Supporting Information File

Bovine Serum Albumin Interactive One Dimensional Hexanuclear Manganese (III) Complex: Synthesis, Structure, Binding and Molecular Docking Studies

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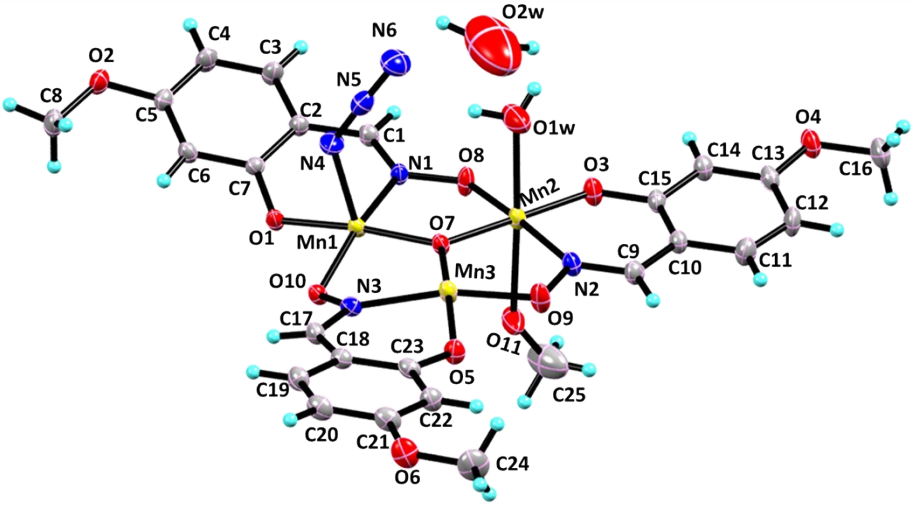

Fig.S1 ORTEP diagram (30% ellipsoidal probability) of the asymmetric unit of the complex with atom numbering scheme.

Table S 1: Crystal data and Refinement parameters for Complex **1**.

Formula	$C_{25}\ H_{26}\ Mn_3\ N_6\ O_{13}\ ,\ H_2O$
Formula Weight	785.35 + 1
Crystal System	Monoclinic
Space group	P21/C (No. 14)
a, b, c [Å]	10.0691(3) 22.5723(6) 13.2877(3)
α, β, γ [˚]	90 90.541(1) 90
V [Å^3]	3019.93(14)
Z	4
D(calc) [g/cm^3]	1.727
Mu(MoKα) [/mm]	1.312
F(000)	1596
Crystal Size [mm]	0.34 × 0.25 × 0.18
Data Collection	
Temperature (K)	273
Radiation [Å]	0.71073
Theta Min-Max [˚]	1.8, 27.5
Dataset	-13: 13 ; -29: 29 ; -17: 17
Tot., Uniq. Data, R(int)	13948, 6916, 0.032
Observed data [I > 2.0 sigma(I)]	4256
Refinement	
N_{ref}, N_{par}	6916, 442
R, wR2, S	0.0441, 0.1178, 1.07

Computational details

The ground and excited state electronic structure calculation in gas phase of complex **1** have been carried out using DFT[1] method associated with the conductor-like polarizable continuum model (CPCM).[2] Becke's hybrid function[3] with the Lee-Yang-Parr (LYP) correlation function[4] was used throughout the study.

For C, H, N, O, and Mn atoms, we employed 6-31+g as basis set for all the calculations. All the calculations were performed with the Gaussian 09W software package.[5] Gauss Sum 2.1 program[6] was used to calculate the molecular orbital contributions from groups or atoms.

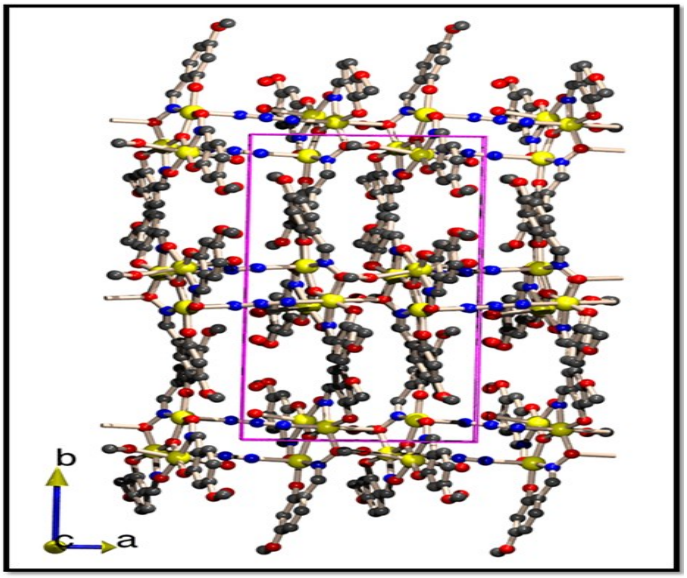

Fig. S2: The packing diagram of the polymeric chains of complex **1.**

Table S2.Selected bond distances (Å)

	Bond Distances
Mn1 -O1	1.882(2)
Mn1 -O7	1.879(2)
Mn1 -O10	1.933(2)
Mn1 -N1	1.978(3)
Mn1 -N4	2.220(3)
Mn1 -O10_b	2.491(2)
Mn2 -O1W	2.304(4)
Mn2 -O3	1.869(2)
Mn2 -O7	1.887(2)
Mn2 -O8	1.911(2)
Mn2 -O11	2.316(3)
Mn2 -N2	1.995(3)
Mn3 -O5	1.861(2)
Mn3 -O7	1.883(2)
Mn3 -O9	1.878(2)
Mn3 -N3	1.988(3)
Mn3 -N6_a	2.213(4)

a = -x,1-y,2-z
b = 1-x,1-y,2-z

Table S3. Selected Bond Angles (˚) of complex-**1**

	Bond Angles
O1 -Mn1 -O7	172.41(9)

O1 -Mn1 -O10	88.01(9)
O1 -Mn1 -N1	90.21(10)
O1 -Mn1 -N4	90.84(10)
O1 -Mn1 -O10_b	84.25(8)
O7 -Mn1 -O10	91.03(9)
O7 -Mn1 -N1	89.16(10)
O7 -Mn1 -N4	96.74(10)
O7 -Mn1 -O10_b	88.16(8)
O10 -Mn1 -N1	167.86(11)
O10 -Mn1 -N4	95.96(11)
O10 -Mn1 -O10_b	81.84(8)
N1 -Mn1 -N4	96.07(12)
O10_b -Mn1 -N1	86.04(10)
O10_b -Mn1 -N4	174.68(9)
O1W -Mn2 -O3	89.35(12)
O1W -Mn2 -O7	89.92(12)
O1W -Mn2 -O8	90.74(13)
O1W -Mn2 -O11	176.12(13)
O1W -Mn2 -N2	94.57(13)
O3 -Mn2 -O7	179.14(9)
O3 -Mn2 -O8	88.51(9)
O3 -Mn2 -O11	94.36(10)
O3 -Mn2 -N2	90.77(10)
O7 -Mn2 -O8	91.96(9)
O7 -Mn2 -O11	86.37(10)
O7 -Mn2 -N2	88.83(10)
O8 -Mn2 -O11	90.52(12)

Table S4. Hydrogen Bond table (Å,˚)

D-H...A	D-H(Å)	H-A(Å)	D-A(Å)	<D-H...A(˚)	symmetry
O1W -H2W1 .. N5	0.8500	2.4600	3.277(5)	162.00	.
O1W -H2W1 .. N6	0.8500	2.3800	3.099(6)	142.00	.
C1 -H1 .. O2	0.9300	2.5200	3.356(4)	149.00	x,1/2-y,-1/2+z
C4 -H4 .. O8	0.9300	2.4700	3.386(4)	168.00	x,1/2-y,1/2+z

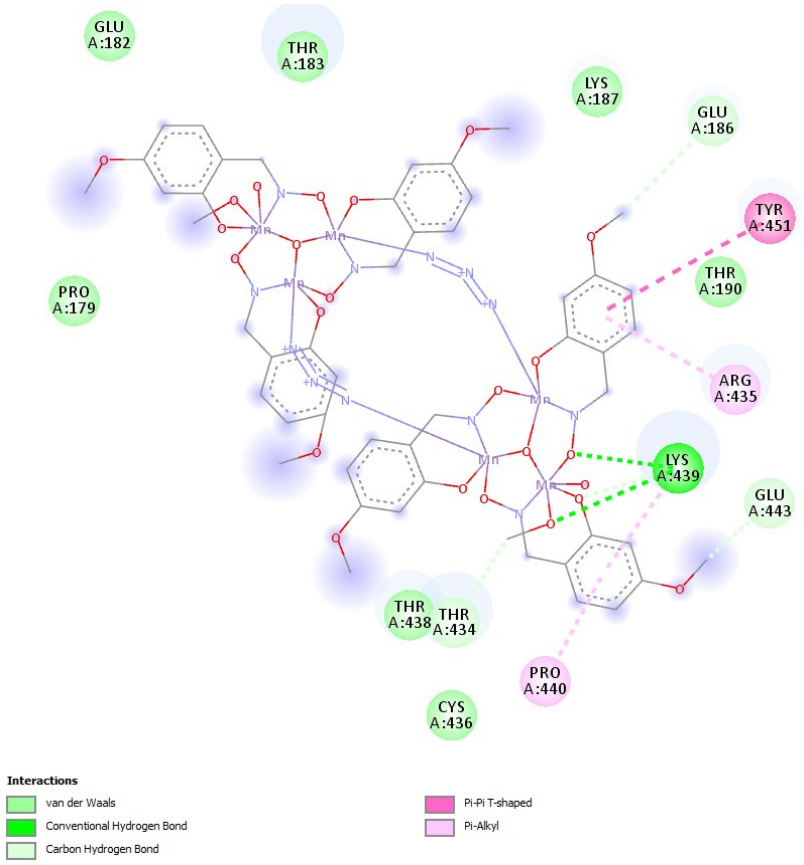

Fig. S3: Interactions of different amino acid residues of BSA with complex **1** in 2D view.

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