Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information for:

Zn^{II} and Hg^{II} binding to a designed peptide that accommodates different coordination geometries

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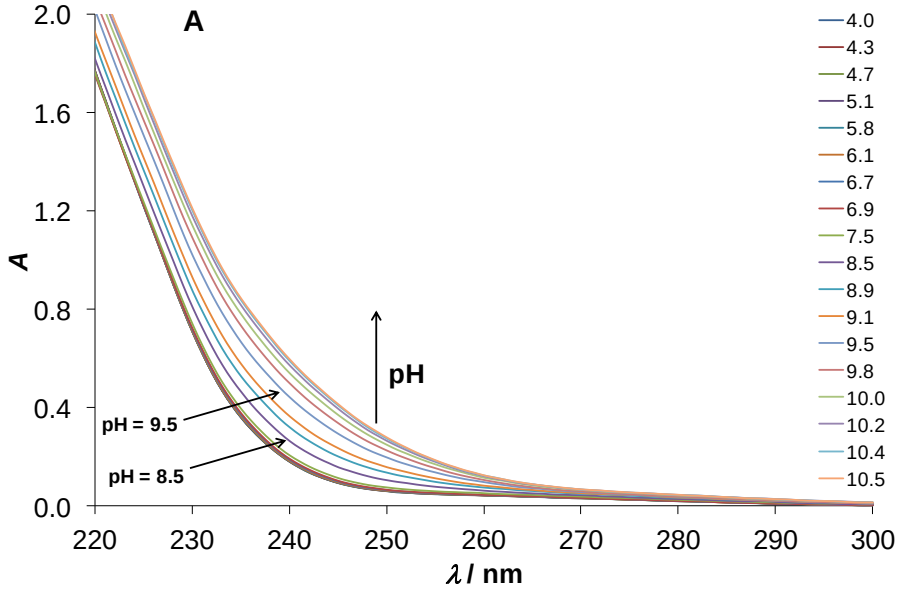

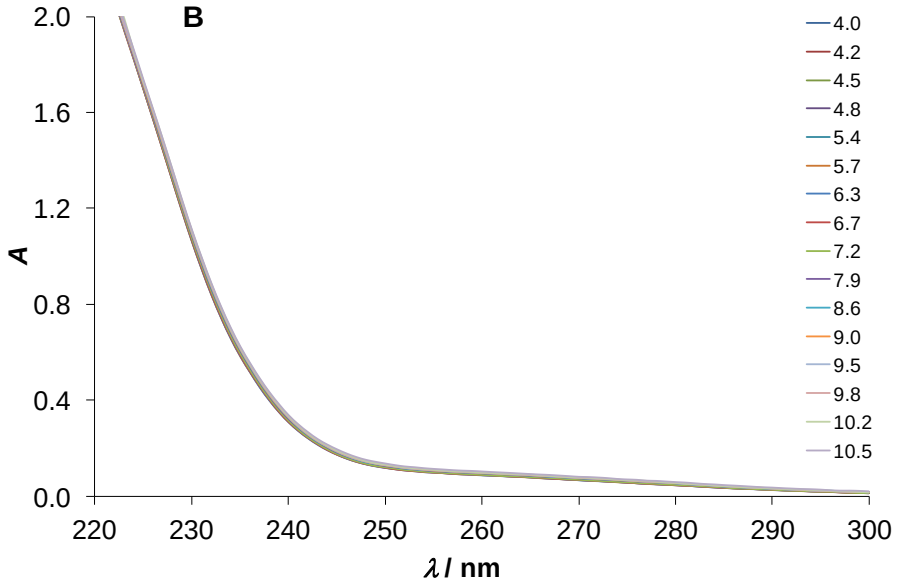

Fig. S1A-B.: UV-spectra recorded for Hg^{II} – **HS** 0.5:1 (A) and 1:1 (B). ($c_{\mathbf{HS}} = 1.0\times10^{-4}$ M (A,B), I = 0.1 M $NaClO_4$, T = 298 K, l = 1.0 cm)

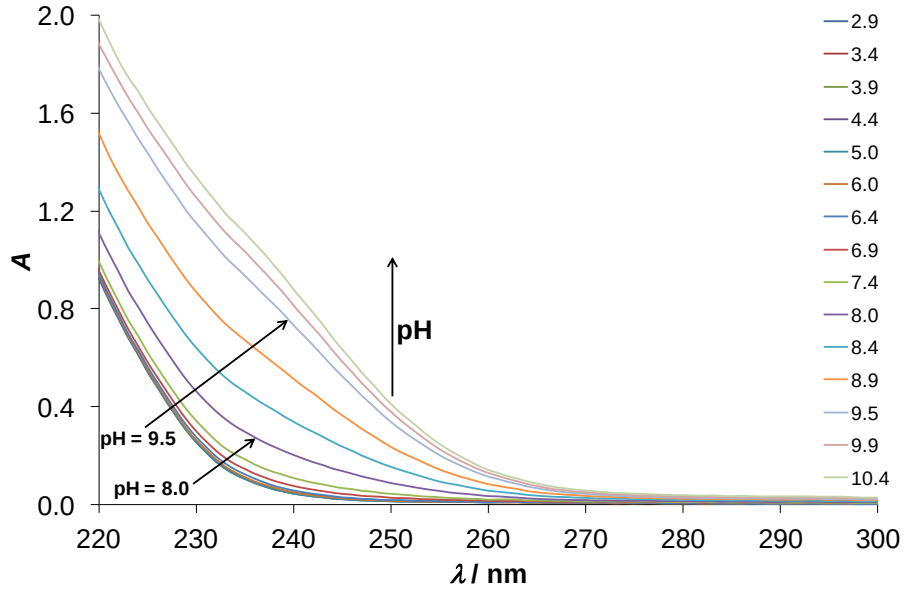

Fig. S2.: UV-spectra recorded for **HS** in the absence of metal ions. ($c_{\mathbf{HS}}$ = 1.0×10^{-4} M, I = 0.1 M $NaClO_4$, T = 298 K, l = 1.0 cm)

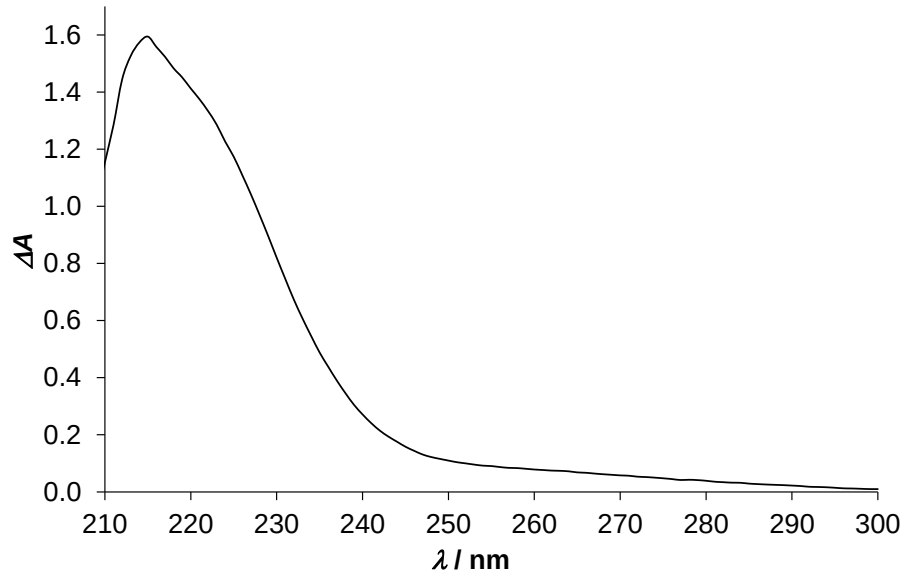

Fig. S3.: Difference of the UV-spectra recorded for Hg^{II}-**HS** 1:1 and **HS** at pH = 4.0. Note that the position of the maximum (λ_{max}) of the observed band has a significant uncertainty due to the large absorbances recorded between 210-220 nm ($c_{\mathbf{HS}} = 1.0\times10^{-4}$ M, I = 0.1 M $NaClO_4$, T = 298 K, l = 1.0 cm)

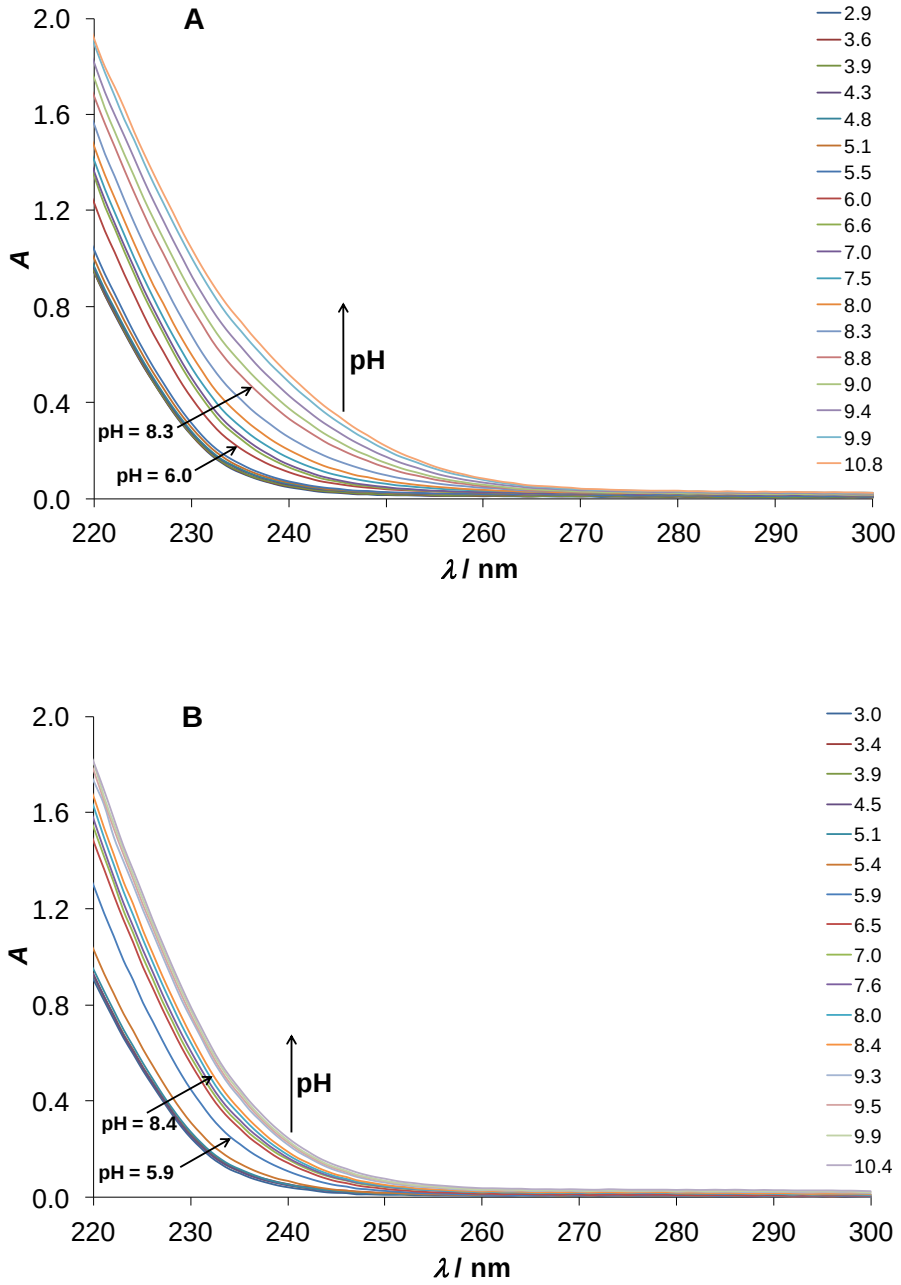

Fig. S4A-B.: UV-spectra recorded for Zn^{II} – **HS** 0.5:1 (A) and 1:1 (B) ($c_{\mathbf{HS}}$ = 1.0×10^{-4} M (A,B), I = 0.1 M $NaClO_4$, T = 298 K, l = 1.0 cm)

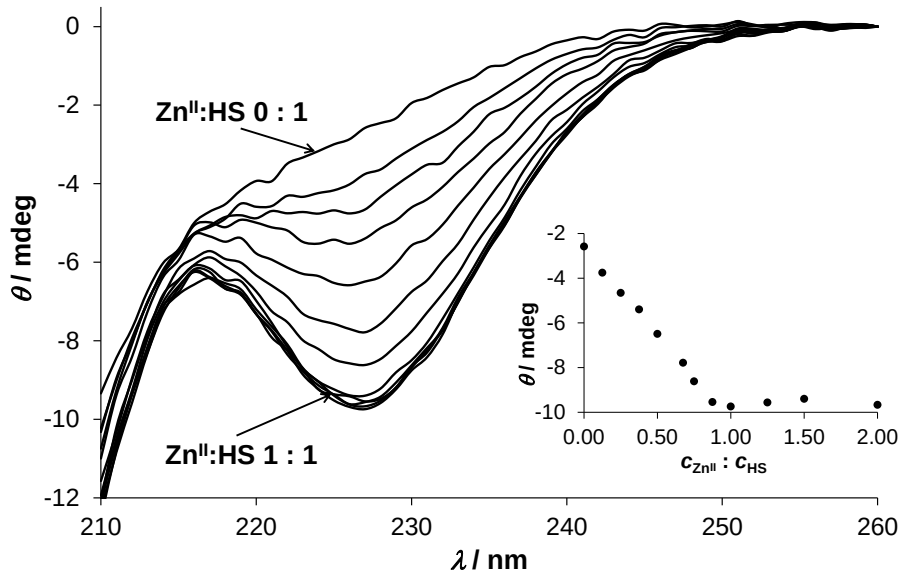

Fig. S5.: SRCD spectra of **HS** as a function of metal ion to ligand ratio in the range of 0:1 to 2:1 at pH = 10.5 ($c_{\mathbf{HS}} = 2.0\times10^{-4}$ M, I = 0.1 M $NaClO_4$, T = 298 K, l = 1 mm). The insert shows the trace of ellipticities at λ = 227 nm.

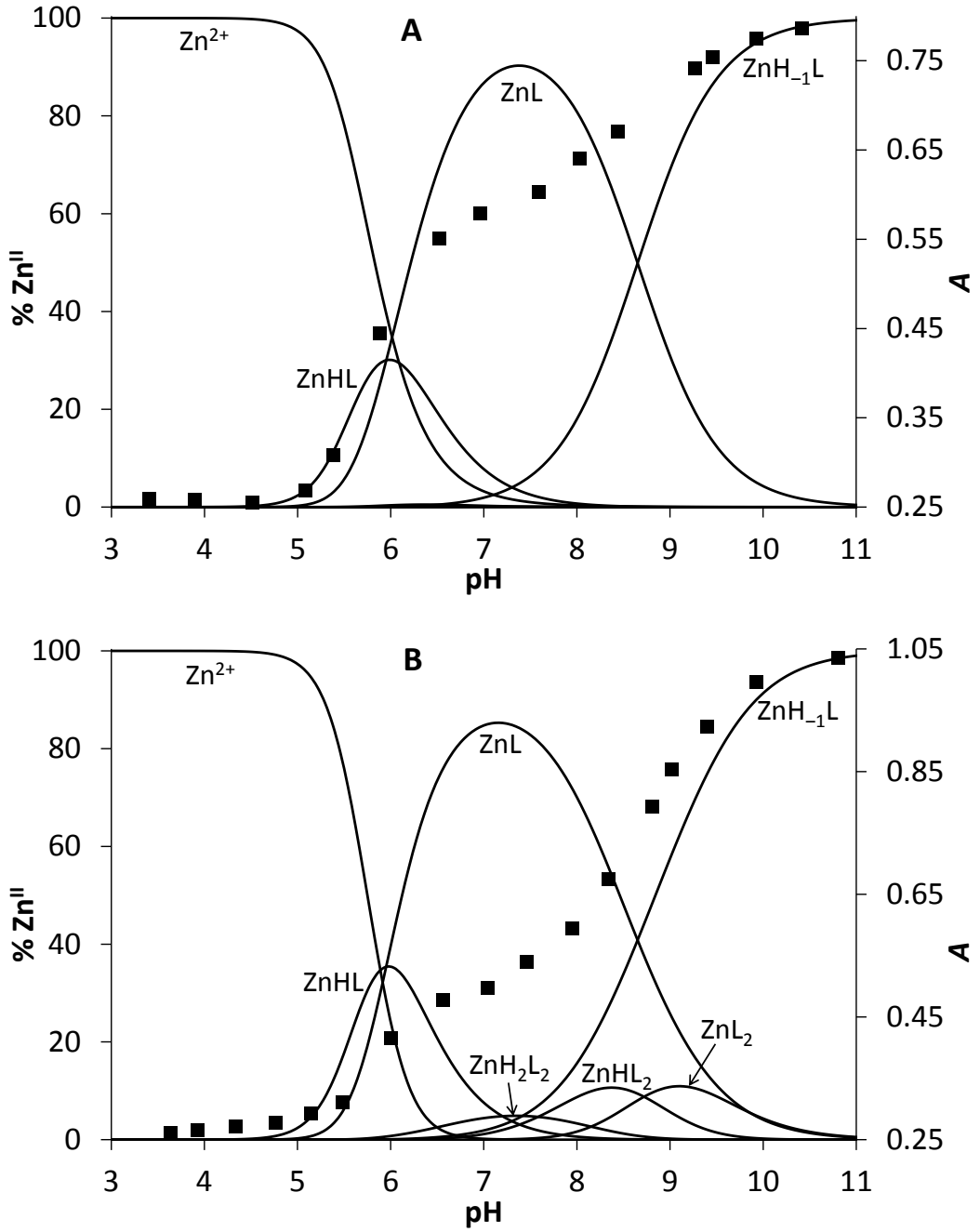

Fig. S6A-B.: Species distribution diagram and for the Zn^{II} : **HS** 1:1 (A) and 0.5:1 (B) systems ($c_{\mathbf{HS}}$ = 1.0×10^{-4} M). The full squares represent the measured absorbances at 230 nm.

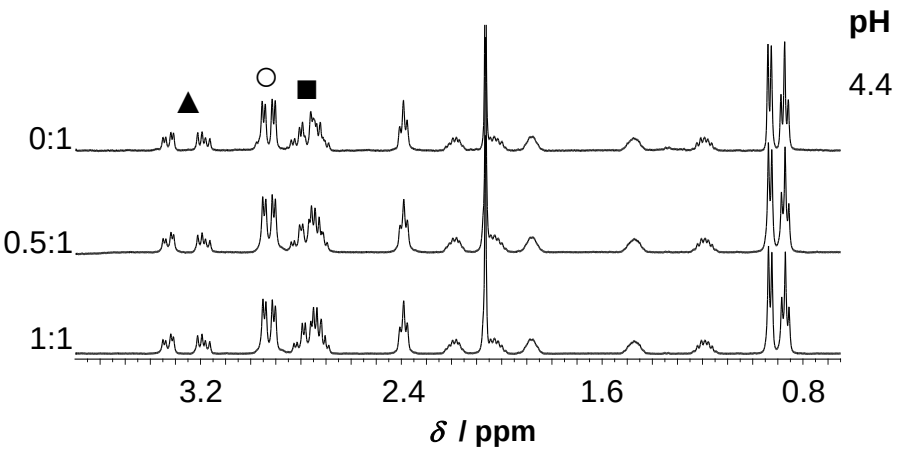

Fig. S7.: Aliphatic region of the ^{1}H NMR spectra of **HS** recorded in the absence of Zn^{II} and in the Zn^{II}:**HS** 0.5:1 and 1:1 systems at pH = 4.4 (H_2O/D_2O = 90:10 %v/v, $c_{\mathbf{HS}} = 1.3\times10^{-3}$ M, T = 298 K). $C_\beta H_2$ resonances of the residues with potential donor groups are indicated by the following symbols: His $C_\beta H_2$: ▲; Cys $C_\beta H_2$: ○; Asp $C_\beta H_2$: ■.