Supporting Information

Homo- and Heterobinuclear Cu^{2+} and Zn^{2+} Complexes of Abiotic Cyclic Hexaazapyridinocyclophanes As SOD Mimics

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Fig. S1 Distribution diagram of receptor **L1**

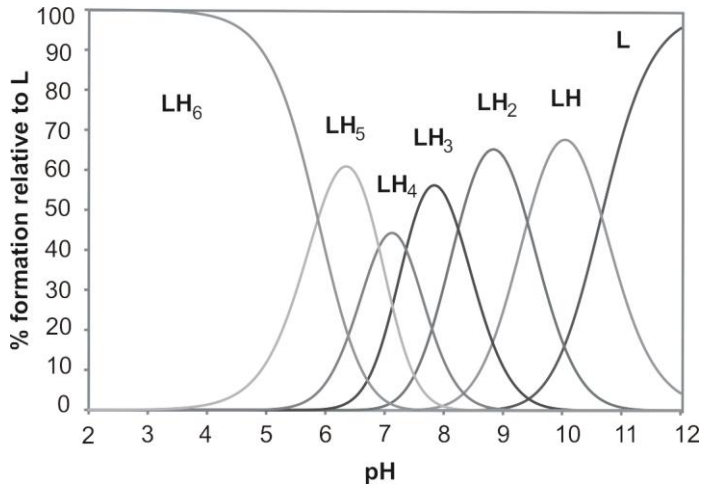

Fig. S2 X-ray crystal structure for $[(CuH_4\mathbf{L2})(H_2O)(ClO_4)]\ (ClO_4)_5 \cdot 3(H_2O)$

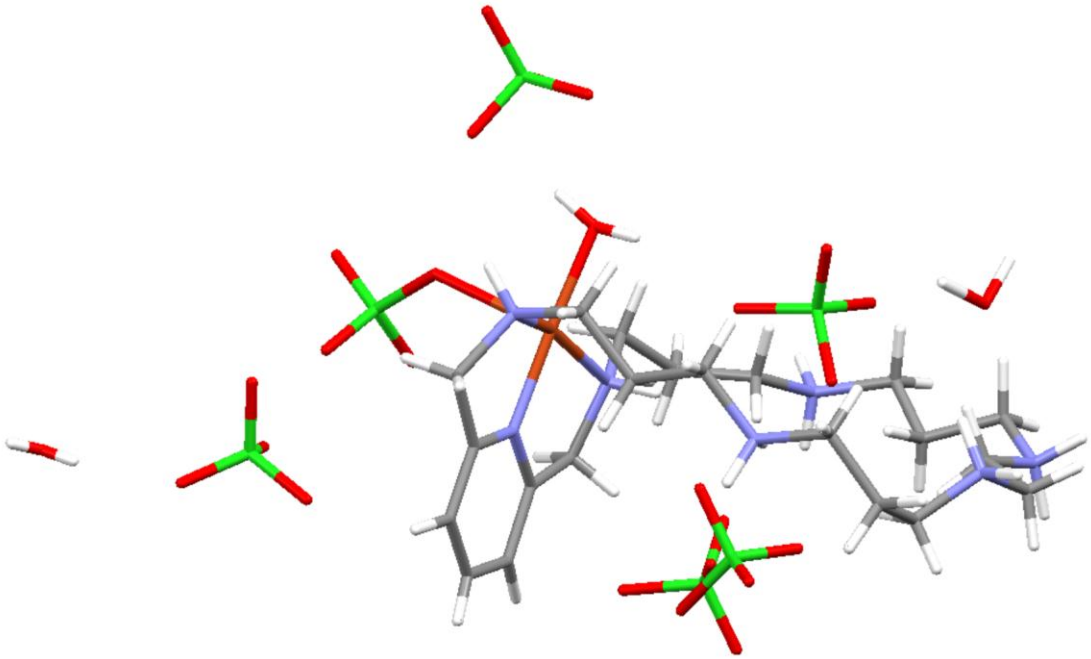

Table S1 Crystallographic Data for $[(CuH_4\mathbf{L2})(H_2O)(ClO_4)]\ (ClO_4)_5 \cdot 3(H_2O)$

	(**1**)
Empirical formula	$C_{21}H_{53}Cl_6CuN_7O_{28}$
Fw	1127.94
Crystal Size,mm	0.20 × 0.10 × 0.06
Cryst.System/s.g.	Pc 2_1 b
T.K	293(2)
a,Å	8.4130(2)
b,Å	18.1930(5)
c, Å	28.4910(9)
α,deg	90º
β, deg	90º
γ, deg	90º
V, Å^3	4360.8(2)
Z	4
d_{calc}, g/cm^3	1.718
μ,mm^{-1}	0.970
Reflect. collected	5746
Unique reflections	4496
Restraints	40
Parameters	578
R1,*w*R2 (all)	0.0588, 0.1569
GOOF	1.067

Fig. S3 Distribution diagram for the system Cu^{2+}-**L1** (A) $[Cu^{2+}] = [L] = 10^{-3}$ M; (B) $[L] = 10^{-3}$ M, $[Cu^{2+}] = 2 \times 10^{-3}$ M

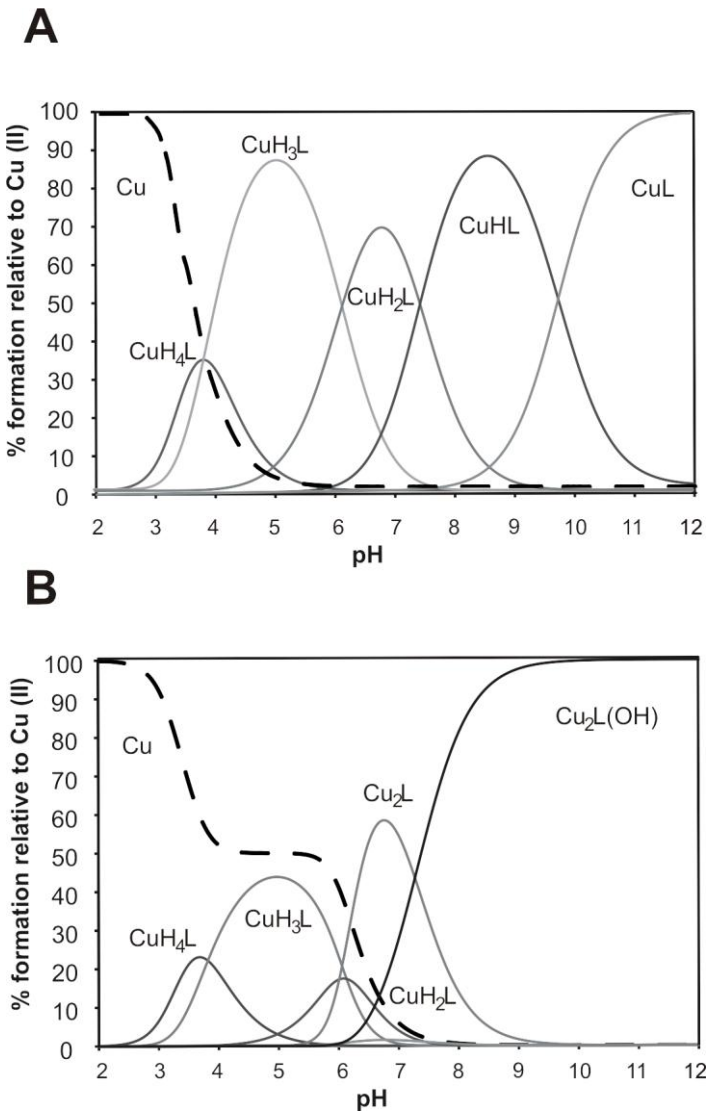

Fig. S4 Distribution diagram for the system Zn^{2+}-**L1** (A) $[Zn^{2+}] = [L] = 10^{-3}$ M; (B) $[L] = 10^{-3}$ M, $[Zn^{2+}] = 2 \times 10^{-3}$ M

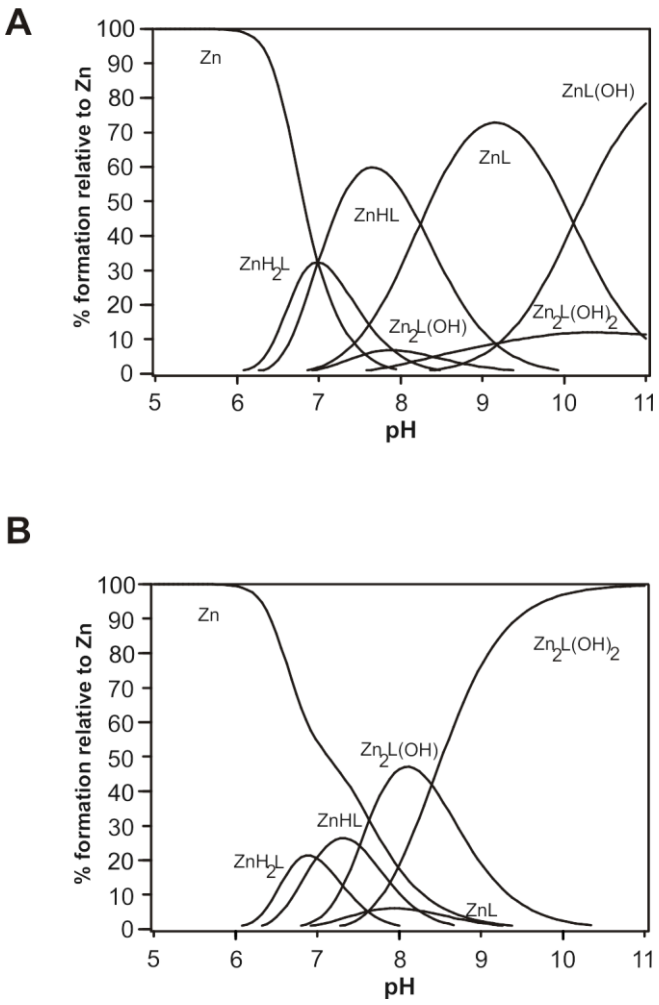

Fig. S5 400 MHz proton NMR spectra in D_2O at 313 K of (A) Cu_2**L2**-Im at pH 7.0 and (B) Cu_2**L2** at pH 7.0. The asterisks mark the residual solvent and impurity signals (*, H_2O; **, HDO)

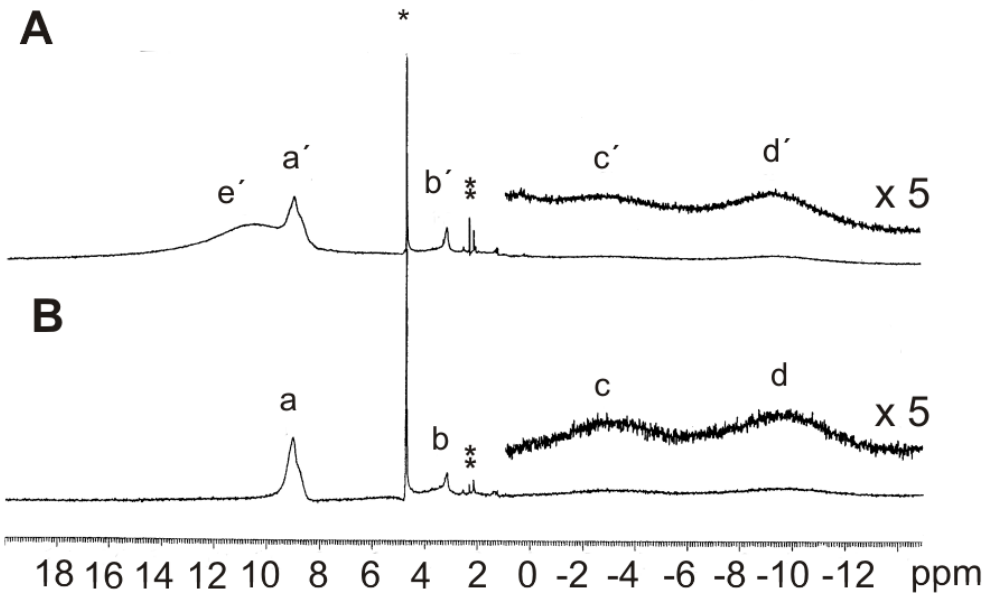

Table S2 ^{1}H NMR hyperfine-shifted resonances of Cu_2**L2**, Cu_2**L2**Im complexes in D_2O at 313 K and pH 7.0.

Syst.	**Sig.**	**δ (ppm)**	**Nº prot**	**Assign.**	**Temperature Dependence**	**T_1 (ms)**	**$\Delta\nu_{1/2}$ (Hz)**	**T_2[a] (ms)**
Cu_2**L2**	a	9.0	8	βCH_2	Anti-Curie	2.1	200	1.6
	b	3.1	3	Hm,p-Py	Anti-Curie	4.3	81	3.9
	c	-3.2	24	αCH_2	Curie	<1	1339	0.24
	d	-9.8			Curie	<1	1339	0.24
Cu_2**L2**Im	e´	10.4	~3x2	αCH-Im	Curie	5.6	~880	~0.36
	a´	9.0	8	βCH_2	Anti-Curie	5.4	278	1.2
	b´	3.2	3	Hm,p-Py	Anti-Curie	7.3	81	3.9
	c´	-3.1	24	αCH_2	Curie	<1	1182	0.27
	d´	-9.9			Curie	<1	1391	0.23

[a] Measured from the line width at half-height

Scheme S1