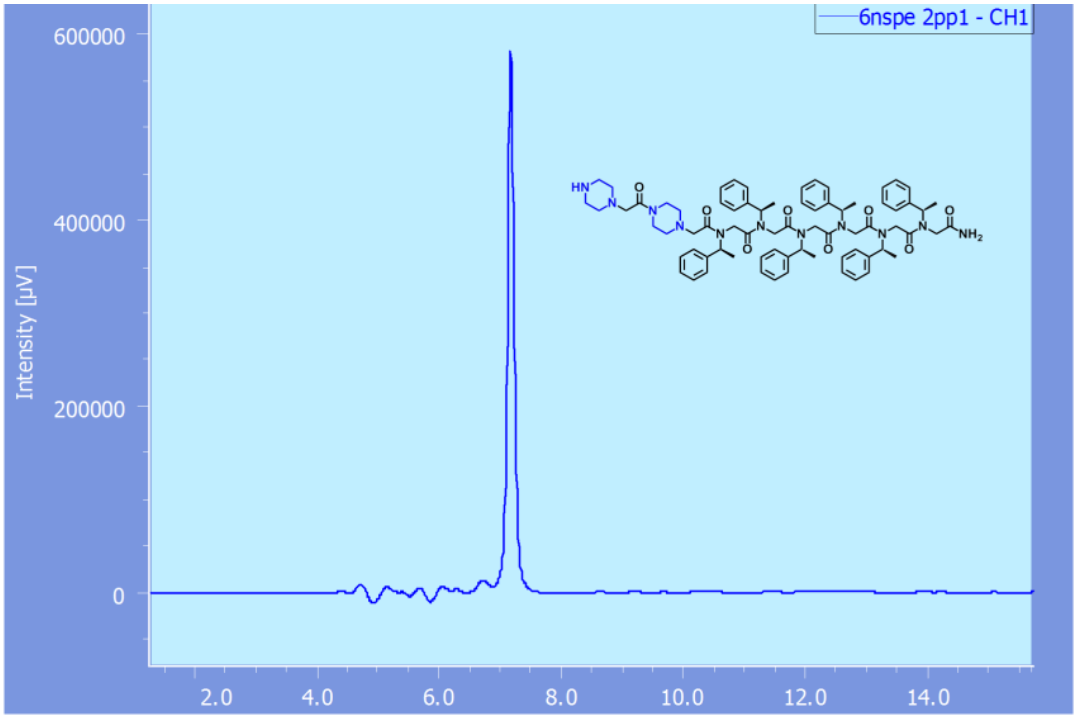



**Figure S14**. HPLC trace of peptoid **P5**

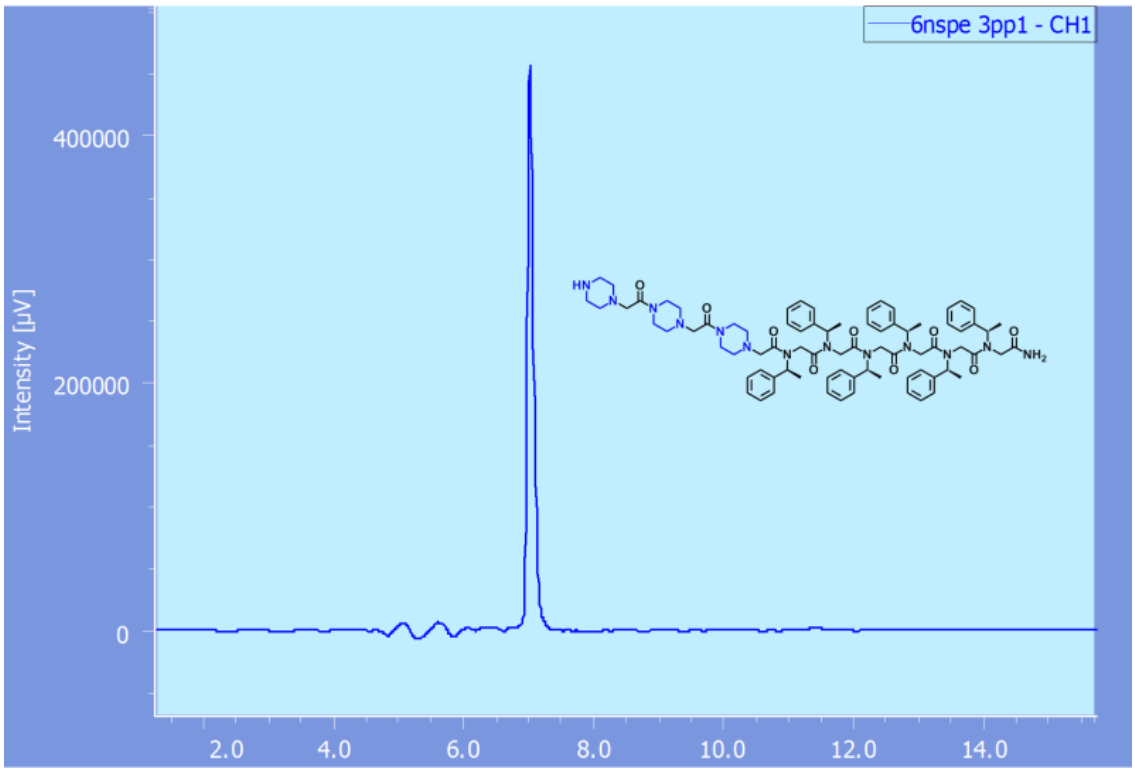



**Figure S15**. HPLC trace of peptoid **P6**

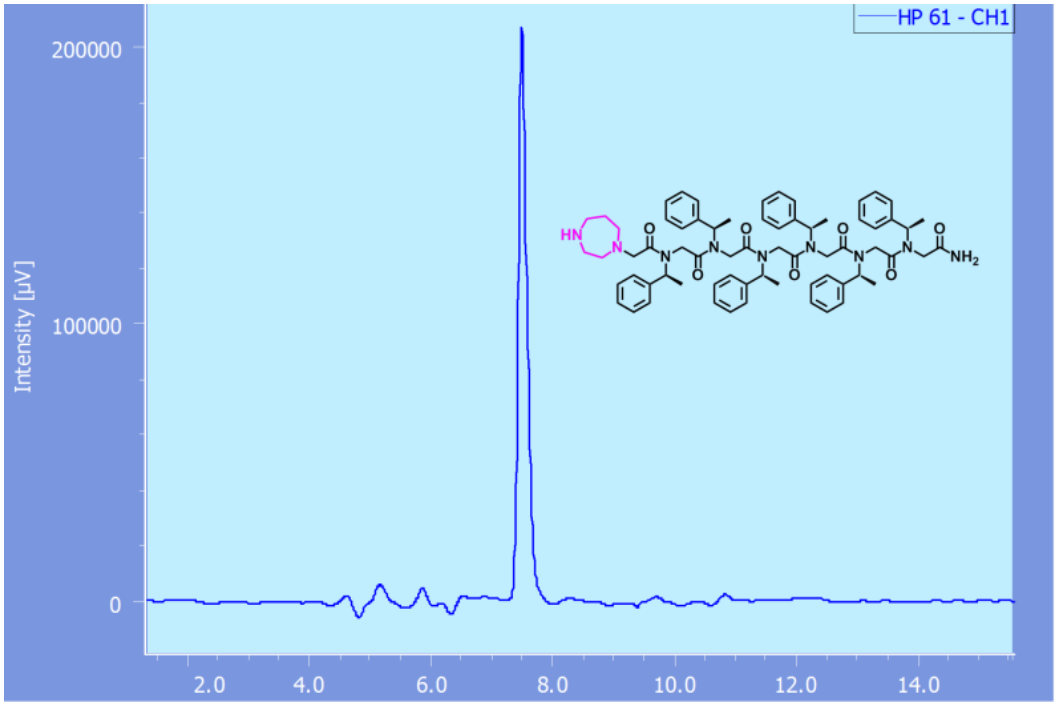



**Figure S16**. HPLC trace of peptoid **P7**

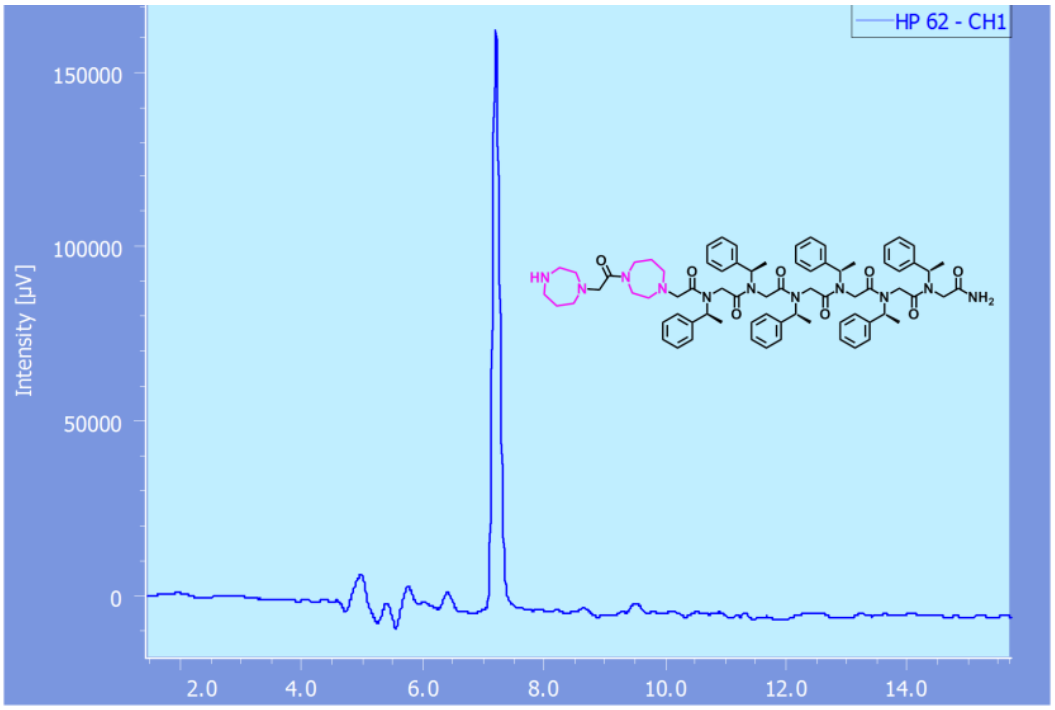



**Figure S17**. HPLC trace of peptoid **P8**

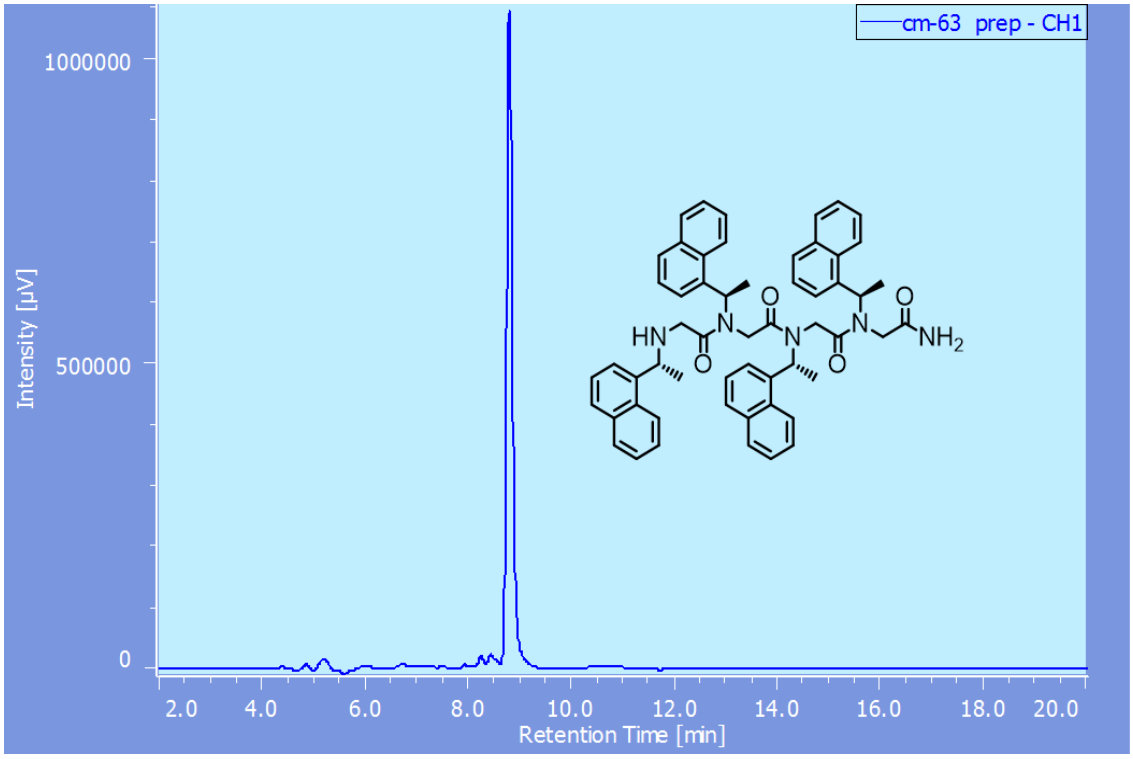



**Figure S18**. HPLC trace of peptoid **P9**

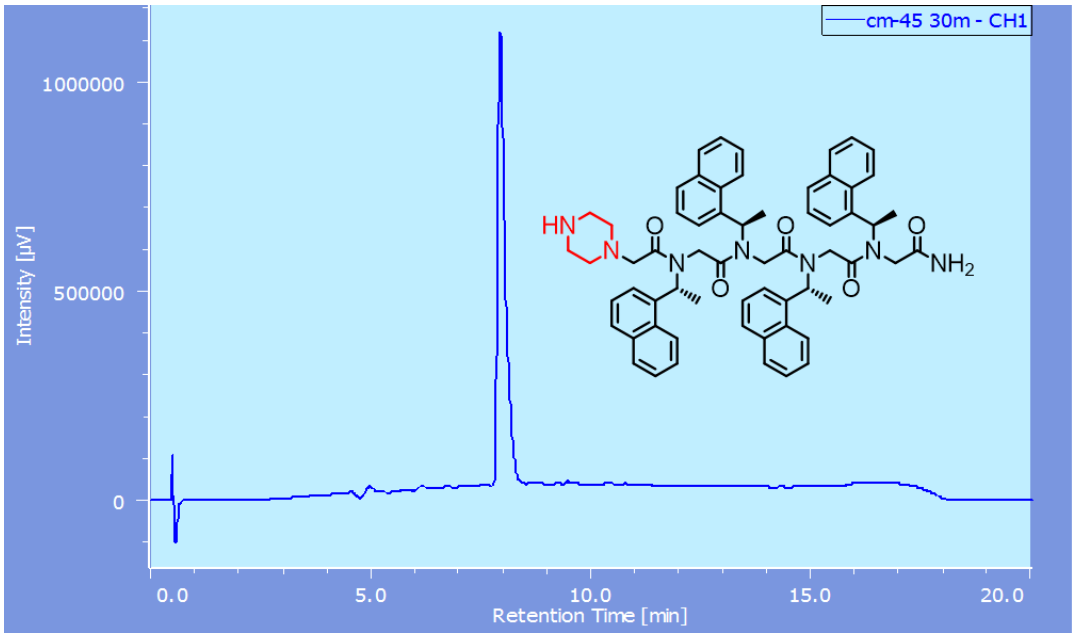



**Figure S19**. HPLC trace of peptoid **P12**

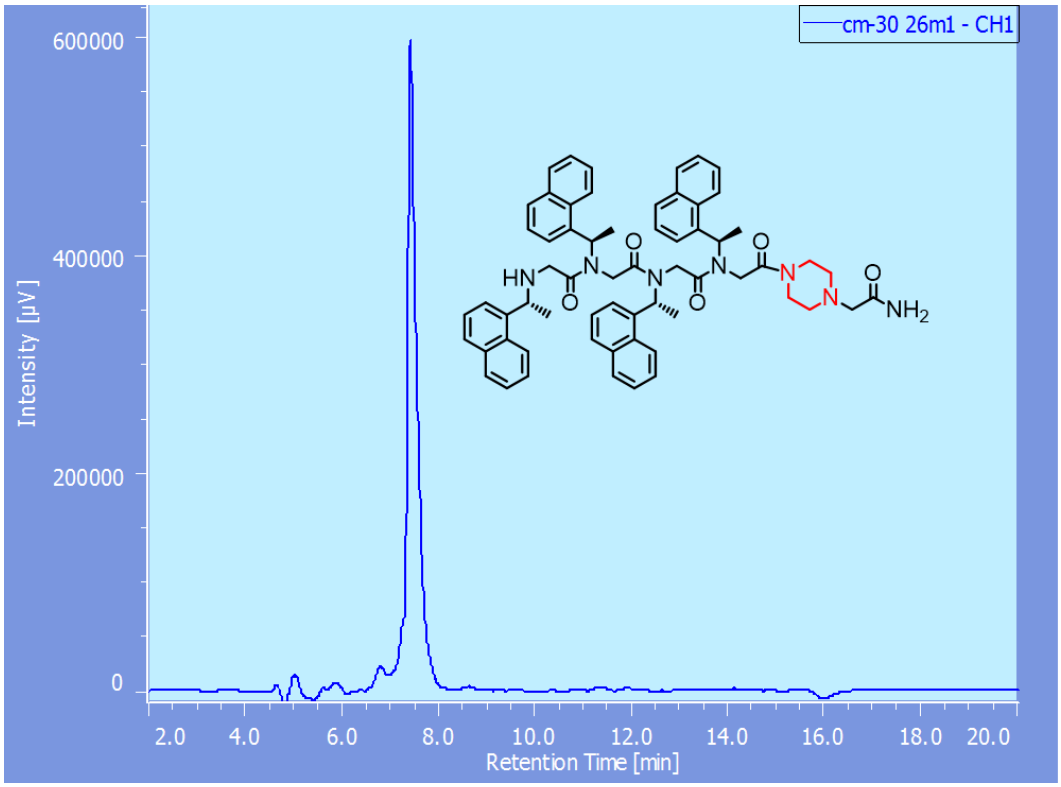



**Figure S20**. HPLC trace of peptoid **P13**

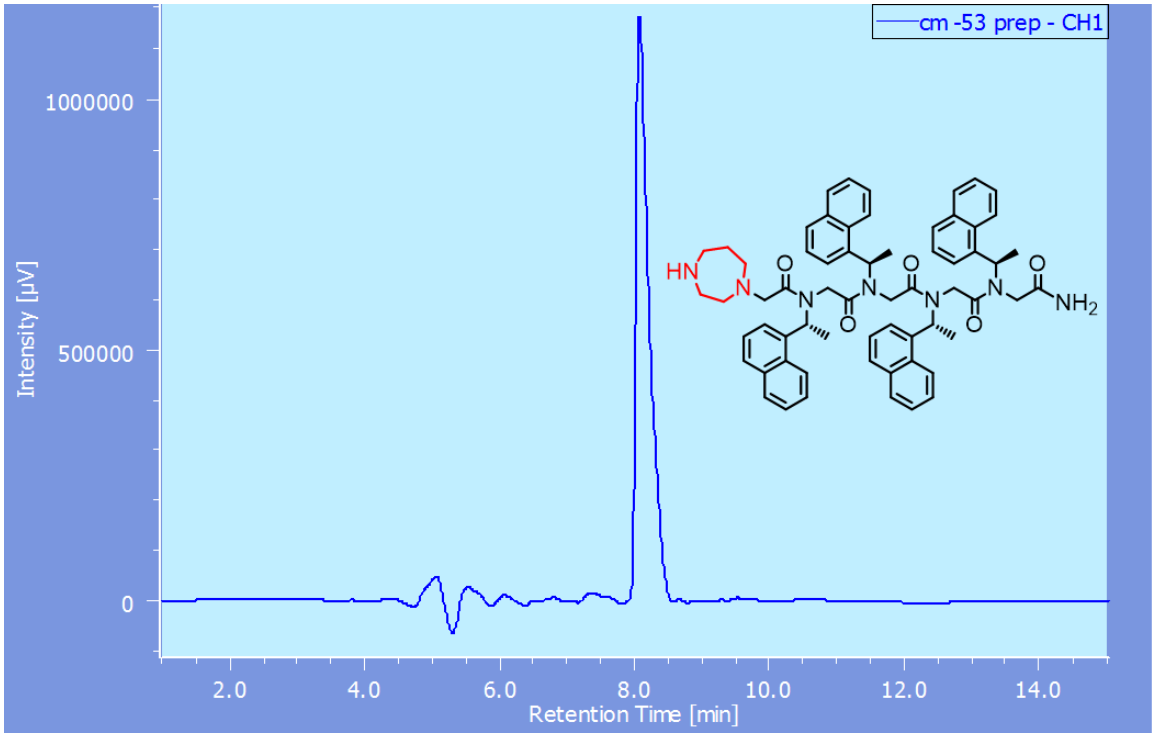



**Figure S21**. HPLC trace of peptoid **P14**

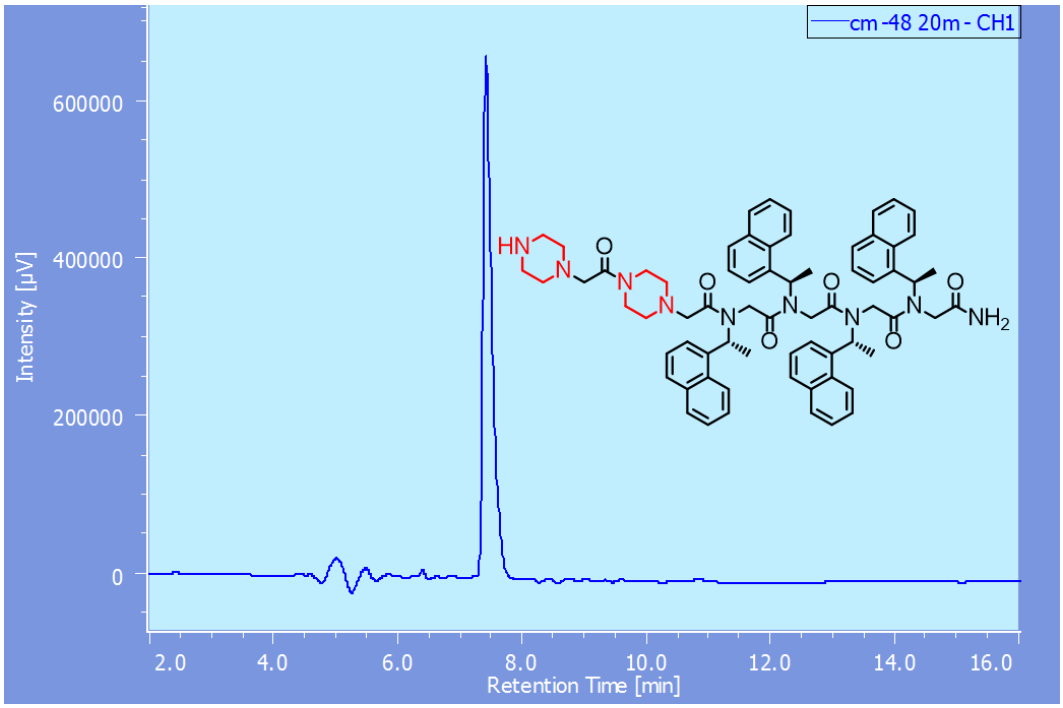



**Figure S22**. HPLC trace of peptoid **P18**

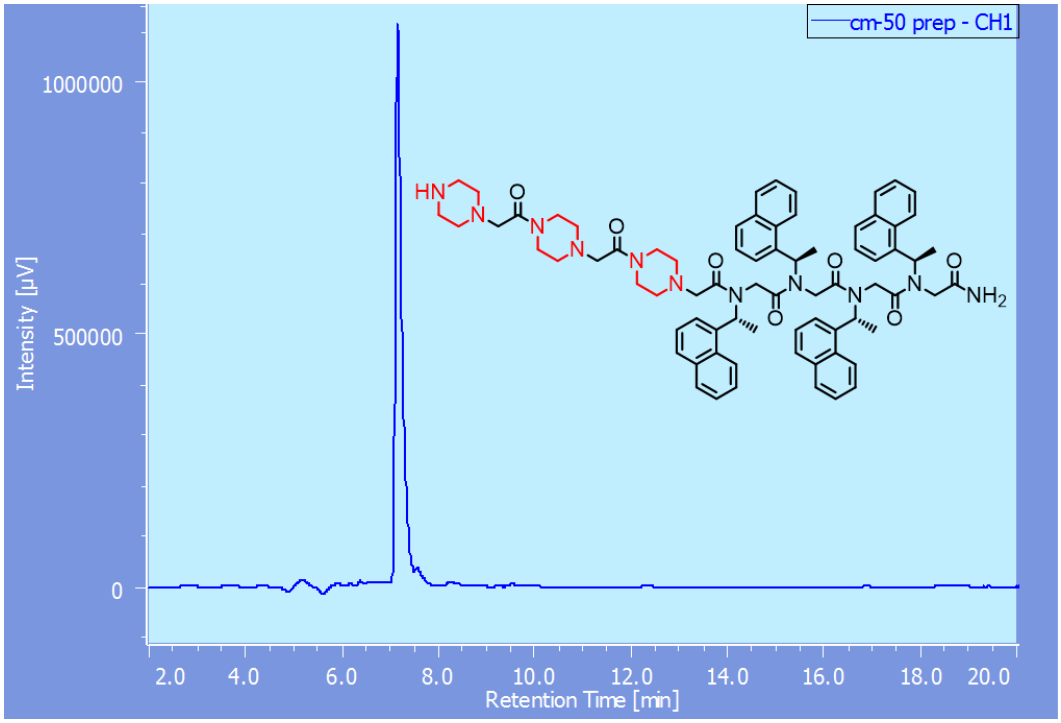



**Figure S23**. HPLC trace of peptoid **P21**

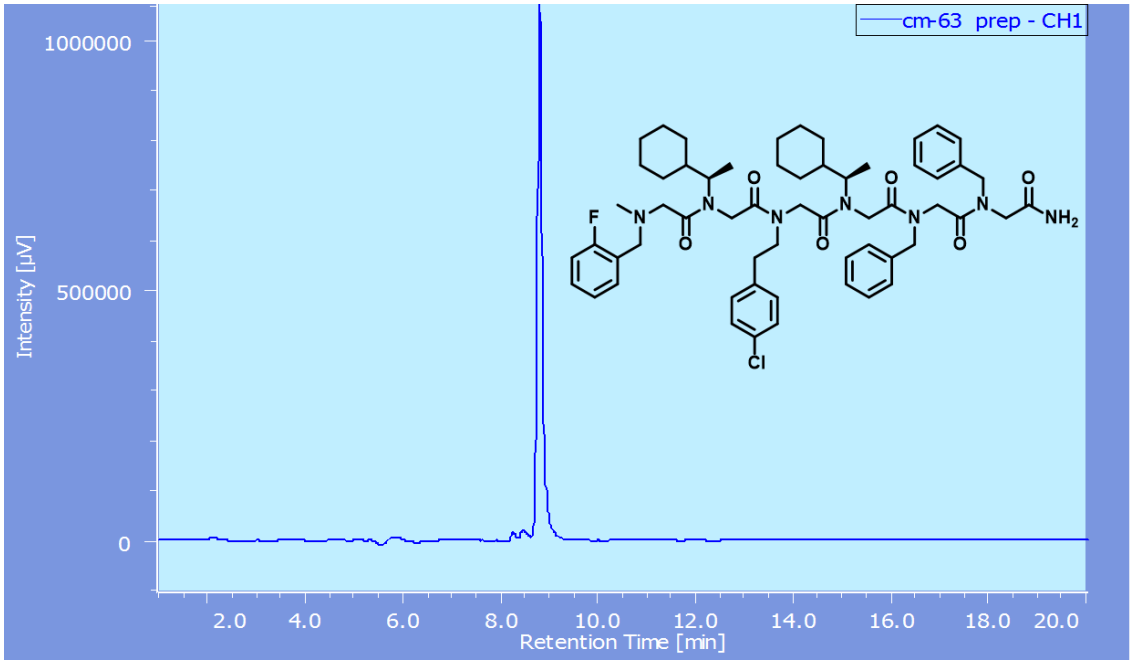



**Figure S24**. HPLC trace of peptoid **P11**

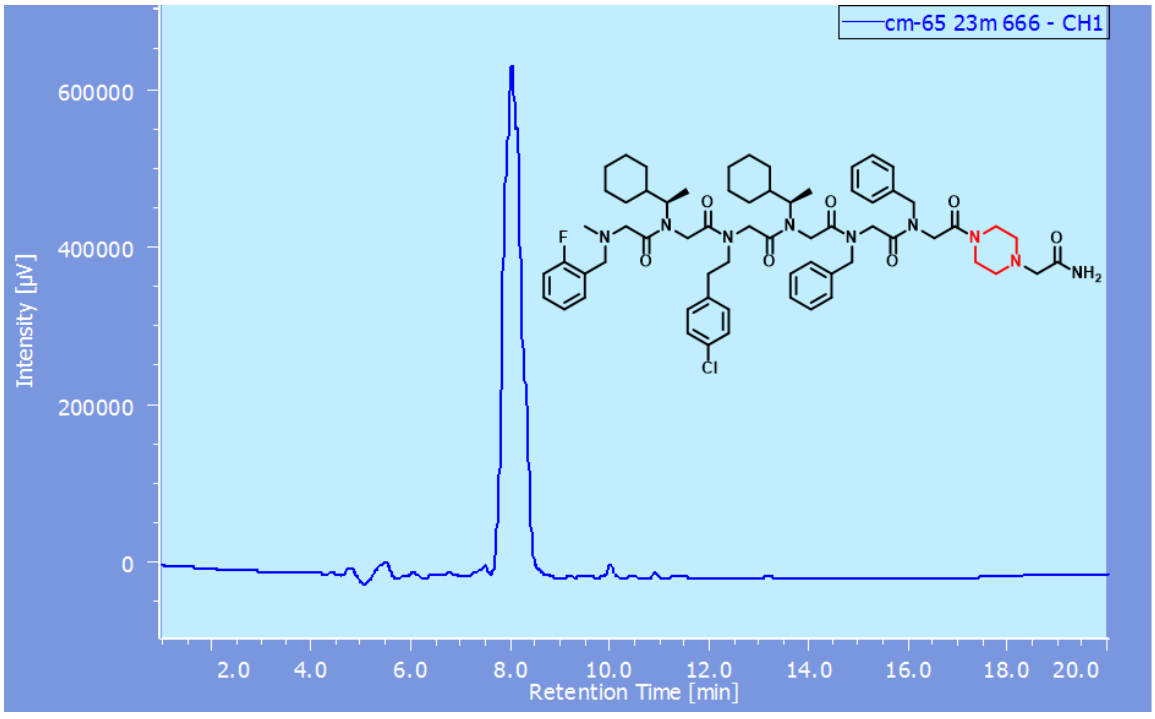



**Figure S25**. HPLC trace of peptoid **P17**

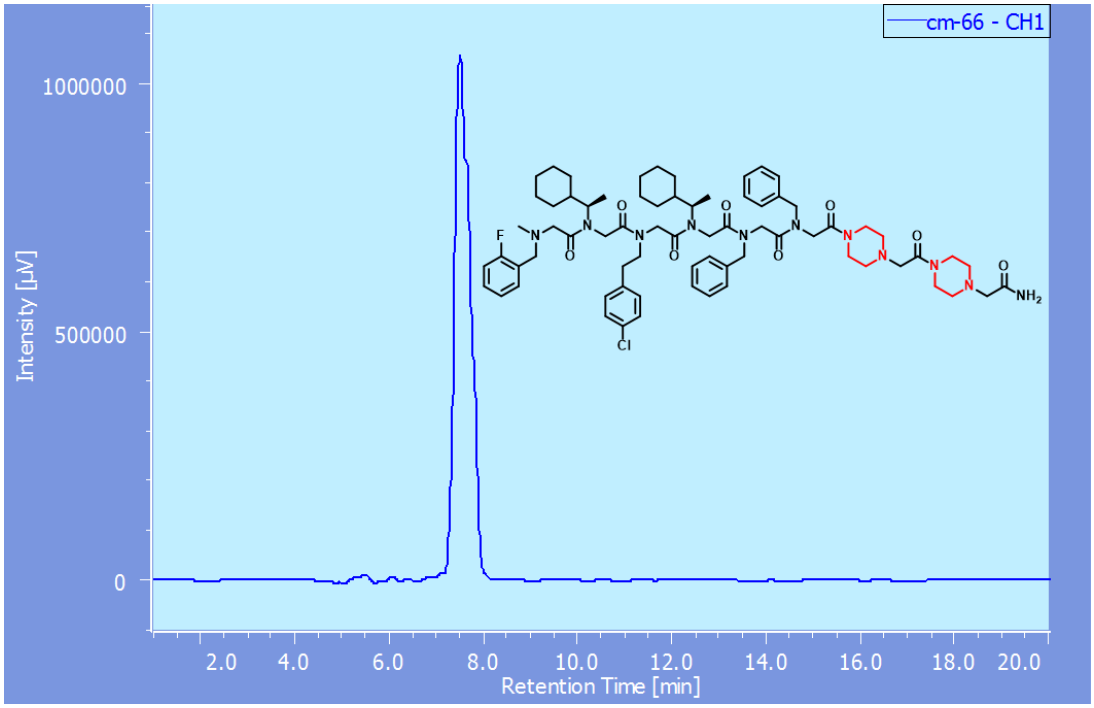



**Figure S26**. HPLC trace of peptoid **P20**

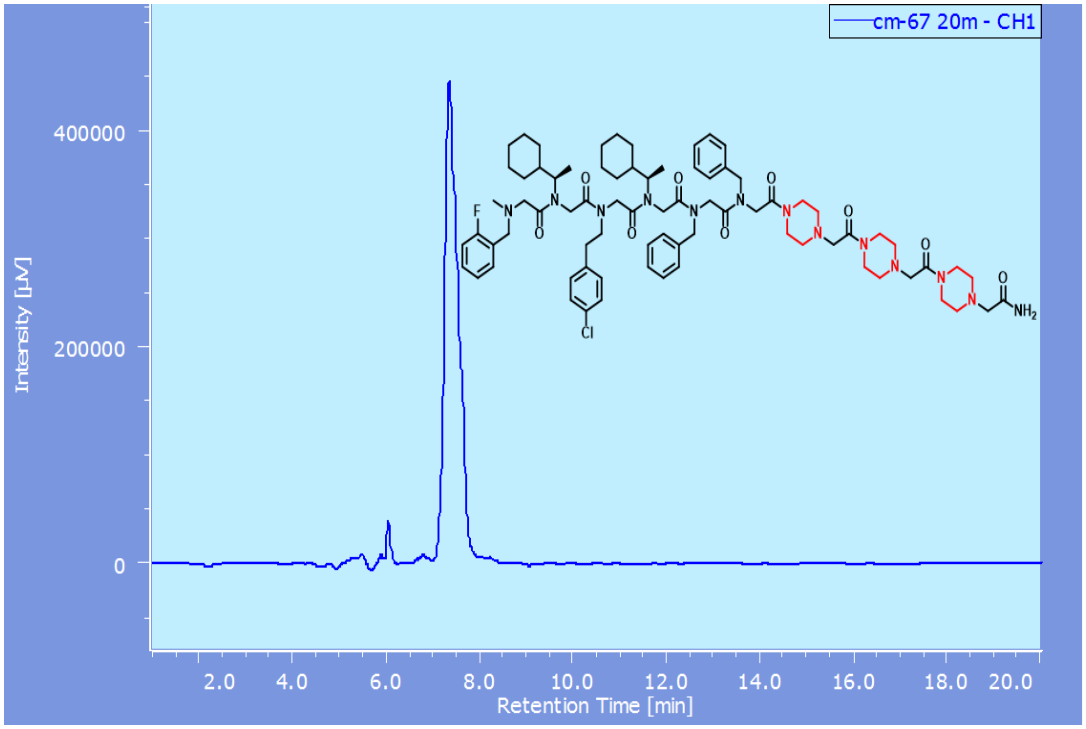



**Figure S27**. HPLC trace of peptoid **P23**

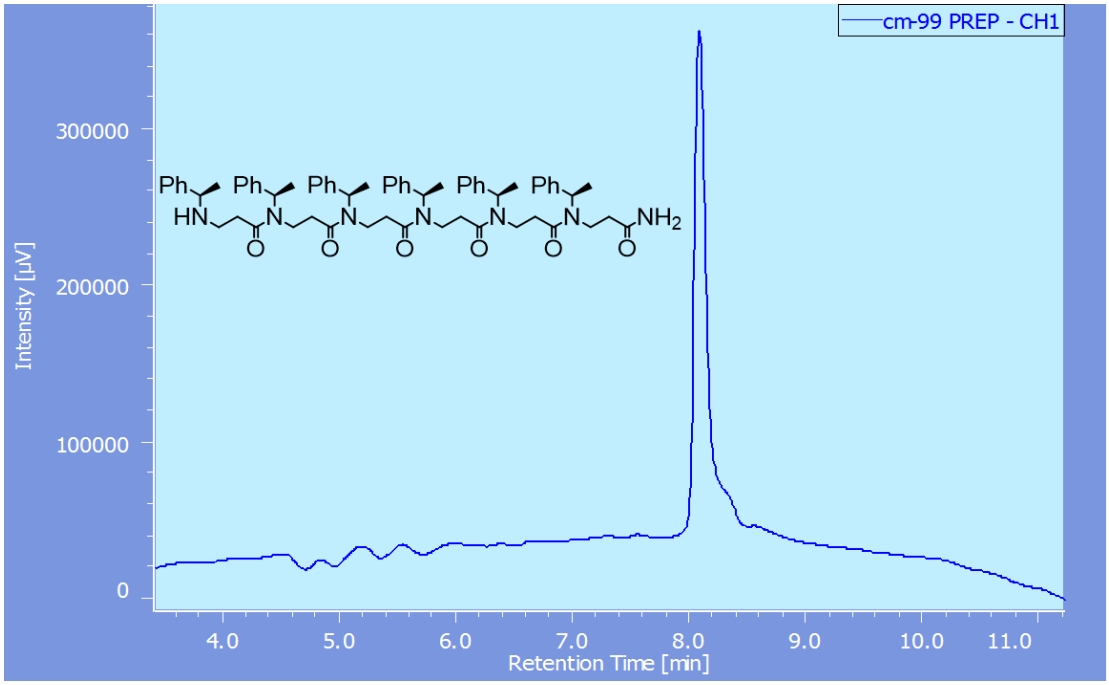



**Figure S28**. HPLC trace of peptoid **P24**

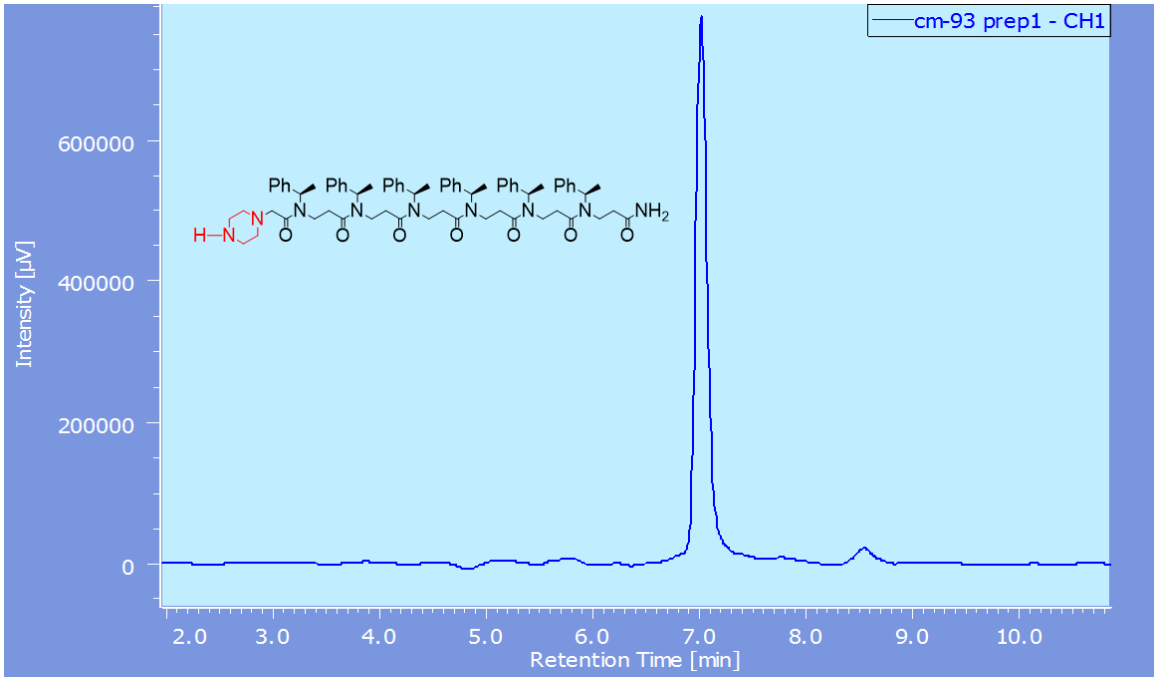



**Figure S29**. HPLC trace of peptoid **P25**

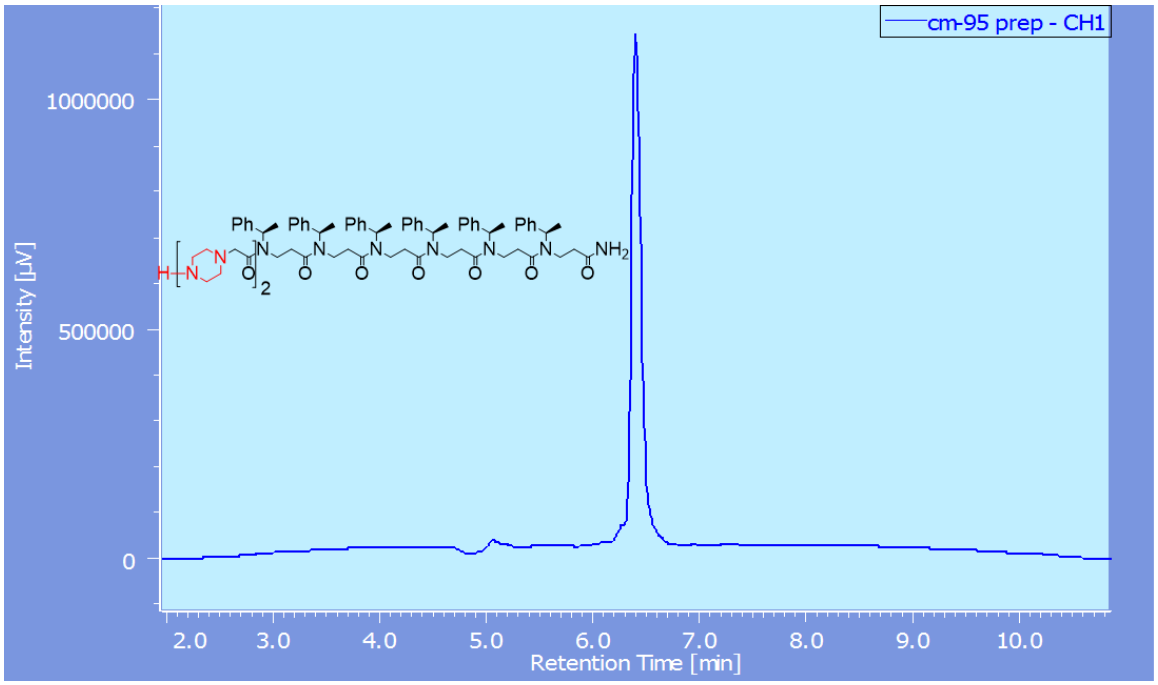



**Figure S30**. HPLC trace of peptoid **P26**

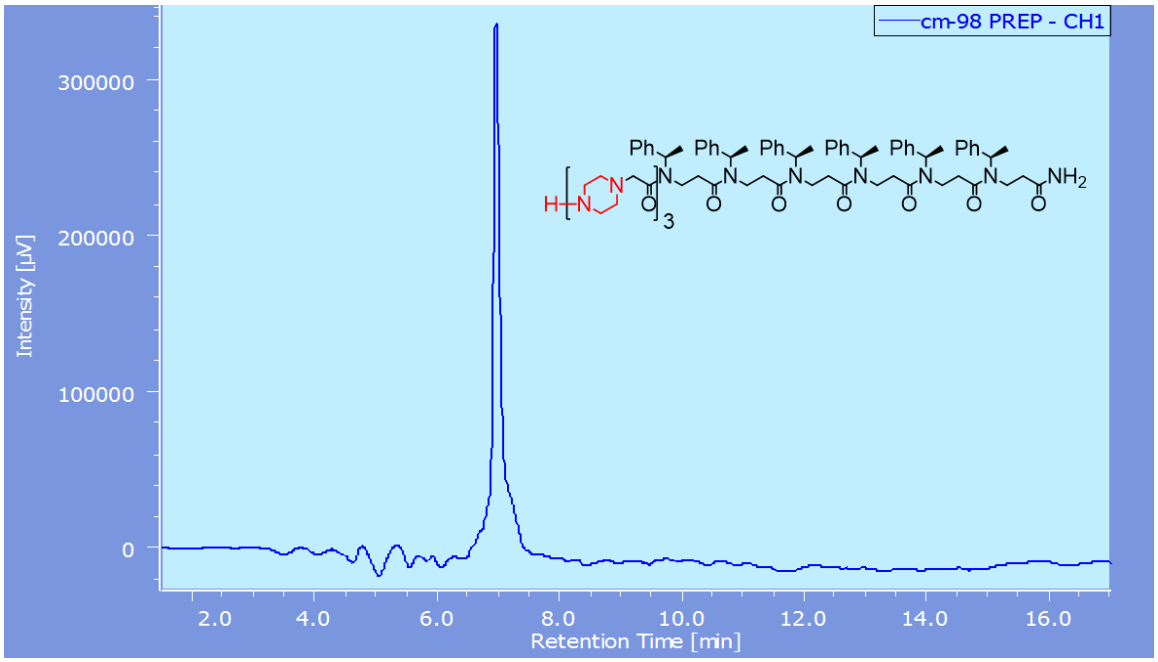



**Figure S31**. HPLC trace of peptoid **P27**

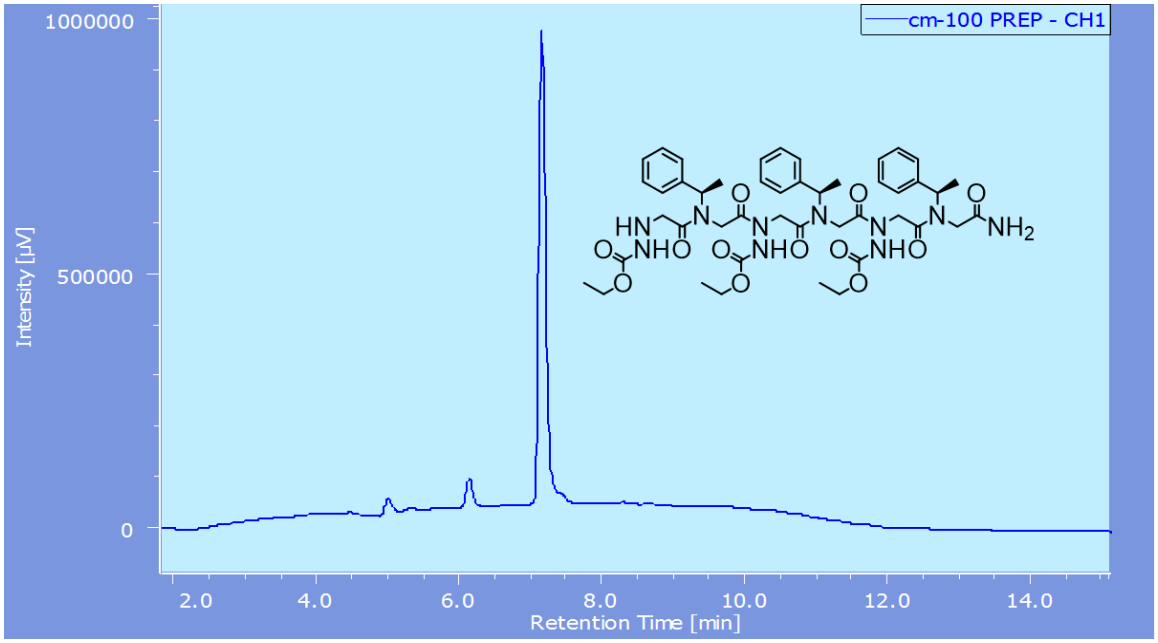



**Figure S32**. HPLC trace of peptoid **P28**

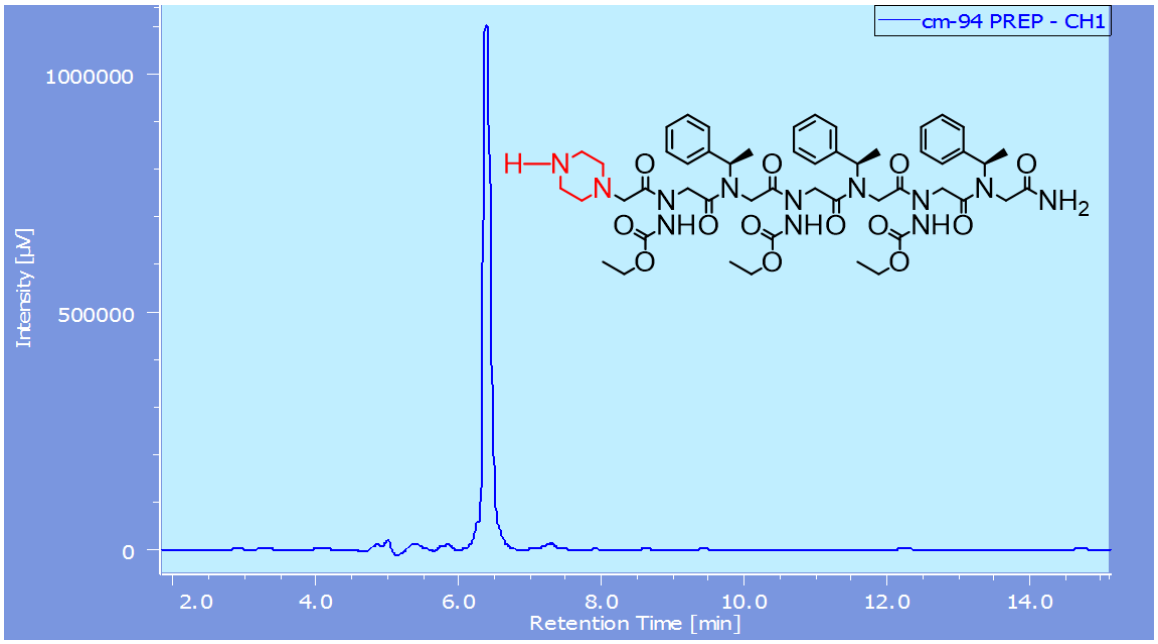



**Figure S33**. HPLC trace of peptoid **P29**

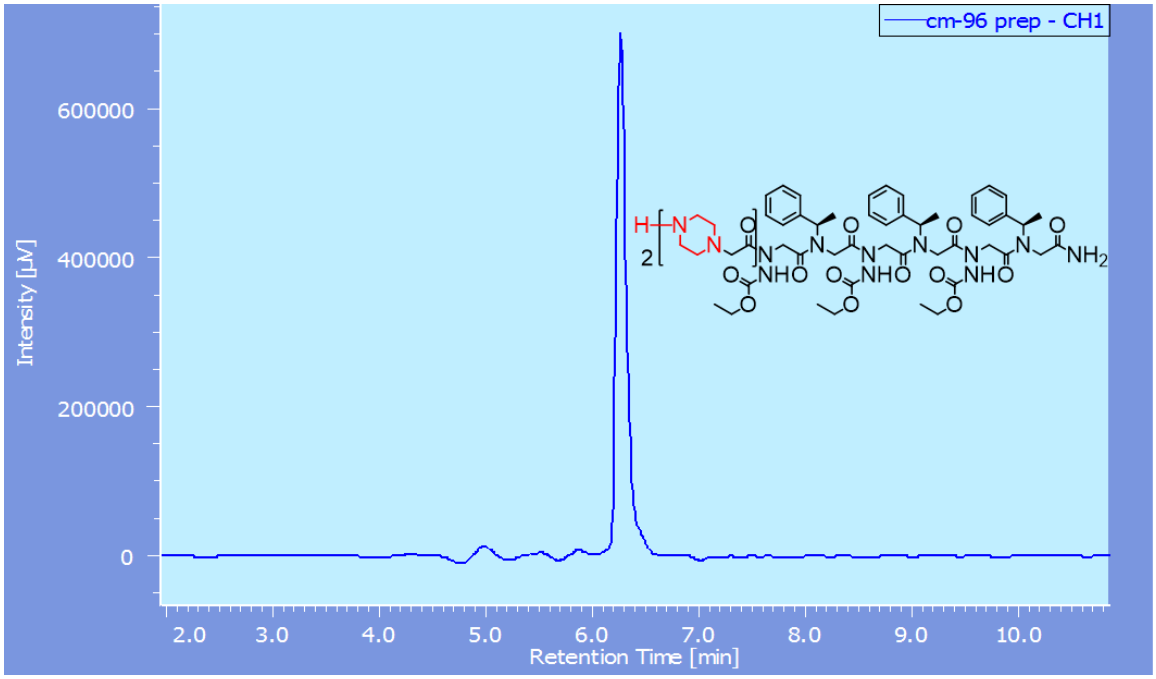



**Figure S34**. HPLC trace of peptoid **P30**

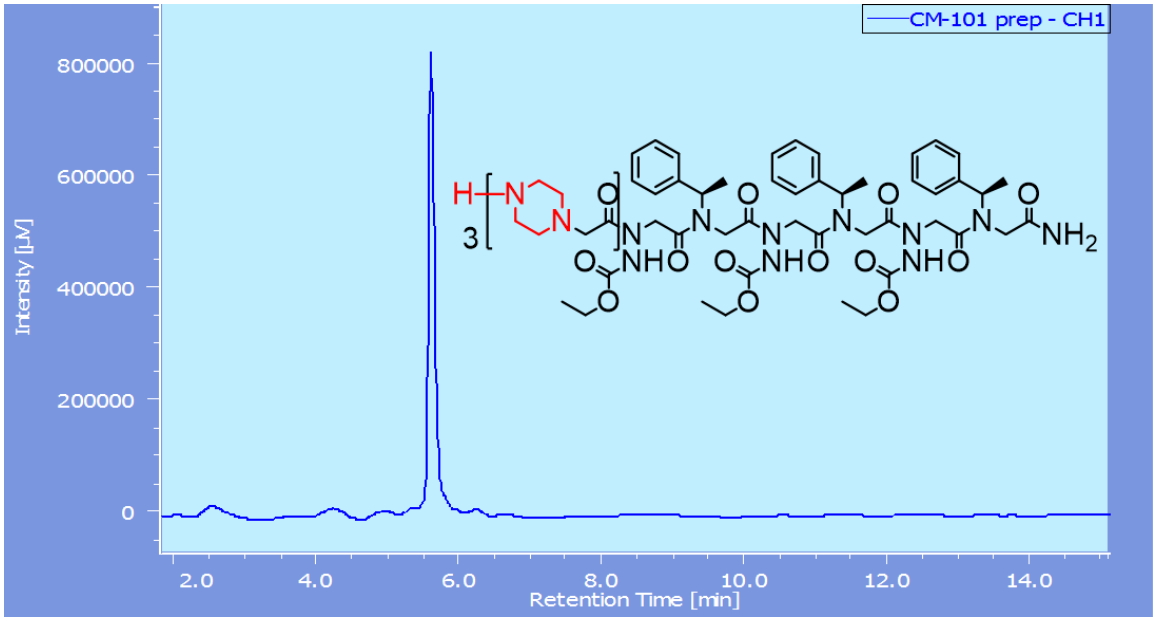



**Figure S35**. HPLC trace of peptoid **P31**

## ESI MS

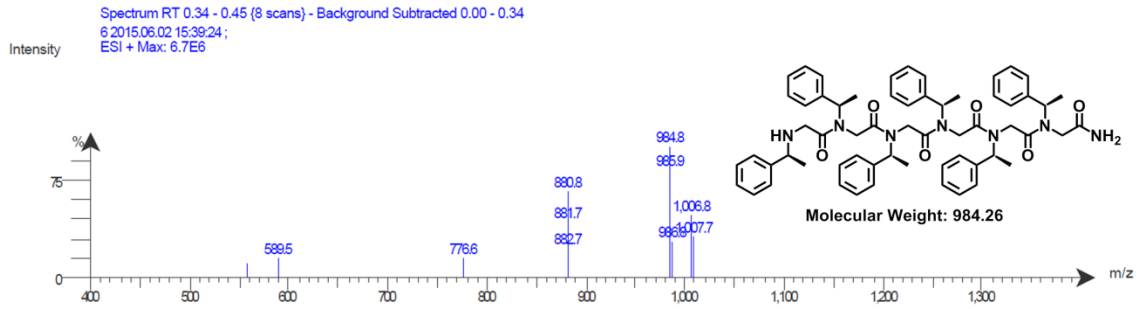



**Figure S36.** ESI MS of peptoid **P1**

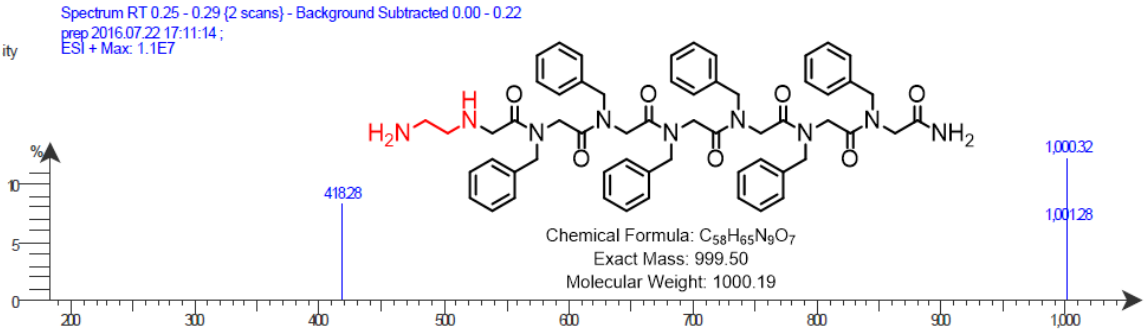



**Figure S37.** ESI MS of peptoid **SP1**

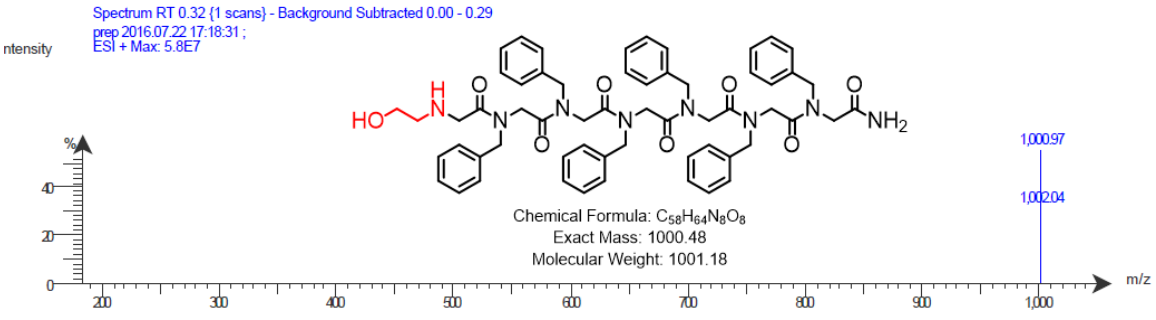



**Figure S38.** ESI MS of peptoid **SP2**

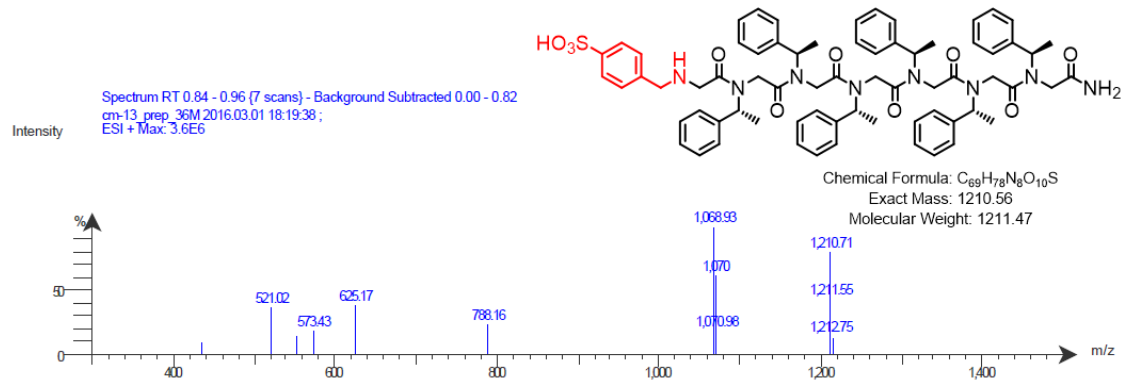



**Figure S39.** ESI MS of peptoid **SP3**

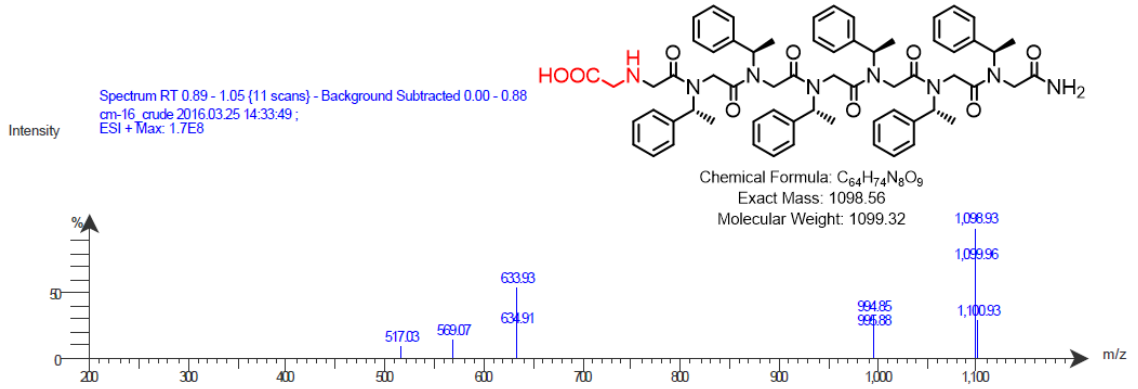



**Figure S40.** ESI MS of peptoid **SP4**

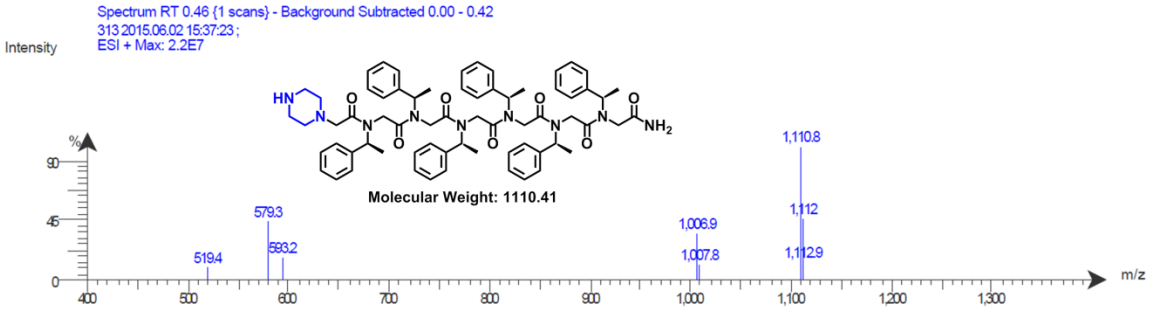



**Figure S41.** ESI MS of peptoid **P2**

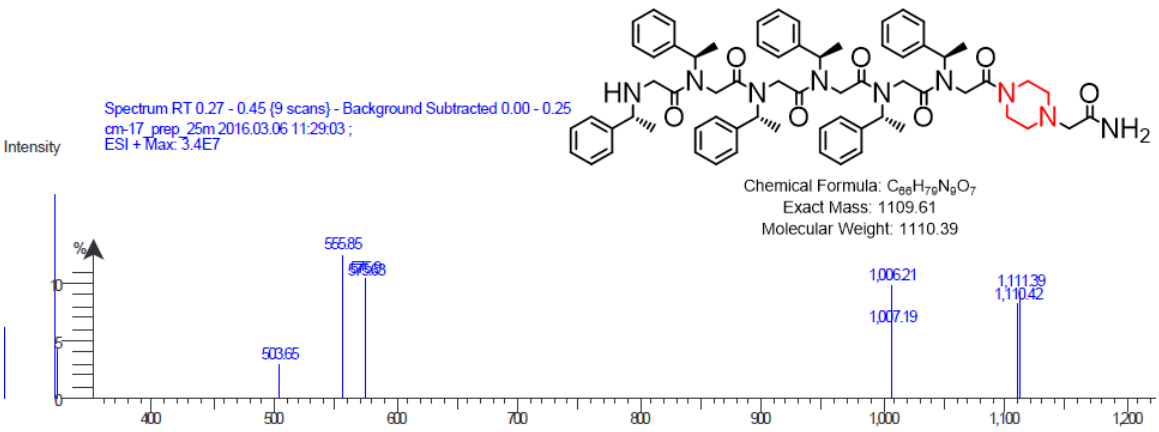



**Figure S42.** ESI MS of peptoid **P3**

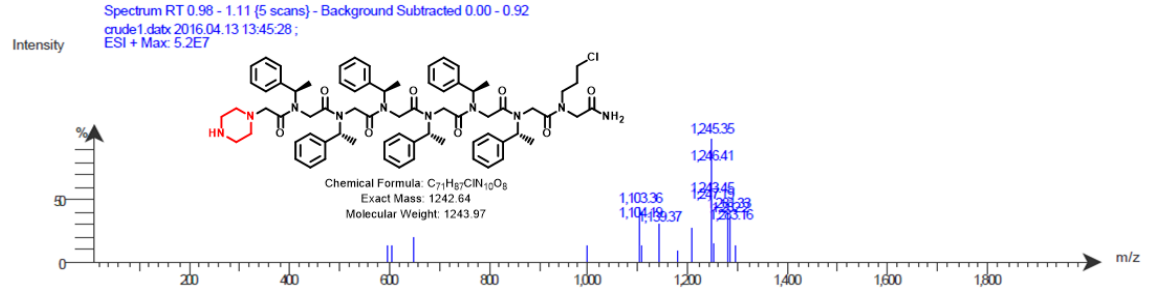



**Figure S43.** ESI MS of peptoid **P linear**

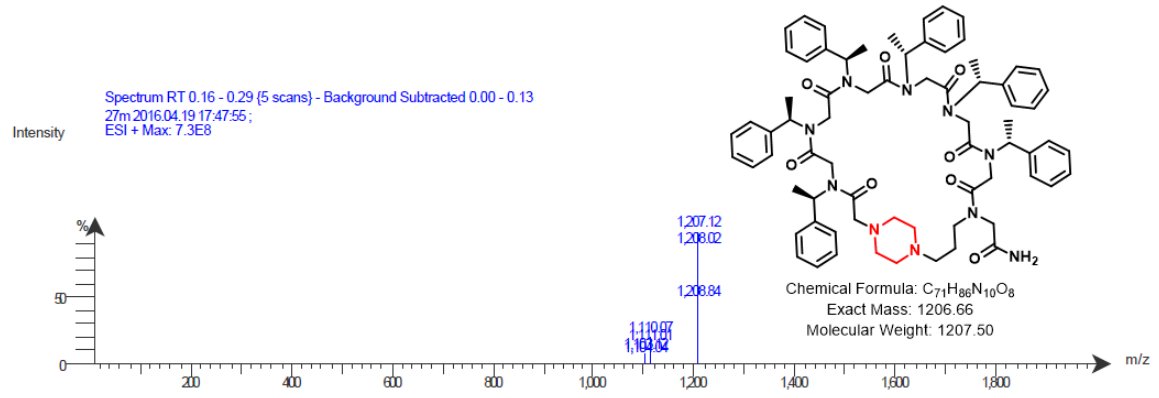



**Figure S44.** ESI MS of peptoid **P4**

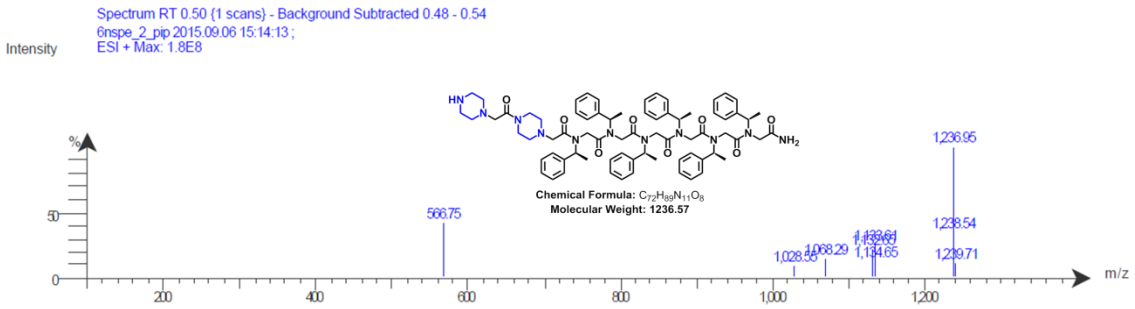



**Figure S45.** ESI MS of peptoid **P5**

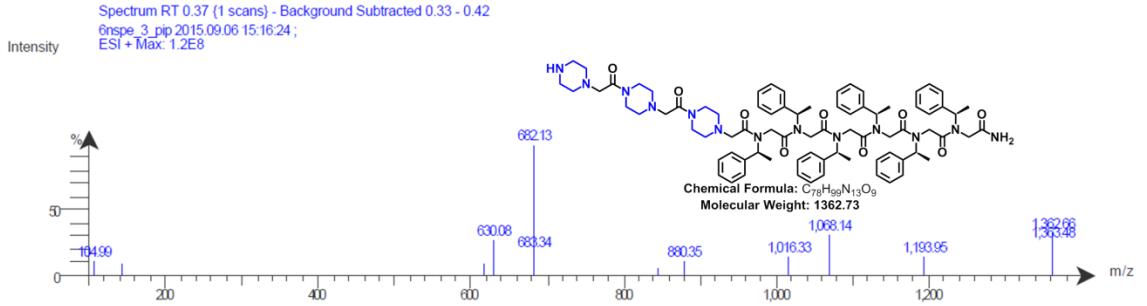



**Figure S46.** ESI MS of peptoid **P6**

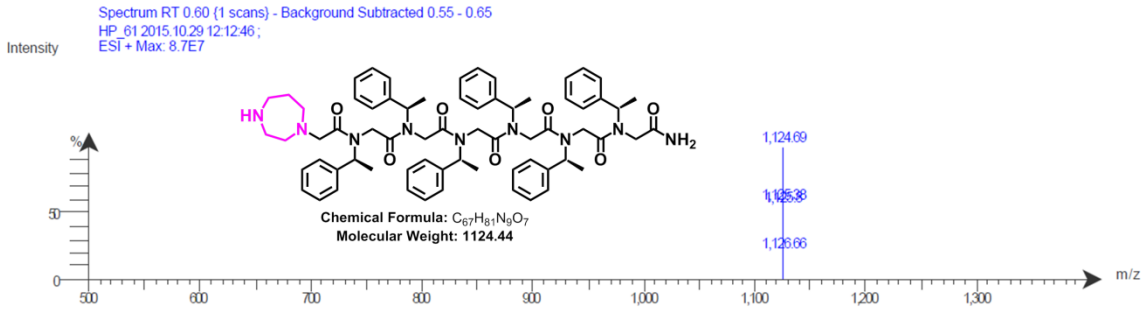



**Figure S47.** ESI MS of peptoid **P7**

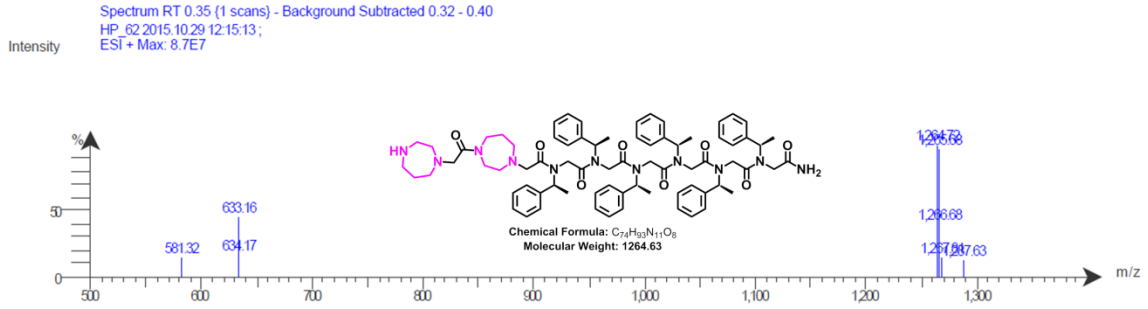



**Figure S58.** ESI MS of peptoid **P8**

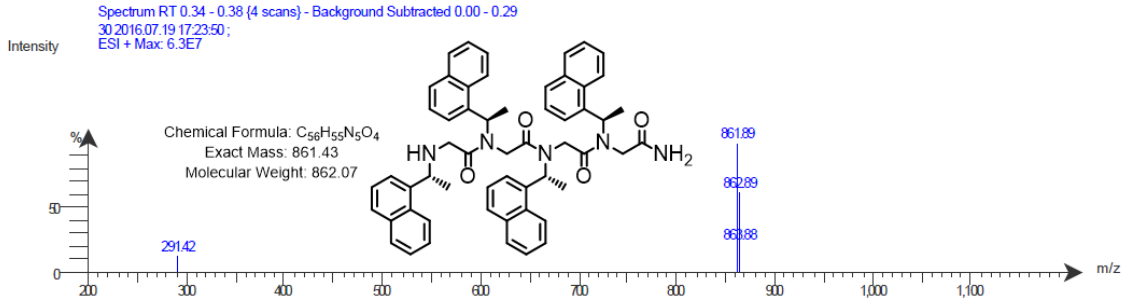



**Figure S59.** ESI MS of peptoid **P9**

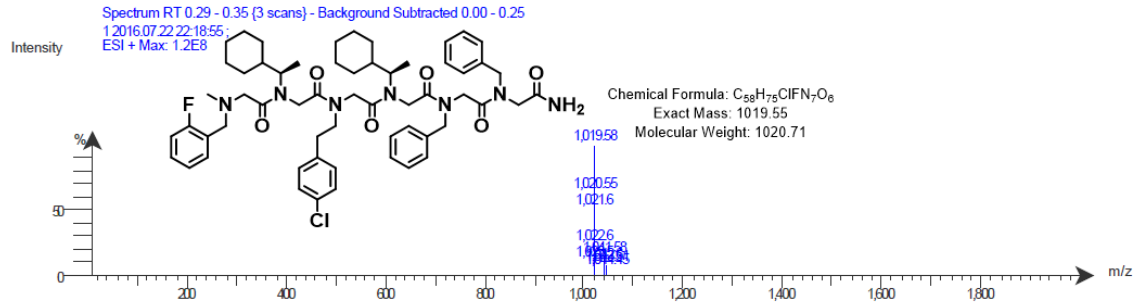



**Figure S50.** ESI MS of peptoid **P11**

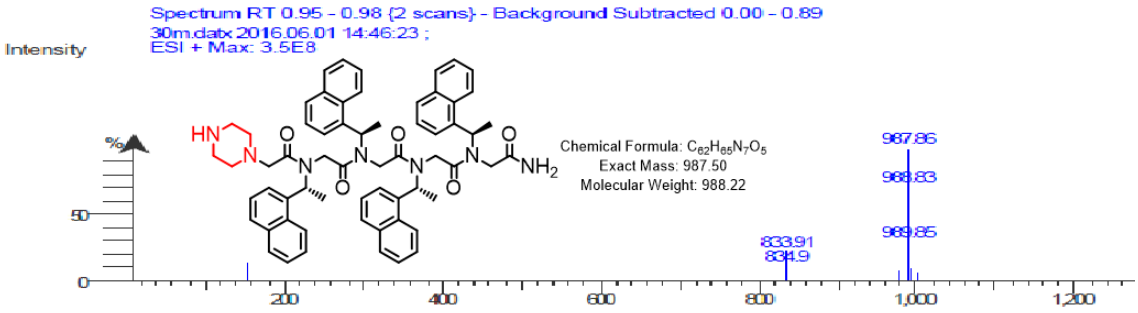



**Figure S51.** ESI MS of peptoid **P12**

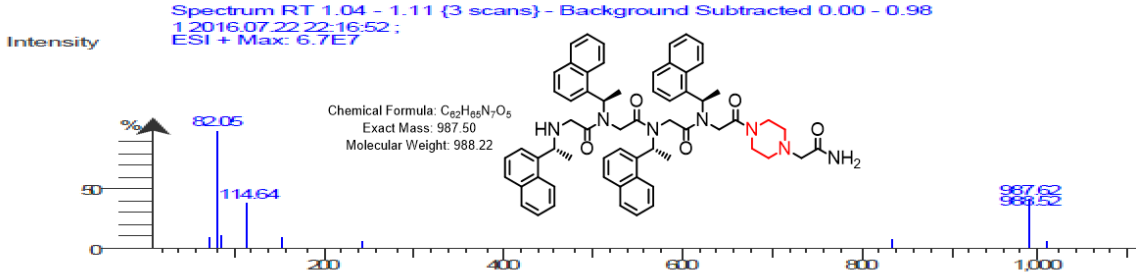



**Figure S52.** ESI MS of peptoid **P13**

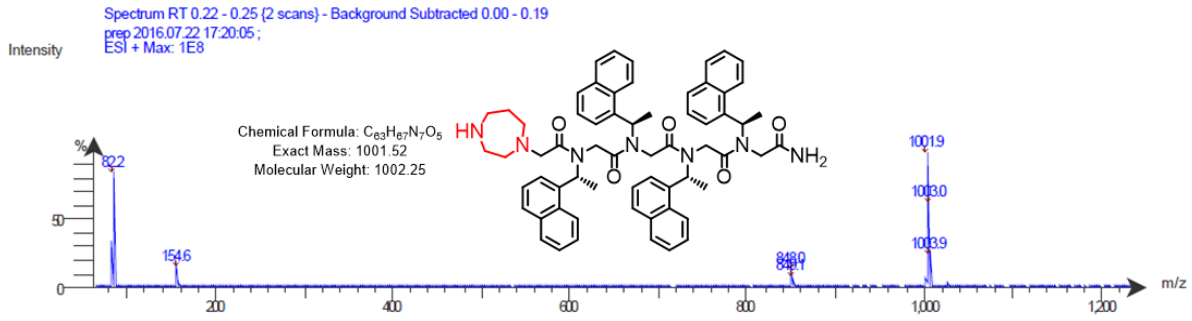



**Figure S53.** ESI MS of peptoid **P14**

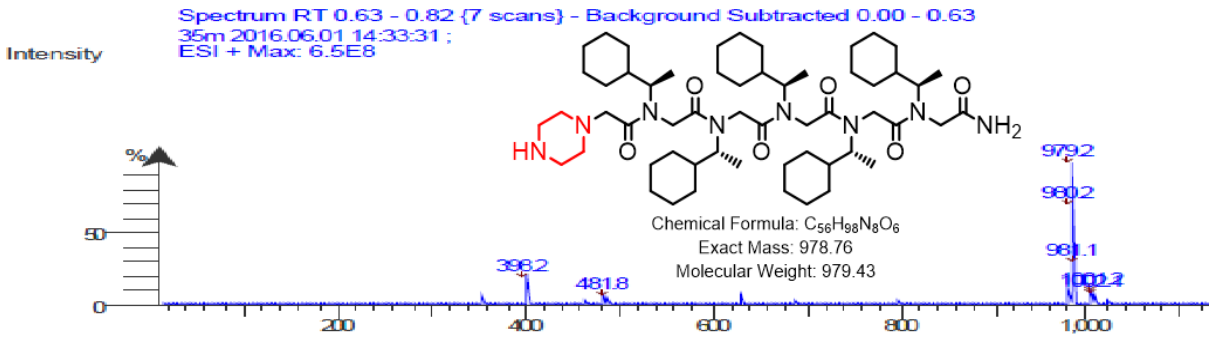



**Figure S54.** ESI MS of peptoid **P15**

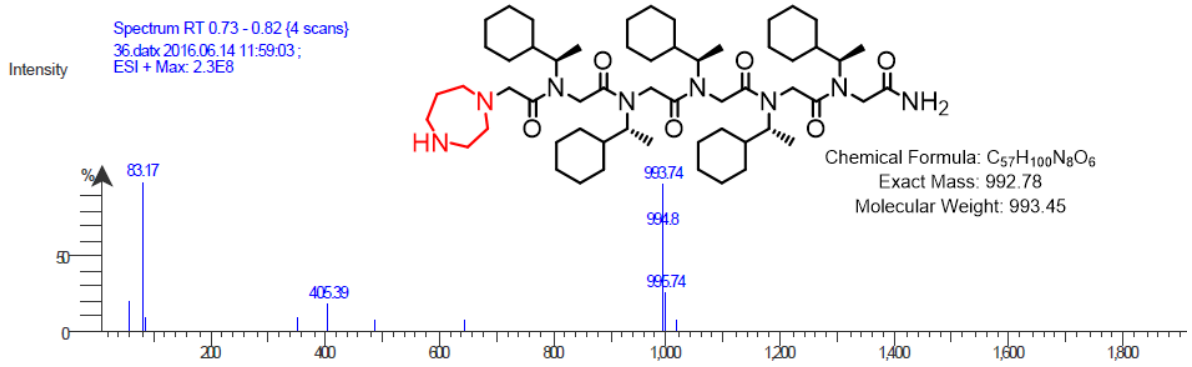



**Figure S55.** ESI MS of peptoid **P16**

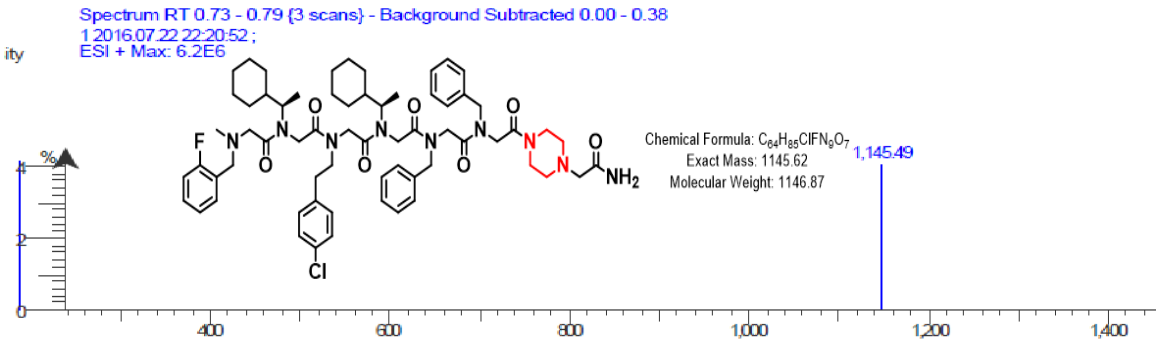



**Figure S56.** ESI MS of peptoid **P17**

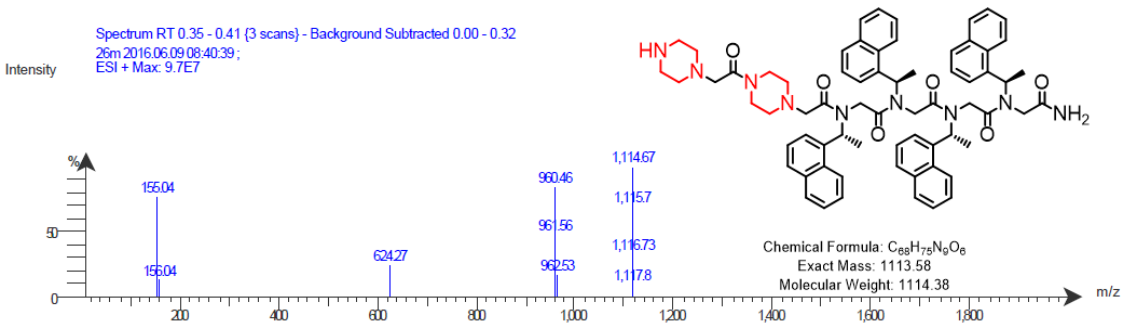



**Figure S57.** ESI MS of peptoid **P18**

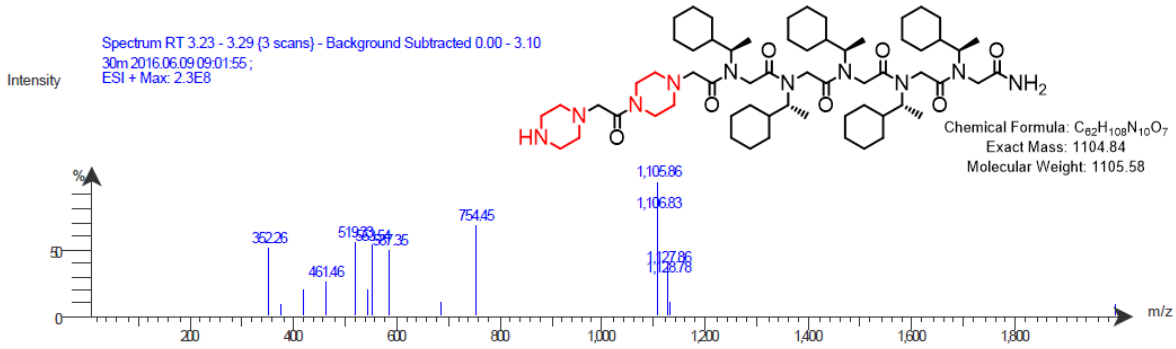



**Figure S58.** ESI MS of peptoid **P19**

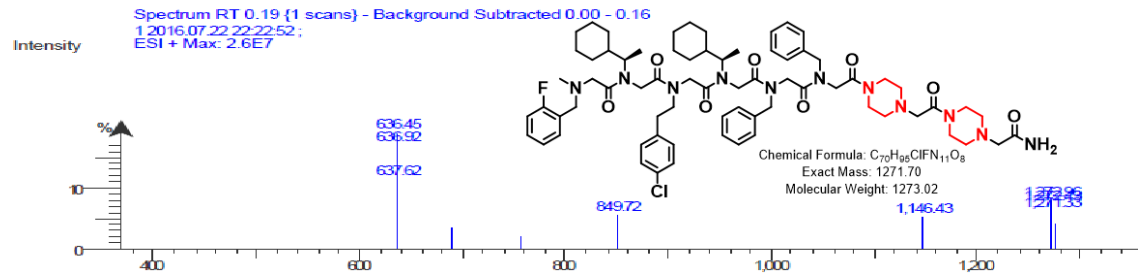



**Figure S59.** ESI MS of peptoid **P20**

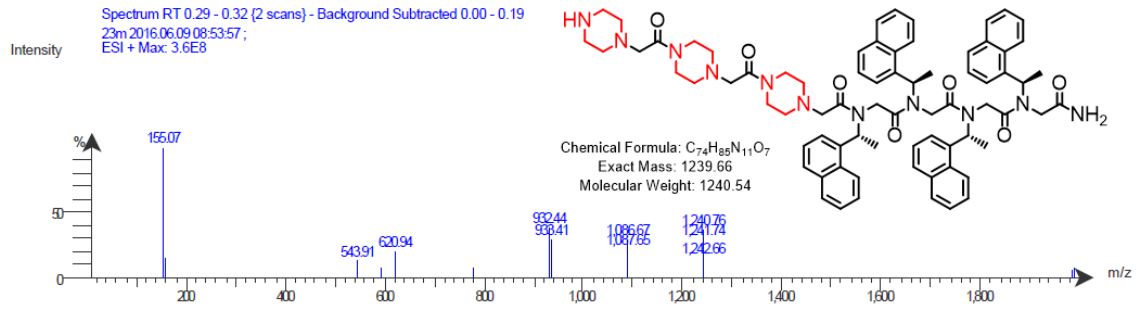



**Figure S60.** ESI MS of peptoid **P21**

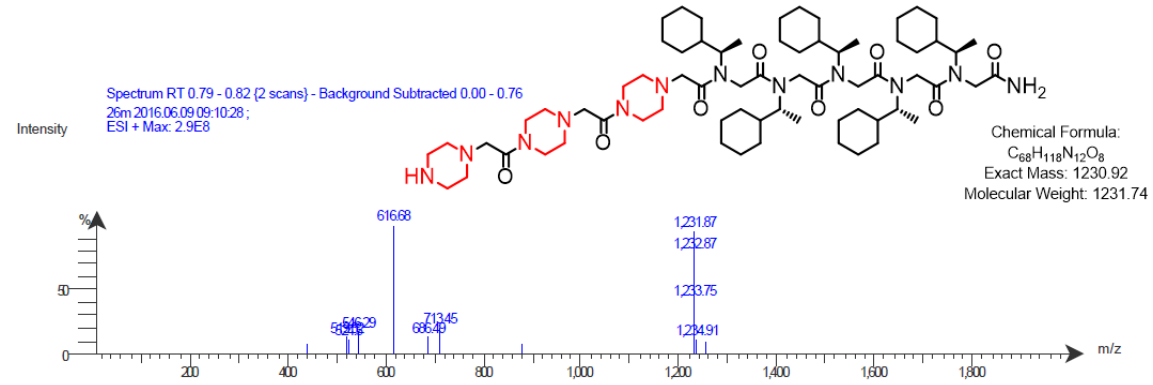



**Figure S61.** ESI MS of peptoid **P22**

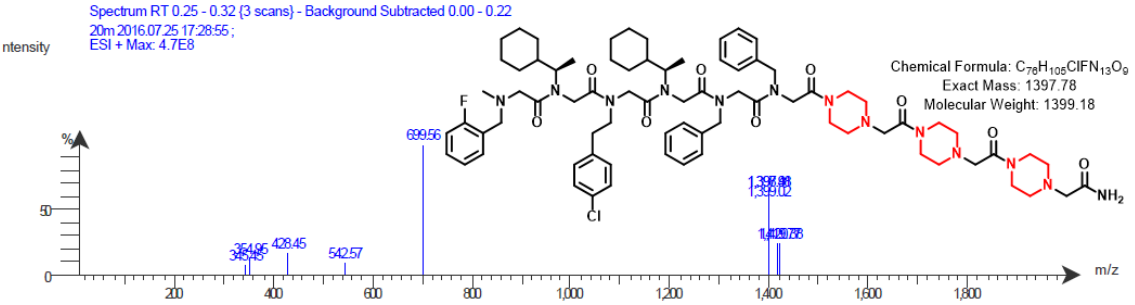



**Figure S62.** ESI MS of peptoid **P23**

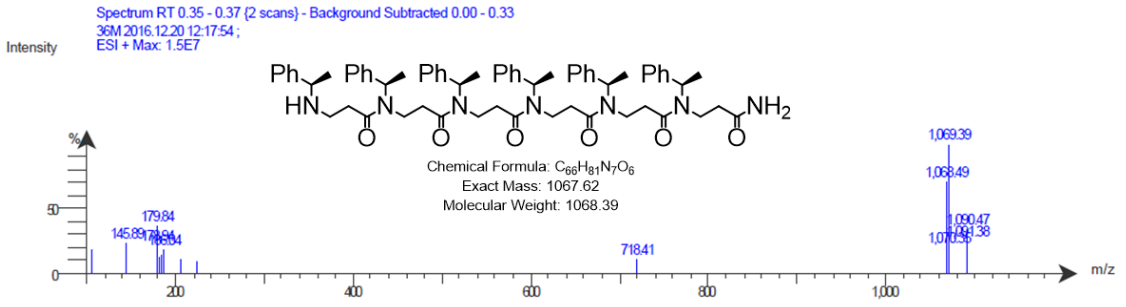



**Figure S63.** ESI MS of peptoid **P24**

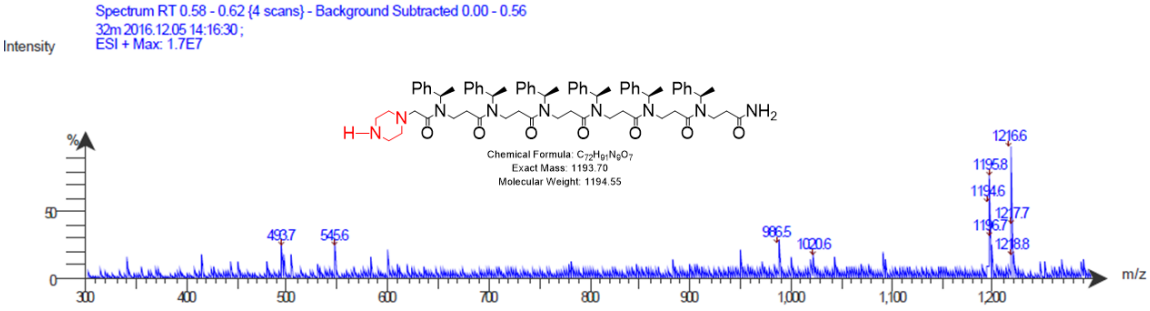



**Figure S64.** ESI MS of peptoid **P25**

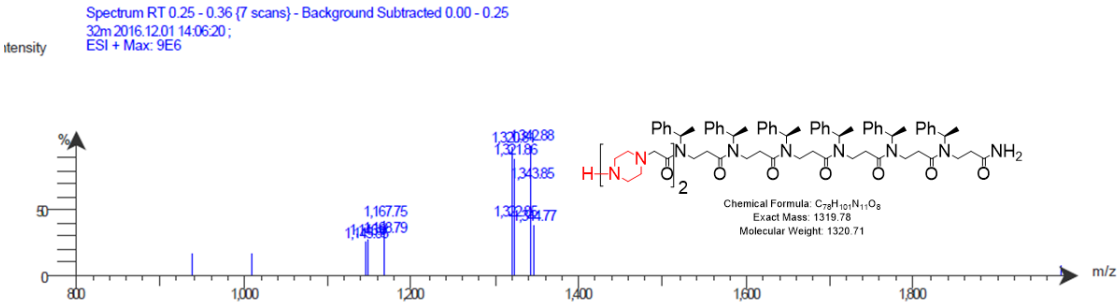



**Figure S65.** ESI MS of peptoid **P26**

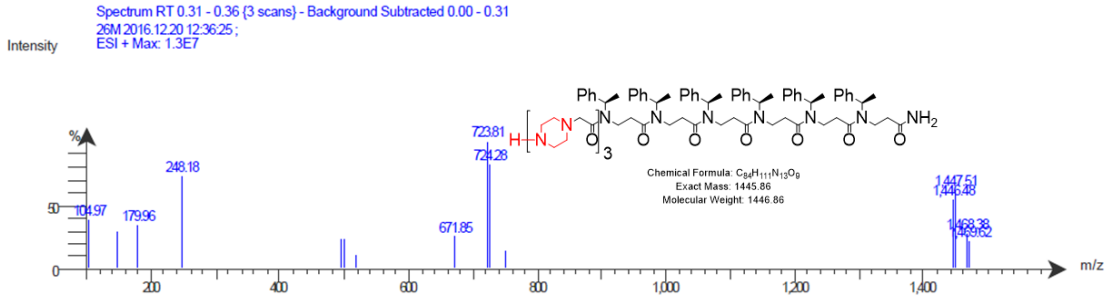



**Figure S66.** ESI MS of peptoid **P27**

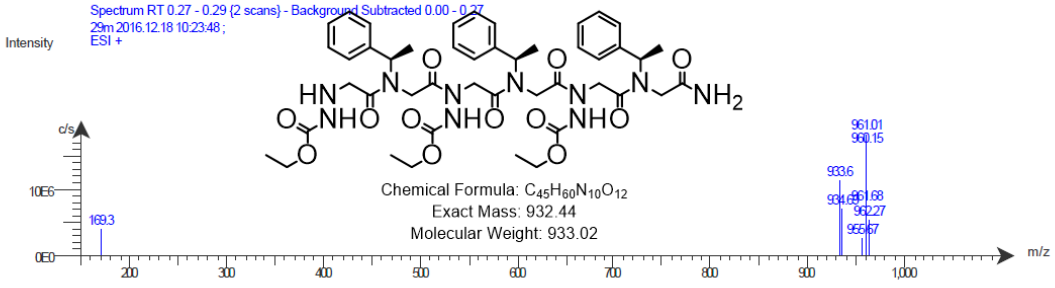



**Figure S67.** ESI MS of peptoid **P28**

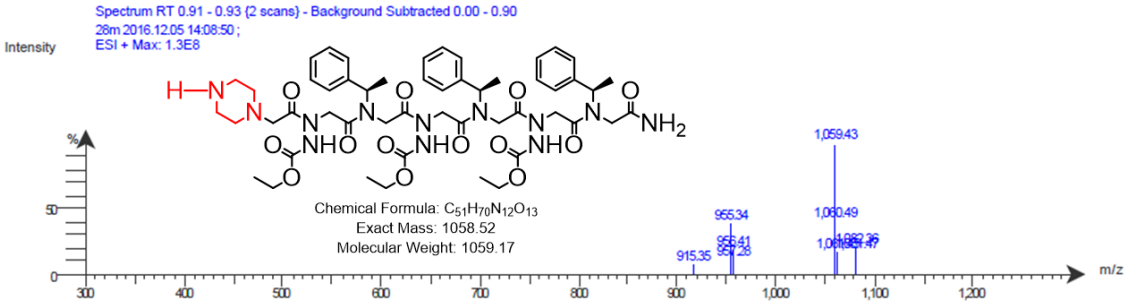



**Figure S68.** ESI MS of peptoid **P29**

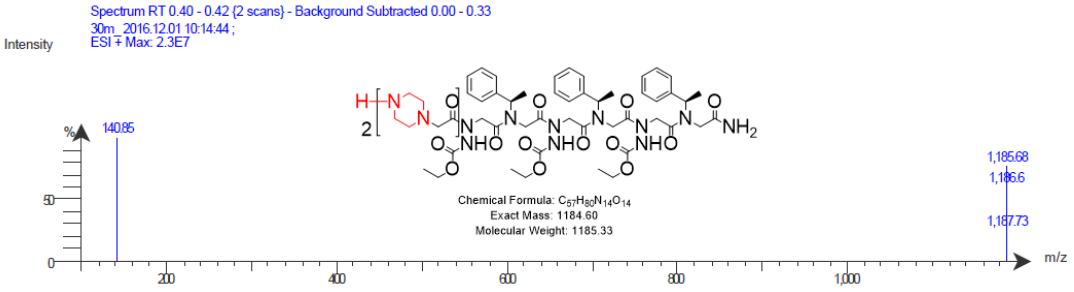



**Figure S69.** ESI MS of peptoid **P30**

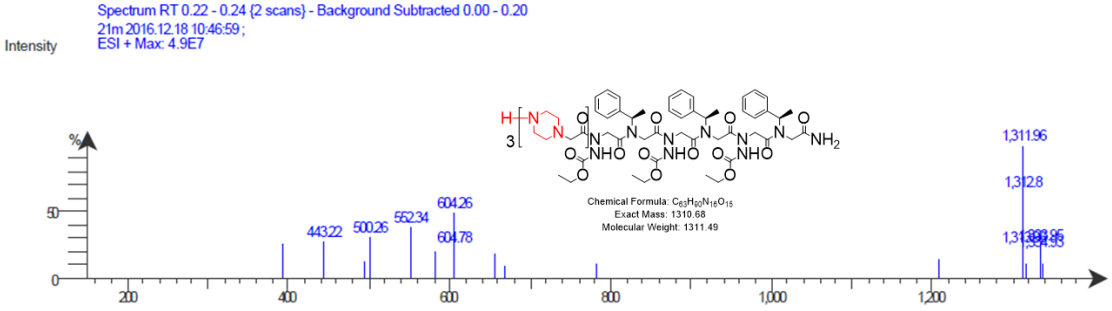



**Figure S70.** ESI MS of peptoid **P31**

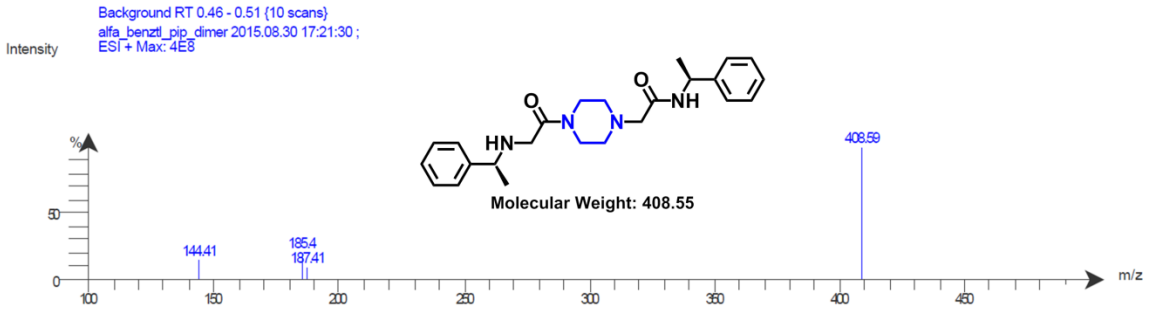
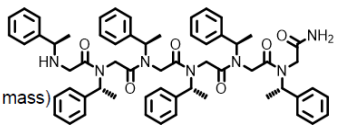



**Figure S71**. ESI MS of peptoid **PD'**

## HRMS of the peptoids

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

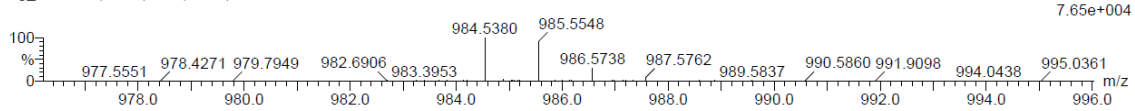


Chemical Formula: $C_{60}H_{69}N_7O_6$
Exact Mass: 983.5309
Molecular Weight: 984.2332

Monoisotopic Mass, Even Electron Ions
549 formula(e) evaluated with 7 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 60-64 H: 64-70 N: 5-17 O: 4-15 Na: 0-1 I: 0-1

P1
Mg_5773 68 (1.141) Cm (68:70)

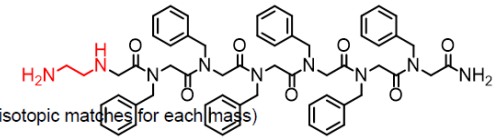
TOF MS ES+
7.65e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 984.5380 | 984.5064 | 31.6 | 32.1 | 34.5 | 171.9 | 1.4 | C64 H66 N5 O5 |
| | 984.5176 | 20.4 | 20.7 | 34.5 | 172.0 | 1.6 | C63 H66 N7 O4 |
| | 984.5040 | 34.0 | 34.5 | 31.5 | 172.4 | 2.0 | C62 H67 N5 O5 Na |
| | 984.5152 | 22.8 | 23.2 | 31.5 | 172.5 | 2.1 | C61 H67 N7 O4 Na |
| | 984.5275 | 10.5 | 10.7 | 29.5 | 172.6 | 2.2 | C61 H70 N5 O7 |
| | 984.5388 | -0.8 | -0.8 | 29.5 | 172.8 | 2.3 | C60 H70 N7 O6 |
| | 984.4911 | 46.9 | 47.6 | 30.5 | 172.9 | 2.5 | C60 H66 N5 O8 |

**Figure S72.** HRMS of peptoid **P1**

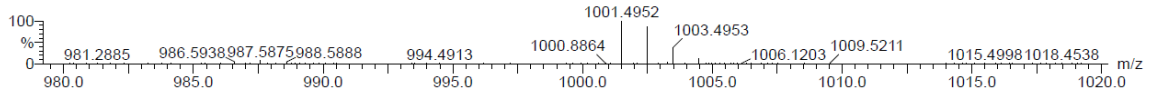
**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Chemical Formula: $C_{58}H_{65}N_9O_7$
Exact Mass: 999.50
Molecular Weight: 1000.19

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 56-58 H: 63-66 N: 5-10 O: 5-10 Na: 0-1
cm-eh
Mg_5758 55 (0.919) Cm (55)

TOF MS ES+
2.65e+003




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1001.4952 | 1001.4925 | 2.7 | 2.7 | 30.5 | 58.0 | 1.1 | C58 H65 N8 O8 |
| | 1001.5038 | -8.6 | -8.6 | 30.5 | 58.1 | 1.2 | C57 H65 N10 O7 |
| | 1001.4901 | 5.1 | 5.1 | 27.5 | 58.5 | 1.6 | C56 H66 N8 O8 Na |
| | 1001.4789 | 16.3 | 16.3 | 27.5 | 58.5 | 1.6 | C57 H66 N6 O9 Na |

**Figure S73.** HRMS of peptoid S**P1**

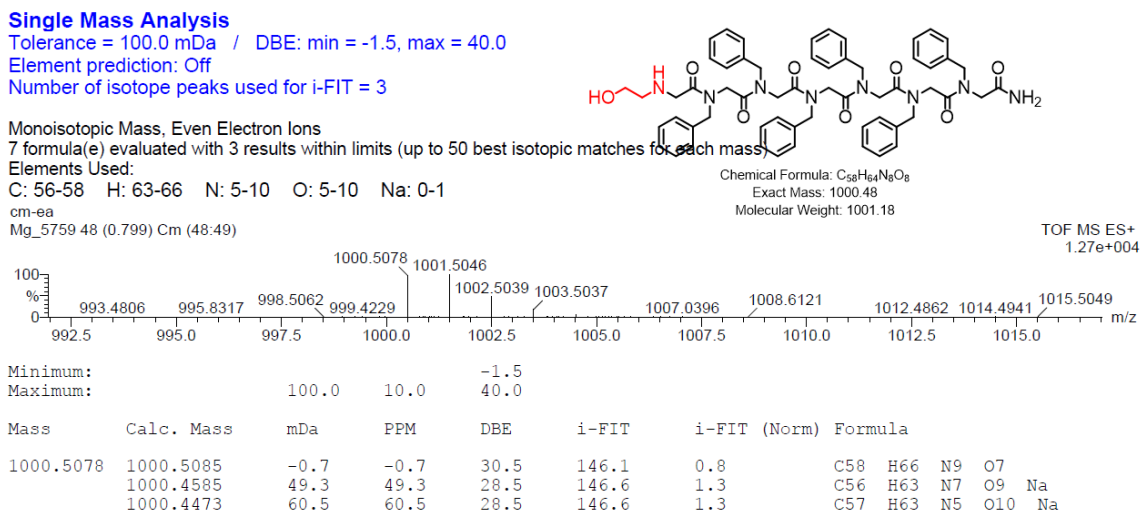



**Figure S74.** HRMS of peptoid **SP2**

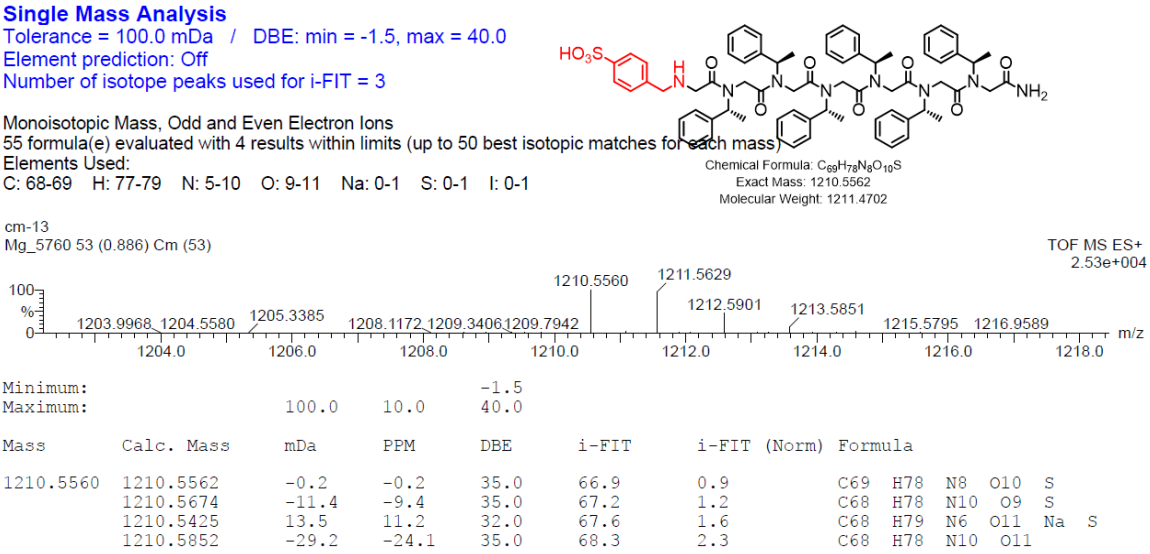
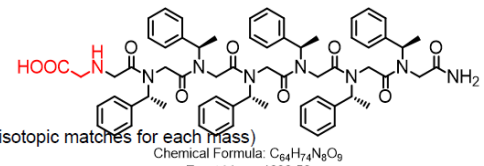



**Figure S75.** HRMS of peptoid **SP3**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

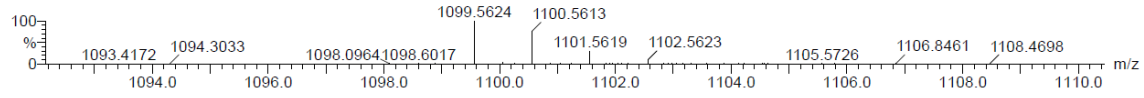



Chemical Formula: $C_{64}H_{74}N_8O_9$
Exact Mass: 1098.56
Molecular Weight: 1099.32

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 62-65 H: 72-75 N: 8-9 O: 7-9 Na: 0-1 I: 0-1

cm-16
Mg_5762 63 (1.056) Cm (63:65)

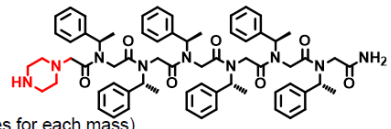
TOF MS ES+
2.87e+004




| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | | | | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | | | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula | | | | | |
| 1099.5624 | 1099.5657 | -3.3 | -3.0 | 31.5 | 108.9 | 0.3 | C64 | H75 | N8 | O9 | | |
| | 1099.5422 | 20.2 | 18.4 | 33.5 | 110.0 | 1.3 | C65 | H72 | N8 | O7 | Na | |

**Figure S76.** HRMS of peptoid S**P4**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

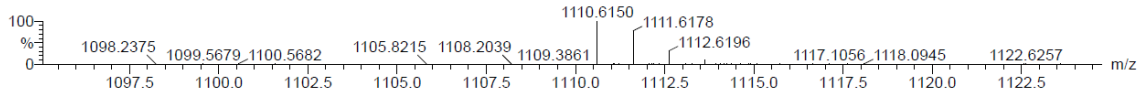



Chemical Formula: $C_{66}H_{79}N_9O_7$
Exact Mass: 1109.6102
Molecular Weight: 1110.3896

Monoisotopic Mass, Even Electron Ions
345 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 63-70 H: 78-80 N: 5-17 O: 6-15 Na: 0-1 I: 0-1

P2
Mg_5770 56 (0.937) Cm (56:58)

TOF MS ES+
2.55e+004




| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | | | | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | | | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula | | | | | |
| 1110.6150 | 1110.6293 | -14.3 | -12.9 | 31.5 | 96.0 | 0.4 | C65 | H80 | N11 | O6 | | |
| | 1110.6181 | -3.1 | -2.8 | 31.5 | 97.2 | 1.6 | C66 | H80 | N9 | O7 | | |
| | 1110.6068 | 8.2 | 7.4 | 31.5 | 98.8 | 3.2 | C67 | H80 | N7 | O8 | | |
| | 1110.5803 | 34.7 | 31.2 | 27.5 | 99.1 | 3.5 | C64 | H80 | N5 | O12 | | |
| | 1110.5916 | 23.4 | 21.1 | 27.5 | 99.7 | 4.1 | C63 | H80 | N7 | O11 | | |
| | 1110.5956 | 19.4 | 17.5 | 31.5 | 100.2 | 4.5 | C68 | H80 | N5 | O9 | | |

**Figure S77.** HRMS of peptoid **P2**

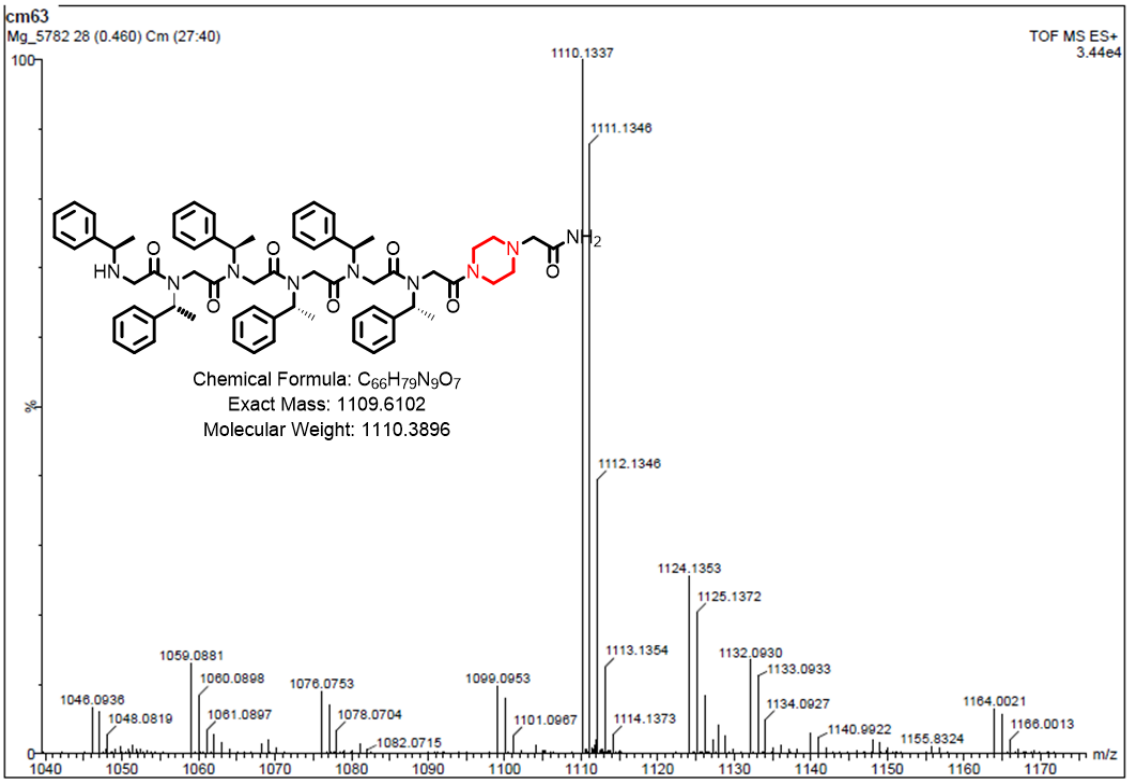



**Figure S78.** HRMS of peptoid **P3**

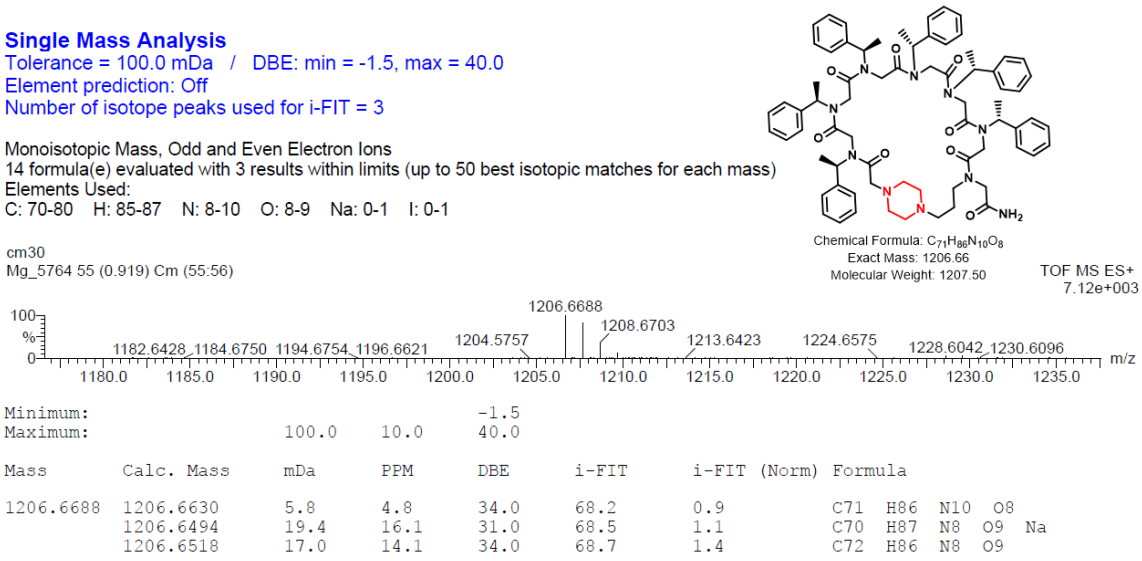
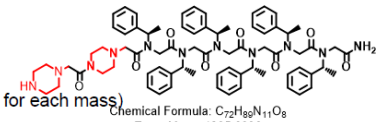


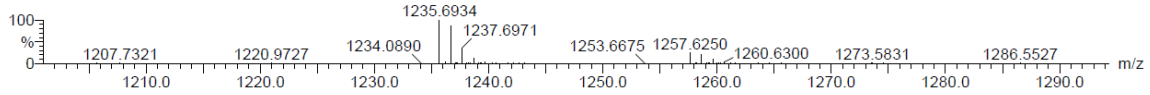

**Figure S79.** HRMS of peptoid **P4**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
138 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 71-73 H: 88-90 N: 5-17 O: 4-15 I: 0-1




P5
Mg_5777 51 (0.851) Cm (51:53)

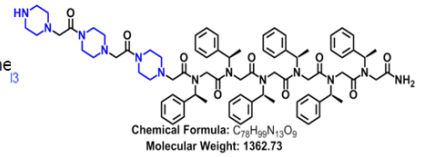



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1235.6934 | 1235.7008 | -7.4 | -6.0 | 34.0 | 66.3 | 0.4 | C71 H89 N13 O7 |
| | 1235.6896 | 3.8 | 3.1 | 34.0 | 67.3 | 1.4 | C72 H89 N11 O8 |
| | 1235.6783 | 15.1 | 12.2 | 34.0 | 68.4 | 2.5 | C73 H89 N9 O9 |
| | 1235.6406 | 52.8 | 42.7 | 30.0 | 69.2 | 3.3 | C71 H89 N5 O14 |
| | 1235.5936 | 99.8 | 80.8 | 29.0 | 70.9 | 5.1 | C71 H90 N5 O6 I |

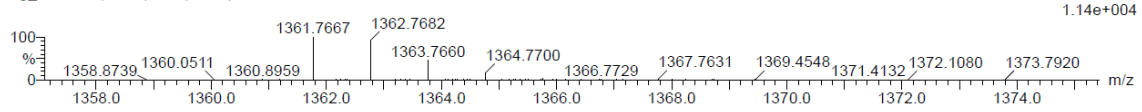
**Figure S80.** HRMS of peptoid **P5**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
199 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matche
Elements Used:
C: 78-79 H: 99-100 N: 5-17 O: 6-15 Na: 0-1 I: 0-1



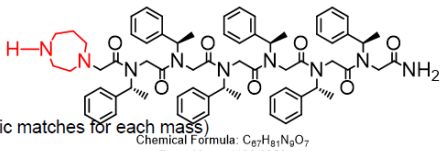

P6
Mg_5771 56 (0.937) Cm (56:60)




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1361.7667 | 1361.7576 | 9.1 | 6.7 | 36.0 | 110.8 | 1.1 | C79 H99 N11 O10 |
| | 1361.7689 | -2.2 | -1.6 | 36.0 | 111.0 | 1.3 | C78 H99 N13 O9 |
| | 1361.7328 | 33.9 | 24.9 | 33.0 | 111.0 | 1.3 | C79 H100 N7 O12 Na |
| | 1361.7440 | 22.7 | 16.7 | 33.0 | 111.6 | 1.9 | C78 H100 N9 O11 Na |

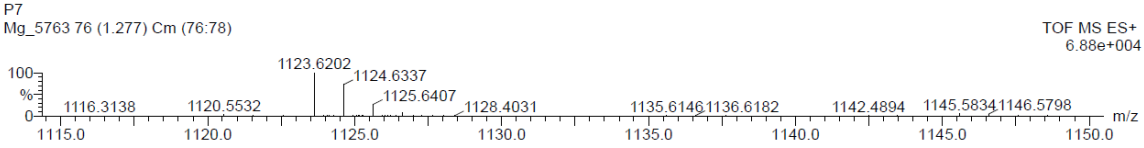
**Figure S81.** HRMS of peptoid **P6**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Odd and Even Electron Ions
15 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 65-70 H: 80-82 N: 8-9 O: 7-9 Na: 0-1 I: 0-1

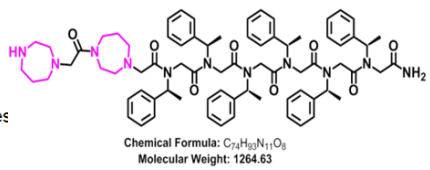
P7
Mg_5763 76 (1.277) Cm (76:78)




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1123.6202 | 1123.5997 | 20.5 | 18.2 | 29.5 | 168.1 | 0.8 | C65 H80 N8 O8 Na |
| | 1123.6235 | -3.3 | -2.9 | 29.0 | 168.2 | 0.9 | C65 H82 N9 O7 Na |
| | 1123.6259 | -5.7 | -5.1 | 32.0 | 169.6 | 2.2 | C67 H81 N9 O7 |

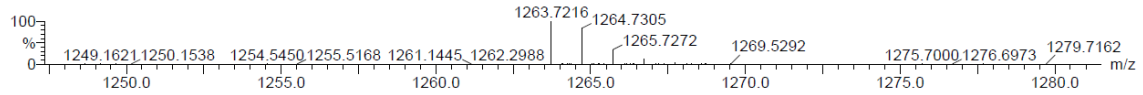
**Figure S82.** HRMS of peptoid **P7**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Odd and Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches
Elements Used:
C: 73-75 H: 92-94 N: 10-11 O: 7-9 Na: 0-1 I: 0-1

P8
Mg_5761 70 (1.174) Cm (70:75)

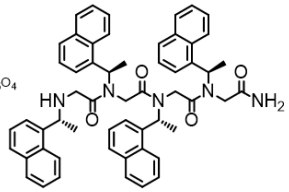


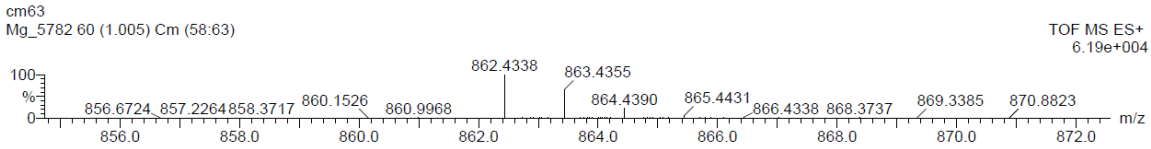

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1263.7216 | 1263.7209 | 0.7 | 0.6 | 34.0 | 163.1 | 0.0 | C74 H93 N11 O8 |

**Figure S83.** HRMS of peptoid **P8**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
295 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 55-57 H: 55-56 N: 5-17 O: 4-15 I: 0-1



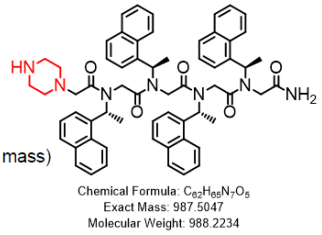



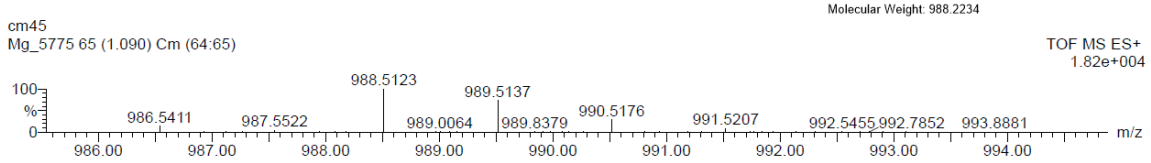

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 862.4338 | 862.4332 | 0.6 | 0.7 | 31.5 | 257.9 | 0.0 | C56 H56 N5 O4 |

**Figure S84.** HRMS of peptoid **P9**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
534 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 60-63 H: 65-66 N: 5-17 O: 4-15 Na: 0-1 I: 0-1



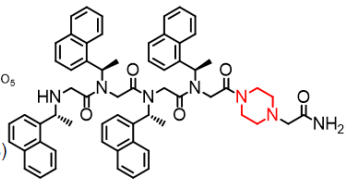




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 988.5123 | 988.5013 | 11.0 | 11.1 | 33.5 | 125.7 | 0.5 | C63 H66 N5 O6 |
| | 988.5125 | -0.2 | -0.2 | 33.5 | 126.6 | 1.3 | C62 H66 N7 O5 |
| | 988.5238 | -11.5 | -11.6 | 33.5 | 127.4 | 2.1 | C61 H66 N9 O4 |

**Figure S85.** HRMS of peptoid **P12**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

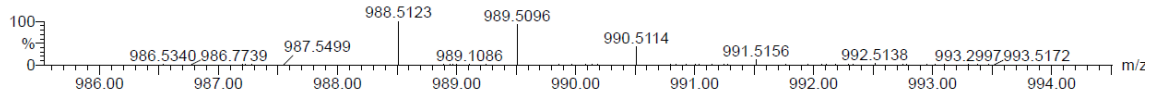
Chemical Formula: $C_{62}H_{66}N_7O_5$
Exact Mass: 987.50
Molecular Weight: 988.22



Monoisotopic Mass, Even Electron Ions
260 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 60-63 H: 65-67 N: 5-17 O: 4-15 I: 0-1

cm54
Mg_5781 52 (0.868) Cm (52:54)

TOF MS ES+
7.69e+00

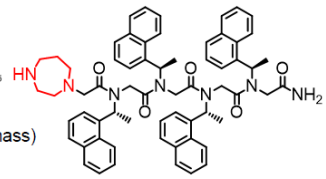



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 988.5123 | 988.5013 | 11.0 | 11.1 | 33.5 | 133.2 | 1.1 | C63 H66 N5 O6 |
| | 988.5125 | -0.2 | -0.2 | 33.5 | 133.3 | 1.1 | C62 H66 N7 O5 |
| | 988.5238 | -11.5 | -11.6 | 33.5 | 133.3 | 1.2 | C61 H66 N9 O4 |

**Figure S86.** HRMS of peptoid **P13**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

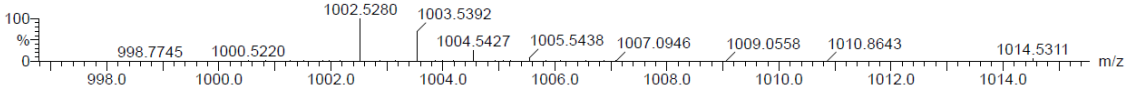
Chemical Formula: $C_{63}H_{67}N_7O_5$
Exact Mass: 1001.52
Molecular Weight: 1002.25



Monoisotopic Mass, Even Electron Ions
549 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 62-64 H: 64-68 N: 5-17 O: 4-15 Na: 0-1 I: 0-1

cm53
Mg_5772 70 (1.175) Cm (70)

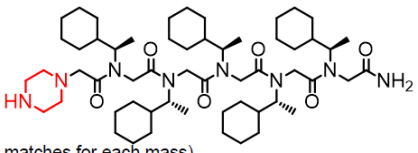
TOF MS ES+
1.83e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1002.5280 | 1002.4918 | 36.2 | 36.1 | 34.5 | 81.9 | 1.0 | C62 H64 N7 O6 |
| | 1002.5394 | -11.4 | -11.4 | 33.5 | 82.4 | 1.5 | C62 H68 N9 O4 |
| | 1002.4806 | 47.4 | 47.3 | 34.5 | 82.6 | 1.7 | C63 H64 N5 O7 |
| | 1002.5282 | -0.2 | -0.2 | 33.5 | 83.0 | 2.0 | C63 H68 N7 O5 |
| | 1002.5170 | 11.0 | 11.0 | 33.5 | 83.5 | 2.6 | C64 H68 N5 O6 |

**Figure S87**. HRMS trace of peptoid **P14**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

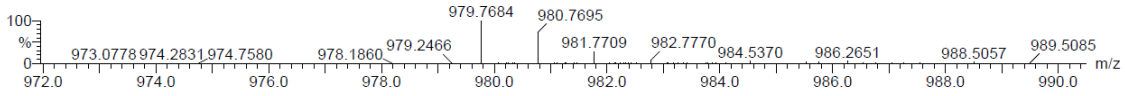



Chemical Formula: $C_{56}H_{98}N_8O_6$
Exact Mass: 978.7609
Molecular Weight: 979.4273

Monoisotopic Mass, Even Electron Ions
209 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 55-57 H: 97-99 N: 5-17 O: 4-15 I: 0-1

cm44
Mg_5780 51 (0.851) Cm (51:54)

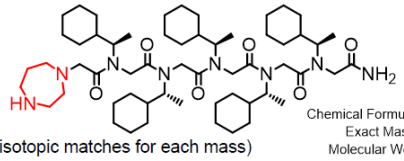
TOF MS ES+
1.60e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 979.7684 | 979.7575 | 10.9 | 11.1 | 11.5 | 146.9 | 0.8 | C57 H99 N6 O7 |
| | 979.7688 | -0.4 | -0.4 | 11.5 | 147.2 | 1.1 | C56 H99 N8 O6 |
| | 979.7800 | -11.6 | -11.8 | 11.5 | 147.5 | 1.5 | C55 H99 N10 O5 |

**Figure S88**. HRMS trace of peptoid **P15**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

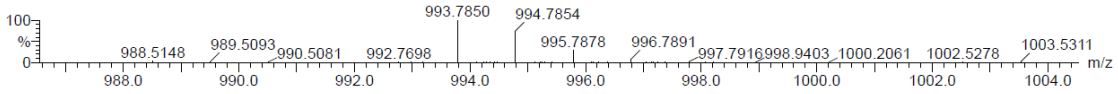



Chemical Formula: $C_{57}H_{100}N_8O_6$
Exact Mass: 992.78
Molecular Weight: 993.45

Monoisotopic Mass, Even Electron Ions
192 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 55-58 H: 100-102 N: 5-17 O: 4-15 I: 0-1

cm51
Mg_5778 55 (0.920) Cm (53:56)

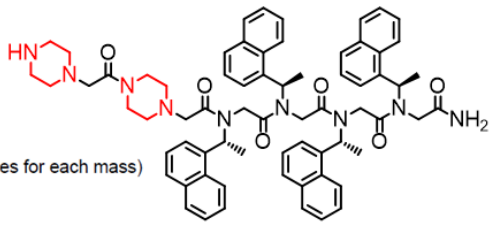
TOF MS ES+
3.29e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 993.7850 | 993.7732 | 11.8 | 11.9 | 11.5 | 162.1 | 1.0 | C58 H101 N6 O7 |
| | 993.7844 | 0.6 | 0.6 | 11.5 | 162.4 | 1.3 | C57 H101 N8 O6 |
| | 993.7956 | -10.6 | -10.7 | 11.5 | 162.7 | 1.6 | C56 H101 N10 O5 |
| | 993.8069 | -21.9 | -22.0 | 11.5 | 163.0 | 1.9 | C55 H101 N12 O4 |

**Figure S89.** HRMS of peptoid **P16**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

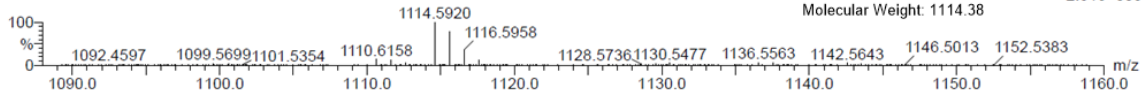


Monoisotopic Mass, Even Electron Ions
222 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 67-69 H: 74-76 N: 5-17 O: 4-15 I: 0-1

cm48
Mg_5783 45 (0.749) Cm (45:47)

Chemical Formula: $C_{68}H_{75}N_9O_6$
Exact Mass: 1113.58
Molecular Weight: 1114.38

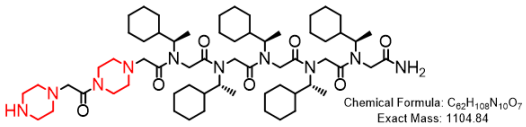
TOF MS ES+
2.31e+003




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1114.5920 | 1114.5806 | 11.4 | 10.2 | 35.5 | 101.7 | 1.0 | C69 H76 N7 O7 |
| | 1114.5919 | 0.1 | 0.1 | 35.5 | 101.8 | 1.1 | C68 H76 N9 O6 |
| | 1114.6031 | -11.1 | -10.0 | 35.5 | 102.0 | 1.3 | C67 H76 N11 O5 |

**Figure S90.** HRMS of peptoid **P18**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

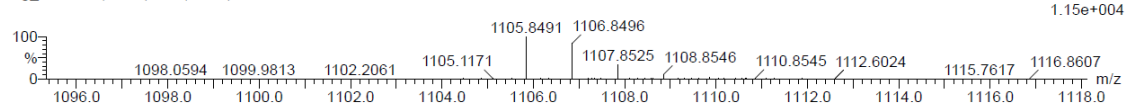


Chemical Formula: $C_{62}H_{108}N_{10}O_7$
Exact Mass: 1104.84
Molecular Weight: 1105.58

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 60-63 H: 100-110 N: 9-11 O: 0-10 Na: 0-1

cm-47
Mg_5752 56 (0.937) Cm (55:56)

TOF MS ES+
1.15e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 50.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1105.8491 | 1105.8245 | 24.6 | 22.2 | 15.5 | 93.4 | 1.0 | C63 H106 N10 O5 Na |
| | 1105.8481 | 1.0 | 0.9 | 13.5 | 93.7 | 1.3 | C62 H109 N10 O7 |
| | 1105.8117 | 37.4 | 33.8 | 14.5 | 94.6 | 2.2 | C61 H105 N10 O8 |
| | 1105.8457 | 3.4 | 3.1 | 10.5 | 94.6 | 2.2 | C60 H110 N10 O7 Na |
| | 1105.7882 | 60.9 | 55.1 | 16.5 | 94.8 | 2.4 | C62 H102 N10 O6 Na |
| | 1105.7753 | 73.8 | 66.7 | 15.5 | 96.1 | 3.7 | C60 H101 N10 O9 |

**Figure S91.** HRMS of peptoid **P19**

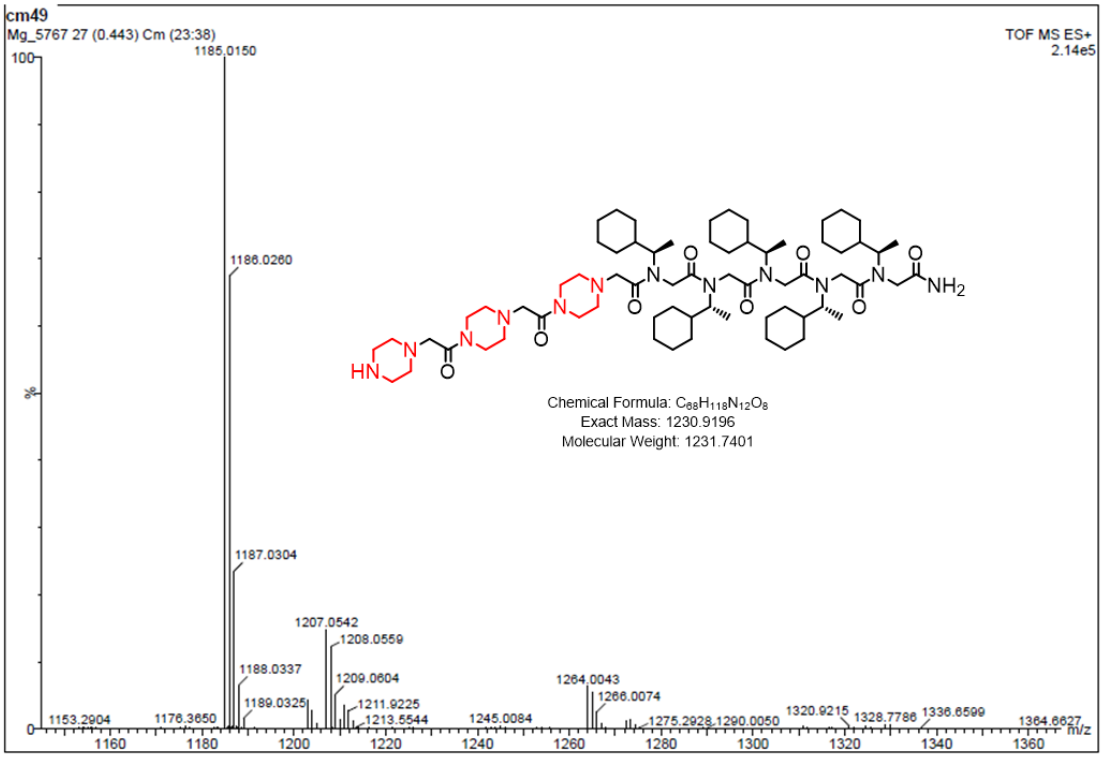



**Figure S96.** HRMS of peptoid **P21**

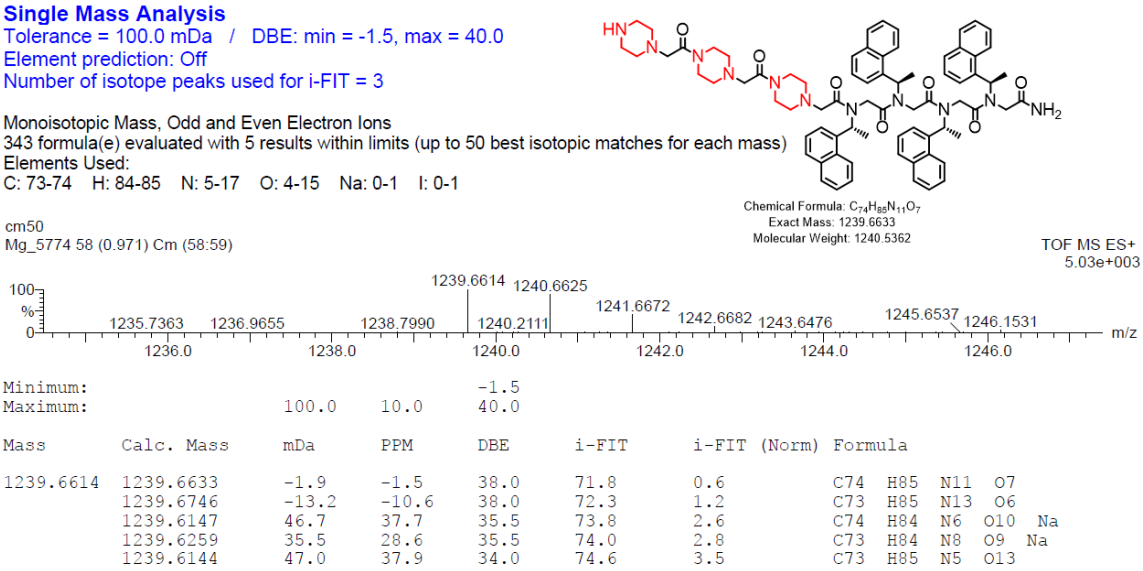
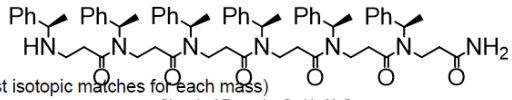



**Figure S92.** HRMS of peptoid **P22**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

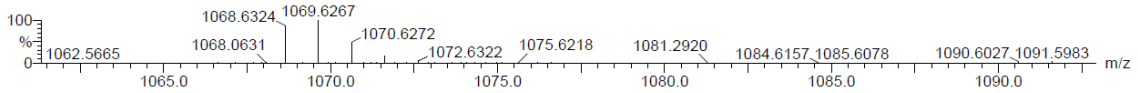


Chemical Formula: $C_{66}H_{81}N_7O_6$
Exact Mass: 1067.62
Molecular Weight: 1068.39

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 65-70 H: 80-82 N: 5-10 O: 5-10 Na: 0-1

cm-99
Mg_5756 65 (1.090) Cm (65)

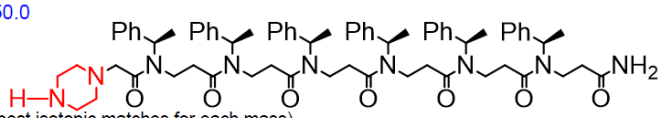
TOF MS ES+
1.35e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| **Mass** | **Calc. Mass** | **mDa** | **PPM** | **DBE** | **i-FIT** | **i-FIT (Norm)** | **Formula** |
| 1068.6324 | 1068.6214 | 11.0 | 10.3 | 29.5 | 69.3 | 1.0 | C67 H82 N5 O7 |
| | 1068.6327 | -0.3 | -0.3 | 29.5 | 69.4 | 1.1 | C66 H82 N7 O6 |
| | 1068.6439 | -11.5 | -10.8 | 29.5 | 69.4 | 1.2 | C65 H82 N9 O5 |

**Figure S93.** HRMS of peptoid **P24**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

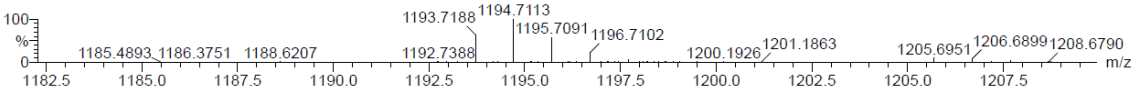


Chemical Formula: $C_{72}H_{91}N_9O_7$
Exact Mass: 1193.70
Molecular Weight: 1194.55

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 71-75 H: 90-93 N: 9-11 O: 0-10 Na: 0-1

cm-93
Mg_5753 54 (0.903) Cm (54:55)

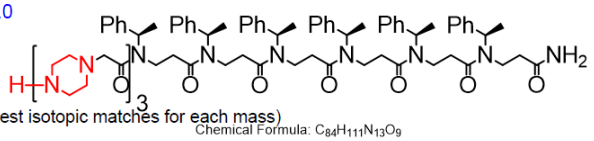
TOF MS ES+
1.65e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 50.0 | | | |
| **Mass** | **Calc. Mass** | **mDa** | **PPM** | **DBE** | **i-FIT** | **i-FIT (Norm)** | **Formula** |
| 1194.7113 | 1194.7232 | -11.9 | -10.0 | 31.5 | 107.7 | 1.4 | C71 H92 N11 O6 |
| | 1194.7120 | -0.7 | -0.6 | 31.5 | 107.8 | 1.5 | C72 H92 N9 O7 |
| | 1194.7361 | -24.8 | -20.8 | 32.5 | 107.9 | 1.6 | C73 H93 N11 O3 Na |
| | 1194.7248 | -13.5 | -11.3 | 32.5 | 108.0 | 1.7 | C74 H93 N9 O4 Na |
| | 1194.7385 | -27.2 | -22.8 | 35.5 | 108.3 | 2.0 | C75 H92 N11 O3 |

**Figure S94.** HRMS of peptoid **P25**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

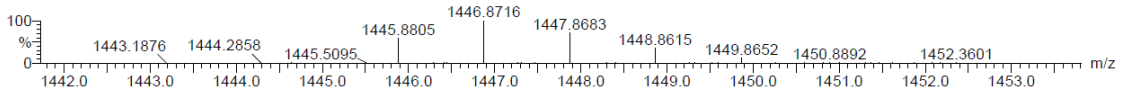



Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 80-85 H: 110-115 N: 9-14 O: 0-10 Na: 0-1

Chemical Formula: $C_{84}H_{111}N_{13}O_9$
Exact Mass: 1445.86
Molecular Weight: 1446.86

cm-98
Mg_5754 65 (1.089) Cm (65:66)

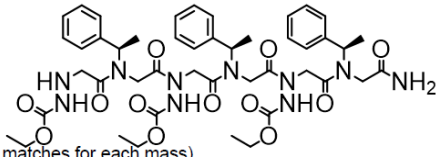
TOF MS ES+
5.24e+003




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 50.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1446.8716 | 1446.8682 | 3.4 | 2.3 | 32.5 | 78.1 | 1.2 | C82 H113 N13 O9 Na |
| | 1446.8570 | 14.6 | 10.1 | 32.5 | 78.2 | 1.3 | C83 H113 N11 O10 Na |
| | 1446.8706 | 1.0 | 0.7 | 35.5 | 78.4 | 1.5 | C84 H112 N13 O9 |
| | 1446.8594 | 12.2 | 8.4 | 35.5 | 78.5 | 1.6 | C85 H112 N11 O10 |

**Figure S96.** HRMS of peptoid **P27**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

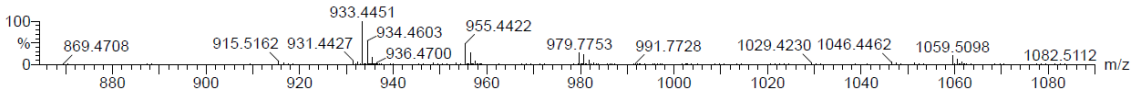



Monoisotopic Mass, Even Electron Ions
68 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 44-45 H: 60-72 N: 10-15 O: 12-15 Na: 0-1 I: 0-1

Chemical Formula: $C_{45}H_{60}N_{10}O_{12}$
Exact Mass: 932.44
Molecular Weight: 933.02

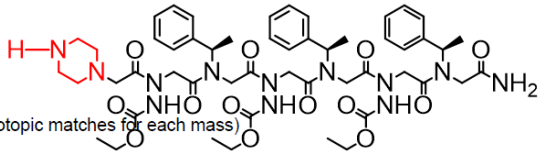
cm100
Mg_5768 48 (0.800) Cm (48:51)

TOF MS ES+
7.97e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 933.4451 | 933.4470 | -1.9 | -2.0 | 20.5 | 205.2 | 0.0 | C45 H61 N10 O12 |

**Figure S96.** HRMS of peptoid **P28**

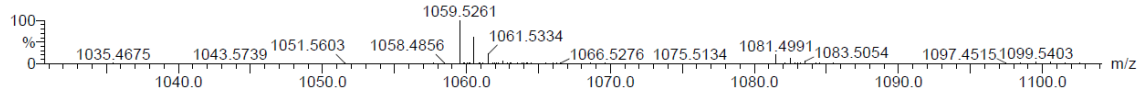


Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 50-55 H: 70-72 N: 10-15 O: 12-15 Na: 0-1 I: 0-1

Chemical Formula: $C_{51}H_{70}N_{12}O_{13}$
Exact Mass: 1058.52
Molecular Weight: 1059.17

cm94
Mg_5766 61 (1.021) Cm (61:62)

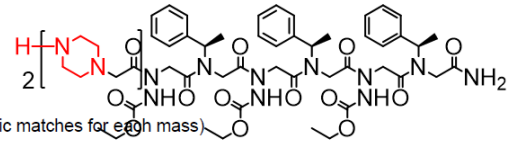
TOF MS ES+
1.75e+004




| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | | | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula | | | | |
| 1059.5261 | 1059.5264 | -0.3 | -0.3 | 22.5 | 120.0 | 1.0 | C51 | H71 | N12 | O13 | |
| | 1059.5151 | 11.0 | 10.4 | 22.5 | 120.4 | 1.5 | C52 | H71 | N10 | O14 | |
| | 1059.5376 | -11.5 | -10.9 | 22.5 | 120.5 | 1.5 | C50 | H71 | N14 | O12 | |
| | 1059.5127 | 13.4 | 12.6 | 19.5 | 120.6 | 1.6 | C50 | H72 | N10 | O14 | Na |

**Figure S97.** HRMS of peptoid **P29**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

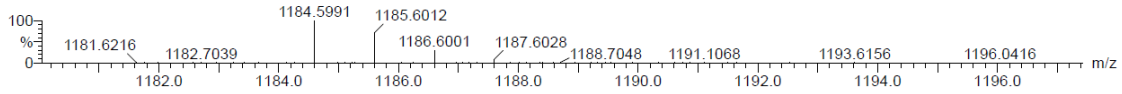


Monoisotopic Mass, Odd and Even Electron Ions
25 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 55-60 H: 80-83 N: 13-15 O: 12-15 Na: 0-1 I: 0-1

Chemical Formula: $C_{57}H_{80}N_{14}O_{14}$
Exact Mass: 1184.60
Molecular Weight: 1185.33

cm96
Mg_5765 85 (1.430) Cm (84:85)

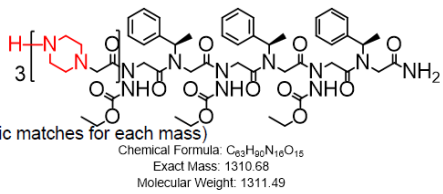
TOF MS ES+
2.84e+003



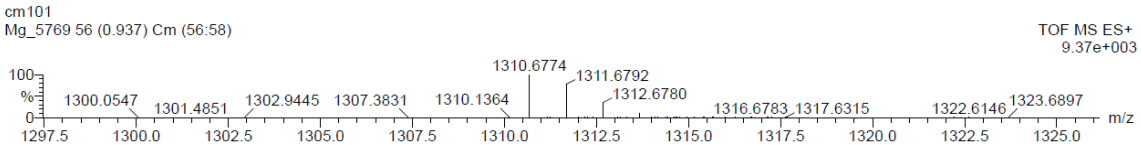

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | | | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula | | | | |
| 1184.5991 | 1184.6104 | -11.3 | -9.5 | 24.5 | 64.8 | 1.1 | C58 | H82 | N13 | O14 | |
| | 1184.5978 | 1.3 | 1.1 | 25.0 | 65.1 | 1.4 | C57 | H80 | N14 | O14 | |
| | 1184.6217 | -22.6 | -19.1 | 24.5 | 65.3 | 1.6 | C57 | H82 | N15 | O13 | |
| | 1184.6080 | -8.9 | -7.5 | 21.5 | 66.2 | 2.5 | C56 | H83 | N13 | O14 | Na |
| | 1184.5954 | 3.7 | 3.1 | 22.0 | 66.7 | 2.9 | C55 | H81 | N14 | O14 | Na |
| | 1184.6192 | -20.1 | -17.0 | 21.5 | 66.8 | 3.0 | C55 | H83 | N15 | O13 | Na |

**Figure S98.** HRMS of peptoid **P30**

**Single Mass Analysis**
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 63-65 H: 90-92 N: 15-17 O: 12-15 Na: 0-1 I: 0-1




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 100.0 | 10.0 | 40.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 1310.6774 | 1310.6897 | -12.3 | -9.4 | 26.5 | 82.4 | 1.0 | C64 H92 N15 O15 |
| | 1310.6900 | -12.6 | -9.6 | 28.0 | 82.7 | 1.4 | C65 H91 N16 O12 Na |
| | 1310.6772 | 0.2 | 0.2 | 27.0 | 82.9 | 1.5 | C63 H90 N16 O15 |
| | 1310.7010 | -23.6 | -18.0 | 26.5 | 83.1 | 1.7 | C63 H92 N17 O14 |

**Figure S99.** HRMS of peptoid **P31**

## 1H NMR Spectra

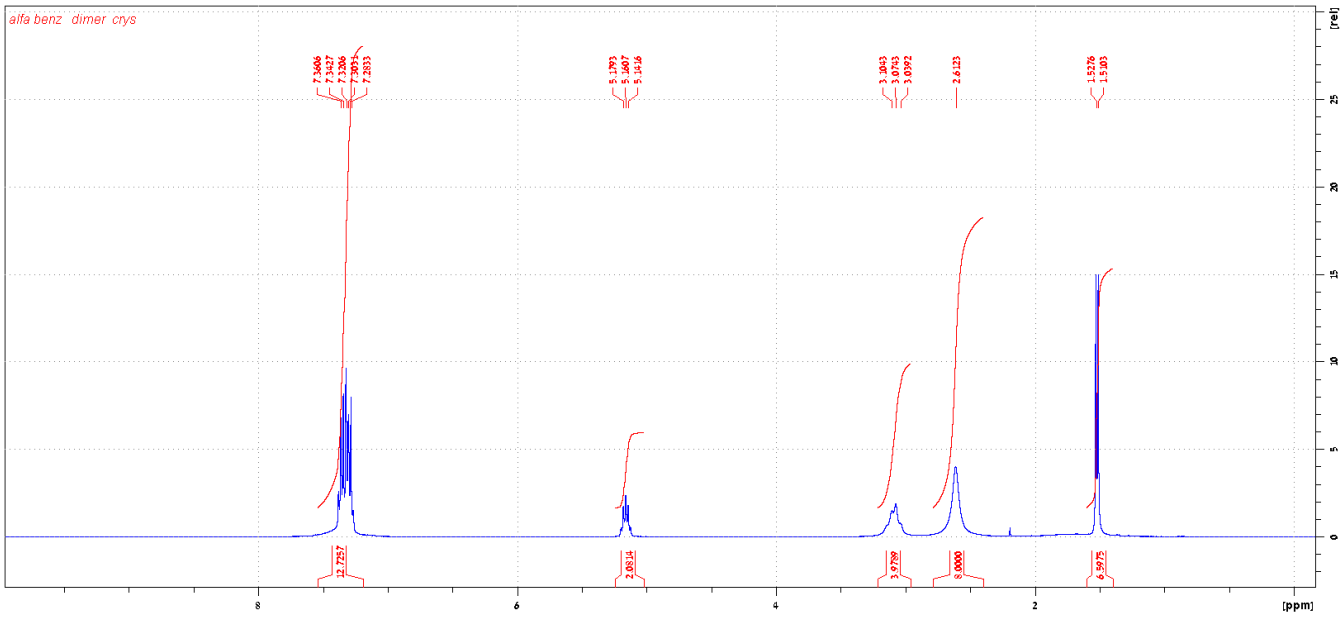



**Figure S100**. 1H NMR spectra of **PD'** in $CD_3OD$