Electron Supplementary Information (ESI)

The curious case of opossum prion: a physicochemical study on the copper (II) binding features of proteins N-terminal domain

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Table S1. Proton Chemical shift of the Op_bis-deca peptide in H_2O, at pH 5.0.

Amino acid	NH	αCH	βCH / γCH	Others
Pro[1]	---	4.26	2.14; 1.85; 1.71	2.01 Ac 3.51 δδ'
His[2]	8.38	4.80	2.99 β; 2.91 β'	8.29 Hδ2; 7.08 Hε1
Pro[3]	---	4.26	2.15; 1.86	3.60 δ; 3.42 δ'
Gly[4]	8.44	3.90 αα'		
Gly[5]	8.18	3.94 αα'		
Ser[6]	8.24	4.34	3.71 ββ'	
Asn[7]	8.36	4.62	2.67; 2.60	7.41 Hδ21; 6.77 Hδ22
Trp[8]	7.97	4.53	3.18 ββ'	7.14 Hδ1 10.05 Hε1 7.39 Hζ2 7.06 Hη2 7.37 Hζ3 7.48 Hε3
Gly[9]	8.09	3.70 αα'		
Gln[10]	7.87	4.48	2.25; 1.96; 1.81	7.42 Hε21; 6.79 Hε22
Pro[11]	---	4.26	2.14; 1.85; 1.71	3.51 δδ'
His[12]	8.38	4.80	2.99 β; 2.91 β'	8.31Hδ2; 7.08 Hε1
Pro[13]	---	4.26	2.15; 1.87	3.60 δ; 3.42 δ'
Gly[14]	8.46	3.90 αα'		
Gly[15]	8.18	3.94 αα'		
Ser[16]	8.24	4.34	3.71 ββ'	
Asn[17]	8.36	4.62	2.67; 2.60	7.41 Hδ21; 6.77 Hδ22
Trp[18]	7.99	4.53	3.18 ββ'	7.14 Hδ1 10.05 Hε1 7.39 Hζ2 7.06 Hη2 7.37 Hζ3 7.48 Hε3
Gly[19]	8.13	3.67-3.74 αα'		
Gln[20]	7.93	4.19	2.23-2.04-1.84	7.52; 7.03 NH_2t 7.42 Hε22; 6.79 Hε21

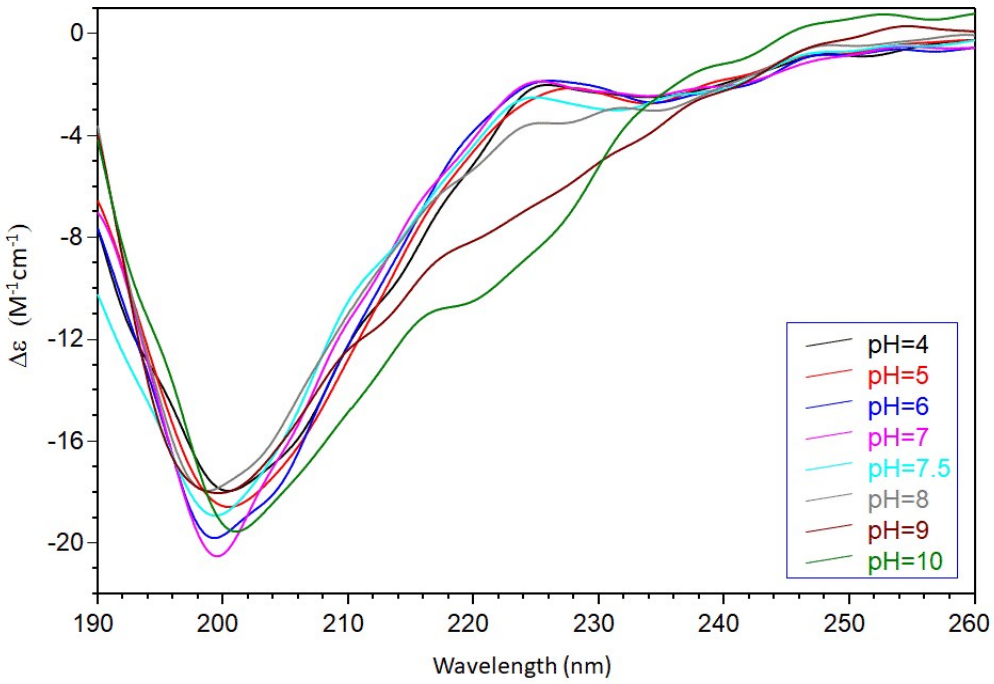

Figure S1. Far UV CD spectra of Cu(II)-Op_bis-deca in H_2O 2:1 metal to ligand molar ratio, [L]= 1 x 10^{-5} M at different pH values.

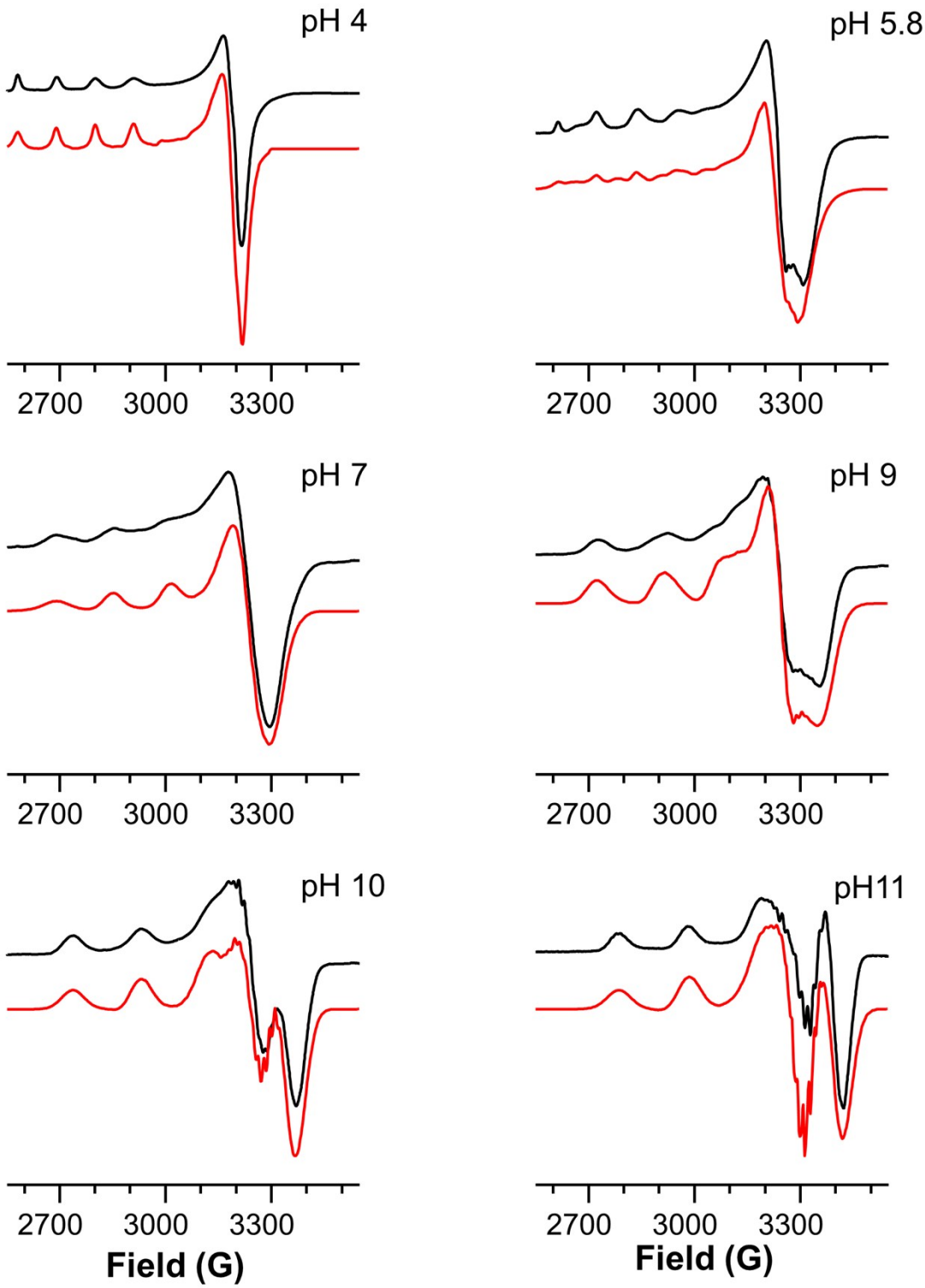

Figure S2. Experimental (black traces) and simulated (red traces) EPR spectra of Cu(II)-Op_bis-deca peptide at Cu(II): L 1:1 molar ratio at different pH values. T= 150 K, [L]=[Cu(II)] = 1 x 10^{-3} M.

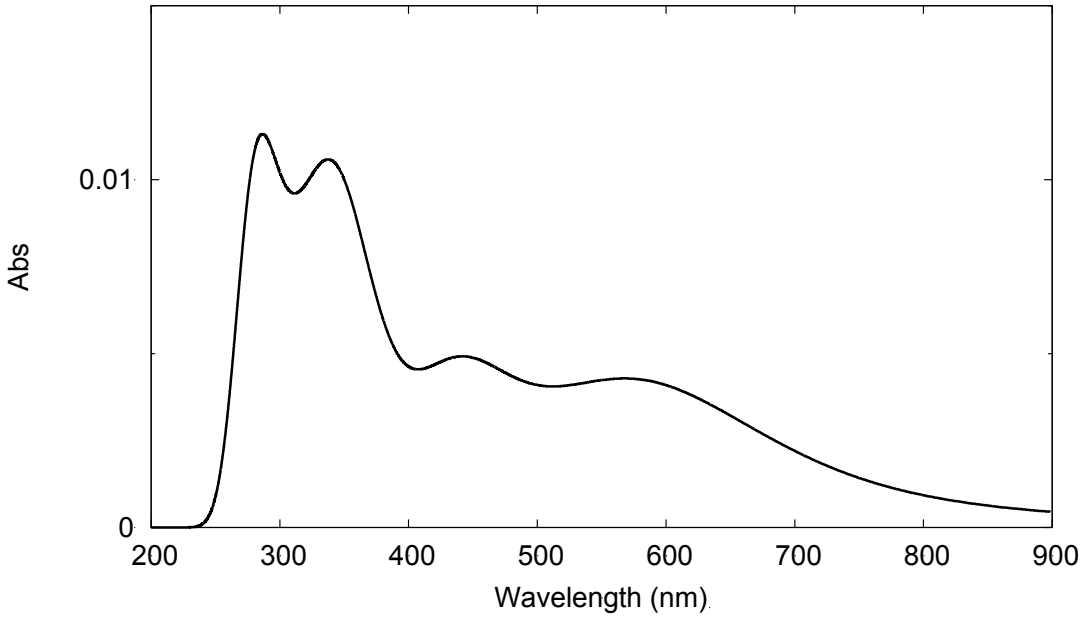

Figure S3. Predicted UV spectrum at the PBE/6-31G* level including the PCM model for the copper(II) coordinated within the ^{2}HPGG^{5} fragment of Op_bis-deca peptide.

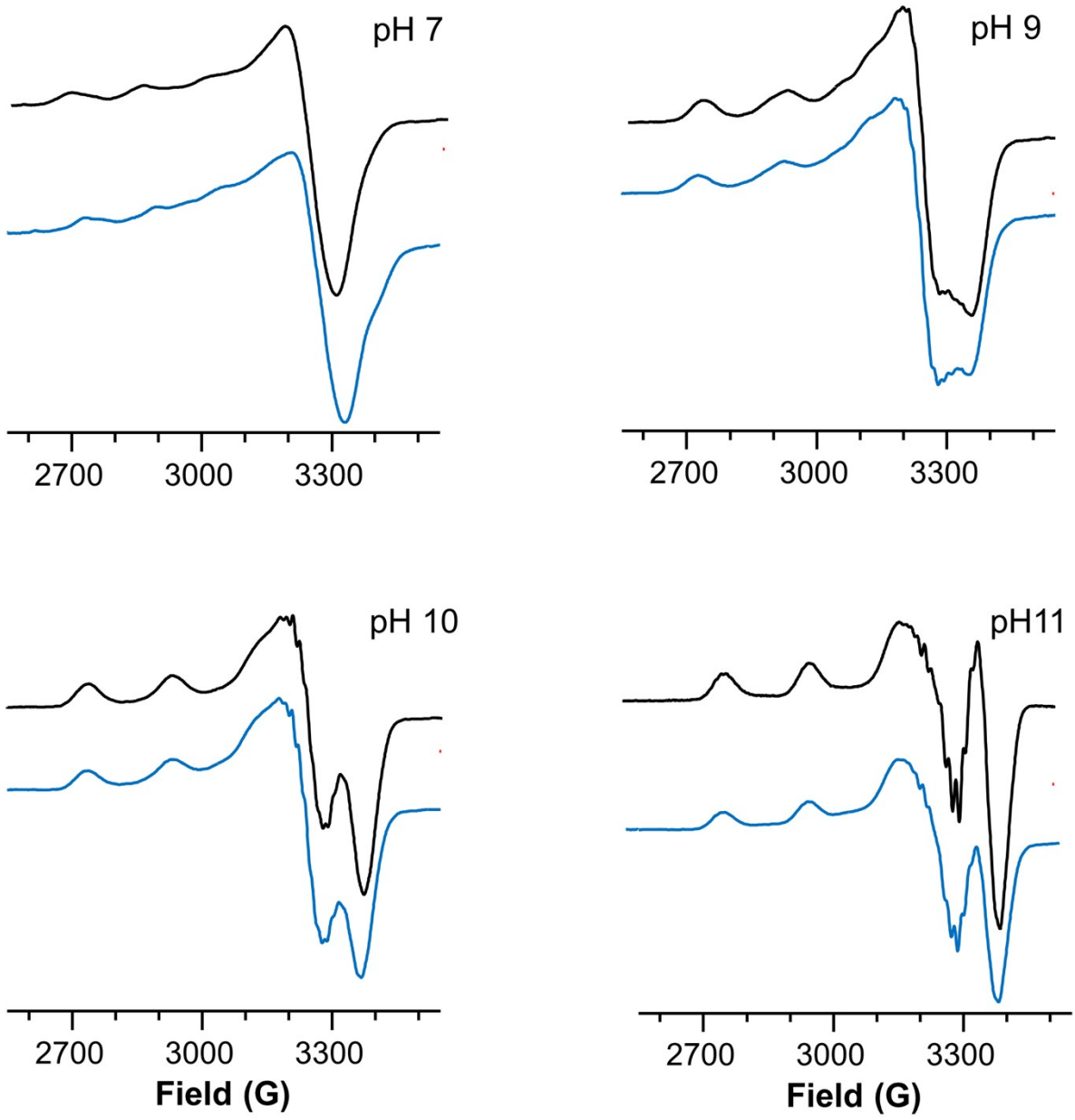

Figure S4. Comparison of EPR spectra of Cu(II)-Op_bis-deca peptide at Cu(II): L 1:1 molar ratio (black traces) with those obtained at Cu(II): L 2:1 molar ratio (blue traces), at different pH values. T= 150 K, [L]= 1 x 10^{-3} M.

Table S2. Coordination parameters for Cu(II) coordinated to Op_bis-deca peptide. Root mean square displacement during geometry optimization is 10^{-3} Å.

Bond	Bond length (Å)	Angle type	Angle (degrees)
Cu^{2+}-O	2.06	N_{im} -Cu^{2+}-N^-	97.63
Cu^{2+}-N_{im}	1.97	N_{im} -Cu^{2+}-O	84.12
Cu^{2+}-N^-	1.91	O-Cu^{2+}-N^-	96.05
Cu^{2+}-N^-	1.93	N^--Cu^{2+}-N^-	86.44

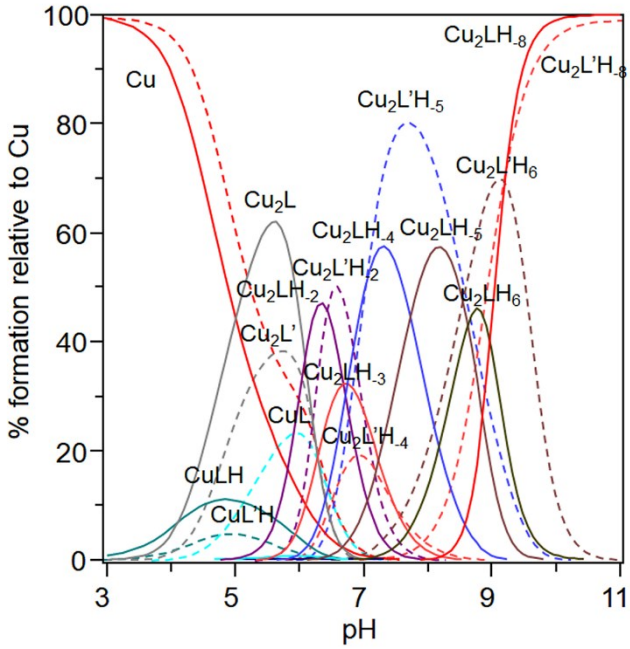

Figure S4. Species distribution diagrams for Cu(II) complexes with L= Op_bis-deca (solid trace) and L'= Hu_bis-octa (dashed trace), 2:1 metal to ligand molar ratio. [L]=[L']= 1 x 10^{-3} M.

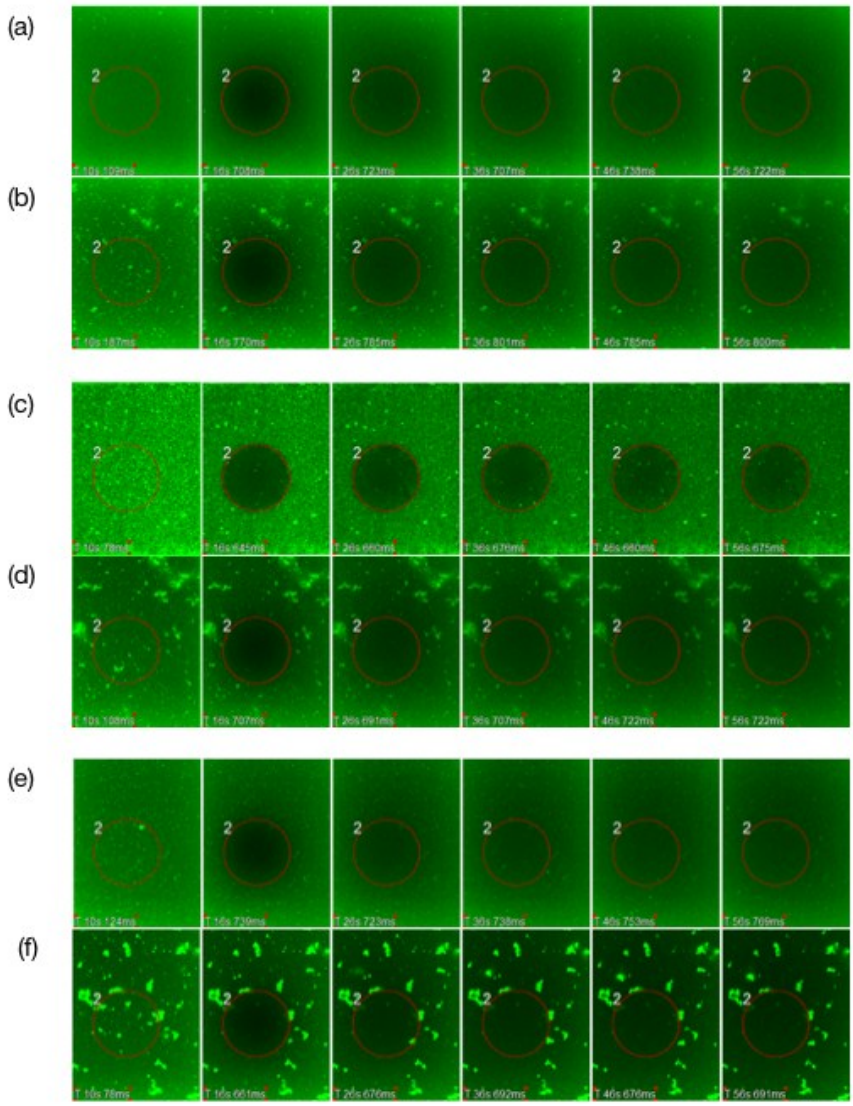

Figure S5. Representative LSM images for the FRAP experiment of SLB made of POPC–NBD formed on glass surfaces and exposed for 30 min to 1 mM peptide solutions. Micrographs recorded before and after bleach at intervals of 5 s. (a) Control bare SLBs; (b) SLB+ 1 mM $CuSO_4$; (b) SLB+ 1 mM $CuSO_4$; (c) SLB+ Op_bis-deca; (d) SLB+ Hu_bis-deca: $CuSO_4$ (1:1); (e) SLB+ Hu_bis-octa; (f) SLB+ Op_bis-deca: $CuSO_4$ (1:1).