Fig. 1S† Concentration distribution of the complexes formed in Cu(II)-to-peptide molar ratio 1:1 as a function of pH. [Cu(II)]=0.001M. (a) Cu(II)-H1A/H9A system (b) Cu(II)-H1A/H6A system
Fig. 2S† Frozen solution EPR spectra (simulated and experimental) of the CuL complexes for the Cu(II)-H1A/H12A (pH 5.5), Cu(II)-H1A/H9A (pH 5.3) and Cu(II)-H1A/H6A (pH 5.6). Metal-to-ligand molar ratio 1:1.
Fig. 3S† ESI mass spectrum for the Cu(II)-H1A/H12A system at 1:1 molar ratio in water solution. Experimental and simulated spectra for the [CuH₁L]⁺ molecular ion with m/z 1195.5 Da.
Fig. 4S† Concentration distribution of the complexes formed in Cu(II)-to-peptide molar ratio 2:1 as a function of pH. [Cu(II)]=0.002M. (a) Cu(II)-H1A/H9A system (b) Cu(II)-H1A/H6A system
Fig. 5S† Concentration distribution of the complexes formed in Cu(II)-to-peptide molar ratio 3:1 as a function of pH. [Cu(II)]=0.003M. (a) Cu(II)-H1A/H9A system (b) Cu(II)-H1A/H6A system
Fig. 6S† CD spectra of the Cu(II)-H1A/H12A, Cu(II)-H1A/H9A and Cu(II)-H1A/H6A systems of the Cu$_2$H$_3$L complexes
Fig. 7S† Frozen solution EPR spectra of the Cu(II)-H1A/H6A, Cu(II)-H1A/H9A and Cu(II)-H1A/H12A systems of the Cu$_3$H$_9$L or Cu$_3$H$_{10}$L complexes formed in 3:1 metal-to ligand molar ratio at pH about 11