Anticancer evaluation of a Manganese Complex on HeLa and MCF-7 Cancer Cells: Design, Deterministic Solvothermal Synthesis Approach, Hirshfeld analysis, DNA Binding, Intracellular Reactive Oxygen Species (ROS) Production, Electrochemical Characterization and Density Functional Theory

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Single crystal X-ray diffraction analysis

Table S1: Experimental data of **($Mn(phen)_2Cl_2$)**.

Empirical formula	$C_{24}H_{16}Cl_2MnN_4$
Formula weight	486.25
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	**a** = 9.1987(4) Å α = 79.964(10)° **b** = 10.7012(5) Å β = 81.224(10)° **c** = 8.4151(4) Å γ = 69.829(10)°
Volume	1071.13(8) $Å^3$
Z	2
Calculated Density	1.508 Mg/m^3
Absorption coefficient	0.885 mm^{-1}
F(000)	494
Crystal size	0.580 x 0.400 x 0.230 mm^3
Theta range for data collection	1.648 to 28.396°.
Index ranges	-12<=h<=12, -13<=k<=13, -16<=l<=16
Reflections collected	14817
Completeness to theta=67.679°	100.0 %
Refinement method	Full-matrix least-squares on F^2
Independent reflections	5317 [R(int) = 0.0241]
Data / restraints / parameters	5317 / 0 / 280
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R_1 = 0.0385, wR_2 = 0.1064
R indices (all data)	R_1 = 0.0450, wR_2 = 0.1120
Extinction coefficient	n/a
Largest diff. peak and hole	0.559 and -0.317 $e.Å^{-3}$

Density functional theory (DFT) calculations

Investigation of the discloses that Investigation of the geometric parameters in Table S1 discloses that, in nearly all cases, the computed geometric parameters match well with the experimentally found geometric parameters (see Table); yet, some of the geometric parameters don't reveal good corroboration. Excitingly, the measured geometric parameters of the monomeric complex diverge further from the experimental information, in comparison to that of the dimeric complex. For instance, the measured Mn-Cl bond length in the monomeric **$(Mn(phen)_2Cl_2)$**. is 2.410 Å (2.480 Å experimental) but the value in the dimeric **$(Mn(phen)_2Cl_2)$**. is improved to 2.452 Å. The perfection in the association amid theory and experiment for the dimeric complex is well observed in bond angles. For instance, the Cl-Mn-Cl bond angle in the X-ray structure is 103.28 degrees while the measured bond angle for the monomer is 114.69^o. Still, the error is decreased for the dimeric complex (the estimated bond angle for the dimeric complex is 108.09^o). Likewise, the Cl-Mn-N (*Anti* to Cl) bond angle in the X-ray geometry is 165.70^o while the measured bond angles in the monomeric and dimeric complexes are 155.60 and 160.39^o. An analogous improved association is noticed for all other bond angles. The contrast of the geometric parameters for the monomeric and dimeric complexes infers that the variance between experiment and theory gets lessened with a rise in the interacting complexes.

Consequently, the alteration (between theory and experiment) is primarily because of the gas phase nature of estimations associated with solid phase nature of X-ray measured geometries.

Table S2. Analysis of the geometric parameters of **($Mn(phen)_2Cl_2$)**.

Parameter	**Exp**	**Theor**	**Parameter**	**Exp**	**Theor**
Bond lengths			**Bond lengths**		
Mn-Cl	2.480	2.410	Mn-Cl	2.480	2.452
Mn-Cl	2.415	2.410	Mn-Cl	2.415	2.405
Mn-N1	2.388	2.390	Mn-N1	2.388	2.391
Mn-N2	2.251	2.307	Mn-N2	2.251	2.312
Mn-N3	2.253	2.308	Mn-N3	2.253	2.290
Mn-N4	2.338	2.391	Mn-N4	2.338	2.380
Bond Angles			**Bond Angles**		
Cl-Mn-Cl	103.28	114.69	Cl-Mn-Cl	103.28	108.09
N-Mn-N (L1)	71.91	70.32	N-Mn-N (L1)	71.91	70.52
N-Mn-N (L2)	71.21	70.34	N-Mn-N (L2)	71.21	70.86
Cl(1)-Mn-N	101.52	100.18	Cl(1)-Mn-N	101.52	101.18
Cl(1)-Mn-N	95.47	91.9	Cl(1)-Mn-N	95.47	92.72
Cl(1)-Mn-N	94.63	85.75	Cl(1)-Mn-N	94.63	89.07
Cl(1)-Mn-N	165.70	155.60	Cl(1)-Mn-N	165.70	160.39
Cl(2)-Mn-N	95.36	91.87	Cl(2)-Mn-N	95.36	90.72
Cl(2)-Mn-N	86.53	85.64	Cl(2)-Mn-N	86.53	87.49
Cl(2)-Mn-N	103.07	100.18	Cl(2)-Mn-N	103.07	107.03
Cl(2)-Mn-N	159.58	155.51	Cl(2)-Mn-N	159.58	156.99