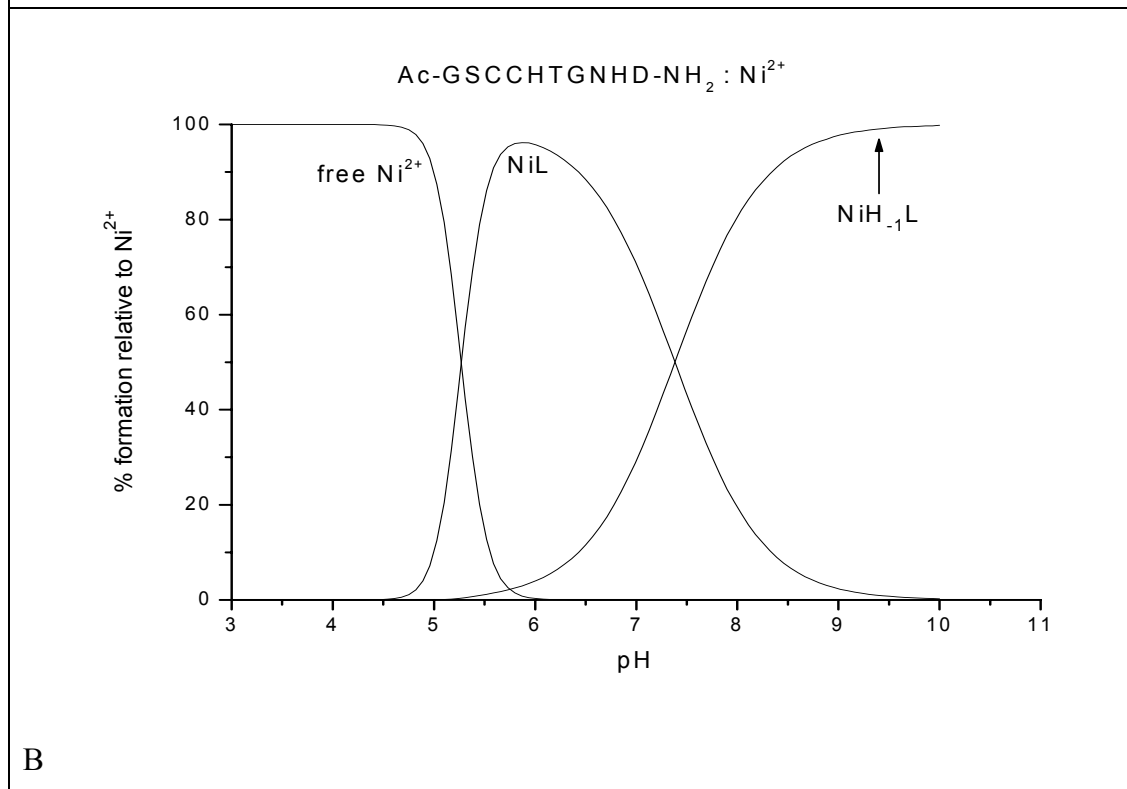
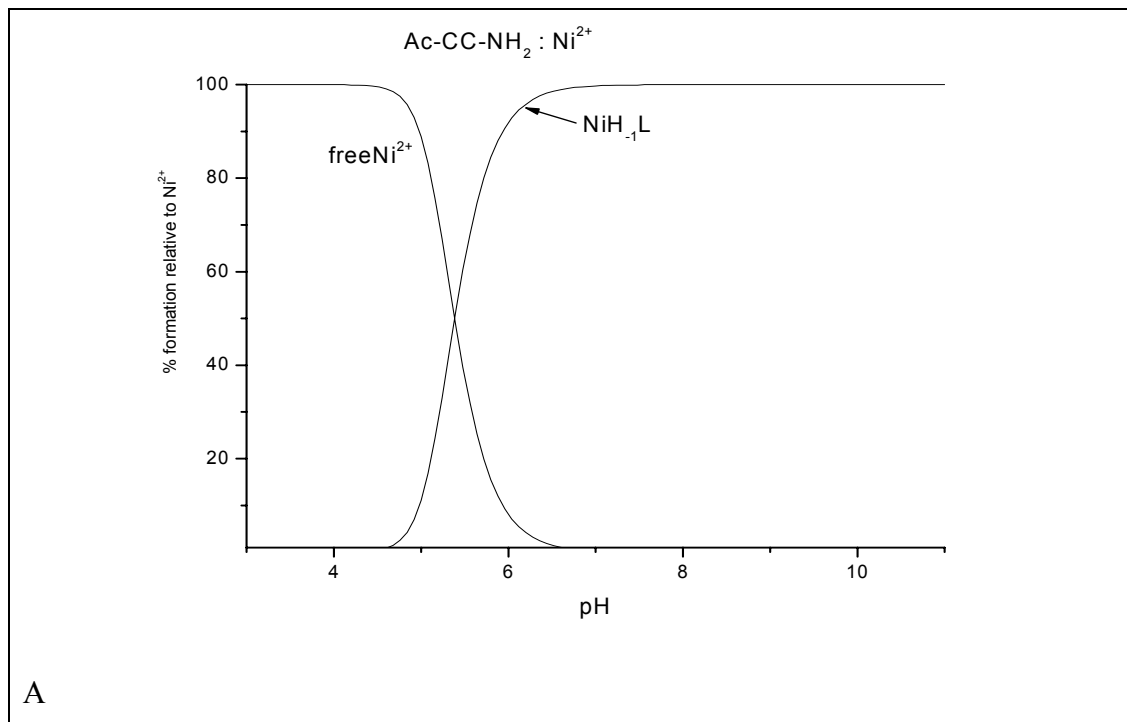
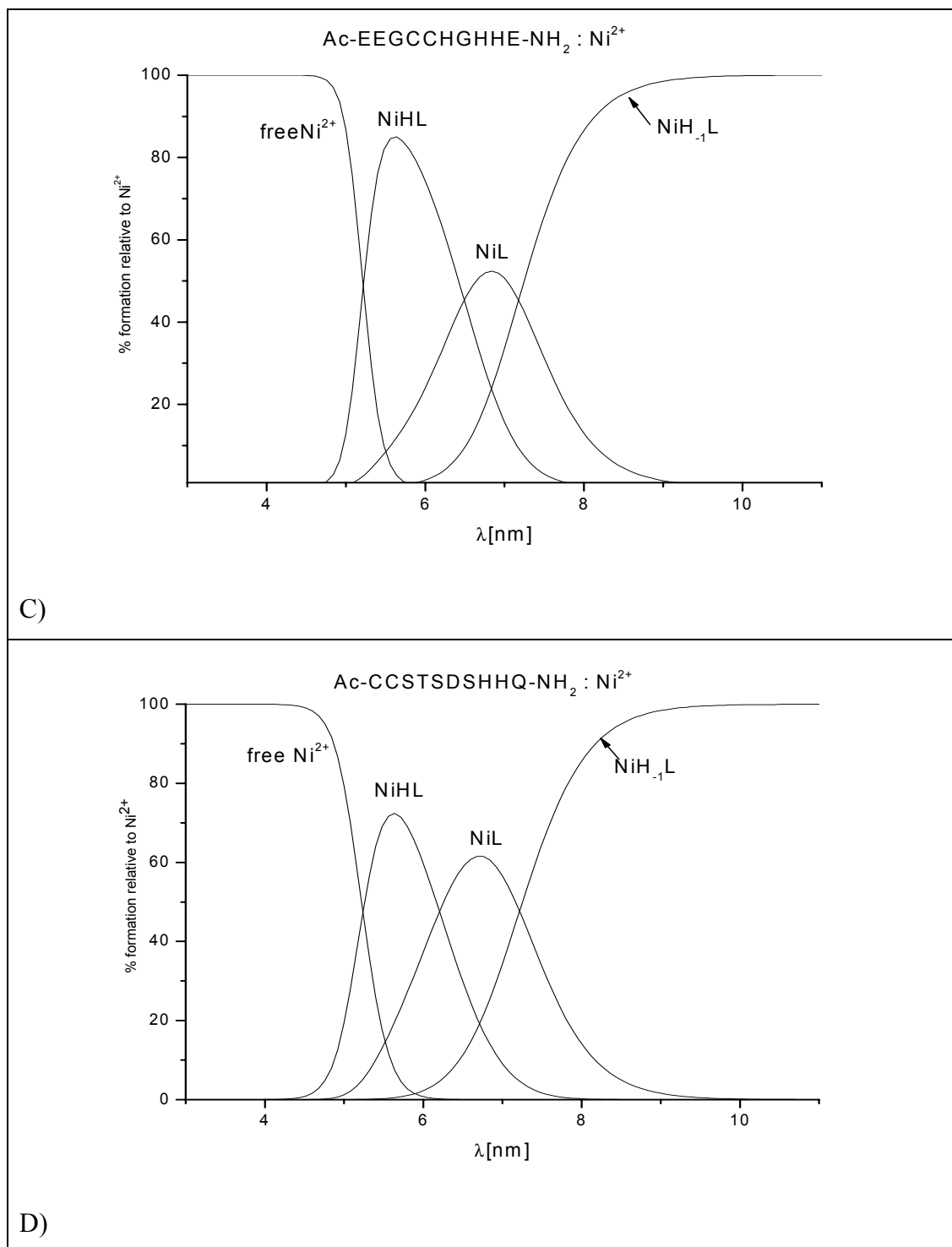
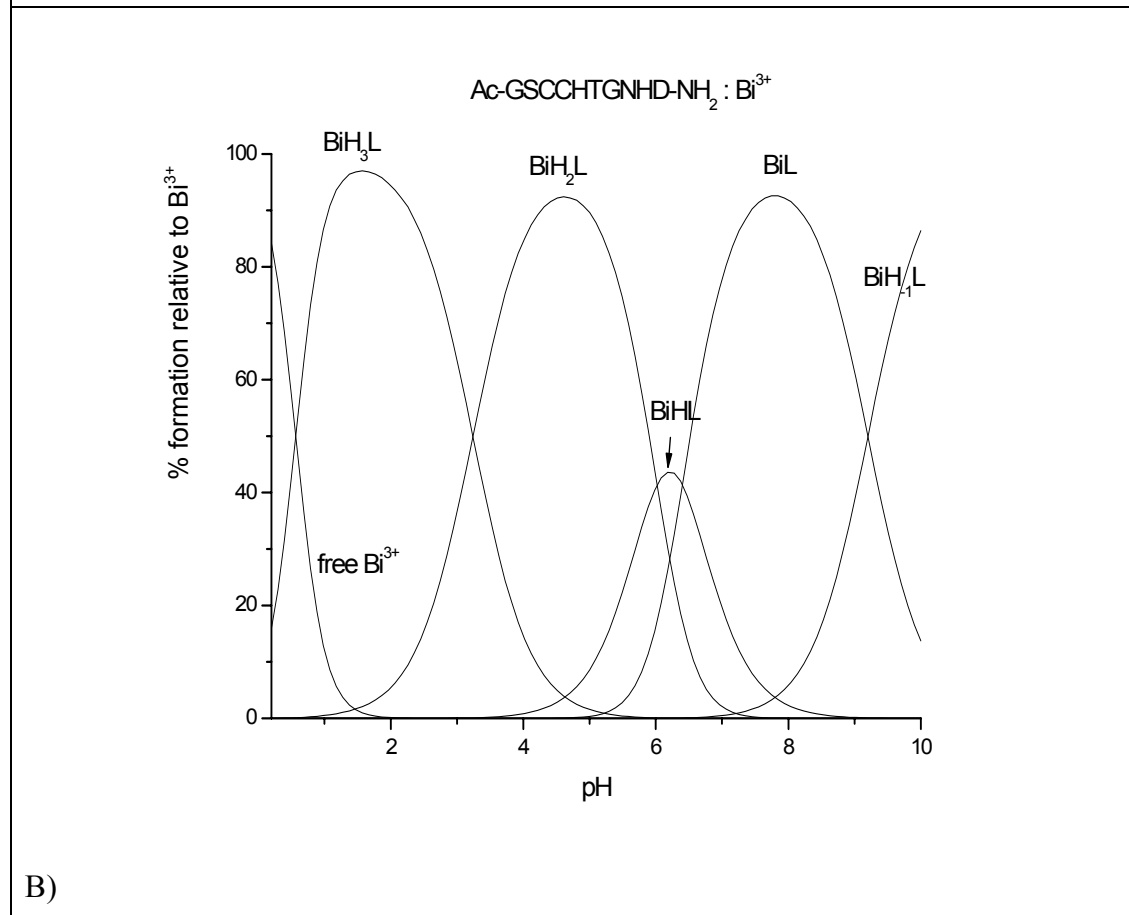
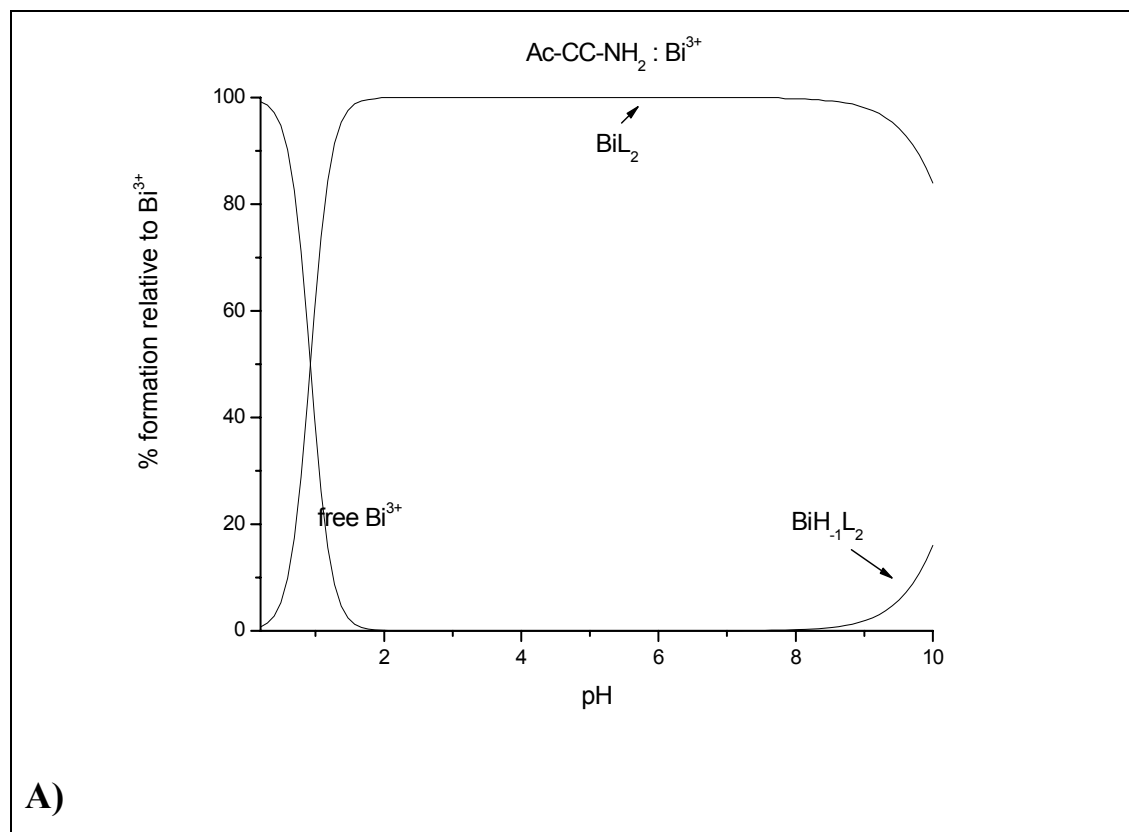


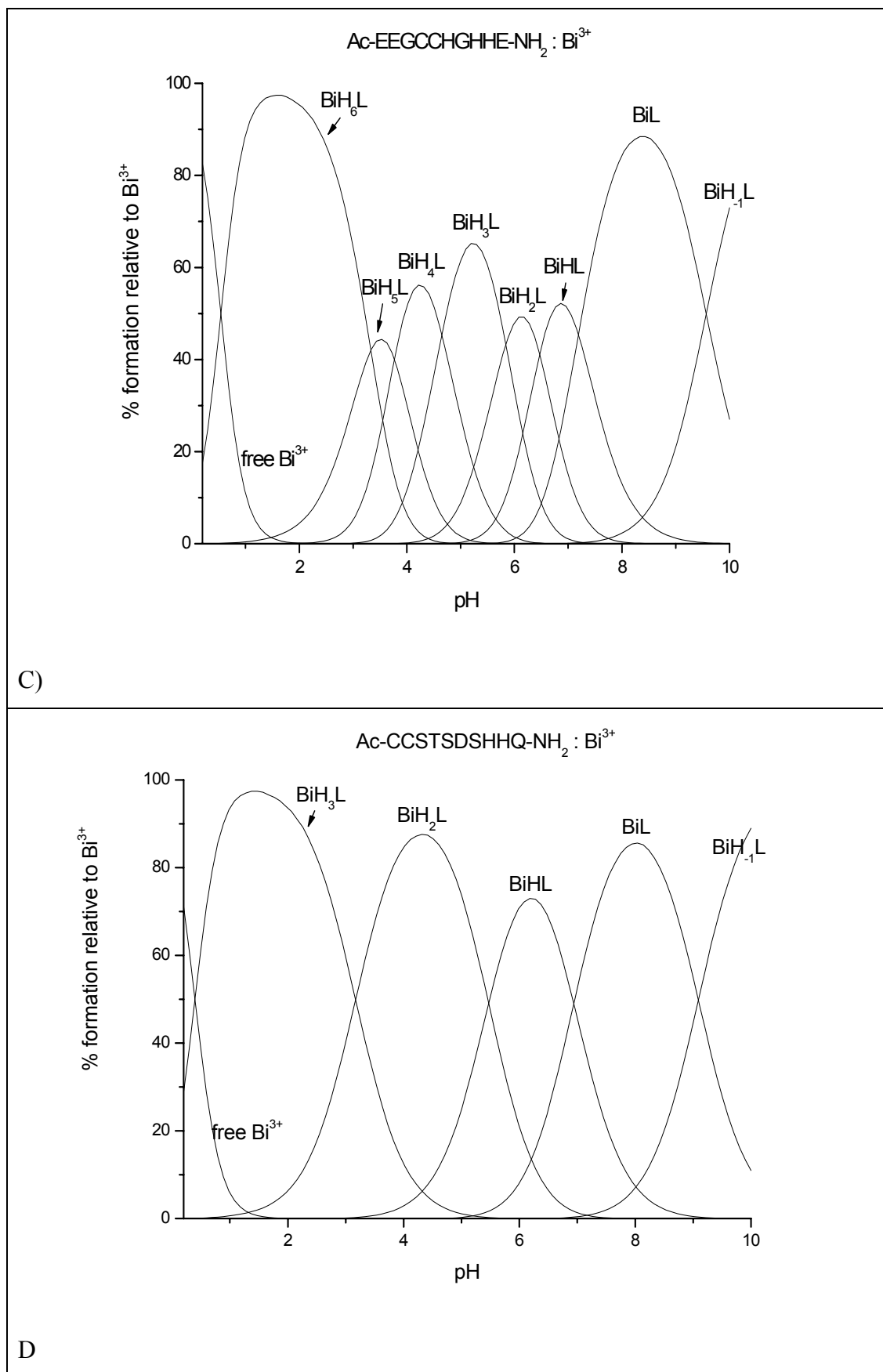
## Supplementary



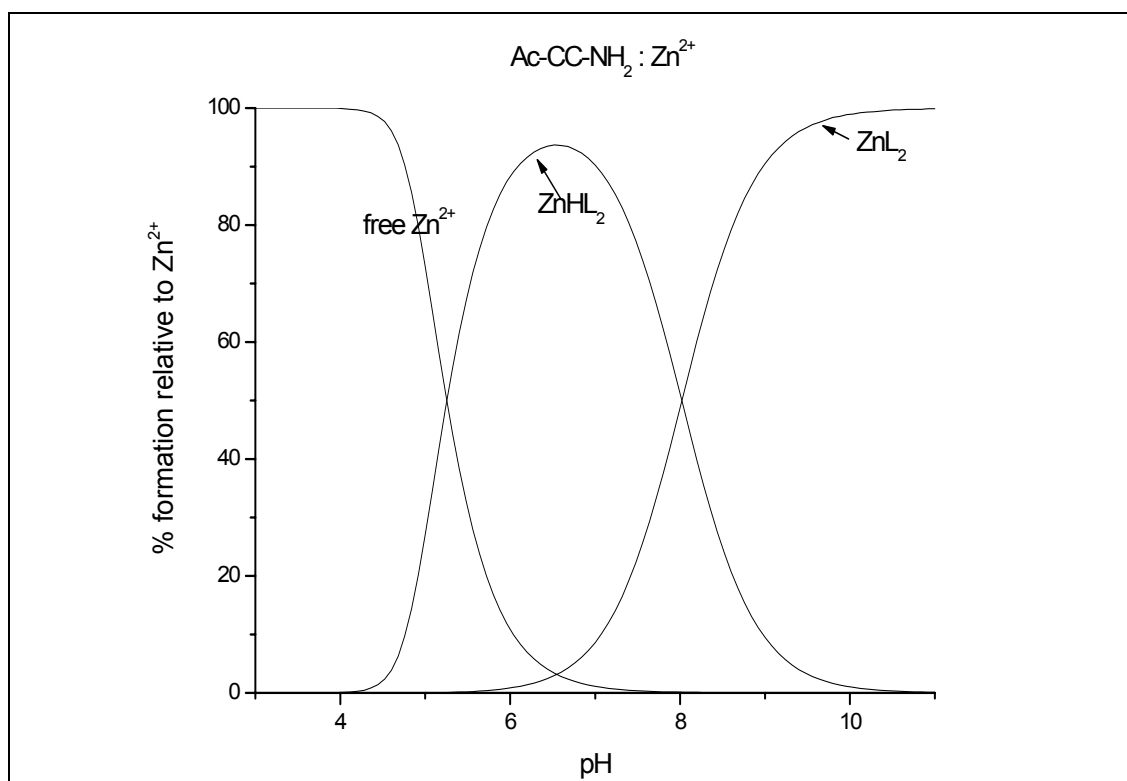


**Fig. S1. Species distribution profiles of Ni<sup>2+</sup> complexes of A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub>, C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub>. Ligand to metal ratio = 1:1.**

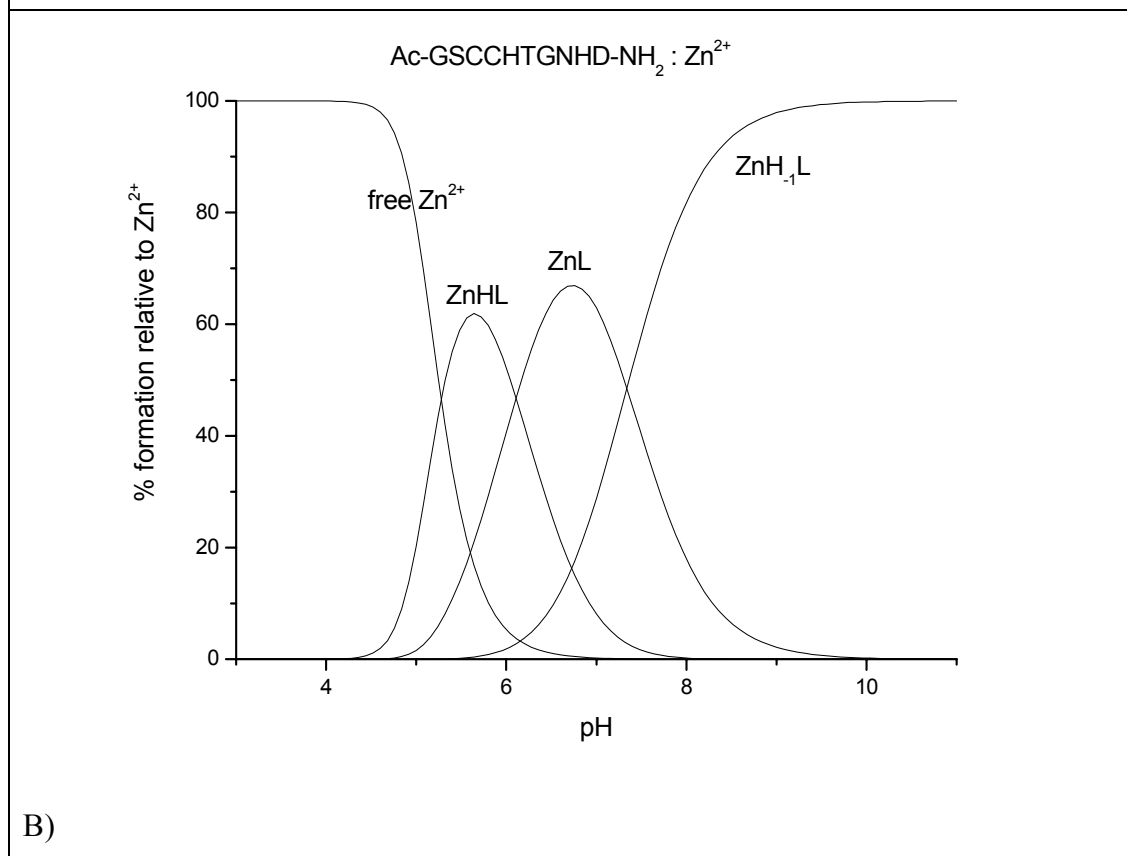




**Fig. S2.** Species distribution profiles of Bi<sup>3+</sup> complexes of A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCHTGNHD-NH<sub>2</sub> C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub>. Ligand to metal ratio = 2:1.



A)



B)

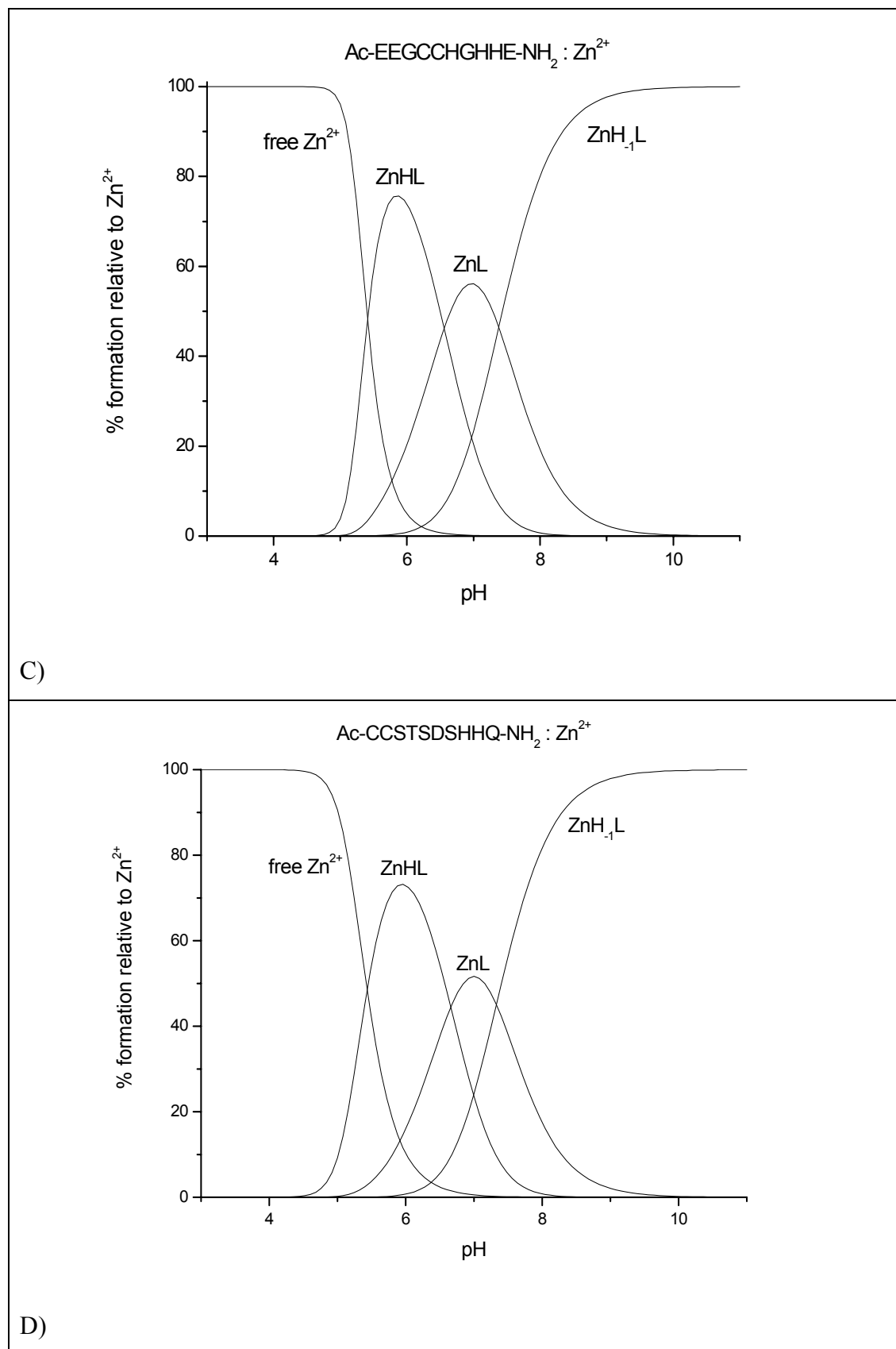
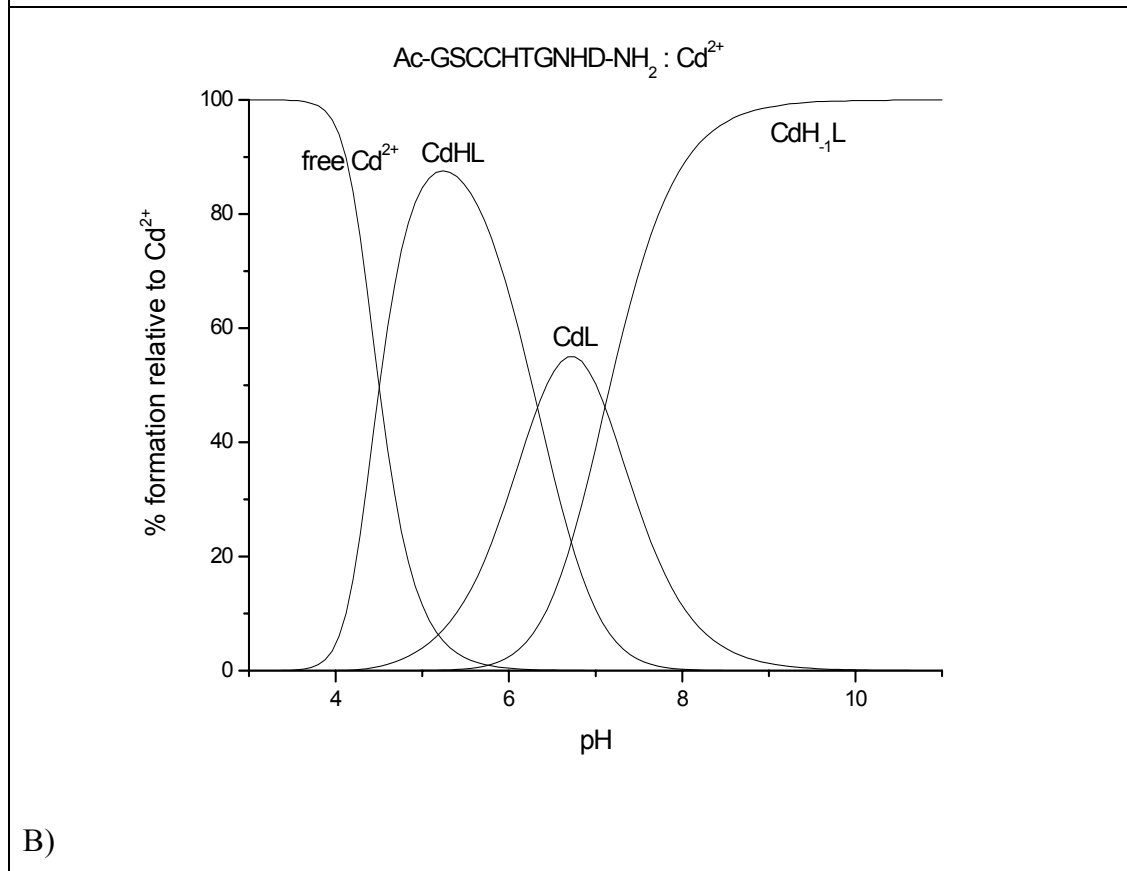
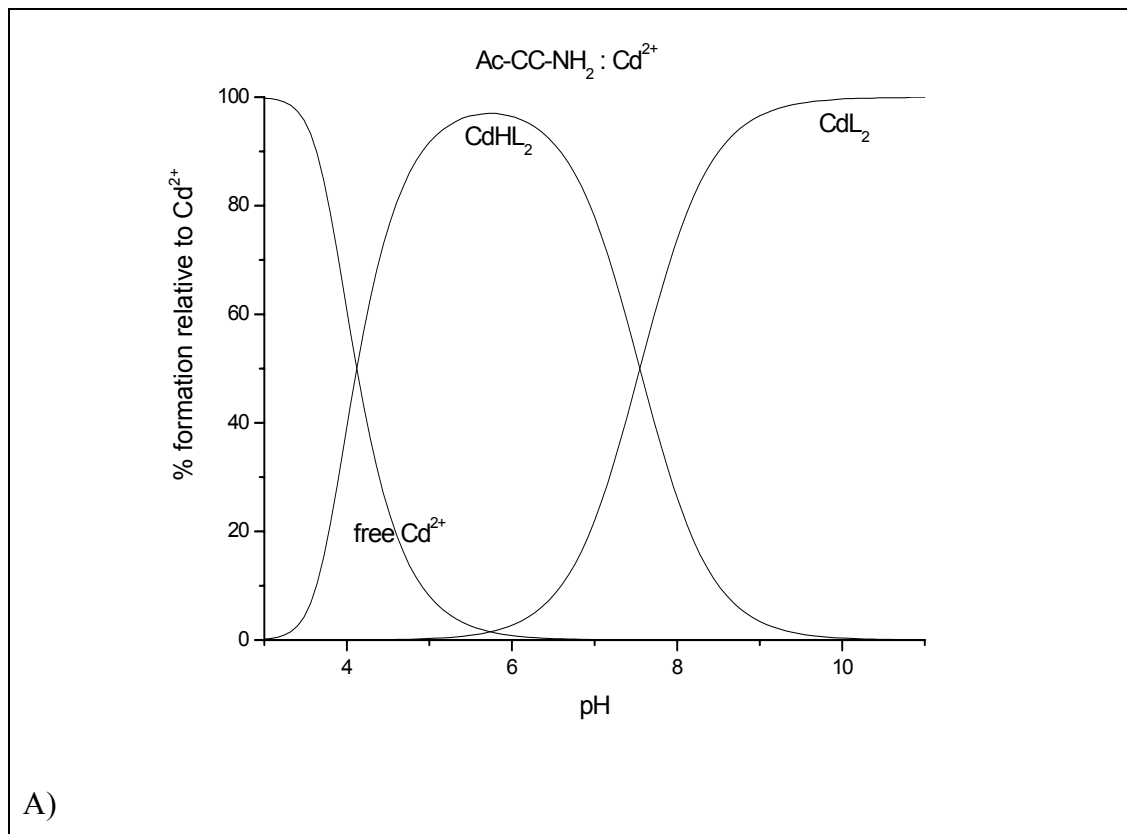
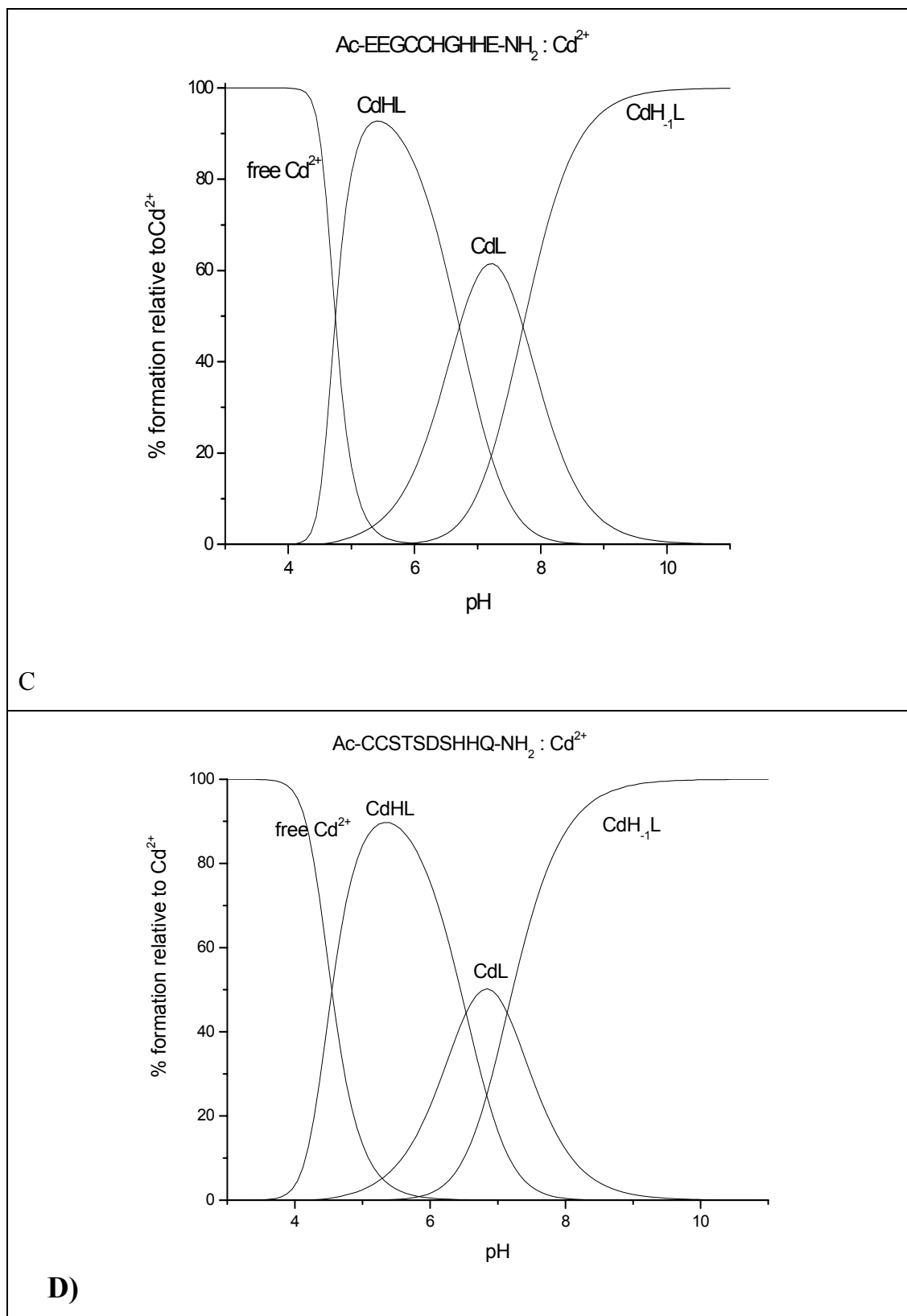


Fig. S3. Species distribution profiles of Zn<sup>2+</sup> complexes of A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCHTGNHD-NH<sub>2</sub>, C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub>. Ligand to metal ratio = 2:1 (A) and 1:1 (B,C,D).





**Fig. S4.** Species distribution profiles of Cd<sup>2+</sup> complexes A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub> C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub>. Ligand to metal ratio = 2:1 (A) and 1:1 (B,C,D).



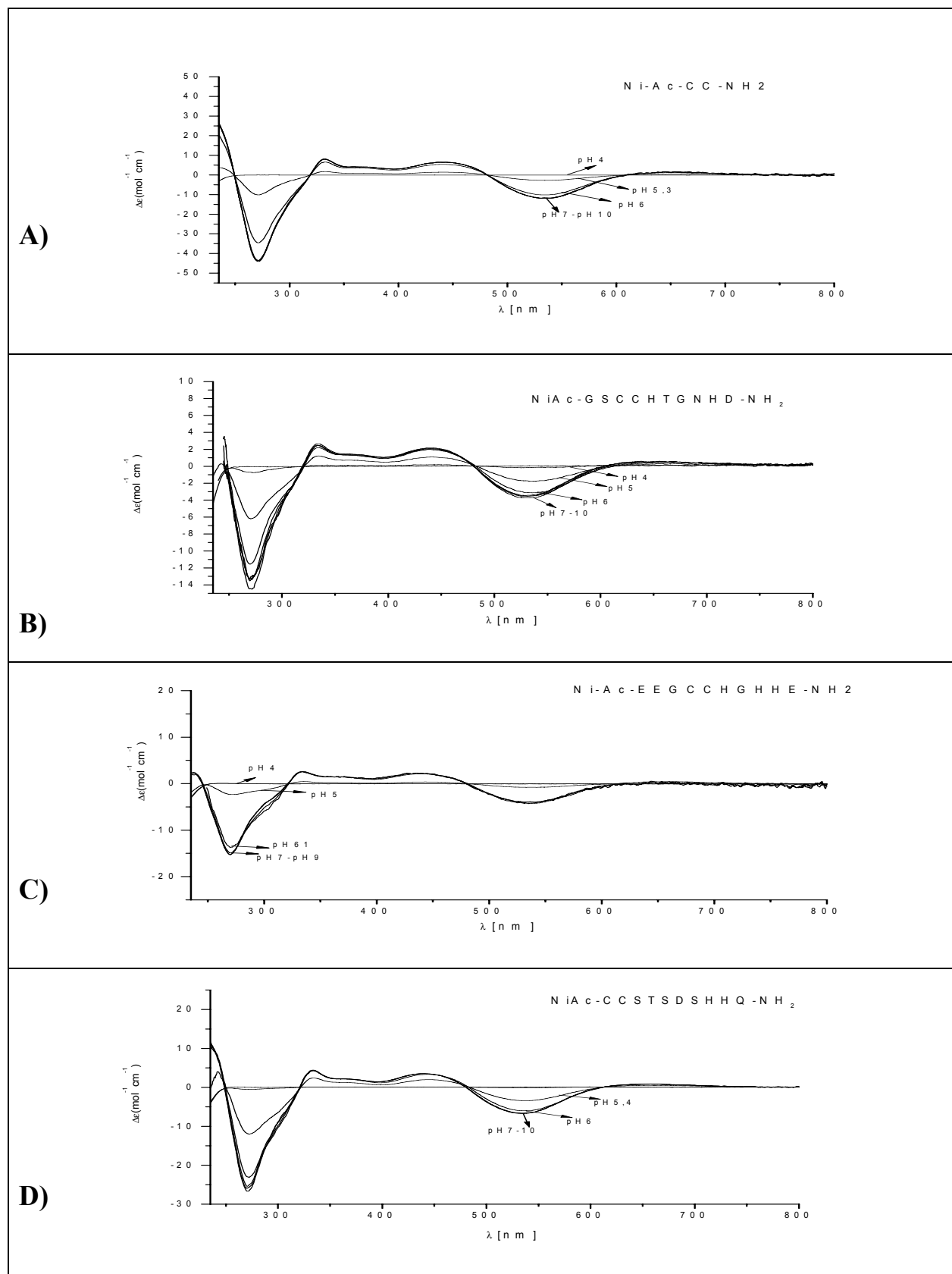


Fig. S5. The CD spectra of  $\text{Ni}^{2+}$  complexes of A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub> C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub>.

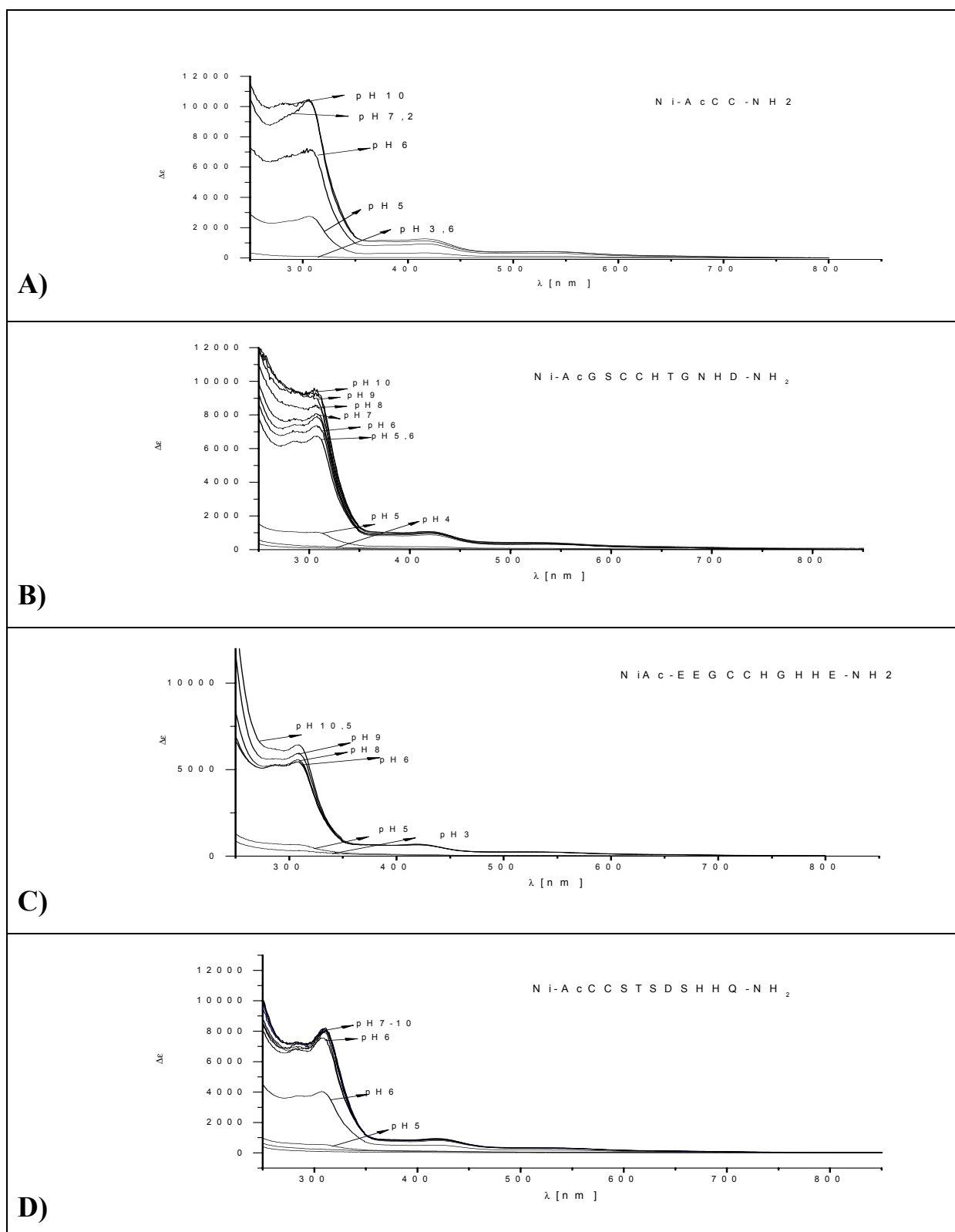
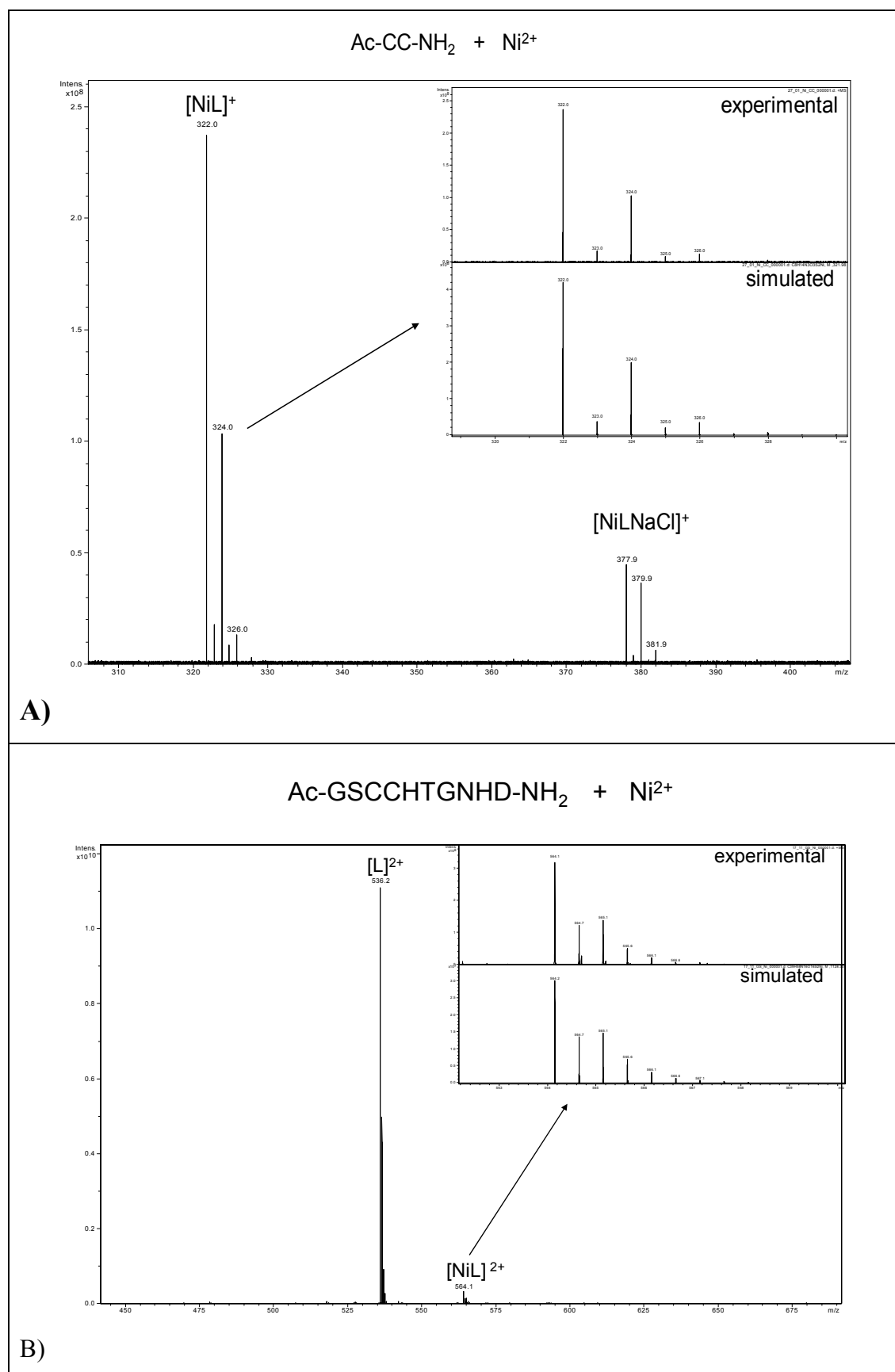
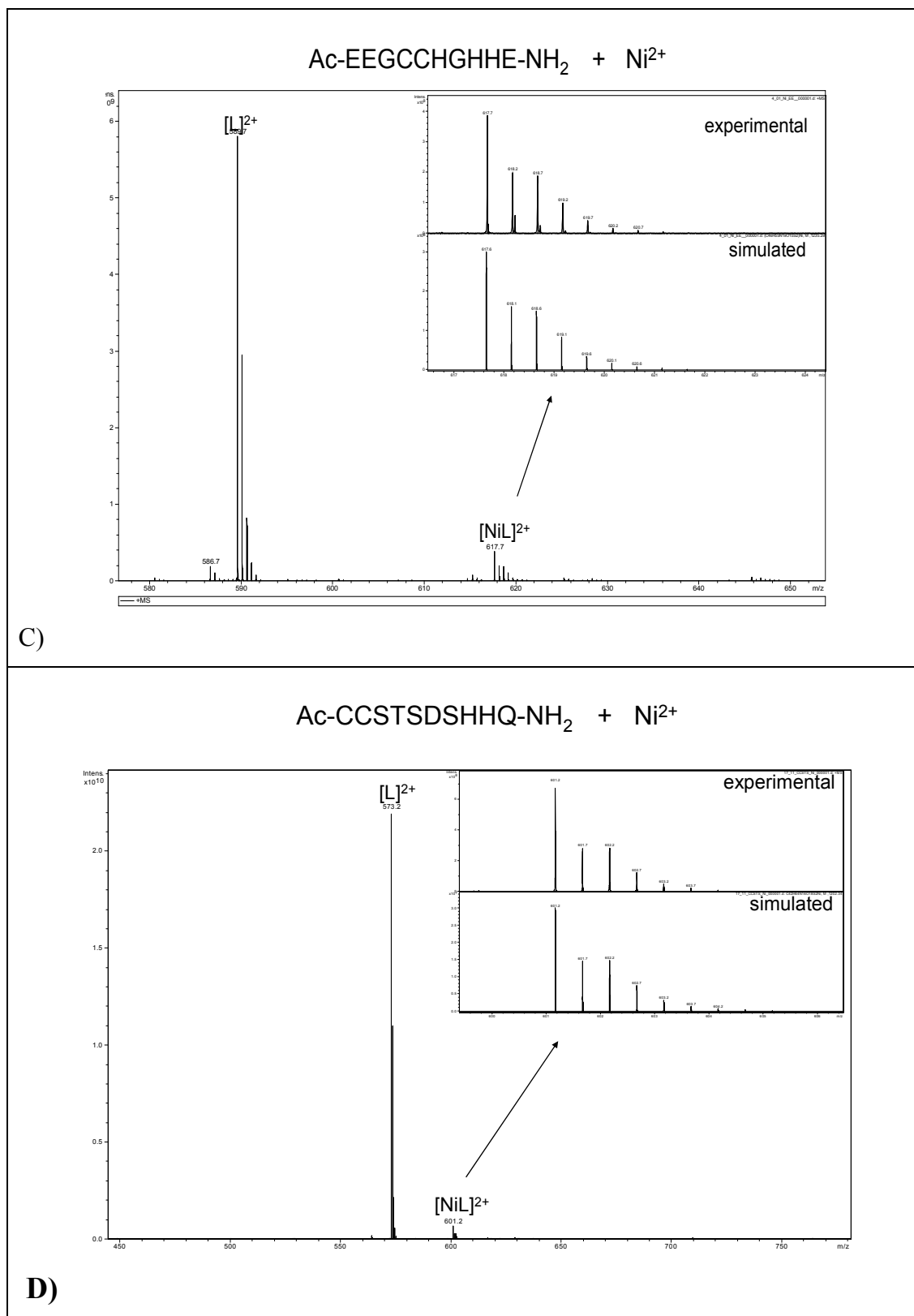
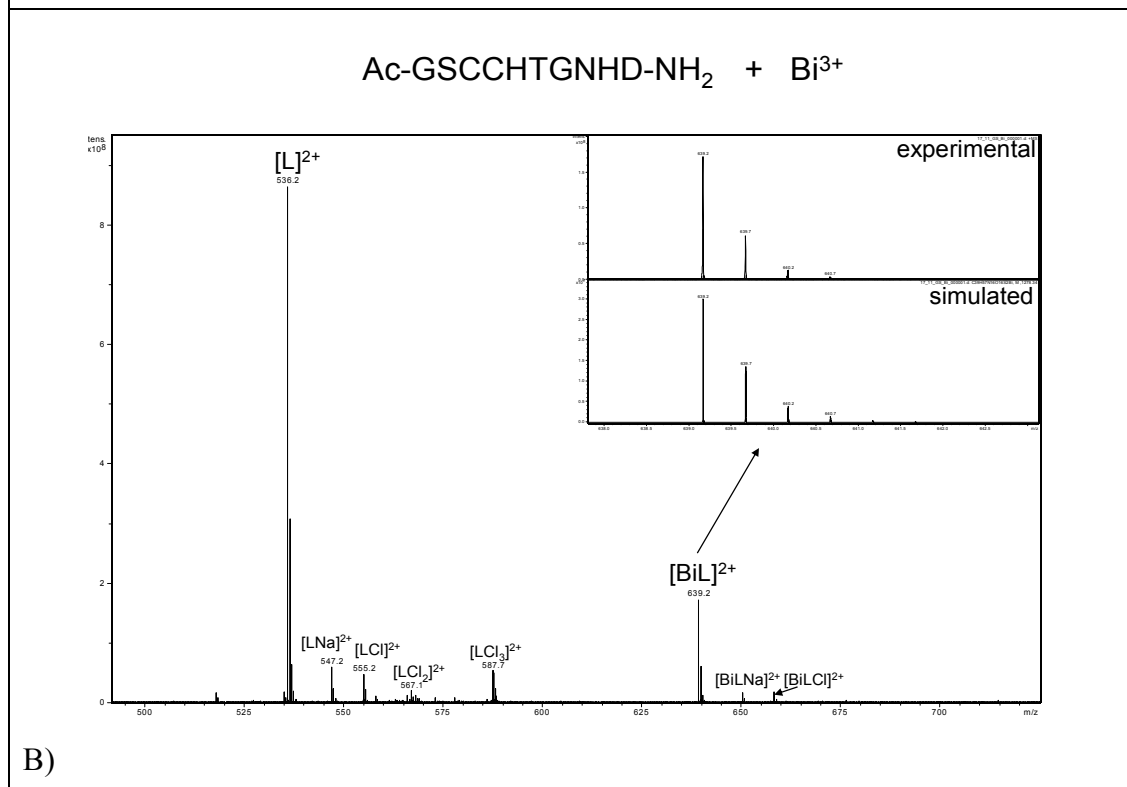
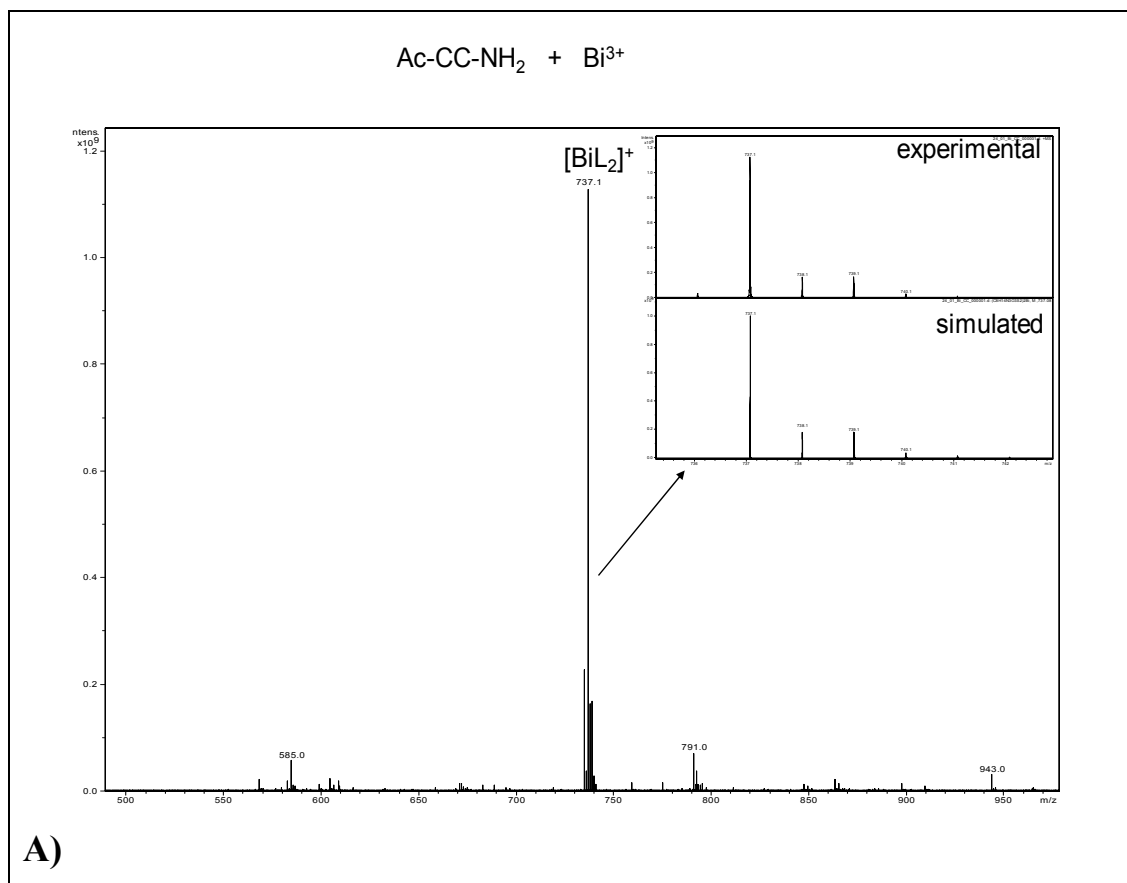


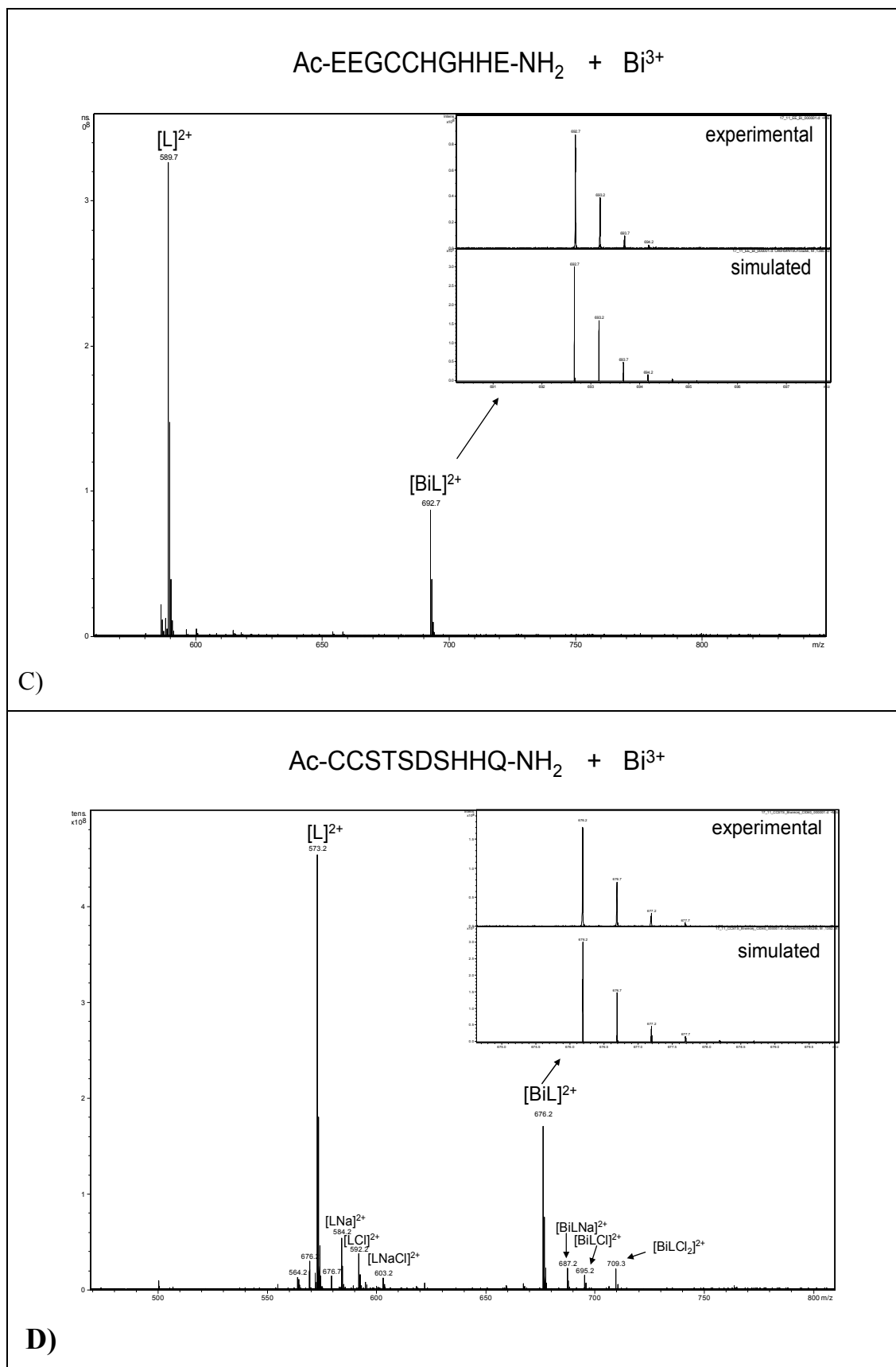
Fig. S6. The UV-Vis spectra of  $Ni^{2+}$  complexes of A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub>, C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub>.



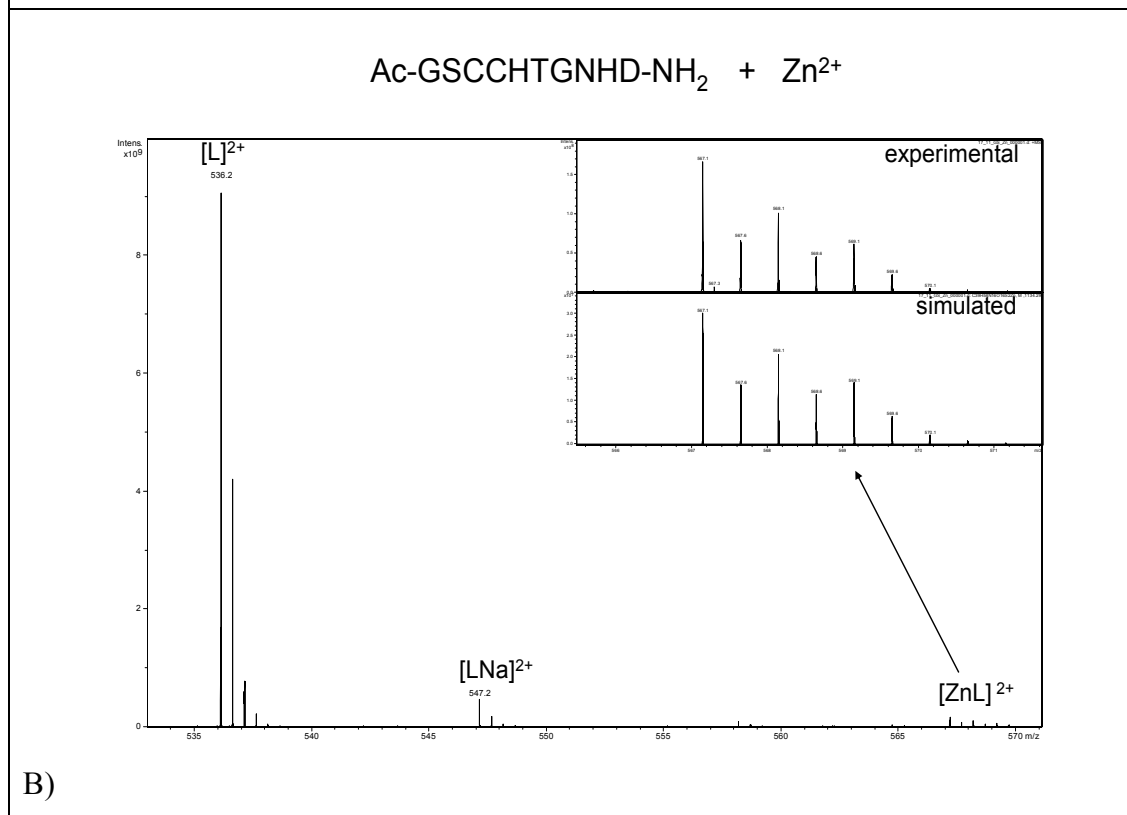
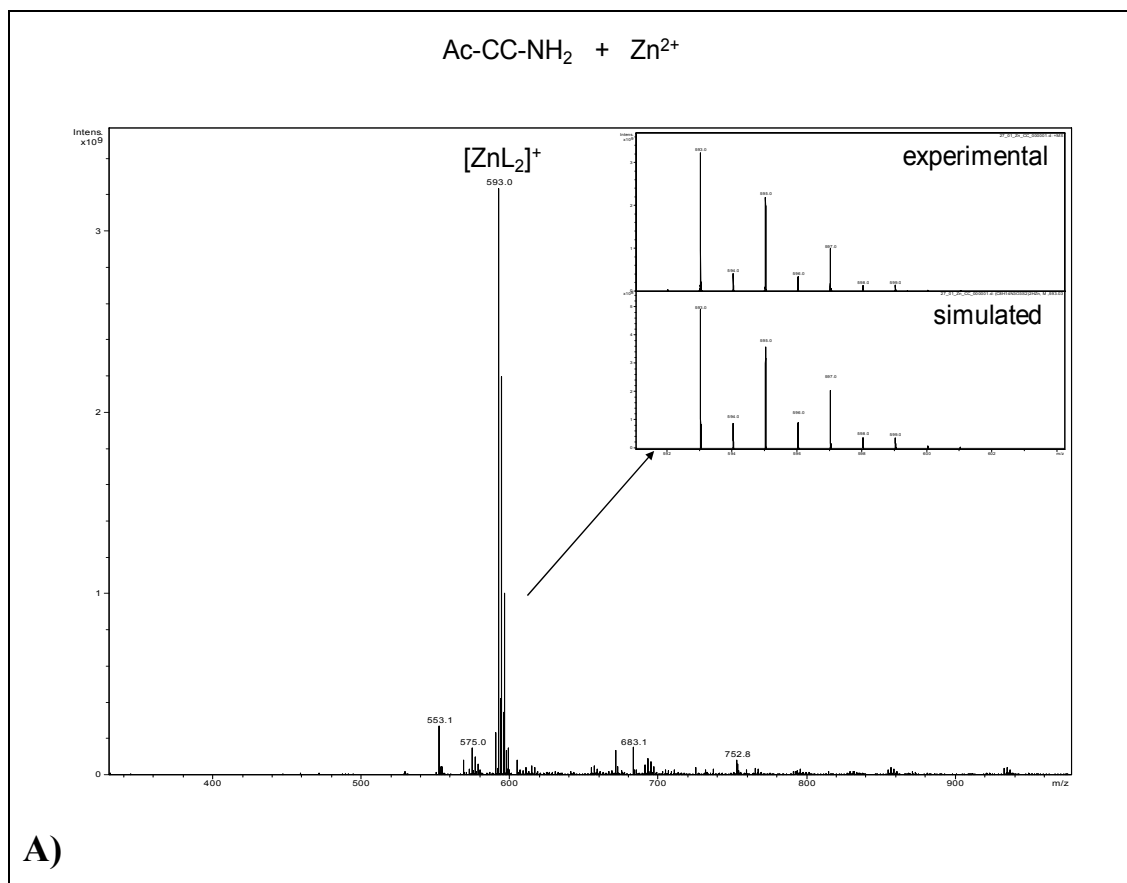


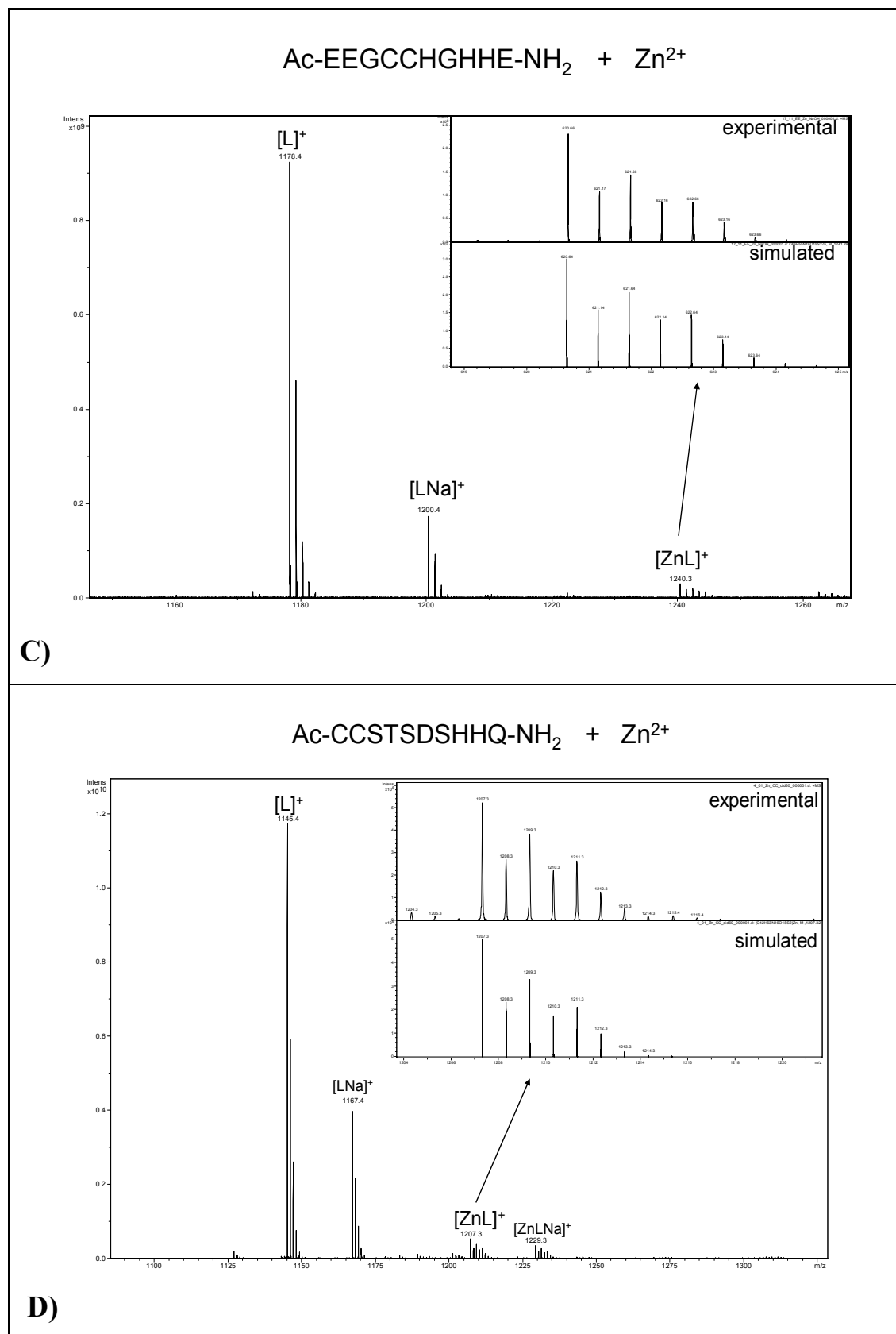
**Fig. S7.** Mass spectra of a system containing Ni<sup>2+</sup> ions A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCHTGNHD-NH<sub>2</sub> C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub> in a 1:1 stoichiometry.





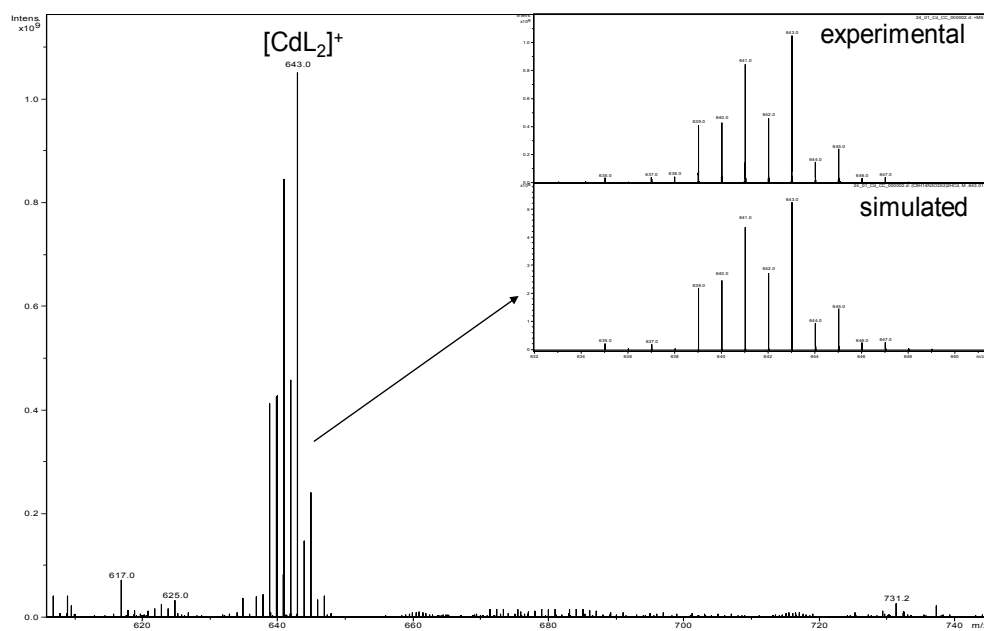
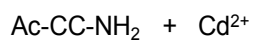
**Fig. S8.** Mass spectra of a system containing Bi<sup>3+</sup> ions and A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub>, C) Ac-EEGCCHGHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub> in a 1:2 stoichiometry.



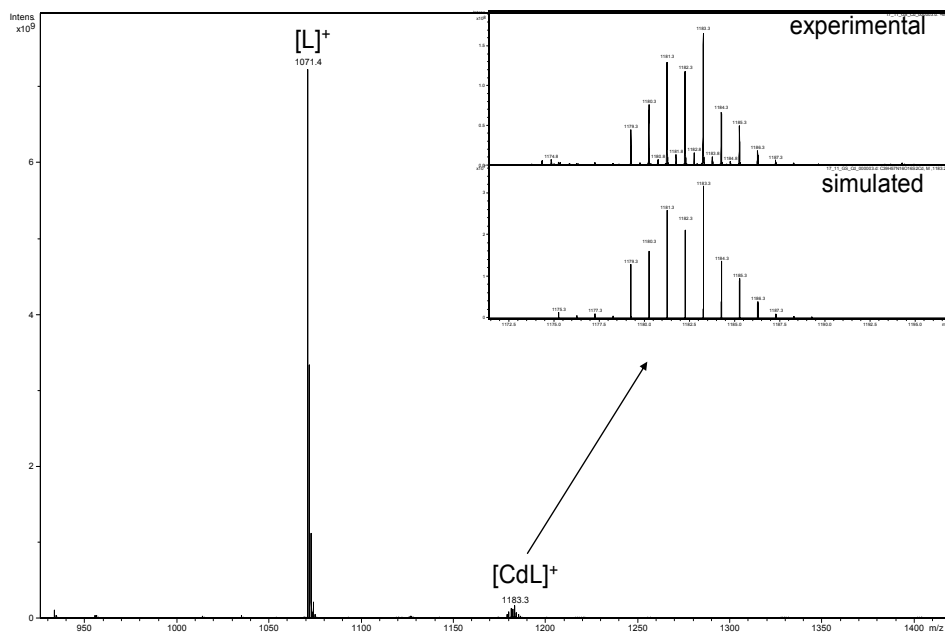


**Fig. S9.** Mass spectra of a system containing Zn<sup>2+</sup> ions and A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub>, C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub> in a 1:1 stoichiometry.

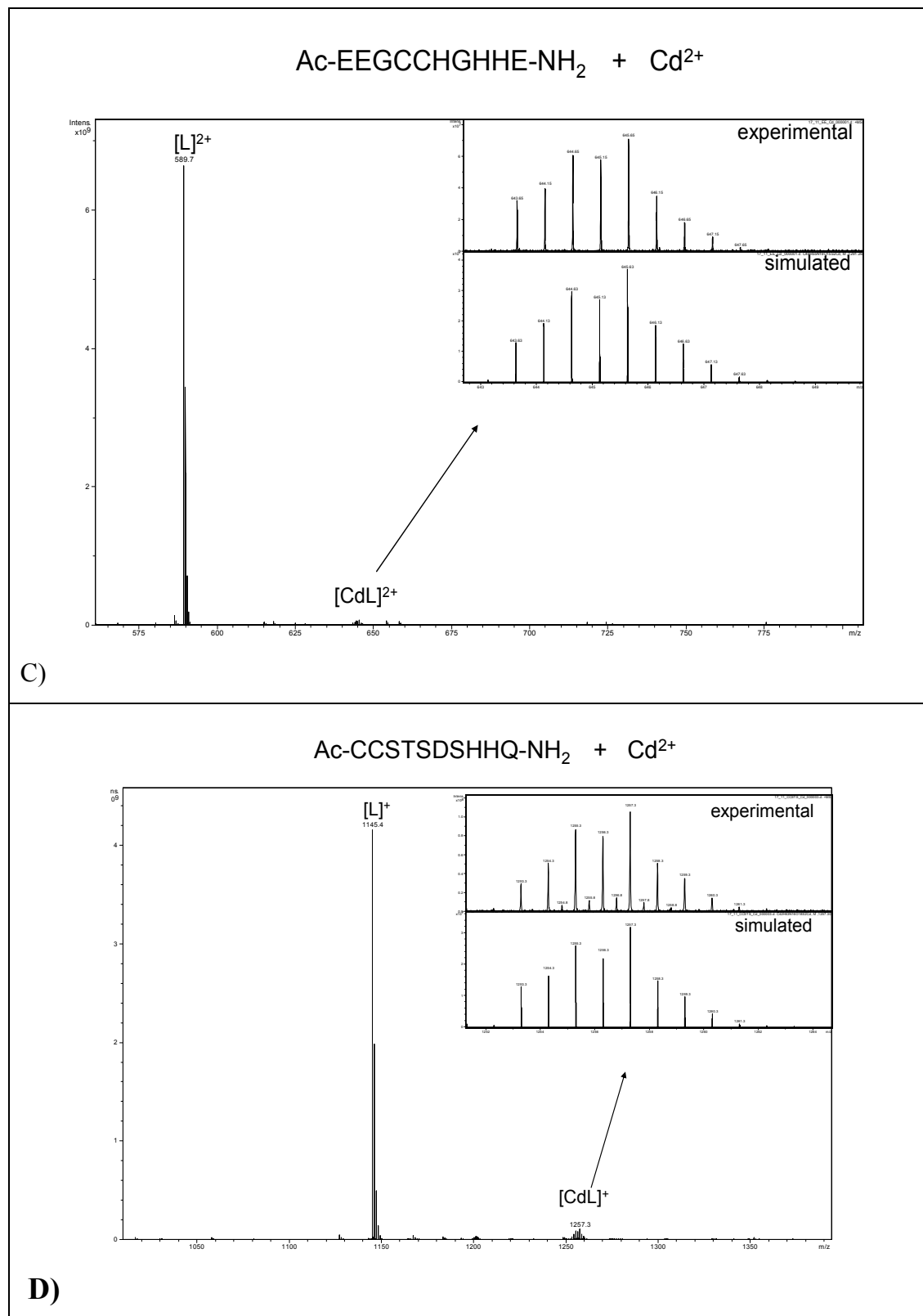




A)



B)



**Fig. S10.** Mass spectra of a system containing Cd<sup>2+</sup> ions and A) Ac-CC-NH<sub>2</sub>, B) Ac-GSCCHTGNHD-NH<sub>2</sub>, C) Ac-EEGCCHGHHE-NH<sub>2</sub>, and D) Ac-CCSTSDSHHQ-NH<sub>2</sub> in a 1:1 stoichiometry.