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 K α radiation, $\lambda = 0.71073$ 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 sp³ 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: <u>http://www.ccdc.cam.ac.uk/</u>

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 μ M 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 cm² 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 H₂O (to get 17 µM concentration) and the UV- Vis spectrum was measured. Afterwards 1 equivalent of Cu²⁺ (10 µL 5mM) or solution containing mixtures of metal ions (1 equiv. Cu²⁺, Co²⁺, Zn²⁺, Mn²⁺, Ni²⁺ and Fe³⁺, 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 acetonitrile) over solvent A (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 ¹H NMR (**S75-S76**).

Peptoid	Monomer sequence	Mw	Crude
		cal:found	purity
P1	(Nspe) ₆	984.26 : 984.80	99
SP1	(Npm) ₆ -Nea	1000.19 :1000.32	80
SP2	(Npm) ₆ -Neh	1001.18 :1002.04	76
SP3	(Nspe) ₆ -Nabs	1211.47:1211.56	73
SP4	(Nspe) ₆ -Naa	1099.32:1099.96	71
P2	(<i>N</i> spe) ₆ - piperazine	1110.41 : 1110.8	85
P3	Piperazine- (<i>Nspe</i>) ₆	1110.41 : 1110.8	71
P-linear	Npl-(Nspe) ₆ - piperazine	1243.94:1243.45	62
P4	<i>N</i> pl-(<i>N</i> spe) ₆ - piperazine	1207.50:1207.12	40
P5	(Nspe) ₆ - (piperazine) ₂	1236.57 : 1236.96	72
P6	(<i>N</i> spe) ₆ - (piperazine) ₃	1362.73 : 1362.66	60
P7	(Nspe) ₆ -homopiperazine	1224.64 : 1124.69	85
P8	(<i>N</i> spe) ₆ -(homopiperazine) ₂	1264.63 :1264.74	82
P9	(Ns1npe) ₄	861.07: 861.89	90
P11	(NPm) ₂ -Nsch-Ncpe-Nsch-Nfpm	1020.77:1020.55	82
P12	(Ns1npe) ₄ -piperazine	988.22:988.83	81
P13	Piperazine -(<i>N</i> s1npe) ₄	988.22:988.52	76
P14	(Ns1npe) ₄ -homopiperazine	1002.25:1003.00	80
P15	(Nsch) ₅ -piperazine	979.43:979.20	75
P16	(Nsch) ₅ -homopiperazine	993.45:993.74	76
P17	Piperazine -(Npm) ₂ -Nsch-Ncpe-Nsch-Nfpm	1146.89:1145.49	70
P18	(<i>N</i> s1npe) ₄ - (piperazine) ₂	1114.38:1114.67	73
P19	(<i>N</i> s1npe) ₄ - (piperazine) ₃	1240.54:1240.26	68
P20	(Nsch) ₅ - (piperazine) ₂	1105.58:1105.86	72
P21	(Nsch) ₅ - (piperazine) ₃	1231.74:1231.87	67
P22	(Piperazine) ₂ -(Npm) ₂ -Nsch-Ncpe-Nsch-Nfpm	1146.89:1145.49	58
P23	(Piperazine) ₃ -(Npm)2-Nsch-Ncpe-Nsch-Nfpm	1273.02:1272.33	47
P24	β-peptoids-(Nspe) ₆	1068.30:1068.49	42
P25	β -peptoids-(<i>N</i> spe) ₆ - piperazine	1194.55:1194.60	35
P26	β-peptoids- (Nspe) ₆ - (piperazine) ₂	1320.71:1320.80	31
P27	β-peptoids- (Nspe) ₆ - (piperazine) ₃	1446.86:1446.48	25
P28	Nspe-NEcz- Nspe-NEcz- Nspe-NEcz	93.02:933.60	90
P29	Nspe-NEcz- Nspe-NEcz- Nspe-NEcz piperazine	1059.17:1059.43	87
P30	<i>N</i> spe- <i>N</i> Ecz- <i>N</i> spe- <i>N</i> Ecz (piperazine) ₂	1185.33:1185.68	82
P31	<i>N</i> spe- <i>N</i> Ecz- <i>N</i> spe- <i>N</i> Ecz (piperazine) ₃	1322.49:1311.96	79

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

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 μ M). (B) Plots of molar ellipticity ([θ]) at 228 nm vs. peptide concentration (40-180 μ M).



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



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



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



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 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

Spectrum RT 0.35 {1 scans} - Background Subtracted 0.32 - 0.40



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



Figure S72. HRMS of peptoid P1

Single Mas Tolerance = Element pred Number of is	s Analysis 100.0 mDa / DE diction: Off sotope peaks used	BE: min = -1 for i-FIT =	1.5, max = 4 3	10.0 H₂N				O MH2	
Monoisotopic 8 formula(e) e Elements Use	Mass, Even Electror valuated with 4 resu d:	lons Its within lim	its (up to 50	best isotopic	matches for	ëach[mass) (Ċ ö	L	
C: 56-58 H cm-eh Mg_5758 55 (0.	: 63-66 N: 5-10 919) Cm (55)	O: 5-10	Na: 0-1		C	Chemical Formula: C ₅₈ H Exact Mass: 999.5 Molecular Weight: 100	₃₅ N ₉ O ₇) 0.19		TOF MS ES+
100 % 981.28 980.0	85 986.5938987.58 985.0	7 <u>5</u> 988.5888 990.0	<u>994.4913</u> 995.0	1000.	1001.4952 8864 1 000.0	1003.4953 	1009.5211 	1015,49981 1015.0	2.65e+003 018.4538 1 m/z 1020.0
Minimum: Maximum:		100.0	10.0	-1.5 40.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula		
1001.4952	1001.4925 1001.5038 1001.4901 1001.4789	2.7 -8.6 5.1 16.3	2.7 -8.6 5.1 16.3	30.5 30.5 27.5 27.5	58.0 58.1 58.5 58.5	1.1 1.2 1.6 1.6	C58 H65 C57 H65 C56 H66 C57 H66	N8 08 N10 07 N8 08 1 N6 09 1	Na Na

Figure S73. HRMS of peptoid SP1

Mg_5759 48	(0.799) Cm (48:49)						j					TOF	MS ES+
100 % 0 993	.4806 995.8317	998.5062 998.5062	00.5078 1001	1.5046 1002.5039 ₁₀	003.5037	1007.0396	1008.6121		1012.48	62 10	14.494	1015.	5049
992.5	995.0	997.5	1000.0	1002.5	1005.0	1007.5	1010.0)	1012.	5	101	5.0	
Minimum: Maximum:		100.0	10.0	-1.5 40.0									
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Form	ula				
1000.5078	1000.5085 1000.4585 1000.4473	-0.7 49.3 60.5	-0.7 49.3 60.5	30.5 28.5 28.5	146.1 146.6 146.6	0.8 1.3 1.3		C58 C56 C57	Н66 Н63 Н63	N9 N7 N5	07 09 010	Na Na	

NH₂

Figure S74. HRMS of peptoid SP2

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 55 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 68-69 H: 77-79 N: 5-10 O: 9-11 Na: 0-1 S: 0-1 I: 0-1 cm-13													
cm-13 Mg_5760 53 (0	.886) Cm (53)											TOF	MS ES+
100 % 0 1203	.9968 1204.5580	1205.3385 12	08.1172.1209.3	12 3406,1209,794	210.5560	1211.5629 1212.5901	1213.5	5851	1215.57	795 12	16.958	9	.53e+004
	1204.0	1206.0	1208.0	1210	.0	1212.0	1214.0	D	11	216.0		121	8.0
Minimum: Maximum:		100.0	10.0	-1.5 40.0									
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Form	ıla				
1210.5560	1210.5562 1210.5674 1210.5425 1210.5852	-0.2 -11.4 13.5 -29.2	-0.2 -9.4 11.2 -24.1	35.0 35.0 32.0 35.0	66.9 67.2 67.6 68.3	0.9 1.2 1.6 2.3		C69 C68 C68 C68	H78 H78 H79 H78	N8 N10 N6 N10	010 09 011 011	S S Na	S

Figure S75. HRMS of peptoid SP3



Single Mas Tolerance = Element pre Number of is	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 Monoisetopic Mass. Even Electron lons												
Monoisotopic 345 formula(e Elements Use C: 63-70 H:	Monoisotopic Mass, Even Electron Ions Image: Control of the second s												
P2 Mg_5770 56 (0).937) Cm ((56:58)								тс	0F MS ES+ 2 55e+004		
100 % 109	8.2375 10	99,5679_11 1100.0	00.5682	1105.8215 1 ⁻ 	108.2039 11(1107.5	1110.6150 09.3861 1110.0	1111.6178 1112.6196 1112.5 111	<u>1117.1056</u> 5.0 1117.5	1118.0945 1120.0	1122.6257	7 m/z		
Minimum: Maximum:			100.0	10.0	$-1.5 \\ 40.0$								
Mass	Calc.	Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm) Form	ula				
1110.6150	1110.6 1110.6 1110.6 1110.5 1110.5 1110.5	5293 5181 5068 5803 5916 5956	-14.3 -3.1 8.2 34.7 23.4 19.4	-12.9 -2.8 7.4 31.2 21.1 17.5	31.5 31.5 31.5 27.5 27.5 31.5	96.0 97.2 98.8 99.1 99.7 100.2	0.4 1.6 3.2 3.5 4.1 4.5	C65 C66 C67 C64 C63 C68	H80 N11 H80 N9 H80 N7 H80 N5 H80 N7 H80 N5	06 07 08 012 011 09			

Figure S77. HRMS of peptoid P2



Figure S78. HRMS of peptoid P3

Single Mas Tolerance = Element pre Number of is	ss Analysis 100.0 mDa / Di diction: Off sotope peaks used	BE: min = - I for i-FIT =	1.5, max = 4 3	40.0							
Monoisotopic 14 formula(e) Elements Use C: 70-80 H:	Vonoisotopic Mass, Odd and Even Electron Ions 14 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 70-80 H: 85-87 N: 8-10 O: 8-9 Na: 0-1 I: 0-1										
cm30 Mg_5764 55 (0).919) Cm (55:56)					с	hemical Formula: Exact Mass: 1 Molecular Weigh	C ₇₁ H ₈₆ N ₁₀ O ₈ 1206.66 tt: 1207.50 TOF MS ES+ 7 12e+003			
100				1206	.6688						
%	1182.6428_1184.6750	1194.6754_11	96,6621 12	204.5757	1208.6703	1213.6423 12	24.6575 12	28,6042,1230.6096			
1180).0 1185.0 11	90.0 1195	5.0 1200.0) 1205.0	1210.0	1215.0 1220.0	1225.0	1230.0 1235.0			
Minimum: Maximum:		100.0	10.0	$^{-1.5}_{40.0}$							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
1206.6688	1206.6630 1206.6494 1206.6518	5.8 19.4 17.0	4.8 16.1 14.1	34.0 31.0 34.0	68.2 68.5 68.7	0.9 1.1 1.4	C71 H86 C70 H87 C72 H86	N10 08 N8 09 Na N8 09			

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

Exact Mass: 1235.6896 Molecular Weight: 1236.5460

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)

TOF MS ES+ 1.69e+004

100- %- 0	7.7321 1210.0	<u>1220.9727</u> 1220.0	1235.6 1234.0890 1230.0	5934 1237.6971 1240.0	1253.6675 12	57.6250 - <mark> - - 1260.6300</mark> - 1260.0 12	<u>1273.583</u> 11773.583 10.0	1280.0	1286.5527	.0
Minimum: Maximum:		100.0	10.0	-1.5 40.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formul	a		
1235.6934	1235.7008 1235.6896 1235.6783 1235.6406 1235.5936	-7.4 3.8 15.1 52.8 99.8	-6.0 3.1 12.2 42.7 80.8	34.0 34.0 34.0 30.0 29.0	66.3 67.3 68.4 69.2 70.9	0.4 1.4 2.5 3.3 5.1	C71 H C72 H C73 H C71 H C71 H	89 N13 89 N11 89 N9 89 N5 90 N5	07 08 09 014 06 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 lons 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 Chemical Formula: C . HaaN Molecular Weight: 1362.73 P6 Mg_5771 56 (0.937) Cm (56:60) TOF MS ES+ 1.14e+004 1362.7682 1361.7667 100-1363.7660 1364.7700 1367.7631 1369.4548_{1371.4132}1372.1080 1373.7920 1364.0 1366.0 1368.0 1370.0 1372.0 1374.0 %-1358.8739 1360.0511 1360.8959 1374.0 E0 1358.0 1360.0 1362.0 Minimum: -1.5 100.0 10.0 40.0 Maximum: -D-

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (No	rm) H	form	ıla			
1361.7667	1361.7576 1361.7689 1361.7328 1361.7440	9.1 -2.2 33.9 22 7	6.7 -1.6 24.9 16.7	36.0 36.0 33.0 33.0	110.8 111.0 111.0 111.6	1.1 1.3 1.3		279 278 279	H99 H99 H100 H100	N11 N13 N7 N9	010 09 012 011	Na Na



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 Exact Mass: 1123 6259 Molecular Weight: 1124.4161 Monoisotopic Mass, Odd and Even Electron Ions

Mg_5763 76 (1.277) Cm (76:78)

P7

TOF MS ES+ 6.88e+004

100- %- 0- 1116.: 1115.0	3138 1120,5532 1120,5532 1120.0	1123.6202 11 1125.	24.6337 	1128.4031 1130.0	<u>1135.61</u> 1135.0	461136.6	182 1140.0	1142.4	894 - 1	1145.58 145.0	34114	6.5798 1150.0
Minimum: Maximum:		100.0	10.0	-1.5 40.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Form	ula			
1123.6202	1123.5997 1123.6235 1123.6259	20.5 -3.3 -5.7	18.2 -2.9 -5.1	29.5 29.0 32.0	168.1 168.2 169.6	0.8 0.9 2.2		C65 C65 C67	H80 H82 H81	N8 N9 N9	08 07 07	Na Na

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 1 Elements Used: Chemical Formula: C₇₄H₉₃N₁₁O₈ Molecular Weight: 1264.63 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) TOF MS ES+ 8.37e+004 1263,7216_1264.7305 100-1265.7272 %-1275.7000.1276.6973 1279.7162 1269.5292 1249.1621.1250.1538 1254.5450.1255.5168 1261.1445 1262.2988 1280.0 0-1270.0 1255.0 1275.0 1250.0 1260.0 1265.0 Minimum: -1.5 Maximum: 100.0 10.0 40.0 Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula Mass

1263.7216	1263.7209	0.7	0.6	34.0	163.1	0.0	C74	Н93	N11	08

Figure S83. HRMS of peptoid P8

Single Mas Tolerance = Element pre- Number of is Monoisotopic 295 formula(e Elements Use C: 55-57 H:	Analysis 100.0 mDa / DE diction: Off sotope peaks used Mass, Even Electror) evaluated with 1 re d: 55-56 N: 5-17 O	BE: min = -1 for i-FIT = n lons sults within l : 4-15 l: 0-	.5, max = 3 imits (up to 1	40.0 50 best isoto	Che M Dipic matches fr	mical Formula: C _{Se} H _{SS} N ₅ O Exact Mass: 861.43 tolecular Weight: 862.07 or each mass)		
cm63 Mg_5782 60 (1	.005) Cm (58:63)							TOF MS ES+ 6 19e+004
100- %- 0	6724_857.2264.858.37 1	17 860.1526 860.0	860.9968	862.4338	863.4355 864.4390 864.0	865.4431 <u>66.4338</u> 866.0 86	68.3737 869.3 8.0 87	3385 870.8823 m/z 0.0 872.0
Minimum: Maximum:		100.0	10.0	-1.5 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	С56 Н56 1	N5 O4

Figure S84. HRMS of peptoid P9

Single Mas Tolerance = Element prec Number of is Monoisotopic I 534 formula(e) Elements Use C: 60-63 H: 0	Single Mass Analysis Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0 Element prediction: Off Jumber of isotope peaks used for i-FIT = 3 Anonoisotopic Mass, Even Electron Ions 34 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass) Elements Used: 35 60-63 H: 65-66 N: 5-17 O: 4-15 Na: 0-1 I: 0-1 m45 Jg_5775 65 (1.090) Cm (64:65) TOF MS ES+											
Mg_5775 65 (1.	090) Cm (64:65)							Т	OF MS ES+			
100 % 0 986.00	986.5411 9{	988 97.5522 988.00	.5123 989.0064 989.00	89.5137 989.8379 990.00	990.5176 	991.5207 992 	2.5455,992.785; T T T T T T T T T T T T T T T T T T T	2 993.8881 994.00	m/z			
Minimum: Maximum:		100.0	10.0	-1.5 40.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula					
988.5123	988.5013 988.5125 988.5238	11.0 -0.2 -11.5	11.1 -0.2 -11.6	33.5 33.5 33.5	125.7 126.6 127.4	0.5 1.3 2.1	C63 H66 C62 H66 C61 H66	N5 06 N7 05 N9 04				

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: Ce₂H_{e6}N₇O₆ Exact Mass: 997.50 Molecular Weight: 988.22 hatches for each mass)

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

000 5400

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

TOF MS ES+ 7.69e+00(

100 % 0 98(986.5340.986.7739	987.5499	989	989.50	96 990.511 990.00	4 991.5	156	992.51	138	993.29 00	<u>97993.5172</u> 994.00	m/z - די
Minimum: Maximum:		100.0	10.0	-1.5 40.0			002.00				001100	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Form	ula			
988.5123	988.5013 988.5125 988.5238	11.0 -0.2 -11.5	11.1 -0.2 -11.6	33.5 33.5 33.5	133.2 133.3 133.3	1.1 1.1 1.2		C63 C62 C61	Н66 Н66 Н66	N5 N7 N9	06 05 04	

Figure S86. HRMS of peptoid P13



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



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

Molecular Weight: 979.4273

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

TOF MS ES+

100- %- 0 972.0	973.0778974.2831.974. 	.7580 978. 976.0	1860 979.246 978.0	979.7684 6 980.0	980.7695 981.7709 982.0	982.7770 984.5370 984.0	986.2651 986.0	988.5057 988.0	989.5085
Minimun Maximun	n: n:	100.0	10.0	-1.5 40.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm) Formula		
979.768	84 979.7575 979.7688 979.7800	10.9 -0.4 -11.6	11.1 -0.4 -11.8	11.5 11.5 11.5	146.9 147.2 147.5	0.8 1.1 1.5	C57 H99 C56 H99 C55 H99	N6 07 N8 06 N10 05	

Figure S88. HRMS trace of peptoid P15

Single Mass Tolerance = Element pre Number of is Monoisotopic 192 formula(e Elements Use C: 55-58 H:	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 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													
cm51 Mg_5778 55 (0	.920) Cm (53:56)								TOF MS ES+ 3.29e+004					
100- %- 0	988.5148 989.509 988.0 990.0	³ 990.5081 	993. 992.7698	.7850 994.7 994.7	854 95.7878 996.7 	891 997.7916998.9 998.0 1	403_1000.206 	1 1002.5278 1002.0	1003.5311 					
Minimum: Maximum:		100.0	10.0	-1.5 40.0										
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula							
993.7850	993.7732 993.7844 993.7956 993.8069	11.8 0.6 -10.6 -21.9	11.9 0.6 -10.7 -22.0	11.5 11.5 11.5 11.5 11.5	162.1 162.4 162.7 163.0	1.0 1.3 1.6 1.9	C58 H101 C57 H101 C56 H101 C55 H101	L N6 07 L N8 06 L N10 05 L N12 04						

Figure S89. HRMS of peptoid P16

cm48

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

 H_2

cm48 Mg_5783 45 (0	.749) Cm (45:47)			Chemical Formula: C ₆₈ H ₇₅ N ₉ O ₆ Exact Mass: 1113.58					, О ₆ Т	OF MS ES+ 2.31e+003		
100 % 0 1092. 1092.	4597 1099,56991 1100.0	101.5354 11 11	1114.59 10.6158 10.0	20 1116.5958 	1128.57361130 113	0.5477 1136.5 	Mol 563 11 1140.0	ecular \ 42.564 0	Weight: 3 114 7 7 7 7	1114.38 6.5013 1150.0	1152.53	:83
Minimum: Maximum:		100.0	10.0	-1.5 40.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Form	ula			
1114.5920	1114.5806 1114.5919 1114.6031	11.4 0.1 -11.1	10.2 0.1 -10.0	35.5 35.5 35.5	101.7 101.8 102.0	1.0 1.1 1.3		C69 C68 C67	H76 H76 H76	N7 N9 N11	07 06 05	

Figure S90. HRMS of peptoid P18

Single Mas Tolerance = Element prec Number of is Monoisotopic 16 formula(e) Elements Use C: 60-63 H	Single Mass Analysis Folerance = 100.0 mDa / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Vonoisotopic 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)				1100 0 100						TOF MS ES+ 1.15e+004		
100 0 1096.0	1098.0594 1099.9 1098.0 1100	8 <u>13 1102.2</u> .0 1102.1	2061 1105. 0 1104.0	1105.8491 1171 0 1106.0	1106.8496	108.8546 1110.8	545 1112 TTTTTTT	2.6024 1114.0	<u>1115.</u> 11	7 <u>617</u> 16.0	1116.8607 		
Minimum: Maximum:		100.0	10.0	-1.5 50.0									
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm) Form	ula					
1105.8491	1105.8245 1105.8481 1105.8117 1105.8457 1105.7882 1105.7753	24.6 1.0 37.4 3.4 60.9 73.8	22.2 0.9 33.8 3.1 55.1 66.7	15.5 13.5 14.5 10.5 16.5 15.5	93.4 93.7 94.6 94.6 94.8 96.1	1.0 1.3 2.2 2.2 2.4 3.7	C63 C62 C61 C60 C62 C60	H106 H109 H105 H110 H102 H101	N10 N10 N10 N10 N10 N10	05 07 08 07 06 09	Na Na Na		

Figure S91. HRMS of peptoid P19



Figure S96. HRMS of peptoid P21

Single Mas Tolerance = Element pre Number of is	es Analysis 100.0 mDa / DE diction: Off sotope peaks used	BE: min = -1 for i-FIT =	1.5, max = 4 3	40.0							
Monoisotopic 343 formula(e Elements Use C: 73-74 H:	Mass, Odd and Ever) evaluated with 5 re d: 84-85 N: 5-17 O	n Electron Io sults within I : 4-15 Na:	ns imits (up to s 0-1 I: 0-1	50 best isoto	pic matches for	r each m	ass)		Ŷ)]	NH ₂
cm50 Mg_5774 58 (0	971) Cm (58:59)					CI	nemical Form Exact Mas Molecular We	ula: C ₇₄ H ₈₈ s: 1239.663 ight: 1240.	N ₁₁ O ₇ 33 5362		TOF MS ES+ 5.03e+003
100-			1239	.6614 1240.66	25						
%	235.7363 1236.965	5 12	238,7990	1240,2111	1241.6672 1	242.6682	1243.647	6	1245.6	⁵³⁷ 1246,153	1 m/z
	1236.0	1238.0		1240.0	1242.0		124	4.0		1246.0	1 1 1 102
Minimum: Maximum:		100.0	10.0	$-1.5 \\ 40.0$							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Formu	la		
1239.6614	1239.6633 1239.6746 1239.6147 1239.6259 1239.6144	-1.9 -13.2 46.7 35.5 47.0	-1.5 -10.6 37.7 28.6 37.9	38.0 38.0 35.5 35.5 34.0	71.8 72.3 73.8 74.0 74.6	0.6 1.2 2.6 2.8 3.5		C74 C73 C74 C73 C73 C73	H85 H85 H84 H84 H85	N11 07 N13 06 N6 010 N8 09 1 N5 013	Na Na

Figure S92. HRMS of peptoid P22

Single Mas Tolerance = Element prec Number of is Monoisotopic 10 formula(e) Elements Use	s Analysis 100.0 mDa / DE diction: Off otope peaks used Mass, Even Electron evaluated with 3 resi d:	BE: min = -1 for i-FIT = lons ults within lir	1.5, max = 4 3 nits (up to 50	40.0 Ph HN. 0 best isotop	Ph Ph N ic matches for Ch	Ph Ph Ph Ph Ph Ph Ph Ph Ph Ph Ph Ph Ph Ph P		h YN O	rNH₂ ⊃	
C: 65-70 H cm-99 Mg_5756 65 (1.	: 80-82 N: 5-10	O: 5-10	Na: 0-1		1	Exact Mass: 1067.6 Molecular Weight: 106	2 8.39		Т	OF MS ES+
100- %- 0-1062.566	1068.6324 5 1068.0631 1065.0	1069.6267 1 1 1070.0	070.6272 	6322 1075.6 1075.0	5218 1081.2 1080.1	920 1084.6157 0 1084.6157	1085.6078 1	3 109	90.6027 <u>109</u> 1090.0	1.35e+004 1.5983 1.5983 m/z
Minimum: Maximum:		100.0	10.0	-1.5 40.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formul	la		
1068.6324	1068.6214 1068.6327 1068.6439	11.0 -0.3 -11.5	10.3 -0.3 -10.8	29.5 29.5 29.5	69.3 69.4 69.4	1.0 1.1 1.2	C67 H C66 H C65 H	H82 N5 H82 N7 H82 N9	07 06 05	

Figure S93. HRMS of peptoid P24

Single Mas Tolerance = Element pre- Number of is	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 lons												
8 formula(e) e Elements Use	ionoisotopic Mass, Even Electron Ions H—N, OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO												
C: 71-75 H	I: 90-93 N: 9-11	O: 0-10	Na: 0-1			Molecular Weig	ht: 1194.55						
Mg_5753 54 (0	.903) Cm (54:55)								TOF MS ES+ 1.65e+004				
100- %- 0	5.4893 1186.3751 118	8.6207	1193.718 1192.738	38 1194.7113 1195.7	⁰⁹¹ 1196.7102	1200.1926/1201.18	63 120	05.6951	6.68991208.6790				
1182.5	1185.0 1187.5	1190.0	1192.5	1195.0	1197.5	1200.0 1202	2.5 1205	.0 120	07.5				
Minimum: Maximum:		100.0	10.0	-1.5 50.0									
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula						
1194.7113	1194.7232 1194.7120 1194.7361 1194.7248 1194.7385	-11.9 -0.7 -24.8 -13.5 -27.2	-10.0 -0.6 -20.8 -11.3 -22.8	31.5 31.5 32.5 32.5 35.5	107.7 107.8 107.9 108.0 108.3	1.4 1.5 1.6 1.7 2.0	C71 H92 C72 H92 C73 H93 C74 H93 C75 H92	N11 O N9 O7 N11 O N9 O4 N11 O	6 3 Na Na 3				

Figure S94. HRMS of peptoid P25



Figure S96. HRMS of peptoid P27

Single Ma Tolerance Element pr Number of	ass Analysis = 100.0 mDa / Df rediction: Off isotope peaks used	3E: min = -1 I for i-FIT =	1.5, max = 4 3	40.0	HN^ O _Y NHC						IH ₂	
Monoisotop 68 formula(Elements U C: 44-45	ic Mass, Even Electron e) evaluated with 1 res sed: H: 60-72 N: 10-15	n Ions sults within Iir O: 12-15 N	mits (up to 50 la: 0-1 I: 0-	0 best isoto 1	pic matches for	each ma Chemica Ei Mole	i ss) I Formula: (xact Mass: 9 cular Weigh	O C ₄₅ H ₆₀ N 932.44 nt: 933.0	₁₀ O ₁₂ 2			
cm100 Mg_5768 48	(0.800) Cm (48:51)											TOF MS ES+
100 % 869. 0	4708 915.516	933.4 2 931.4427 920	451 934.4603 936.4700 940	955.4422 9 960	991.7 991.7 980 10	728 1 	029.4230 	1046.44	62 1 	059.509 	18 • • • • • •	1082.5112 1080
Minimum: Maximum:		100.0	10.0	-1.5 40.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Form	ıla			
933.4451	933.4470	-1.9	-2.0	20.5	205.2	0.0		C45	H61	N10	012	

Figure S96. HRMS of peptoid P28



Figure S97. HRMS of peptoid P29



Figure S98. HRMS of peptoid P30

Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 40.0Element 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

Chemical Formula: C₆₃H₉₀N₁₆O₁₅ Exact Mass: 1310.68 Molecular Weight: 1311.49

cm101 Mg_5769 56 (0.937) Cm (56:58)

TOF MS ES+ 9.37e+003

100 % 1300.0 0 1297.5	0547 <u>1301.4851 1303</u> 1300.0 1302.5	2.9445 1307. 1305.0	3831 1310 	1310.6774 0.1364 1310.0	1311.6792 1312.678 1312.5 13	0 <u>1316.</u> 315.0	6 <u>783_131</u> 1317.5	7.6315	0.0	1322.6 1322.	146/132 5	3.6897 1325.0	m/z
Minimum: Maximum:		100.0	10.0	-1.5 40.0									
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Form	ula				
1310.6774	1310.6897 1310.6900 1310.6772 1310.7010	-12.3 -12.6 0.2 -23.6	-9.4 -9.6 0.2 -18.0	26.5 28.0 27.0 26.5	82.4 82.7 82.9 83.1	1.0 1.4 1.5 1.7		C64 C65 C63 C63	H92 H91 H90 H92	N15 N16 N16 N17	015 012 015 014	Na	

Figure S99. HRMS of peptoid P31





Figure S100. 1H NMR spectra of PD' in CD₃OD