

Bis-maltol-polyamine Family: Structural Modifications at Strategic Positions. Synthesis, Coordination and Antineoplastic Activity of Two New Ligands

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1. Ancillary information for description of the structure

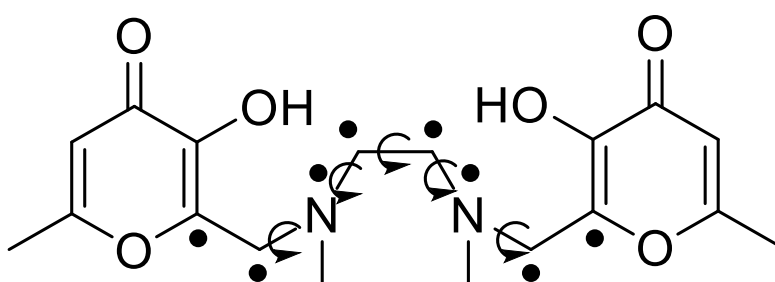


Fig. S1 Dihedral angles used to define the conformation of the chain that connects the two rings.

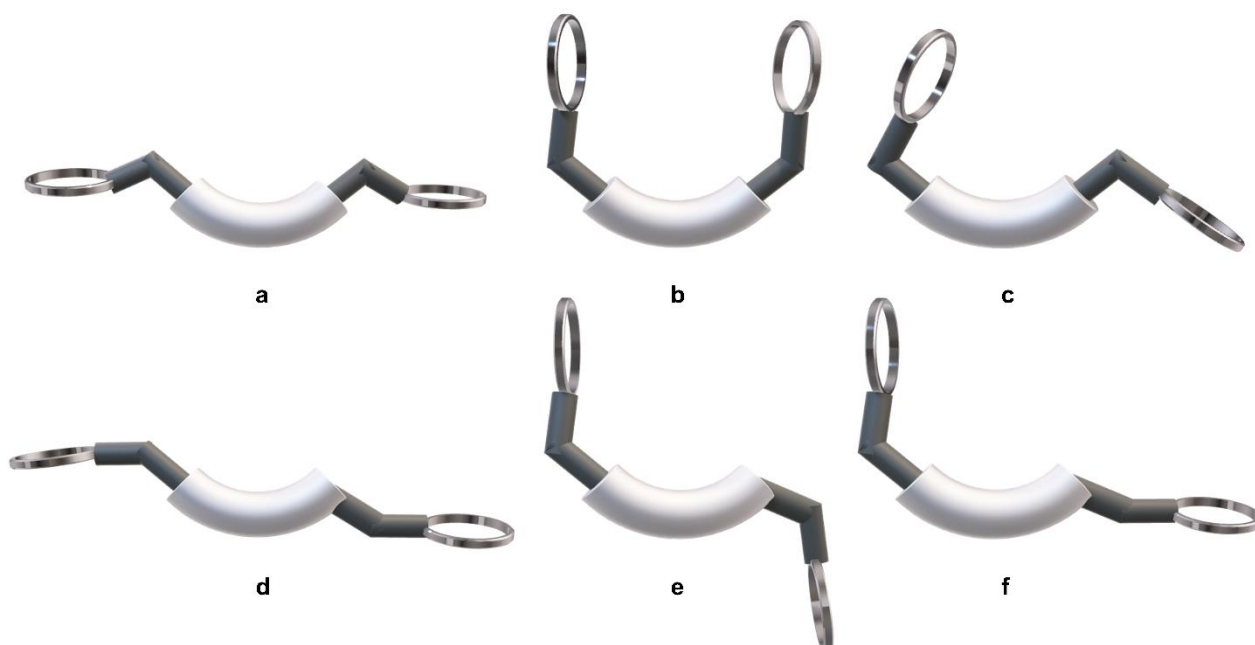


Fig. S2 Possible orientations of the Side Arms: (a) Open; (b) Face-to-Face; (c) Bent; (d) p_Up-Down; (e) o_Up-Down; (f) p-o_Up-Down (see ref. 23d in the main text).

2. Crystal packing and crystallographic data

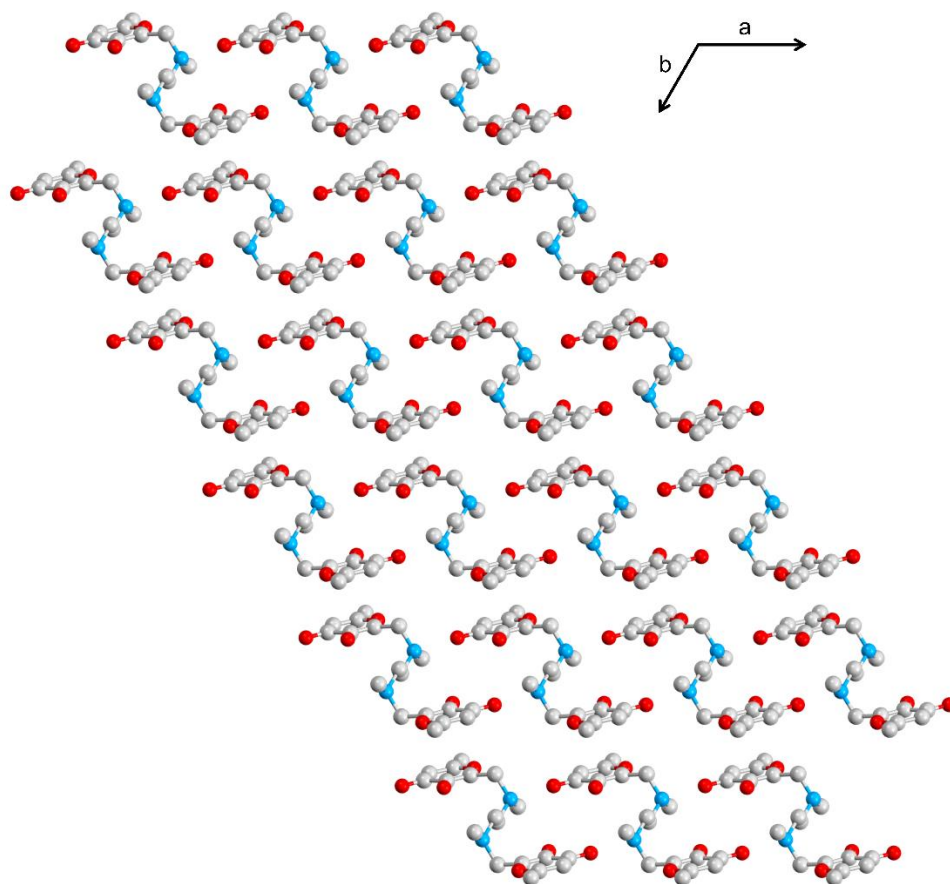


Fig. S3 Parallel chains of $[H_2L1]^{2+}$ cations in **6**.

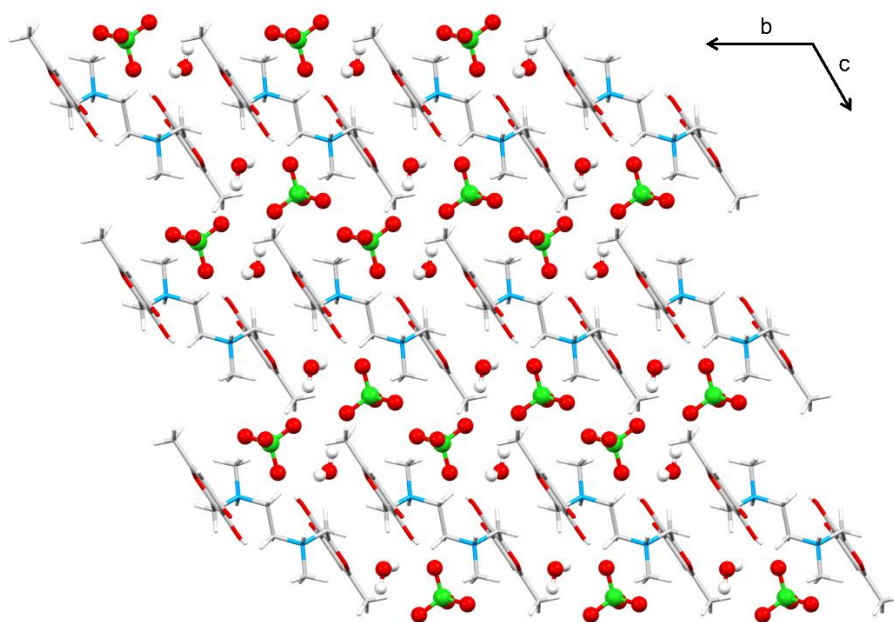


Fig. S4 Crystal packing of compound **6**.

Table S1 Crystallographic data and refinement parameters for compound **6**.

Formula	[H ₂ L1](ClO ₄) ₂ ·2(H ₂ O)
MW	601.34
T (K)	100
λ (Å)	0.71073
Crystal system, space group	Triclinic, P-1
Unit cell dimensions (Å, °)	a = 8.0335(7), α = 104.296(9) b = 8.3743(8), β = 104.670(8) c = 10.408(1), γ = 105.419(8)
Volume (Å ³)	614.8(1)
Z, D _c (mg/cm ³)	1, 1.624
μ (mm ⁻¹)	0.348
Crystal size (mm)	0.28x0.22x0.18
2 θ range (°)	8.51-59.06
Reflections collected /unique	8107 / 2905
Data / parameters	2905 / 218
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0505, wR2 = 0.1325
R indices (all data)	R1 = 0.0606, wR2 = 0.1371
GOF's	1.188