Chiral Cu(II), Co(II) and Ni(II) complexes based on 2,2’-bipyridine modified peptoids

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Supporting Information

Table S1. Peptoid oligomer sequences and their molecular weights.

Ns1npe = (S)-N-(1-naphthylethyl)glycine, Nbp-(2,2’-bipyridine-3’-yloxy) ethylamine, Ns1tbe -

<table>
<thead>
<tr>
<th>Peptoid oligomers</th>
<th>Molecular weight</th>
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<tr>
<td></td>
<td>Calc: Found (gr/mol)</td>
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<tr>
<td>6P1 (Ns1tbe-Nbp-Ns1tbe-Ns1tbe-Nbp-Ns1tbe)</td>
<td>1092.42 : 1092.77</td>
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<tr>
<td>6P1Ac (Ns1tbe-Nbp-Ns1tbe-Ns1tbe-Nbp-Ns1tbe-Ac)</td>
<td>1134.45 : 1135.47</td>
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<td>4P1 (Nbp-Ns1tbe-Ns1tbe-Nbp)</td>
<td>810.00 : 810.58</td>
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<tr>
<td>4P1Ac (Nbp-Ns1tbe-Ns1tbe-Nbp-Ac)</td>
<td>852.03 : 852.66</td>
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<tr>
<td>6P2 (Ns1npe-Nbp-Ns1npe-Ns1npe-Nbp-Ns1npe)</td>
<td>1372.61 : 1372.55</td>
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<tr>
<td>6P2Ac (Ns1npe-Nbp-Ns1npe-Ns1npe-Nbp-Ns1npe-Ac)</td>
<td>1414.65 : 1414.78</td>
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<td>4P2Ac (Nbp-Ns1npe-Ns1npe-Nbp-Ac)</td>
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(S)-N-(1-tert-butylethyl)glycine, Ac= acetylated.

Electronic Supplementary Material (ESI) for Dalton Transactions.
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**Table S2.** Molecular weights of the Peptoid metal complexes.

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<td>(C3B)Co</td>
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<td>(R-C3B)Cu</td>
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<tr>
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HPLC of peptoid oligomers

Figure S1. HPLC traces of purified peptoid oligomer 6P1 at 214nm.

Figure S2. HPLC traces of purified peptoid oligomer 6P1Ac at 214nm.
Figure S3. HPLC traces of purified peptoid oligomer 4P1 at 214nm.

Figure S4. HPLC traces of purified peptoid oligomer 4P1Ac at 214nm.
Figure S5. HPLC traces of purified peptoid oligomer 6P2 at 214nm.

Figure S6. HPLC traces of purified peptoid oligomer 6P2Ac at 214nm.
Figure S7. HPLC traces of purified peptoid oligomer 4P2 at 214nm.

Figure S8. HPLC traces of purified peptoid oligomer 4P2Ac at 214nm.
UV-VIS Spectroscopy

Figure S9. UV-Vis titration of L2B (17 µM) with Cu$^{2+}$ acetate in ACN.

Figure S10. UV-Vis titration of L2B (17 µM) with Co$^{2+}$ acetate in ACN.
**Figure S11.** UV-Vis titration of L2B (17 μM) with Ni$^{2+}$ acetate in ACN.

**Figure S12.** UV-Vis titration of R-L2B (17 μM) with Cu$^{2+}$ acetate in ACN.
Figure S13. UV-Vis titration of R-L2B (17 µM) with Co$^{2+}$ acetate in ACN.

Figure S14. UV-Vis titration of R-L2B (17 µM) with Ni$^{2+}$ acetate in ACN.
Figure S15. UV-Vis titration of C3B (17 µM) with Cu$^{2+}$ acetate in ACN.

Figure S16. UV-Vis titration of C3B (17 µM) with Co$^{2+}$ acetate in ACN.
Figure S17. UV-Vis titration of C3B (17 µM) with Ni^{2+} acetate in ACN.

Figure S18. UV-Vis titration of R-C3B (17 µM) with Cu^{2+} acetate in ACN.
Figure S19. UV-Vis titration of R-C3B (17 μM) with Co\(^{2+}\) acetate in ACN.

Figure S20. UV-Vis titration of R-C3B (17 μM) with Ni\(^{2+}\) acetate in ACN.
Figure S21. UV-Vis titration of 6P1 (17 µM) with Cu$^{2+}$ acetate in ACN.

Figure S22. UV-Vis titration of 6P1 (17 µM) with Co$^{2+}$ acetate in ACN.
**Figure S23.** UV-Vis titration of 6P1 (17 µM) with Ni²⁺ acetate in ACN.

**Figure S24.** UV-Vis titration of 6P2 (17 µM) with Cu²⁺ acetate in ACN.
**Figure S25.** UV-Vis titration of 6P2 (17 µM) with Co$^{2+}$ acetate in ACN.

**Figure S26.** UV-Vis titration of 6P2 (17 µM) with Ni$^{2+}$ acetate in ACN.
Figure S27. UV-Vis titration of 4P1 (17 μM) with Cu\(^{2+}\) acetate in ACN.

Figure S28. UV-Vis titration of 4P1 (17 μM) with Co\(^{2+}\) acetate in ACN.
Figure S29. UV-Vis titration of 4P1 (17 µM) with Ni^{2+} acetate in ACN.

Figure S30. UV-Vis titration of 4P2 (17 µM) with Cu^{2+} acetate in ACN.
Figure S31. UV-Vis titration of 4P2 (17 µM) with Co^{2+} acetate in ACN.

Figure S32. UV-Vis titration of 4P2 (17 µM) with Ni^{2+} acetate in ACN.
Figure S33. UV-Vis titration of 4P1Ac (17 µM) with Cu$^{2+}$ acetate in ACN.

Figure S34. UV-Vis titration of 4P1Ac (17 µM) with Co$^{2+}$ acetate in ACN.
**Figure S35.** UV-Vis titration of 4P1Ac (17 µM) with Ni$^{2+}$ acetate in ACN.

**Figure S36.** UV-Vis titration of 4P2Ac (17 µM) with Cu$^{2+}$ acetate in ACN.
**Figure S37.** UV-Vis titration of 4P2Ac (17 µM) with Co$^{2+}$ acetate in ACN.

**Figure S38.** UV-Vis titration of 4P2Ac (17 µM) with Ni$^{2+}$ acetate in ACN.
**Job plot data**

**Figure S39.** Job-plot of peptoid oligomers with metal ions measured in acetonitrile (22-66 µM total concentration).
**CD data**

**Figure S40.** CD spectra of the peptoid oligomer 4P1 and its metal complexes measured at the concentration of 100 µM in ACN solution.

**Figure S41.** CD spectra of the peptoid oligomer 4P2 and its metal complexes measured at the concentration of 100 µM in ACN solution.
**Figure S42.** CD spectra of the peptoid oligomer 6P1Ac and its metal complexes measured at the concentration of 100 µM in ACN solution.

**Figure S43.** CD spectra of the peptoid oligomer 6P2Ac and its metal complexes measured at the concentration of 100 µM in ACN solution.
FTIR data

Figure S44. ATR-FTIR spectra of the peptoid oligomer 4P1 and its Cu$^{2+}$ complex.

Figure S45. ATR-FTIR spectra of the peptoid oligomer 6P1 and its Cu$^{2+}$ complex.
ESI-MS of the peptoid oligomers:

Figure S46. ESI-MS traces of peptoid oligomer 6P1

Figure S47. ESI-MS traces of peptoid oligomer 6P1Ac
Figure S48. ESI-MS traces of peptoid oligomer 4P1

Figure S49. ESI-MS traces of peptoid oligomer 4P1Ac
Figure S50. ESI-MS traces of peptoid oligomer 6P2

Figure S51. ESI-MS traces of peptoid oligomer 6P2Ac
Figure S52. ESI-MS traces of peptoid oligomer 4P2

Figure S53. ESI-MS traces of peptoid oligomer 4P2Ac
ESI-MS of the metallopeptoids:

Figure S54. ESI-MS traces of L2BCu complex.

Figure S55. ESI-MS m/z traces of [L2BCu+TFA]^+ (bottom) and calculated ESI-MS spectrum (top).
Figure S56. ESI-MS traces of L2BCo complex

Figure S57. ESI-MS m/z traces of L2BCo (bottom) and calculated ESI-MS spectrum (top).
Figure S58. ESI-MS traces of L2BNi complex.

Figure S59. ESI-MS m/z traces of L2BNi (bottom) and calculated ESI-MS spectrum (top).
Figure S60. ESI-MS traces of R-L2BCu complex.

Figure S61. ESI-MS m/z traces of R-L2BCu (bottom) and calculated ESI-MS spectrum (top).
Figure S62. ESI-MS traces of R-L2BCo complex.

Figure S63. ESI-MS m/z traces of R-L2BCo (bottom) and calculated ESI-MS spectrum (top).
Figure S64. ESI-MS traces of R-L2BNi complex.

Figure S65. ESI-MS m/z traces of R-L2BNi (bottom) and calculated ESI-MS spectrum (top).
Figure S66. ESI-MS traces of C3BCu complex.

Figure S67. ESI-MS m/z traces of C3BCu (bottom) and calculated ESI-MS spectrum (top).
Figure S68. ESI-MS traces of C3BCo complex.

Figure S69. ESI-MS m/z traces of [C3BCo-TFA]^+ (bottom) and calculated ESI-MS spectrum (top).
Figure S70. ESI-MS traces of C3B Ni complex.

Figure S71. ESI-MS m/z traces of [C3B Ni-TFA]⁺ (bottom) and calculated ESI-MS spectrum (top).
Figure S72. ESI-MS traces of R-C3BCu complex.

Figure S73. ESI-MS m/z traces of [R-C3BCu-TFA]$^+$ (bottom) and calculated ESI-MS spectrum (top).
Figure S74. ESI-MS traces of R-C3BCo complex.

Figure S75. ESI-MS m/z traces of [R-C3BCo-TFA]⁺ (bottom) and calculated ESI-MS spectrum (top).
Figure S76. ESI-MS traces of R-C3B Ni complex.

Figure S77. ESI-MS m/z traces of R-C3B Ni (bottom) and calculated ESI-MS spectrum (top).
Figure S78. ESI-MS traces of 6P1Cu complex.

Figure S79. ESI-MS m/z traces of 6P1Cu (bottom) and calculated ESI-MS spectrum (top).
Figure S80. ESI-MS traces of 6P1Co complex.

Chemical Formula: \( C_{60}H_{89}CoN_{11}O_8 \)
Exact Mass: 1150.62
Molecular Weight: 1151.35

Figure S81. ESI-MS m/z traces of 6P1Co (bottom) and calculated ESI-MS spectrum (top).
Figure S82. ESI-MS traces of 6P1Ni complex.

Figure S83. ESI-MS m/z traces of 6P1Ni (bottom) and calculated ESI-MS spectrum (top).
**Figure S84.** ESI-MS traces of 6P1AcCu complex.

**Figure S85.** ESI-MS m/z traces of 6P1AcCu (bottom) and calculated ESI-MS spectrum (top).
Figure S86. ESI-MS traces of 6P1AcCo complex.

Figure S87. ESI-MS m/z traces of 6P1AcCo (bottom) and calculated ESI-MS spectrum (top).
Figure S88. ESI-MS traces of 6P1AcNi complex.

Figure S89. ESI-MS m/z traces of 6P1AcNi (bottom) and calculated ESI-MS spectrum (top).
Figure S90. ESI-MS traces of 4P1Cu complex.

Figure S91. ESI-MS m/z traces of 4P1Cu (bottom) and calculated ESI-MS spectrum (top).
Figure S92. ESI-MS traces of 4P1Co complex.

Figure S93. ESI-MS m/z traces of 4P1Co (bottom) and calculated ESI-MS spectrum (top).
Figure S94. ESI-MS traces of 4P1Ni complex.

Figure S95. ESI-MS m/z traces of 4P1Ni (bottom) and calculated ESI-MS spectrum (top).
Figure S96. ESI-MS traces of 4P1AcCu complex.

Figure S97. ESI-MS m/z traces of 4P1AcCu (bottom) and calculated ESI-MS spectrum (top).
Figure S98. ESI-MS traces of 4P1AcCo complex.

Figure S99. ESI-MS m/z traces of 4P1AcCo (bottom) and calculated ESI-MS spectrum (top).
**Figure S100.** ESI-MS traces of 4P1AcNi complex.

**Figure S101.** ESI-MS m/z traces of 4P1AcNi (bottom) and calculated ESI-MS spectrum (top).
Figure S102. ESI-MS traces of 6P2Cu complex.

Figure S103. ESI-MS m/z traces of [6P2Cu-TFA]⁺ (bottom) and calculated ESI-MS spectrum (top).
Figure S104. ESI-MS traces of 6P2Co complex.

Figure S105. ESI-MS m/z traces of [6P2Co-TFA]+ (bottom) and calculated ESI-MS spectrum (top).
**Figure S106.** ESI-MS traces of 6P2Ni complex.

**Figure S107.** ESI-MS m/z traces of [6P2Ni-TFA]$^+$ (bottom) and calculated ESI-MS spectrum (top).
Figure S108. ESI-MS traces of 6P2AcCu complex.

Figure S109. ESI-MS m/z traces of 6P2AcCu (bottom) and calculated ESI-MS spectrum (top).
Figure S110. ESI-MS traces of 6P2AcCo complex.

Figure S111. ESI-MS m/z traces of 6P2AcCo (bottom) and calculated ESI-MS spectrum (top).
Figure S112. ESI-MS traces of 6P2AcNi complex.

Figure S113. ESI-MS m/z traces of 6P2AcNi (bottom) and calculated ESI-MS spectrum (top).
Figure S114. ESI-MS traces of 4P2Cu complex.

Figure S115. ESI-MS m/z traces of 4P2Cu (bottom) and calculated ESI-MS spectrum (top).
Figure S116. ESI-MS traces of 4P2Co complex.

Figure S117. ESI-MS m/z traces of [4P2Co-TFA]$^+$ (bottom) and calculated ESI-MS spectrum (top).
Figure S118. ESI-MS traces of 4P2Ni complex.

Figure S119. ESI-MS m/z traces of $[4P2Ni\text{-TFA}]^+$ (bottom) and calculated ESI-MS spectrum (top).
Figure S120. ESI-MS traces of 4P2AcCu complex.

Figure S121. ESI-MS m/z traces of 4P2AcCu (bottom) and calculated ESI-MS spectrum (top).
Figure S122. ESI-MS traces of 4P2AcCo complex.

Figure S123. ESI-MS m/z traces of 4P2AcCo (bottom) and calculated ESI-MS spectrum (top).
Figure S124. ESI-MS traces of 4P2AcNi complex.

Figure S125. ESI-MS m/z traces of 4P2AcNi (bottom) and calculated ESI-MS spectrum (top).