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Supporting Information for:

Folding of Unstructured Peptoids and Formation of Hetero-bimetallic Peptoid Complexes upon Side-chains-to-Metal Coordination

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Materials:

8-hydroxy-2-quinolinecarbonitrile and (S)-(-)-1-phenylethylamine (Nspe) were supplied by Acros; Rink Amide resin was supplied by Novabiochem; Zinc acetate dehydrate, (S)-(-)-1-methoxy-2-propylamine (Nsmp), Trifluoroacetic acid (TFA) were supplied by Alfa Aesar; bromoacetic acid, cobalt acetate tetrahydrate and copper acetate monohydrate were supplied by MERCK; Water HPLC grade, acetonitrile HPLC grade, N,N'diisopropylcarbodiimide (DIC), piperidine, zinc trifluoromethanesulfonate was supplied by Sigma-Aldrich; Dimethylforamide (DMF) and methanol (MeOH) solvents were purchased from Bio-Lab Itd. Solvents and reagents were used without additional purification. 8-hydroxy-2 quinolinemethylamine (*N*hq) and 2,2':6',2''-Terpyridineamine (Nterpy) were synthesized according to previously published procedure.[1]

Instrumentation:

Peptoid oligomers were analyzed by reversed-phase HPLC (analytical C18(2) column, Phenomenex, Luna 5µm, 100 Å, 2.0x50 mm) on a Jasco UV-2075 PLUS detector using a linear gradient of 5–95% ACN in water (0.1% TFA) over 10 min at a flow rate of 0.7 mL/min. Peptoid olygomers were purified by preparative HPLC using a AXIA Packed C18(2) column (Phenomenex, Luna 15µm, 100 Å, 21.20x100mm). Peaks were eluted with a linear gradient of 5–95% ACN in water (0.1% TFA) over 50 min at a flow rate of 5 mL/min. Mass spectrometry analysis of peptoid oligomers and their metal complexes was performed on Advion expression CMS mass spectrometer under electrospray ionization (ESI), direct probe ACN, flow rate 0.2 ml/min, Waters LCT Premier, Waters Acquity and Bruker maXis impact mass spectrometers under electrospray ionization (ESI), ACN:H_2O (70:30), flow rate 0.3 ml/min. UV measurements were carried out on Agilent Cary 60 UV-Vis spectrophotometer. CD measurements were performed using a circular dichroism spectrometer Applied Photophysics Chirascan. NMR measurements were conducted on a Bruker DRX700 spectrometer equipped with cryogenic triple-resonance TCI probe with *z*-axis pulsed field gradients. EPR spectra were recorded on a Bruker EMX-10/12 X-band (ν=9.4 GHz) digital EPR Spectrometer. Spectra processing and simulation were performed with Bruker WIN-EPR and SimFonia Software. Data processing for publication was done with the softwares Excel and KaleidaGraph.

Preparation of the peptoid oligomers:

Peptoids were synthesized manually at room temperature on Rink amide resin using the submonomer approach[2] that involves two main steps: acetylation and halide displacement by amine to form N-substituted glycine oligomer. This two-step addition cycle was modified as follows: for 100 mg resin after incorporation of 8-hydroxy-2-quinolinemethylamine, 0.17 ml of a 1.2 M solution of bromoacetic acid, 0.04 ml of neat *N, N*'-diisopropylcarbodiimide (DIC) and 0.29 ml of DMF were added to the resin and mixed at room temperature for 20 minutes.[3] Bromoacetylations and amine displacement steps were repeated until the peptoids were obtained. For analysis, approximately 5 mg of resin was treated with 95% TFA in water (40 mL g^{-1} resin) for 10 minutes. The cleavage cocktail was evaporated and the peptoid oligomers were re-suspended in 0.5 mL 50 % HPLC grade acetonitrile in HPLC grade water. For full cleavage of peptoids from solid support the resin was treated with 5 ml 95% TFA in water for 30 min. TFA was evaporated under low pressure, crude peptoids were re-suspended in 2 mL HPLC solvent 50% water in ACN, lyophilized overnight and then purified by preparative HPLC.

Characterization of the peptoid oligomers

The peptoid oligomers were characterized by analytical HPLC using a C18 column. The analysis was performed using a solvent gradient consist of 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}. Additional characterization was conducted by ESI-MS. The peptoids were further purified by RP-HPLC and lyophilized overnight.

UV-VIS Spectroscopy

Titration experiments of peptoid oligomers with the metal ions Zn^{2+}, Co^{2+} and Cu^{2+} were followed by UV-VIS measurements. In the typical experiment 10 μL of a peptoid solution (2.5-5 mM in 4:1 MeOH:H_2O) was diluted in 3 ml 4:1 MeOH:H_2O solution and then sequentially titrated with about 20-30 μL aliquots of a metal ion (5 mM in H_2O), in multiple steps, until the binding was completed. Job plot experiment was determined using UV-Vis spectrometry by varying mole fraction of metal ion Cu^{2+} and peptoid **12P1** using 7 μM total molar concentration in 4:1 MeOH:H_2O solution. Raw data were processed for publication using Microsoft Excel and KaleidaGraph.

Synthesis of metal complexes for MS analysis

Shortly before MS analysis, solutions of peptoid oligomers (100-200 µL 0.5 mM) in MeOH was treated with a solution of metal ions Cu^{2+}, Co^{2+} or Zn^{2+} (in H_2O) and the mixture was stirred for 30 minutes. The metal complexes were analyzed by mass spectrometry using Waters LCT Premier, Waters Acquity or Bruker maXis impact mass spectrometers under electrospray ionization (ESI), ACN:H_2O (70:30), flow rate 0.3 ml/min.

Synthesis of Cu^{2+} complexes for EPR analysis

Copper complexes for EPR were prepared in methanol (0.4 ml) by addition of 1 equivalent of copper acetate to peptoids **12P5** (8.6 mg, 0.0041 mmol) **12P6** (5.0 mg, 0.0024 mmol), **12P1a** (5.67 mg, 0.0031), **12P1b** (4.11 mg, 0.0028 mmol) and by addition of 2 equivalents of copper acetate to peptoids **12P1** (5.73 mg, 0.0029 mmol), **12P2** (5.28 mg, 0.0027 mmol), **12P3** (5.25 mg, 0.0027 mmol) **12P4** (5.05 mg, 0.0026 mmol) **12P5** (4.43 mg, 0.0021 mmol) **12P6** (3.84 mg, 0.0018 mmol) and the solutions were stirred for 1 hour. In the synthesis of (**12P5**)CuCo and (**12P5**)CuZn, after the addition of 1 equivalent of Cu^{2+} to the peptoid **12P5** (6.1 mg, 0.0029 mmol) 1 equiv. of cobalt acetate or zinc acetate were added and the solutions were stirred for another 1 hour. Green solids were precipitated by addition of NH_4PF_6 (0.1 ml of a 1 M aqueous solution). The precipitates were isolated by centrifugation, washed with water and lyophilized overnight. Yields of the complexes were as followed: (**12P1**)Cu_2 61% (3.61 mg), (**12P2**)Cu_2 64% (3.12 mg), (**12P3**)Cu_2 65% (4.7 mg), (**12P4**)Cu_2 62% (3.56 mg), (**12P5**)Cu 51% (4.47 mg), (**12P5**)CuCo 73% (7.7 mg), (**12P5**)CuZn 85% (5.6 mg), (**12P5**)Cu_2 76% (3.79 mg), (**12P6**)Cu 59% (3.24 mg), (**12P6**)Cu_2 65% (2.76 mg), (**12P1a**)Cu 51% (2.99 mg) and (**12P1b**)Cu 79% (3.35 mg). EPR measurements were carried out on a Bruker EMX-10/12 X-band (ν=9.4 GHz) digital EPR Spectrometer from solid state at room temperature with (2,2,6,6-Tetramethyl-1-piperidinyl)oxidanyl (TEMPO, g=2.0059) in an inner tube for determination of the g-factor. Spectra simulation and processing were performed with Bruker WIN-EPR and SimFonia Software.

Structural characterization of peptoid oligomers and their metal complexes by Circular Dichroism (CD) Spectroscopy.

Shortly before CD analysis solutions of lyophilized peptoid powders (5 mM 500 µL) in MeOH:H_2O 4:1 were prepared. CD scans were performed at room temperature using 100µM concentration of each measured sample (free ligand peptoids and metal-peptoid complexes). Scans were performed over the 340 to 190 nm region at a step of 1nm (scan rate=1 sec/step) in a fused quartz cell with a path length of 0.1 cm. CD spectra were obtained after averaging 4 scans per sample. After the CD measurement of the free peptoids 1-2 equivalents of metal ion Cu^{2+}, Co^{2+} or Zn^{2+} were added and the CD was measured again.

NMR Spectroscopy

NMR measurements were conducted on a Bruker DRX700 spectrometer equipped with cryogenic triple-resonance TCI probe with *z*-axis pulsed field gradients. All experiments were conducted at 16.4 T and 298 K. Peptoid conformations were characterized in this study using two-dimensional homonuclear method, COSY experiment. Typical acquisition parameters were 256-300 complex points and an acquisition time of 30.5-35.7 ms in the indirect ^1H dimension, and 2048 complex points and an acquisition time of 209 ms in the observed ^1H dimension. All spectra were processed and analyzed using the Topspin 3.2 software suite (Bruker BioSpin, Karlsruhe, Germany).

Binding constants calculations

The binding constants for Zn^{2+} and Co^{2+} metal ions were measured using UV-Vis spectroscopy by titration of 2-5 µL aliquots of a metal ion solution (2 mM in H_2O) into a 3 ml solution of the peptoids complexes (**12P5**)Cu and (**12P6**)Cu (typically 6-7µM) in MeOH:H_2O 1:1. To the solution of 3 ml peptoid oligomer **12P5** or **12P6** 1 equivalent of Cu^{2+} acetate was added and the solutions were titrated with 2-5 µL aliquots of a metal ion (2 mM in H_2O) in multiple steps. The binding was followed by recording the UV-Vis spectrum as a function of the total added metal ions. The results were fitted by a nonlinear regression (curve fit) [3-4] using GraphPad Prism® software.

References

1. G. Maayan, B. Yoo and K. Kirshenbaum, *Tetrahedron Letters*, 2008, **49**, 335-338.

2. R. N. Zuckermann, J. M. Kerr, S. B. W. Kent and W. H. Moos *J. Am. Chem. Soc.* 1992, **114**, 10646-10647.

3. G. Maayan, K. Kirshenbaum and M. D. Ward, *Chem. Comm*., 2009, 56-58.

4. M. Baskin and G. Maayan, *Chem. Sci*., 2016, **7**, 2809–2820.

Table S1. Peptoid oligomer sequences and their molecular weights.

*N*spe = (S)-(-)-1-phenylethylamine, *N*hq = 8-hydroxy-2-quinolinemethylamine,

*N*smp = (S)-(+)-1-methoxy-2-propylamine. Nterpy = 2,2':6',2''-Terpyridineamine.

Peptoid	Sequence	Molecular weight Calc: Found (gr/mol)
12P1	Nspe-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nspe	1971.25: 1972.10
12P2	Nspe-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nhq-Nsmp-Nsmp-Nhq-Nspe-Nsmp	1971.25 : 1971.49
12P3	Nsmp-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nhq-Nsmp-Nsmp-Nhq- Nspe -Nspe	1971.25: 1972.10
12P4	Nspe-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nhq-Nsmp-Nsmp-Nhq- Nsmp - Nsmp	1939.21: 1939.08
12P5	Nspe-Nterpy-Nsmp-Nsmp-Nhq-Nsmp-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nspe	2089.39 : 2090.97
12P6	Nsmp-Nterpy-Nsmp-Nsmp-Nhq-Nsmp-Nhq-Nsmp-Nsmp-Nhq- Nspe -Nspe	2089.39 : 2090.02
12P1a	Nspe-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nsmp-Nsmp-Nsmp-Nsmp-Nsmp-Nspe	1801.13: 1801.73
12P1b	Nspe-Nsmp-Nsmp-Nsmp-Nsmp-Nsmp-Nhq-Nsmp-Nsmp-Nhq-Nsmp-Nspe	1801.13: 1801.51

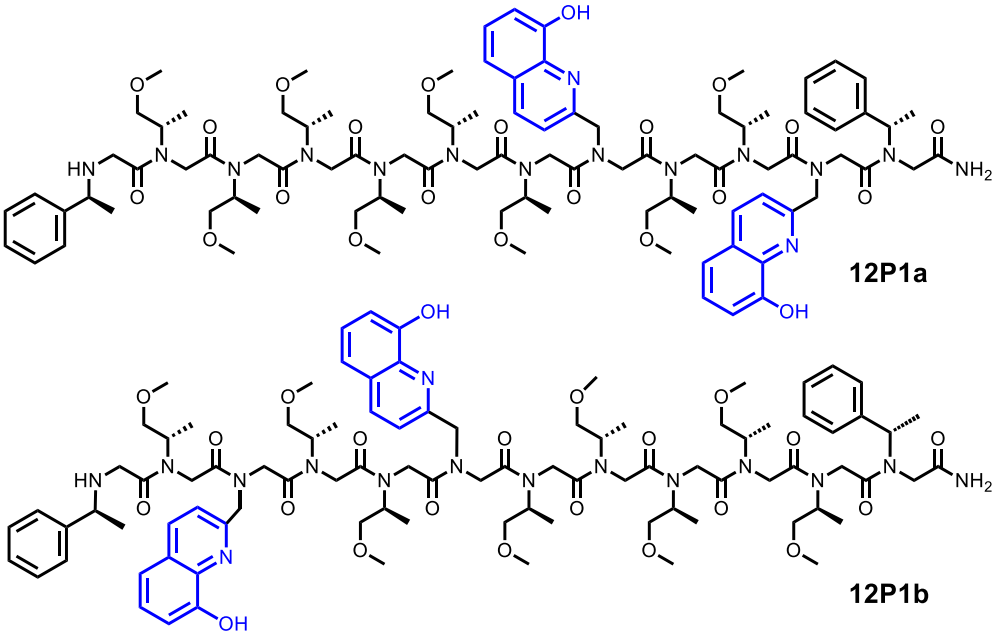


Figure S1. Chemical structure of peptoid oligomers **12P1a** and **12P1b**.

Table S2. Molecular weights of the Peptoid metal complexes.

Peptoid -Metal complex	Molecular weight Calc.: Found (gr/mol)
(**12P1**)Co_2	2085.09 : 2085.05
(**12P1**)Cu_2	2094.31 : 2093.78
(**12P1**)Zn_2	2097.98 : 2096.94
(**12P2**)Cu_2	2094.31 : 2094.94
(**12P2**)Zn_2	2097.98 : 2096.94
(**12P2**)Co_2	2085.09 : 2083.94
(**12P3**)Cu_2	2094.31 : 2092.92
(**12P3**)Zn_2	2097.98 : 2097.94
(**12P3**)Co_2	2085.09 : 2083.94
(**12P4**)Cu_2	2062.27 : 2063.57
(**12P4**)Co_2	2053.04 : 2054.54
(**12P4**)Zn_2	2065.94 : 2067.57
(**12P5**)Cu	2151.93 : 2151.95
(**12P5**)CuCo	2208.86 : 2208.86
(**12P5**)CuZn	2213.85 : 2213.86
(**12P6**)Cu	2151.93 : 2152.11
(**12P6**)CuCo	2208.86 : 2208.86
(**12P6**)CuZn	2213.85 : 2213.85
(**12P1a**)Cu	1862.66 : 1862.96
(**12P1a**)Co	1858.05 : 1858.96
(**12P1a**)Zn	1861.89 : 1861.95
(**12P1b**)Cu	1862.66 : 1862.95
(**12P1b**)Co	1858.05 : 1858.96
(**12P1b**)Zn	1861.89 : 1861.17

EPR data of Cu complexes

Table S3. EPR parameters of the copper complexes:

Copper complex	$A_{\parallel}[G]$	$g_{\perp}$	$g_{\parallel}$
(**12P1**)Cu_2	149	2.082	2.276
(**12P2**)Cu_2	148	2.084	2.279
(**12P3**)Cu_2	147	2.080	2.275
(**12P4**)Cu_2	151	2.085	2.245
(**$H_2$6**)Cu	150	2.071	2.250
(**12P5**)Cu	165	2.069	2.240
(**12P5**)Cu_2	159	2.072	2.20
(**12P5**)CuCo	165	2.068	2.245
(**12P5**)CuZn	165	2.068	2.245
(**12P6**)Cu	163	2.067	2.240
(**12P6**)Cu_2	158	2.072	2.225
(**12P1a**)Cu	155	2.067	2.250
(**12P1b**)Cu	156	2.065	2.248

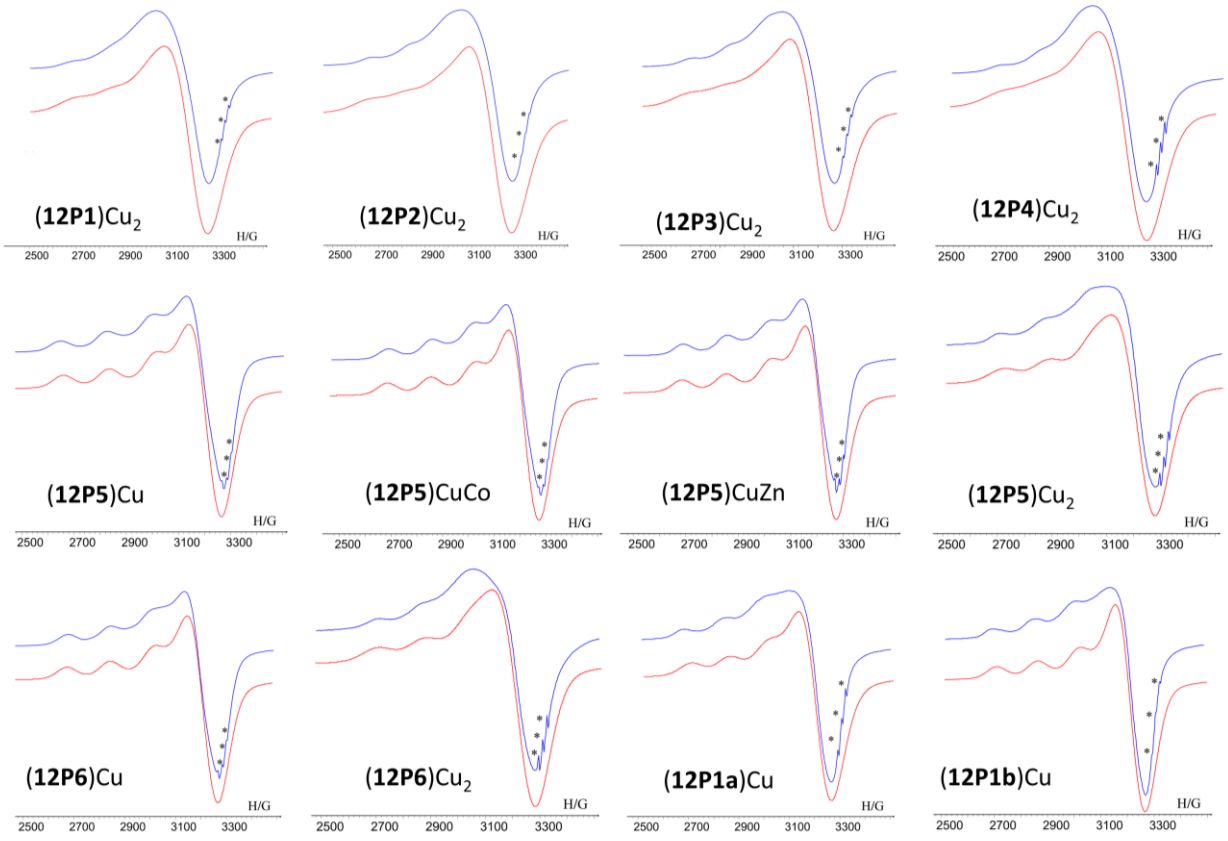


Figure S2. Room temperature X-band EPR spectra of peptoid copper complexes in solid state (blue line) and the corresponding simulated spectra (red line). Reference- TEMPO (marked by *, g = 2.0058).

HPLC data of peptoid oligomers

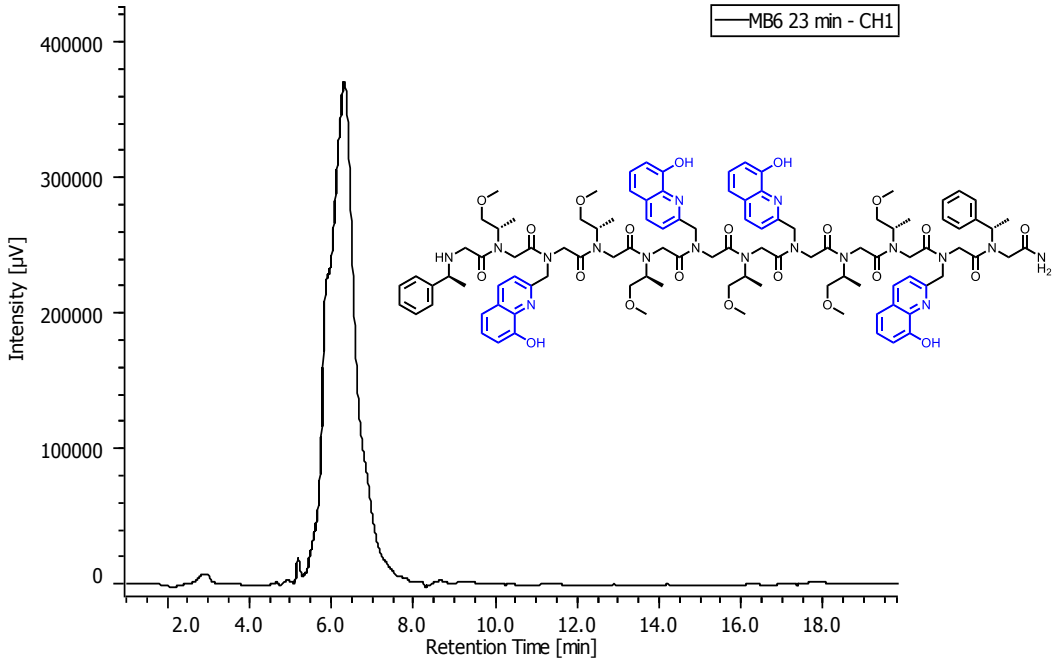


Figure S3. HPLC traces of purified peptoid **12P1** at 214nm.

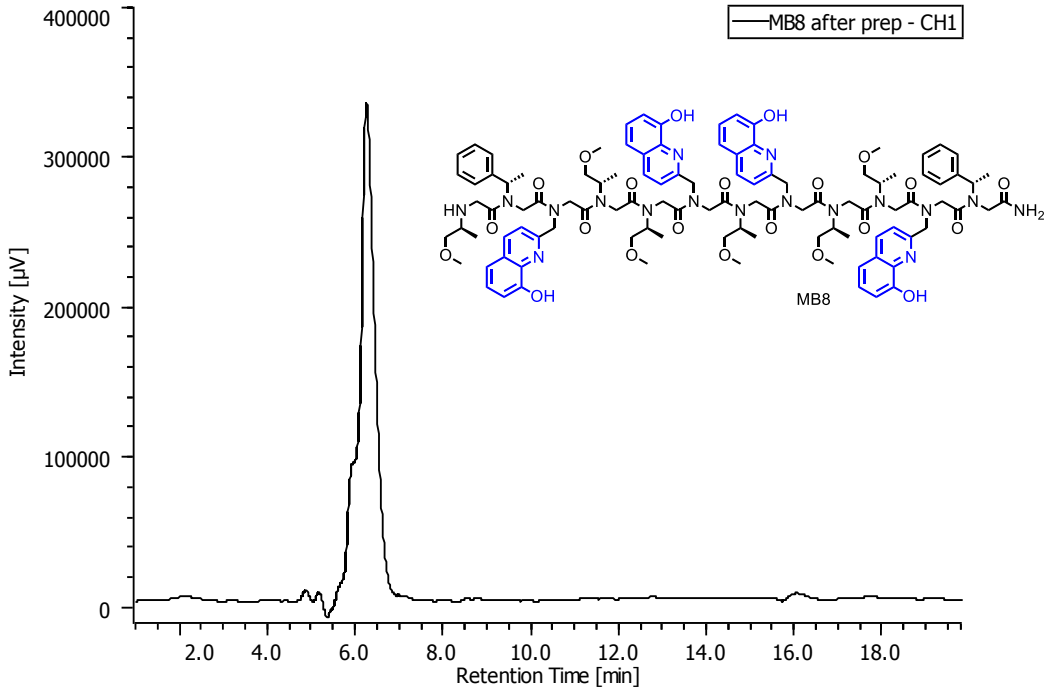


Figure S4. HPLC traces of purified peptoid oligomer **12P2** at 214nm.

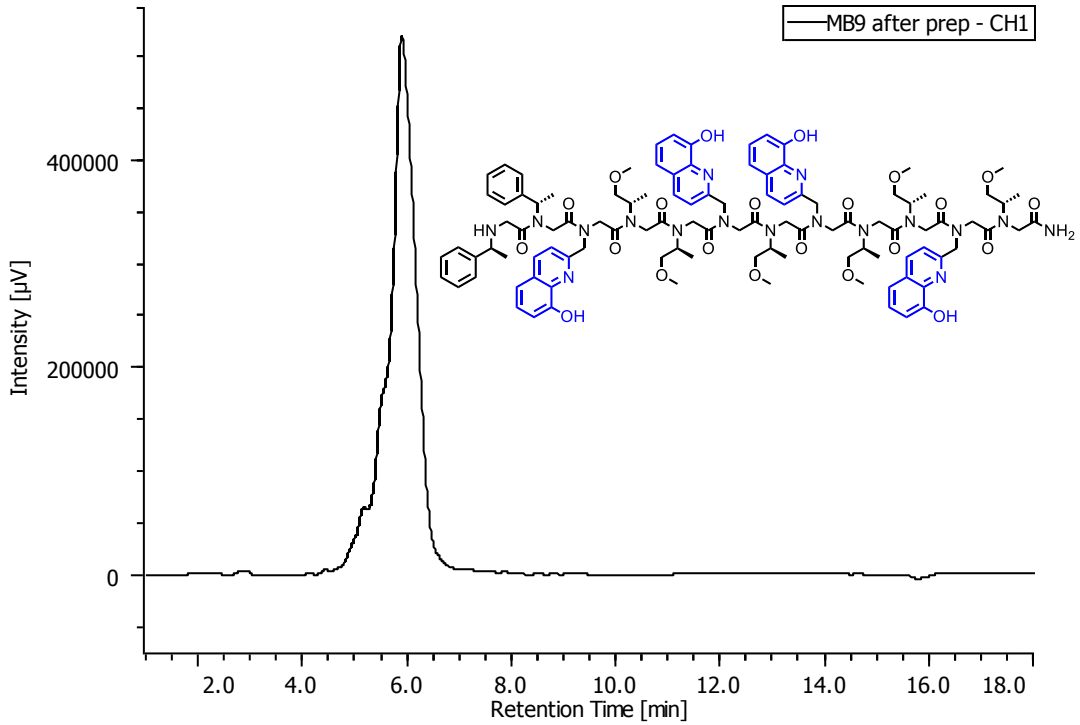


Figure S5. HPLC traces of purified peptoid oligomer **12P3** at 214nm.

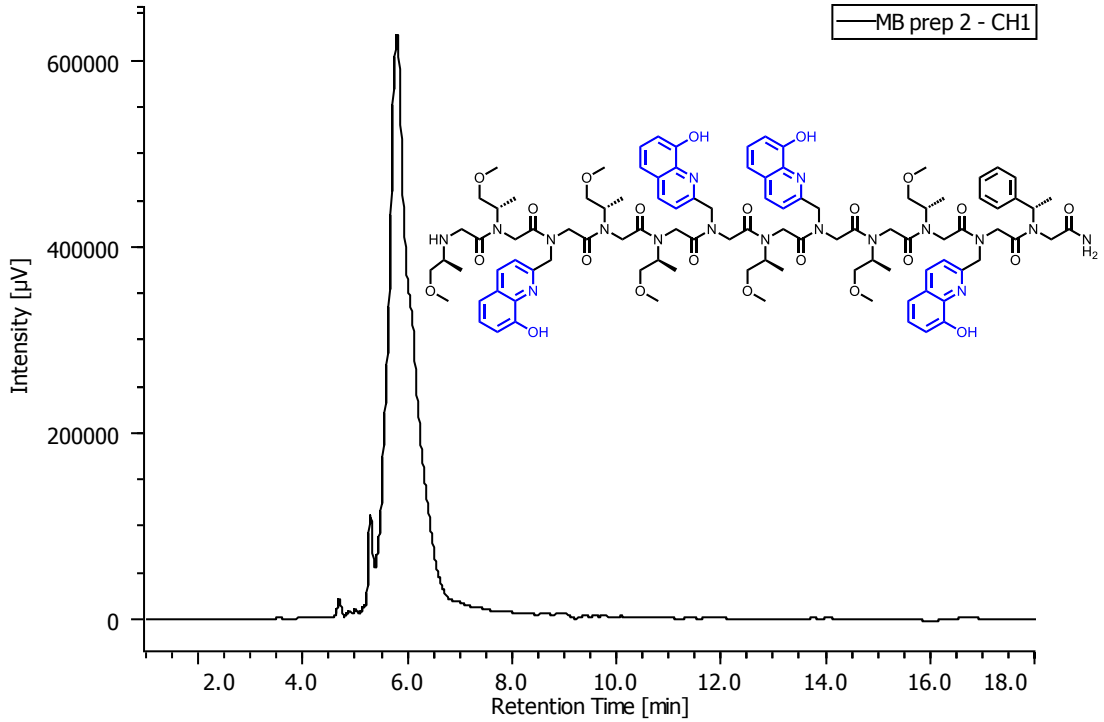


Figure S6. HPLC traces of purified peptoid oligomer **12P4** at 214nm.

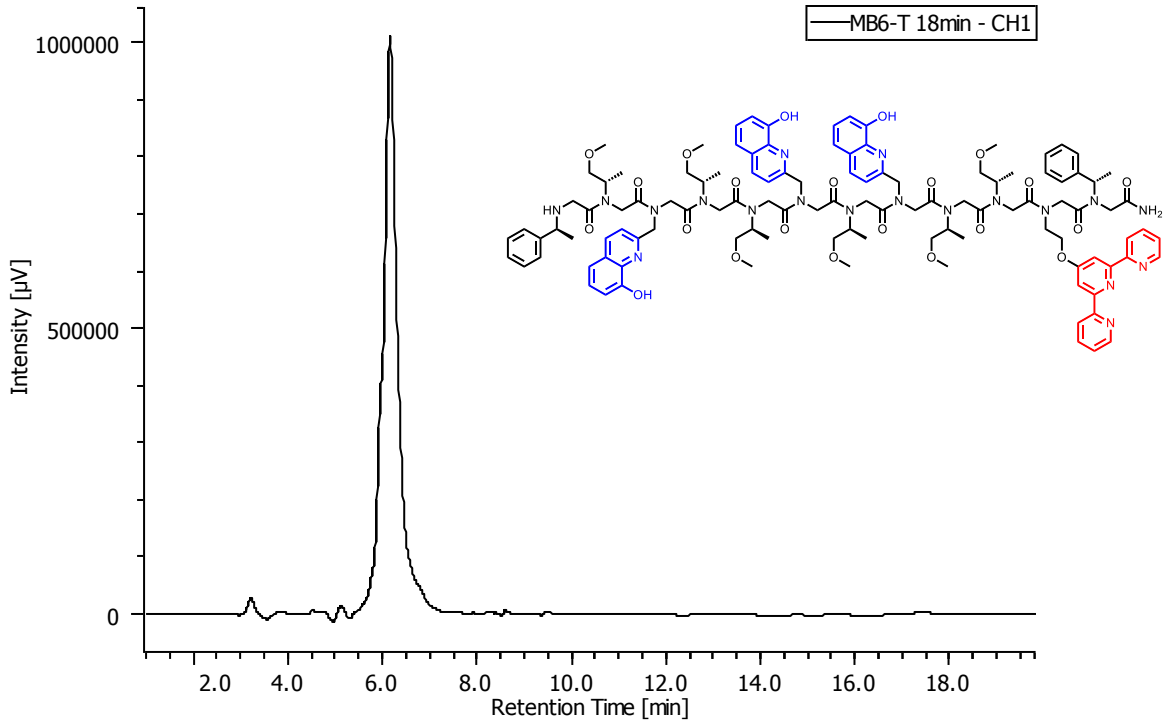


Figure S7. HPLC traces of purified peptoid oligomer **12P5** at 214nm.

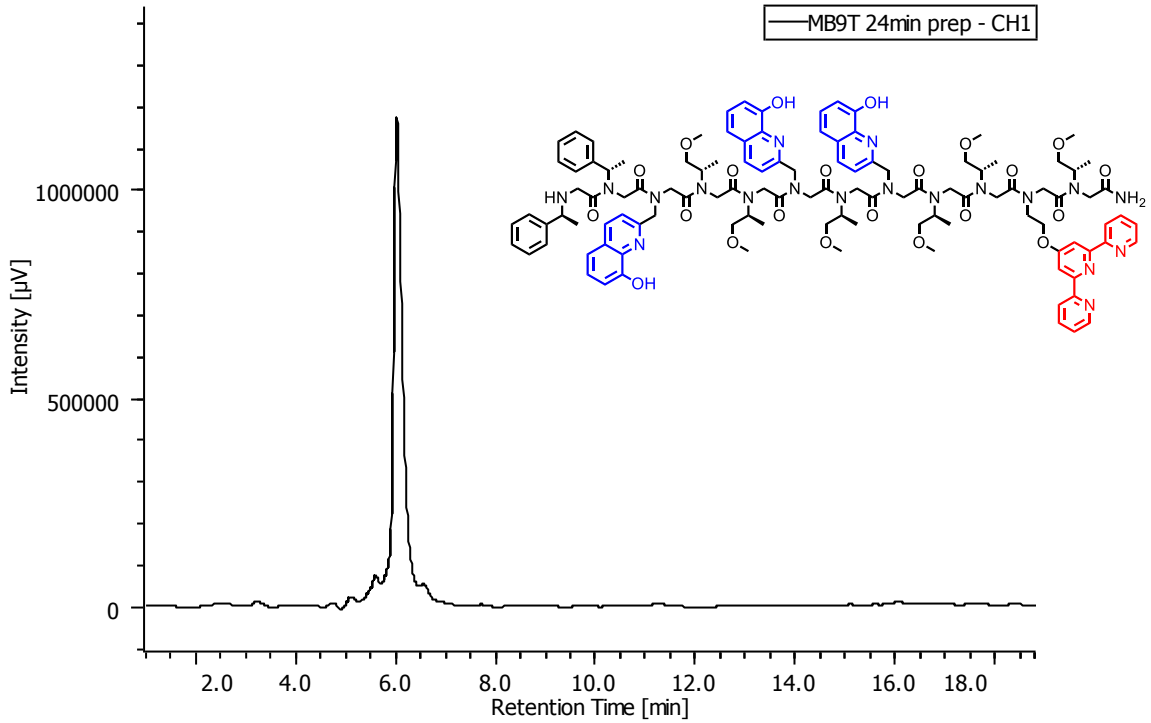


Figure S8. HPLC traces of purified peptoid oligomer **12P6** at 214nm.

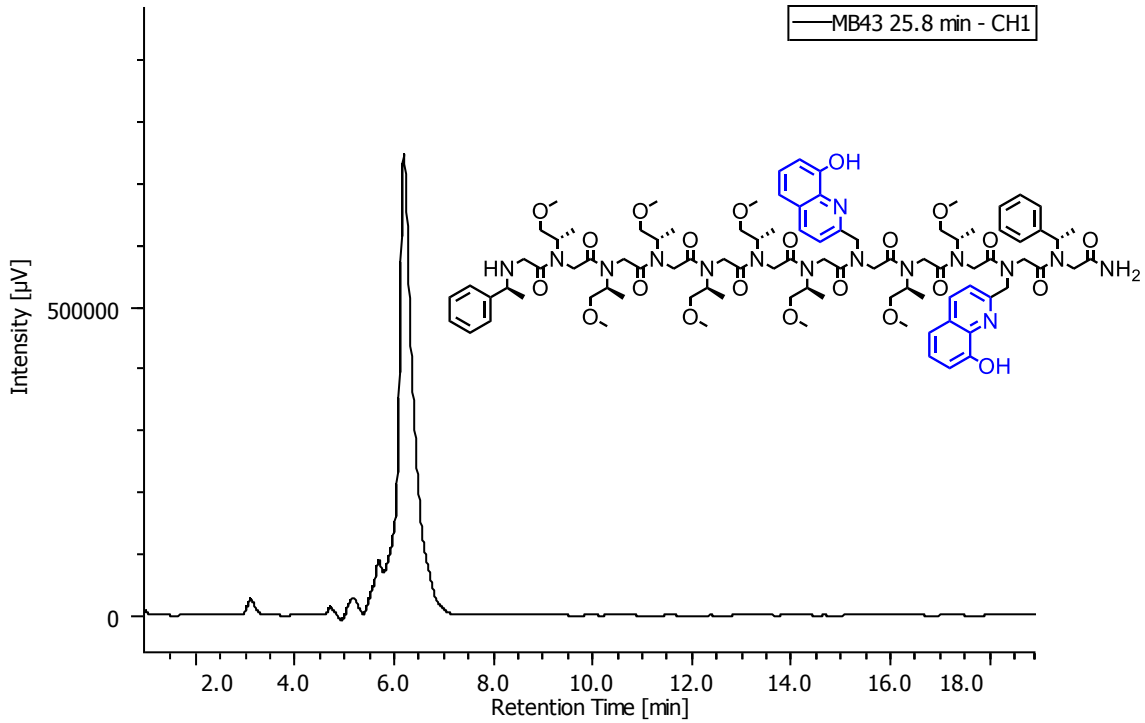


Figure S9. HPLC traces of purified peptoid oligomer **12P1a** at 214nm.

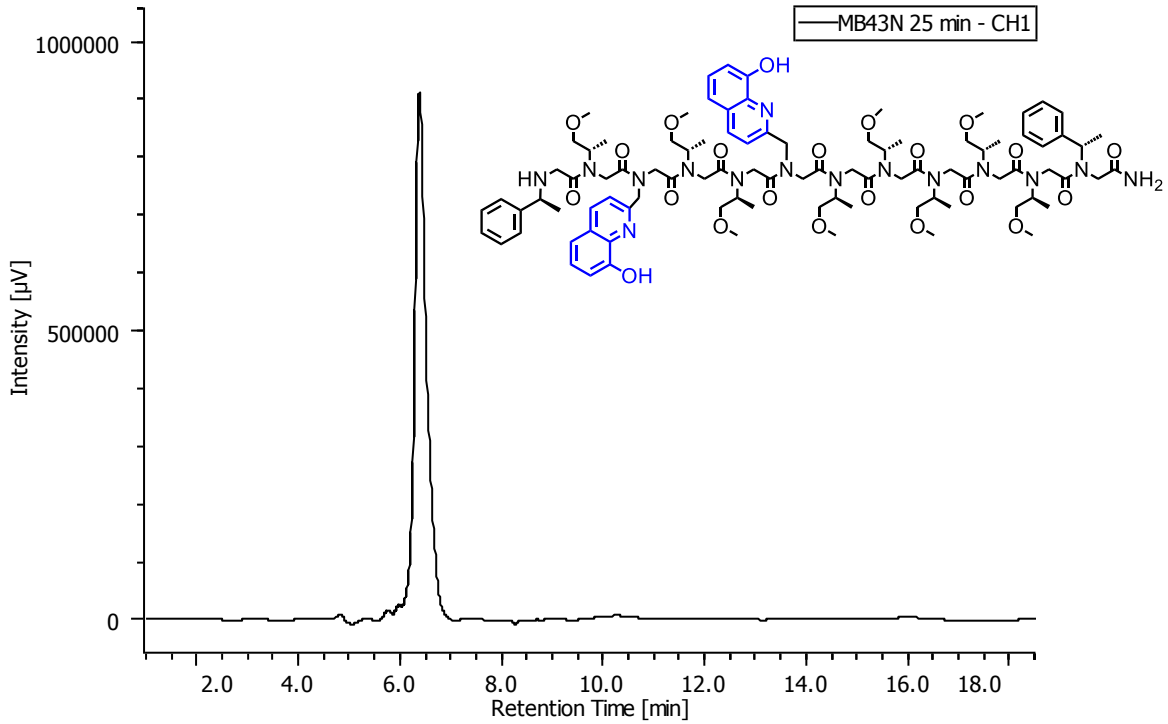


Figure S10. HPLC traces of purified peptoid oligomer **12P1b** at 214nm.

UV-VIS data

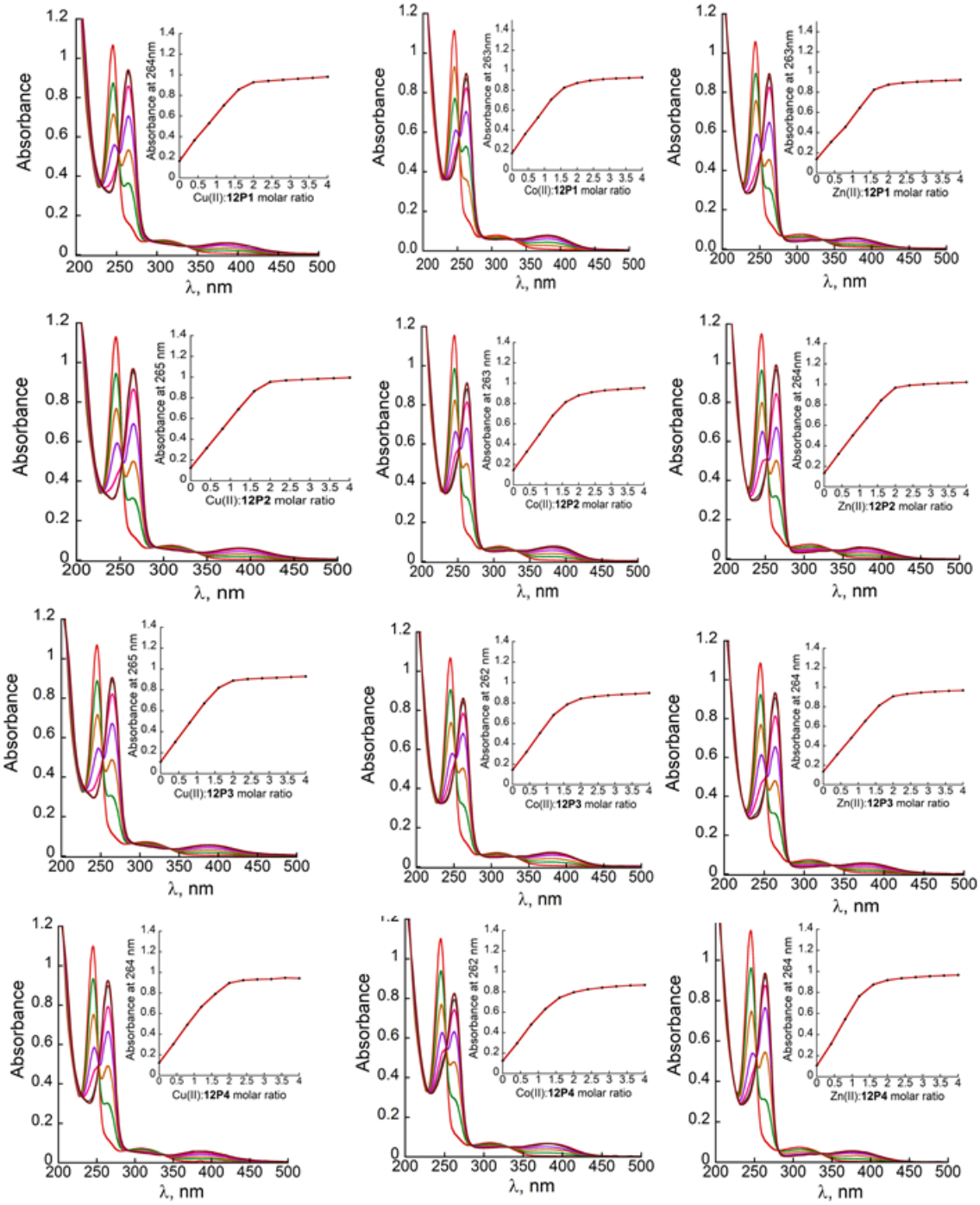


Figure S11. UV-VIS spectra of peptoid oligomers **12P1-12P4** and the formation of their (**12P**)M_2 complexes. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 8.5μM.

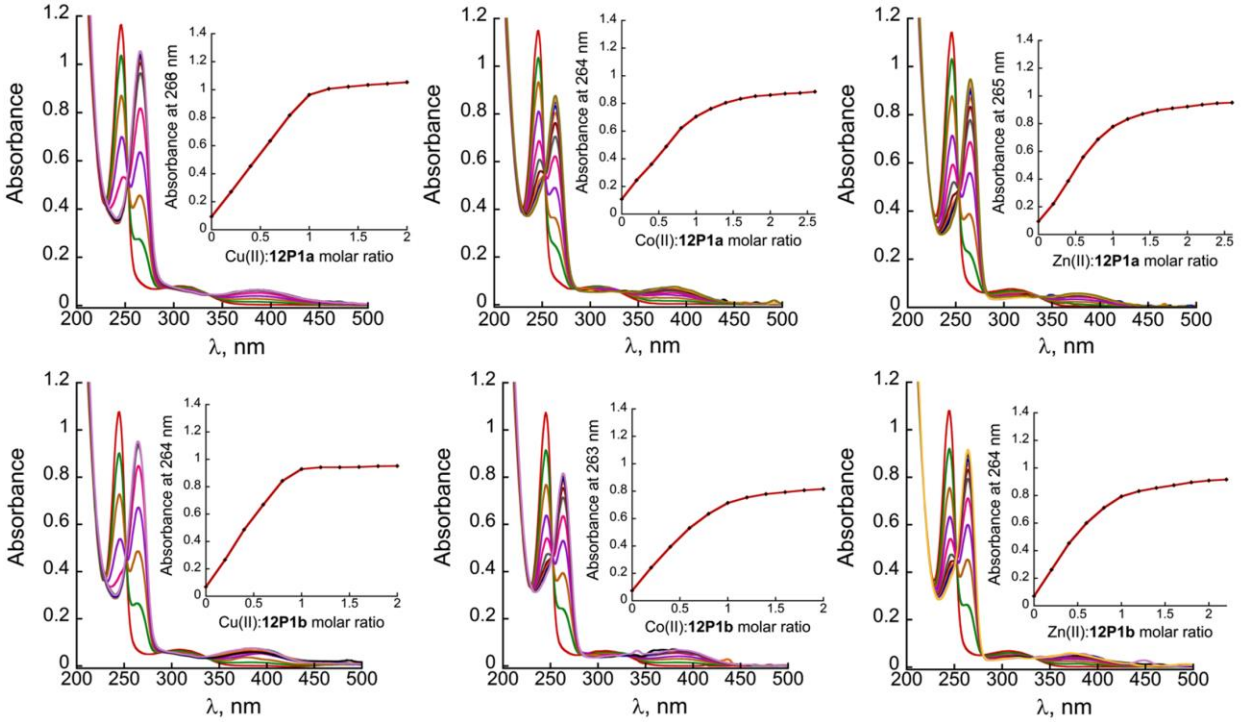


Figure S12. UV-VIS spectra of peptoid oligomers **12P1a** and **12P1b** and the formation of their (**12P**)M complexes. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17µM.

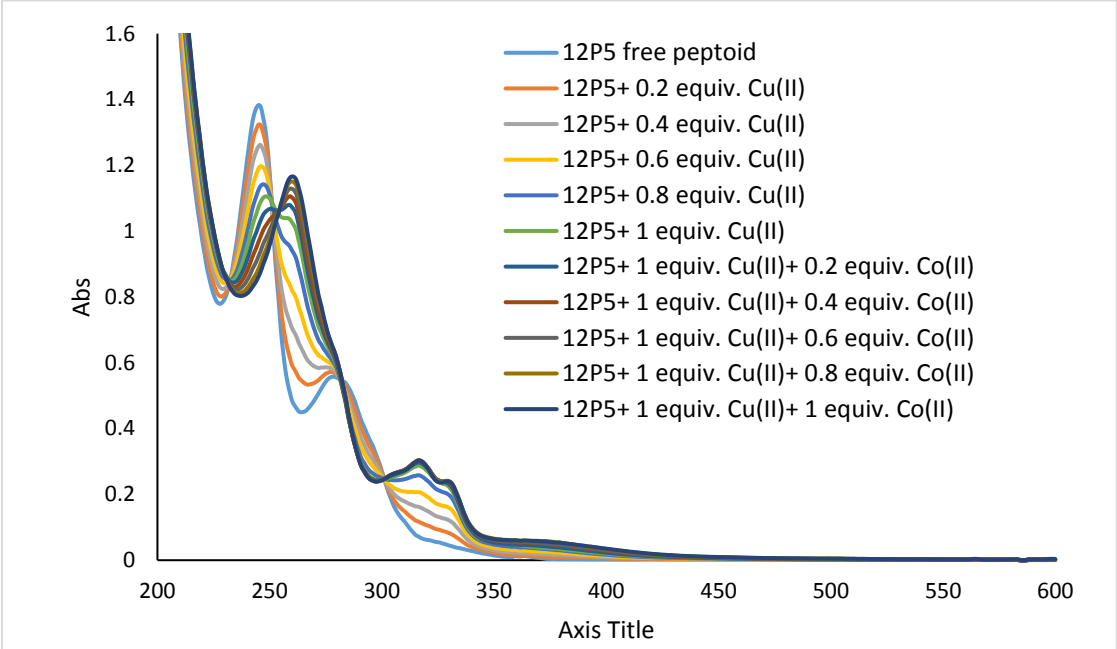


Figure S13. UV-VIS titration of peptoid oligomer **12P5** with first 1 equiv. of Cu^{2+} followed by titration with Co^{2+} towards the formation of (**12P5**)CuCo complex. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17µM.

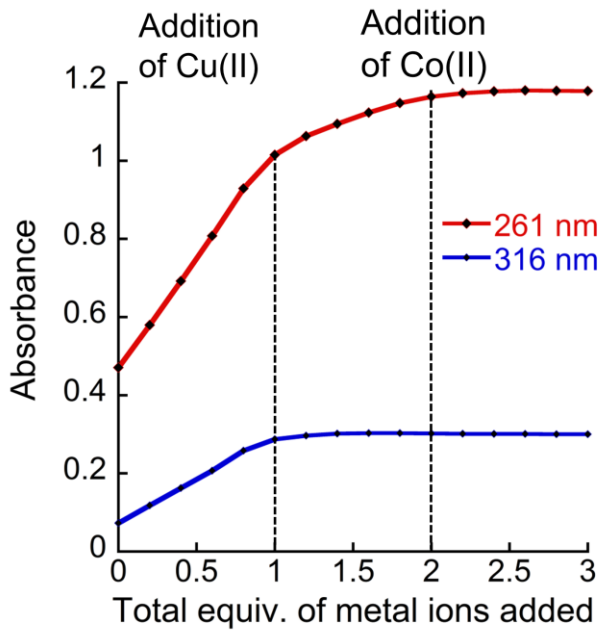


Figure S14. Absorbance at 261 nm and 316 nm of titration of oligomer **12P5** with first 1 equiv. of Cu^{2+} followed by titration with Co^{2+} towards the formation of (**12P5**)CuCo complex.

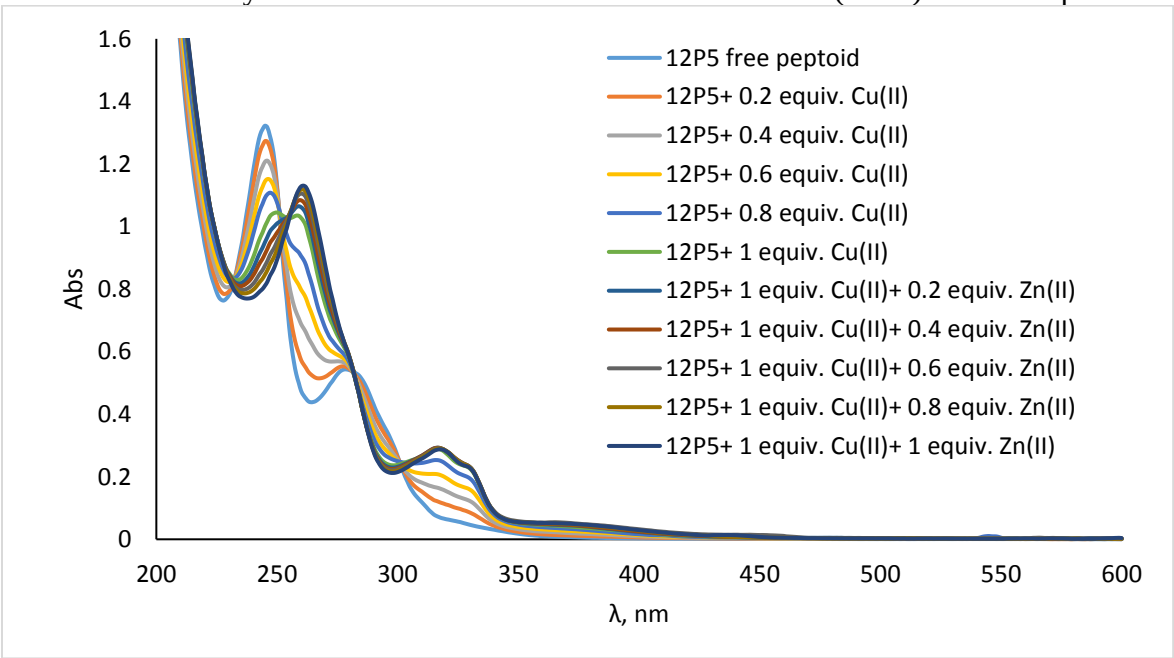


Figure S15. UV-VIS titration of peptoid oligomer **12P5** with first 1 equiv. of Cu^{2+} followed by titration with Zn^{2+} towards the formation of (**12P5**)CuZn complex. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17μM.

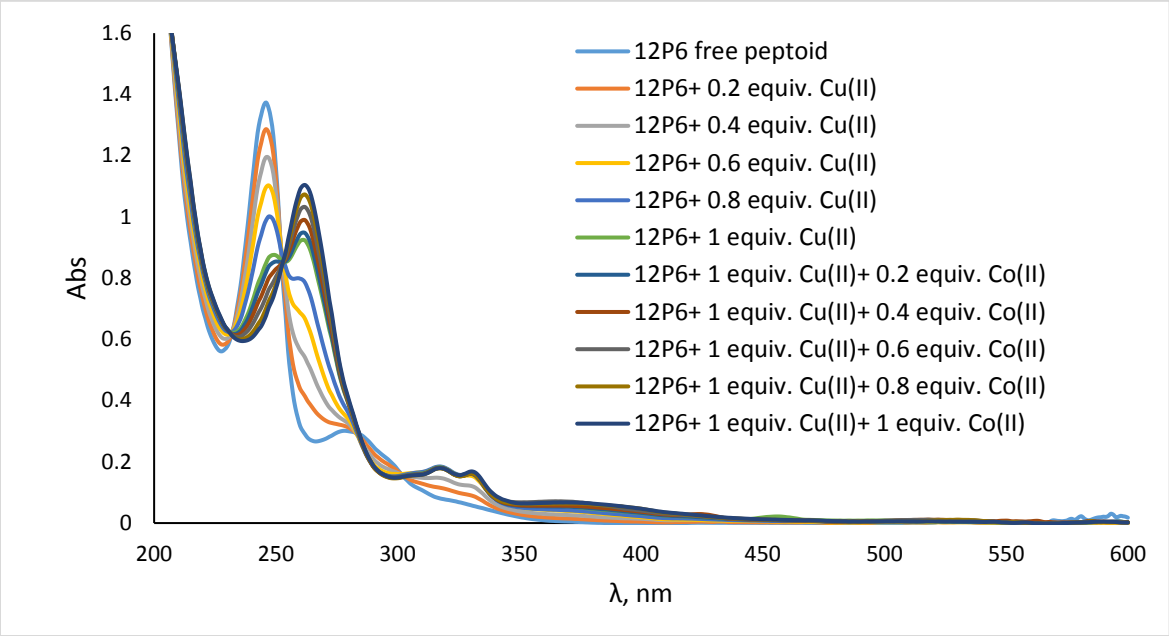


Figure S16. UV-VIS titration of peptoid oligomer **12P6** with first 1 equiv. of Cu^{2+} followed by titration with Co^{2+} towards the formation of (**12P6**)CuCo complex. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17µM.

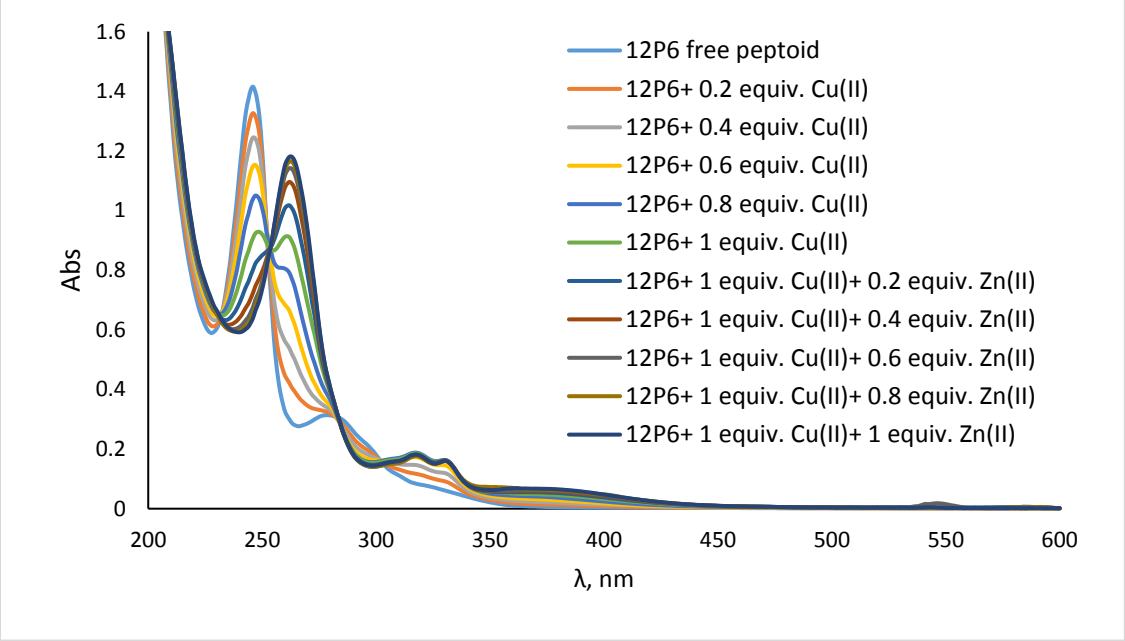


Figure S17. UV-VIS titration of peptoid oligomer **12P6** with first 1 equiv. of Cu^{2+} followed by titration with Zn^{2+} towards the formation of (**12P6**)CuZn complex. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17µM.

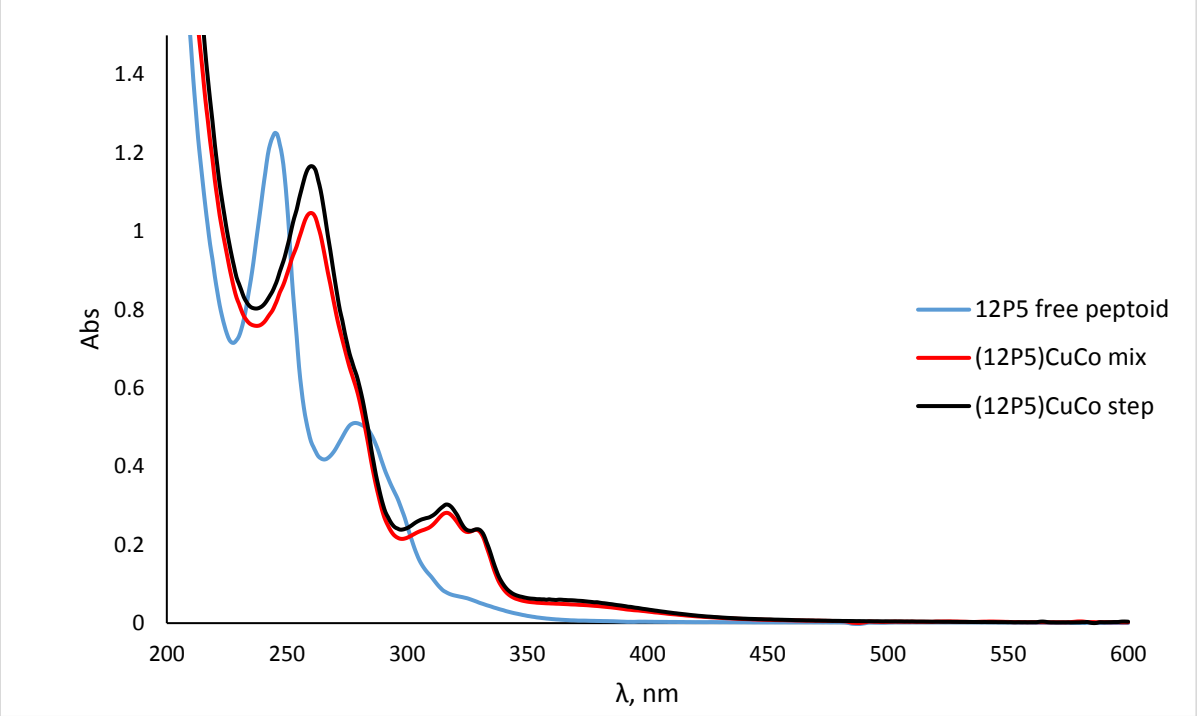


Figure S18. UV-Vis spectra of (**12P5**)CuCo complex obtained by a step approach (addition of 1 equiv. of Cu^{2+} followed by addition of 1 equiv. of Co^{2+}) or by a mix approach (addition of mixture of Cu^{2+} and Co^{2+}).

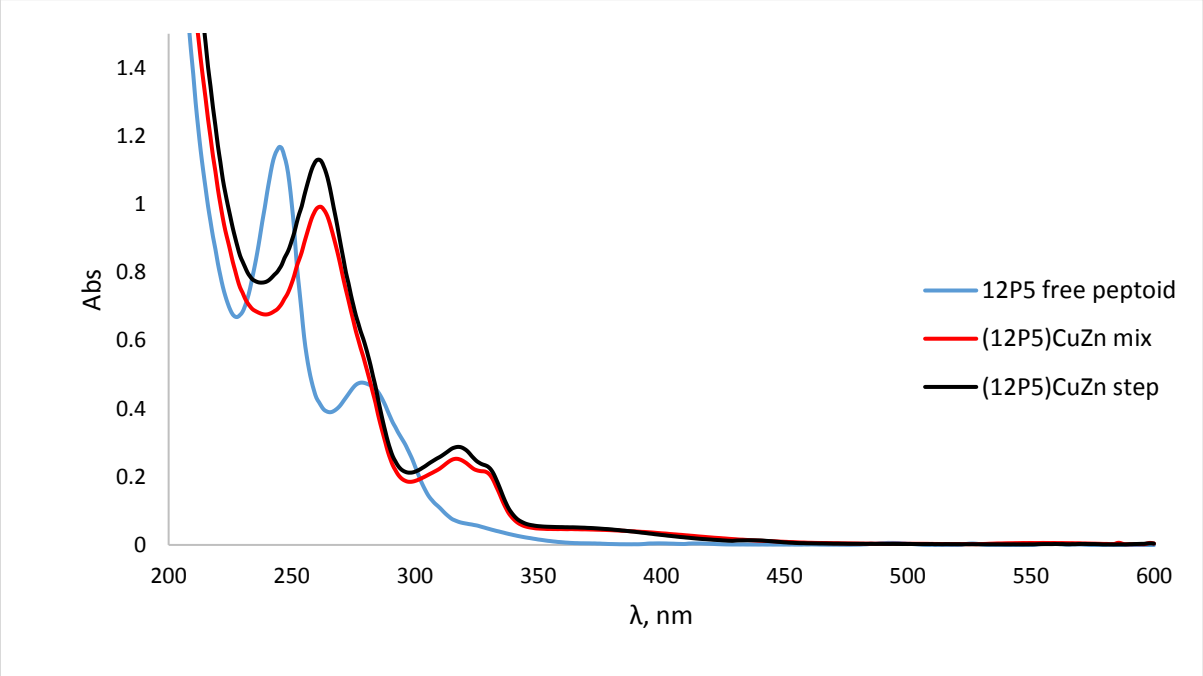


Figure S19. UV-Vis spectra of (**12P5**)CuZn complex obtained by a step approach (addition of 1 equiv. of Cu^{2+} followed by addition of 1 equiv. of Zn^{2+}) or by a mix approach (addition of mixture of Cu^{2+} and Zn^{2+}).

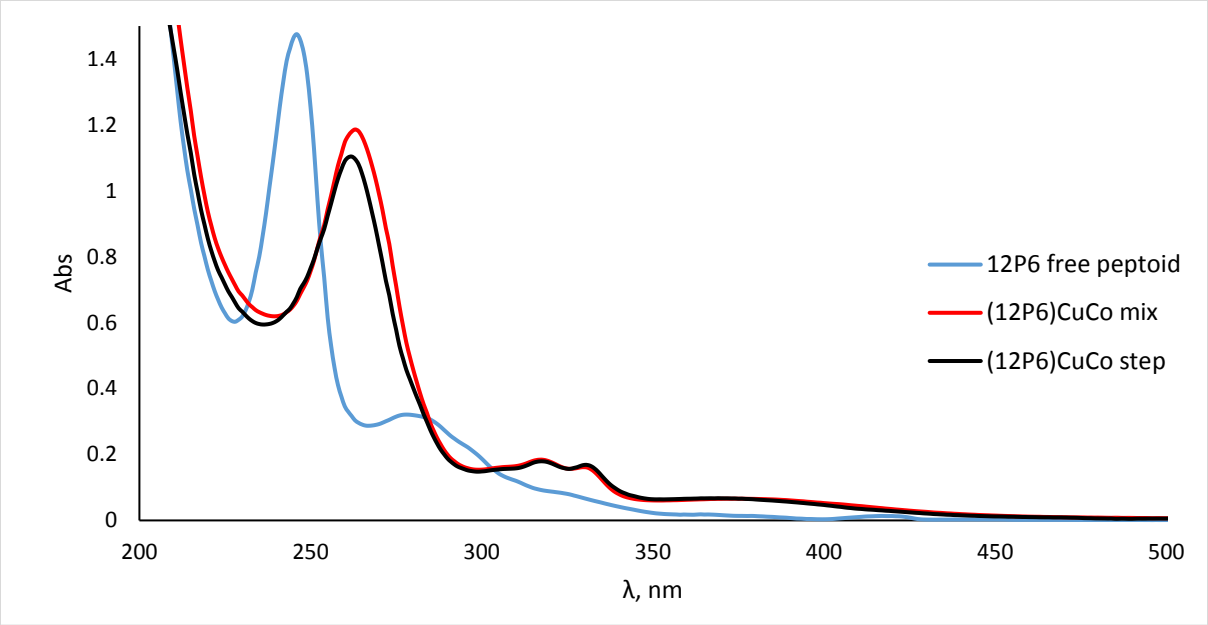


Figure S20. UV-Vis spectra of (**12P6**)CuCo complex obtained by a step approach (addition of 1 equiv. of Cu^{2+} followed by addition of 1 equiv. of Co^{2+}) or by a mix approach (addition of mixture of Cu^{2+} and Co^{2+}).

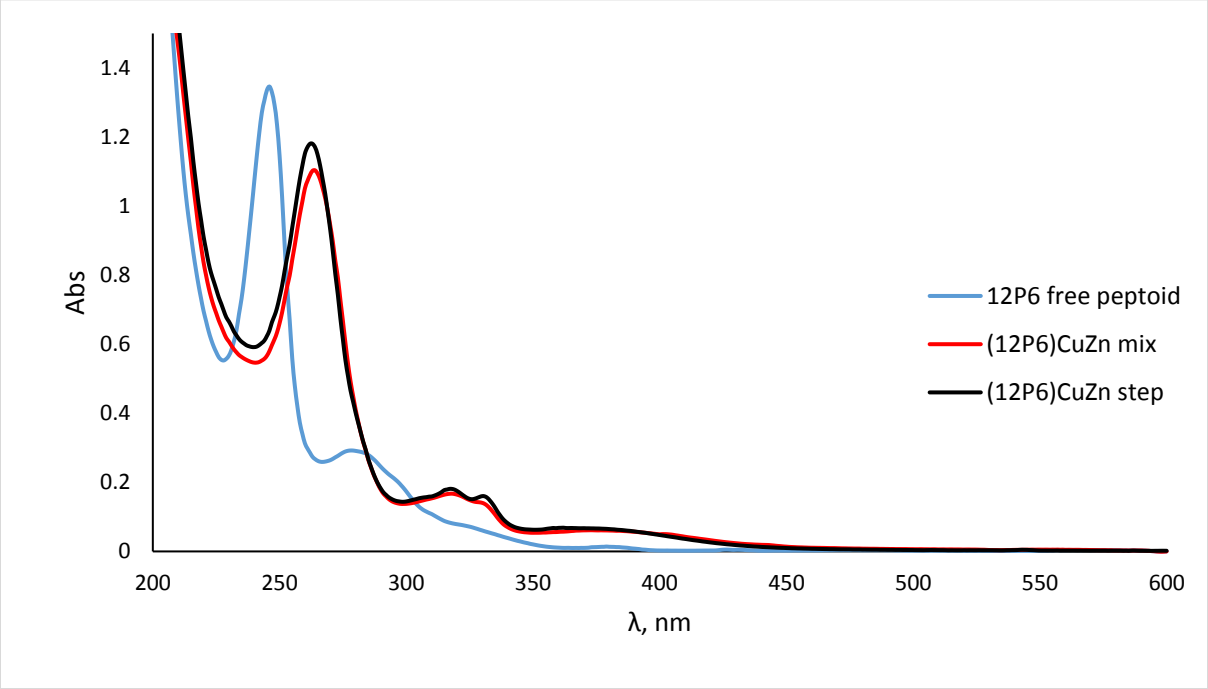


Figure S21. UV-Vis spectra of (**12P6**)CuZn complex obtained by a step approach (addition of 1 equiv. of Cu^{2+} followed by addition of 1 equiv. of Zn^{2+}) or by a mix approach (addition of mixture of Cu^{2+} and Zn^{2+}).

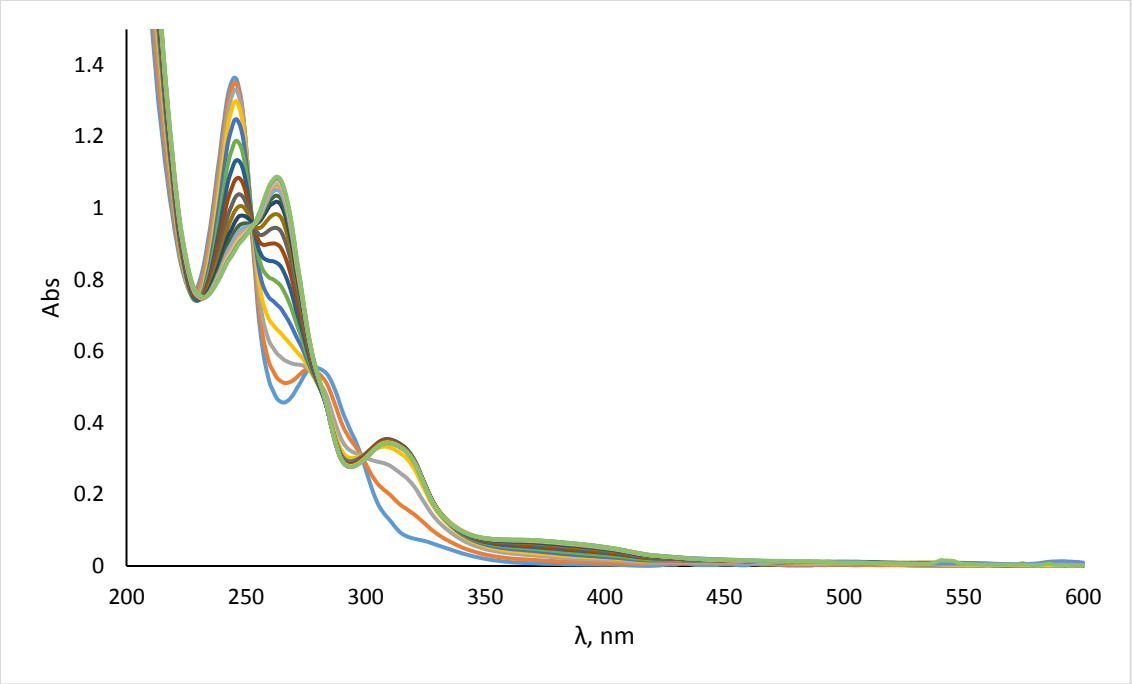


Figure S22. UV-VIS titration of peptoid oligomer **12P5** with Co^{2+} towards the formation of (**12P5**)Co_2 complex. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17µM.

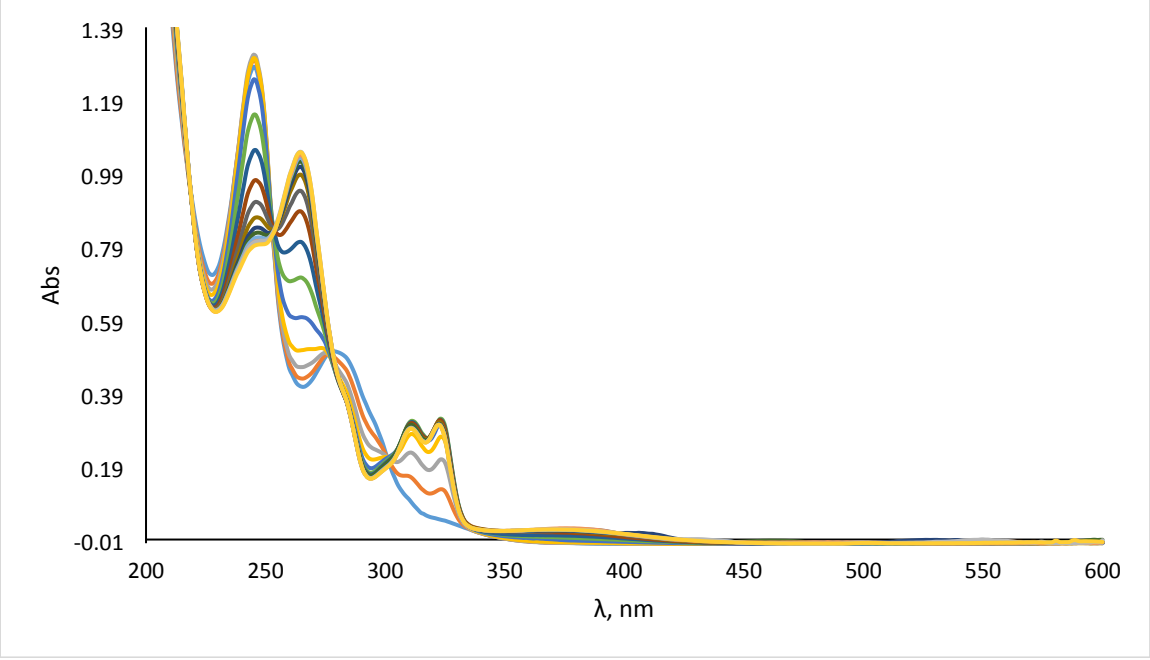


Figure S23. UV-VIS titration of peptoid oligomer **12P5** with Zn^{2+} towards the formation of (**12P5**)Zn_2 complex. The spectra were recorded at room temperature, in a MeOH:H_2O (4:1) solution at initial concentration of 17µM.

CD Data

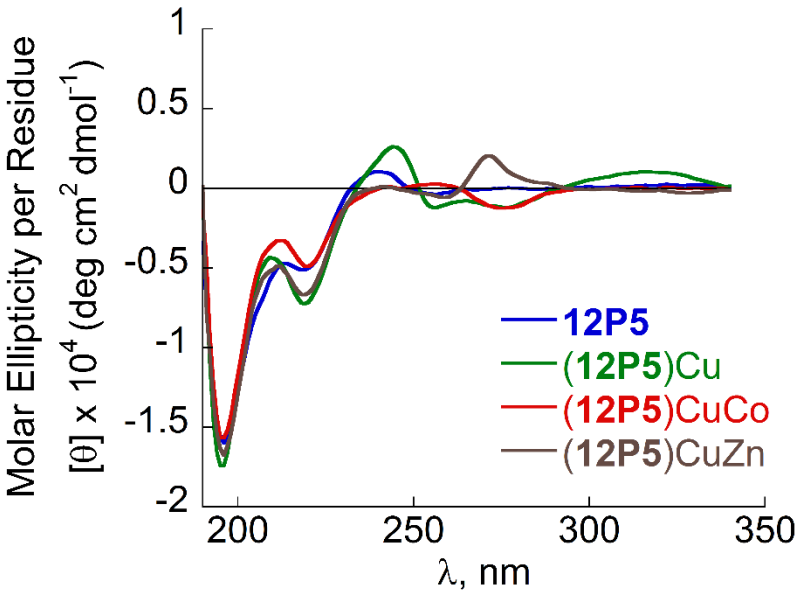


Figure S24. CD spectra of **12P5** and its (**12P5**)CuCo and (**12P5**)CuZn complexes at concentration of 100μM in MeOH/H_2O 4:1.

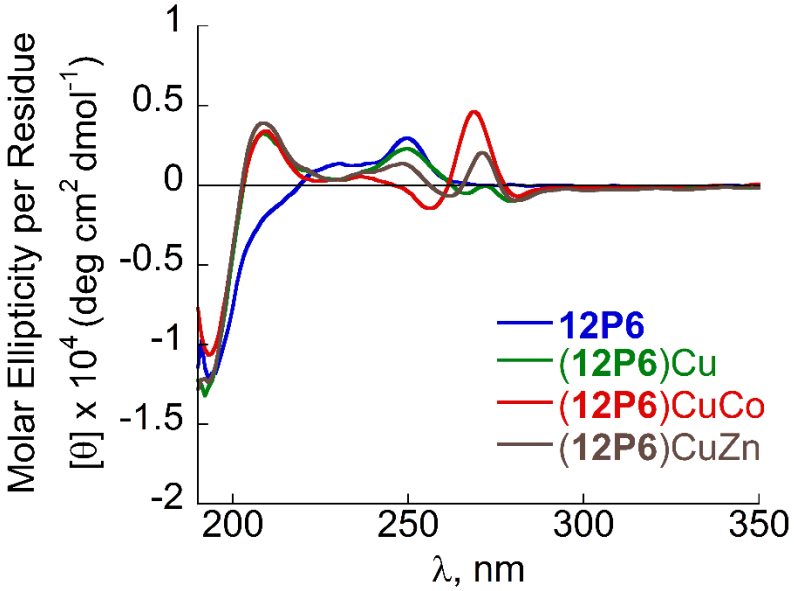


Figure S25. CD spectra of **12P6** and its (**12P6**)CuCo and (**12P6**)CuZn complexes at concentration of 100μM in MeOH/H_2O 4:1.

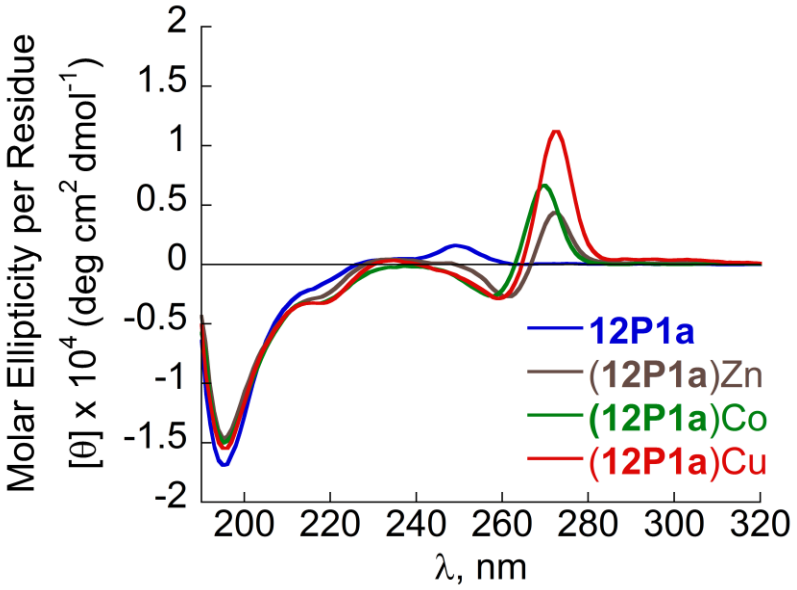


Figure S26. CD spectra of **12P1a** and its metal complexes at concentration of 100μM in MeOH/H_2O 4:1.

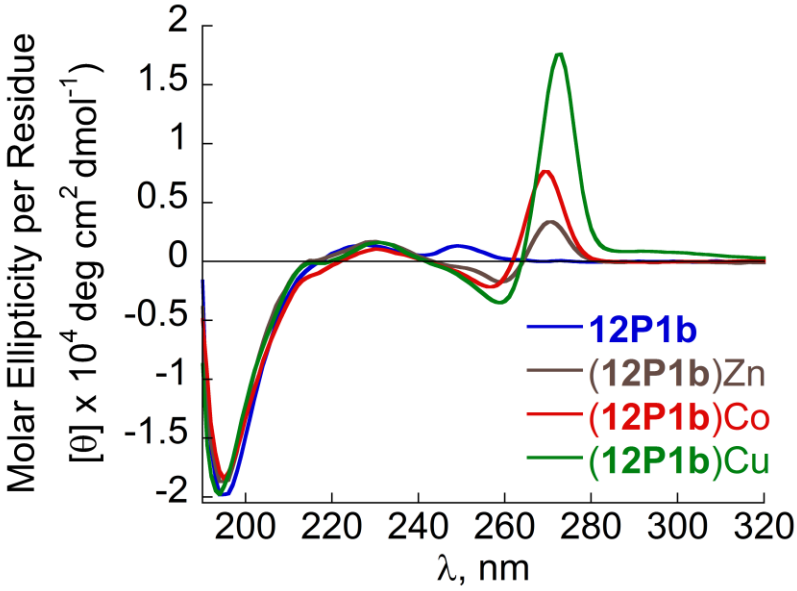


Figure S27. CD spectra of **12P1-b** and its metal complexes at concentration of 100μM in MeOH/H_2O 4:1.

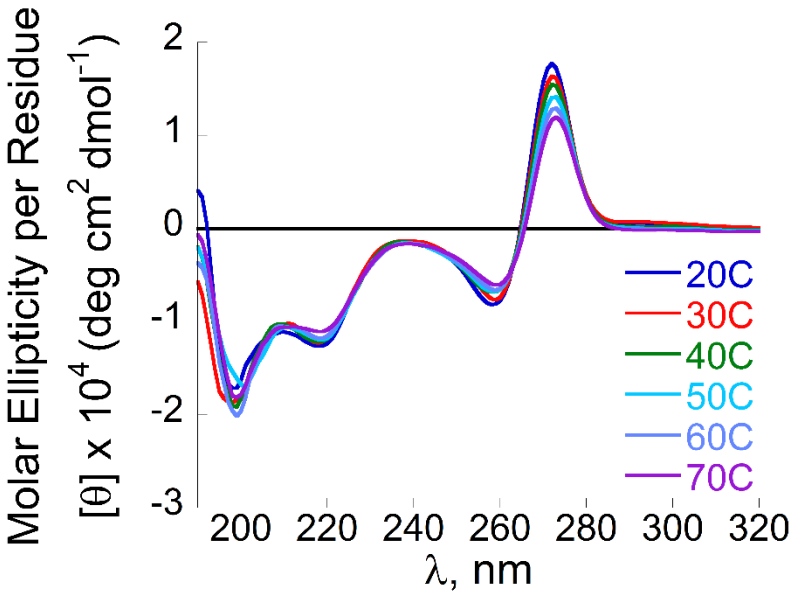


Figure S28. CD spectra of (**12P1**)Cu_2 complex in different temperatures at concentration of 100μM in MeOH/H_2O 4:1.

ESI-MS data of peptoids

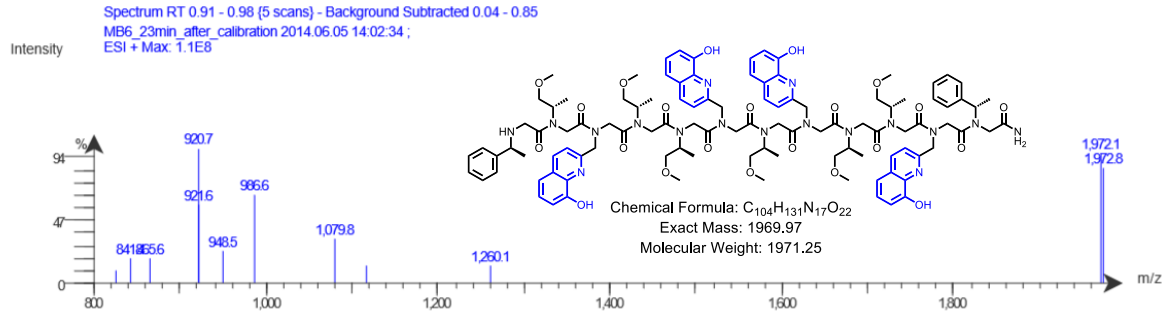


Figure S29. ESI-MS traces of peptoid oligomer **12P1**.

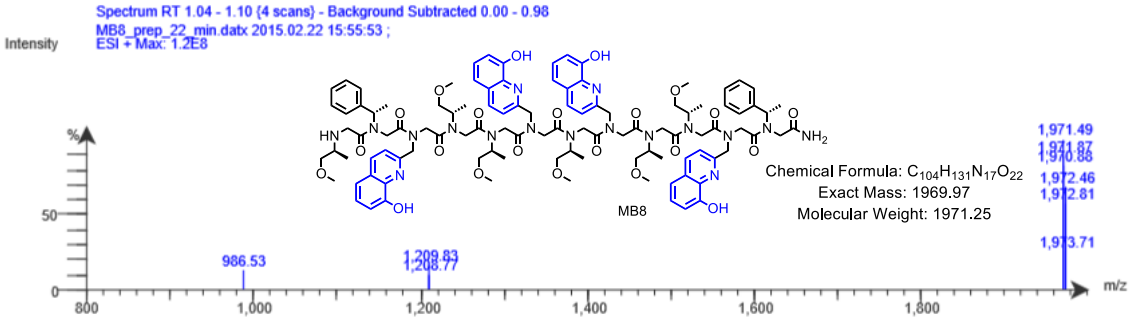


Figure S30. ESI-MS traces of peptoid oligomer **12P2**.

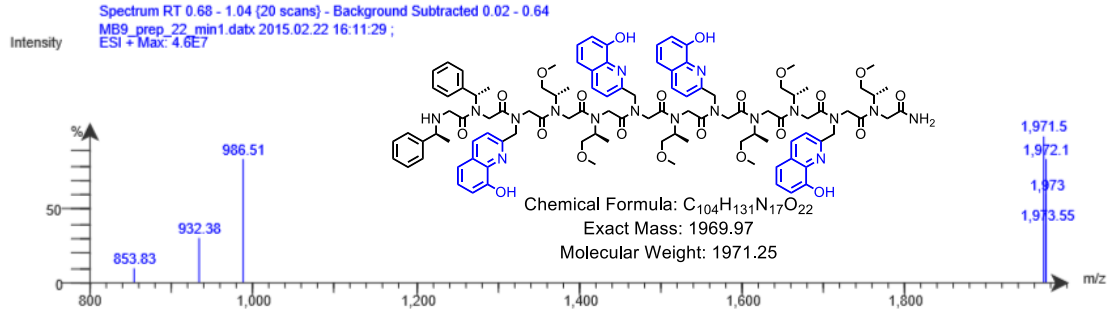


Figure S31. ESI-MS traces of peptoid oligomer **12P3**.

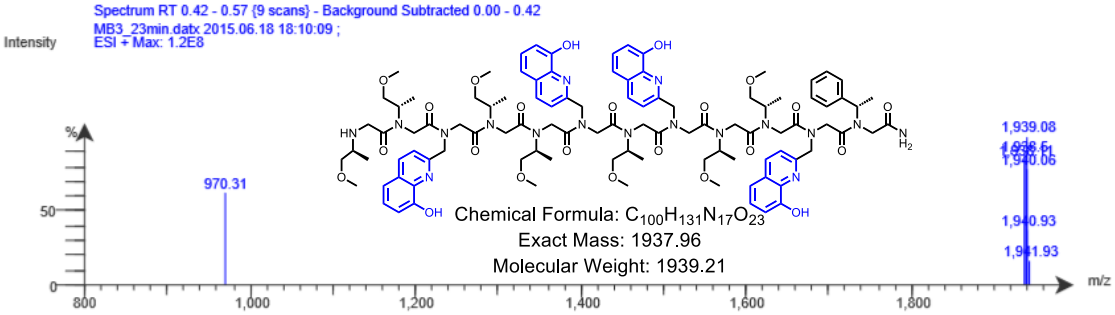


Figure S32. ESI-MS traces of peptoid oligomer **12P4**.

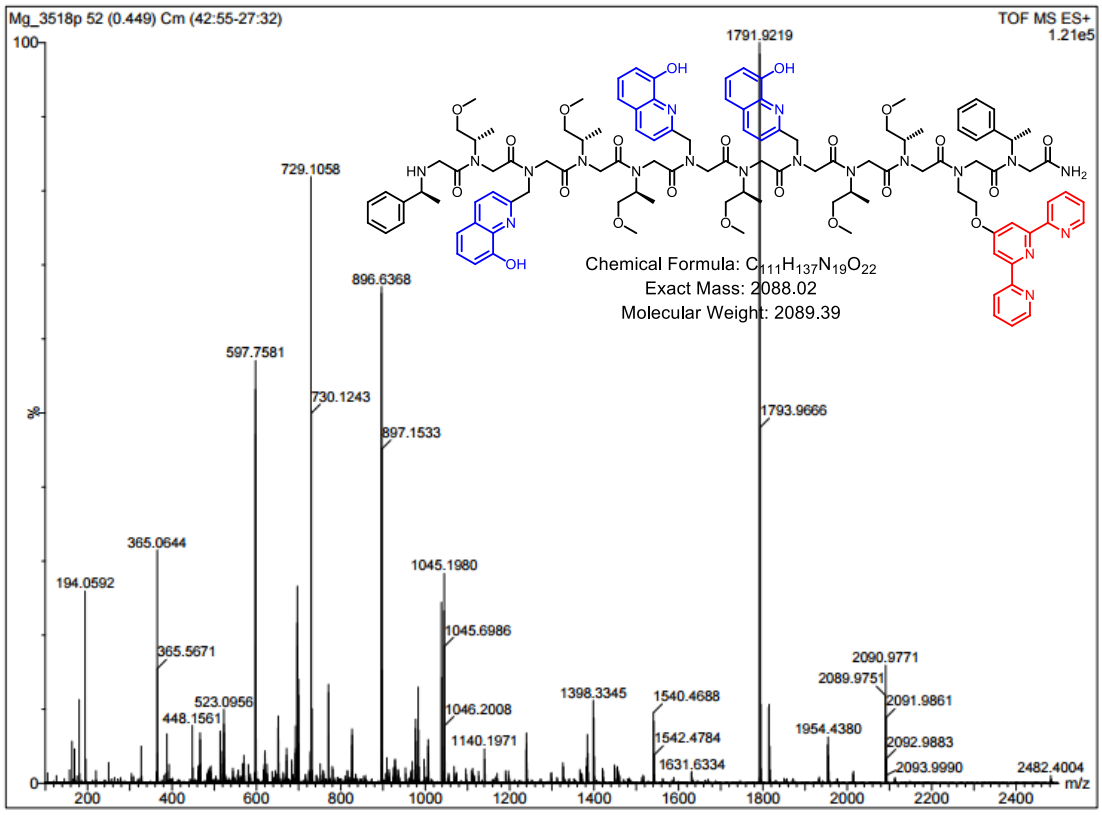


Figure S33. ESI-MS traces of peptoid oligomer **12P5**.

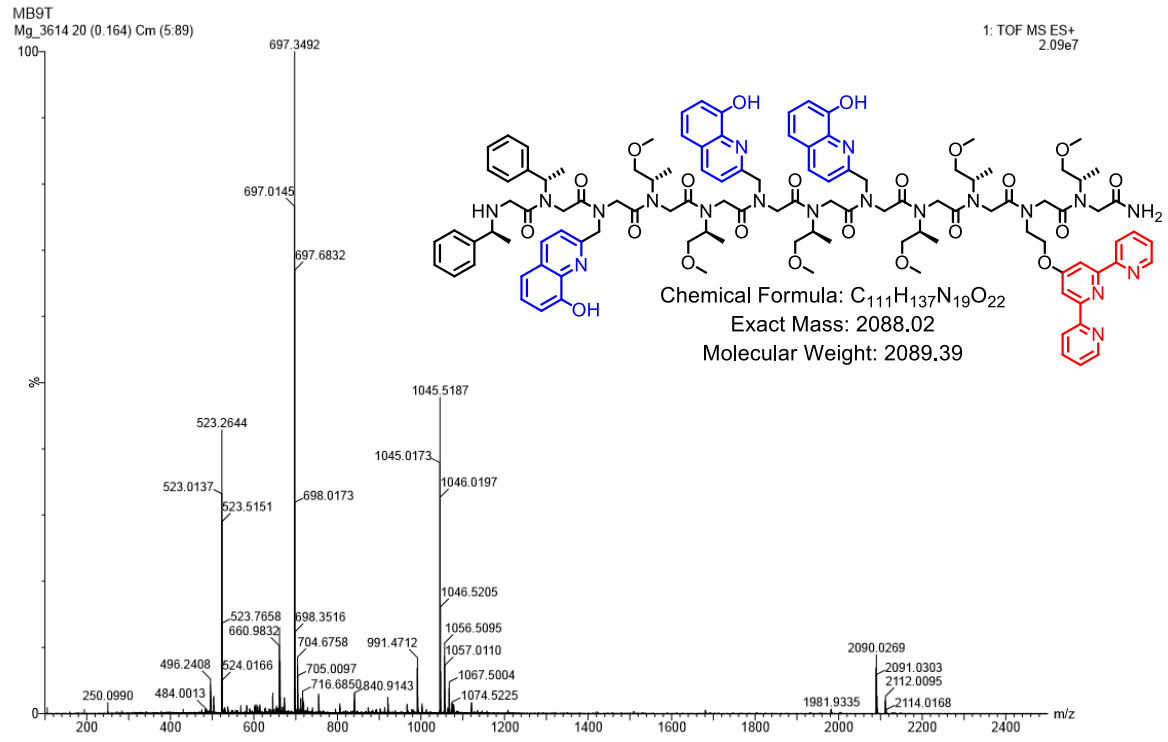


Figure S34. ESI-MS traces of peptoid oligomer **12P6**.

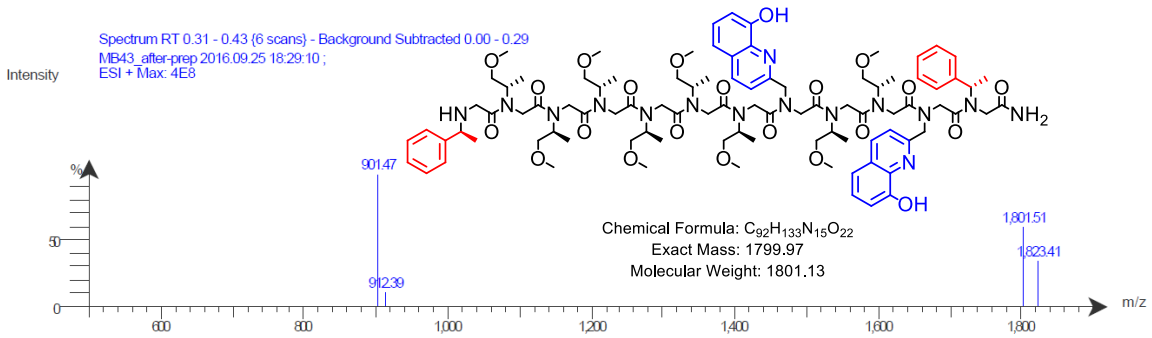


Figure S35. ESI-MS traces of peptoid oligomer **12P1a**.

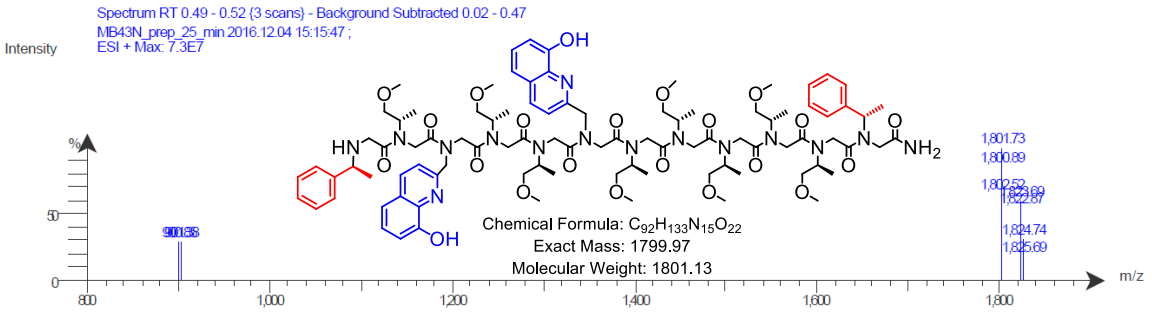


Figure S36. ESI-MS traces of peptoid oligomer **12P1b**.

ESI-MS data of peptoids-metal complexes

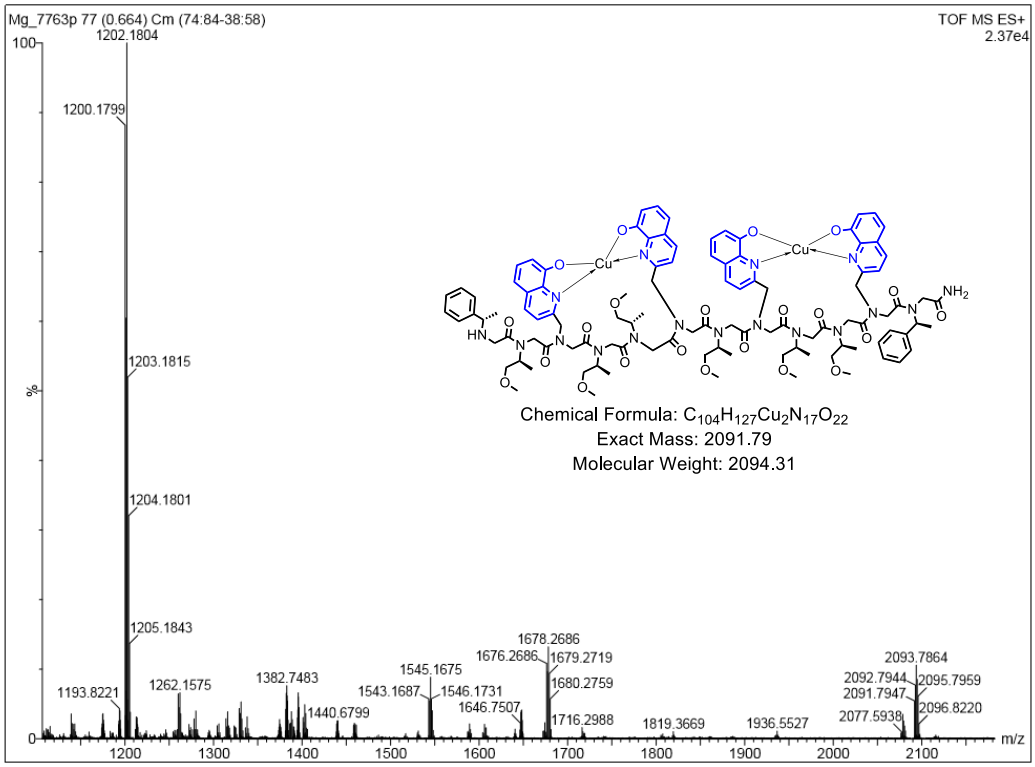


Figure S37. ESI-MS traces of peptoid oligomer (**12P1**)Cu_2 complex.

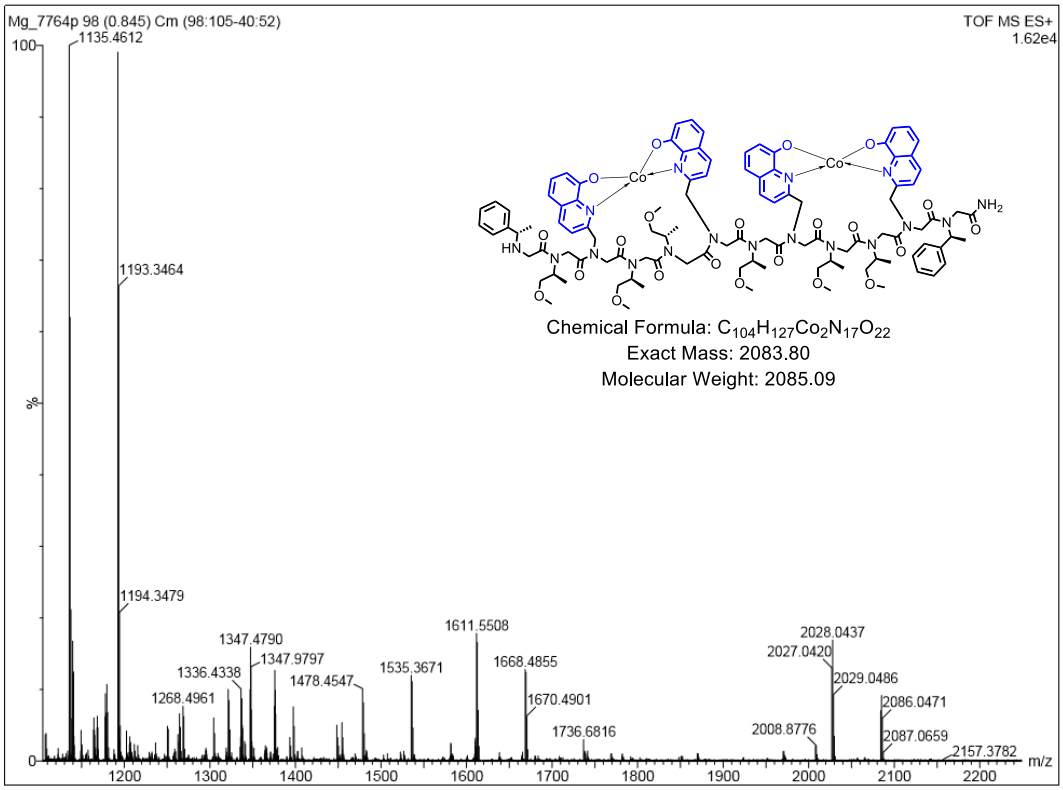


Figure S38. ESI-MS traces of peptoid oligomer (**12P1**)Co_2 complex.

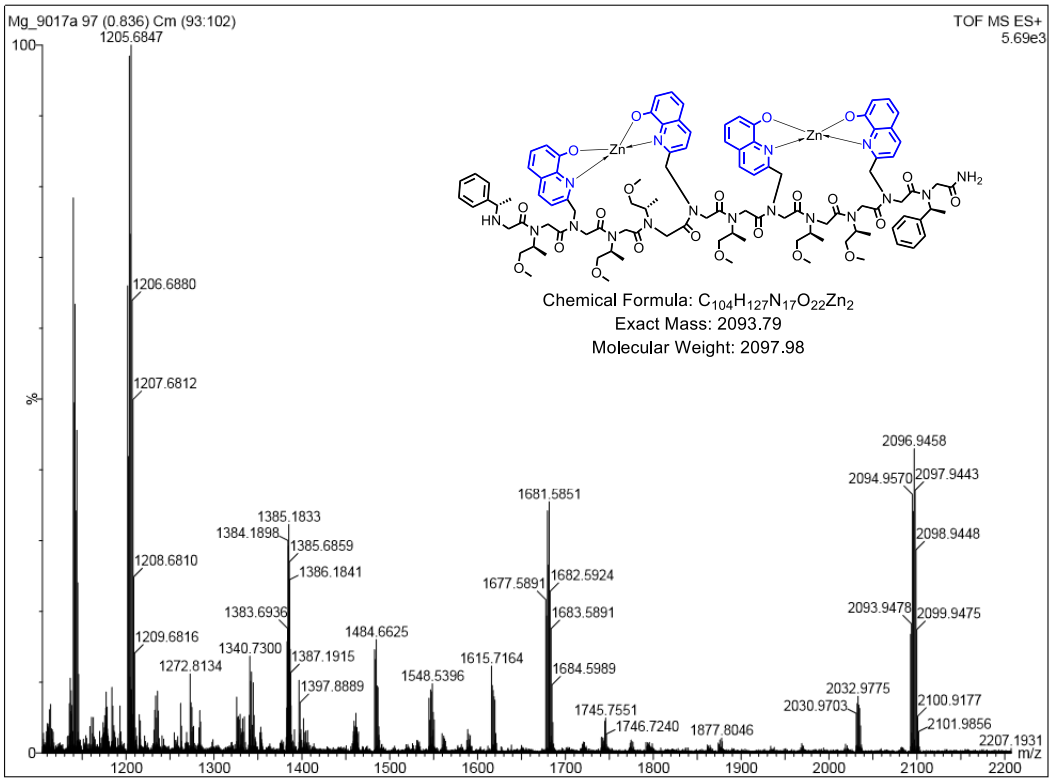


Figure S39. ESI-MS traces of peptoid oligomer (**12P1**)Zn_2 complex.

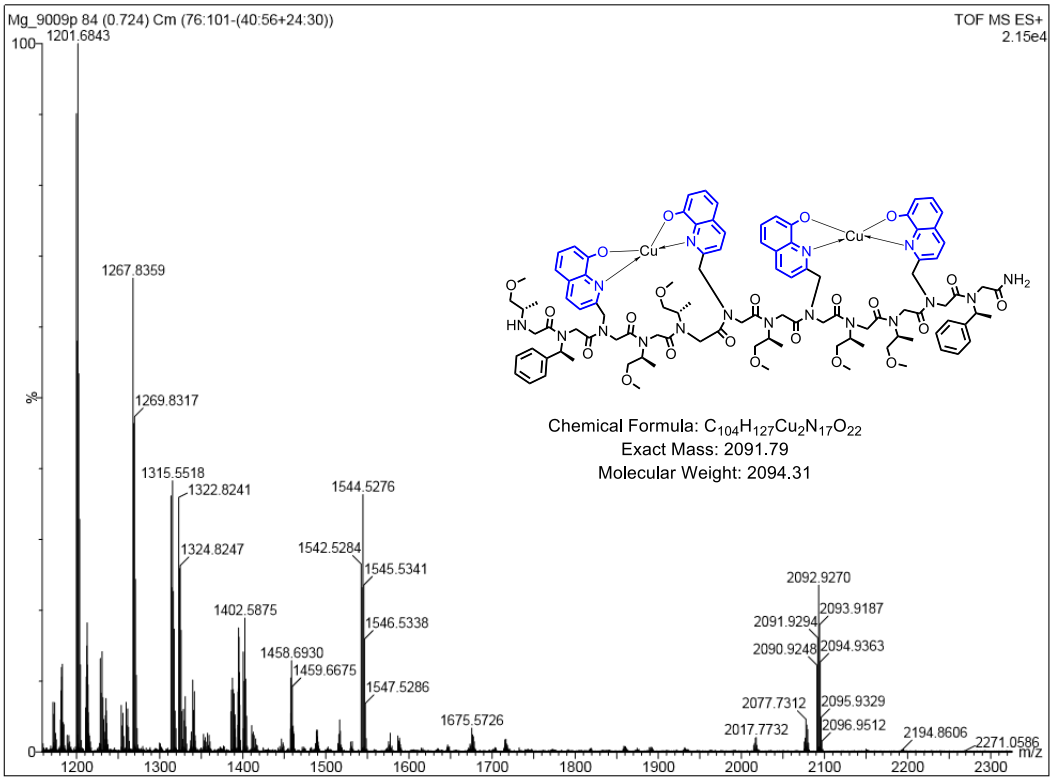


Figure S40. ESI-MS traces of peptoid oligomer (**12P2**)Cu_2 complex.

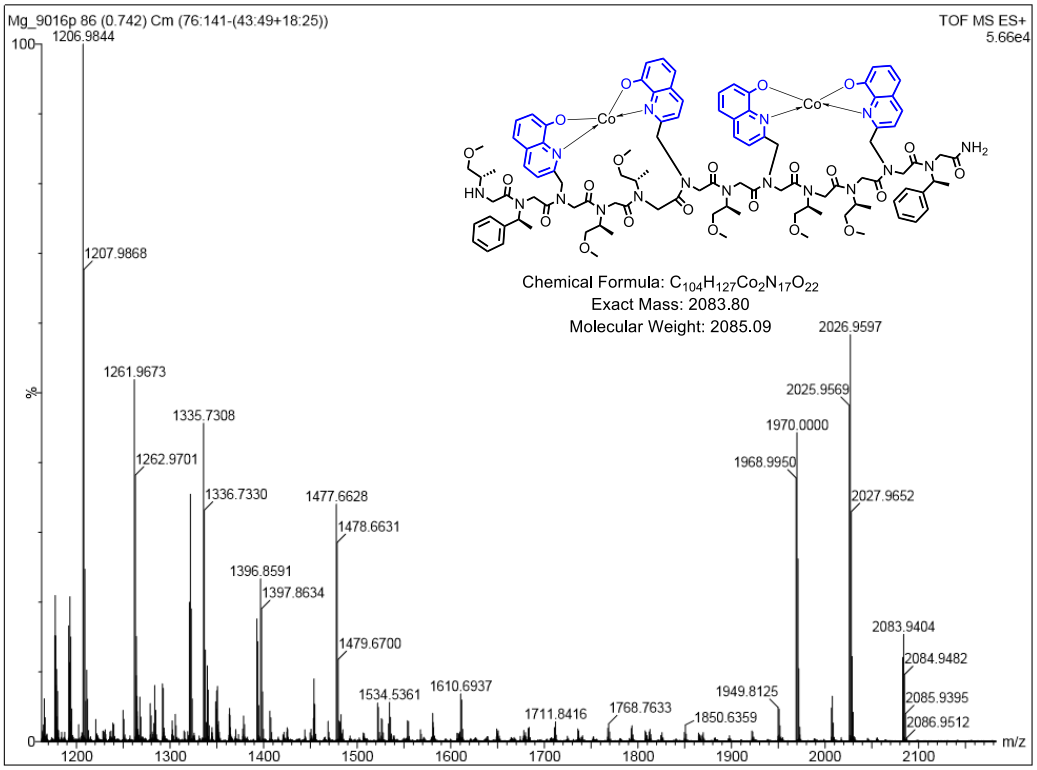


Figure S41. ESI-MS traces of peptoid oligomer (**12P2**)Co_2 complex.

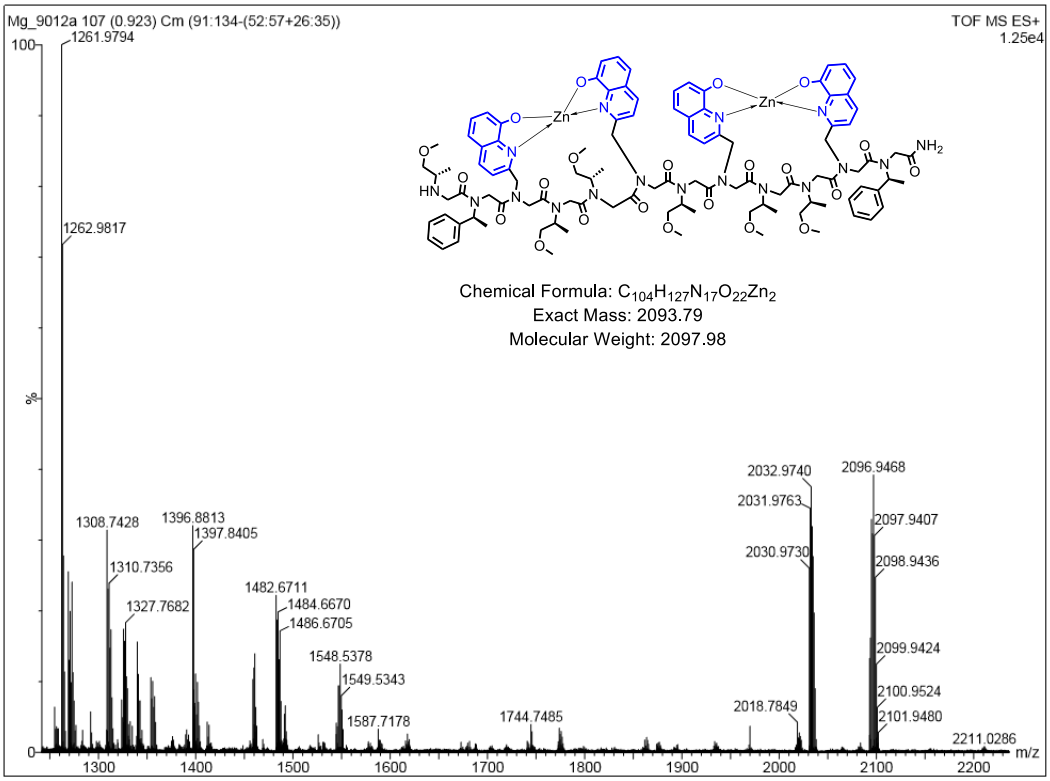


Figure S42. ESI-MS traces of peptoid oligomer (**12P2**)Zn_2 complex.

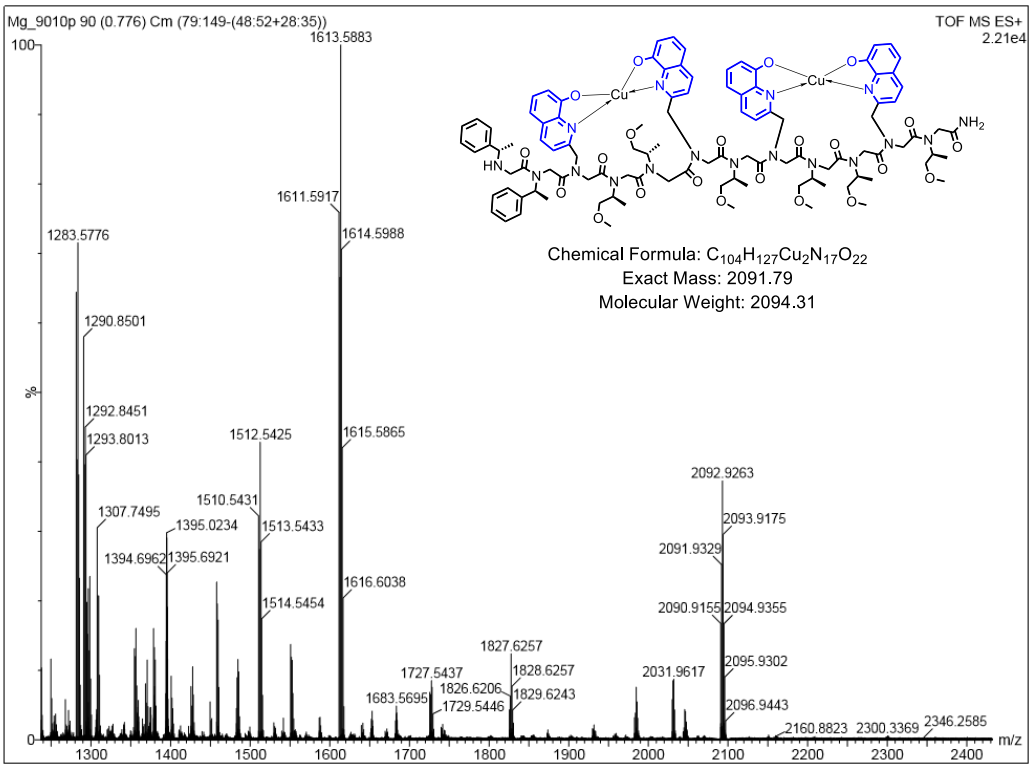


Figure S43. ESI-MS traces of peptoid oligomer (**12P3**)Cu_2 complex.

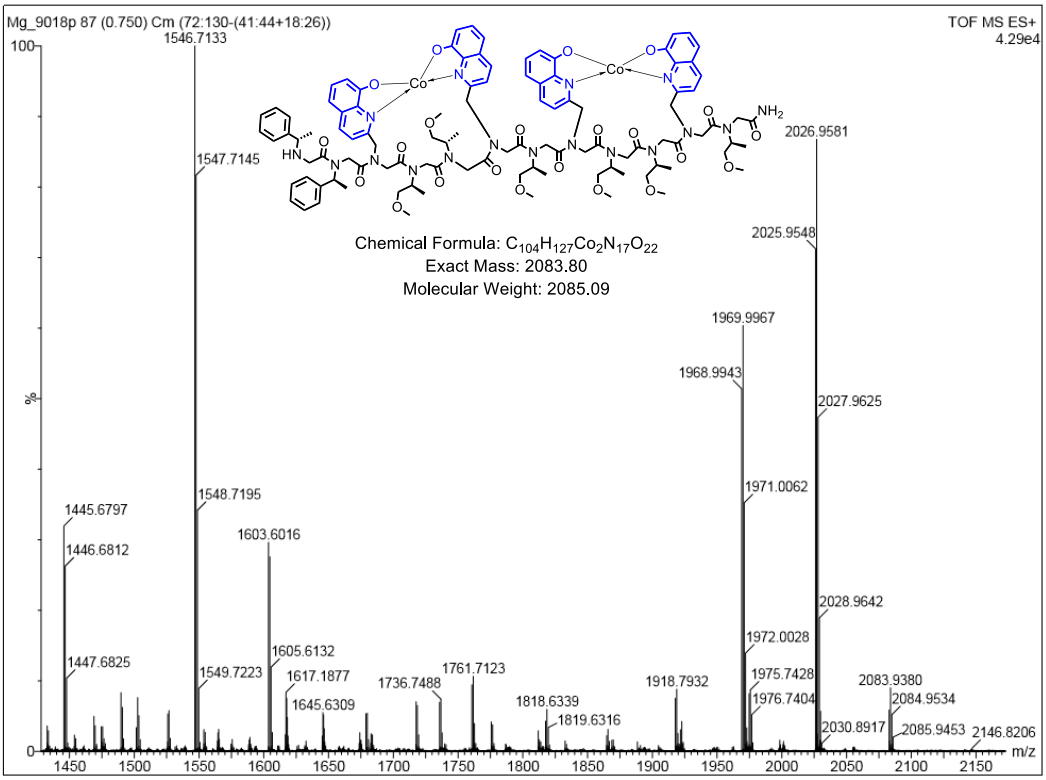


Figure S44. ESI-MS traces of peptoid oligomer (**12P3**)Co_2 complex.

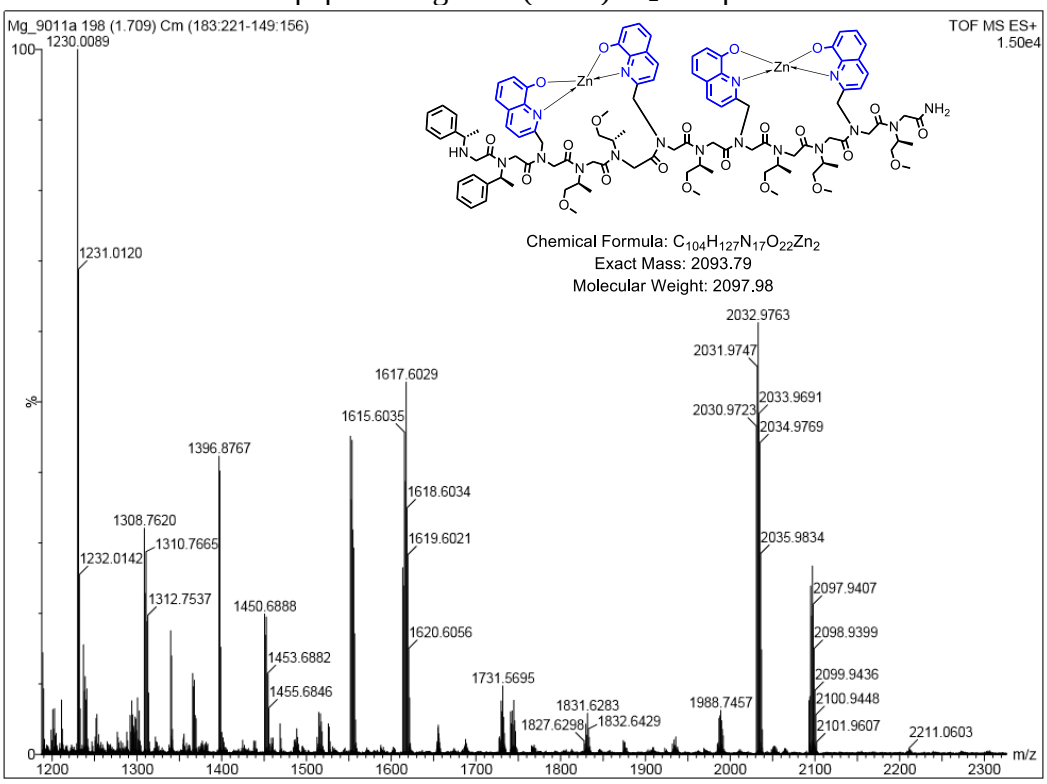


Figure S45. ESI-MS traces of peptoid oligomer (**12P3**)Zn_2 complex.

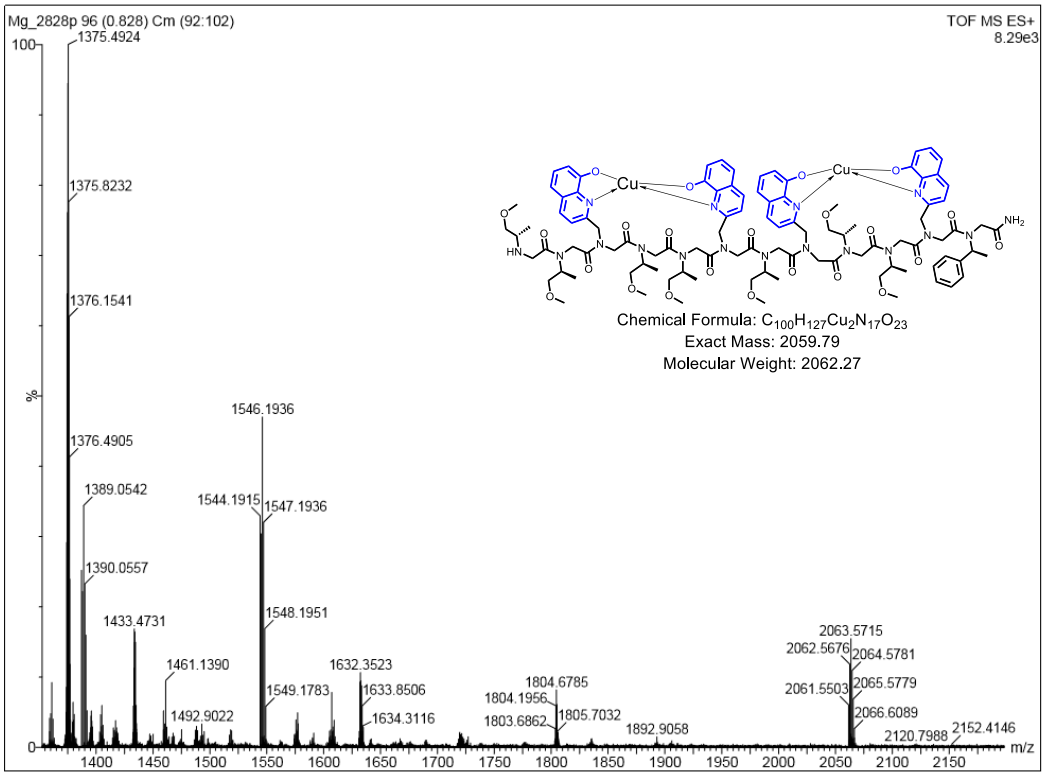


Figure S46. ESI-MS traces of peptoid oligomer (**12P4**)Cu_2 complex.

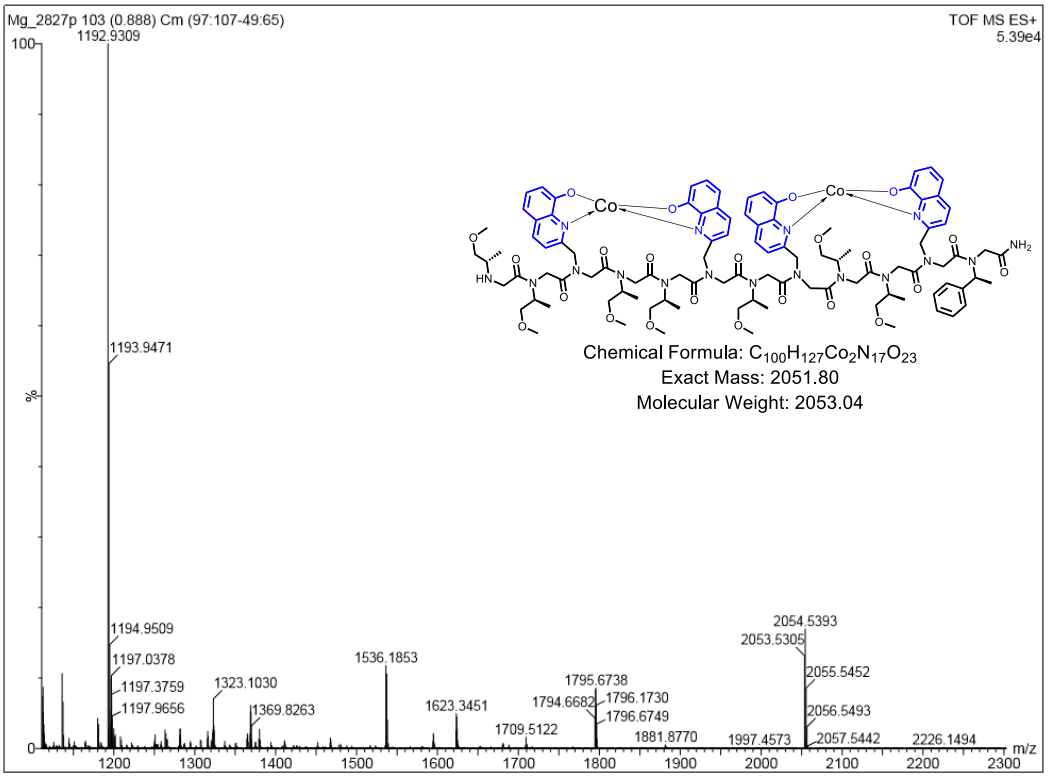


Figure S47. ESI-MS traces of peptoid oligomer (**12P4**)Co_2 complex.

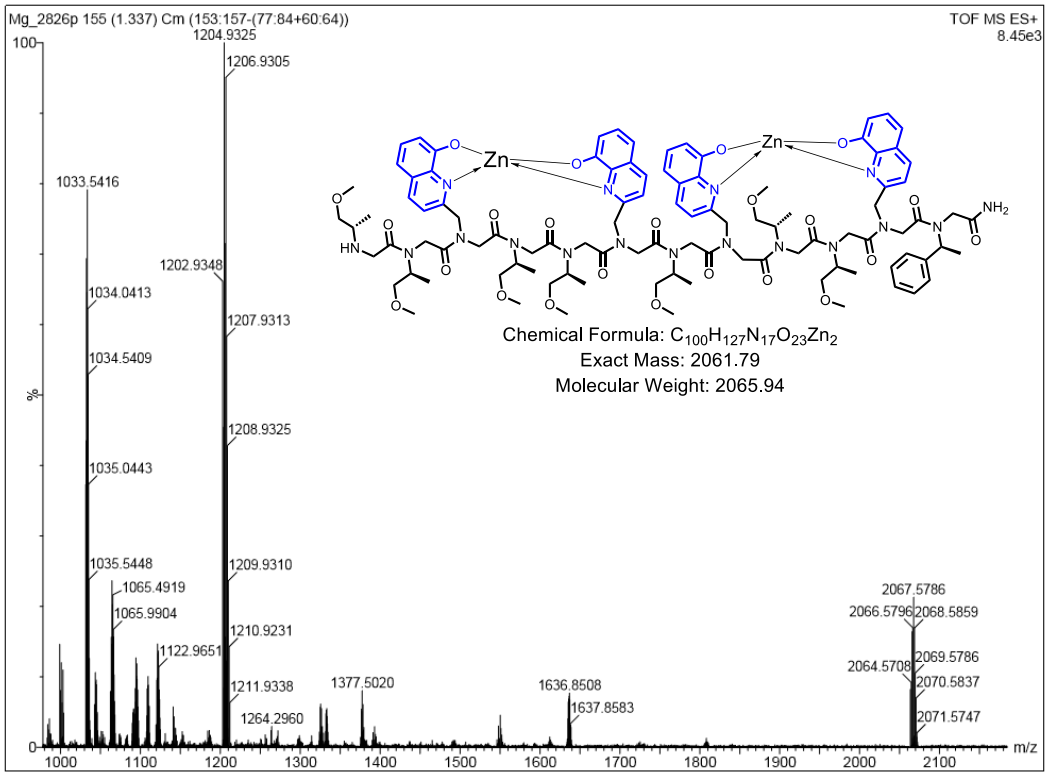


Figure S48. ESI-MS traces of peptoid oligomer (**12P4**)Zn_2 complex.

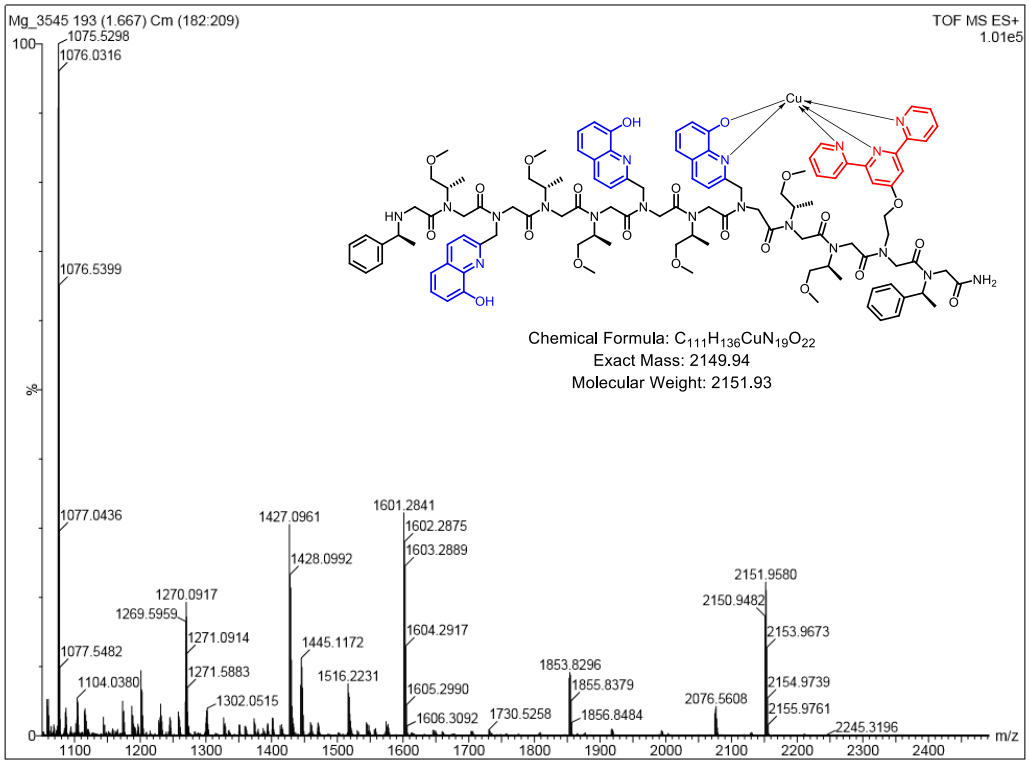


Figure S49. ESI-MS traces of peptoid oligomer (**12P5**)Cu complex.

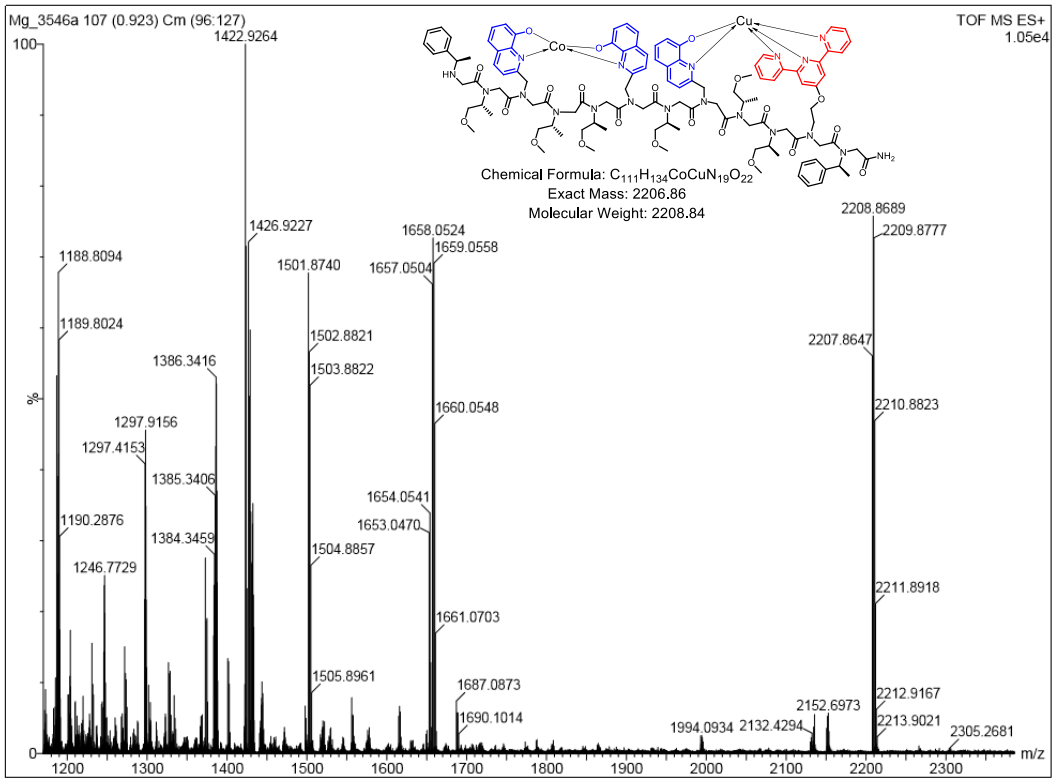


Figure S50. ESI-MS traces of peptoid oligomer (**12P5**)CuCo complex.

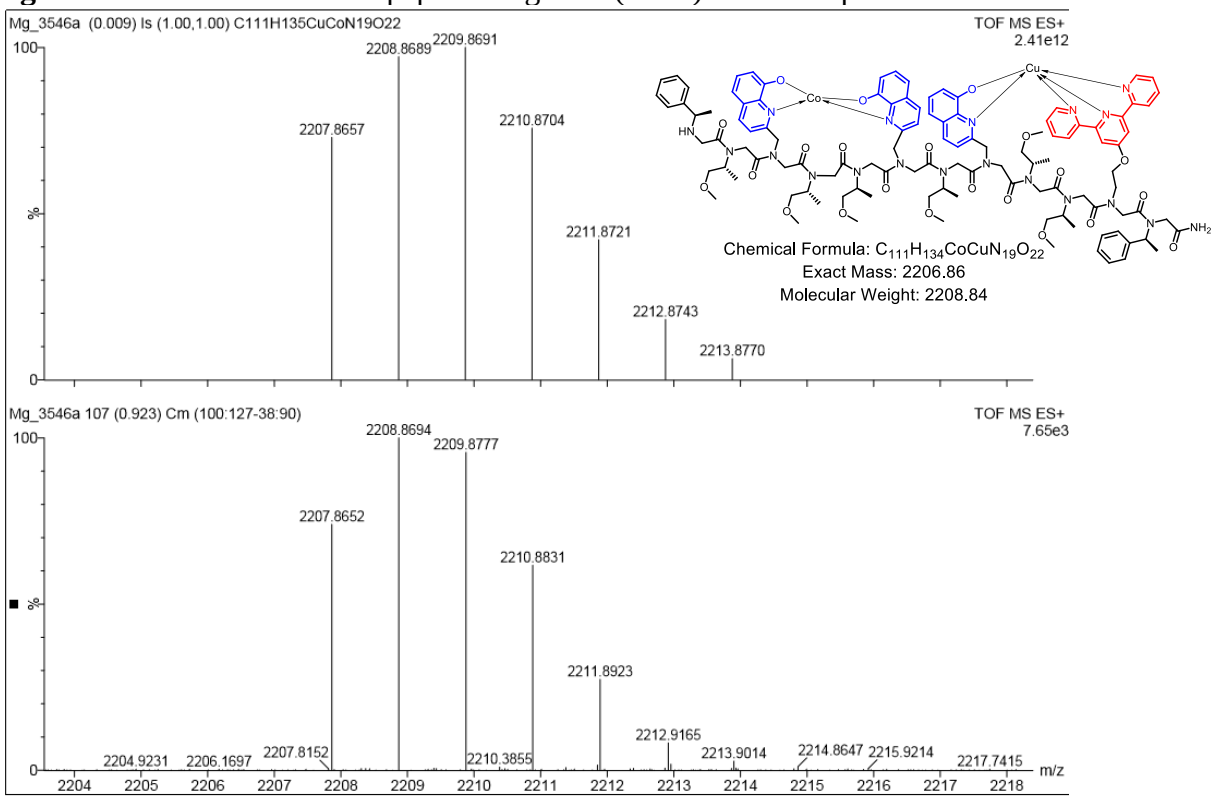


Figure S51. Experimental isotopic analysis by ESI-MS of (**12P5**)CuCo complex (bottom) and calculated ESI-MS spectrum (top).

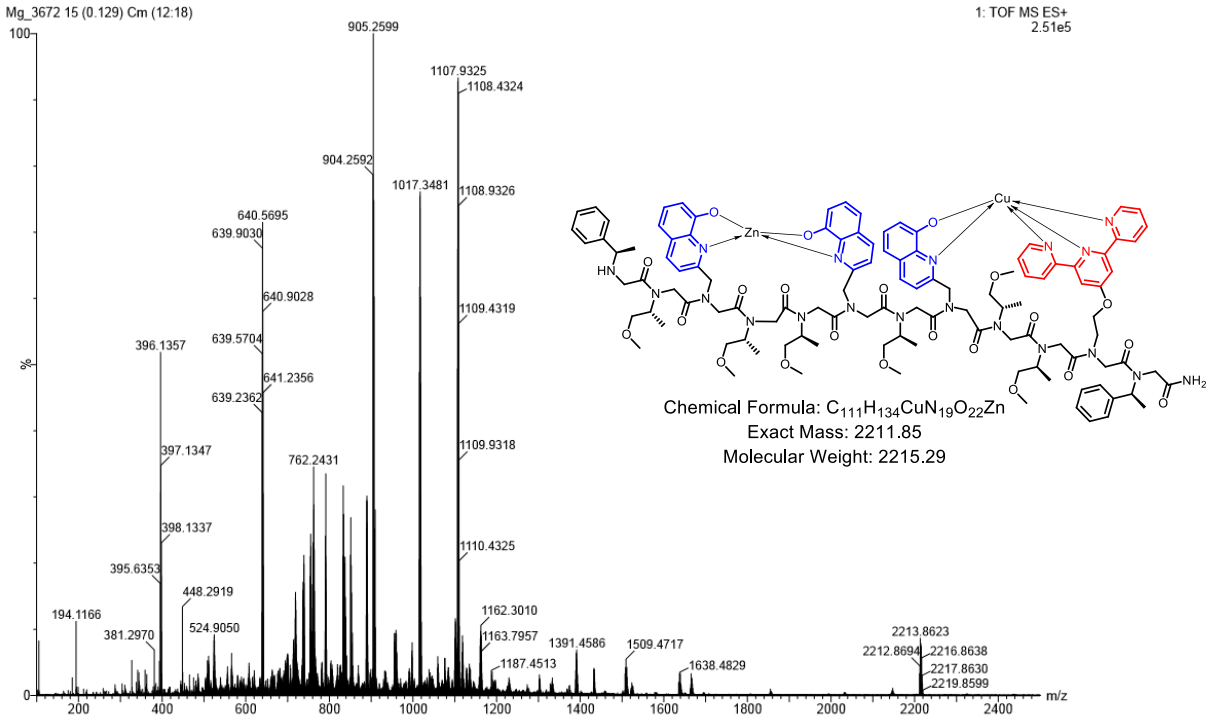


Figure S52. ESI-MS traces of peptoid oligomer (**12P5**)CuZn complex.

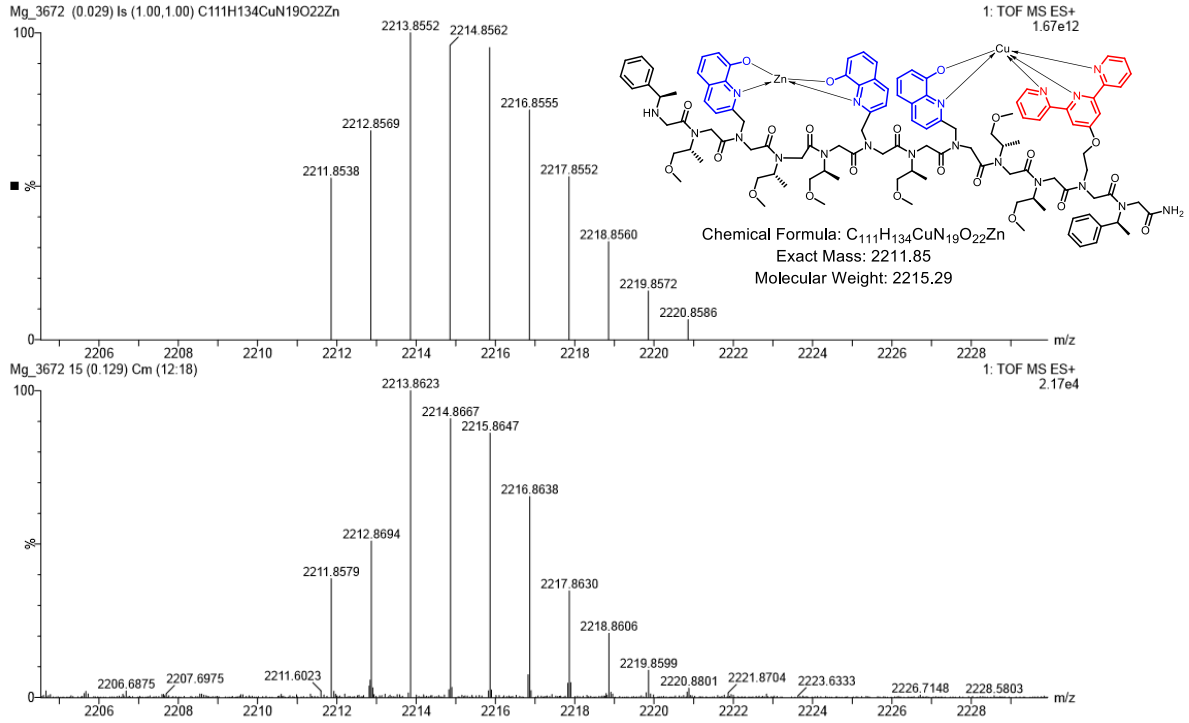


Figure S53. Experimental isotopic analysis by ESI-MS of (**12P5**)CuZn complex (bottom) and calculated ESI-MS spectrum (top).

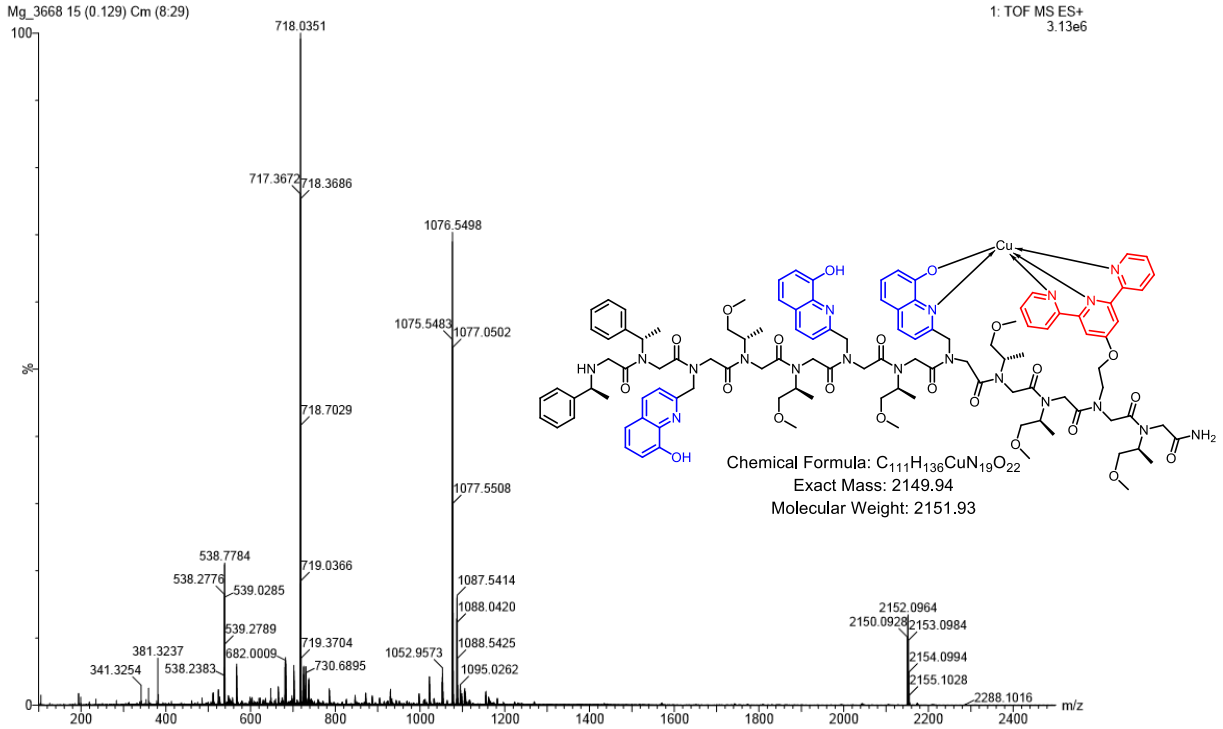


Figure S54. ESI-MS traces of peptoid oligomer (**12P6**)Cu complex.

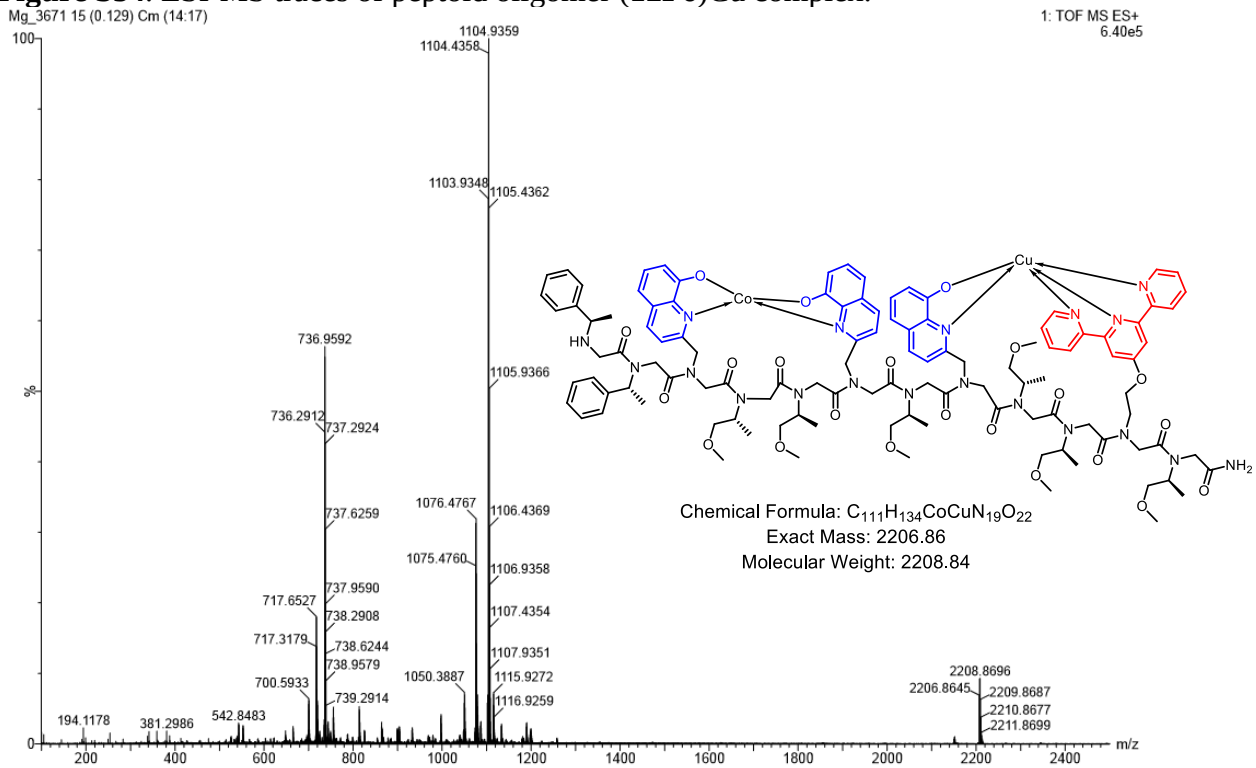


Figure S55. ESI-MS traces of peptoid oligomer (**12P6**)CuCo complex.

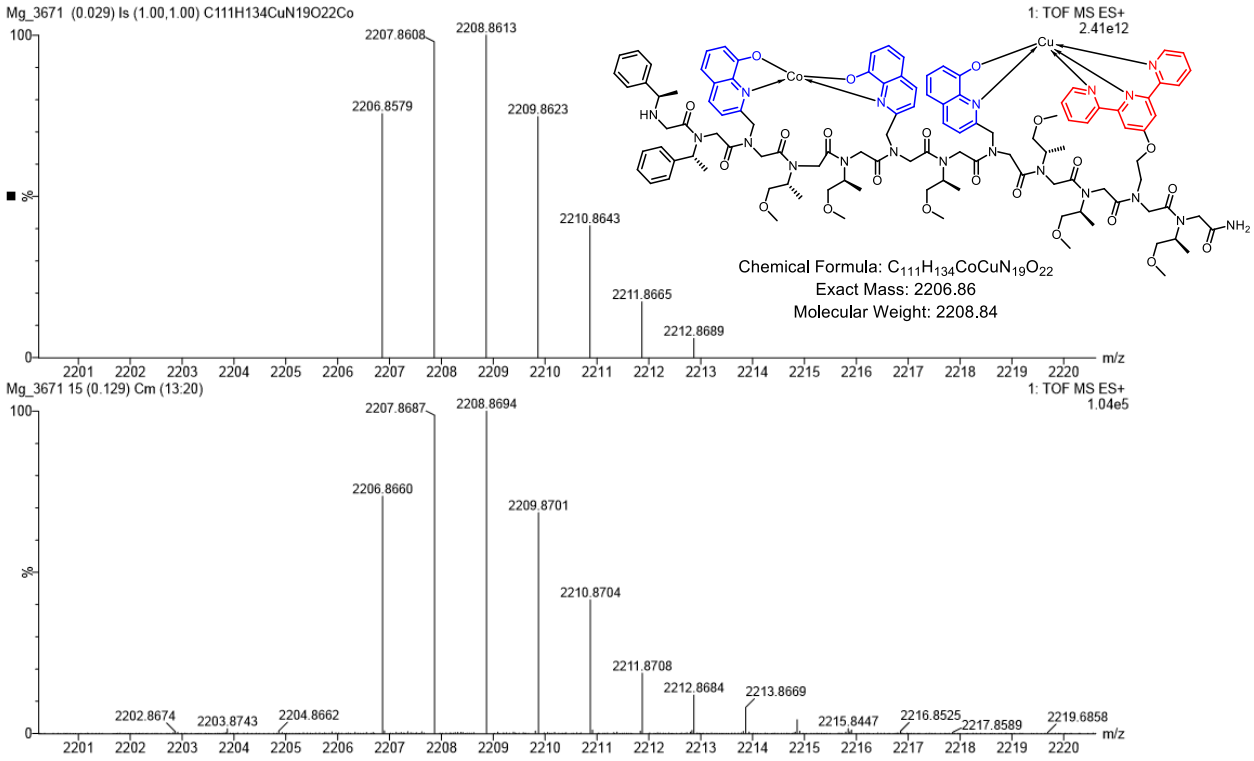


Figure S56. Experimental isotopic analysis by ESI-MS of (**12P6**)CuCo complex (bottom) and calculated ESI-MS spectrum (top).

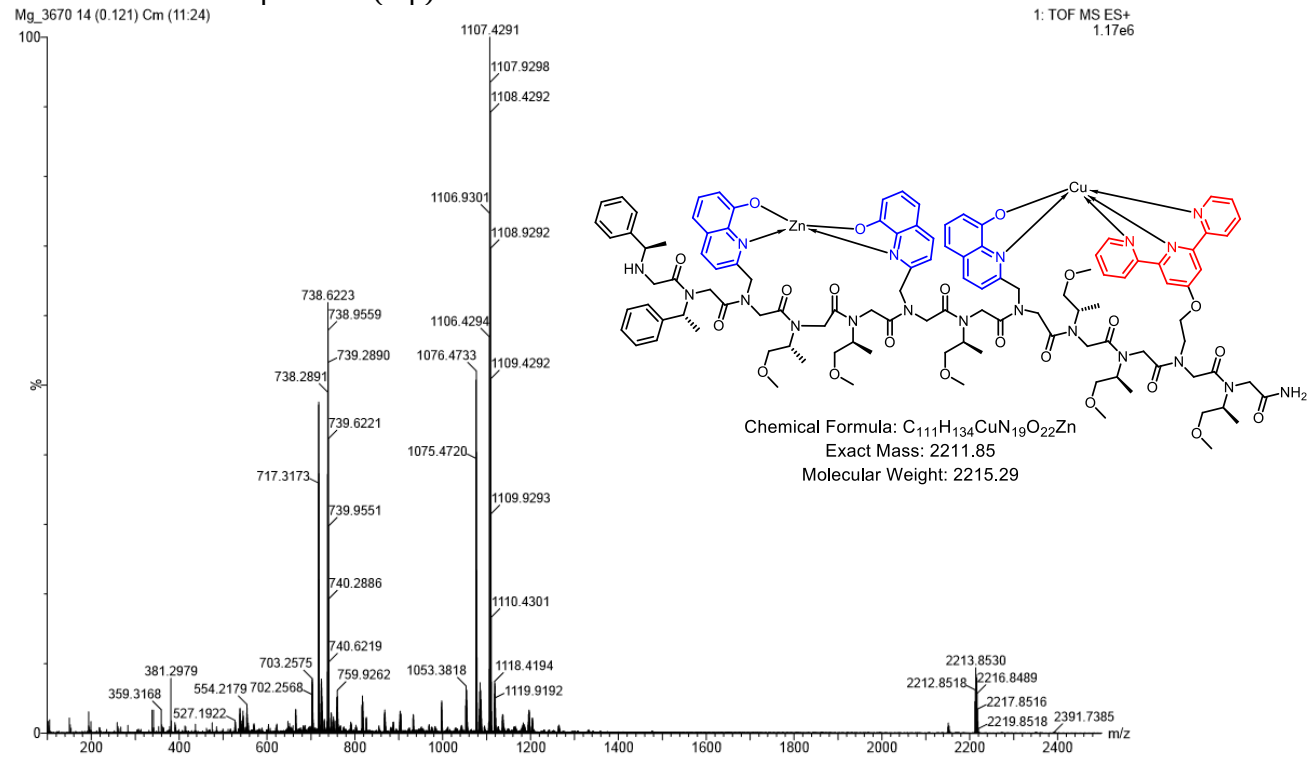


Figure S57. ESI-MS traces of peptoid oligomer (**12P6**)CuZn complex.

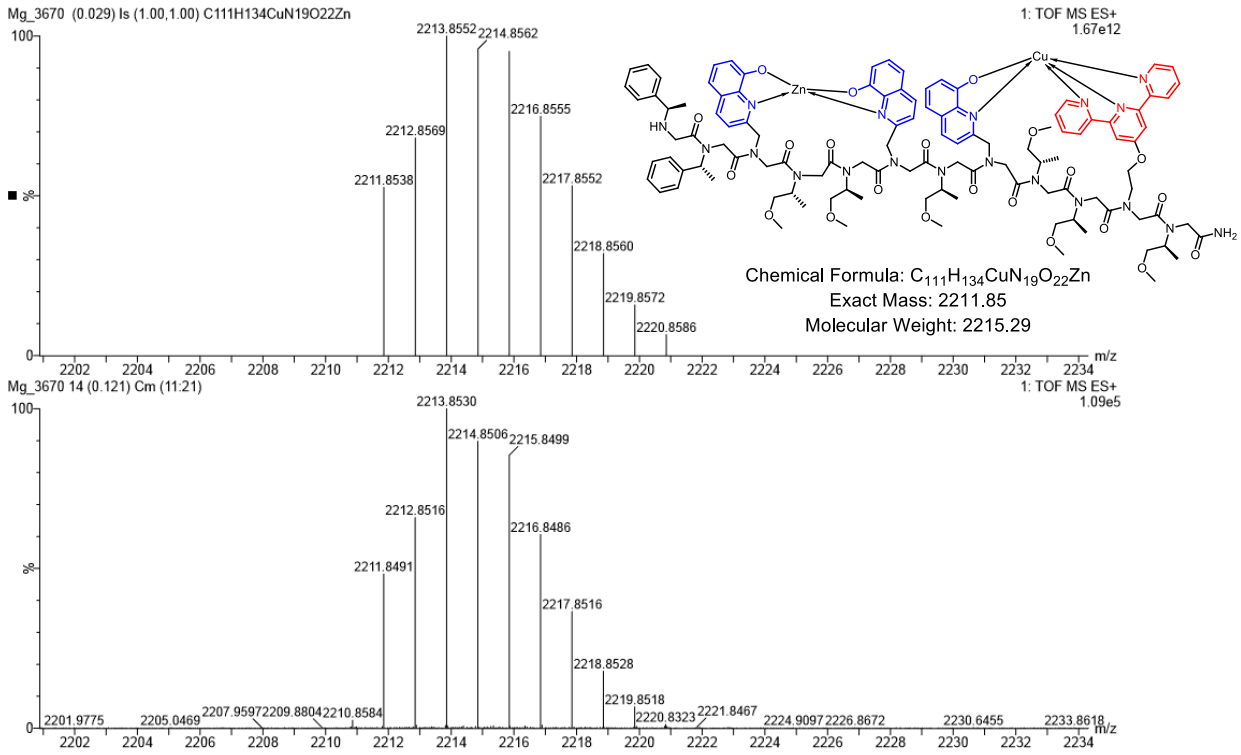


Figure S58. Experimental isotopic analysis by ESI-MS of (**12P6**)CuZn complex (bottom) and calculated ESI-MS spectrum (top).

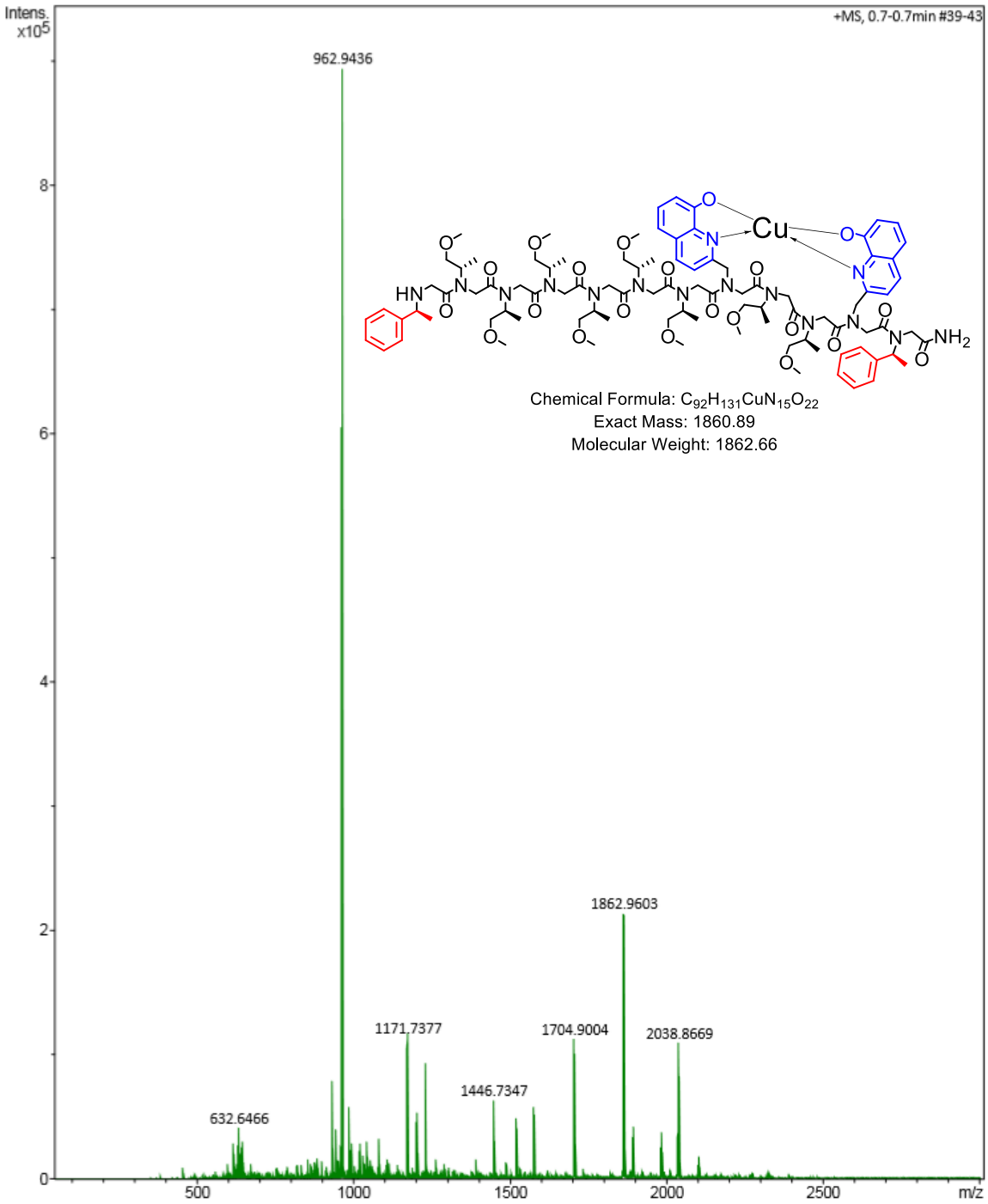


Figure S59. ESI-MS traces of peptoid oligomer (**12P1a**)Cu complex.

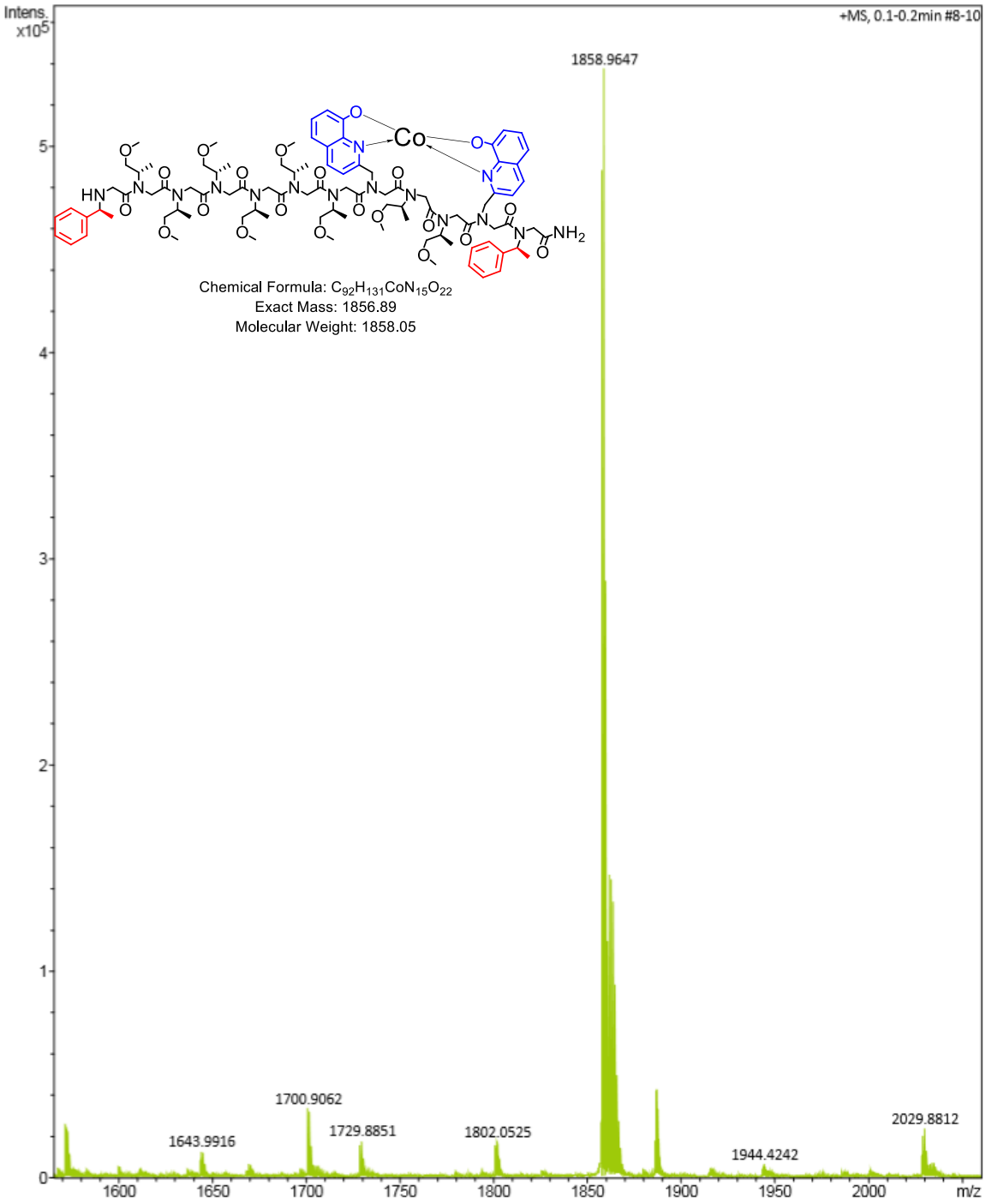


Figure S60. ESI-MS traces of peptoid oligomer (**12P1a**)Co complex.

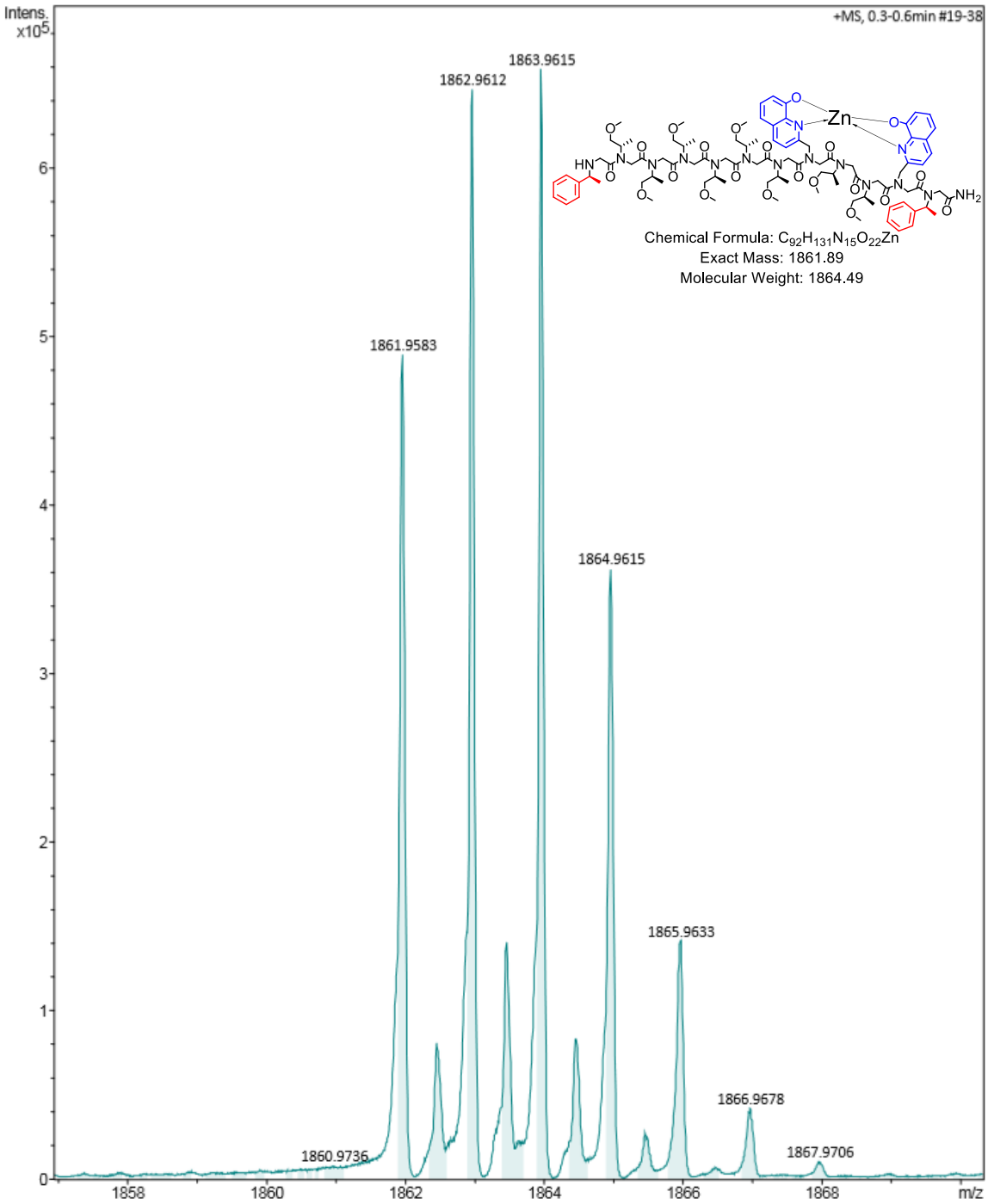


Figure S61. ESI-MS traces of peptoid oligomer (**12P1a**)Zn complex.

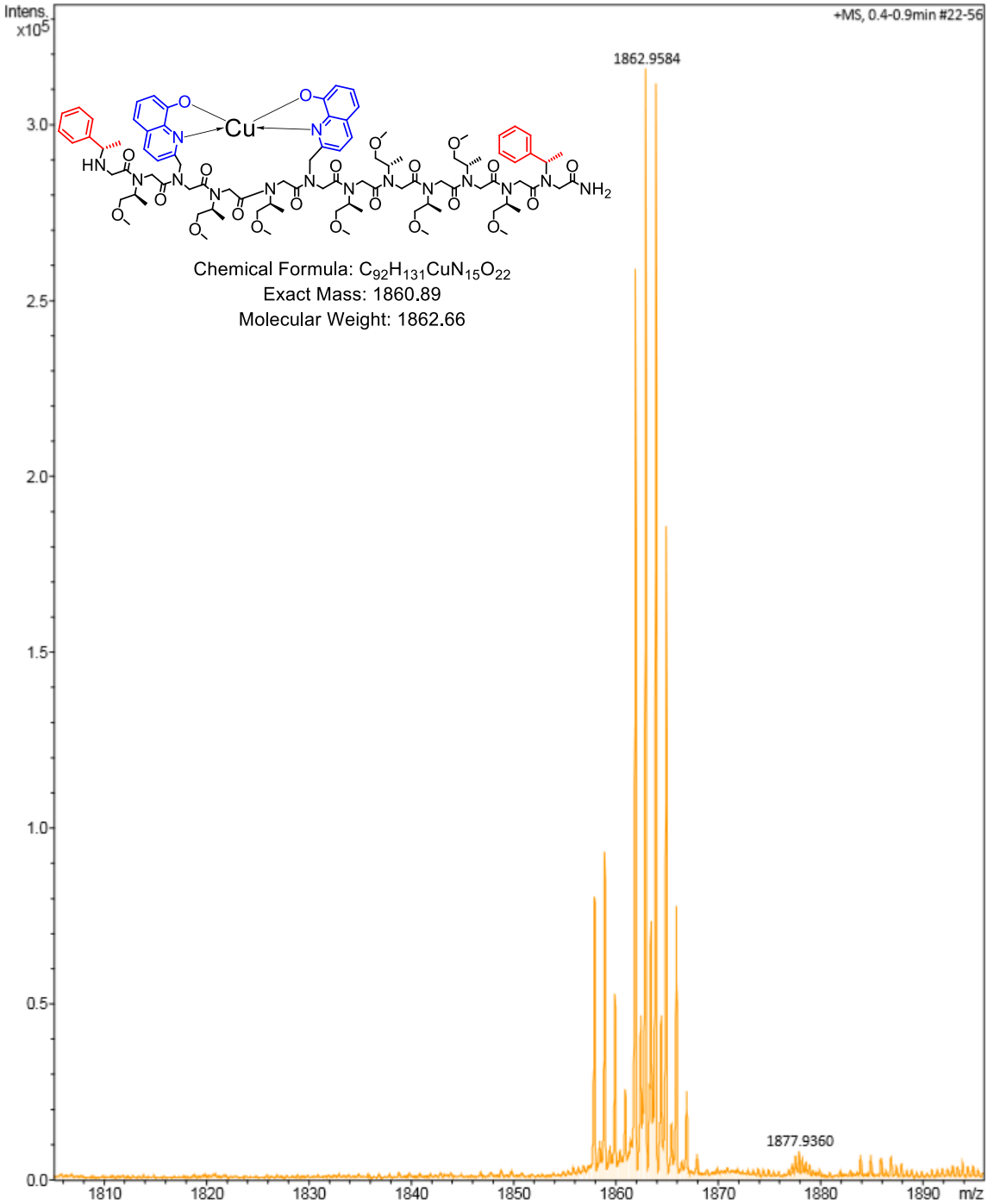


Figure S62. ESI-MS traces of peptoid oligomer (**12P1b**)Cu complex.

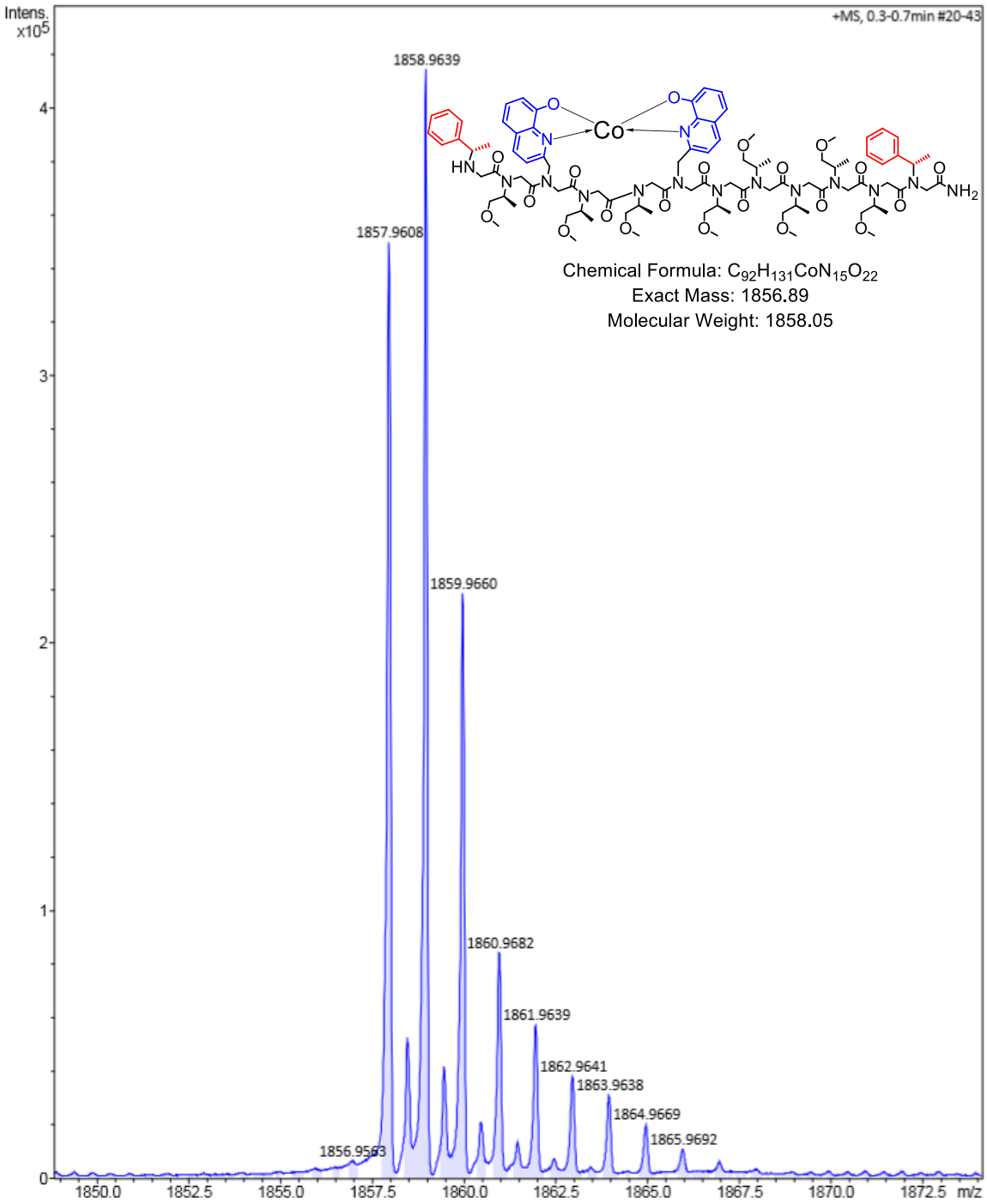


Figure S63. ESI-MS traces of peptoid oligomer (**12P1b**)Co complex.

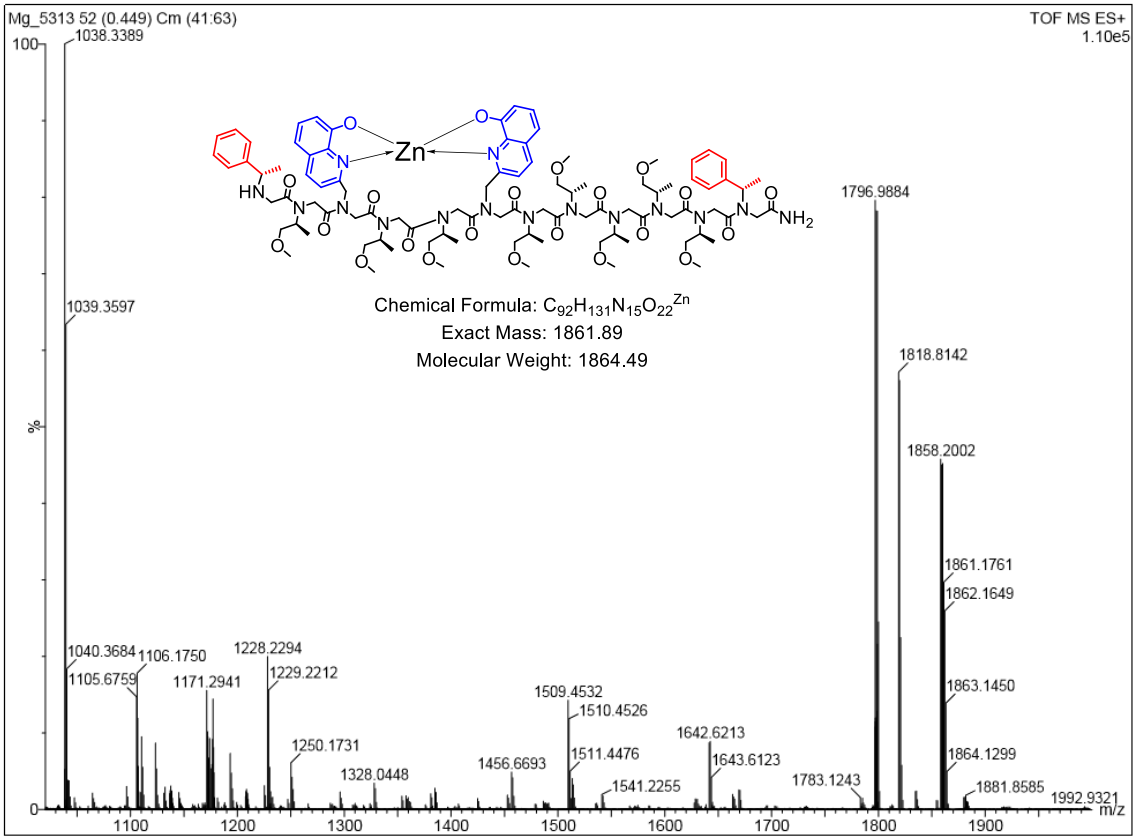


Figure S64. ESI-MS traces of peptoid oligomer (**12P1b**)Zn complex.

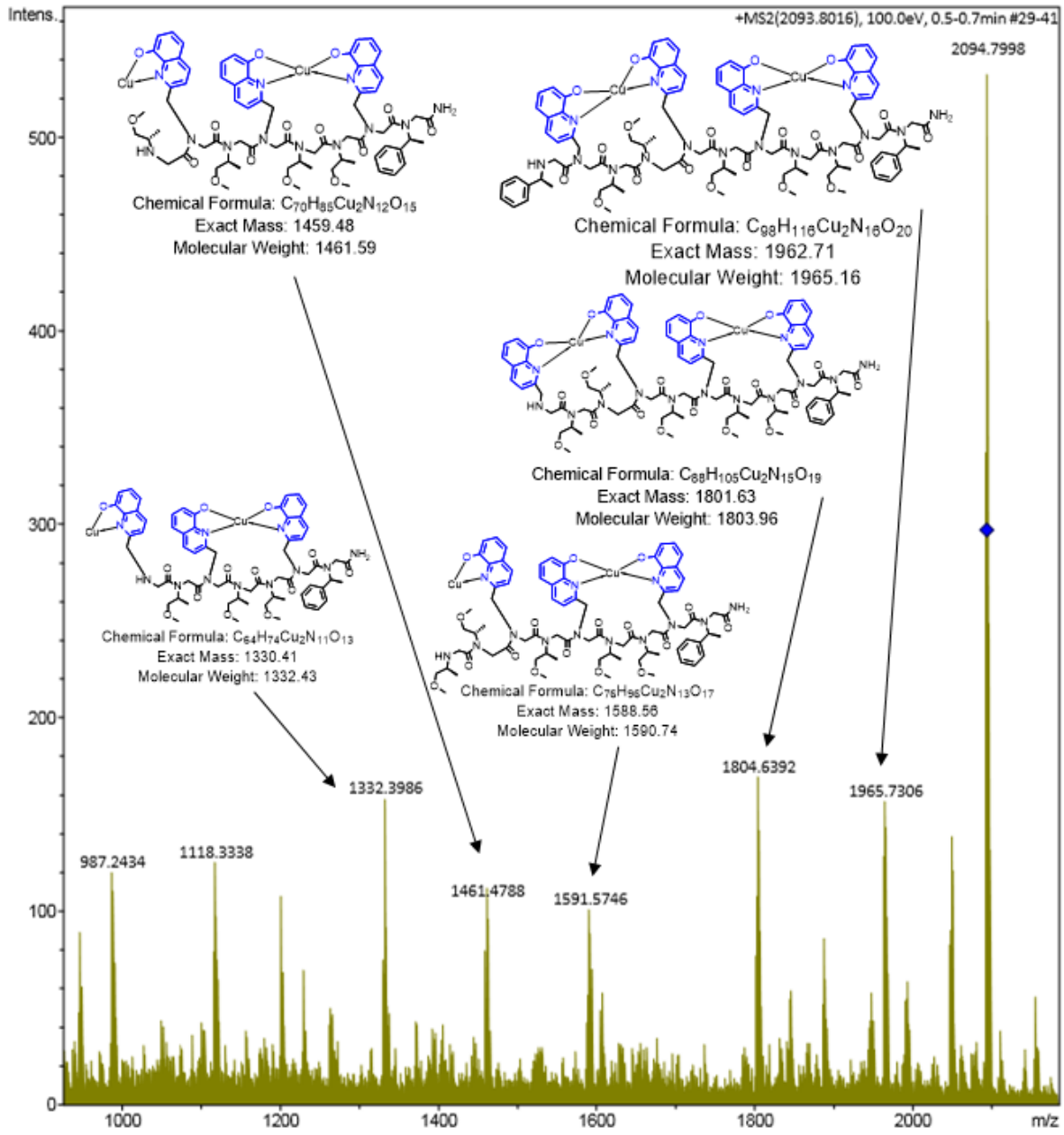


Figure S65. MS/MS analysis of peptoid oligomer (**12P2**)Cu_2 complex.

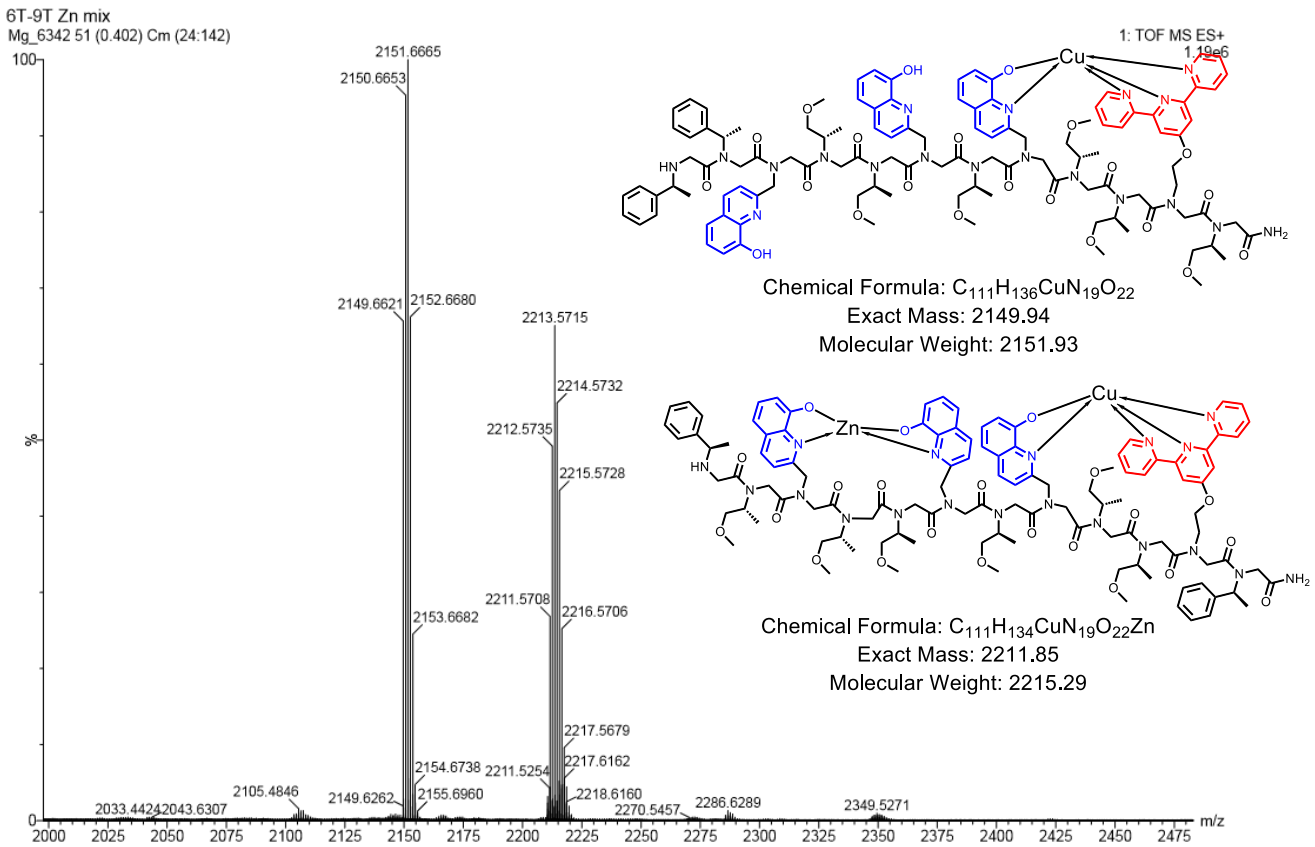


Figure S66. ESI-MS traces of (**12P5**)CuZn and (**12P6**)Cu complexes obtained from competition experiment: addition 1 equiv. of Co^{2+} to the mixture of (**12P5**)Cu and (**12P6**)Cu.

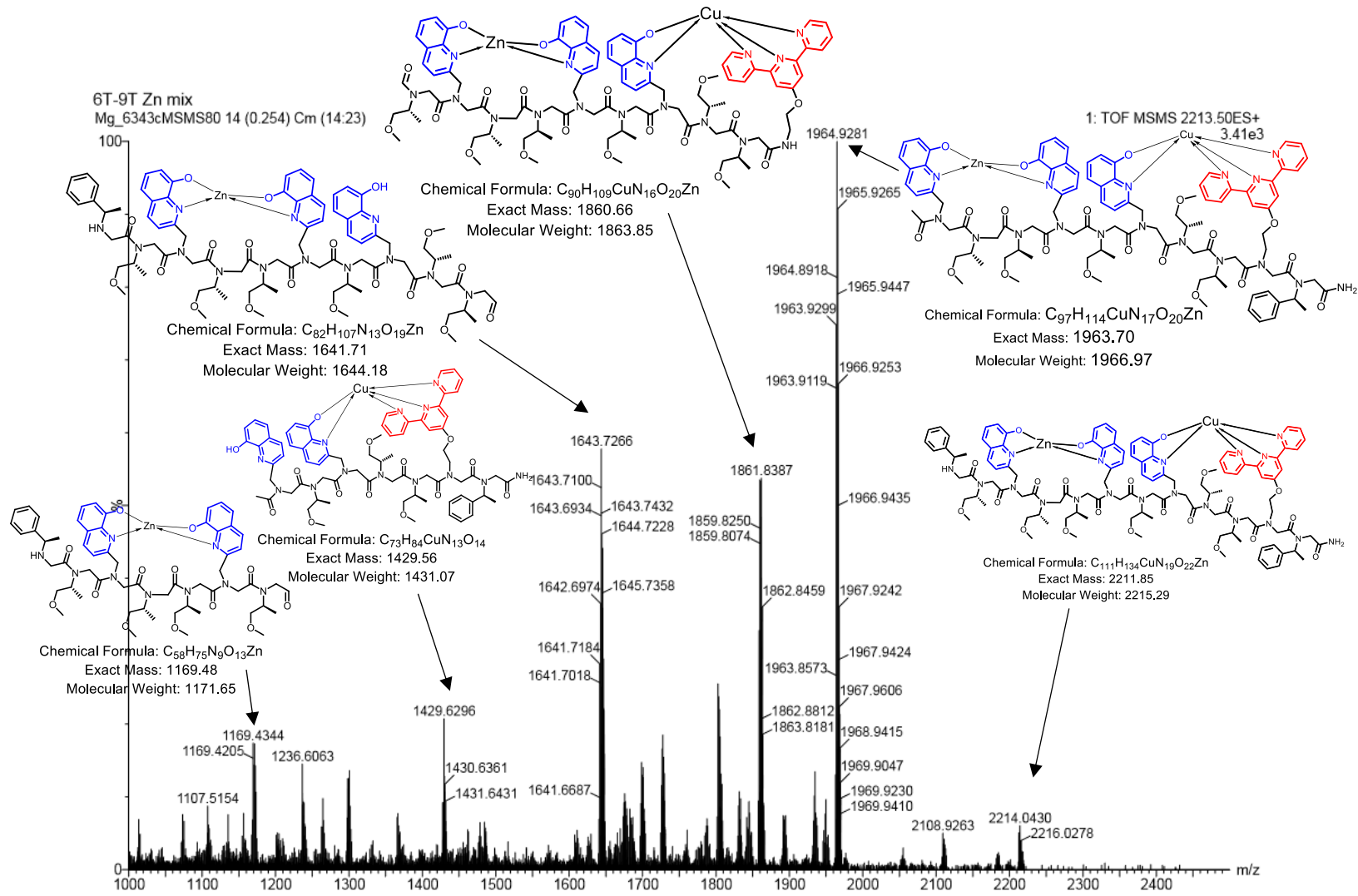


Figure S67. MS/MS analysis of (**12P5**)CuZn complex obtained from the competition experiment: addition 1 equiv. of Zn^{2+} to the mixture containing (**12P5**)Cu and (**12P6**)Cu, 0.5mM in MeOH:H_2O 4:1 soultion.

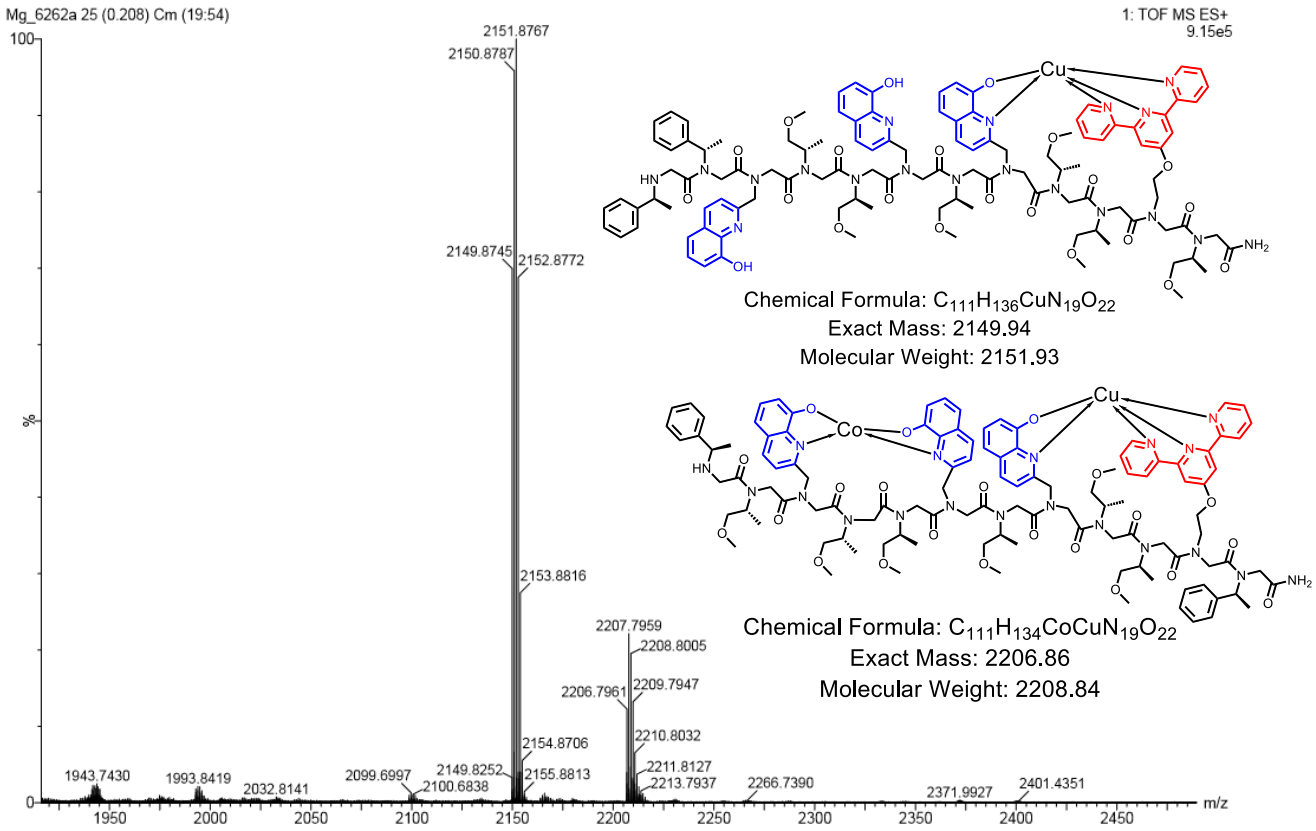


Figure S68. ESI-MS traces of (**12P5**)CuCo and (**12P6**)Cu complexes obtained from competition experiment: addition 1 equiv. of Co^{2+} to the mixture containing (**12P5**)Cu and (**12P6**)Cu, 0.5mM in MeOH:H_2O 4:1 soultion.

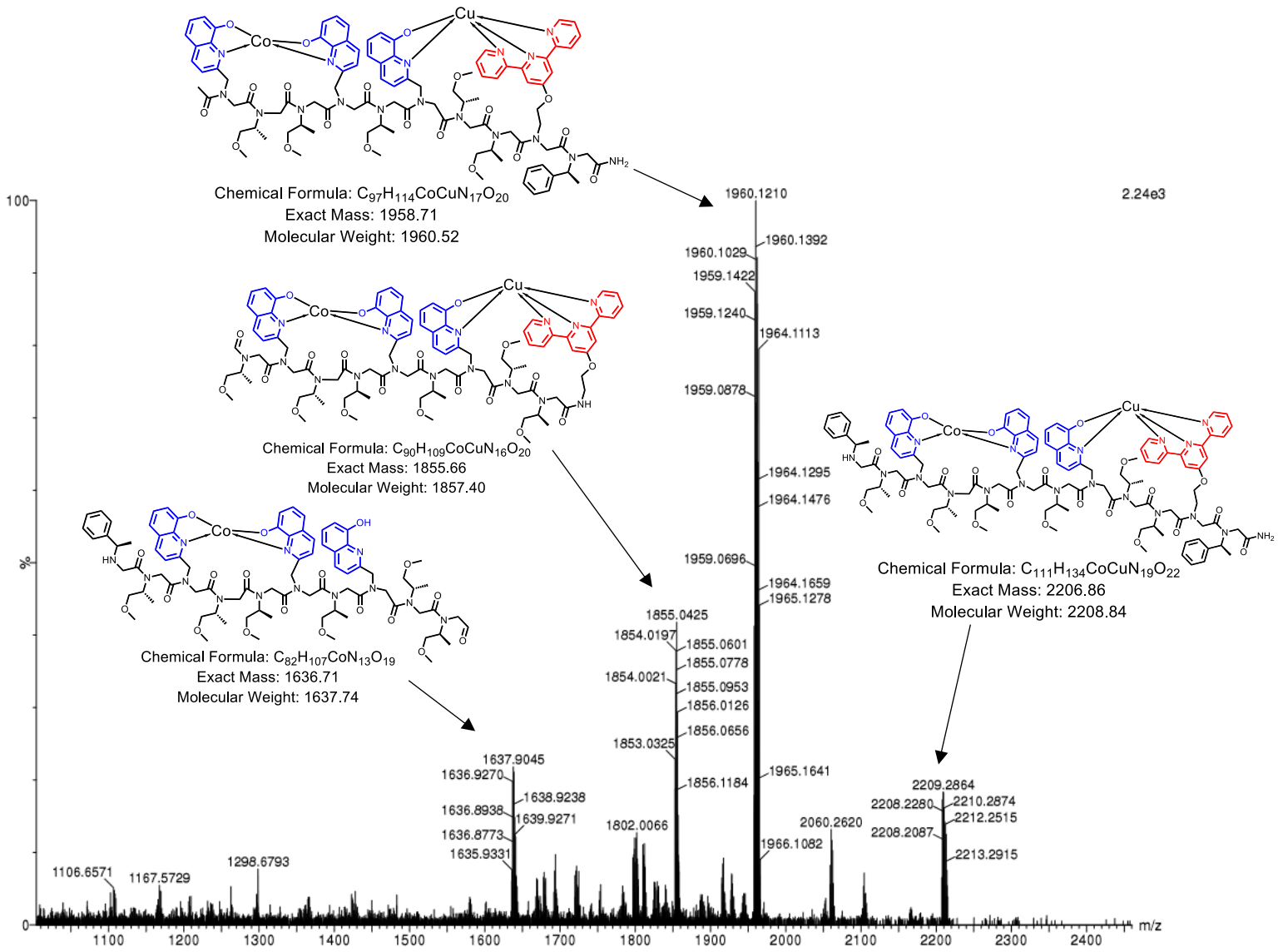


Figure S69. MS/MS analysis of (**12P5**)CuCo complex obtained from the competition experiment: addition 1 equiv. of Co^{2+} to the mixture containing (**12P5**)Cu and (**12P6**)Cu, 0.5mM in MeOH:H_2O 4:1 soultion.

NMR data

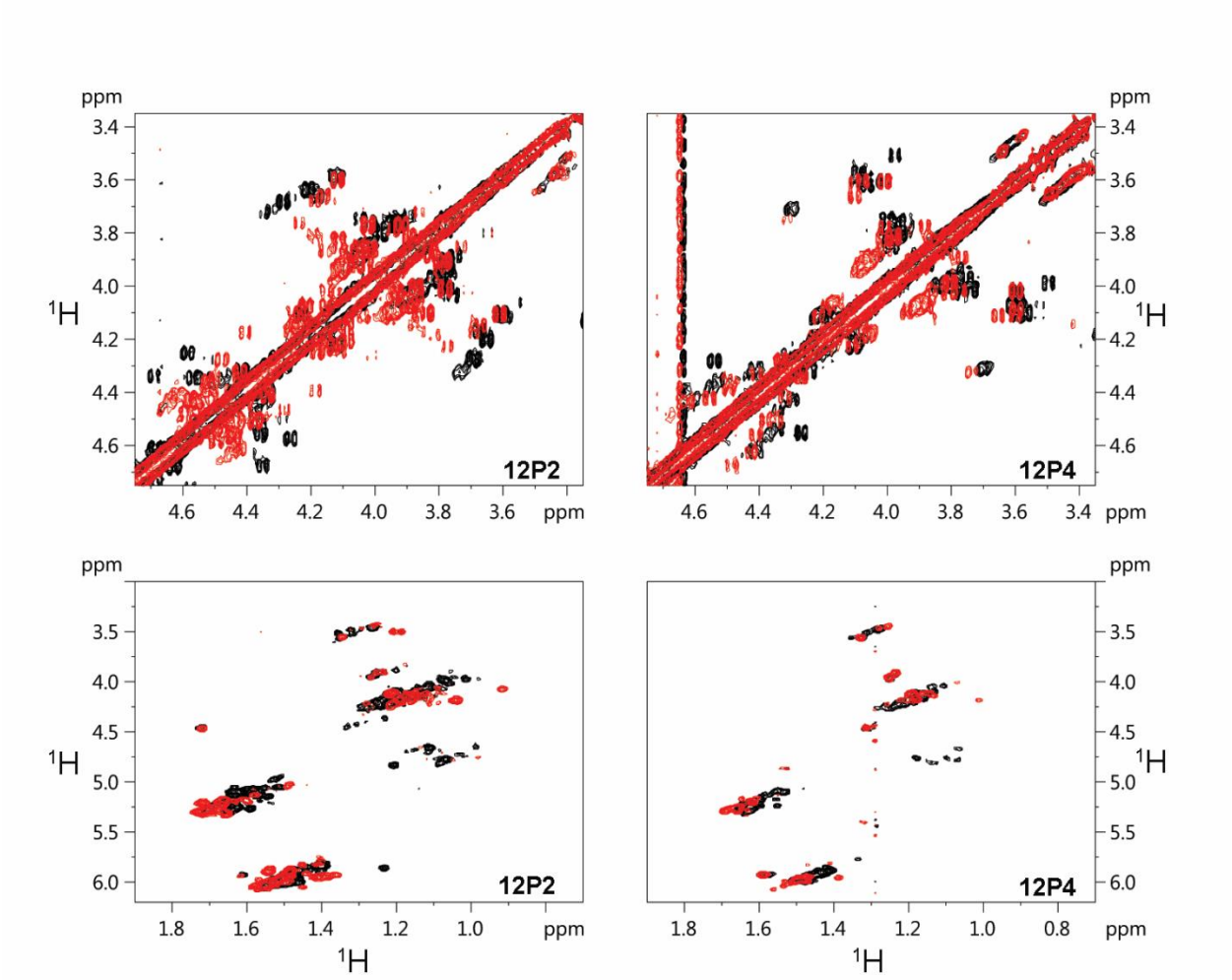
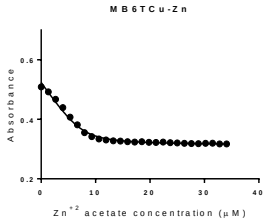
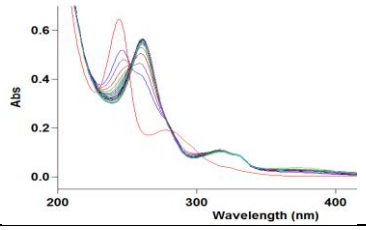
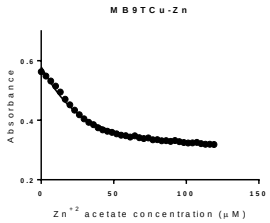
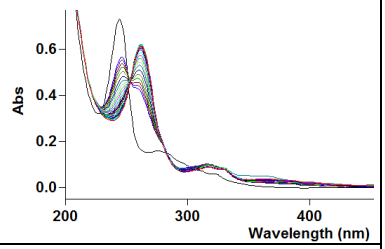
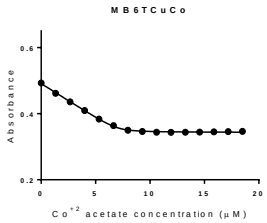
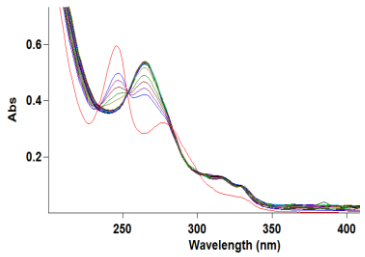
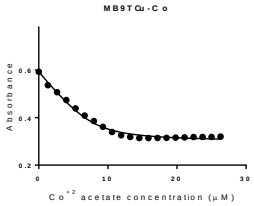
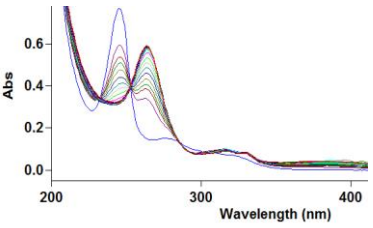


Figure S70. NMR spectra of ^{1}H-^{1}H COSY (700 MHz) experiment of the free peptoids **12P2** and **12P4** (black) and their corresponding (**12P2**)Zn_2 and (**12P4**)Zn_2 complexes measured at 283 K at 4mM concentration in CD_3OD.

Table S4. The association constants, non-linear regression fit and UV-Vis spectra for the titration of (**12P5**)Cu and (**12P6**)Cu with metal ions Zn^{2+} and Co^{2+} (typically 6-7μM in MeOH:H_2O 1:1).

Peptoid-M	Binding constant	R square	Fitting curve	UV titration
(**12P5**)Cu-Zn	$(4.019\pm0.592)\times10^{11}$	0.9917		
(**12P6**)Cu-Zn	$(7.162\pm0.611)\times10^{9}$	0.9931		
(**12P5**)Cu-Co	$(3.955\pm0.902)\times10^{12}$	0.9988		
(**12P6**)Cu-Co	$(2.900\pm0.521)\times10^{11}$	0.9909		

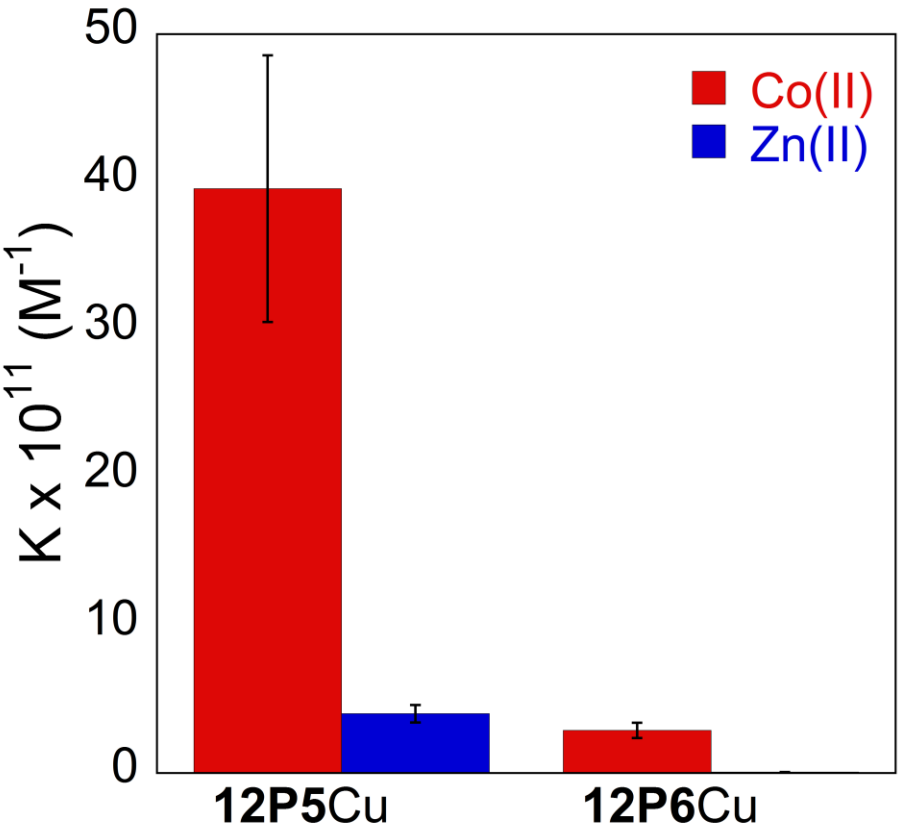


Figure S71. Association constants for the coordination of Zn^{2+} and Co^{2+} to (**12P5**)Cu and (**12P6**)Cu for the formation of the heterobimetallic complexes in MeOH:H_2O 1:1.

DFT Calculations

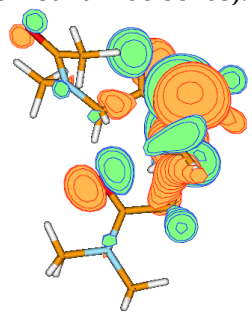
Table S5. Geometry angles of **(HQ)**$_2$Zn metal centers in metallopeptoid (**12P1**)Zn_2 based on DFT analysis.

angles	N-terminus	C-terminus
N1-Zn-N2	127.38	131.94
N1-Zn-O1	84.97	85.057
N1-Zn-O2	118.013	111.98
O1-Zn-O2	125.456	132.171
O1-Zn-N2	120.992	117.708

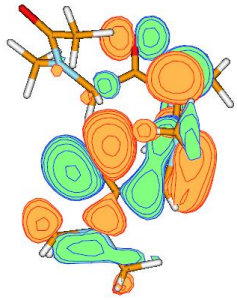
Table S6. Bond distances of geometry centers of **(HQ)**$_2$Zn in metallopeptoid (**12P1**)Zn_2 based on DFT analysis.

distances	N-terminus [Å]	C-terminus [Å]
N1-Zn	2.039	2.043
N2-Zn	2.033	2.037
O1-Zn	1.965	1.957
O2-Zn	1.965	1.977

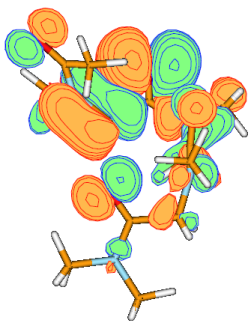
Figure S72. BHLYP/def2-TZVP+COSMO(methanol) computed frontier molecular orbitals (MO, at 0.02 a.u. contour) of right-handed, cis-PPI 4-mer peptoid model (**p4c**). Each MO is labeled by the order number used for excitation notations, the energy level (in eV), the labeling relative to the HOMO (H-) and LUMO (L+), and the bonding nature (i.e., σ, π and n orbitals) and amide site labeling from N-terminus (i.e., a1-4 for four amide bonds).



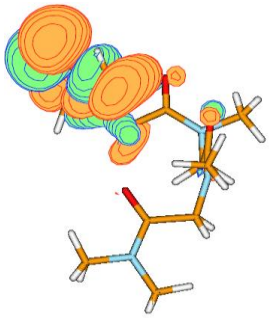
36 -9.554 H-7 *n*O a3



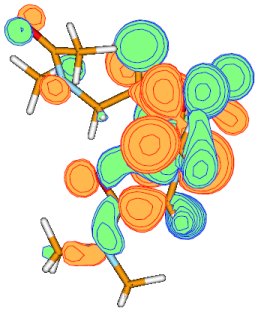
37 -9.486 H-6 *n*O a4



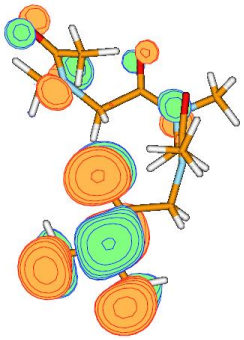
38 -9.458 H-5 *n*O a2



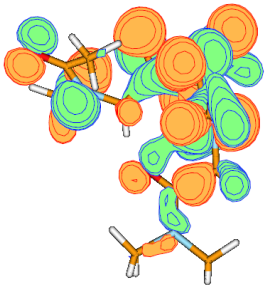
39 -9.101 H-4 *n*O a1



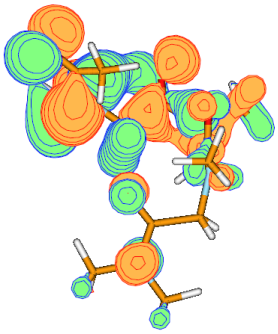
40 -8.597 H-3 π a3



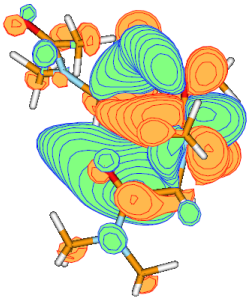
41 -8.471 H-2 π a4



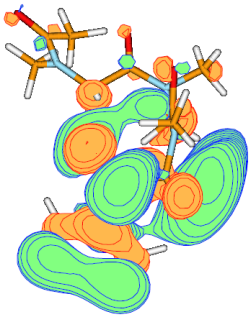
42 -8.452 H-1 π a2



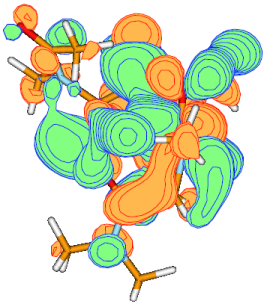
43 -8.246 HOMO π a1



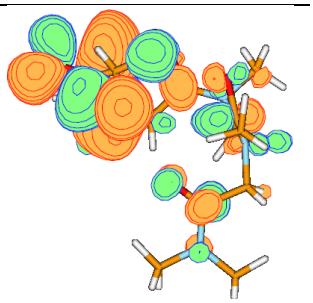
44 1.334 LUMO π* a3



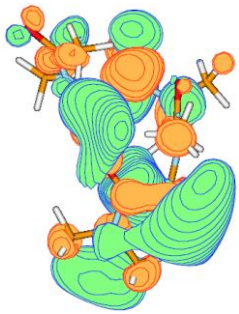
45 1.425 L+1 π* a4



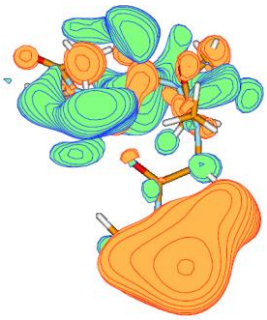
46 1.485 L+2 π* a2



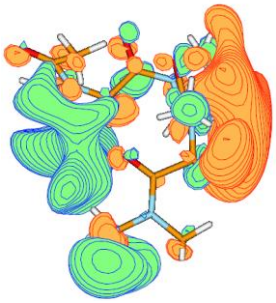
48 1.815 L+4 π* a1



47 1.601 L+3 Ry*

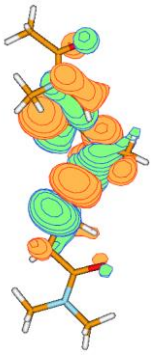


49 2.139 L+5 Ry*



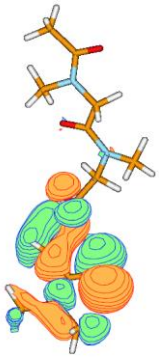
50 2.333 L+6 Ry*

Figure S73. BHLYP/def2-TZVP+COSMO(methanol) computed frontier molecular orbitals (MO, at 0.02 a.u. contour) of left-handed, trans-PPII 4-mer peptoid model (**p4t**). See Figure S1 for other details.



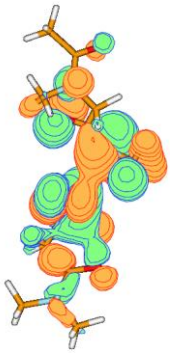
36 -9.418 H-7 *n*O a32

37 -9.389 H-6 *n*O a23



38 -9.317 H-5 *n*O a4

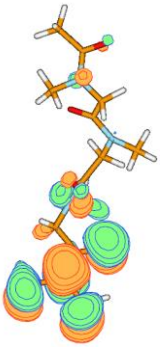
39 -9.157 H-4 *n*O a1



40 -8.427 H-3 π a23

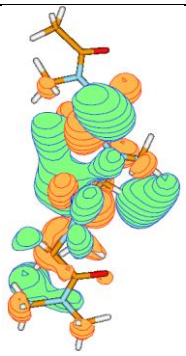
41 -8.370 H-2 π a32

42 -8.330 H-1 π a1

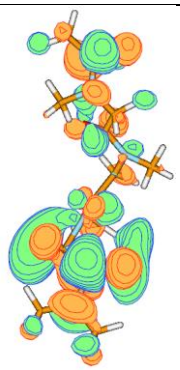


43 -8.307 HOMO π a4

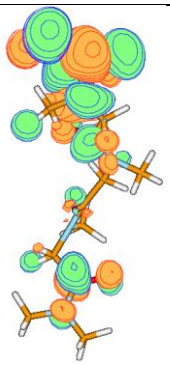
44 1.613 LUMO π* a23



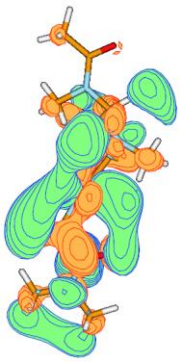
45 1.639 L+1π* a32



47 1.724 L+3π* a4



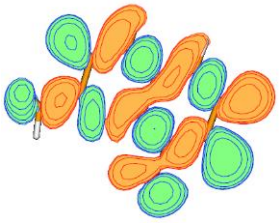
48 1.753 L+4π* a1



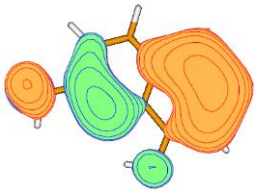
46 1.706 L+2Ry* a23

49 1.914 L+5 Ry* 14

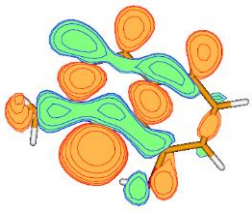
Figure S74. BHLYP/def2-TZVP+COSMO(methanol) computed frontier molecular orbitals (MO, at 0.02 a.u. contour) of free **HQ**. Each MO is labeled by the order used for excitations, the energy level (in eV), the labeling relative to the HOMO (H-) and LUMO (L+), and the bonding nature (i.e., σ, π and n orbitals).



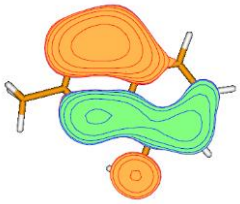
18 -11.25 H-5 *n*O



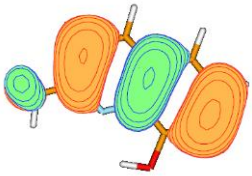
19 -10.68 H-4 π3



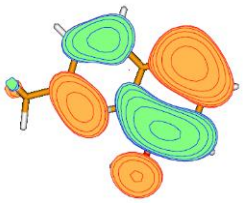
21 -9.401 H-2 *n*N



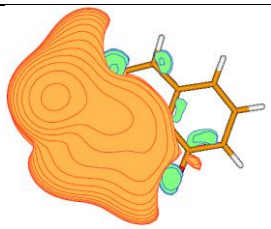
20 -9.505 H-3 π2



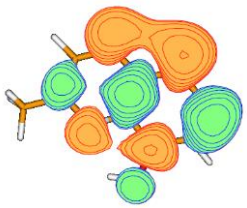
22 -7.960 H-1 π1



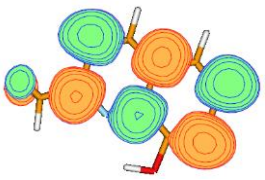
23 -7.058 HOMO π0



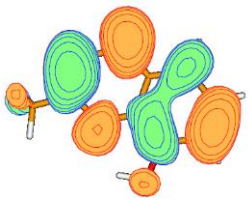
27 2.098 L+3 Ry*



26 1.632 L+2 π2*



25 0.301 L+1 π1*



24 -0.579 LUMO π0*

Figure S75. BHLYP/def2-TZVP+COSMO(methanol) computed frontier molecular orbitals (MO, at 0.02 a.u. contour) of free **ZnQ$_2$** complex. Due to the *C*$_2$-symmetry, the MOs are further distinguished as symmetric and antisymmetric (a and b, respectively). See Figure S1 for other details.

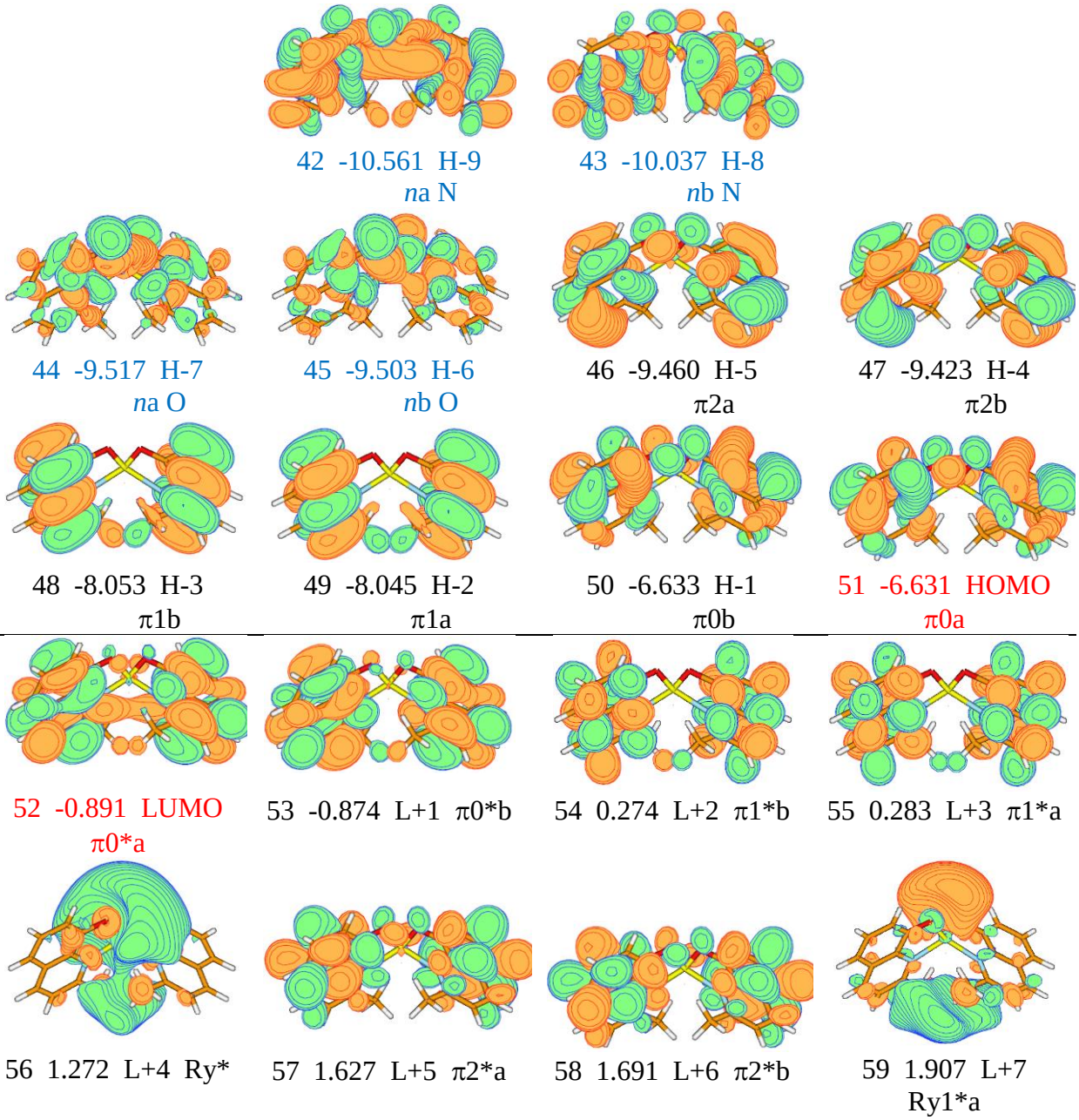
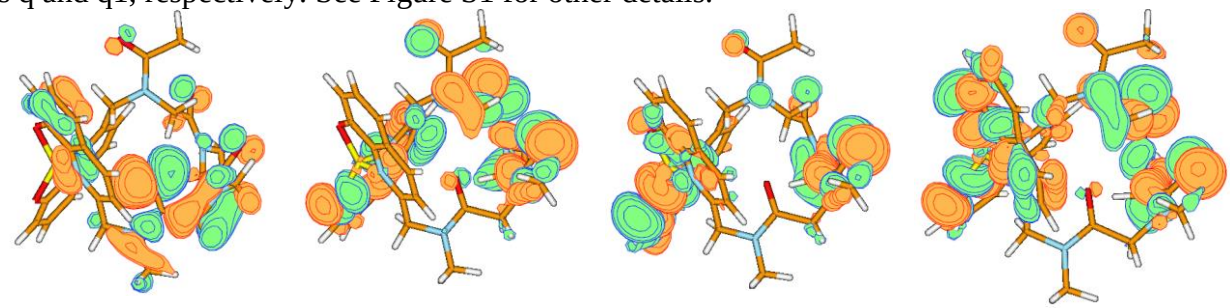
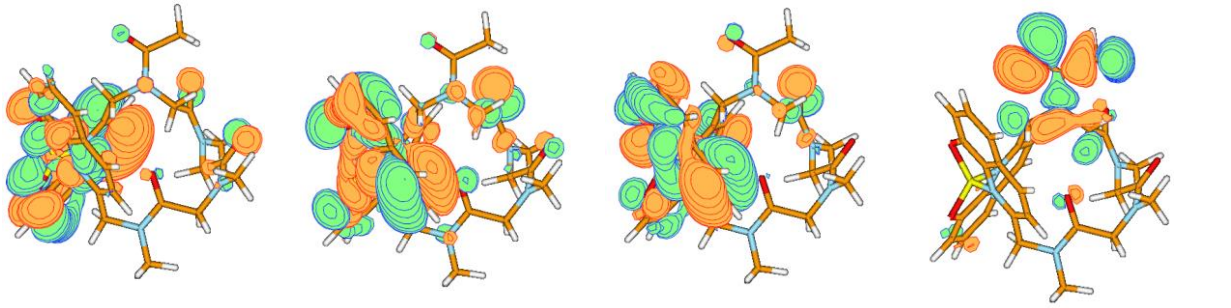


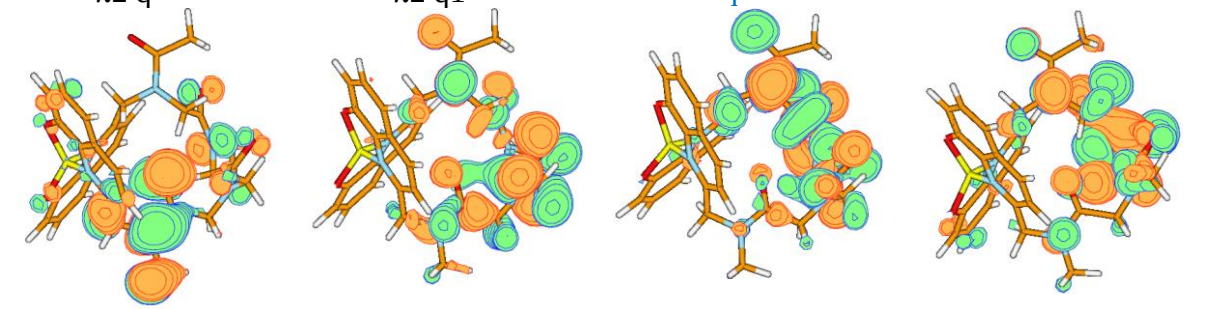
Figure S76. BHLYP/def2-TZVP+COSMO(methanol) computed frontier molecular orbitals (MO, at 0.02 a.u. contour) of free **ZnQ$_2$c** complex. The inner and outer **Q** ligand site are labeled as q and q1, respectively. See Figure S1 for other details.



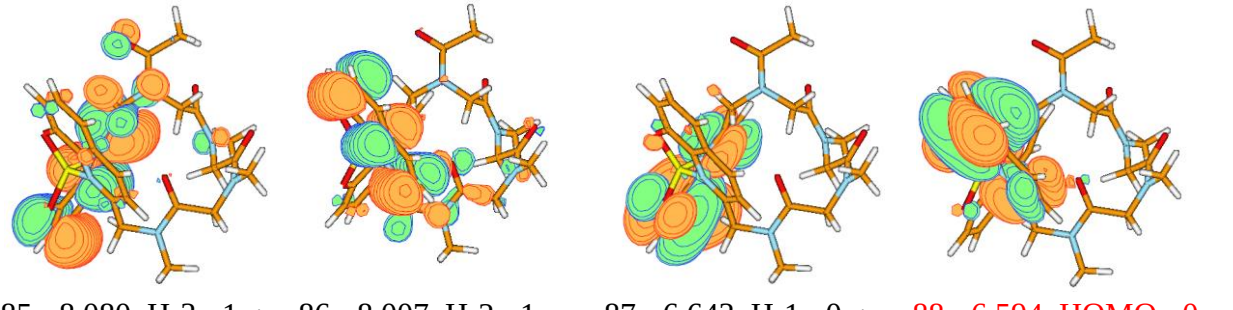
73 -9.804 H-15 *n* a4 | 74 -9.619 H-14 *n* a2 | 75 -9.557 H-13 *n* q, a3 | 76 -9.513 H-12 *n* q, a3



77 -9.478 H-11 π2 q | 78 -9.454 H-10 π2 q1 | 79 -9.413 H-9 *n* q1 | 80 -9.264 H-8 *n* a1



81 -8.919 H-7 π a4 | 82 -8.699 H-6 π a3 | 83 -8.600 H-5 π a1 | 84 -8.553 H-4 π a2



85 -8.080 H-3 π1 q | 86 -8.007 H-2 π1 q1 | 87 -6.643 H-1 π0 q | 88 -6.594 HOMO π0 q1

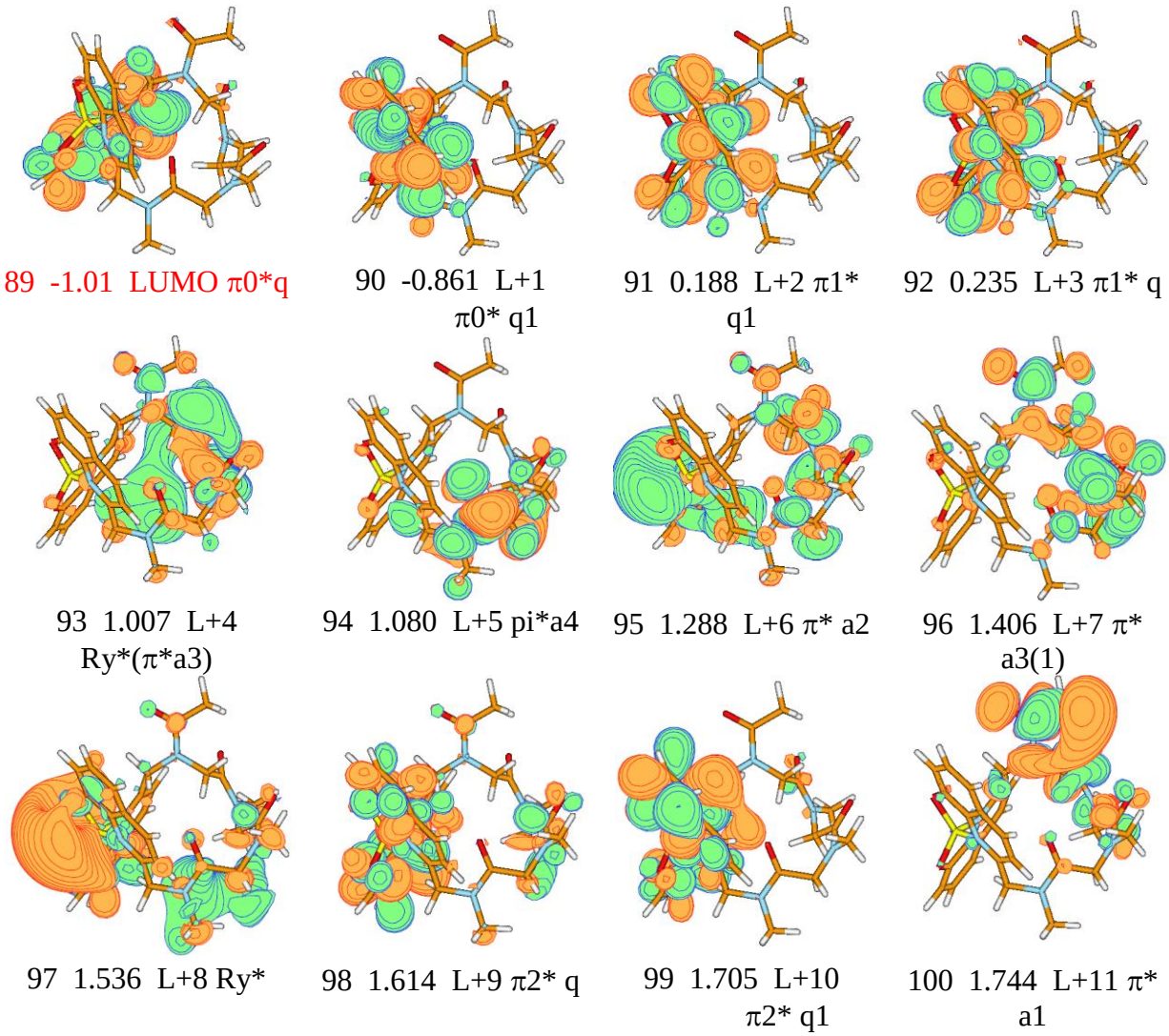


Table S7. The sTD-BHLYP-D3/def2-TZVP + COSMO computed excitation energies and UV and CD intensities computed at level, along with detailed electronic assignment of the free **HQ**, **ZnQ_2**, **p4c** (cis-PPI) and **p4t** (trans-PPII) model systems based on the labeled frontier MOs as shown in Figure S1. The excites states most relevant for assignment are highlighted as bold rows in red.

States	Energy	λ	UV	CD	transitions			Assignment
HQ	eV	nm						
1	**3.649**	**339.8**	**0.049**	**0.181**	**0.93(23-> 24)**	**--**	**--**	**π0-π0***
2	3.910	317.1	0.003	-0.168	0.51(23-> 25)	0.45(22-> 24)	--	π0-π1*, π1-π0*
3	4.861	255.1	0.007	0.581	0.95(21-> 24)	--	--	*n*N-π0*
4	**5.172**	**239.7**	**0.910**	**-7.591**	**0.45(22-> 24)**	**0.40(23-> 25)**	**--**	**π1-π0*, π0-π1***
5	5.412	229.1	0.042	-0.353	0.58(22-> 25)	0.29(23-> 26)	0.11(20-> 24)	π1-π1*
6	**5.944**	**208.6**	**0.145**	**4.520**	**0.61(23-> 26)**	**0.22(20-> 24)**	**0.11(22-> 25)**	**π0-π2***
7	5.966	207.8	0.004	0.287	0.66(23-> 27)	0.18(23-> 29)	0.11(23-> 28)	π0-Ry*
8	6.056	204.7	0.001	-2.534	0.98(21-> 25)	--	--	*n*N-π0*
9	**6.242**	**198.6**	**0.339**	**0.816**	**0.62(20-> 24)**	**0.25(22-> 25)**	**--**	**π2-π0***

10	6.259	198.1	0.000	0.561	0.80(23-> 28)	0.11(23-> 29)	--	π0-Ry1*
11	**6.411**	**193.4**	**0.509**	**5.546**	**0.56(22-> 26)**	**0.19(20-> 25)**	**--**	**π1-π2***
12	6.743	183.9	0.000	0.444	0.37(23-> 29)	0.25(23-> 30)	0.14(23-> 27)	π0-Ry2*
13	6.858	180.8	0.000	2.172	0.74(22-> 27)	0.13(23-> 30)	--	π1-Ry*
14	6.966	178.0	0.065	-2.582	0.50(20-> 25)	0.25(22-> 26)	0.20(19-> 24)	π2-π1*
ZnQ2								
1	**2.911**	**425.9**	**0.097**	**-0.995**	**0.50(50-> 52)**	**0.48(51-> 53)**	**--**	**π0-π0* ba**
2	**2.961**	**418.7**	**0.020**	**1.350**	**0.49(51-> 52)**	**0.48(50-> 53)**	**--**	**π0-π0* aa**
3	3.586	345.7	0.000	0.044	0.49(50-> 53)	0.48(51-> 52)	--	π0-π0* aa0
4	3.592	345.2	0.000	-0.116	0.49(51-> 53)	0.48(50-> 52)	--	π0-π0* ba0
5	3.710	334.2	0.002	0.802	0.31(51-> 55)	0.30(50-> 54)	0.18(48-> 53)	π0-π1* aa0
6	3.716	333.6	0.004	-0.905	0.31(50-> 55)	0.30(51-> 54)	0.18(49-> 53)	π0-π1* ba0
7	**4.816**	**257.4**	**0.945**	**-101.406**	**0.30(50-> 55)**	**0.26(48-> 52)**	**0.25(49-> 53)**	**π1-π0* ba**
8	**4.821**	**257.2**	**0.587**	**113.798**	**0.31(49-> 52)**	**0.24(48-> 53)**	**0.21(50-> 54)**	**π1-π0* aa**
9	4.838	256.3	0.008	1.346	0.53(51-> 55)	0.44(50-> 54)	--	π0-π1* aa
10	**4.840**	**256.2**	**0.068**	**-6.282**	**0.60(51-> 54)**	**0.33(50-> 55)**	**--**	**π0-π1* ab**
11	5.036	246.2	0.002	0.357	0.88(51-> 56)	--	--	π0-π2* aa
12	**5.045**	**245.8**	**0.051**	**-4.904**	**0.78(50-> 56)**	**0.10(48-> 52)**	**--**	**π0-π2* ba**
13	5.061	245.0	0.011	-1.124	0.49(49-> 53)	0.39(48-> 52)	--	π1-π0* ba
14	5.064	244.8	0.002	0.281	0.51(48-> 53)	0.44(49-> 52)	--	π1-π0* aa
15	5.276	235.0	0.020	-2.196	0.26(50-> 57)	0.22(51-> 58)	0.20(49-> 54)	π0-π2* ba
16	5.279	234.9	0.006	2.190	0.25(51-> 57)	0.22(49-> 55)	0.22(48-> 54)	π1-π2* aa
17	5.310	233.5	0.001	-0.001	0.48(44-> 52)	0.37(45-> 53)	--	*n*-π0* aa
18	5.311	233.4	0.004	-0.054	0.46(44-> 53)	0.39(45-> 52)	--	*n*-π* ab
19	**5.597**	**221.5**	**0.188**	**-5.560**	**0.27(47-> 52)**	**0.25(46-> 53)**	**0.17(50-> 57)**	**π2-π0* ba**
20	**5.600**	**221.4**	**0.005**	**3.582**	**0.28(46-> 52)**	**0.27(47-> 53)**	**0.17(51-> 57)**	**π2-π0* aa**
21	5.773	214.8	0.009	-1.425	0.61(43-> 52)	0.14(42-> 53)	0.13(45-> 52)	*n*1-π0* ba
22	5.779	214.5	0.007	1.142	0.60(43-> 53)	0.16(42-> 52)	0.12(45-> 53)	*n*1-π0* aa
23	5.852	211.9	0.010	-0.078	0.72(51-> 59)	0.21(50-> 60)	--	π0-Ry1* aa
24	5.853	211.8	0.012	-0.075	0.72(50-> 59)	0.20(51-> 60)	--	π0-Ry1* ba
25	5.896	210.3	0.000	0.000	0.15(50-> 63)	0.13(51-> 62)	0.10(51-> 63)	π0-Ry**
26	5.897	210.2	0.000	-0.018	0.15(51-> 63)	0.13(50-> 62)	0.10(50-> 63)	π0-Ry**
27	6.025	205.8	0.080	2.329	0.41(51-> 60)	0.25(51-> 61)	0.10(50-> 59)	π0-Ry2*
28	6.029	205.6	0.001	-0.234	0.43(50-> 60)	0.25(50-> 61)	0.10(51-> 59)	π0-Ry2*
29	6.130	202.3	0.084	-1.358	0.46(51-> 61)	0.10(51-> 60)	--	π0-Ry3*
30	6.133	202.2	0.003	-0.426	0.51(50-> 61)	0.09(50-> 60)	--	π0-Ry3*
31	6.164	201.1	0.015	1.854	0.42(44-> 52)	0.34(45-> 53)	--	*n*-π0* aa
32	6.175	200.8	0.116	0.075	0.47(44-> 53)	0.41(45-> 52)	--	*n*-π0* ab
33	6.225	199.2	0.057	-0.387	0.44(50-> 57)	0.31(51-> 58)	0.13(51-> 61)	π0-π2* ba
34	6.229	199.0	0.001	0.041	0.43(51-> 57)	0.41(50-> 58)	--	π0-π2* aa
35	**6.266**	**197.9**	**1.032**	**-13.816**	**0.25(51-> 58)**	**0.25(49-> 54)**	**0.18(47-> 52)**	**π0-π2* ab**
36	6.296	196.9	0.001	0.134	0.50(49-> 55)	0.49(48-> 54)	--	π1-π1* aa
37	6.304	196.7	0.015	0.274	0.56(48-> 55)	0.42(49-> 54)	--	π1-π1* ba
38	**6.354**	**195.1**	**0.253**	**15.422**	**0.19(46-> 52)**	**0.19(48-> 54)**	**0.19(49-> 55)**	**π1-π1* aa**

39	6.364	194.8	0.005	-0.238	0.35(46-> 53)	0.27(47-> 52)	0.16(47-> 53)	π2-π0*
40	6.365	194.8	0.007	0.146	0.34(47-> 53)	0.28(46-> 52)	0.19(46-> 53)	π2-π0*
41	6.532	189.8	0.022	-0.253	0.22(50-> 64)	0.21(51-> 65)	0.13(51-> 67)	π0-Ry**
42	6.534	189.8	0.005	0.218	0.22(51-> 64)	0.21(50-> 65)	0.15(50-> 67)	π0-Ry**
43	**6.589**	**188.2**	**0.331**	**-15.008**	**0.18(49-> 58)**	**0.18(48-> 57)**	**0.17(45-> 55)**	**π1-π2* aa**
44	6.593	188.1	0.003	-0.084	0.47(44-> 55)	0.46(45-> 54)	--	*n*-π1* aa
45	6.595	188.0	0.130	-5.061	0.40(44-> 54)	0.30(45-> 55)	--	*n*-π1* ba
46	**6.608**	**187.6**	**0.101**	**18.082**	**0.23(48-> 58)**	**0.23(49-> 57)**	**0.20(49-> 56)**	**π1-π2* ba**
47	6.635	186.9	0.014	2.124	0.73(49-> 56)	--	--	π1-Ry* aa
48	6.644	186.6	0.073	-3.533	0.79(48-> 56)	--	--	π1-Ry* ba

P4c

1	**5.867**	**211.3**	**0.012**	**-1.165**	**0.19(43-> 46)**	**0.15(38-> 47)**	**0.15(43-> 47)**	**n-π* a2**
2	**5.878**	**210.9**	**0.015**	**-1.145**	**0.24(36-> 44)**	**0.20(42-> 44)**	**0.12(36-> 46)**	**n-π* a3**
3	**5.973**	**207.6**	**0.007**	**-0.728**	**0.81(39-> 48)**	**--**	**--**	**n-π* a1**
4	5.990	207.0	0.007	0.134	0.38(37-> 45)	0.14(40-> 45)	0.11(42-> 45)	n-π* a4
5	**6.515**	**190.3**	**0.023**	**-0.853**	**0.28(41-> 47)**	**0.22(41-> 45)**	**0.20(41-> 44)**	**π-π* a4**
6	**6.606**	**187.7**	**0.010**	**-1.492**	**0.19(43-> 44)**	**0.12(43-> 46)**	**0.11(43-> 49)**	**π-π* a2**
7	**6.707**	**184.9**	**0.026**	**2.011**	**0.28(42-> 46)**	**0.19(42-> 45)**	**0.08(42-> 44)**	**π-π* a2**
8	6.716	184.6	0.050	-0.722	0.35(40-> 44)	0.15(36-> 44)	0.14(42-> 44)	π-π*
9	6.817	181.9	0.003	0.198	0.23(40-> 45)	0.19(42-> 45)	0.19(37-> 45)	π-π*
10	6.838	181.3	0.094	2.574	0.19(40-> 44)	0.15(40-> 45)	0.13(42-> 47)	π-π*
11	6.990	177.4	0.035	0.063	0.15(43-> 47)	0.14(43-> 49)	0.10(43-> 50)	π-Ry*
12	**7.015**	**176.7**	**0.363**	**13.195**	**0.24(40-> 44)**	**0.13(42-> 44)**	**0.09(43-> 44)**	**π-π* a23**
13	7.061	175.6	0.105	-2.350	0.22(41-> 44)	0.14(42-> 44)	0.13(43-> 46)	π-π*

P4t

1	**5.910**	**209.8**	**0.008**	1.000	**0.17(41-> 44)**	**0.15(37-> 44)**	**0.12(36-> 44)**	**n-π* a23**
2	5.934	208.9	0.005	0.156	0.20(42-> 44)	0.14(42-> 45)	0.14(37-> 45)	n-π* a32
3	**5.946**	**208.5**	**0.010**	1.552	**0.65(39-> 48)**	**0.13(39-> 47)**	**0.06(42-> 48)**	**n-π* a4**
4	6.045	205.1	0.006	0.253	0.34(38-> 47)	0.16(41-> 47)	0.15(38-> 46)	n-π* a1
5	6.532	189.8	0.030	0.246	0.34(43-> 49)	0.25(43-> 45)	0.20(43-> 46)	π-Ry* a4
6	6.714	184.7	0.023	0.511	0.27(41-> 45)	0.17(41-> 46)	0.12(41-> 47)	π-π* a32
7	**6.715**	**184.6**	**0.059**	**2.882**	**0.34(42-> 49)**	**0.19(42-> 45)**	**0.11(40-> 44)**	**π-Ry* a14**
8	6.754	183.6	0.022	-0.604	0.28(40-> 45)	0.17(40-> 44)	0.07(40-> 49)	π-π* a23
9	6.799	182.4	0.030	1.115	0.18(42-> 46)	0.11(42-> 49)	0.09(42-> 44)	π-Ry* a1
10	6.835	181.4	0.016	0.442	0.33(40-> 46)	0.11(40-> 44)	0.09(36-> 44)	π-π* a23
11	6.924	179.1	0.001	0.054	0.24(38-> 47)	0.19(41-> 47)	0.14(41-> 46)	π-Ry*
12	7.048	175.9	0.522	-0.378	0.22(40-> 44)	0.15(41-> 45)	0.10(41-> 44)	π-π* a3
13	**7.137**	**173.7**	**0.157**	-5.650	**0.45(41-> 44)**	**0.11(40-> 45)**	**0.06(42-> 44)**	**π-π* a23**
14	7.229	171.5	0.008	0.522	0.45(43-> 44)	0.15(43-> 46)	0.15(43-> 45)	π-π* CT
15	**7.283**	**170.2**	**0.067**	-3.159	**0.24(40-> 45)**	**0.18(41-> 45)**	**0.10(40-> 46)**	**π-π* a23**

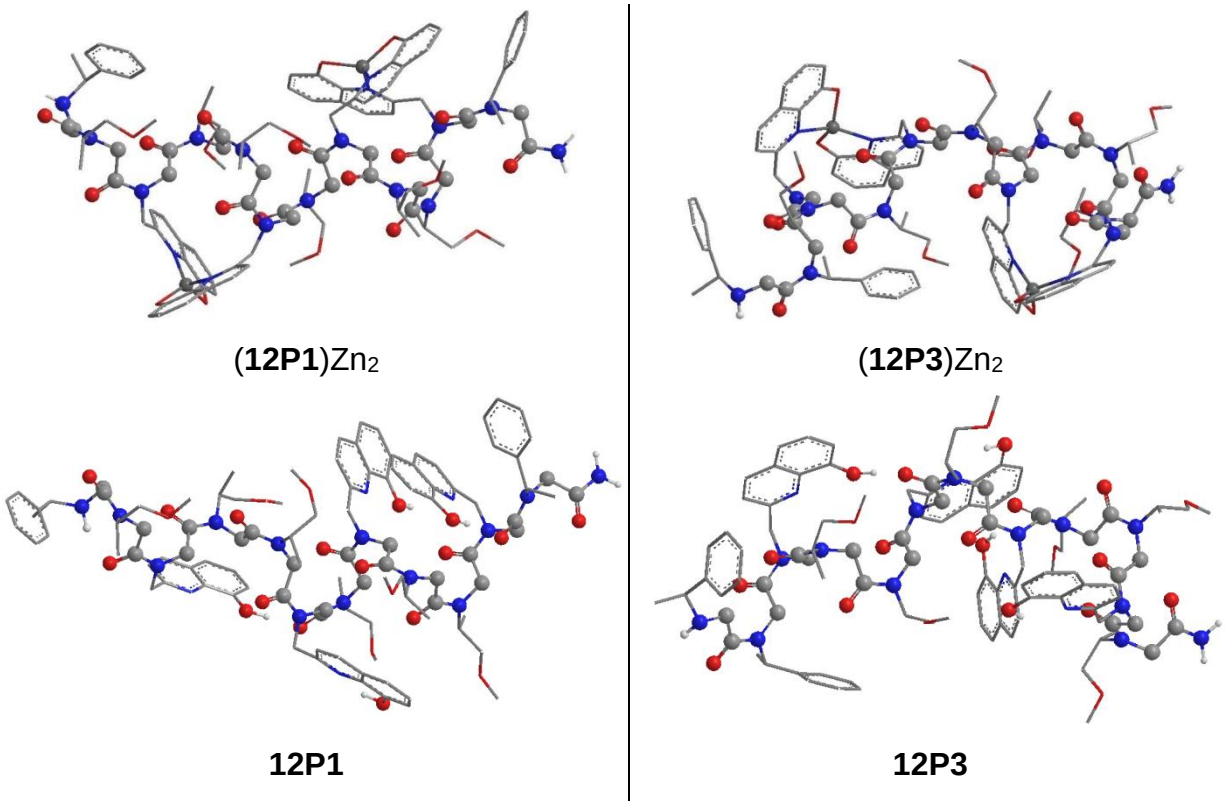
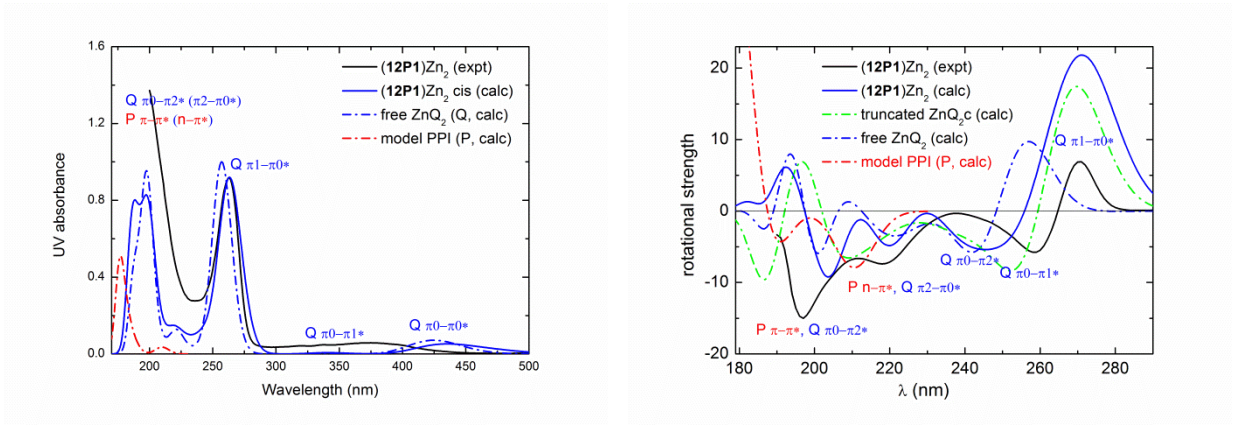
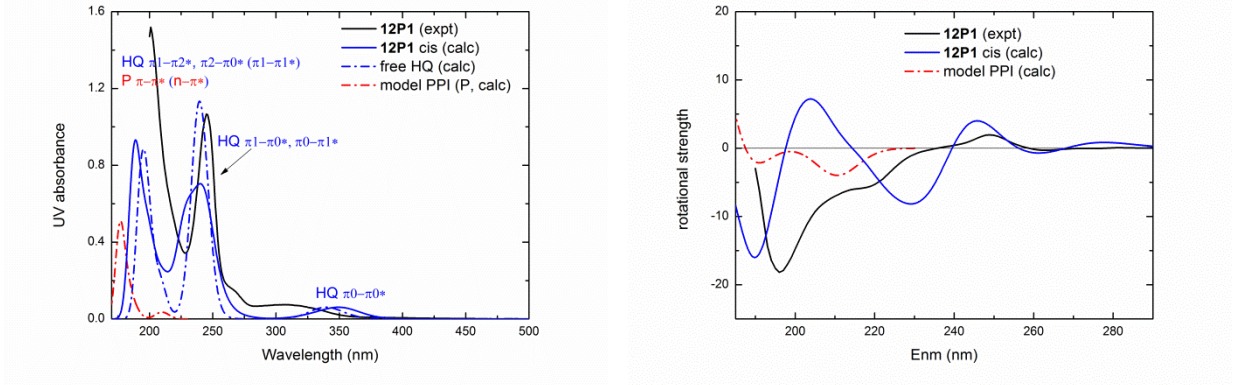


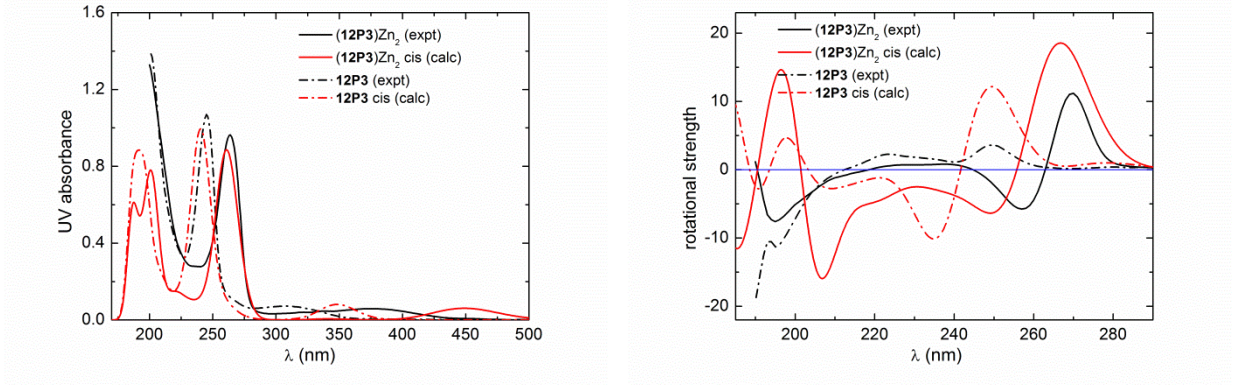
Figure S77. The TPSS-D3/def2-TZVP + COSMO (methanol) optimized **12P1** and **12P3** peptoids assuming the right-handed cis-PPI helical structures, with (top) and without (bottom) Zn(II)-coordination. The main-chain C, N, O atoms and acidic H atoms (HQ hydroxyl and amide NH groups) are high-lighted as grey, blue, red and white balls, respectively.



(**12P1**)Zn_2, right-handed cis-PPI helix

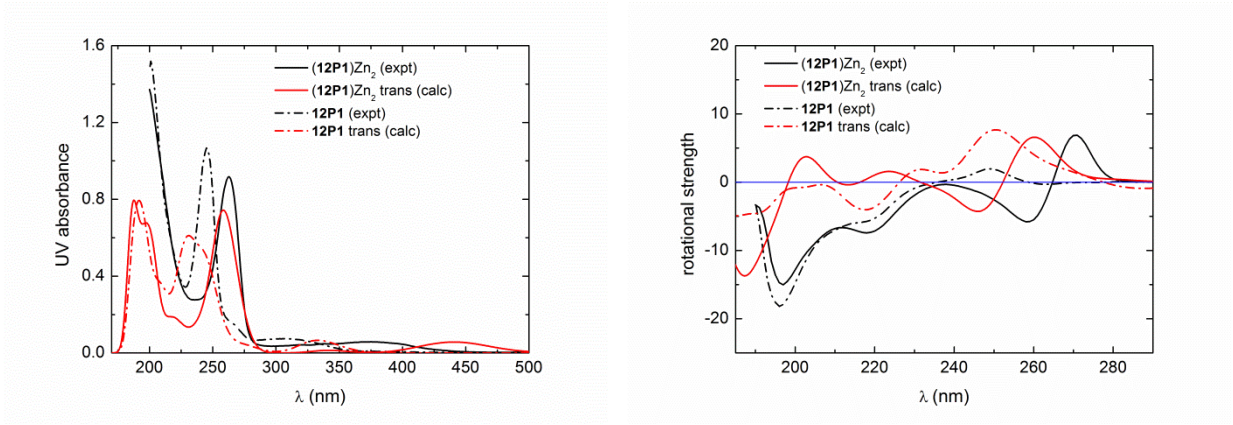


12P1, right-handed cis-PPI helix

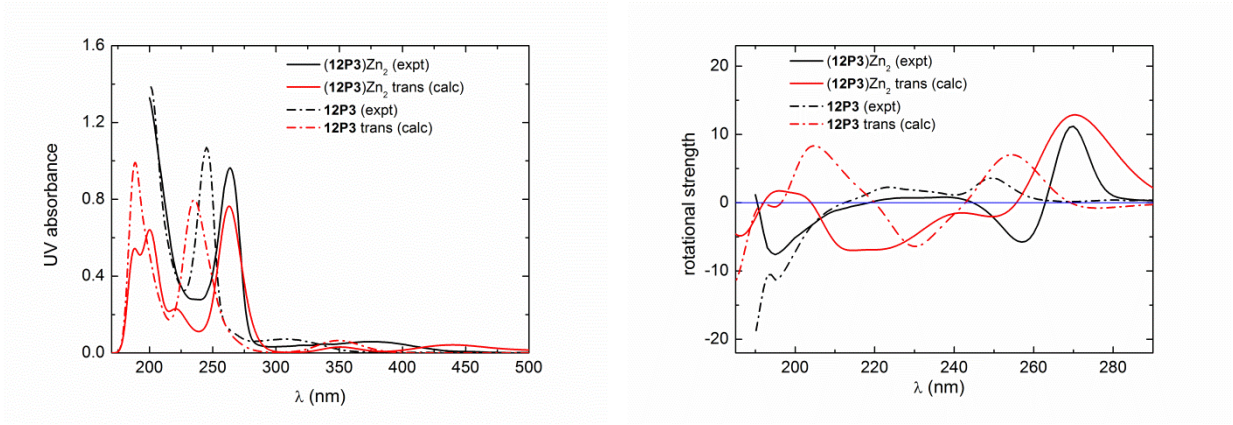


12P3 and (**12P3**)Zn_2, right-handed cis-PPI helix

Figure S78. Comparison of the sTD-BHLYP/def2-TZVP+COSMO computed and experimental UV (left) and CD (right) spectra of peptoids **12P1** and **12P3** with and without Zn(II)-coordination. The assignment of bands to excited electronic states is based on smaller model systems of free HQ, ZnQ_2, p4c and truncated ZnQ_2c molecules.



12P1 and (**12P1**)Zn_2, left-handed trans-PPII



12P3 and (**12P3**)Zn_2, left-handed trans-PPII

Figure S79. Comparison of the experimental and the sTD-BHLYP/def2-TZVP + COSMO computed UV-vis (left) and CD (right) spectra of **12P1** (top) and **12P3** (bottom) with and without Zn(II)-coordination, assuming high-lying left-handed, trans-PPII structures.

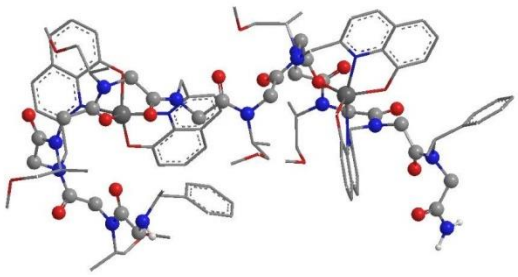
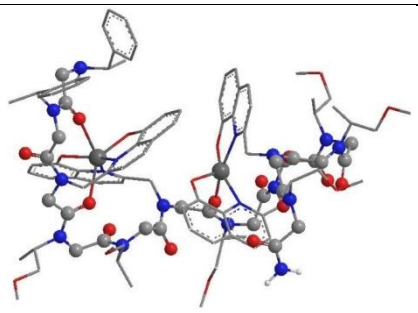
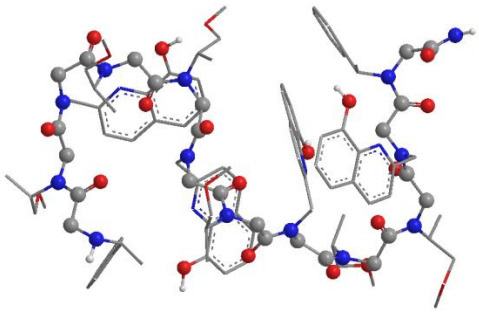
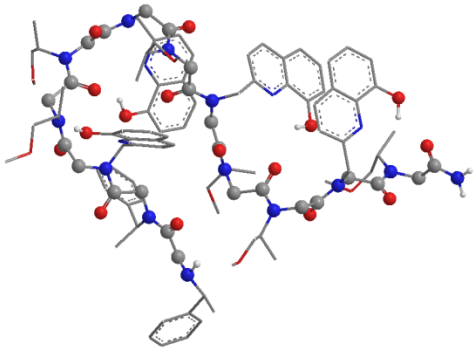
	
(**12P1**)Zn_2: trans PPII, 15.3 kal/mol	(**12P3**)Zn_2: trans PPII, 40.9 kcal/mol
	
12P1: trans PPII, 34.6 kal/mol	**12P3**: trans PPII, 12.3 kcal/mol

Figure S80. The TPSS-D3/def2-TZVP + COSMO (methanol) optimized **12P1** and **12P3** complexes assuming the left-handed trans-PPII helical structures, with (top) and without Zn(II)-coordination. The energies in kcal/mol are given relative to the corresponding cis-PPI structures. The main-chain C, N, O atoms and acidic H atoms (HQ hydroxyl and amide NH groups) are highlighted as grey, blue, red and white balls, respectively.

Table S8. The TPSS-D3/def2-TZVP + COSMO(methanol) optimized Cartesian coordinates (in Å, in the form of two-column list) of various structures, including the cis-PPI and trans-PPII structures of **12P1**, (**12P1**)Zn_2, **12P3** and (**12P3**)Zn_2 complexes as well as the **HQ**, **ZnQ_2**, **ZnQ_2c**, **p4c** and **p4t** model systems. For each structure, the number of atoms and total electronic energy at the TPSS-D3/def2-TZVP + COSMO(methanol) level are given, followed by the list of detailed atomic coordinate.

12P1_cis-PPI.xyz
274
Energy = -6631.948297450

N	-11.5372797	-18.1658676	2.4174691
C	-12.4297787	-16.9891868	2.6063978
C	-12.1844497	-19.4688427	2.3908380
H	-11.7446410	-16.1410802	2.6798044
H	-11.5821402	-20.2186612	2.9109095
C	-12.4435745	-19.9648366	0.9566631
O	-11.7716943	-19.5573366	0.0052863
C	-10.2599333	-17.9596957	2.0128896
C	-9.3492030	-19.1687443	1.7524588
O	-9.7805832	-16.8183706	1.8749881
N	-8.2321928	-19.2214894	2.6952085
H	-8.9687429	-19.0598848	0.7367741
C	-8.4519117	-19.8144663	4.0130030
H	-7.5617293	-20.3856312	4.2910411
H	-9.2904265	-20.5146449	3.9332866
C	-7.0359837	-18.6041359	2.4965207
C	-6.8295315	-17.8602873	1.1596641
O	-6.1523133	-18.6241904	3.3566294
N	-5.5579377	-17.1551692	1.1597678
H	-7.6625838	-17.1703203	1.0025148
C	-4.3921315	-17.7417907	0.4654525
H	-3.5352563	-17.1799345	0.8399043
C	-5.3655581	-16.0879298	1.9822114
C	-6.6313667	-15.5006942	2.6446937
O	-4.2607442	-15.5707506	2.1796944
N	-6.2845138	-14.3837413	3.5031623
H	-7.1661814	-16.2606732	3.2193306
C	-6.1870963	-12.9977480	2.9711899
H	-5.2118187	-12.6186522	3.2894753
C	-5.7489805	-14.6024912	4.7279608
C	-5.8087269	-16.0337556	5.2929507
O	-5.2593358	-13.6843343	5.4010902
N	-4.9784488	-16.1464489	6.4759489
H	-5.5398727	-16.7951289	4.5589277
C	-5.5652827	-15.9401954	7.7917596
H	-6.5045477	-15.3946238	7.6710335
H	-4.9026619	-15.3183963	8.3974644
C	-3.6656348	-16.4555867	6.4167711
C	-3.0905639	-16.7455442	5.0176682
O	-2.9422964	-16.4748824	7.4165849
N	-1.6389051	-16.6163327	5.0506478
H	-3.5117918	-16.0983196	4.2439282
C	-0.8097962	-17.8419015	4.9935861
H	0.2170128	-17.5008357	5.1377179
C	-1.0929048	-15.4255029	5.3719301
C	-2.0306506	-14.2163051	5.2653069
O	0.1210190	-15.2841356	5.6285192
N	-1.4858048	-13.0055177	5.8485562
H	-3.0109201	-14.4131982	5.6895981
C	-0.5673626	-12.2310082	4.9929208
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H    -3.7177113   -6.5825587   -0.4946576
H    -3.8374251   -5.5266672    0.9307319
H    -5.1794326   -5.6275342   -0.2418485
C    -3.8155317   -4.5634289   -2.4182803
H    -3.4617563   -5.5089130   -2.8596862
H    -3.3324667   -3.7301051   -2.9497814
C    -5.6266514   -4.3218202   -3.9068926
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H    -5.2412979   -3.3819243   -4.3298561
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H    -5.9185798   -3.8198854    5.8248987
H    -6.1934441   -4.4583411    4.1807617
C    -8.5266253   -3.9649425    5.0582058
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H    -9.4880720   -3.4479877    5.0405821
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O    -7.5229488   -2.9832400    4.7947652
H    -8.8094458    1.2217454    0.9044893
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O    -2.3406752    4.2371964   -0.5740125
C    -8.9068940   -2.5371428   -2.6672130
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H    -9.9387717   -2.8418208   -2.4631783
C    -9.6171861   -0.2080374   -3.4972141
C   -10.0858487    1.0609699   -3.1346974
C    -9.9121940   -0.6813623   -4.7822197
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H    -9.5575112   -1.6565829   -5.0997045
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(**12P1**)Zn_2_trans-PPII.xyz

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H	7.1366440	-8.2990195	-3.7826030
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H	-12.6095679	0.4201998	1.1773318

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H	-5.9581977	5.6672286	5.7718818
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C	7.0098699	1.4305794	4.8468675
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C   -12.2974589  -15.8412250    1.1237609
O   -11.1751003  -15.9131610    0.6181688
C   -10.2640896  -16.4487944    3.5115994
C   -10.4676669  -17.9072422    3.0333679
O    -9.1792495  -16.1150689    4.0021745
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H	-5.8076668	-17.9201892	-0.9991029
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H	-4.9630574	-3.0553892	4.6446587
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H	-2.5736734	-2.5356313	2.7851325
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H     5.2916440    1.2566152   -4.0056136
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HQ.xyz

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21
Energy = -516.7976260657
C     2.6100591    0.5014322   -1.3576495
H     3.6223846    0.5518174   -0.9382391
H     2.1023288   -0.3744934   -0.9492106
C     1.8417548    1.7502442   -1.0245400
C     0.0952514    2.7708206    0.0998480
C     1.5446772    4.1497648   -1.2416855
C     0.4201323    4.0699416   -0.3800808
H     1.8442002    5.1137819   -1.6450614
C    -1.0213990    2.5956707    0.9672977
C    -1.7855613    3.6827109    1.3448436
C    -1.4516136    4.9695734    0.8615820
C    -0.3767935    5.1733617    0.0176669
H    -2.6352688    3.5447946    2.0066230
H    -2.0636891    5.8130854    1.1681482
C     2.2423417    3.0080930   -1.5581945
H     3.1044807    3.0516228   -2.2172771
H    -0.1334023    6.1677084   -0.3459744
N     0.7926807    1.6430090   -0.2181534
O    -1.2934942    1.3322388    1.3975187
H     2.7151726    0.3870193   -2.4423098
H    -0.5941529    0.7772698    0.9725717
```

ZnQ$_2$.xyz

```
41
Energy = -2811.914939566
Zn   -0.0003387    0.0000109    0.9388335
N     0.7260262    1.5526840   -0.1660020
N    -0.7263541   -1.5527376   -0.1660838
O     1.1188151   -1.3540726    1.8044190
O    -1.1194561    1.3542341    1.8042122
C     0.0529734    2.6856536    0.1984921
C    -0.0530282   -2.6855825    0.1983432
C     0.4316455   -5.0758353   -0.0058076
C    -0.4312168    5.0760193   -0.0055676
C     0.2974153    3.9381639   -0.4308093
C    -0.2971543   -3.9380976   -0.4310606
C     0.9190866   -2.5416651    1.2520596
C    -0.9193558    2.5418499    1.2520303
C     1.3625886   -4.9344117    1.0082909
C    -1.3623552    4.9346988    1.0083609
C     1.2747665    3.9460901   -1.4579806
C    -1.2744495   -3.9461708   -1.4582960
```

```
C     1.6385653    1.5741585   -1.1372368
C    -1.6387870   -1.5743400   -1.1374055
C     1.6107234   -3.6945137    1.6332303
C    -1.6108445    3.6947951    1.6331592
C     1.9327531    2.7864483   -1.8051721
C    -1.9326621   -2.7866596   -1.8054499
C     2.3047693    0.2798521   -1.5037601
C    -2.3049858   -0.2801278   -1.5042472
H     0.2531740   -6.0366074   -0.4792173
H    -0.2523906    6.0368177   -0.4787900
H     1.5012043    4.8784645   -1.9688031
H    -1.5006638   -4.8785667   -1.9691791
H     1.9273028   -5.8021723    1.3399216
H    -1.9268851    5.8025629    1.3400344
H     2.4002206   -0.3663780   -0.6259423
H    -2.3980380    0.3674076   -0.6271430
H     2.3519772   -3.6221566    2.4244828
H    -2.3522373    3.6225261    2.4242891
H     1.7062777   -0.2532101   -2.2535959
H    -1.7079124    0.2514471   -2.2562670
H     2.6824515    2.7865387   -2.5895929
H    -2.6823144   -2.7868615   -2.5899162
H     3.2948573    0.4550502   -1.9308199
H    -3.2961642   -0.4553067   -1.9288101
```

ZnQ$_2$c_cis-PPI.xyz

```
76
Energy = -3761.254458930
C     0.5432778   -2.8843300    1.2705917
N     1.9848947   -2.7235699    1.0527281
H    -0.0219686   -2.3112744    0.5388195
C     2.8755578   -3.5356467    1.8916633
H     2.2515469   -4.2960374    2.3703020
H     3.3211962   -2.9202364    2.6825871
C     2.5651409   -1.7373542    0.3246634
C     1.6466445   -0.7683677   -0.4428860
O     3.7951666   -1.5970397    0.2984795
N     2.3572071   -0.0344206   -1.4763802
H     1.1859566   -0.0796991    0.2729675
C     3.1210262    1.0602967   -1.2244901
C     3.2016004    1.5055500    0.2482319
O     3.7393729    1.6699792   -2.1036061
N     4.2350298    2.5059235    0.4683048
H     3.3853130    0.6346726    0.8822575
C     5.5557732    2.2599258    0.2764612
C     5.9703553    0.8579417   -0.2058542
O     6.4096245    3.1423925    0.4472859
N     7.2239183    0.3930431    0.3835867
H     6.0654521    0.9290812   -1.2927006
C     7.1322959   -0.6234313    1.4271968
H     8.1574400   -0.9385777    1.6441752
H     6.5780377   -1.4882037    1.0407388
O     9.4980922    0.3106259    0.4349472
H     5.2120593    0.0977756   -0.0067201
C     6.4617595   -0.1604353    2.6975733
C     5.2881127   -0.7984132    4.6260406
C     5.7918551    1.5368350    4.2744955
C     5.1789427    0.5468347    5.0815814
H     5.7572486    2.5761991    4.5908693
C     4.7563454   -1.9029367    5.3835306
C     4.0902208   -1.5892636    6.5707705
C     3.9670213   -0.2535873    7.0072744
C     4.4973523    0.8077186    6.2953221
H     3.6705462   -2.3971040    7.1638902
H     3.4431586   -0.0616322    7.9402998
C     6.4357596    1.1892701    3.1060102
H     6.9153998    1.9374513    2.4852774
H     4.4057997    1.8293923    6.6513359
N     5.9056725   -1.1100062    3.4481169
O     4.9184912   -3.1391894    4.9393875
H     2.2449497    1.9398001    0.5488004
```

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H     0.8294119   -1.3033669   -0.9298970
H     0.2805215   -3.9400041    1.1673778
C     3.9808875   -4.2056125    1.1131355
C     3.7344751   -4.9084124   -0.0861241
C     6.2552963   -4.7630579    1.0111210
C     4.7762323   -5.5271764   -0.7402481
H     2.7255238   -4.9440299   -0.4833338
C     6.0913405   -5.4755660   -0.2102037
H     4.5985801   -6.0653040   -1.6676941
N     5.2029300   -4.1480917    1.6289838
C     7.5362588   -4.6417750    1.6597487
C     7.2238415   -6.0778164   -0.8087036
C     8.4549220   -5.9555419   -0.1866886
H     9.3294286   -6.4141064   -0.6415777
C     8.6207760   -5.2542446    1.0248530
H     9.6037631   -5.1802397    1.4816012
H     7.1137490   -6.6231142   -1.7411919
O     7.6325357   -3.9759766    2.7984410
Zn    5.9088638   -3.1474683    3.2499226
C     2.3709905   -0.6452649   -2.8077713
H     1.3449812   -0.7849190   -3.1601269
H     2.9112667    0.0154027   -3.4830191
H     2.8747213   -1.6178704   -2.7645304
C     8.4626999    0.7299350   -0.1026418
C     8.5110490    1.5903662   -1.3471333
H     8.1154605    1.0323967   -2.2047552
H     7.9202872    2.5003010   -1.2237759
H     9.5526086    1.8440951   -1.5442747
C     3.8367682    3.8871316    0.7652591
H     4.5057206    4.3019652    1.5207768
H     3.8910045    4.5098883   -0.1346018
H     2.8131246    3.8801732    1.1407006
H     0.2681815   -2.5443041    2.2752288
```

p4c_cis-PPI.xyz

```
45
Energy = -1030.428072211
C     0.7641806   -2.8226235    1.0251673
N     2.1842852   -2.6965613    0.6992905
H     0.2010031   -1.9609787    0.6733601
C     3.0522481   -3.7332579    1.2585914
H     2.7987998   -4.7092060    0.8289908
H     2.9119270   -3.7763993    2.3434221
C     2.7076073   -1.7455572   -0.1081737
C     1.7313931   -0.6817825   -0.6657997
O     3.9131978   -1.6831848   -0.3929605
N     2.4050830    0.2171501   -1.5868751
H     1.2800399   -0.1185916    0.1559189
C     3.2541532    1.1831871   -1.1478193
C     3.2190880    1.4921315    0.3655339
O     4.0004849    1.8192717   -1.8994066
N     4.2069405    2.4961377    0.7203774
H     3.3844507    0.5801269    0.9430315
C     5.5290818    2.1836978    0.8086456
C     5.8627373    0.6803762    0.8752940
O     6.4183535    3.0392045    0.8787063
N     7.2925594    0.4373457    0.8701356
H     5.3859795    0.1341346    0.0596567
C     7.9841214    0.5365453    2.1547905
H     9.0270644    0.2617857    2.0052044
H     7.5170205   -0.1462709    2.8720493
O     9.2388743    0.1904900   -0.2885887
H     5.4483470    0.2708449    1.8041153
H     2.2301076    1.8713531    0.6406344
H     0.9136584   -1.1624351   -1.2081405
H     0.3510931   -3.7295237    0.5686086
C     2.4811307   -0.2139097   -2.9850748
H     1.4816989   -0.5023066   -3.3198331
H     2.8518151    0.6156284   -3.5848106
H     3.1615756   -1.0674767   -3.0850509
C     8.0009262    0.3088532   -0.2874559
```

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C     7.2088859    0.2911509   -1.5814338
H     6.5359725   -0.5730934   -1.6170013
H     6.5903782    1.1873099   -1.6926156
H     7.9153699    0.2290084   -2.4091676
C     3.8091308    3.8985035    0.5785103
H     4.5648521    4.5238933    1.0517816
H     3.7225824    4.1687318   -0.4798556
H     2.8439667    4.0407163    1.0713505
H     0.6505359   -2.8930021    2.1117719
H     7.9221903    1.5604549    2.5379315
H     4.0851664   -3.4830569    1.0235847
```

p4t_trans-PPII.xyz

```
45
Energy = -1030.426915564
C    -2.7292144  -13.9363025    8.0202620
N    -2.9111917  -13.5322363    9.4138941
H    -2.1174408  -14.8365079    7.9948906
C    -3.7265040  -12.3359527    9.6157153
H    -3.9217920  -12.1675826   10.6726177
C    -2.2941092  -14.2201568   10.4064232
C    -2.5051733  -13.7035393   11.8452529
O    -1.5903743  -15.2193610   10.2011091
N    -1.7788037  -14.5198883   12.8020828
H    -3.5668837  -13.7389799   12.0992371
C    -0.3511092  -14.2398706   12.9689280
H     0.0107777  -14.6542383   13.9094956
C    -2.3752369  -15.6621424   13.2353406
C    -1.5159906  -16.5984236   14.1032835
O    -3.5505040  -15.9410482   12.9702521
N    -2.2630101  -17.7817680   14.4907731
H    -1.1980762  -16.0755150   15.0083810
C    -2.3616255  -18.8581952   13.5024538
H    -3.1016152  -18.6165181   12.7313168
H    -2.6291938  -19.7966063   13.9872986
C    -3.0667609  -17.6902618   15.5840233
C    -3.9894030  -18.8897724   15.8568206
O    -3.0539205  -16.7083596   16.3362122
N    -4.8308249  -18.6585600   17.0160172
H    -3.3862312  -19.7825843   16.0383615
C    -6.0129583  -17.8226538   16.8060532
H    -6.6887271  -17.9022914   17.6555878
C    -4.3448794  -19.0023221   18.2420673
C    -5.1802624  -18.6453627   19.4556439
O    -3.2634253  -19.6050776   18.3600746
H    -6.1769144  -19.0960653   19.4035373
H    -5.3071624  -17.5608827   19.5402569
H    -4.6312226  -19.0709290   14.9887885
H    -0.6254436  -16.9118082   13.5502545
H    -2.1559022  -12.6709253   11.9353986
H    -3.7052689  -14.1342532    7.5641361
H    -4.6844352  -12.4621779    9.1001511
H    -3.2189830  -11.4564152    9.2017621
H    -0.2138673  -13.1561270   12.9980890
H     0.2290536  -14.6531002   12.1362807
H    -1.3831465  -18.9843438   13.0326524
H    -6.5364648  -18.1734495   15.9118975
H    -5.7252955  -16.7747670   16.6649720
H    -4.6647644  -19.0168435   20.3413595
H    -2.2340167  -13.1341620    7.4608929
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