

SUPPLEMENTARY INFORMATION

Structural Models for Cu(II) Bound to the Fragment 92-96 of the Human Prion Protein

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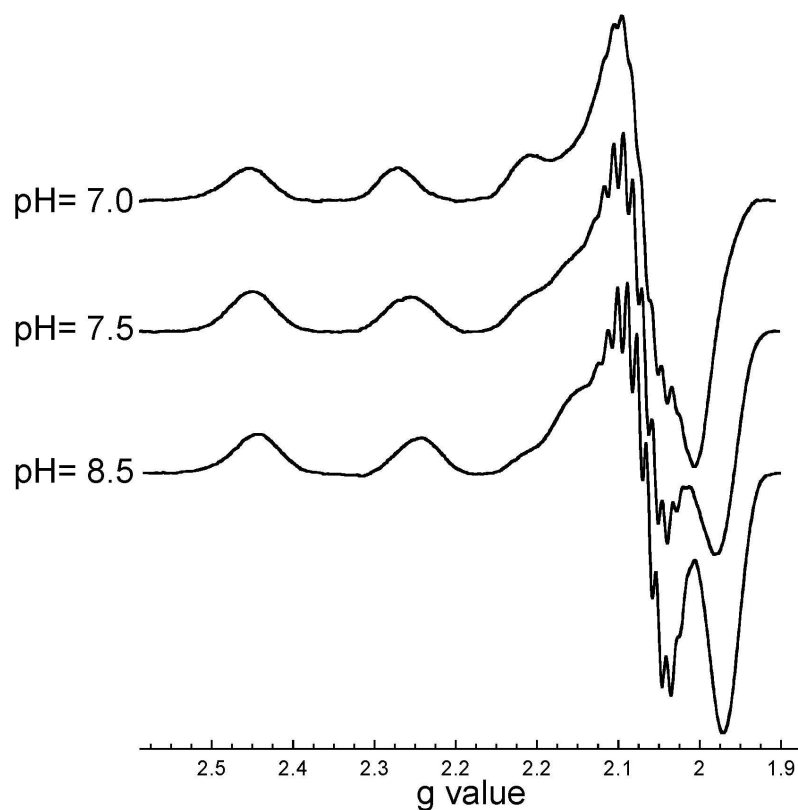


Figure S1. EPR spectra of the Cu(II) complexes formed with the PrP(92-115) at pH 8.5, 7.5 and 7.0. All spectra were collected as described in the experimental section at 150 K.

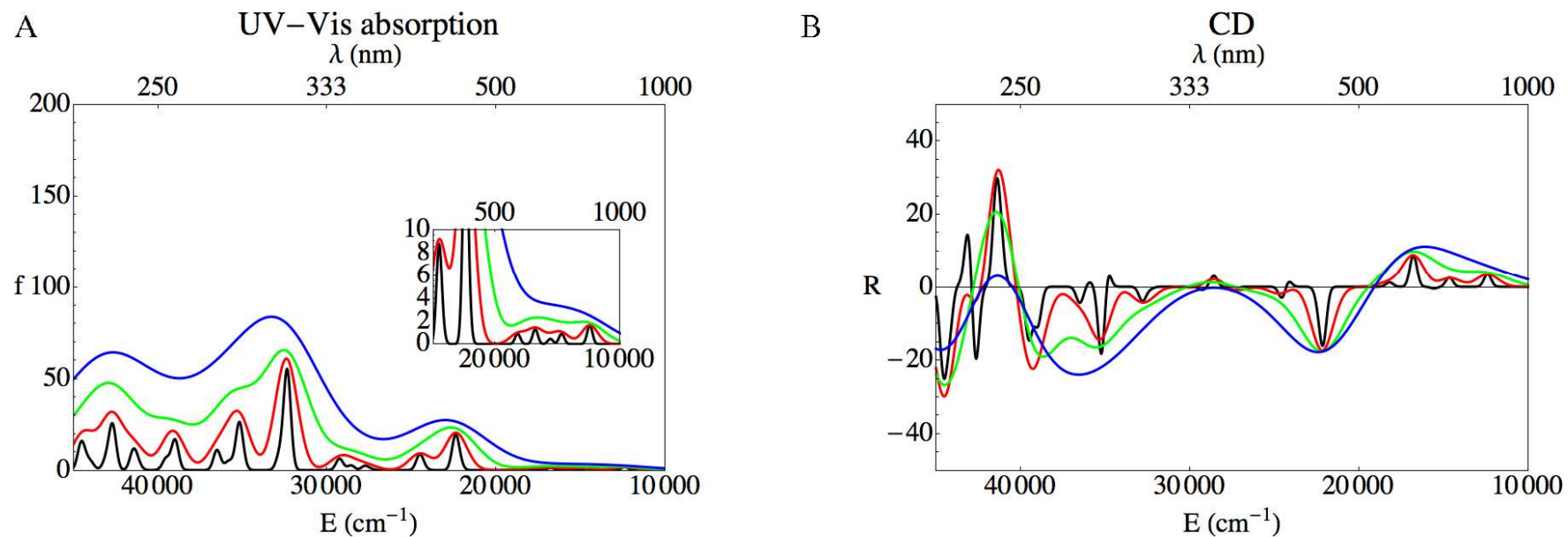


Figure S2. UV-Vis absorption (**A**) and CD (**B**) spectra of the Cu(II)-PrP(92-96) complex with a 2N2O coordination mode calculated with the PBE0 functional. The simulation was done with a FWHM of 500 (black line), 1500 (red line), 3000 (green line) and 5000 cm^{-1} (blue line)

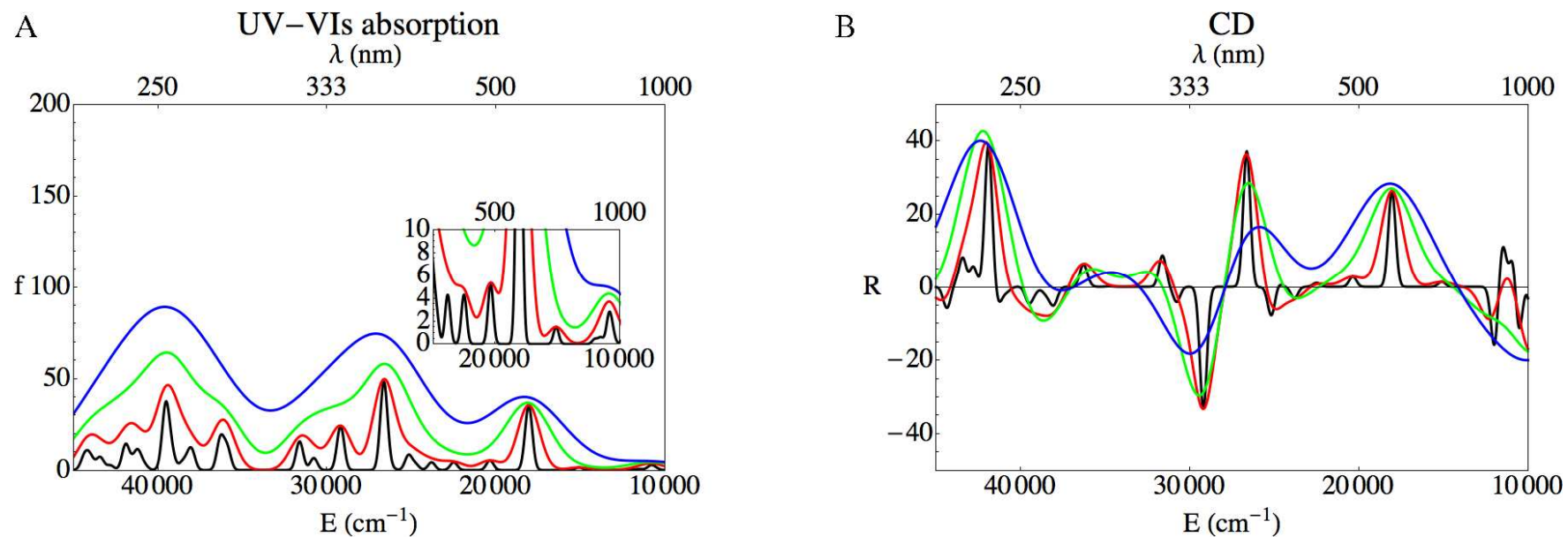


Figure S3. UV-Vis absorption and CD spectra of the Cu(II)-PrP(92-96) complex with a N3O coordination mode calculated with the PBE0 functional. The simulation was done with a FWHM of 500 (black line), 1500 (red line), 3000 (green line) and 5000 cm⁻¹ (blue line)