Supporting information

Structural Characterization and Antimicrobial Activity of the Zn(II) Complex with P-113 (Demegen), a Derivative of Histatin 5

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Table 1S. ^{1}H NMR chemical shift of P113 and Ac-P113.

Figure 1S. ^{1}H 1D spectra of P113 1.0 mM, pH 7.0, in H_2O/D_2O 9:1 mixture at (a) T= 278 and (b) T=298 K.

Figure 2S. CD spectra of P113 in absence (solid line) and in presence of 3.0 (dot-dash line) or 6.0 (dash line) Zn(II) eqs. All the samples were 0.06 mM, in water, pH 7.0, T=298.

Figure 3S. Selected regions of ^{1}H 1D NMR spectra at T=318 K in absence and in presence of Zn(II) of (A) AcP113, (B) P113. The peptide solutions were 2.0 mM, in DMSO-d_6.

Figure 4S. Selected regions of ^{1}H-^{1}H TOCSY spectra in absence (black) and in presence (green) of 6.0 Zn(II) eqs. (A) AcP113, (B) P113. The peptide solutions were 2.0 mM, in DMSO-d_6.

Figure 5S. Selected regions of ^{1}H 1D NMR spectra at T=278 K of P113 in presence of different amount of Zn(II). The peptide solutions were 1.0 mM, in H_2O/D_2O (9:1). * and # labels correspond to the signals of the apo and Zn(II) bound forms respectively.

Figure 6S. Comparison of the (A) P113-Zn(II) and (B) P113-Cu(II) structures. In both cases the first 11 structures, fitted on the backbone of residues 1-5, are shown. Figure was created with MOLMOL 2K.1.0.

Table 1S. ^{1}H NMR resonance assignments of P113 and AcP113 in DMSO (T=318 K) and in water (T=278 K).

Residue	Proton	AcP113(DMSO) Free	P113 (DMSO) Free	P113(H_2O) Free
Ac	CH_3	1.89	-	-
	HN	8.04	-	-
Ala1	Hα	4.25	3.80	4.00
	Hβ	1.23	1.34	1.47
	HN	7.91	8.39	-
	Hα	4.26	4.33	4.29
Lys2	Hβ	1.74	1.72	1.76
	Hγ	1.36	1.34	1.41
	Hδ	1.56	-	-
	Hε	2.79	-	2.98
	HN	7.89	8.06	8.62
	Hα	4.28	4.28	4.28
Arg3	Hβ	1.71	1.52	1.72
	Hγ	1.52	1.52	1.53
	Hδ	3.12	3.13	3.09
	NHε	-	7.67	-
	HN	7.91	7.94	8.55
	Hα	4.46	4.48	4.53
His4	Hβ1	2.92	2.91	3.03
	Hβ2	2.92	2.91	3.03
	Hδ	6.84	6.84	6.94
	Hε	7.52	7.52	7.72
	HN	8.07	8.12	8.31
	Hα	4.43	4.45	4.56
His5	Hβ1	3.03	3.04	3.03
	Hβ2	2.90	2.89	3.03
	Hδ	6.83	6.83	6.96
	Hε	7.57	7.58	7.62
Gly6	HN	8.73	8.75	8.56
	Hα	3.73	3.74	3.90
	HN	8.14	8.16	8.22
	Hα	4.46	4.49	4.52
Tyr7	Hβ1	2.98	2.97	3.00
	Hβ2	2.75	2.74	3.00
	Hδ	6.67	6.68	7.10
	Hε	7.04	7.03	6.81
	HN	8.0	8.04	8.34
	Hα	4.26	4.28	4.24
Lys8	Hβ	1.74	1.70	1.67
	Hγ	1.36	1.36	1.28
	Hδ	1.56	1.55	1.34
	Hε	2.79	2.79	2.96
Arg9	HN	7.89	7.93	8.37

	Hα	4.28	4.28	4.19
	Hβ	1.71	1.70	1.75
	Hγ	1.52	1.53	1.58
	Hδ	3.12	3.12	3.16
	NHε	-	7.53	-
Lys10	HN	7.89	7.90	8.49
	Hα	4.22	4.21	4.24
	Hβ	1.54	1.52	1.67
	Hγ	1.28	1.52	1.28
	Hδ	1.54	1.27	1.34
	Hε	2.76	2.76	2.96
Phe11	HN	7.96	7.98	8.51
	Hα	4.51	4.50	4.60
	Hβ1	3.05	3.06	3.04
	Hβ2	2.85	2.86	3.04
	Harom	7.04	7.07	7.30
His12	HN	8.03	8.05	8.35
	Hα	4.43	4.44	4.49
	Hβ1	2.90	2.94	3.08
	Hβ2	2.90	2.87	2.97
	Hδ	6.83	6.83	6.96
	Hε	7.57	7.58	7.77
NH_2	HN1	7.1	7.12	7.14
	HN2	6.99	7.00	7.05

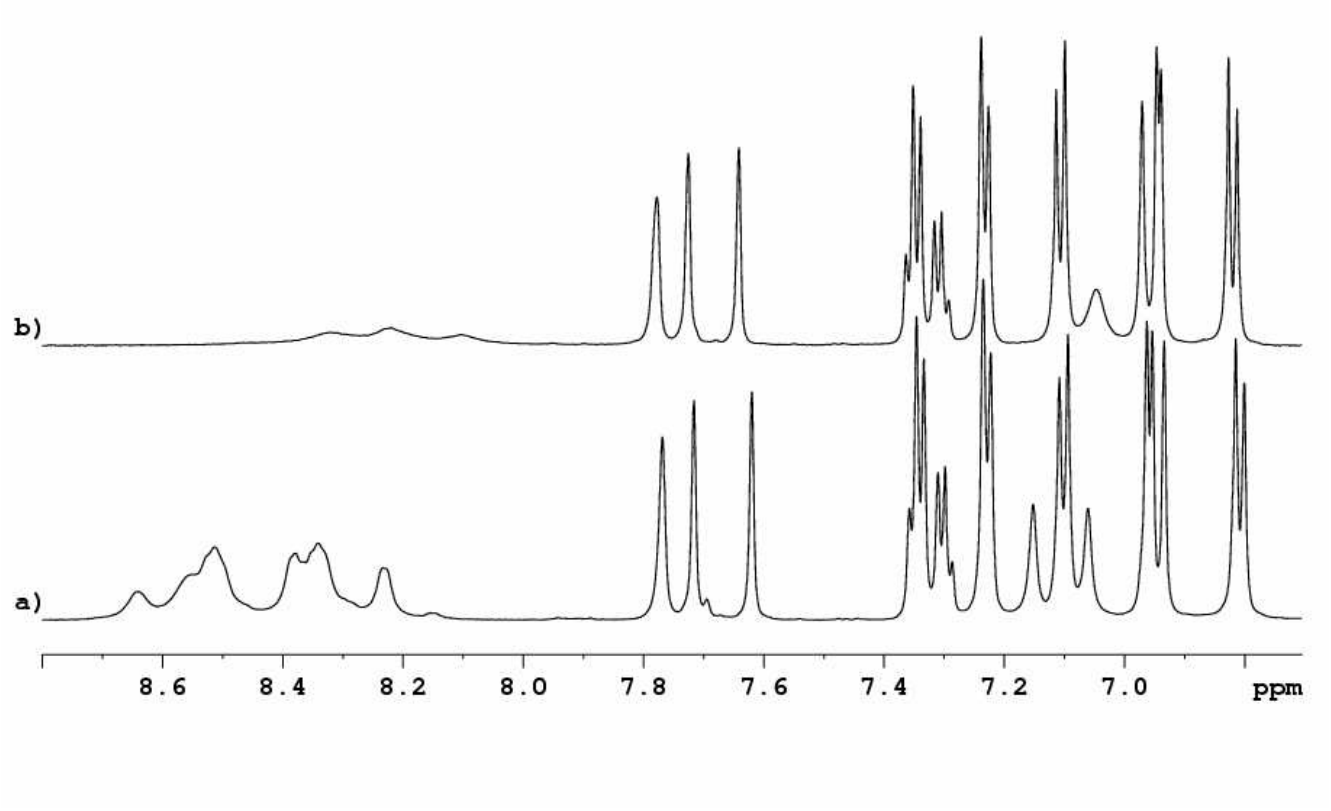

Figure 1S. ^{1}H 1D spectra of P-113 1.0 mM, pH 7.0, in H_2O/D_2O 9:1 mixture at (a) T= 278 and (b) T=298 K.

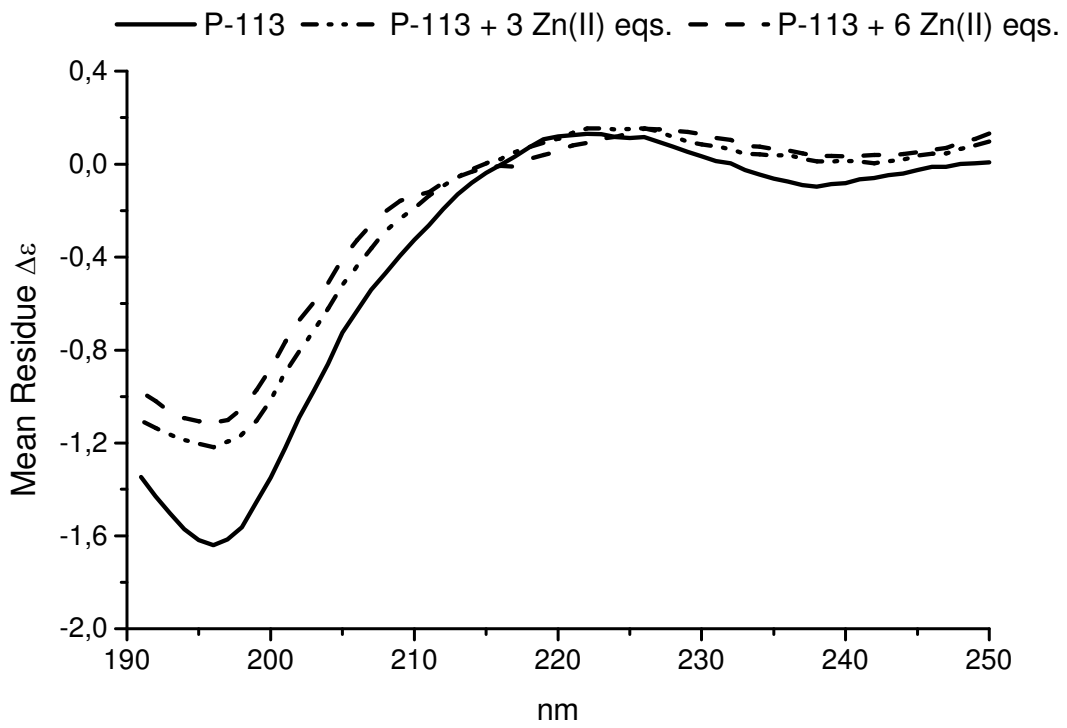

Figure 2S. CD spectra of P-113 in absence (solid line) and in presence of 3.0 (dot-dash line) or 6.0 (dash line) Zn(II) eqs. All the samples were 0.06 mM, in water, pH 7.0, T=318.

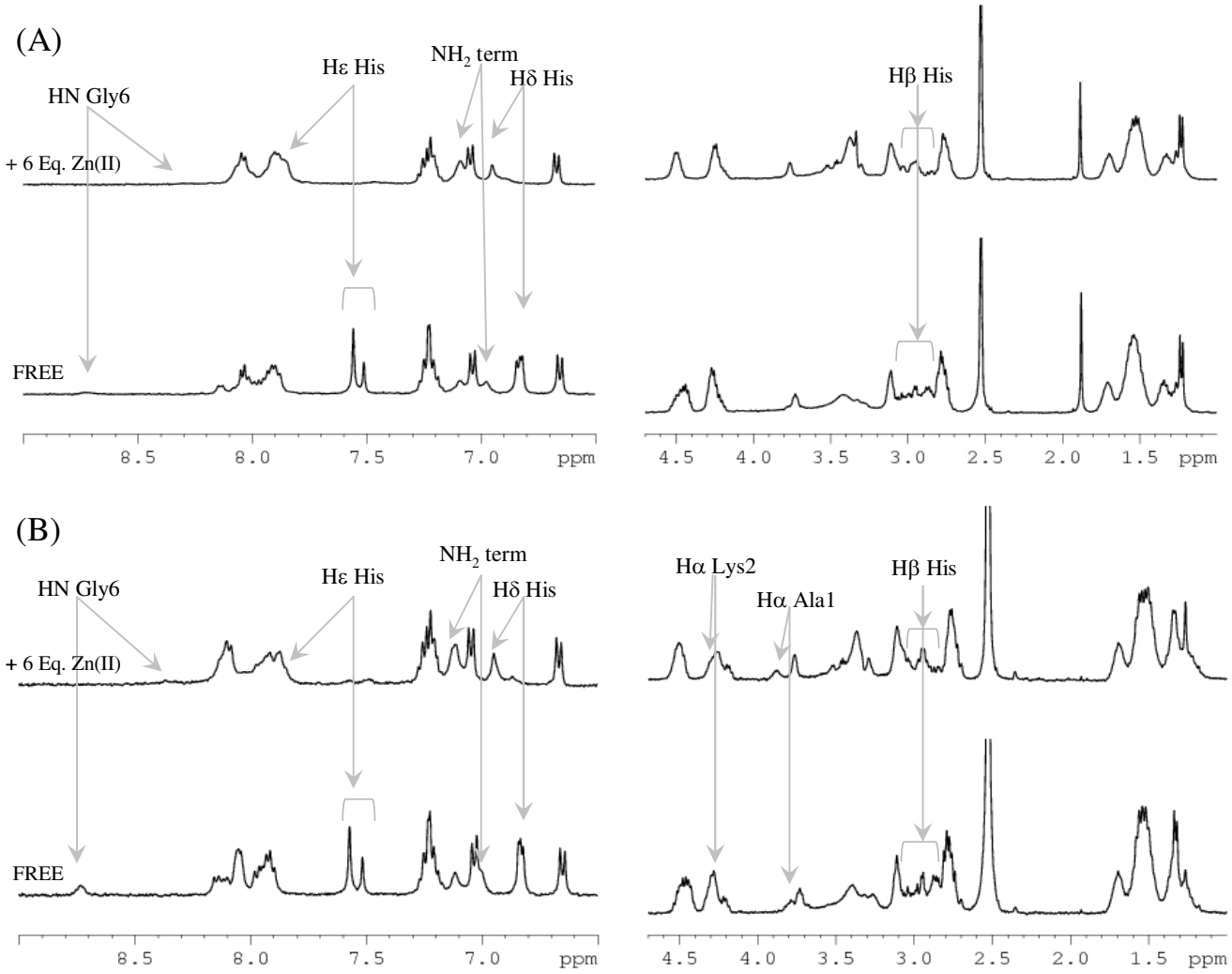

Figure 3S. Selected regions of ^{1}H 1D NMR spectra at T=318 K of (A) Ac-P113, (B) P-113. The peptide solutions were 2.0 mM, in DMSO-d_6.

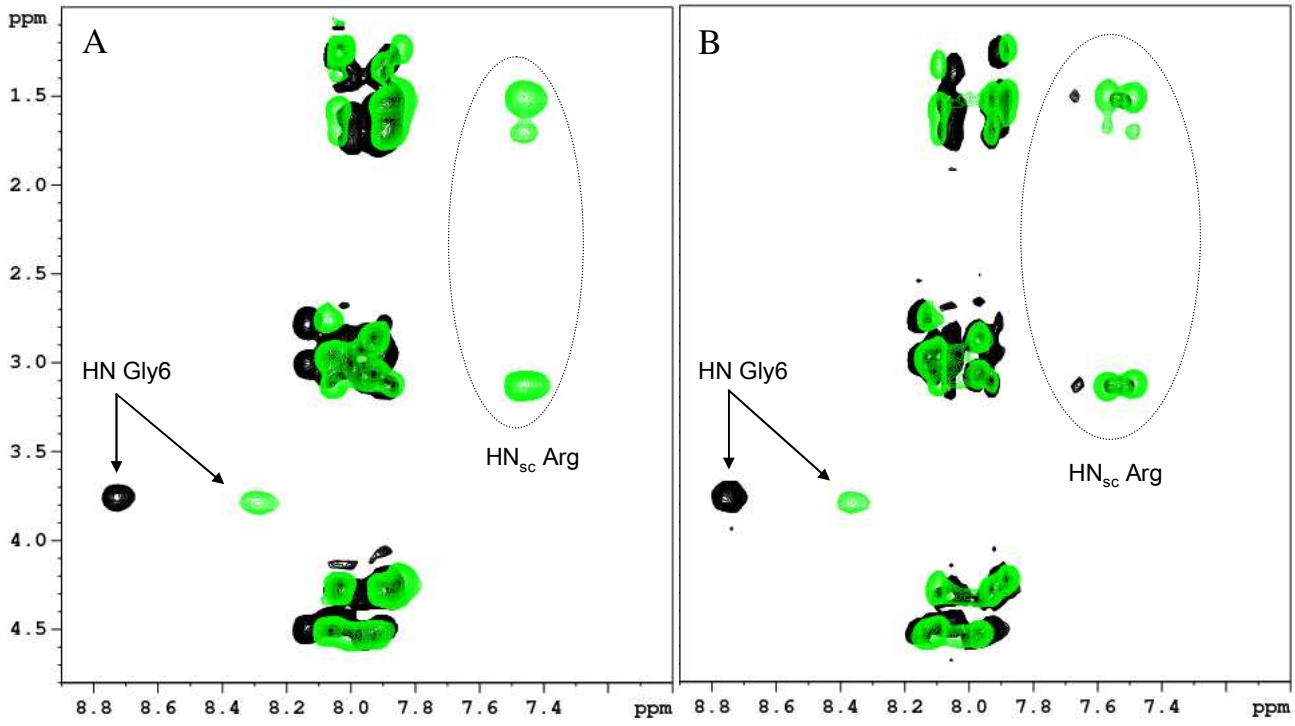

Figure 4S. Selected regions of ^{1}H-^{1}H TOCSY spectra in absence (black) and in presence (green) of 6.0 Zn(II) eqs. (A) Ac-P113, (B) P-113. The peptide solutions were 2.0 mM, in DMSO-d_6.

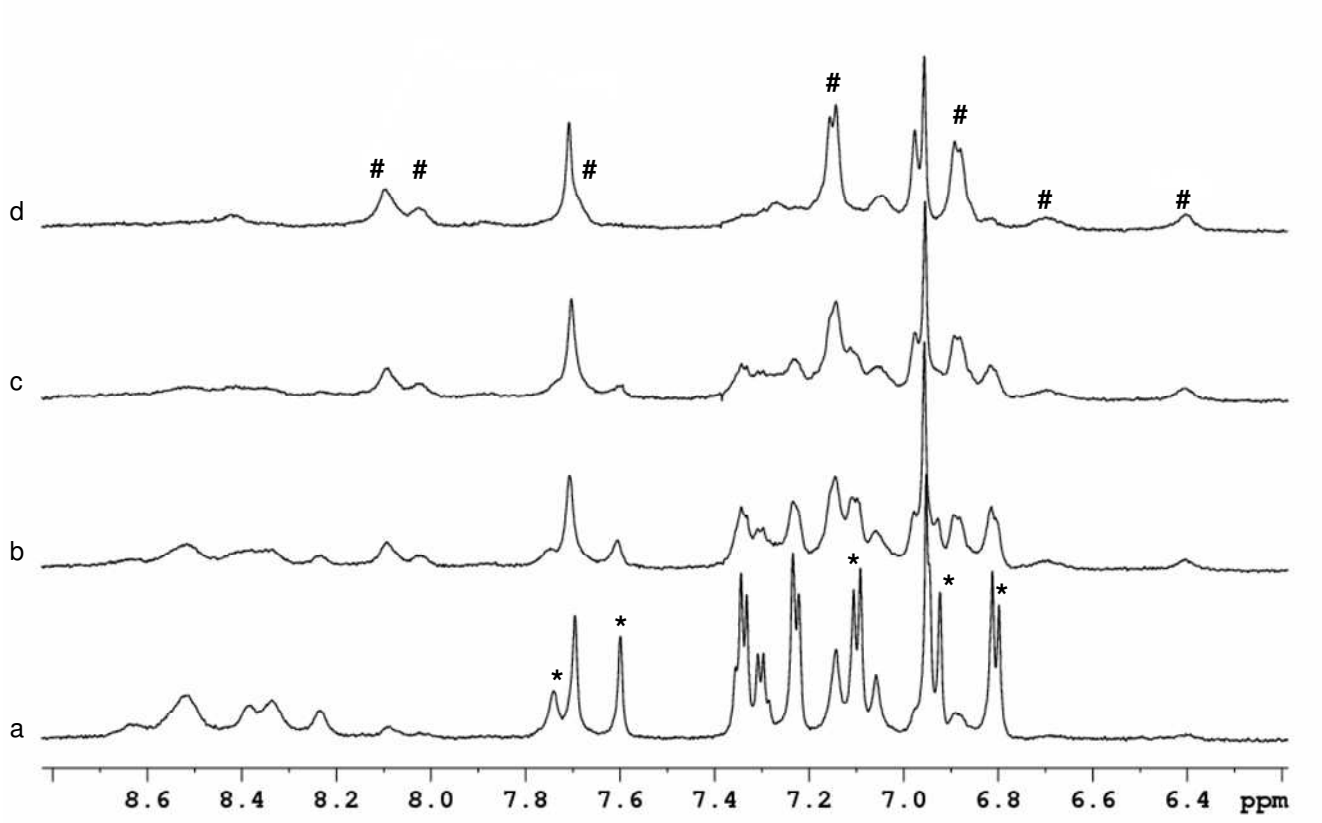

Figure 5S. Selected region of ^{1}H 1D NMR spectra at T=278 K of P113 in presence of a) 0.25 Zn(II) eqs.; b) 0.50 Zn(II) eqs.; c) 1.0 Zn(II) eqs.; d) 2.0 Zn(II) eqs. The peptide solutions were 1.0 mM, in H_2O/D_2O (9:1). * and # labels correspond to the signals of the apo and Zn(II) bound forms respectively.

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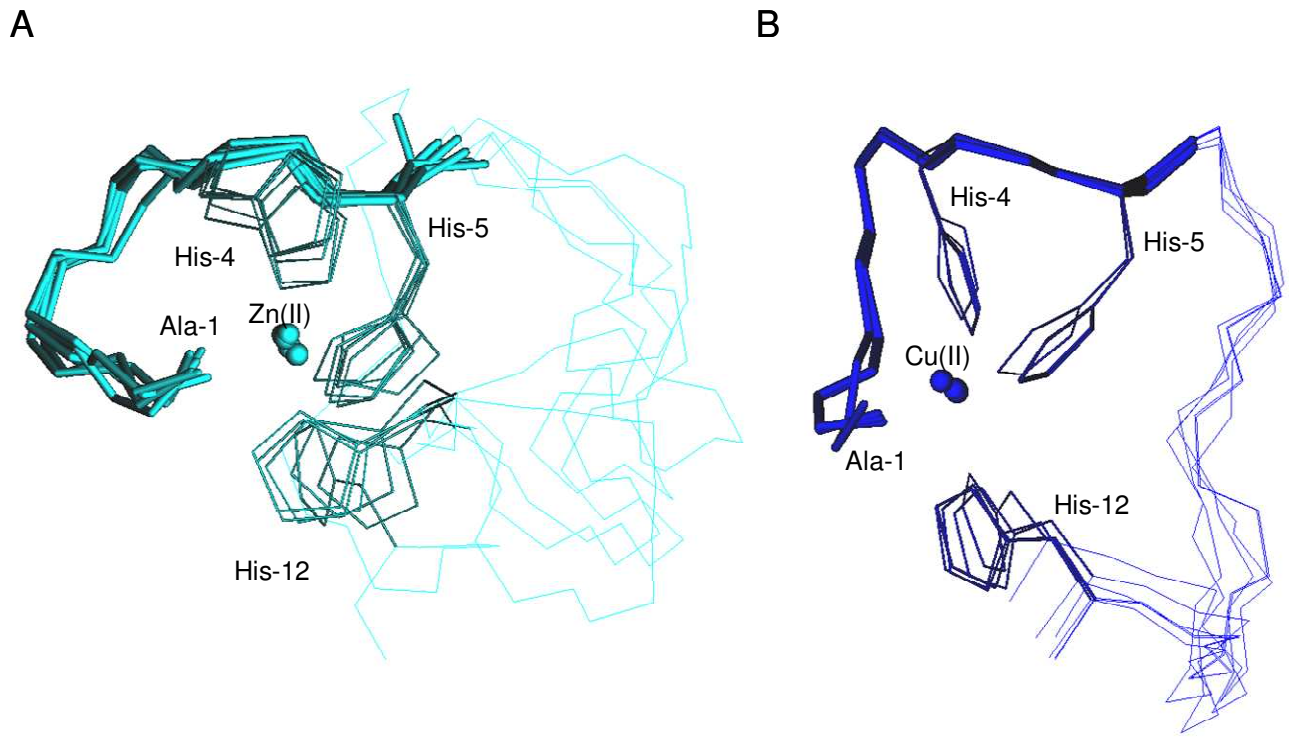

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