Supplementary Material (ESI) for Dalton Transactions

"Competition between histamine-like and poli-imidazole coordination sites for Cu^{2+} and Zn^{2+} ions in zebra-fish peptide of prion-like protein"

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SUPPLEMENTARY INFORMATION

Table 1S. 1H chemical shift (ppm) of zf74-86 1.0 mM, pH 7.5, T=298K in D_2O

	Hα	Hβ	Hγ	others
His 74	3.95	3.03		Hε 7.72 Hδ 6.98
Thr 75,78,81	4.33	4.22	1.16	
Gly 76,79,82,85	4.02 3.95 ~3.92 ~ 3.88			
His 86	4.58	3.11-3.04		Hε 7.75 Hδ 6.97
His 77*	4.70	3.10		Hε 7.72 Hδ 6.96
His 80*	4.70	3.07		Hε 7.69 Hδ 6.95
Ser 83	4.52	3.92-3.86		
Ser 84	4.49	3.89		

The *label indicates that the assignment of His 77 and His 80 can be also exchanged

Table 2S. ^{13}C chemical shift (ppm) of zf74-86 1.0 mM, pH 7.5, T=298K, in D_2O

	Cα	Cβ	Cγ	others
His 74	54.2	30.8		Cε 136.07 Cδ 116.90
Thr 75,78,81	59.13	66.85	18.4	
Gly 76,79,82,85	42.4			
His 86	53.3	28.6		Cε 136.07 Cδ 116.90
His 77,80	53.8	28.6		Cε 136.07 Cδ 116.90
Ser 83	55.4	60.94		
Ser 84	55.8	60.86		

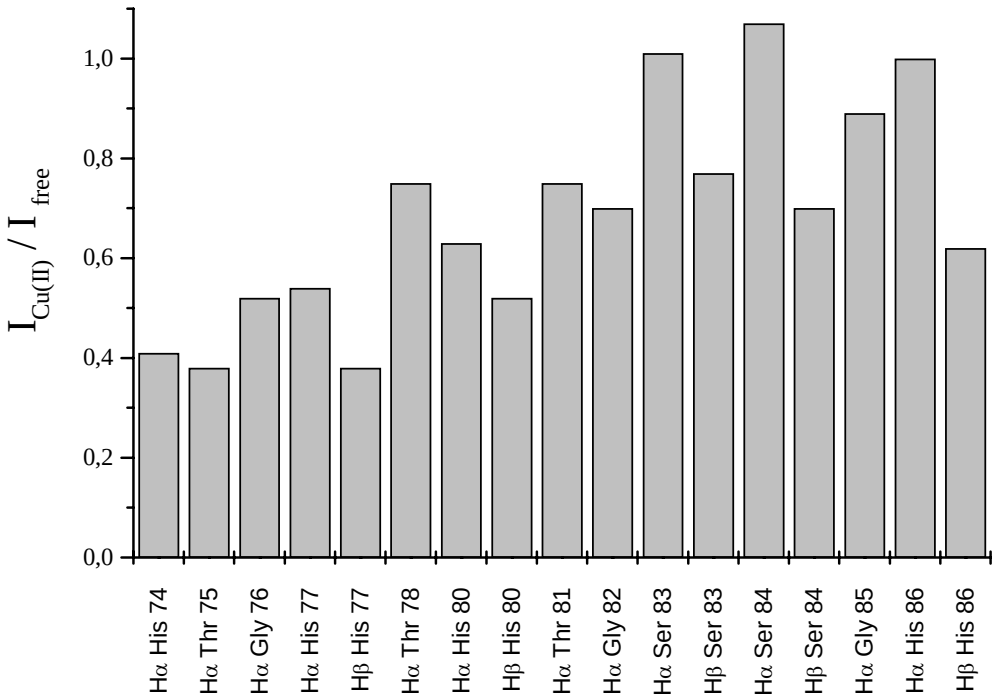

Figure 1S. Intensity reduction of ^{1}H-^{1}H TOCSY cross -peaks of zf74-86 1.0 mM solutions induced by 0.3 eqs. of Cu^{2+} pH 3.3, T=298.

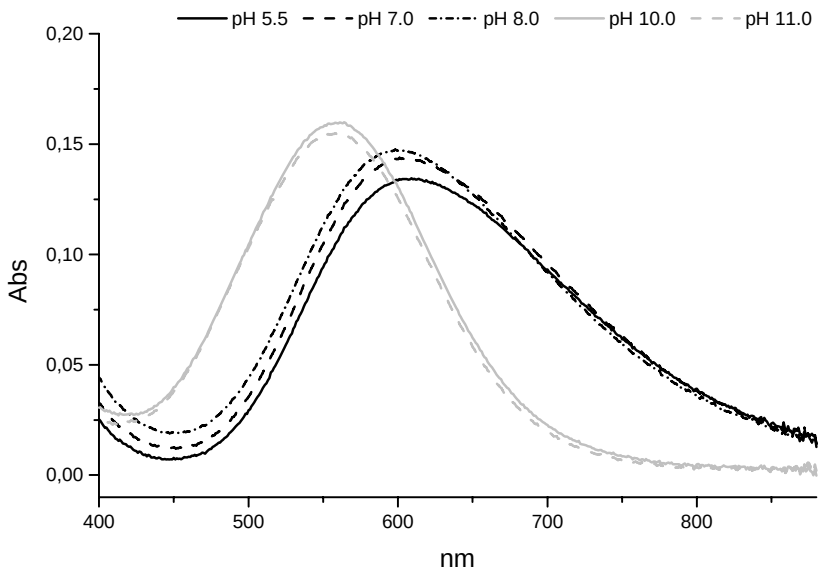

Figure 2S. UV-Vis spectra of Cu^{2+} -zf74-86 complexes at different pH. Metal to ligand ratio=1:1.1.

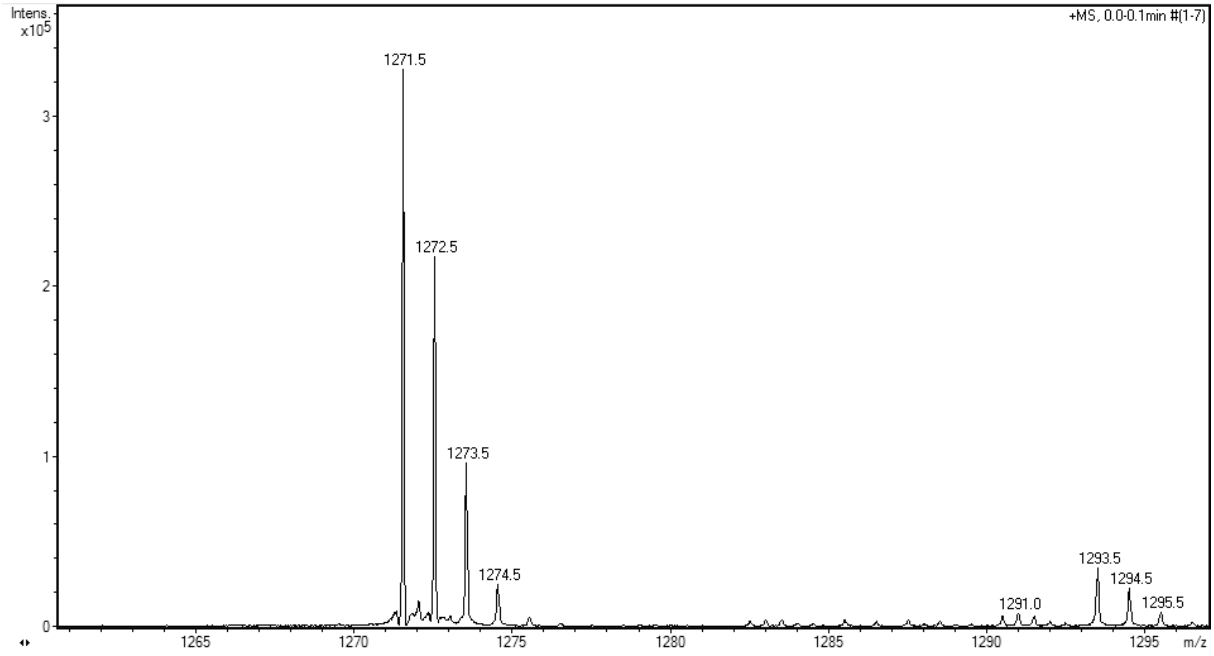

Figure 3S. ESI-MS spectra of zf74-86 in positive mode.