Electronic Supplementary Information

Unusual binding modes in the copper(II) and palladium(II) complexes of peptides containing both histidyl and cysteinyl residues

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Figure Captions

Figure S1. Circular dichroism spectra recorded in the Cu(II):AAHAAC-NH_2 1:1 system. c_L = 2 mM.

Figure S2. Calculated ECD spectra and optimized structure of the different $PdLH_{-1}$ complexes, L = AAHAAC-NH_2.

Figure S3. EPR spectra of Cu(II):AHAAAC-NH_2 1:1 at pH 7.93.

Figure S4. Concentration distribution curve of the complexes formed in the Pd(II):AHAAAC-NH_2 1:1 system. The stepwise protonation constants are also marked. c_L = 2 mM.

Figure S5. pH-dependent CD spectra recorded in the Pd(II):AHAAAC-NH_2 1:1 system.

Figure S6. Calculated ECD spectrum of the MLH_{-1} complex formed in the Pd(II):AHAAAC-NH_2 system.

Figure S1. Circular dichroism spectra recorded in the Cu(II):AAHAAC-NH_2 1:1 system. c_L = 2 mM.

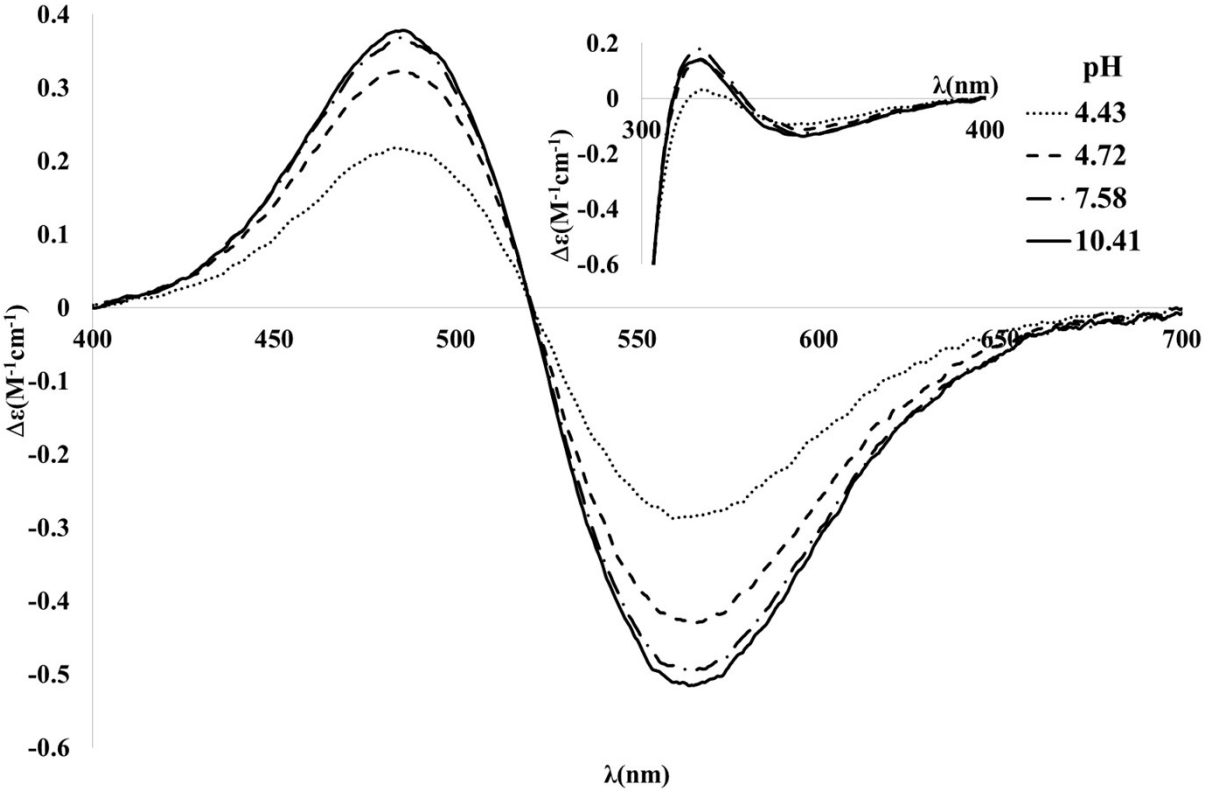
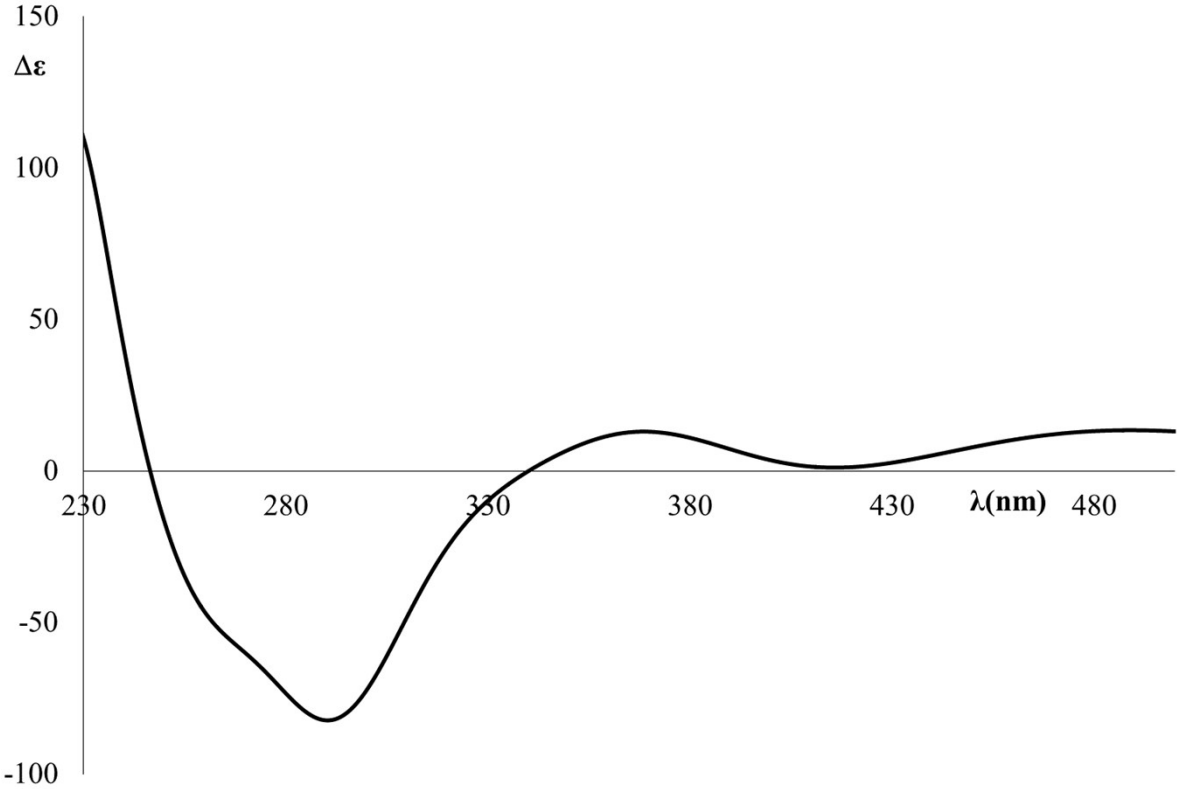
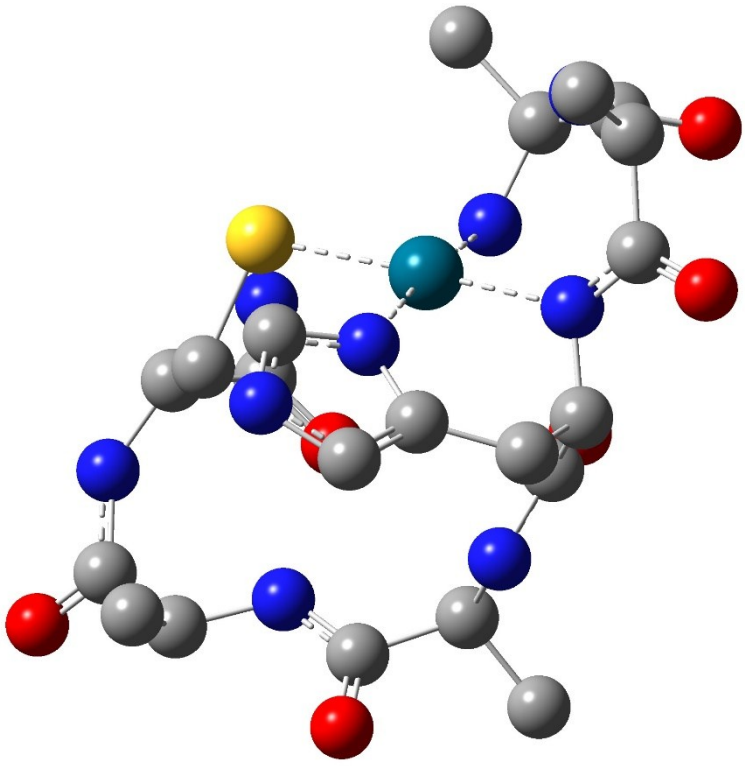


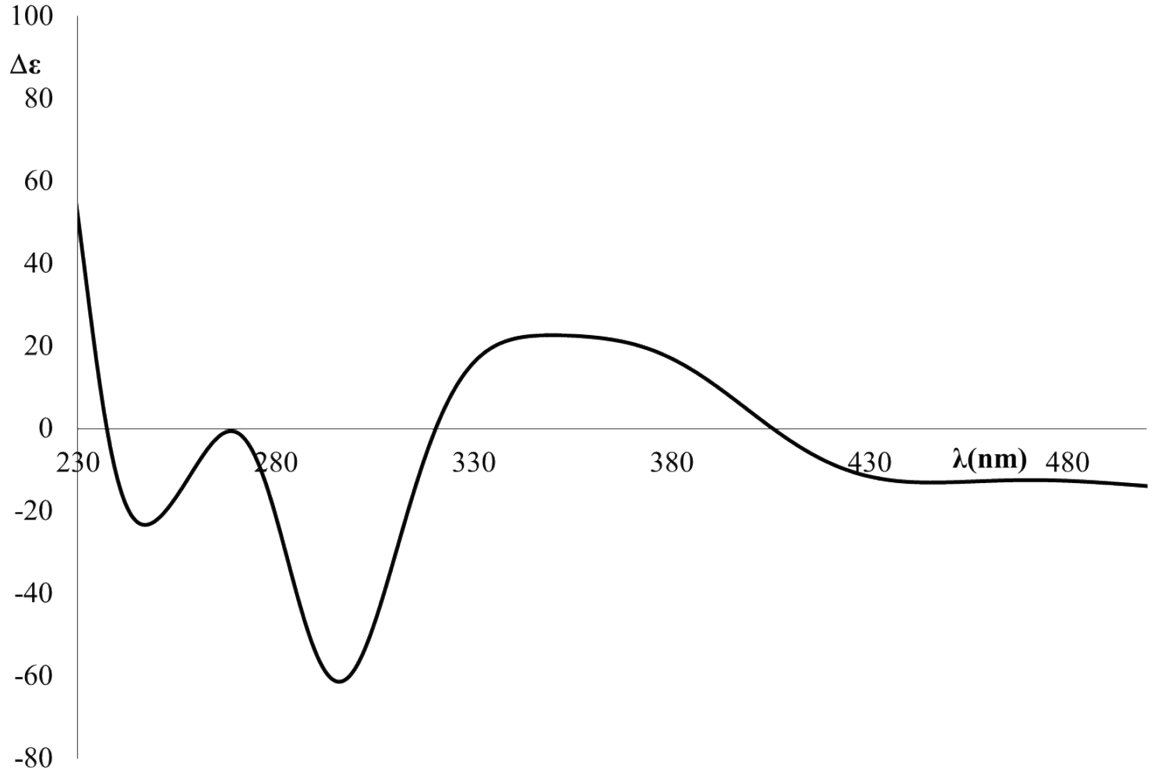
Figure S2. Calculated ECD spectra and optimized structure of the different $PdLH_{-1}$ complexes, L = AAHAAC-NH_2.

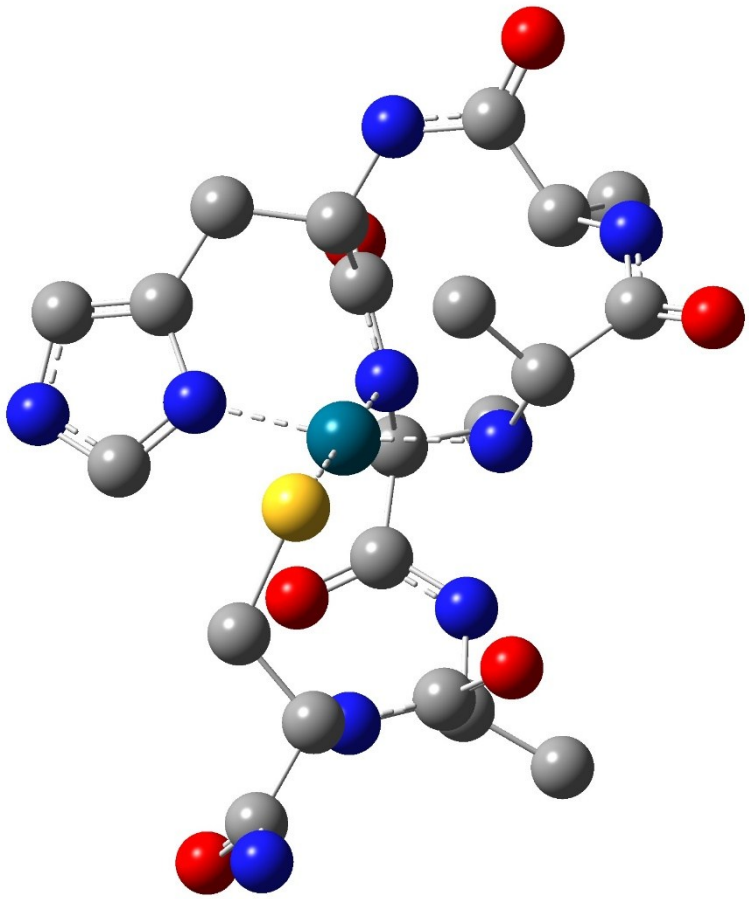
N(2) coordination



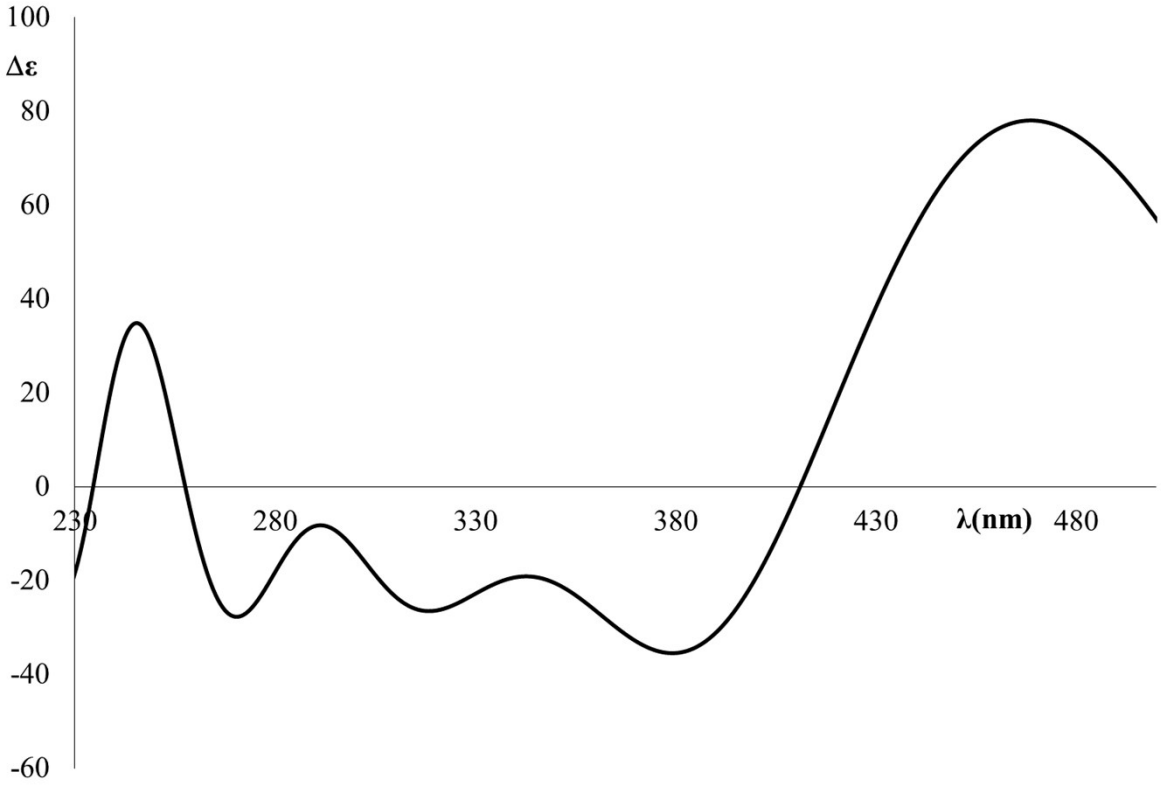


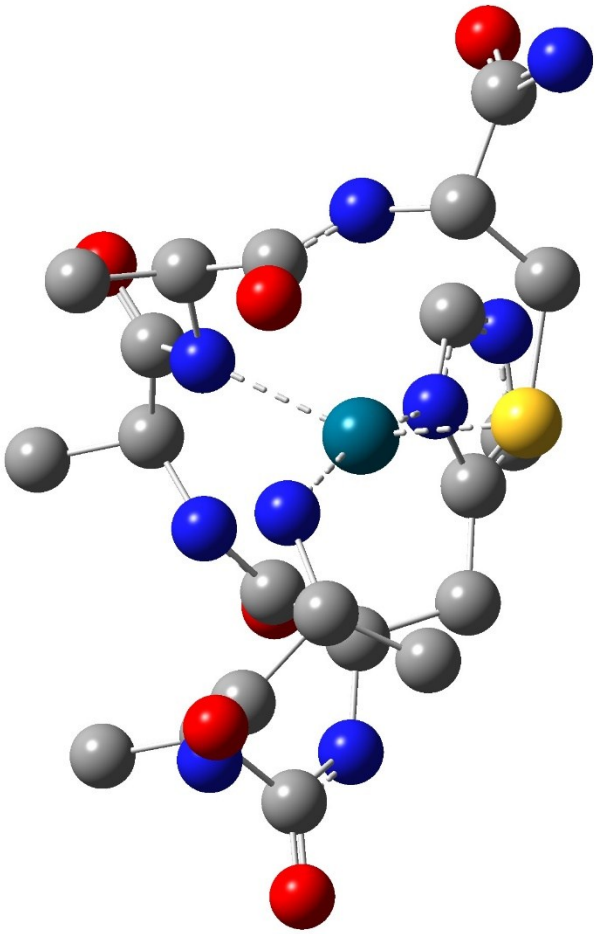
N(3) coordination





N(4) coordination





N(5) coordination

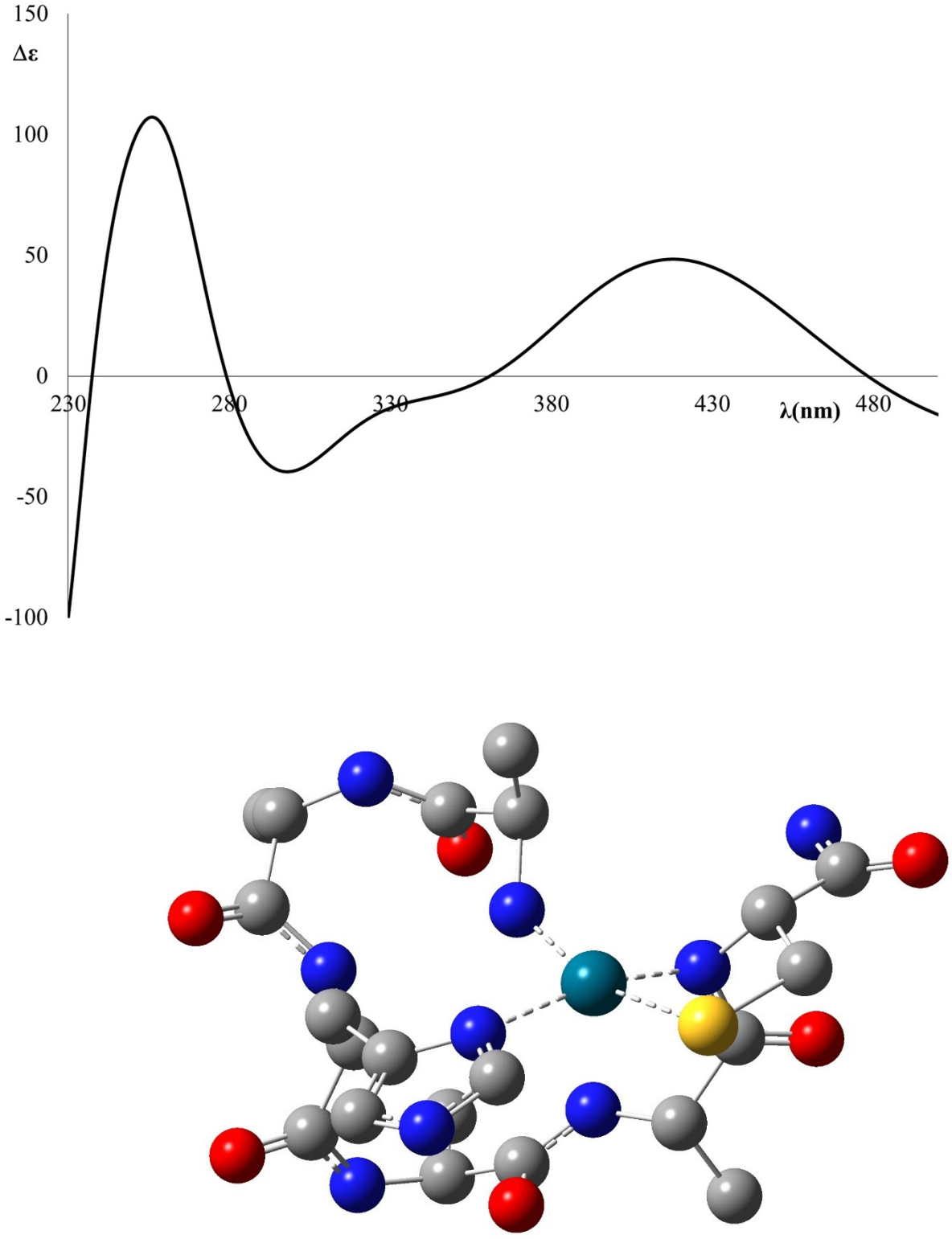


Figure S3. EPR spectra of Cu(II):AHAAAC-NH_2 1:1 at pH 7.93.

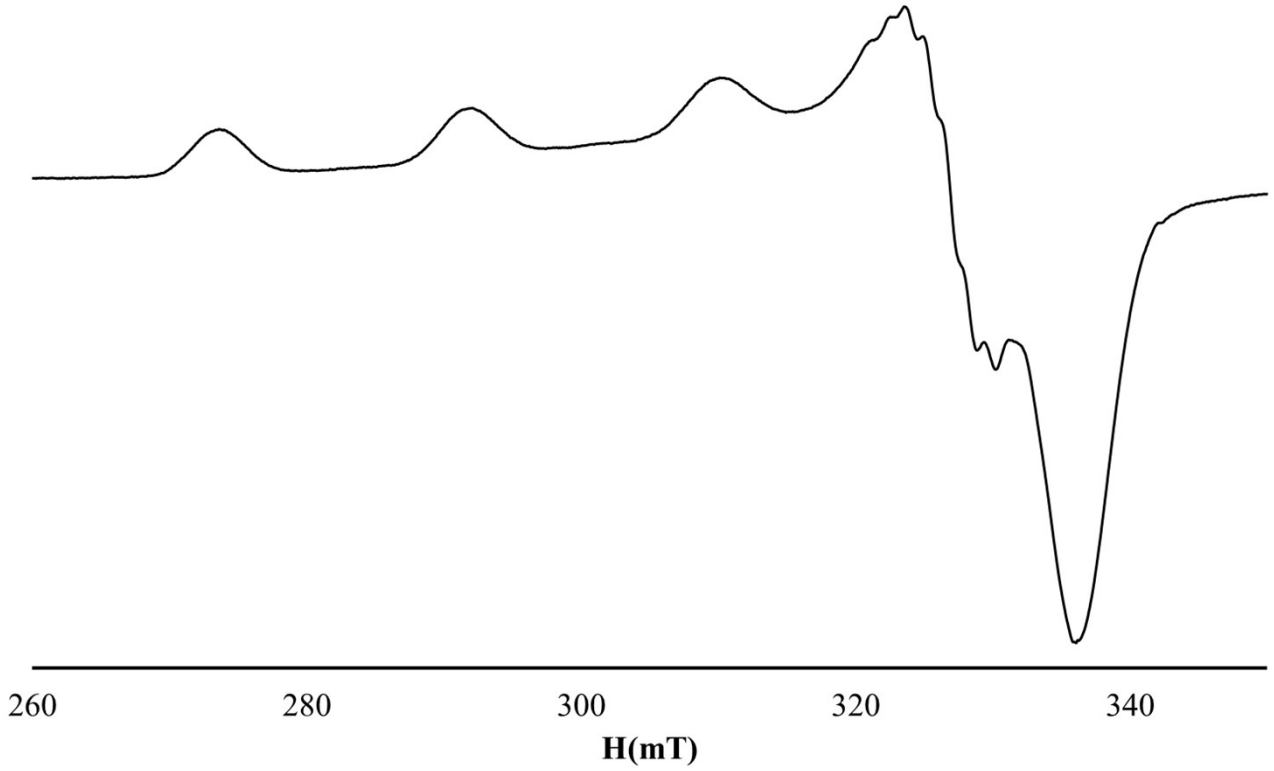

260
280
300
320
340
H(mT)

Figure S4. Concentration distribution curve of the complexes formed in the Pd(II):AHAAAC-NH_2 1:1 system. The stepwise protonation constants are also marked. c_L = 2 mM.

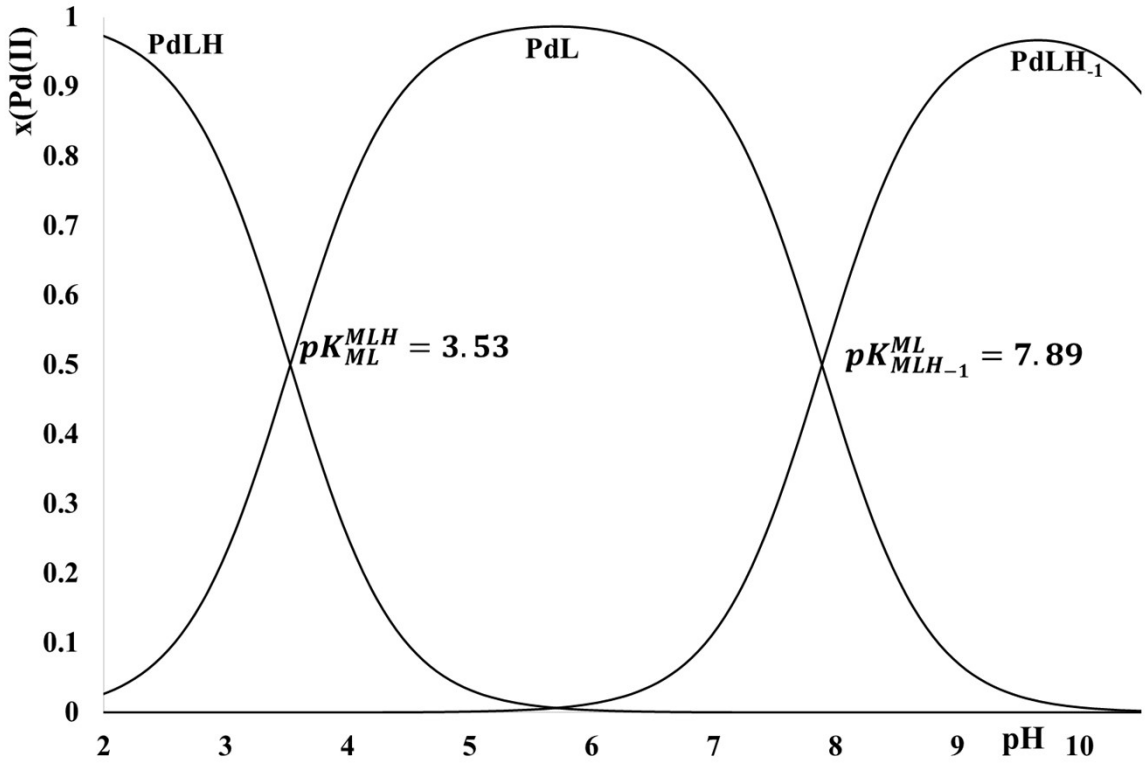


Figure S5. pH-dependent CD spectra recorded in the Pd(II):AHAAAC-NH_2 1:1 system.

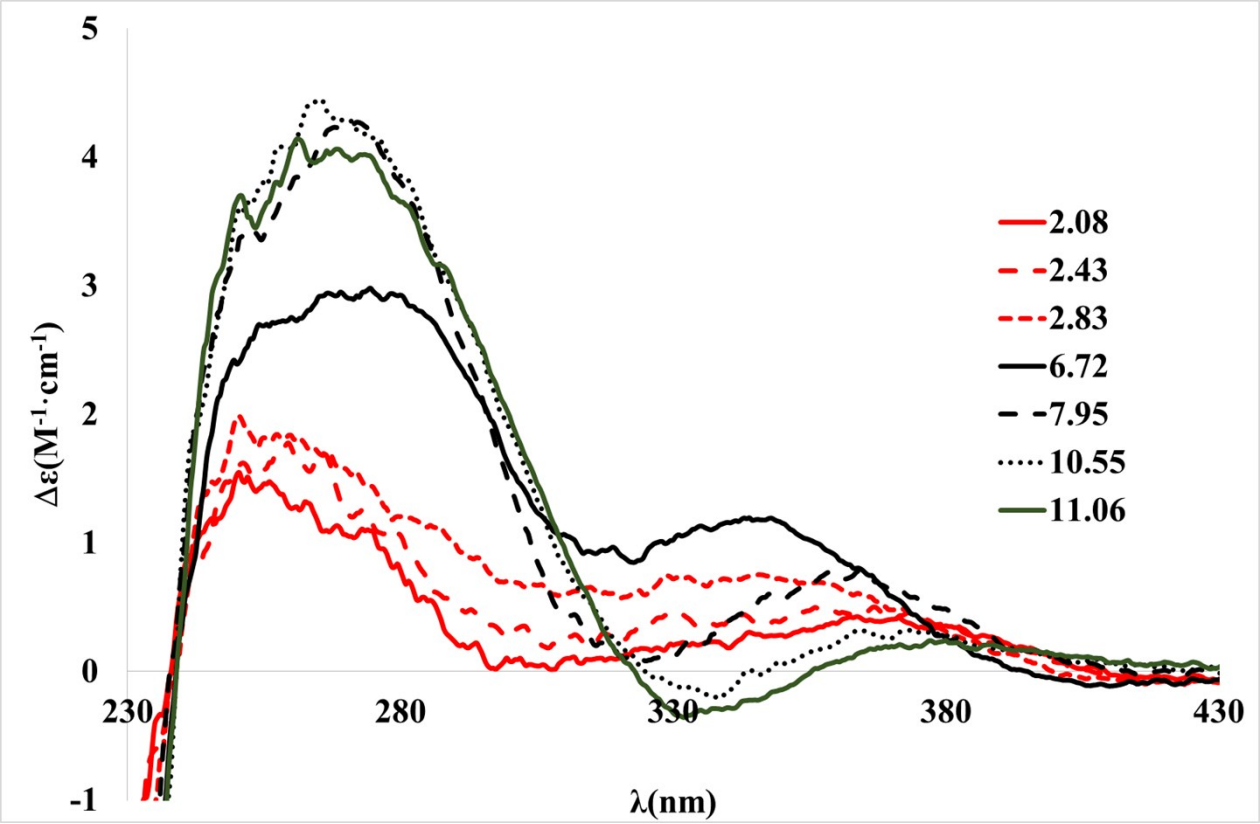


Figure S6. Calculated ECD spectrum of the MLH_{-1} complex formed in the Pd(II):AHAAAC-NH_2 system.