Synthesis, Structural characterization, DFT and Molecular Dynamics Simulations of Dinuclear (μ-hydroxo) Bridged triethanolamine Copper (II) complexes: Efficient Candidates Towards Visible Light Mediated Photo-Fenton Degradation of Organic Dyes

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Supplementary Information

Table S1: Electrochemical data of complexes **1-3**.

Complex ID	E_{pa} (V)	E_{pc} (V)	I_{pc} (A)	I_{pa} (A)	I_{pa}/I_c	$\Delta E = E_{pa} - E_{pc}$
Complex **1**	-1.1914	-1.2207	3.21×10^{-5}	1.329×10^{-5}	1.56	+0.0293
Complex **2**	-0.6159	-0.79031	-2.44×10^{-5}	4.4168×10^{-5}	1.810	+0.1744
Complex **3**	-0.72021	-0.90332	-6.451×10^{-5}	3.317×10^{-5}	1.194	+0.1830

Table S2: General surface information for complexes **1-3**

General surface information	Complex 1	Complex 2	Complex 3
Iso-value	0.5	0.5	0.5
Volume (Å³)	716.79	716.07	793.13
Area (Å²)	574.22	577.45	645.00
Globularity	0.675	0.670	0.642
Asphericity	0.257	0.316	0.499

Table S3: Surface property information for complexes **1-3**.

Name (property)	Complex 1			Complex 2			Complex 3		
	Min	**Mean**	**Max**	**Min**	**Mean**	**Max**	**Min**	**Mean**	**Max**
d_i (Å)	0.671	1.636	2.569	0.675	1.649	2.586	0.678	1.582	2.530

d_e (Å)	0.757	1.643	2.526	0.757	1.648	2.662	0.767	1.590	2.397
d_{norm}	-0.707	0.479	1.417	-0.701	0.448	1.206	-0.697	0.482	1.367
Shape index	-0.997	0.183	0.998	-0.994	0.193	0.996	-1.000	0.182	0.998
Curvedness	-3.993	-0.988	0.414	-3.792	-0.953	0.463	-3.947	-0.922	0.475

Table S4: Analysing the fingerprint based on the type of elements present, we calculate the ratio of the surface area where atoms interact closely, both within and outside the surface, in relation to the overall surface area.

	Inside atom	**Outside atoms**						
		Cu	**O**	**F**	**H**	**N**	**C**	
Complex 1	**C**	0	0	0.6	6.0	0	3.7	10.2
	Cu	0	0	0	0	0	0	0.00
	F	0	0.8	2.8	11.7	0	0.5	15.7
	H	0	6.6	10.9	43.3	0	4.8	65.6
	N	0	0	0	0	0	0	0.00
	O	0	0	0.8	7.7	0	0	8.5
		0.00	7.4	15.1	68.7	0.00	8.9	
	Inside atom	**Outside atoms**						
		Cu	**Cl**	**O**	**H**	**N**	**C**	
Complex 2	**C**	0	1.4	0	7.4	0	1.8	10.6
	Cl	0	1.1	0	9.2	0	1.4	11.7
	Cu	0	0	0	0	0	0	0.00
	H	0	5.7	7.6	50.9	0	5.0	69.3
	N	0	0	0	0	0	0	0.00
	O	0	0	0	8.5	0	0	8.5
		0.00	8.2	7.6	75.9	0.00	8.2	
	Inside atom	**Outside atoms**						
		Cu	**O**	**H**	**N**	**C**		
Complex 3	**C**	0	0.2	8.9	0	0	9.1	
	Cu	0	0	0	0	0	0.00	
	H	0	8.7	65.9	0	6.5	81.1	
	N	0	0	0	0	0	0.00	
	O	0	0.1	9.5	0	0.2	9.8	
		0.00	9.0	84.3	0.00	6.7		

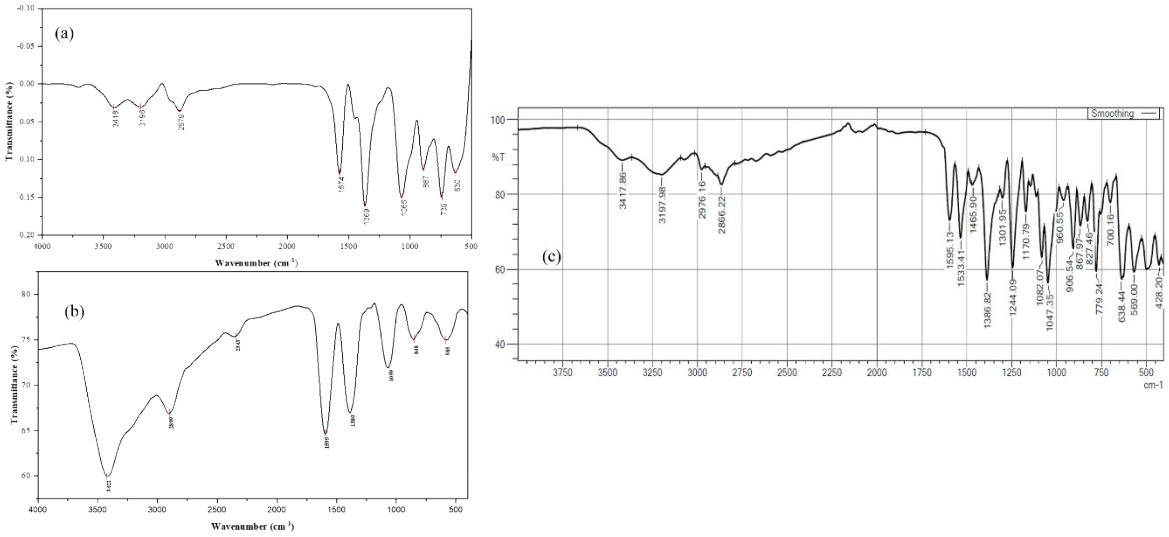

Figure S1: IR spectra of complexes **1-3** (a-c)

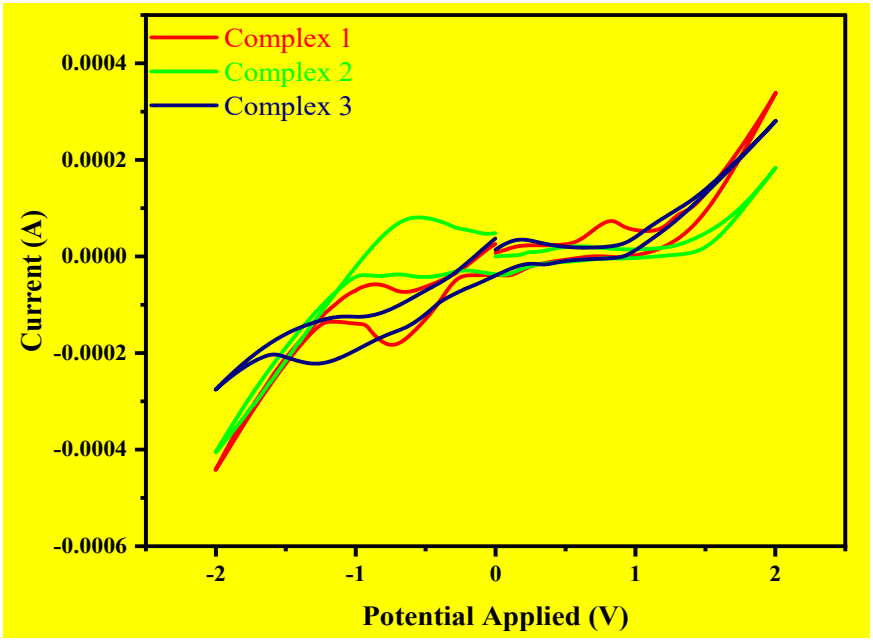

Figure S2: Electrochemical behaviour of complexes **1-3**

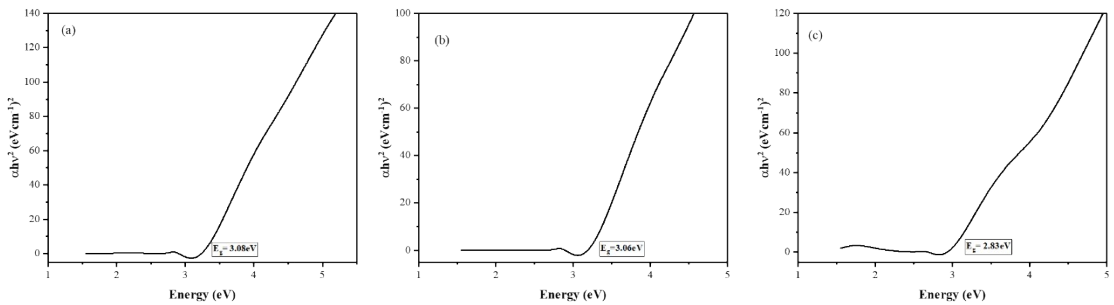

Figure S3: Tauc's plot of the complexes **1-3** (a-c) calculated using UV-Vis spectroscopy

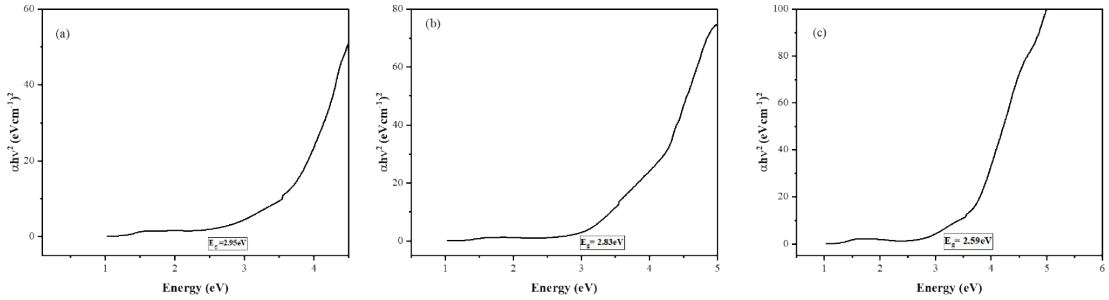

Figure S4: Tauc's plot of the complexes **1-3** (a-c) calculated using DRS

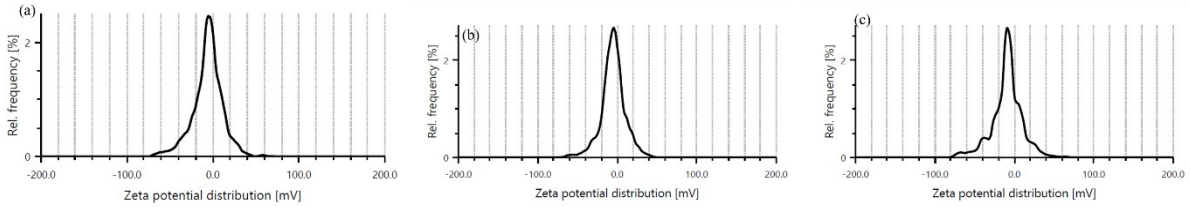

Figure S5: Zeta potential for complexes **1-3** (a-c)

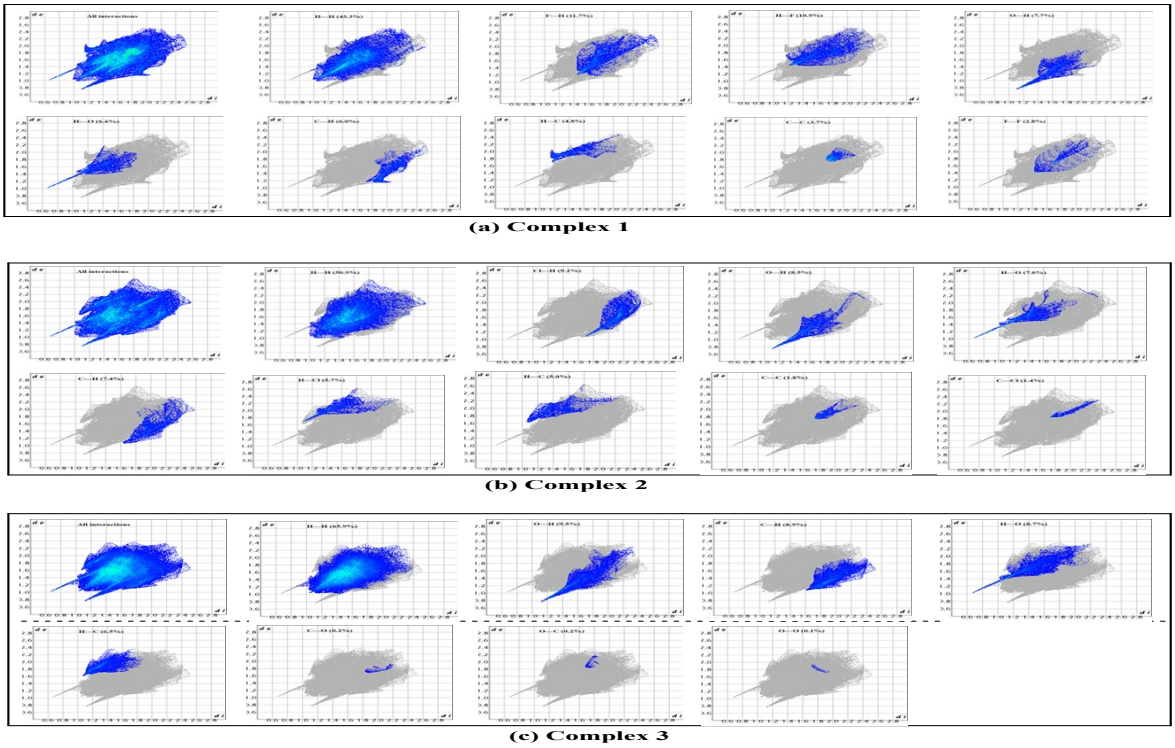

Figure S6: Fingerprint diagrams depicting different non-covalent interactions within single crystals of complexes **1-3**.

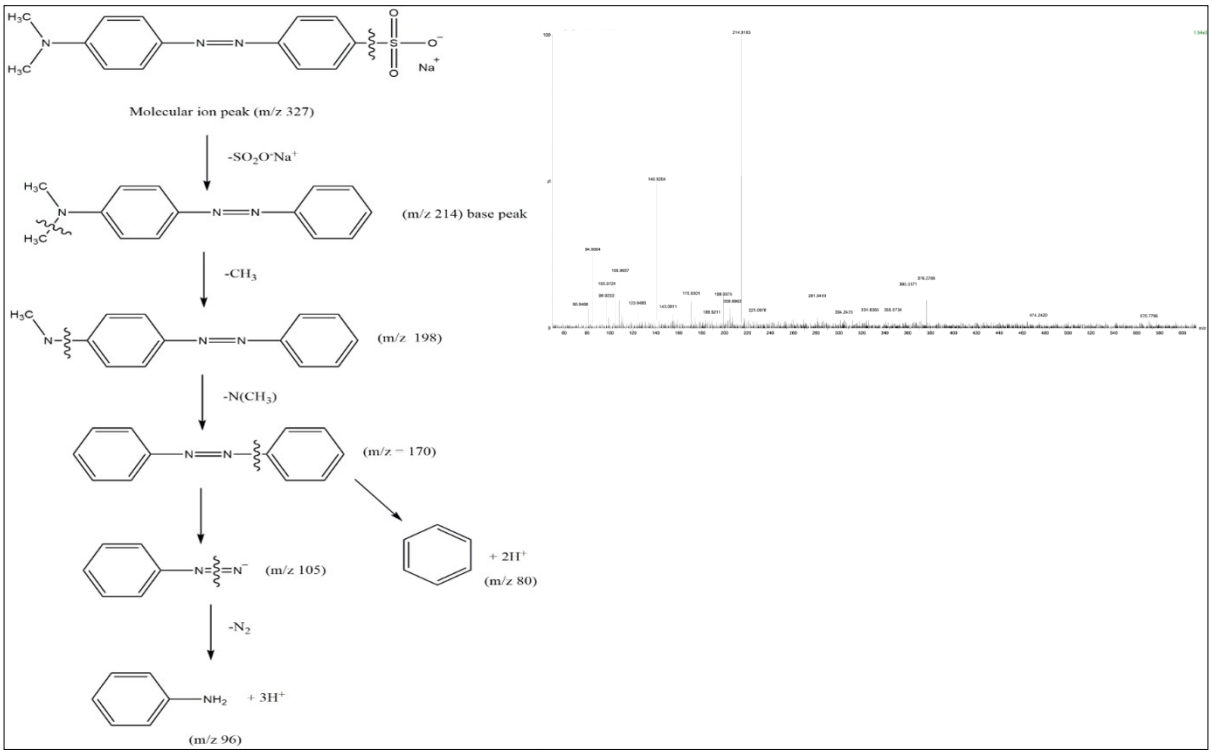

Figure S7: Degradation pattern of MO by complex **3** interpreted through mass spectra

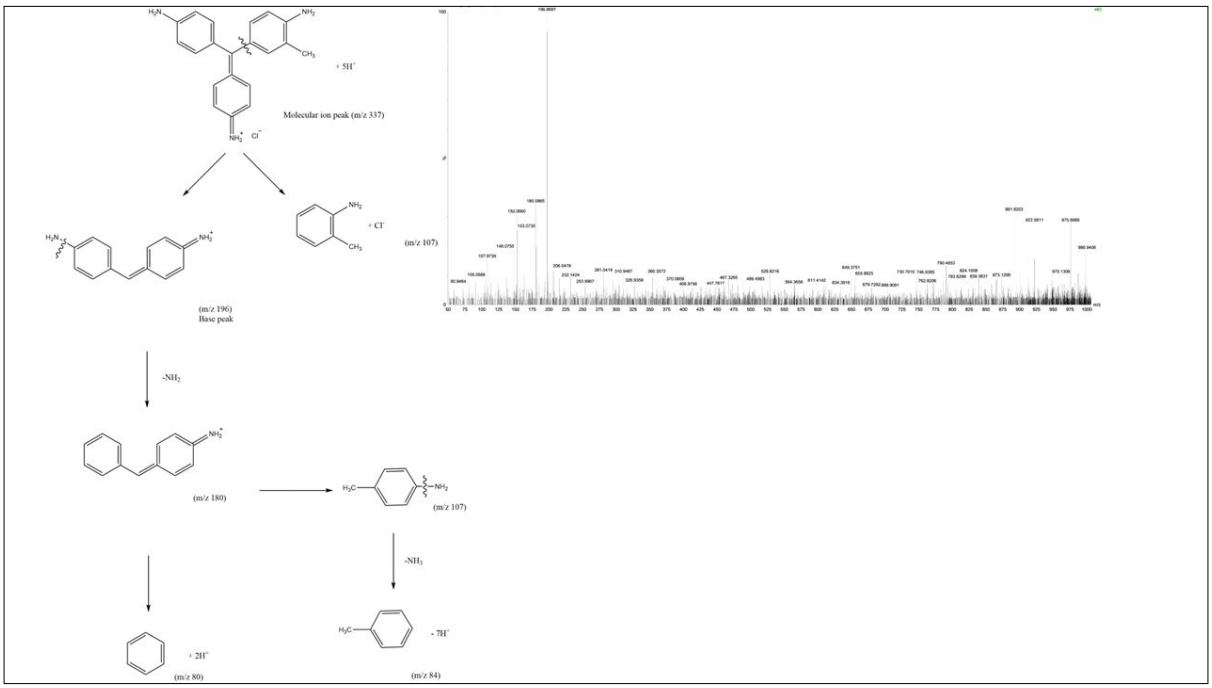

Figure S8: Degradation pattern of FB by complex **3** interpreted through mass spectra.

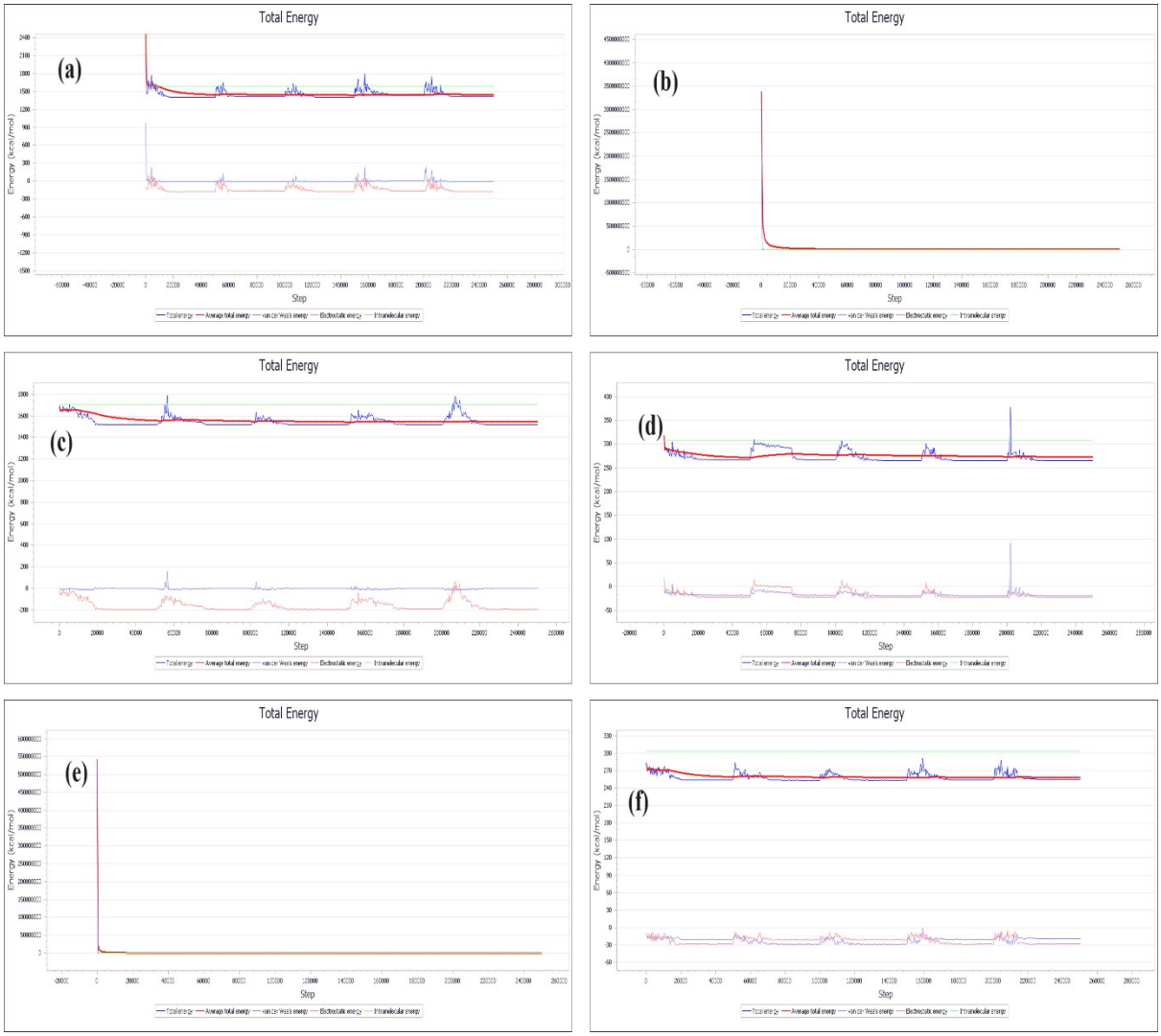

Figure S9: Total energy distribution for (a) MO/complex **1**, (b) MO/complex **2**, (c) MO/complex **3**, (d) FB/complex **1**, (e) FB/complex **2**, (f) FB/complex **3**.

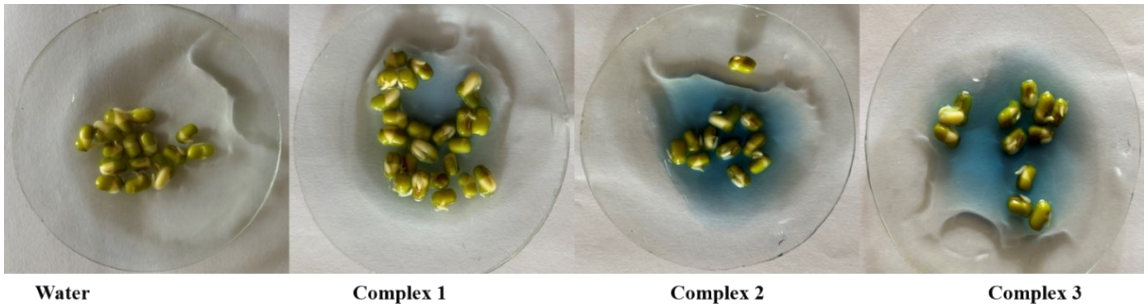

Figure S10: Phytotoxicity assessment: seed germination assay of *Vigna radiata* with complexes **1-3**.