Supplementary Information

Dipicolylamine as a unique structural switching element for helical peptides

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Fig. S1. The molar ellipticities of peptide 1 at 222 nm ($[\theta]_{222}$) as a function of the ratio of metal ions to each peptide [Fe(II), orange; Cu(II), blue; Ni(II), green; Co(II), red; Zn(II), purple]. The sample contained 30 µM peptide in 10 mM MOPS containing 100 mM NaCl (pH 7.0).



Fig. S2. (a) The $[\theta]_{222}$ of peptide **2** (30 µM) is shown in the absence (black) or presence of 150 µM metal ions [Fe(II), orange; Cu(II), blue; Co(II), red; Zn(II), purple] and after addition of excess EDTA (1 mM). (b) Changes in the CD spectra of peptide **2** are shown in the absence (black) or presence of 150 µM of Ni(II) (green) and after the addition of excess EDTA (1 mM) (blue). The inset shows these spectra around 260 nm. The peak around 260 nm, which was induced by the addition of Ni(II), disappeared after the addition of EDTA.



Fig. S3. ITC measurement in the complex of peptide 2 with (a) Fe(II) and (b) Co(II). The sample contained 30 μ M peptide in 10 mM MOPS containing 100 mM NaCl (pH 7.0).



Fig. S4. Thermal denaturing curve of (a) peptides 2 and (b) 1 in the absence (black) or presence (green) of Ni(II) (1.2 equivalents). Insets show these of the temperature derivatives. The samples contained 30 μ M peptide and 36 μ M Ni(II) in 10 mM MOPS containing 100 mM NaCl (pH 7.0).



Fig. S5. Difference values of $[\theta]_{222}$ of the Fe(II)-peptide **2** complex are given before and after the addition of other metal ions. The Fe(II)-peptide **2** complex was formed in the presence of two equivalents of Fe(II) prior to the addition of other metal ions [Ni(II), Cu(II), Co(II), Zn(II), Al(III), Mn(II), Pb(II), Cd(II) and Ag(I) (20 equivalents per peptide); Ca(II) and Mg(II) (10,000 equivalents)]. Each $\Delta[\theta]_{222}$ was calculated by subtracting the $[\theta]_{222}$ value after the addition of a metal ion from that of the Fe(II)-peptide **2** complex in the absence of metals. The samples contained 30 μ M peptide and 60 μ M Fe(II) in 10 mM MOPS containing 100 mM NaCl (pH 7.0).



Fig. S6. (a) Effects of metal ion addition on $[\theta]_{222}$ of the Ni(II)-peptide 2 complex. The Ni(II)-peptide 2 complex was formed in the presence of one equivalent of Ni(II) prior to the addition of other metal ions [Fe(II), orange; Cu(II), blue; Co(II), red; Zn(II), purple]. (b) CD spectral changes of the Ni(II)-peptide 2 complex by addition of Cu(II). The samples contained 30 μ M peptide and 30 μ M Ni(II) in 10 mM MOPS containing 100 mM NaCl (pH 7.0).