Electronic Supplementary Material (ESI) for Dalton Transactions

SUPPLEMENTARY INFORMATION

Copper(II) coordination properties of decapeptides containing three His residues: the impact of cyclization and Asp residue coordination.

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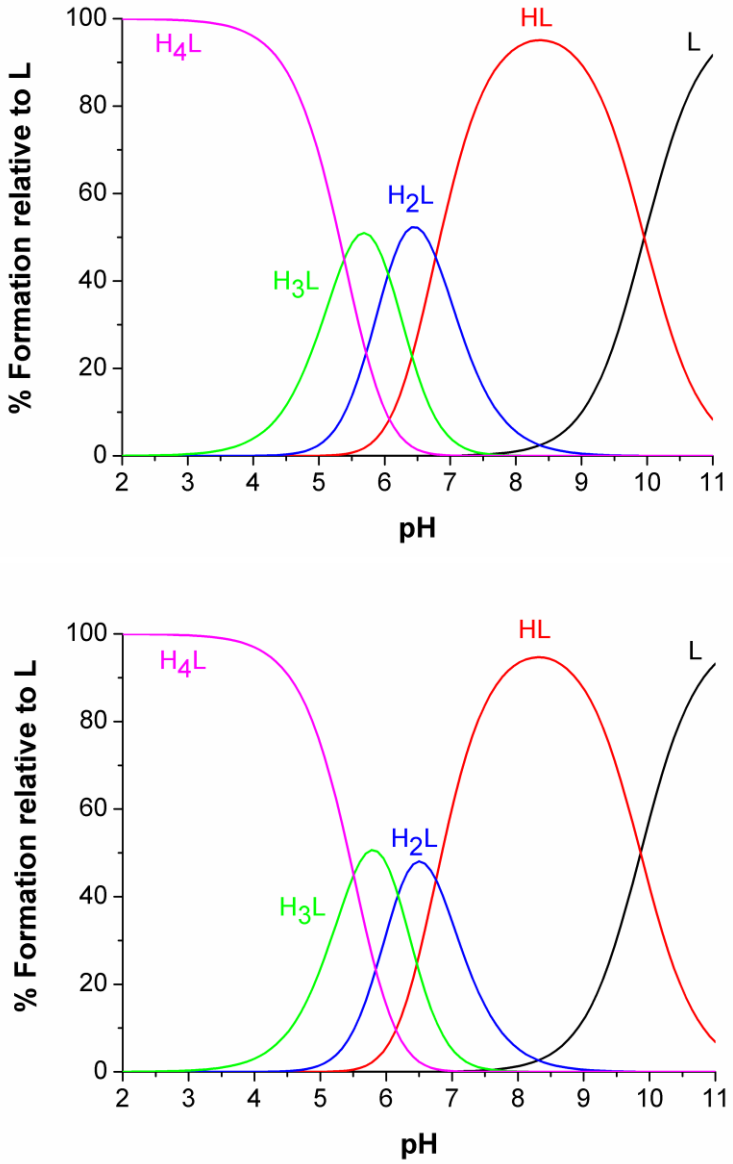

Figure S1. Species distribution diagrams for the C-Asn (upper) and O-Asn (lower) peptides at 298.2 K, I = 0.1 M KNO_3 and [Peptide] = 1.0×10^{-3} M. Charges are omitted for simplicity.

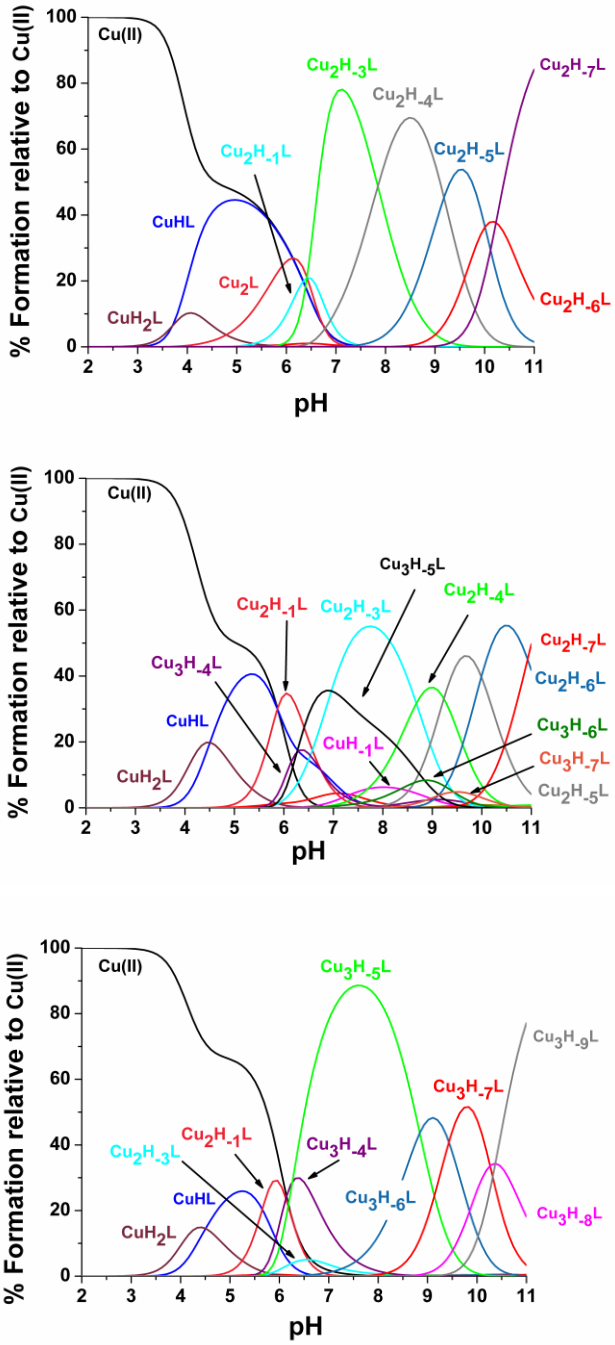

Figure S2. Species distribution diagrams for the copper(II) complexes of (upper) C-Asn (1.0×10^{-3} M) with 2 equiv of $Cu(NO_3)_2$; (middle) O-Asn (1.0×10^{-3} M) with 2 equiv of $Cu(NO_3)_2$ and (lower) O-Asn (1.0×10^{-3} M) with 3 equiv of $Cu(NO_3)_2$ at 298.2 K and I = 0.1 M KNO_3. Charges are omitted for simplicity.

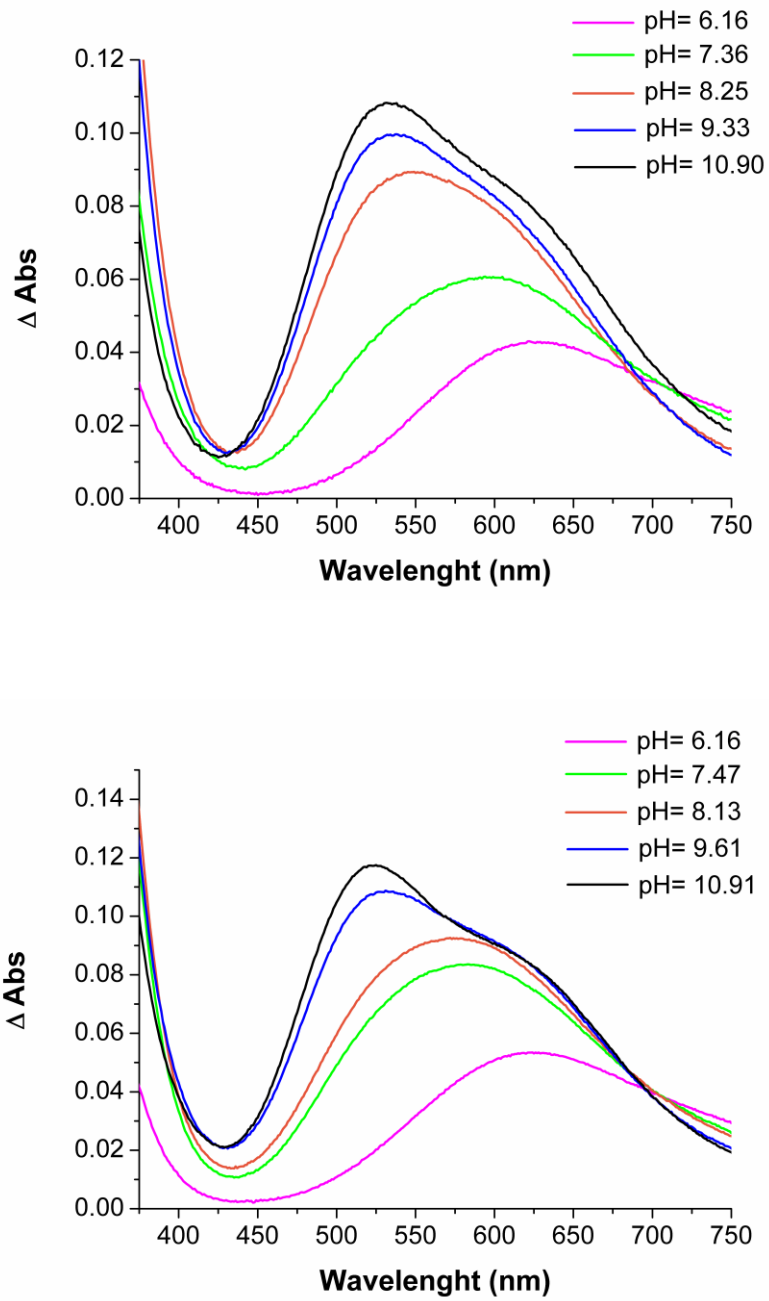

Figure S3. UV-Vis spectra of the copper(II) complexes formed with C-Asn (upper) and O-Asn (lower) at a 1:1 ratio (1.0×10^{-3} M) at different pH values and 298.2 K.

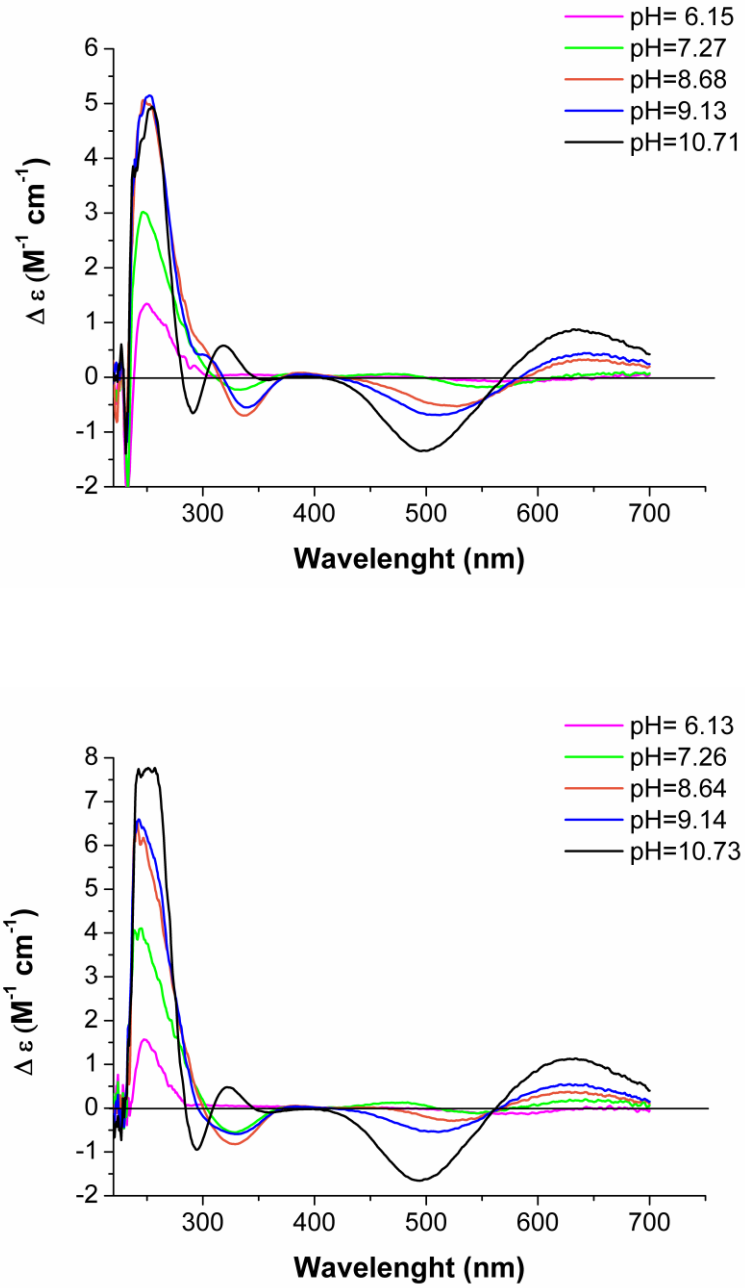

Figure S4. CD spectra of the copper(II) complexes formed with C-Asn (upper) and O-Asn (lower) at a 1:1 ratio (0.5×10^{-3} M) at different pH values and 298.2 K.

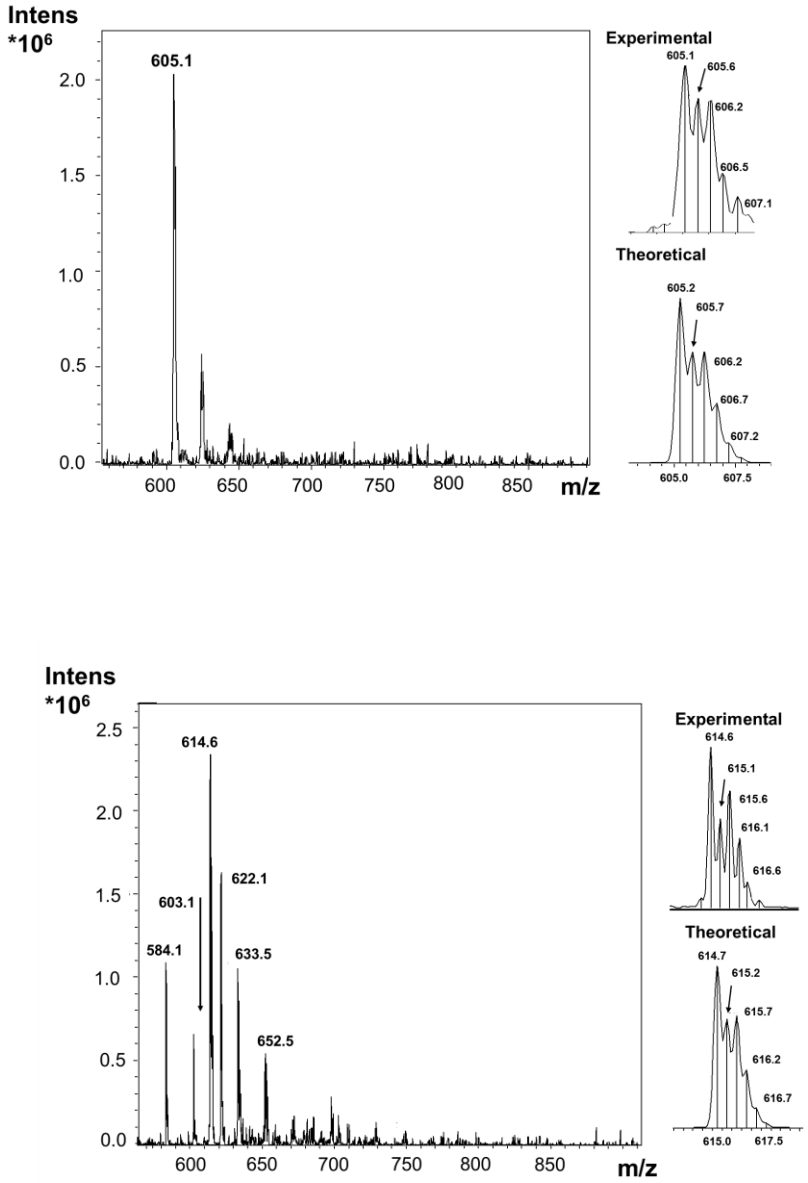

Figure S5. ESI-MS spectra of the C-Asn (upper) and O-Asn (lower) peptides with one equiv of Cu^{2+} at 1.0×10^{-3} M concentration and pH 6.0. Spectra were recorded in the positive detection mode.