Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary materials

Specificity of the Zn^{2+}, Cd^{2+} and Ni^{2+} ion binding sites in the loop domain of the HypA protein

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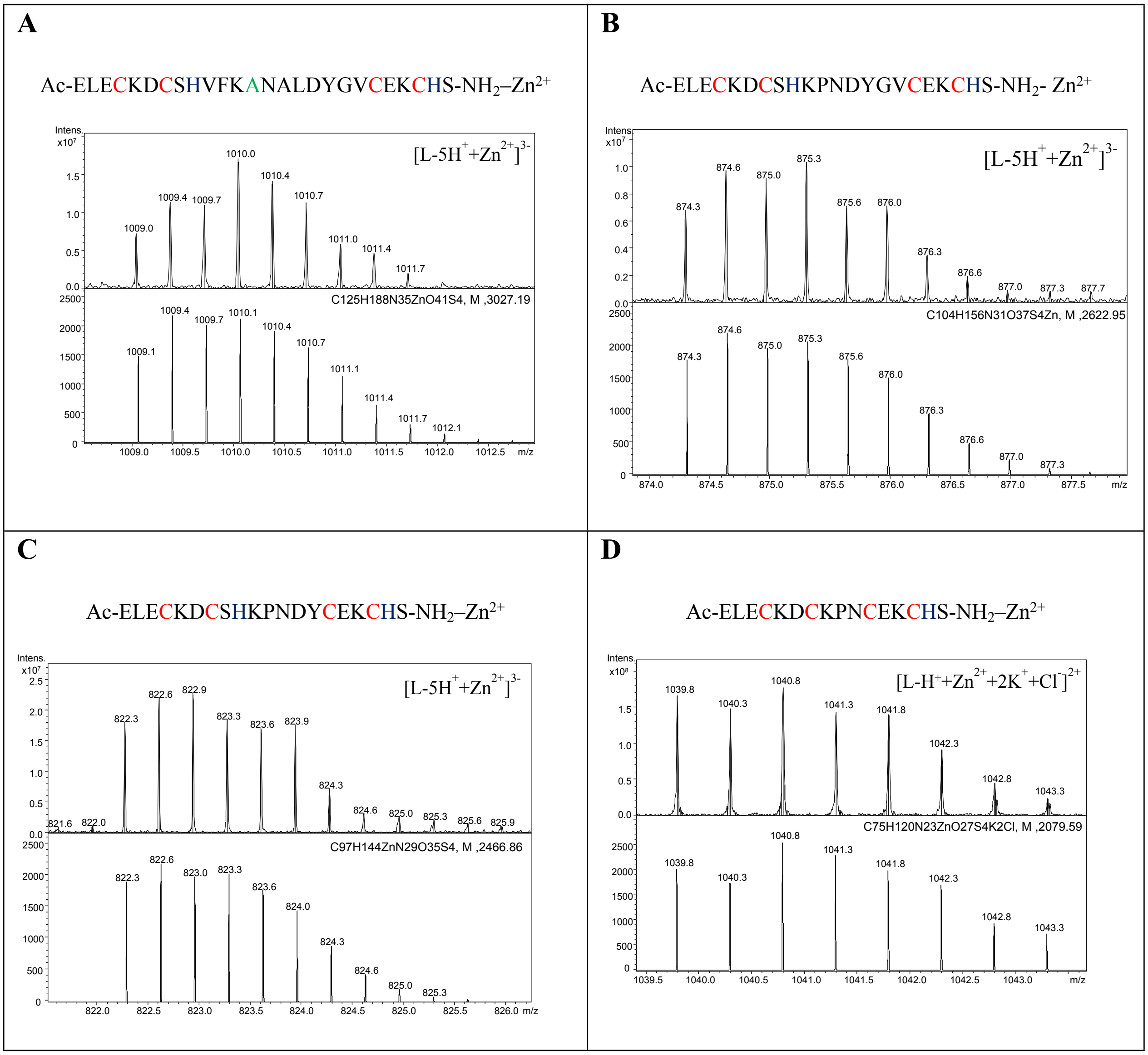

Fig. S1. Mass spectra of a system containing Zn^{2+} and A) HypA1, B) HypA2, C) HypA3 and D) HypA4 peptide. Upper spectrum- experimental, spectrum below- simulated.

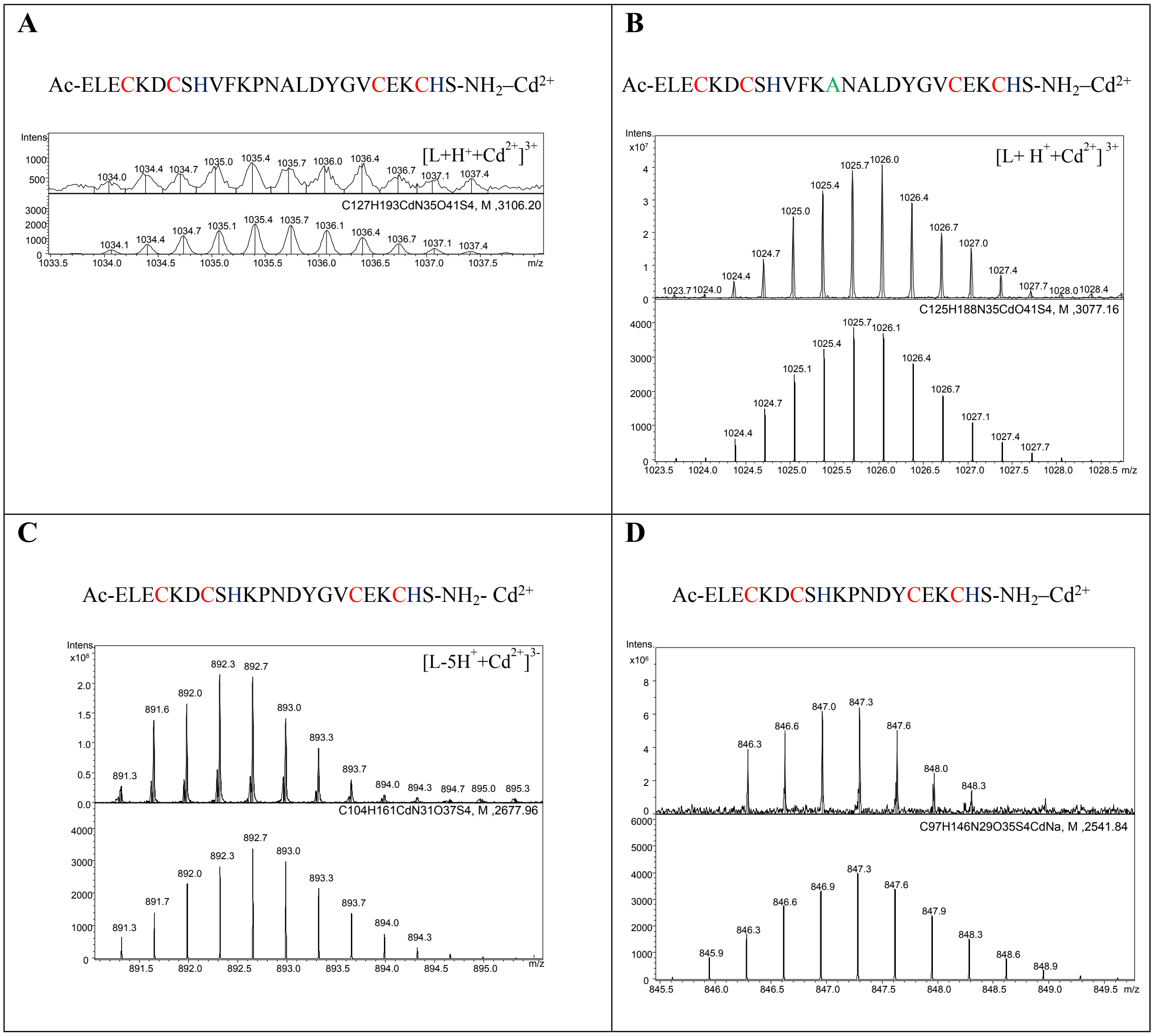

Fig. S2. Mass spectra of a system containing Cd^{2+} and A) HypA WT, B) HypA1, C) HypA2 and D) HypA3 peptide. Upper spectrum- experimental, spectrum below- simulated.

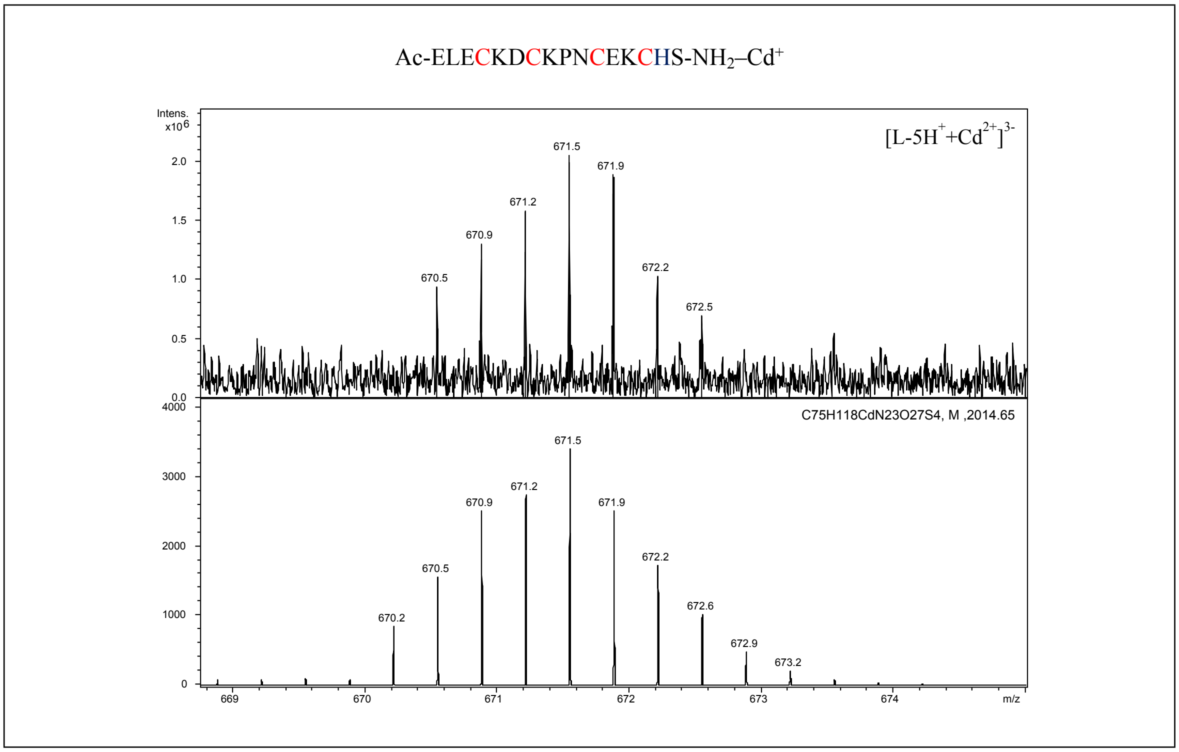

Fig. S3. Mass spectra of a system containing Cd^{2+} and HypA4 peptide. Upper spectrum- experimental, spectrum below- simulated.

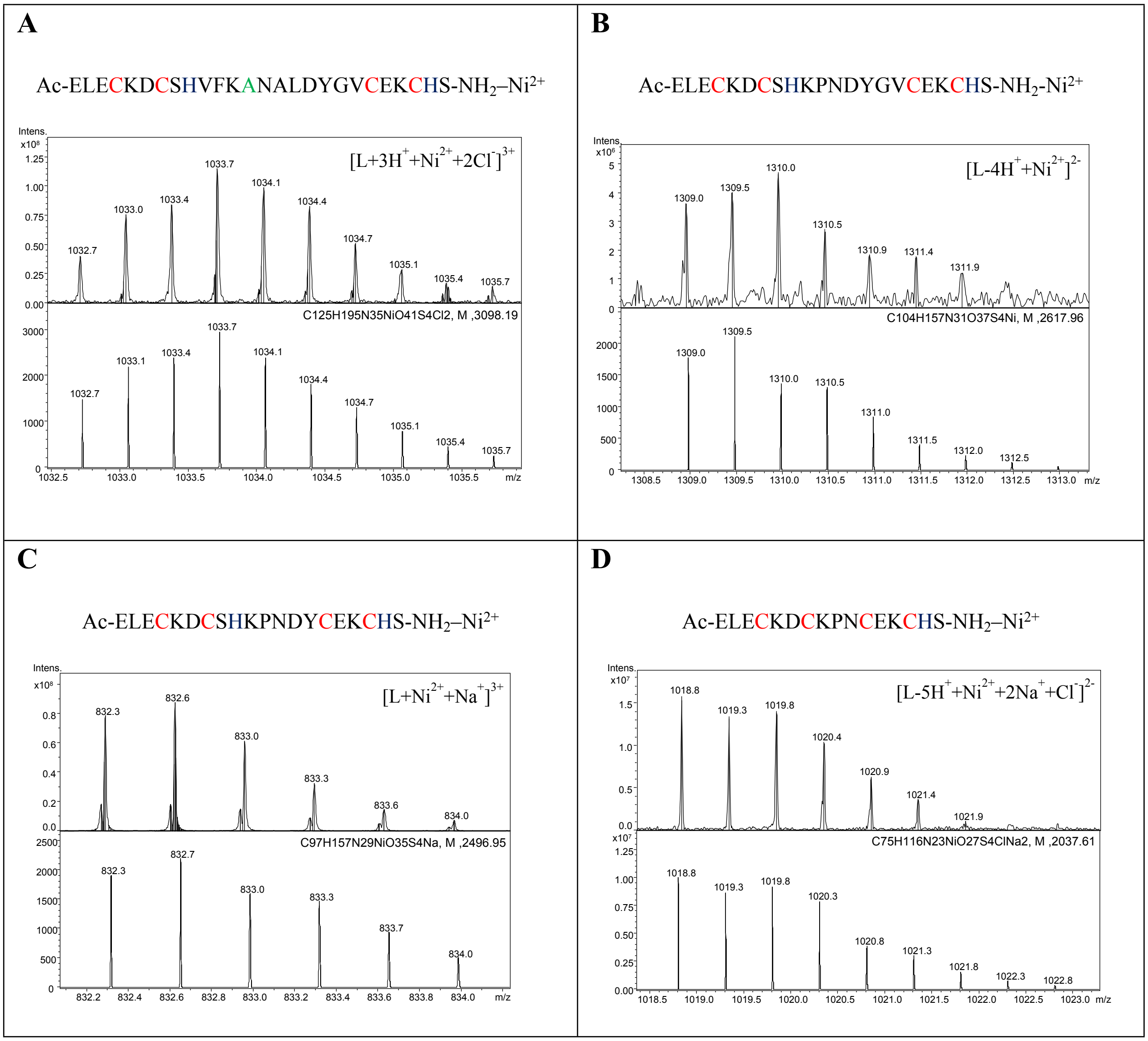

Fig. S4. Mass spectra of a system containing Ni^{2+} and A) HypA1, B) HypA2, C) HypA3 and D) HypA4 peptide. Upper spectrum- experimental, spectrum below- simulated.

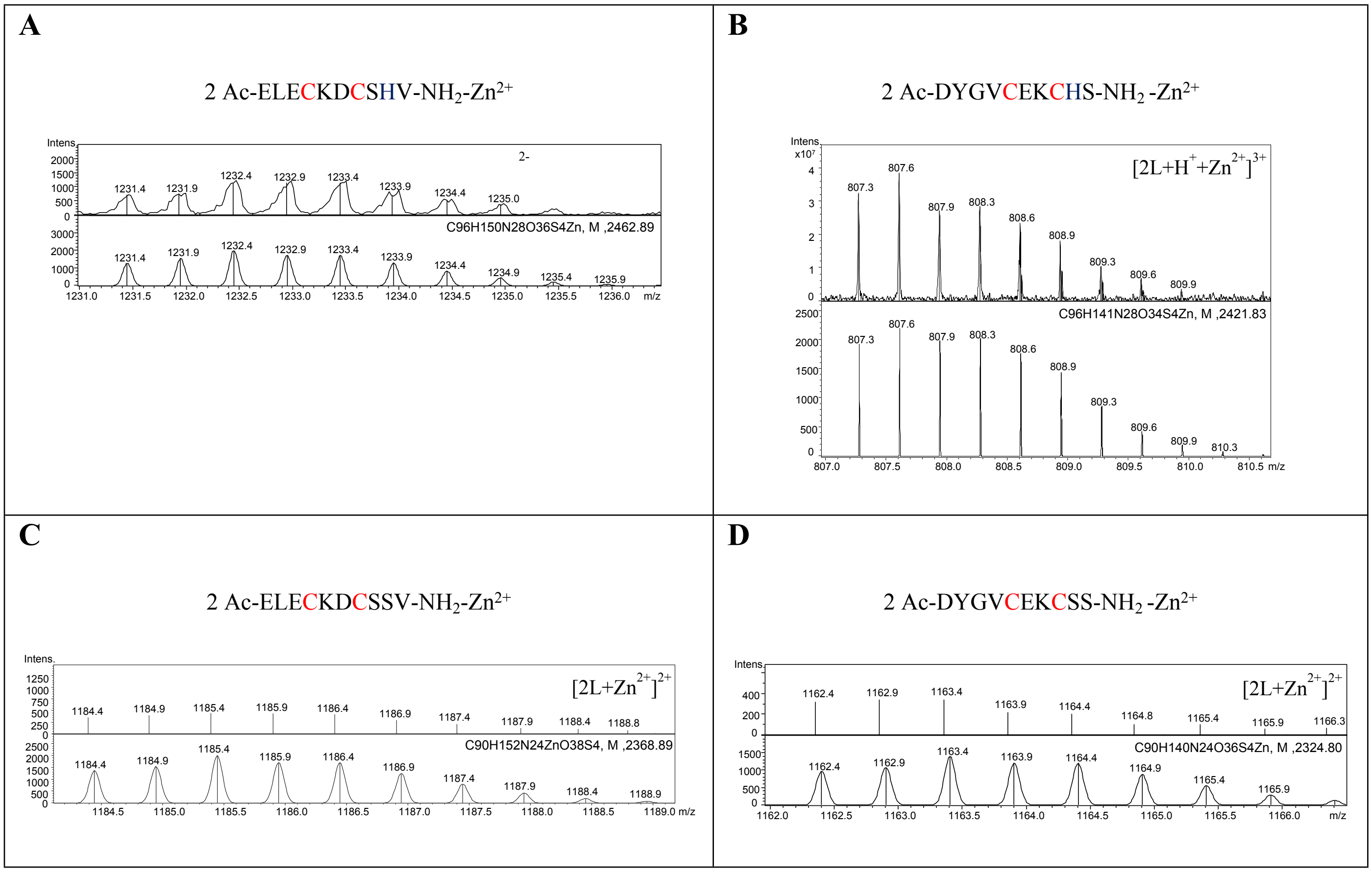

Fig. S5. Mass spectra of a system containing Zn^{2+} and A) ELE, B) DYG, C) ELES and D) DYGS peptide. Upper spectrum- experimental, spectrum below- simulated.

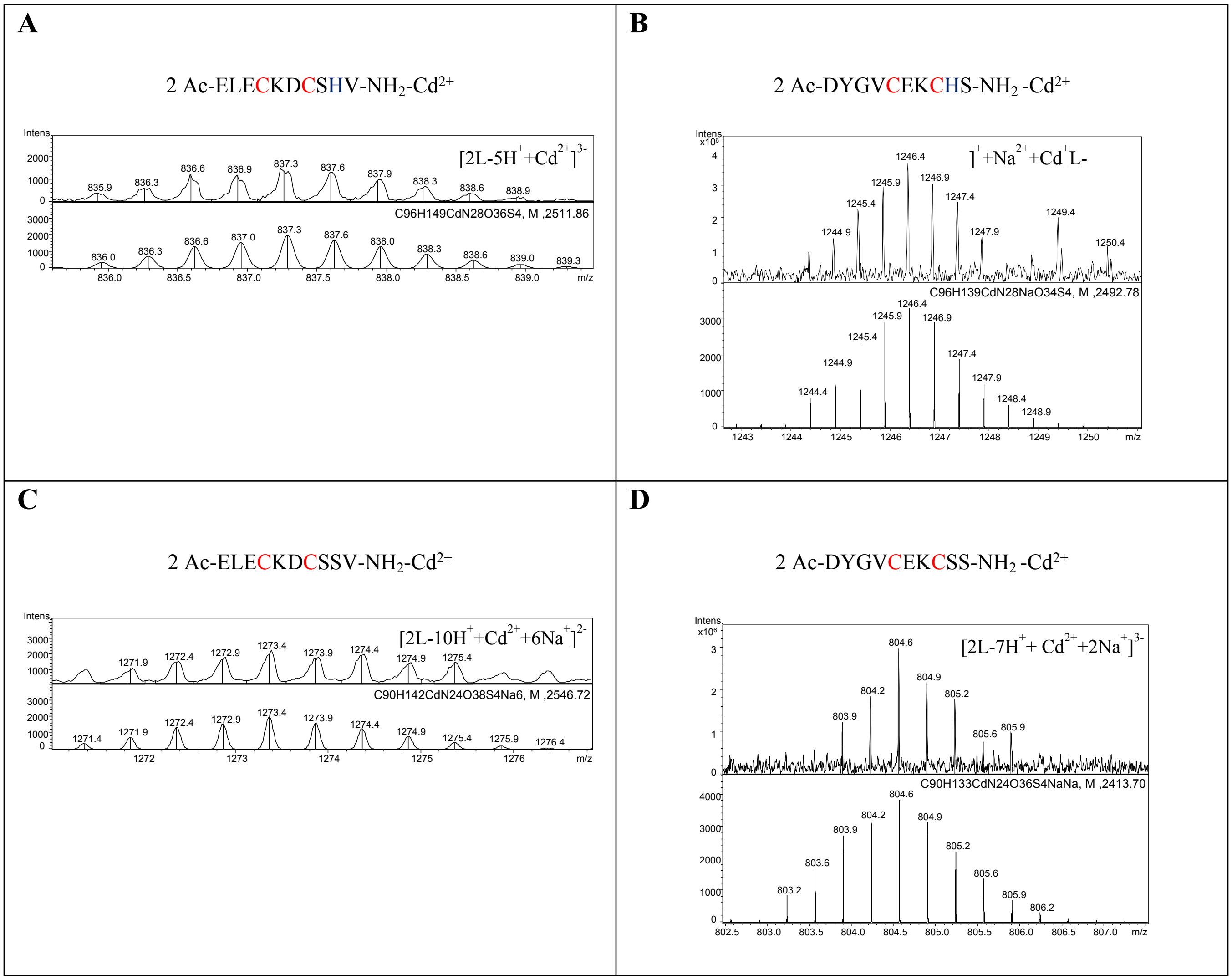

Fig. S6. Mass spectra of a system containing Cd^{2+} and A) ELE, B) DYG, C) ELES and D) DYGS peptide. Upper spectrum- experimental, spectrum below- simulated.

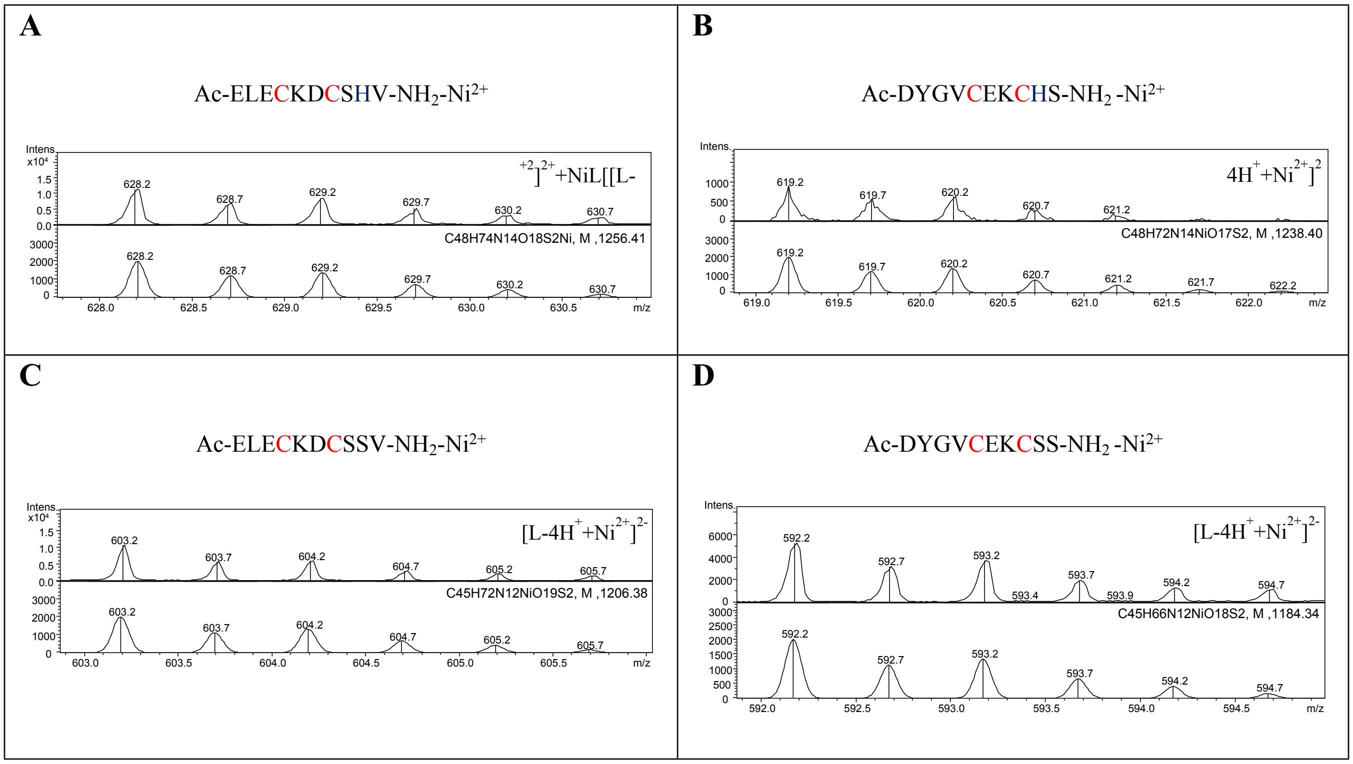

Fig. S7. Mass spectra of a system containing Ni^{2+} and (A) ELE, (B) DYG, (C) ELES and (D) DYGS peptide. Upper spectrum- experimental, spectrum below- simulated.

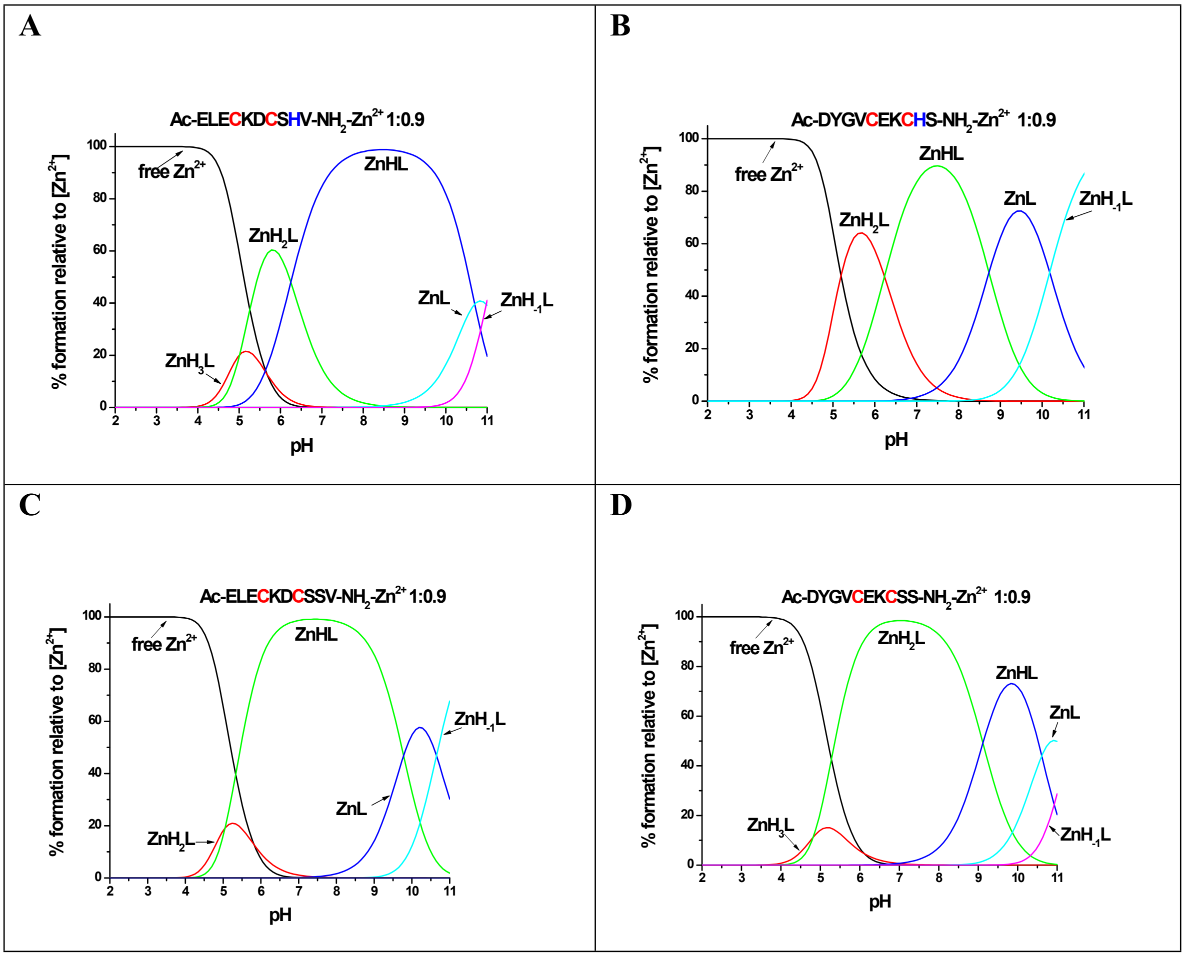

Fig. S8. Species distribution profiles for Zn^{2+} complexes of (A) ELE, (B) DYG, (C) ELES, (D) DYGS peptide. Ligand to metal ratio = 1:0.9; $[Zn^{2+}]$ = 0.9 mM.

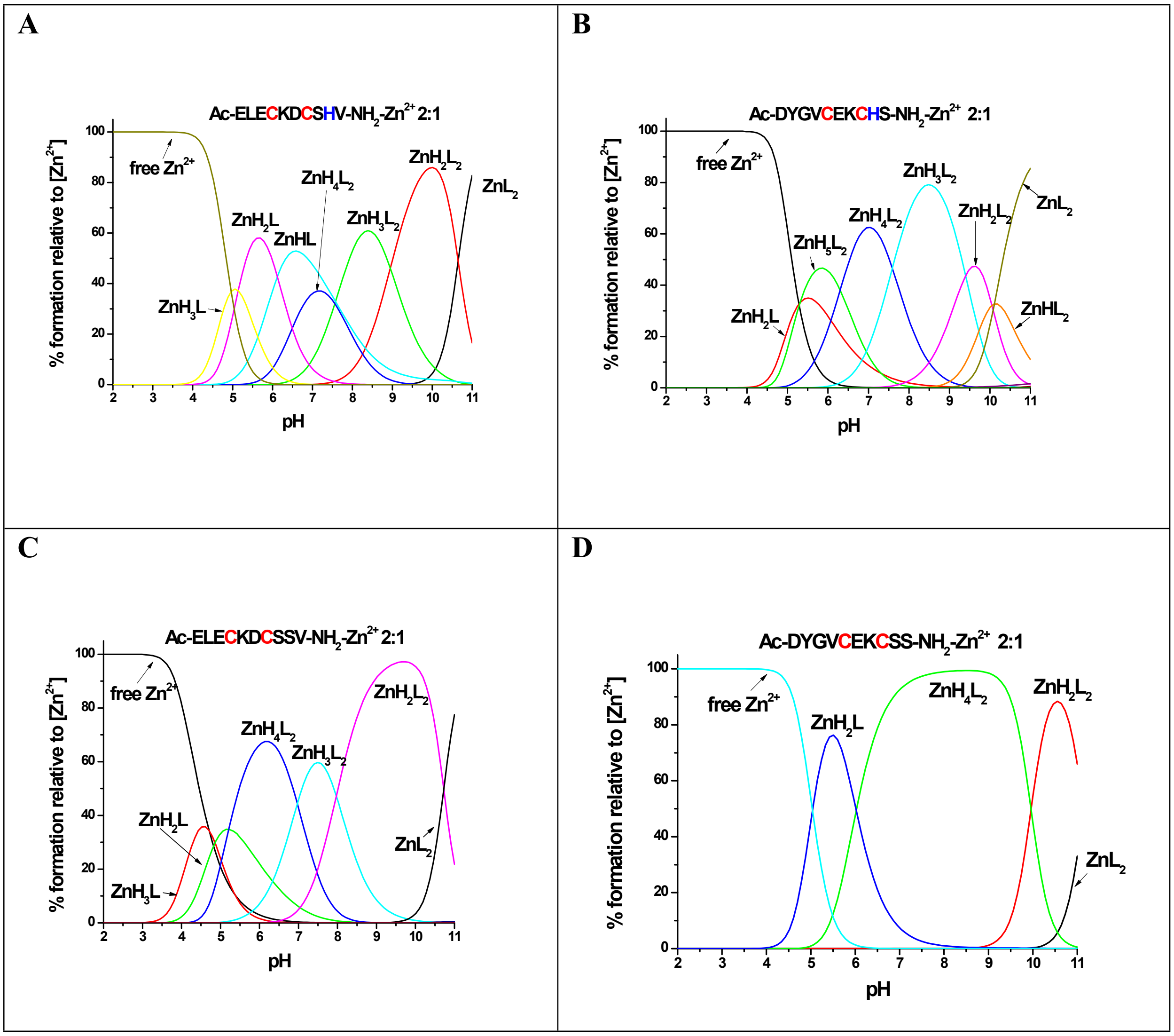

Fig. S9. Species distribution profiles for Zn^{2+} complexes of (A) ELE, (B) DYG, (C) ELES, (D) DYGS peptide. Ligand to metal ratio = 2:1; [Zn^{2+}] = 0.5 mM.

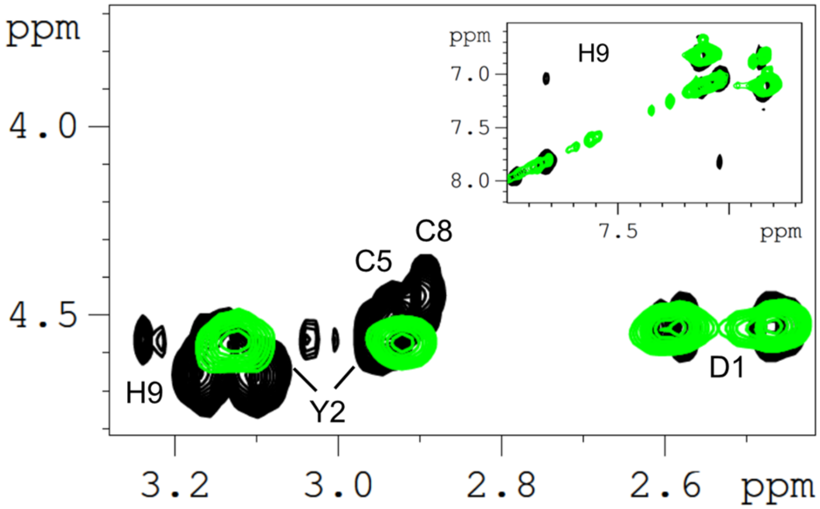

Fig. S10. Selected aliphatic and aromatic regions of the ^{1}H–^{1}H TOCSY spectra of DYG at $1{\times}10^{-3}$ M, pH 7.4 and T 303 K in the absence (black contours) and in the presence (green contours) of 0.6 Zn^{2+} equivalents.

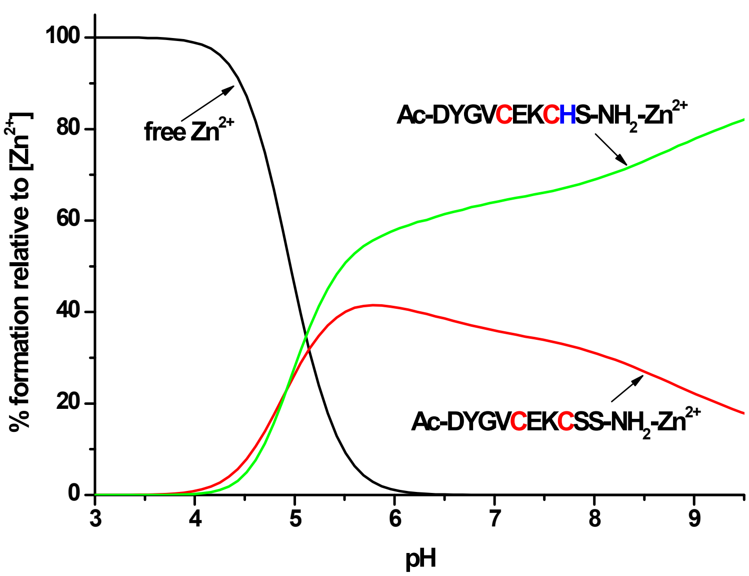

Fig. S11. A Competition plot of Zn^{2+} complexes with DYG and DYGS (1 : 1 : 1 molar ratio).

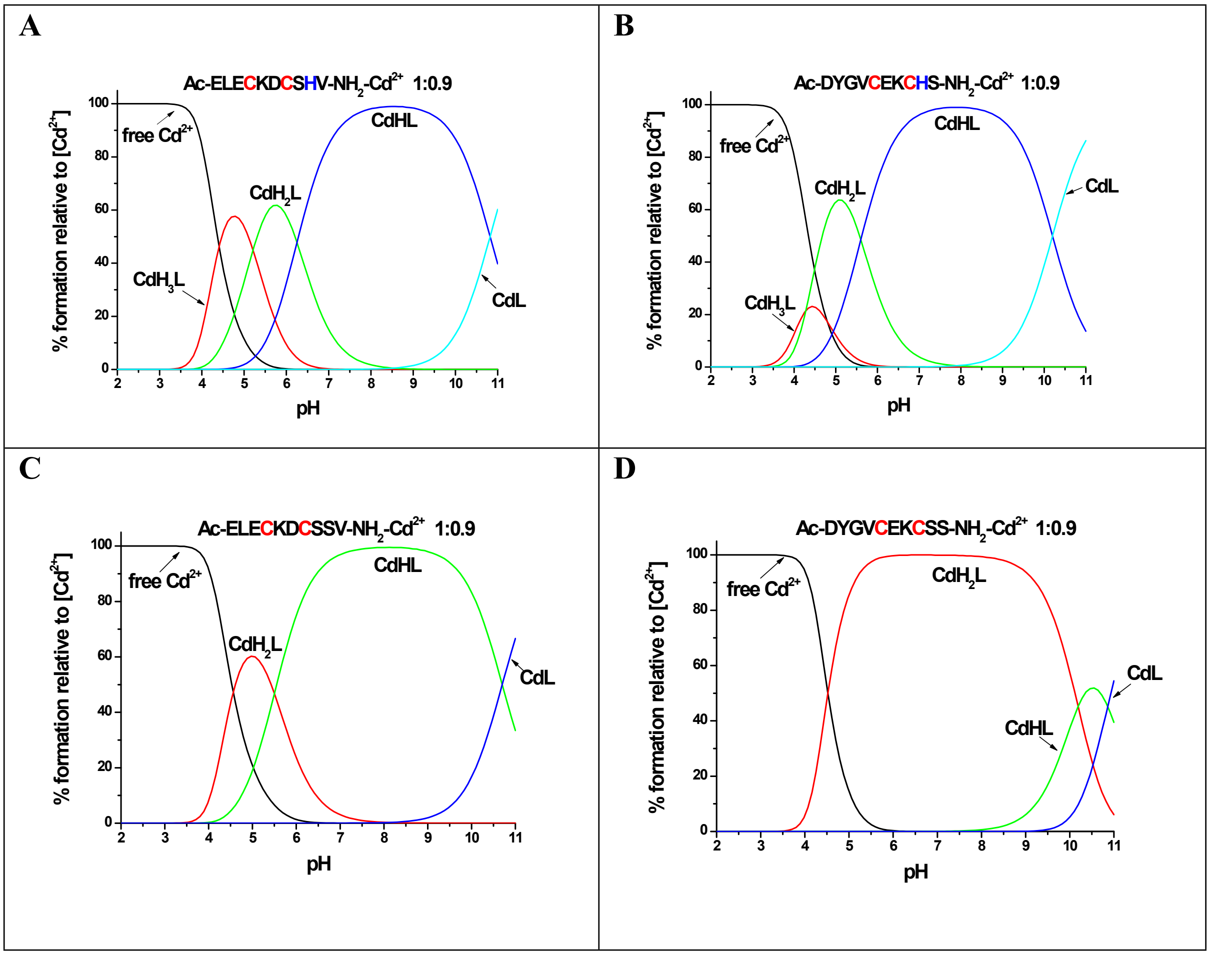

Fig. S12. Species distribution profiles for Cd^{2+} complexes of (A) ELE, (B) DYG, (C) ELES, (D) DYGS peptide. Ligand to metal ratio = 1:0.9; $[Cd^{2+}]$ = 0.9 mM.

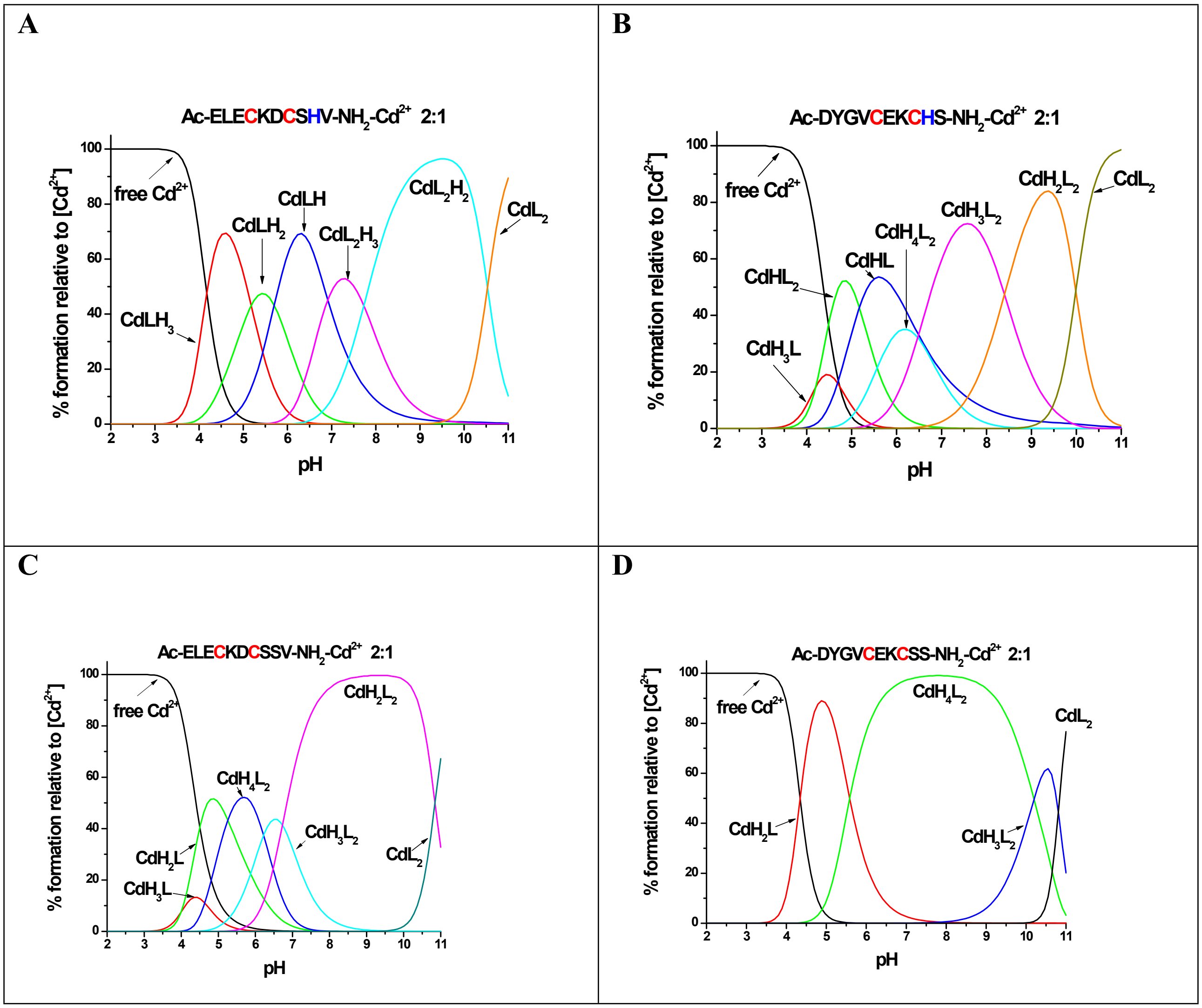

Fig. S13. Species distribution profiles for Cd^{2+} complexes of (A) ELE, (B) DYG, (C) ELES, (D) DYGS peptide. Ligand to metal ratio = 2:1; $[Cd^{2+}]$ = 0.5 mM.

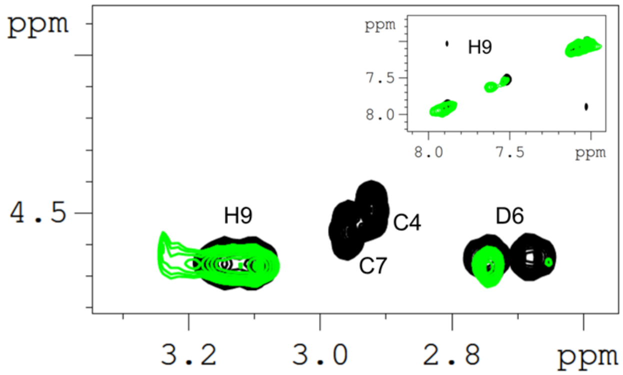

Fig. S14. Selected aliphatic and aromatic regions of the ^{1}H–^{1}H TOCSY spectra of ELE at 1×10^{-3} M, pH 7.4 and T 303 K in the absence (black contours) and in the presence (green contours) of 0.6 Cd^{2+} equivalents.

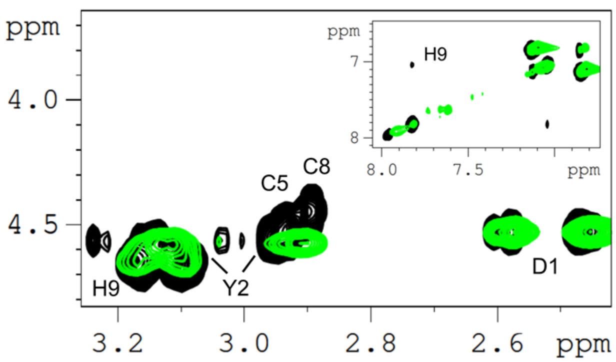

Fig. S15. Selected aliphatic and aromatic regions of the ^{1}H–^{1}H TOCSY spectra of DYG at 1×10^{-3} M, pH 7.4 and T 303 K in the absence (black contours) and in the presence (green contours) of 0.6 Cd^{2+} equivalents.

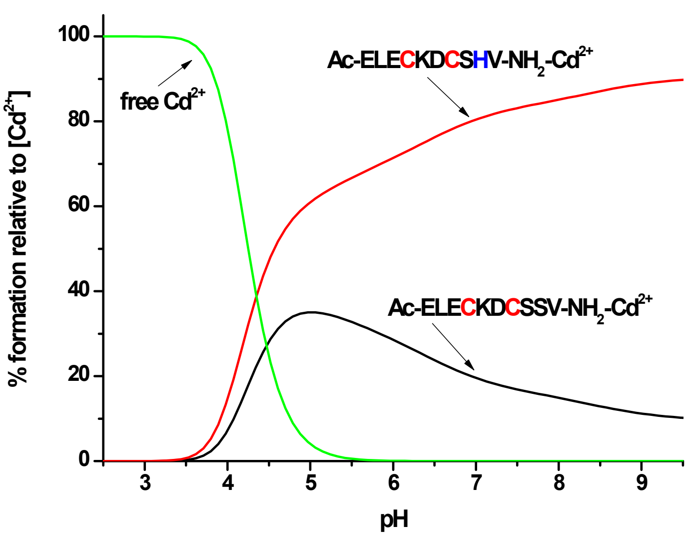

Fig. S16. A competition plot of Cd^{2+} complexes with ELE and ELES (1 : 1 : 1 molar ratio).

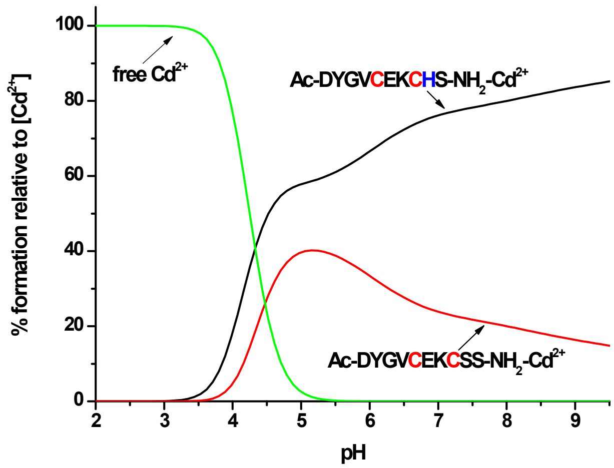

Fig. S17. A competition plot of Cd^{2+} complexes with DYG and DYGS (1 : 1 : 1 molar ratio).

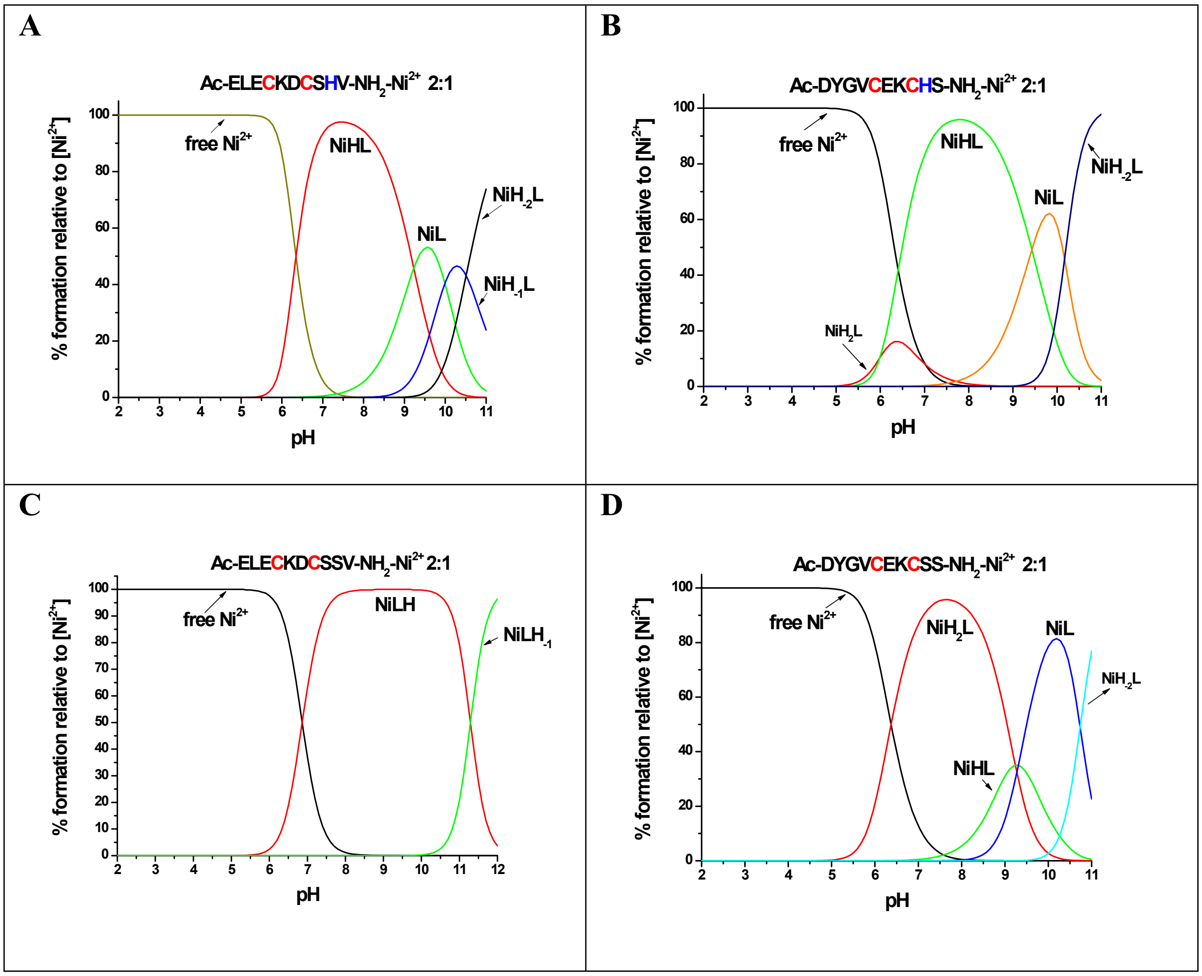

Fig. S18. Species distribution profiles for Ni^{2+} complexes of (A) ELE, (B) DYG, (C) ELES, (D) DYGS peptide. Ligand to metal ratio = 2:1; $[Ni^{2+}]$ = 0.5 mM.

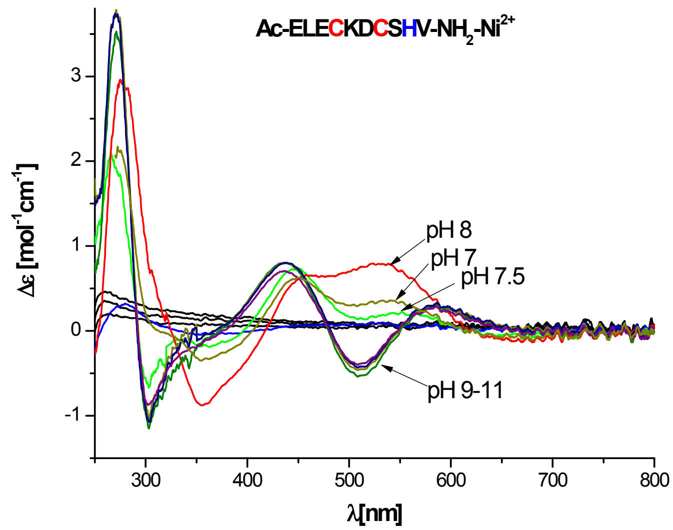

Fig. S19. CD spectra for Ni^{2+} complexes of ELE peptide. Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1×10^{-3} M and ligand to metal molar ratios were 2:1 and 1:0.9.

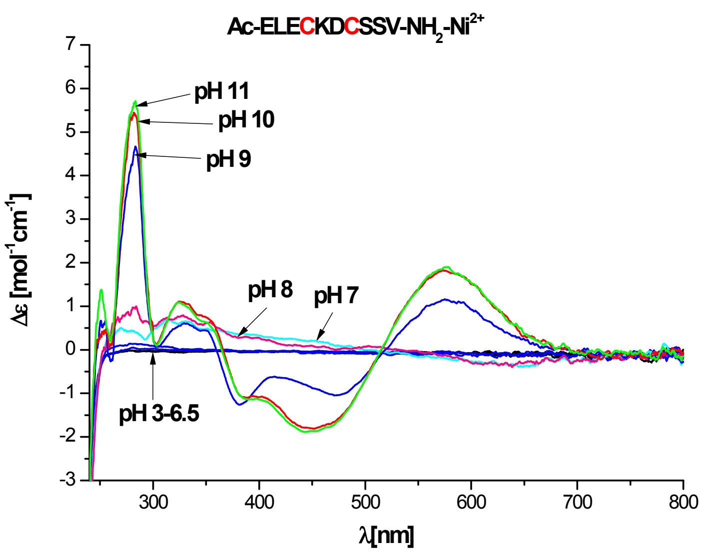

Fig. S20. CD spectra for Ni^{2+} complexes of ELES peptide. Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1×10^{-3} M and ligand to metal molar ratios were 2:1 and 1:0.9.

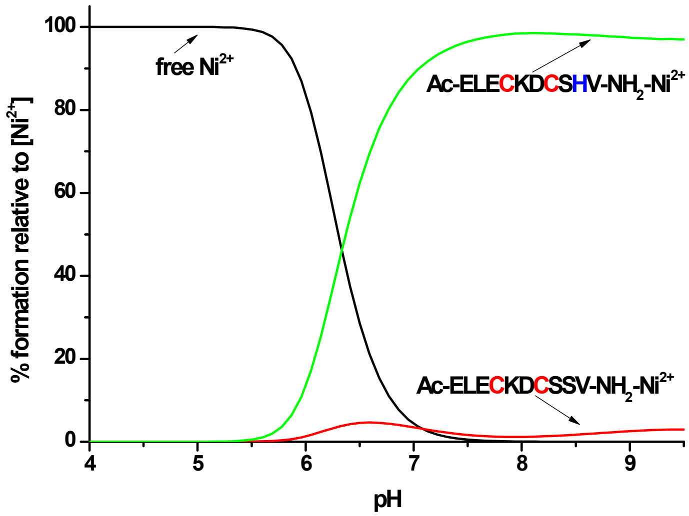

Fig. S21. A competition plot of Ni^{2+} complexes with ELE and ELES (1 : 1 : 1 molar ratio).

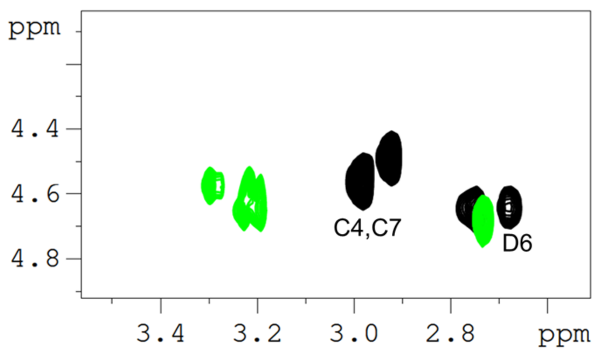

Fig. S22. Selected aliphatic regions of the ^{1}H–^{1}H TOCSY spectra of ELES at 1×10^{-3} M, pH 8.9 and T 303 K in the absence (black contours) and in the presence (green contours) of 0.7 Ni^{2+} equivalents.

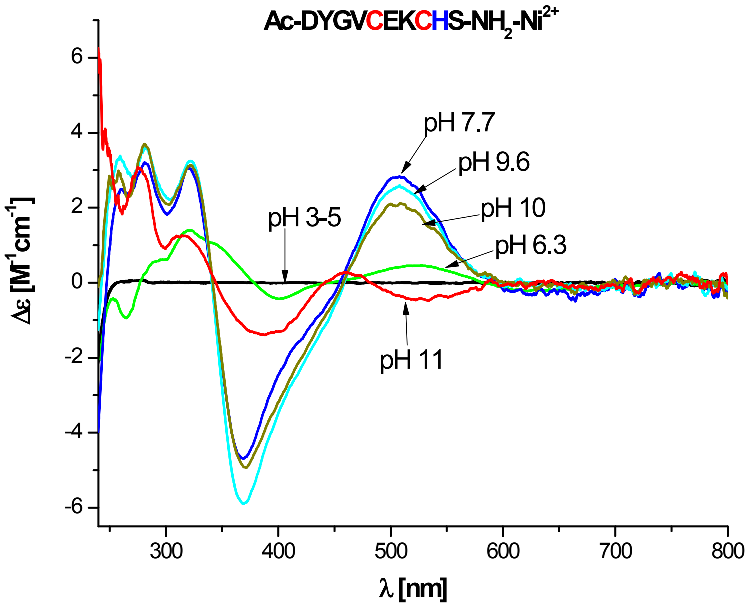

Fig. S23. CD spectra for Ni^{2+} complexes of DYG peptide. Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1×10^{-3} M and ligand to metal molar ratios were 2:1 and 1:0.9.

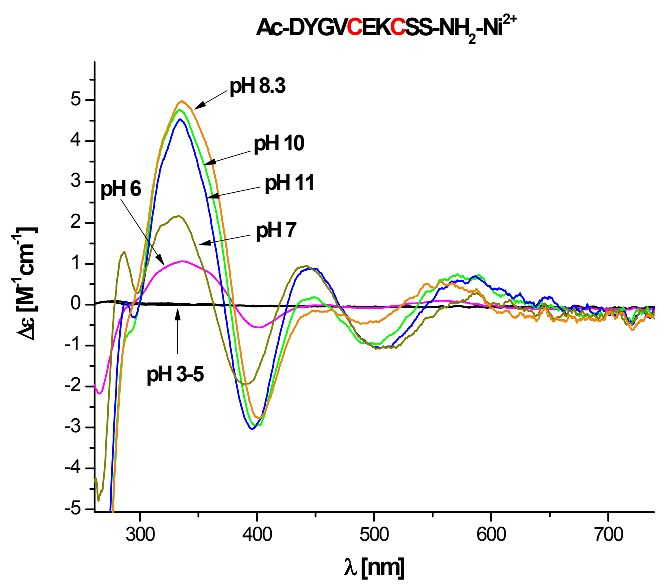

Fig. S24. CD spectra for Ni^{2+} complexes of DYGS peptide. Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1×10^{-3} M and ligand to metal molar ratios were 2:1 and 1:0.9.

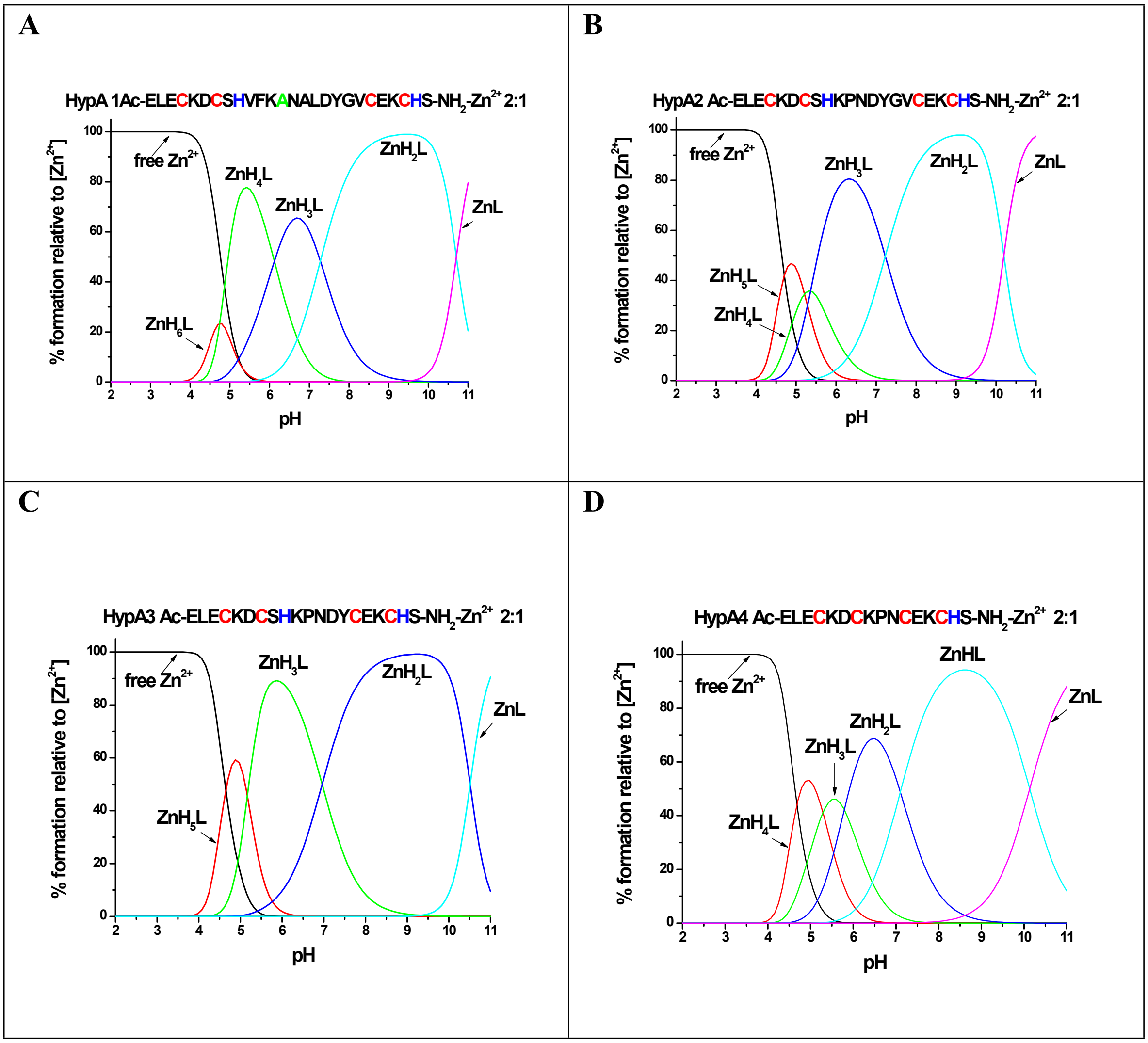

Fig. S25. Species distribution profiles for Zn^{2+} complexes of (A) HypA1, (B) HypA2, (C) HypA3, (D) HypA4 peptide. Ligand to metal ratio = 2:1; $[Zn^{2+}] = 0.5$ mM.

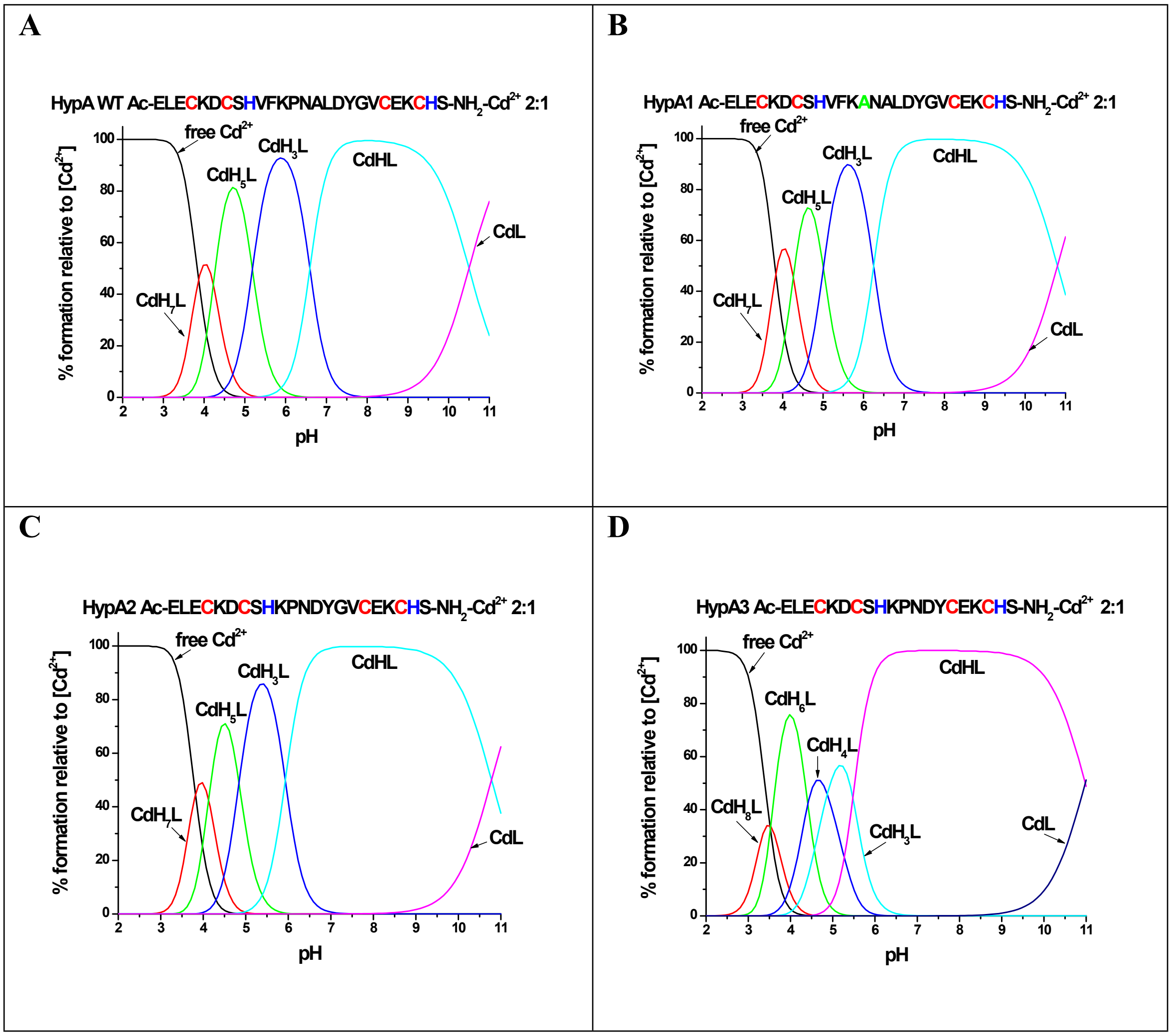

Fig. S26. Species distribution profiles for Cd^{2+} complexes of (A) HypA WT, (B) HypA1, (C) HypA2, (D) HypA3 peptide. Ligand to metal ratio = 2:1; $[Cd^{2+}]$ = 0.5 mM.

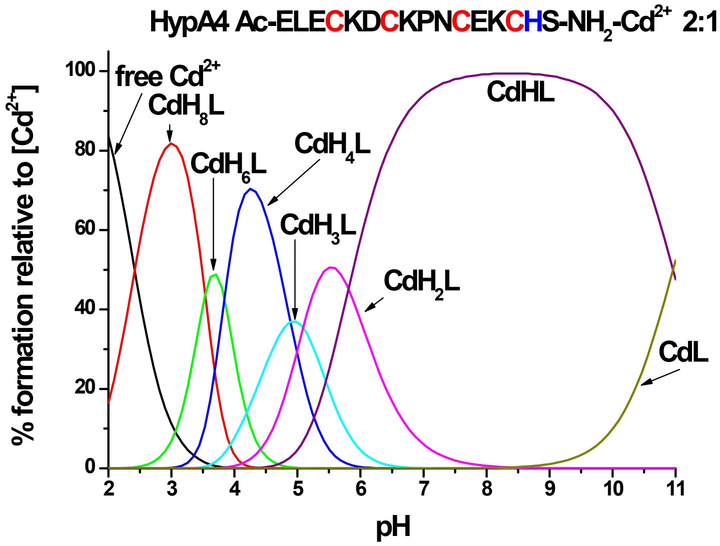

Fig. S27. Species distribution profiles for Cd^{2+} complexes of HypA4 peptide. Ligand to metal ratio = 2:1; $[Cd^{2+}]$ = 0.5 mM.

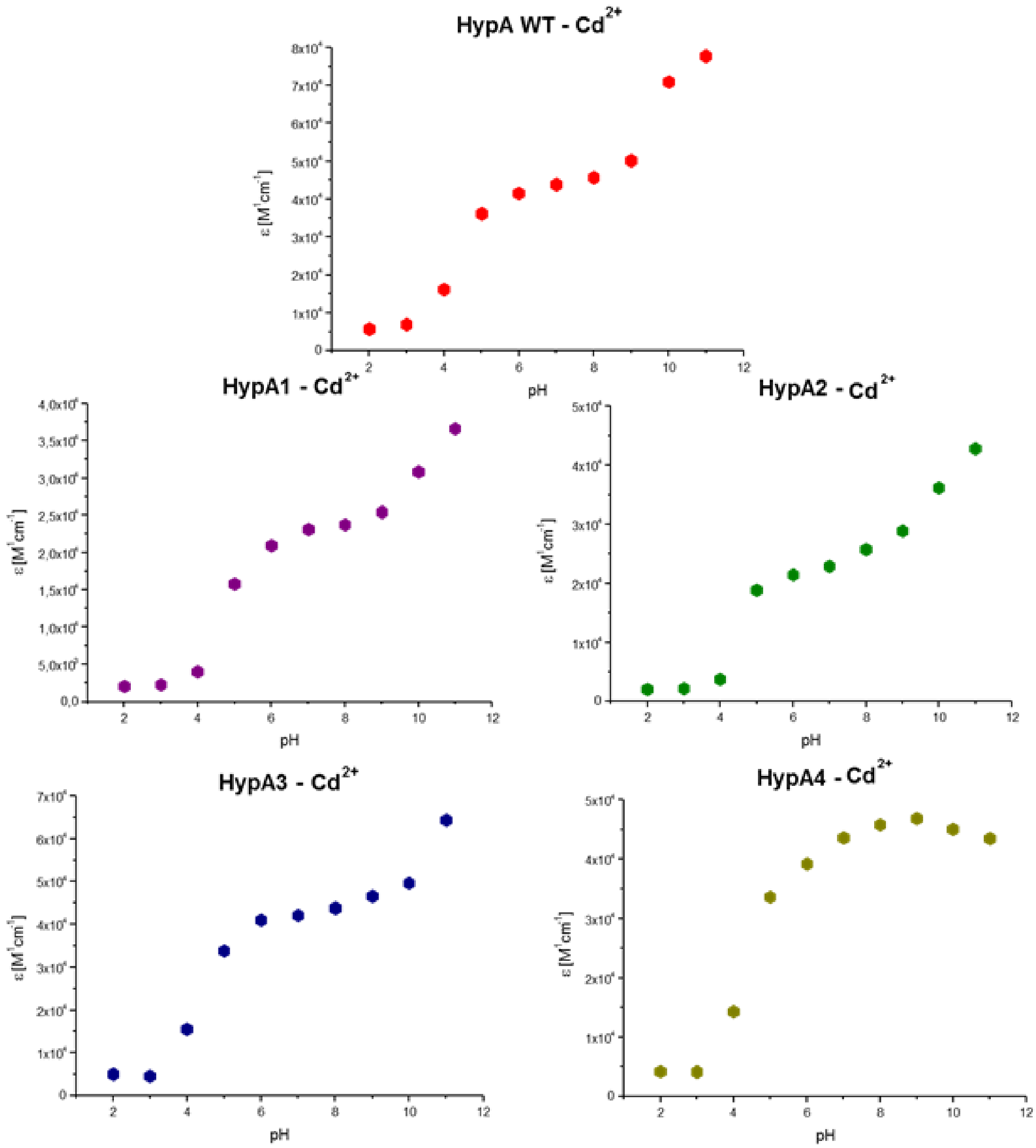

Fig. S28. The dependence of the extinction coefficient on the pH for the transition at 250 nm for Cd^{2+} complexes of HypA WT, HypA1, HypA2, HypA3 and HypA4 peptide.

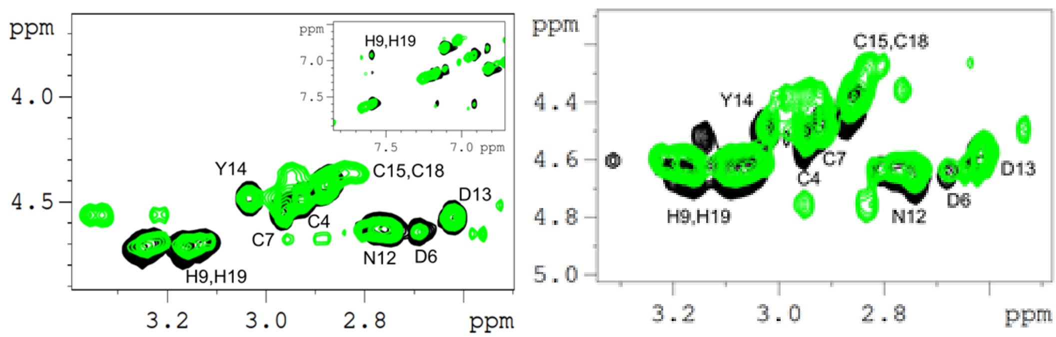

Fig. S29. Selected aliphatic and aromatic regions of the ^{1}H–^{1}H TOCSY spectra of HypA3 at 1×10^{-3} M, pH 6.4 (left), pH 8.0 (right) and T 303 K in the absence (black contours) and in the presence (green contours) of 0.5 Cd^{2+} equivalents.

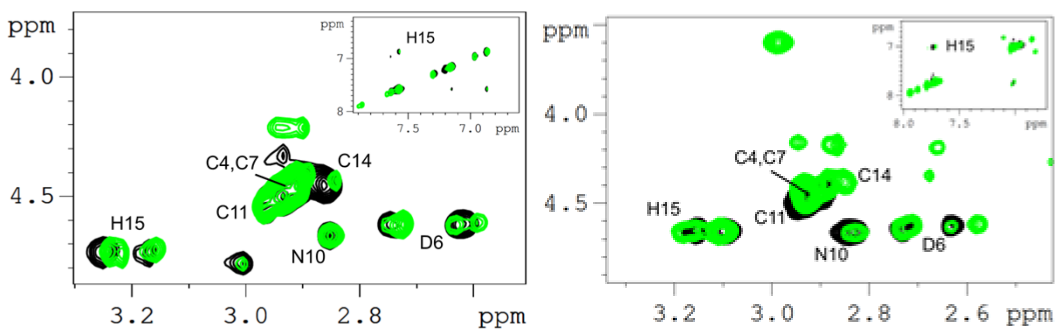

Fig. S30. Selected aliphatic and aromatic regions of the ^{1}H–^{1}H TOCSY spectra of HypA4 at 1×10^{-3} M, pH 6.4 (left), pH 8.0 (right) and T 303 K in the absence (black contours) and in the presence (green contours) of 0.5 Cd^{2+} equivalents.

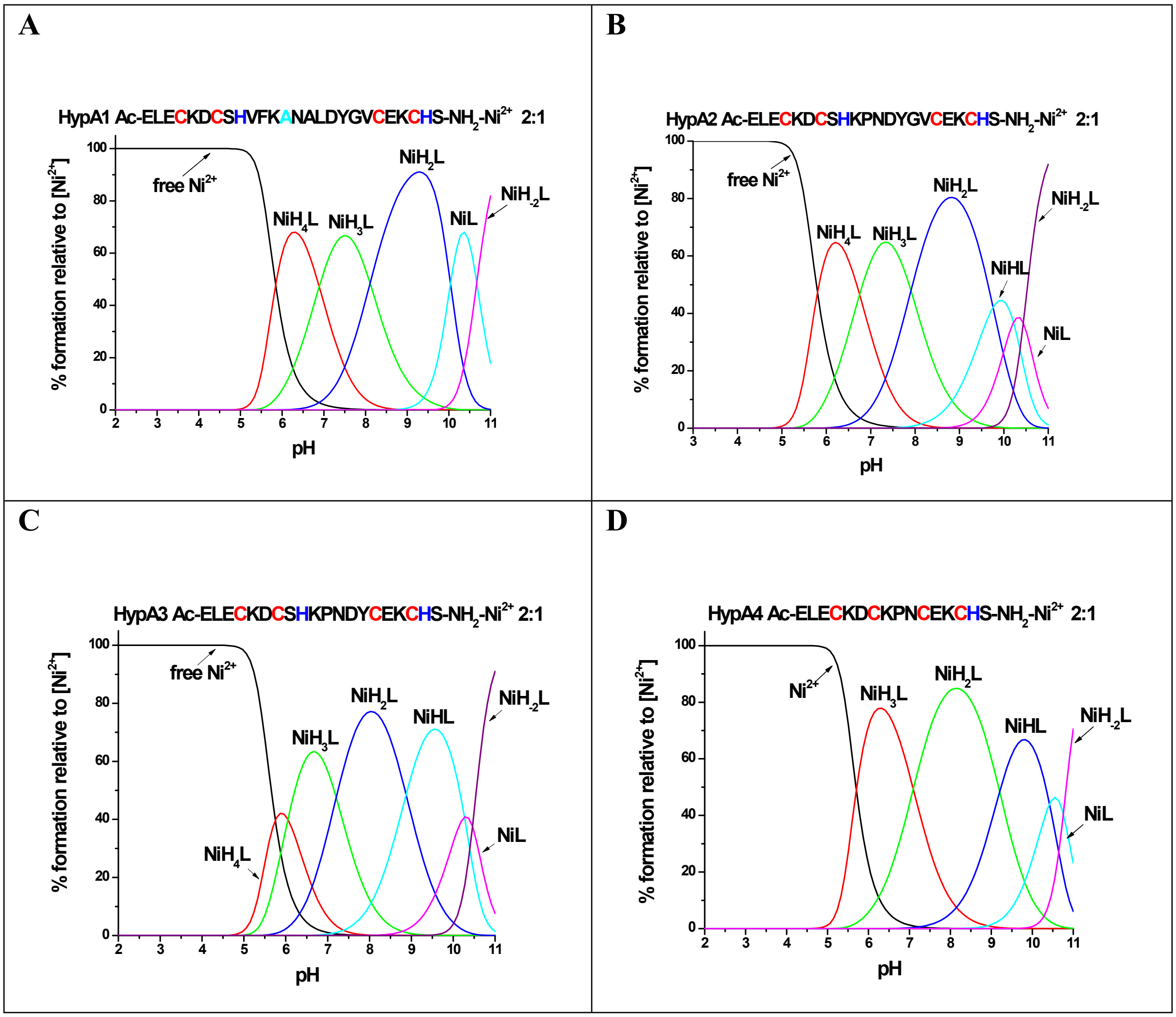

Fig. S31. Species distribution profiles for Ni^{2+} complexes of (A) HypA1, (B) HypA2, (C) HypA3, (D) HypA4 peptide. Ligand to metal ratio = 2:1; $[Ni^{2+}]$ = 0.5 mM.

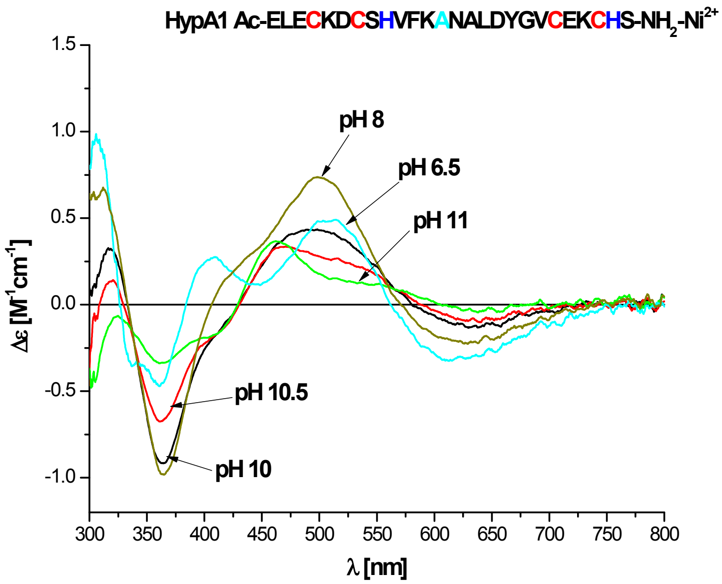

Fig. S32. CD spectra for Ni^{2+} complexes of HypA1 peptide. Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1×10^{-3} M and ligand to metal molar ratios were 2:1 and 1:0.9.

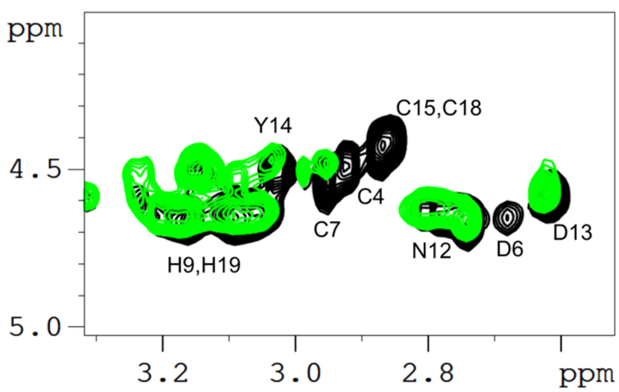

Fig. S33. Selected aliphatic regions of the ^{1}H–^{1}H TOCSY spectra of HypA3 at 1×10^{-3} M, pH 7.4 and T 303 K in the absence (black contours) and in the presence (green contours) of 0.7 Ni^{2+} equivalents.

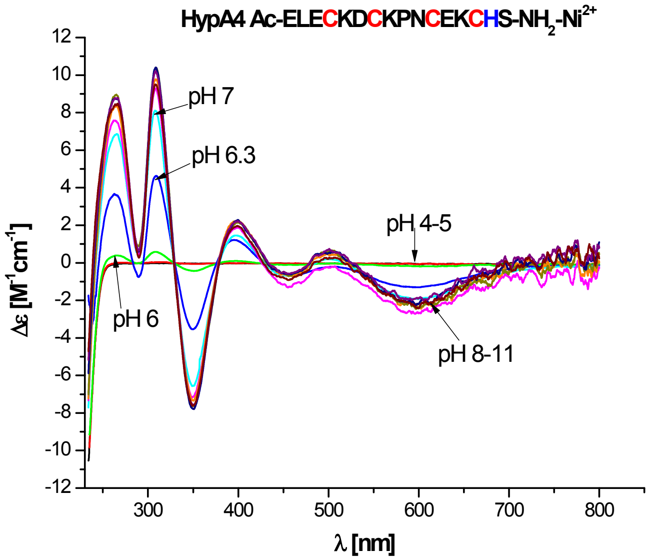

Fig. S34. CD spectra for Ni^{2+} complexes of HypA4 peptide. Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1×10^{-3} M and ligand to metal molar ratios were 2:1 and 1:0.9.