Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Metal binding selectivity of an N-terminally free multihistidine peptide NH_2-HAVAHHH-NH_2

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Figure S1
The HPLC chromatogram (a) and MS spectrum (b) of NH_2-HAVAHHH-NH_2 ($[C_{35}H_{51}N_{16}O_7]^+$ (M_r = 807.412)

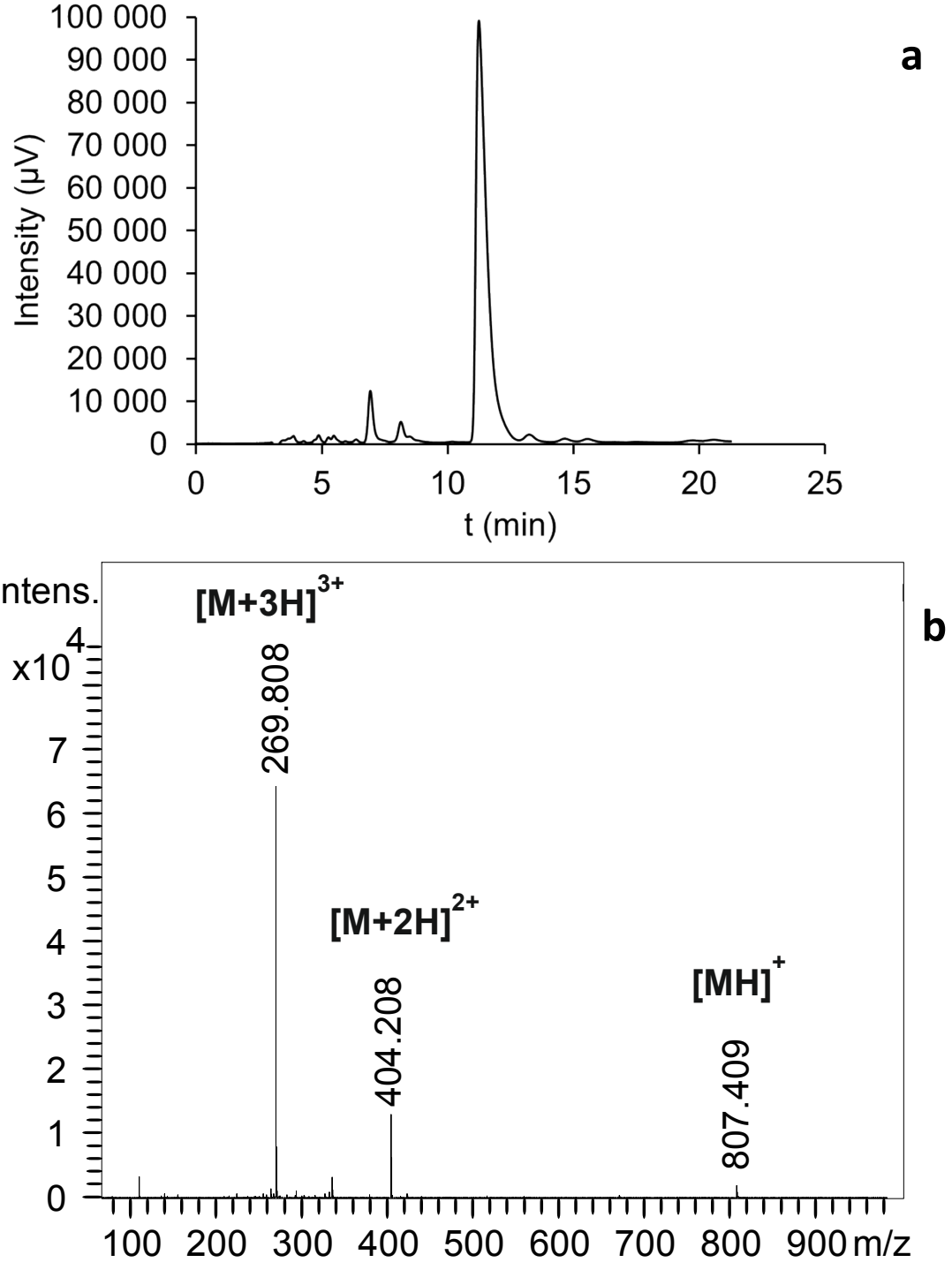

Figure S2
Metal ion speciation of the copper(II)–NH_2-HAVAHHH-NH_2 system ($c_{Cu(II)}$ = 2.0 mM c_L = 4.0 mM)

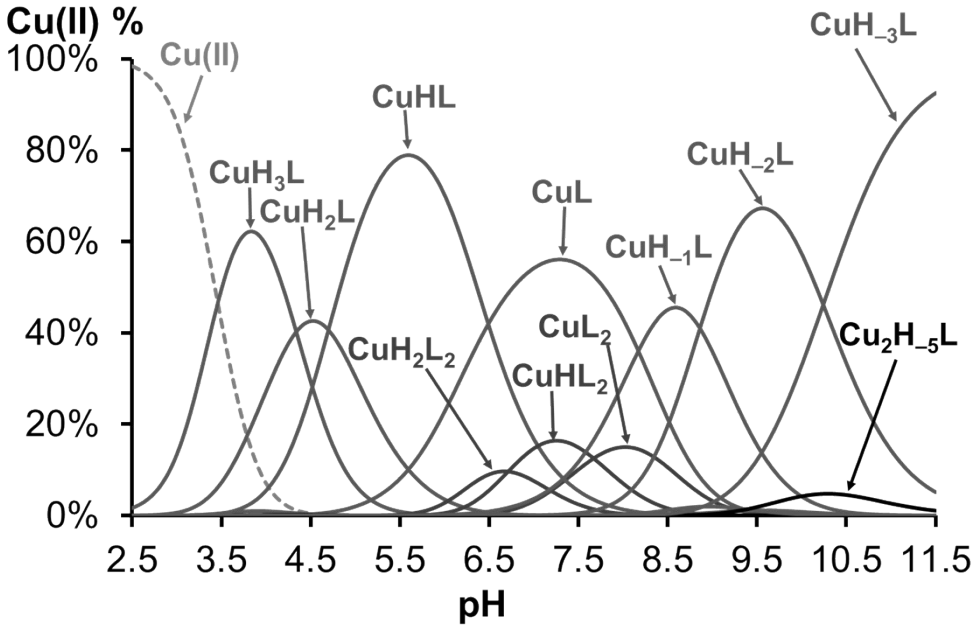

Figure S3

Metal ion speciation of the copper(II)–NH_2-HAVAHHH-NH_2 system ($c_{Cu(II)}$ = 4.0 mM c_L = 2.0 mM)

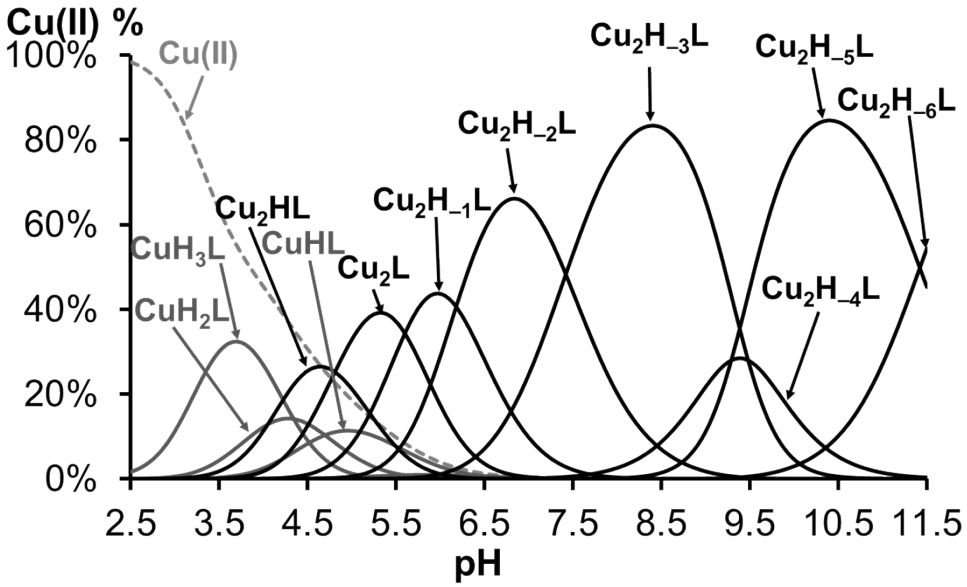

Figure S4:
Metal ion speciation of the nickel(II)–NH_2-HAVAHHH-NH_2 system ($c_{Ni(II)}$ = 2.0 mM c_L = 1.0 mM)

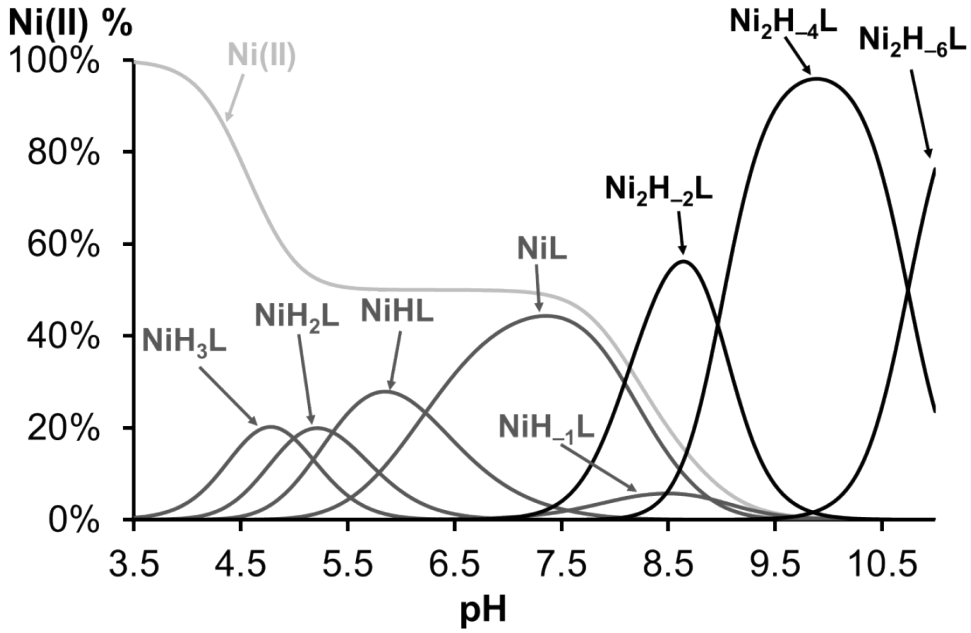

Figure S5
Speciation of the model system containing nickel(II), histamine (A), Ac-HHGH (B) and tetraalanine (C) in equimolar concentration (2.0 mM). Data from ref. 36, 41, 42.

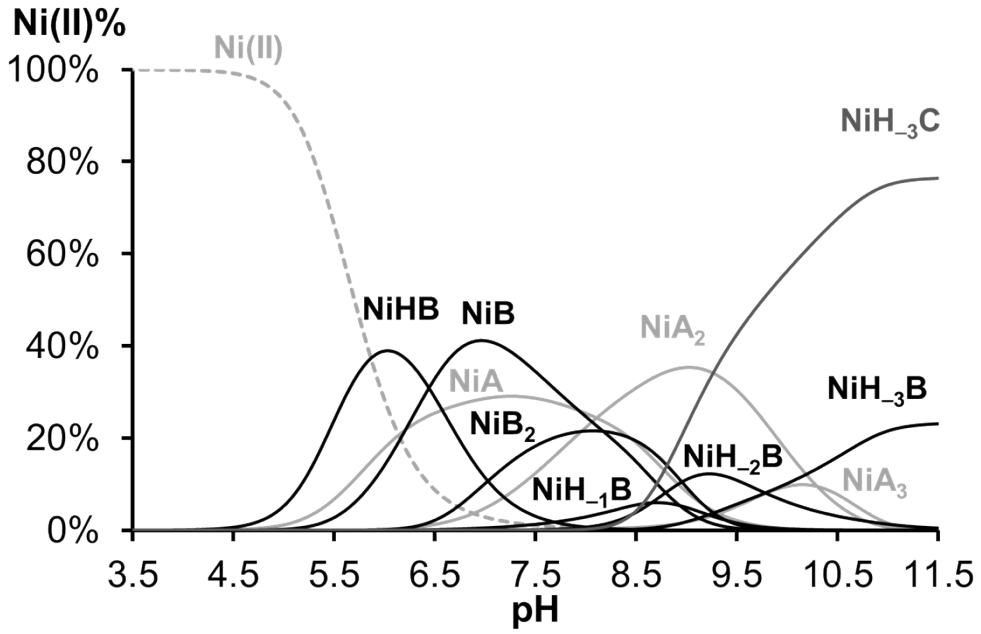

Figure S6

CD spectra of the [$NiH_{-3}L$] complex of tetraalanine[42], the prion fragment Ac-KTNMKHMAG [44] and NH_2-HAVAHHH-NH_2 (pH = 10.95).

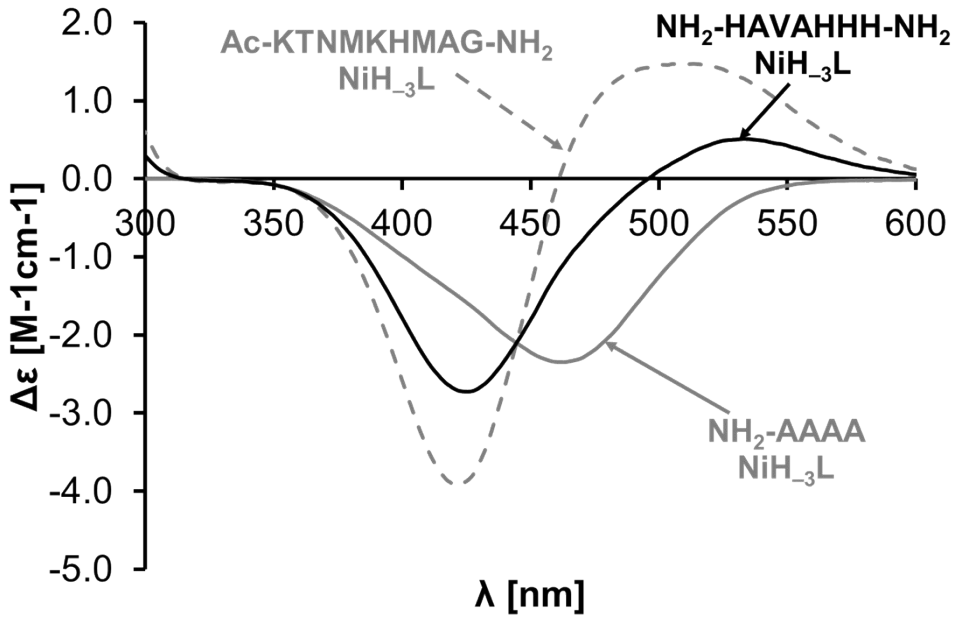

Figure S7

Selected aliphatic region of the $^{1}H–^{1}H$ COSY spectrum of the free ligand (green) and that of the $[NiH_{-3}L]^{-}$ complex (red) at pH = 11.5 ($c_L = c_{Ni}$ = 10.0 mM).

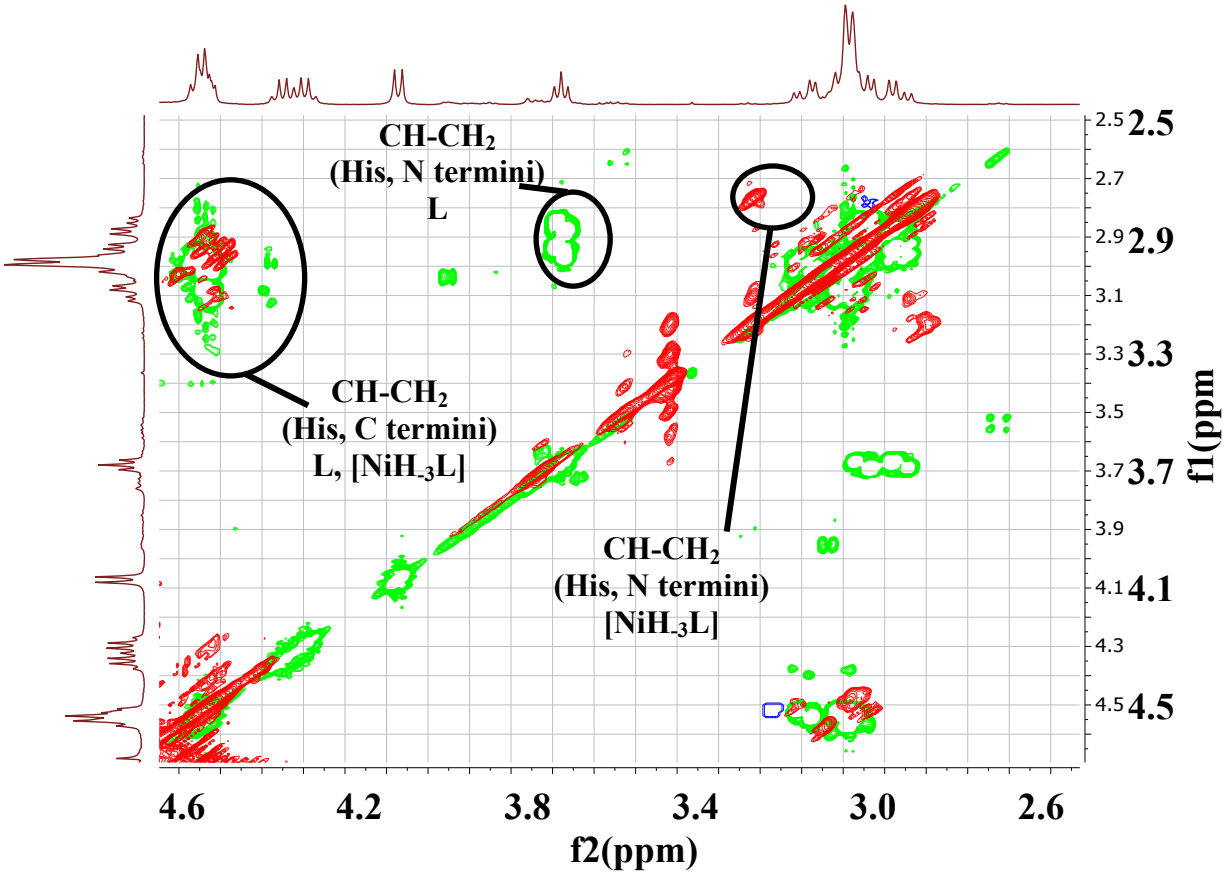

Figure S8

Selected region of ESI-MS spectrum recorded in the nickel(II)–NH_2-HAVAHHH-NH_2 = 2:1 system at pH 11.0 (a) and the calculated spectrum for the species $[Ni_2H_{-6}L]^{2-}$ = $[C_{35}H_{44}N_{16}O_7Ni_2]^{2-}$ (M_r = 916.230) (b)

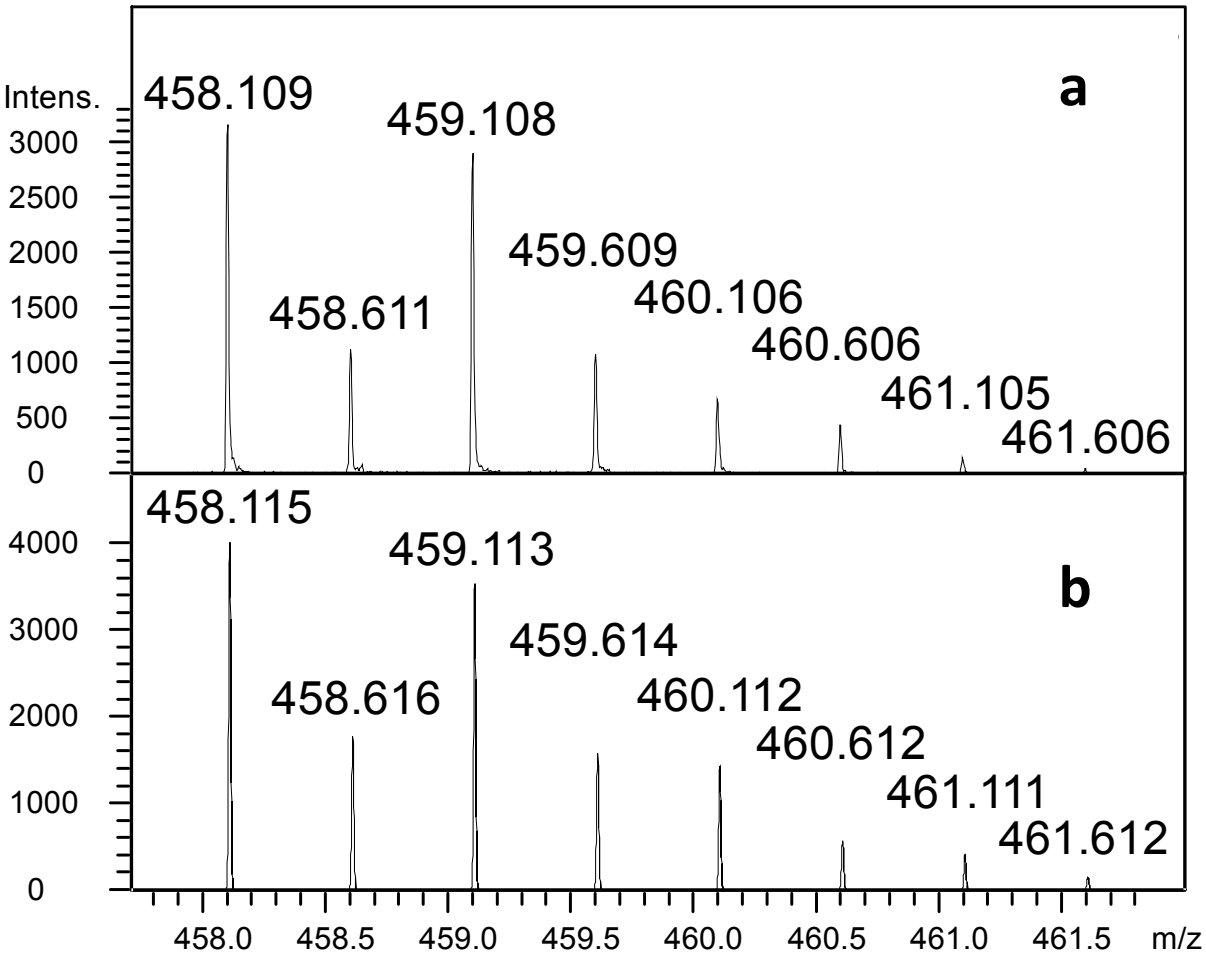

Figure S9

CD spectrum of the $[CuNiH_{-5}L]^{-}$ mixed metal complex of NH_2-HAVAHHH-NH_2 (pH = 10.92) together with CD spectra of dinuclear copper(II) and nickel(II) complexes and the superposition of latter two spectra.

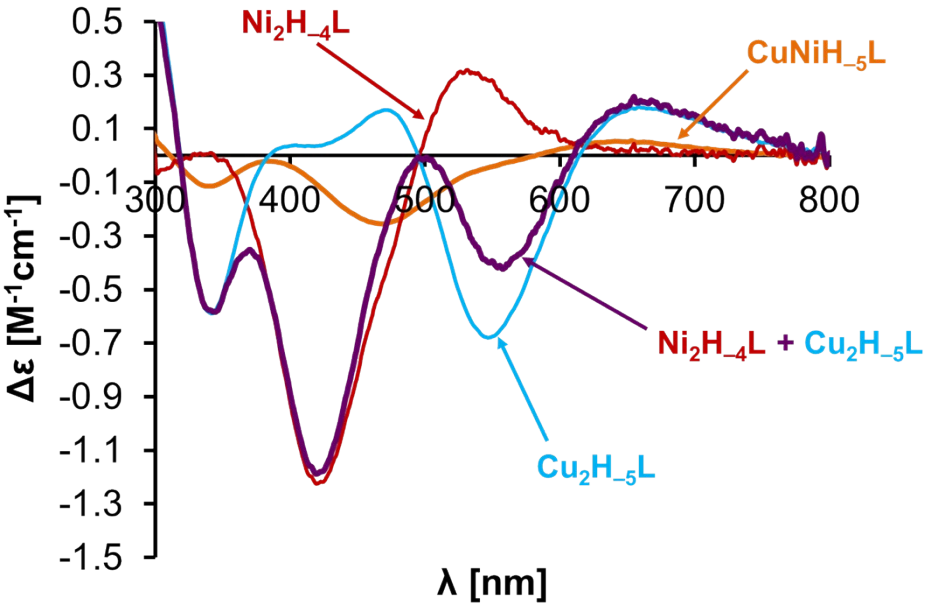

Figure S10

UV-Vis spectra of the major species formed in the $[(\eta^6\text{-}p\text{-cym})Ru(H_2O)_3]^{2+}$–$NH_2$-HAVAHHH-$NH_2$ system at 1:1 (pH = 2.54) (a), 2:1 (pH = 2.70) (b) ratios and the spectra of $[(\eta^6\text{-}p\text{-cym})Ru(H_2O)_3]^{2+}$ solution at pH = 2.11 (c) and pH = 3.12 (d)

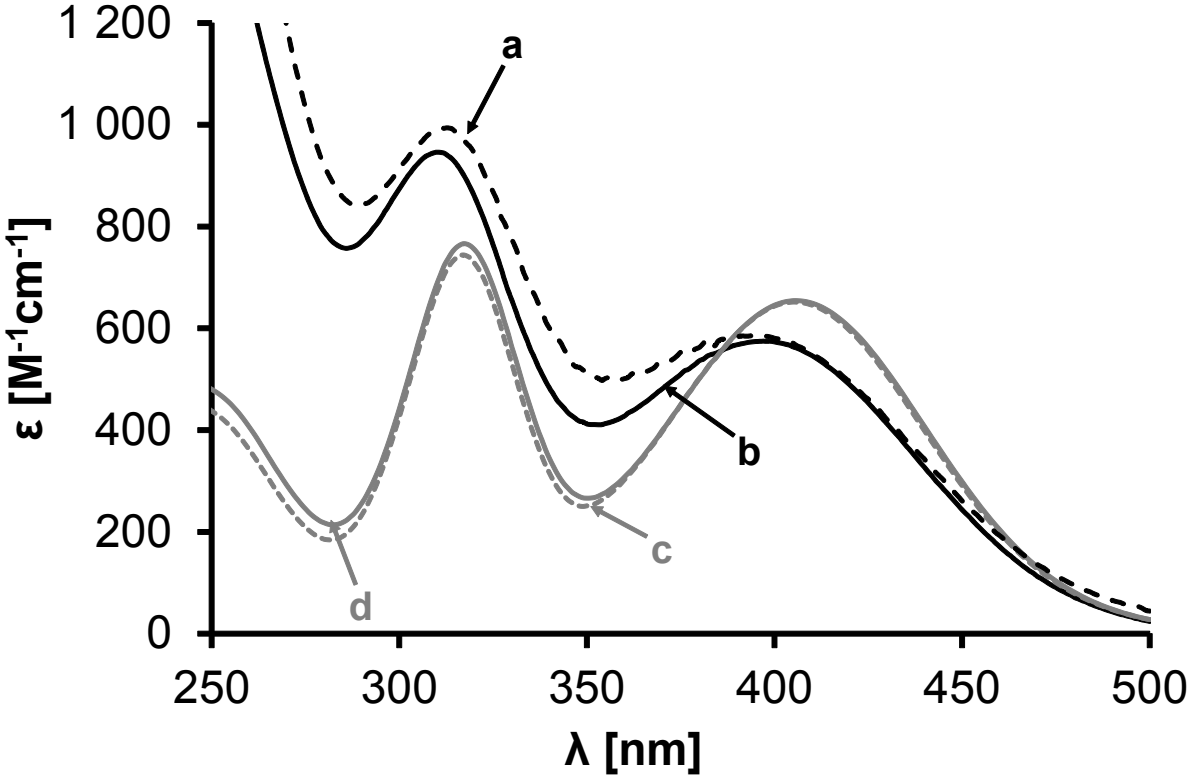

Figure S11

pH-dependent ^{1}H NMR spectra of the $[(\eta^{6}\text{-}p\text{-cym})Ru(H_2O)_3]^{2+}$–$NH_2$-HAVAHHH-$NH_2$ system.

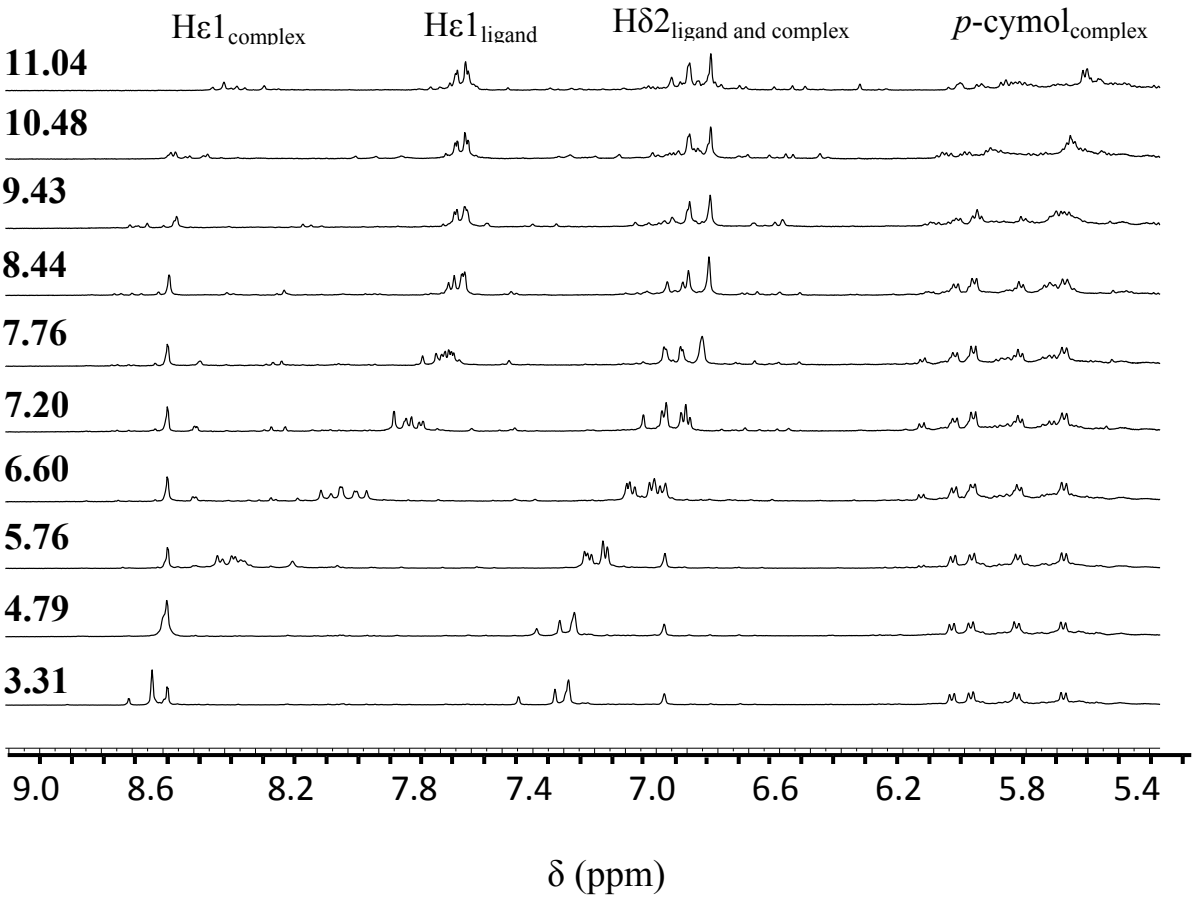

Figure S12

Selected region of ESI-MS spectrum recorded in the $[(\eta^6\text{-}p\text{-cym})Ru(H_2O)_3]^{2+}$–$NH_2$-HAVAHHH-$NH_2$ = 1:1system at pH 2.54 (b) and calculated spectrum for the species $[(MH_2L)Cl]^{3+}$ = $[C_{35}H_{52}N_{16}O_7(RuC_{10}H_{14})Cl]^{3+}$ (M_r = 1079.403) (b)