Electronic Supporting Information (ESI†)

for

Mitochondrial selectivity and remarkable photocytotoxicity of a ferrocenyl neodymium(III) complex of terpyridine and curcumin in cancer cells

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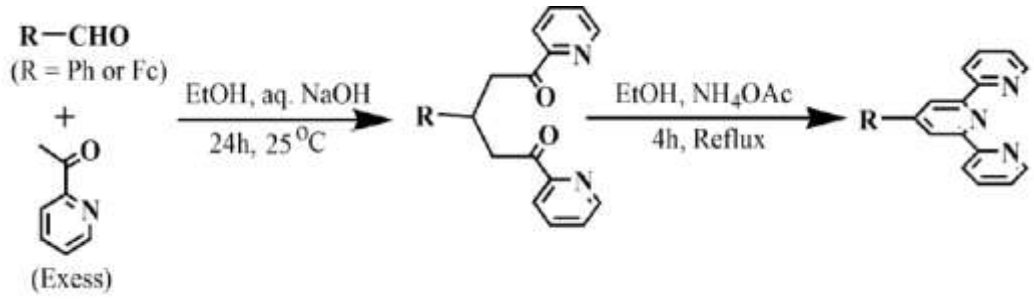

Fig. S1: Synthetic scheme for the preparation of Ph-tpy and Fc-tpy ligands.

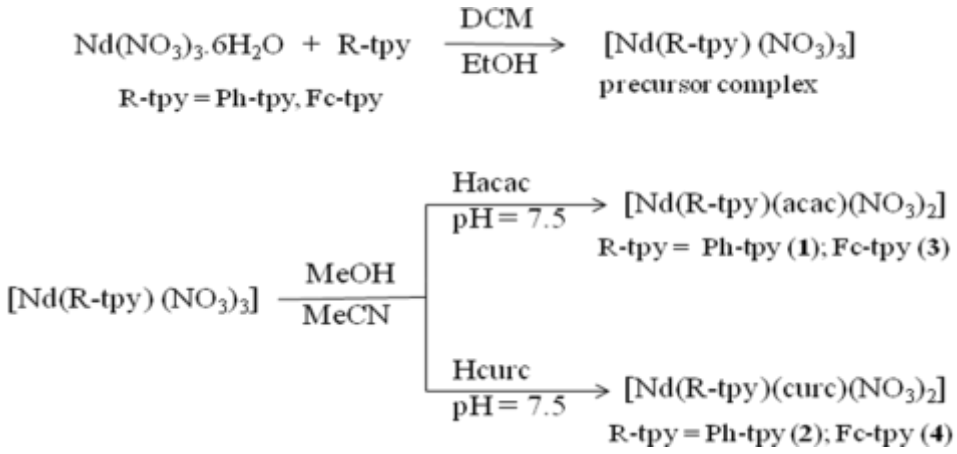

Fig. S2: Synthetic scheme for the preparation of the complexes **1-4**.

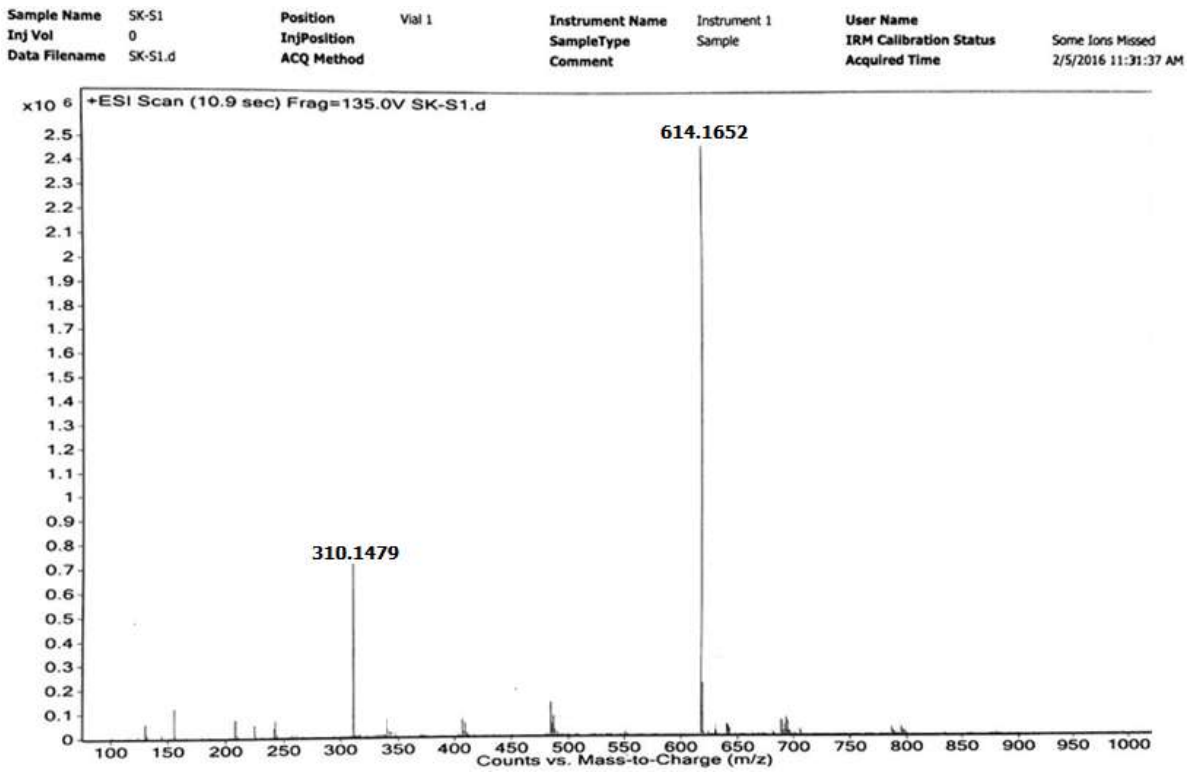

Fig. S3. The ESI-MS spectrum of the complex [Nd(Ph-tpy)(acac)$(NO_3)_2$] (**1**) showing the prominent $[M–(NO_3^-)]^+$ peak at *m/z* = 614.1652. The peak at 310.1479 corresponds to M +1 species for the Ph-tpy ligand.

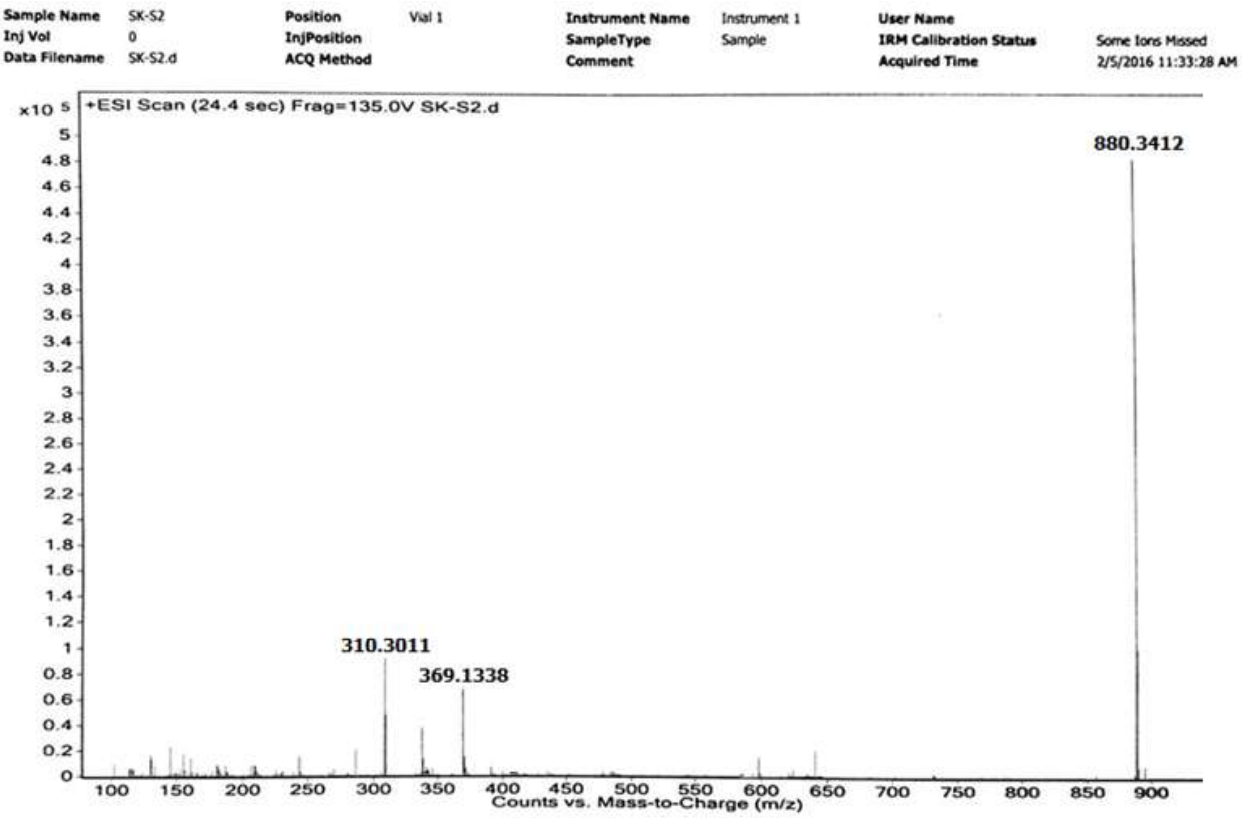

Fig. S4. The ESI-MS spectrum of the complex [Nd(Ph-tpy)(curc)(NO_3)$_2$] (**2**) showing the prominent [M–(NO_3^-)]$^+$ peak at *m*/*z* = 880.3412. The peaks at 310.3011 and 369.1338 correspond to M +1 species for the Ph-tpy and Hcurc ligands respectively.

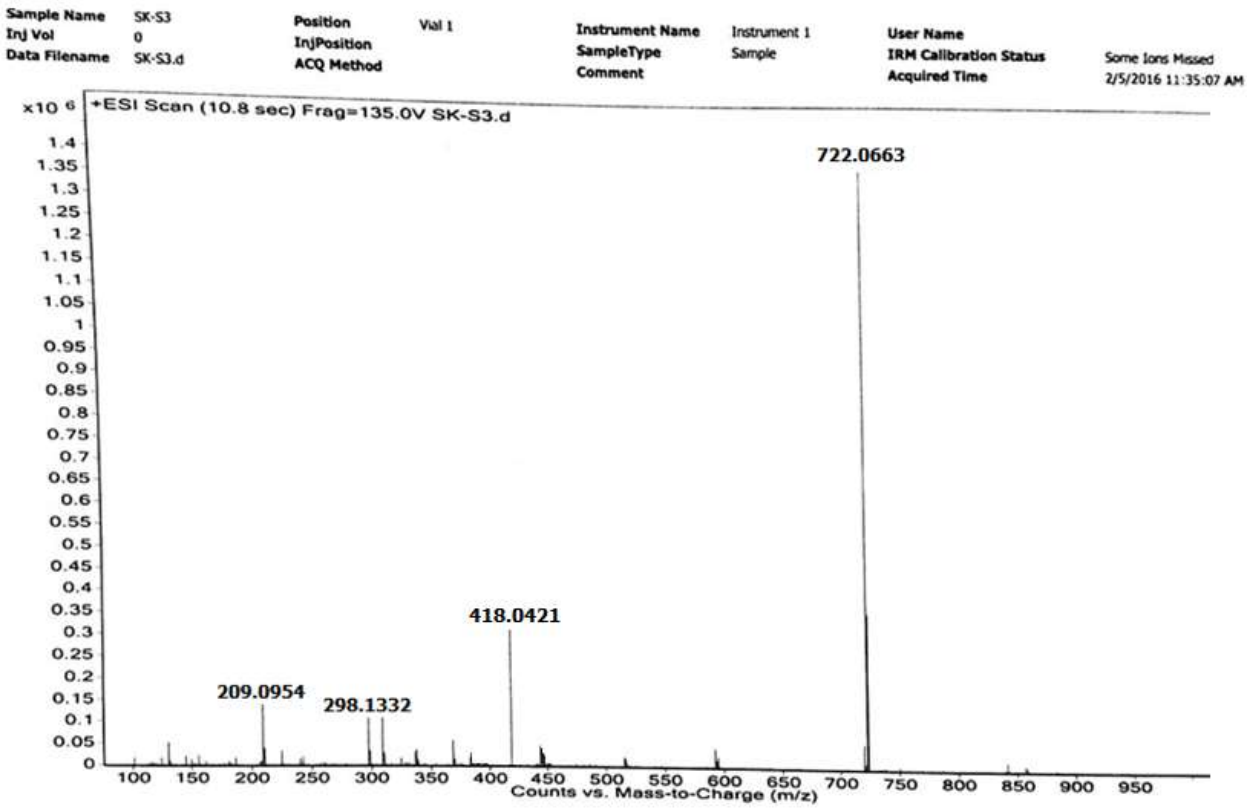

Fig. S5. The ESI-MS spectrum of the complex [Nd(Fc-tpy)(acac)(NO_3)$_2$] (**3**) showing the prominent [M–(NO_3^-)]$^+$ peak at *m*/*z* = 722.0663. The peak at 418.0421 corresponds to M +1 species for the Fc-tpy ligand.

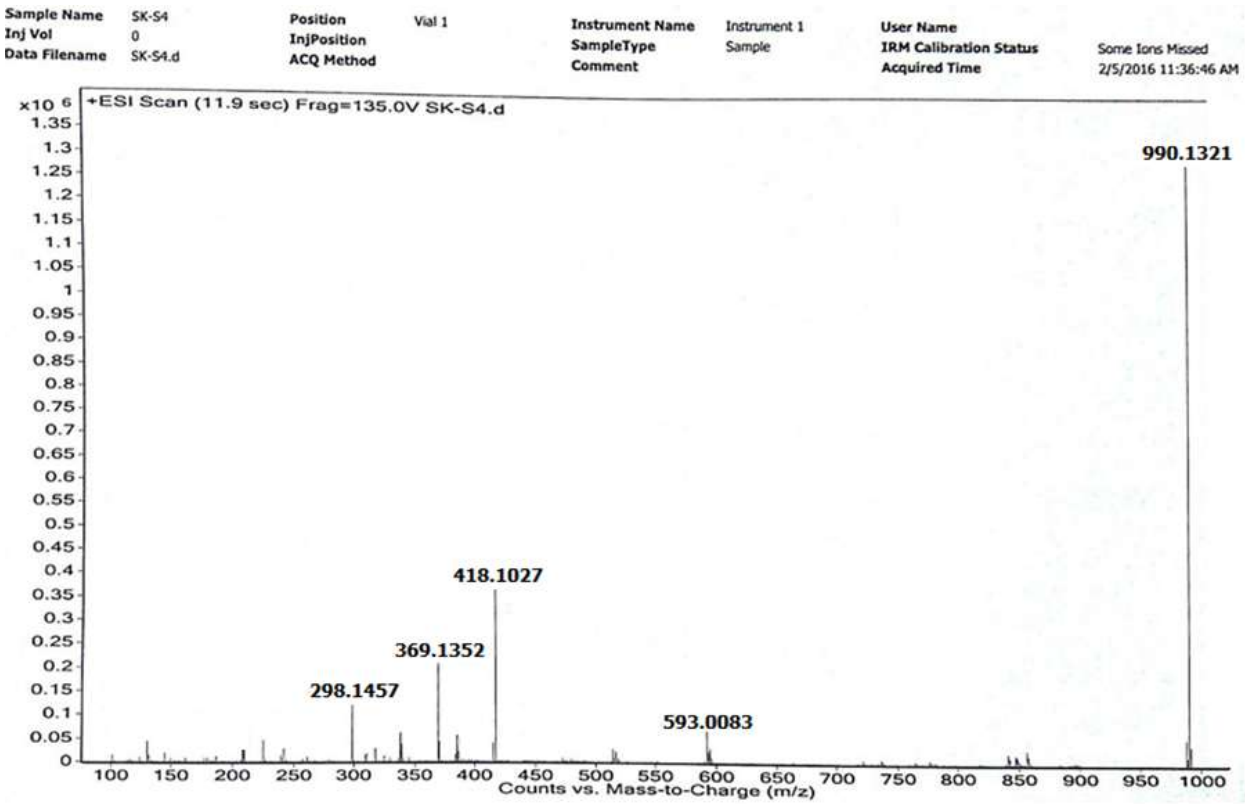

Fig. S6. The ESI-MS spectrum of the complex [Nd(Fc-tpy)(curc)(NO_3)$_2$] (**4**) showing the prominent [M–(NO_3^-)]$^+$ peak at *m*/*z* = 990.1321. The peaks at 418.1027 and 369.1352 correspond to M +1 species for the Fc-tpy and Hcurc ligands respectively.

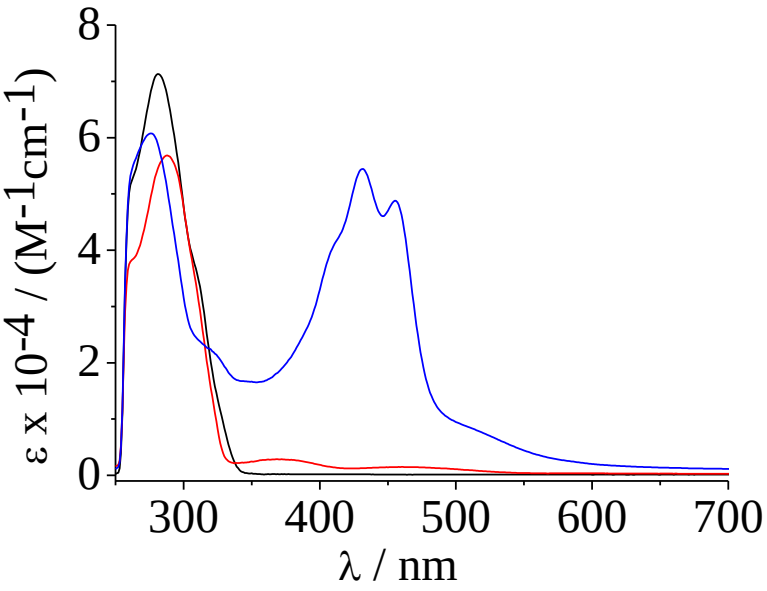

Fig. S7. The electronic absorption spectra of complexes **1** (red), **2** (blue) and **3** (black) recorded in DMF.

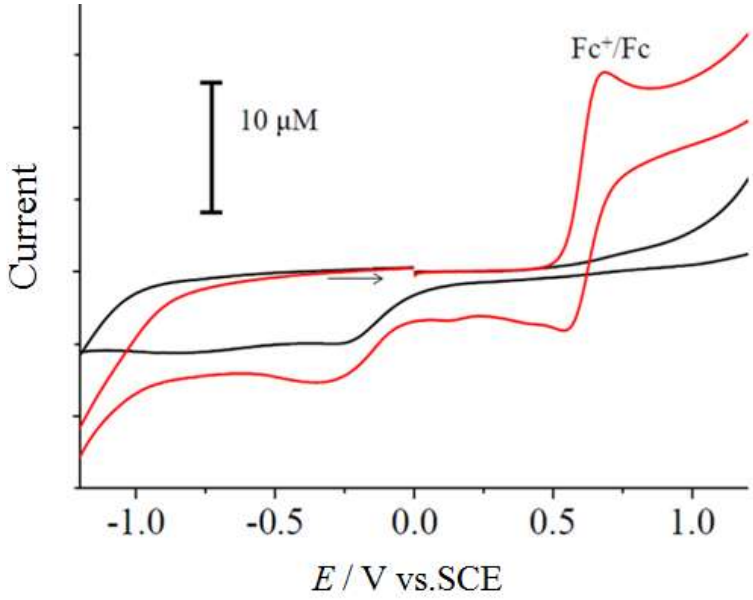

Fig. S8. Cyclic voltammograms of complexes **1** (black) and **3** (red curve) recorded in DMF in the presence of 0.1 M TBAP as supporting electrolyte.

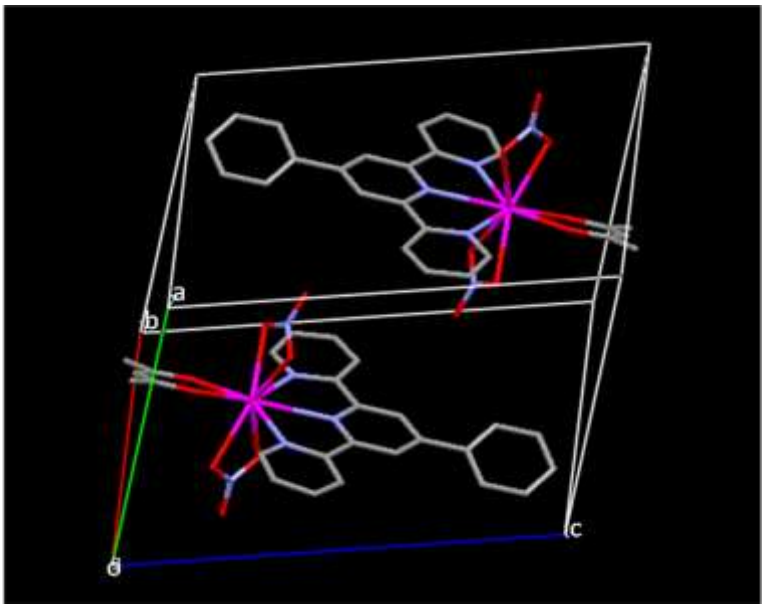

Fig. S9. The unit cell packing diagram for complex **1** in the solid state.

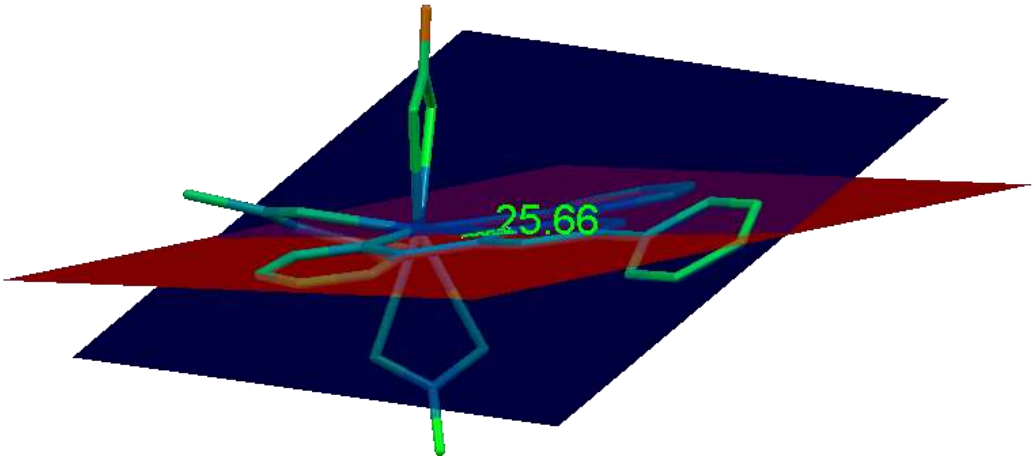

Fig. S10. Diagram showing the dihedral angle made by the pendant phenyl moiety of the Ph-tpy ligand with the terpyridine moiety in the crystal structure of complex **1**.

Table S1. Selected bond distances (Å) and angles (°) for the complex **1** with estimated standard deviations (e.s.d.) in the parentheses.

Nd(1)-O(1)	2.3407(19)	O(6)-Nd(1)-O(8)	48.83(7)
Nd(1)-O(2)	2.3391(18)	N(1)-Nd(1)-O(1)	150.62(7)
Nd(1)-O(3)	2.528(2)	N(1)-Nd(1)-O(2)	84.31(7)
Nd(1)-O(5)	2.566(2)	N(1)-Nd(1)-O(3)	90.34(8)
Nd(1)-O(6)	2.562(2)	N(1)-Nd(1)-O(5)	74.16(8)
Nd(1)-O(8)	2.566(2)	N(1)-Nd(1)-O(6)	117.03(7)
Nd(1)-N(1)	2.578(2)	N(1)-Nd(1)-O(8)	68.28(7)
Nd(1)-N(2)	2.635(2)	N(2)-Nd(1)-O(1)	142.33(7)
Nd(1)-N(3)	2.607(2)	N(2)-Nd(1)-O(2)	144.02(6)
O(1)-Nd(1)-O(2)	73.59(7)	N(2)-Nd(1)-O(3)	72.12(7)
O(1)-Nd(1)-O(3)	86.74(8)	N(2)-Nd(1)-O(5)	104.85(8)
O(1)-Nd(1)-O(5)	81.97(9)	N(2)-Nd(1)-O(6)	94.74(7)
O(1)-Nd(1)-O(6)	81.91(8)	N(2)-Nd(1)-O(8)	74.81(7)
O(1)-Nd(1)-O(8)	124.73(7)	N(3)-Nd(1)-O(1)	82.09(7)
O(2)-Nd(1)-O(3)	124.72(7)	N(3)-Nd(1)-O(2)	148.64(7)
O(2)-Nd(1)-O(5)	76.78(8)	N(3)-Nd(1)-O(3)	72.05(7)
O(2)-Nd(1)-O(6)	87.98(8)	N(3)-Nd(1)-O(5)	119.56(7)
O(2)-Nd(1)-O(8)	80.40(7)	N(3)-Nd(1)-O(6)	68.95(7)
O(3)-Nd(1)-O(5)	49.15(8)	N(3)-Nd(1)-O(8)	98.22(7)
O(3)-Nd(1)-O(6)	140.47(8)	N(1)-Nd(1)-N(2)	62.53(6)
O(3)-Nd(1)-O(8)	146.25(8)	N(1)-Nd(1)-N(3)	124.60(7)
O(5)-Nd(1)-O(6)	160.38(10)	N(2)-Nd(1)-N(3)	62.09(7)
O(5)-Nd(1)-O(8)	137.52(8)		

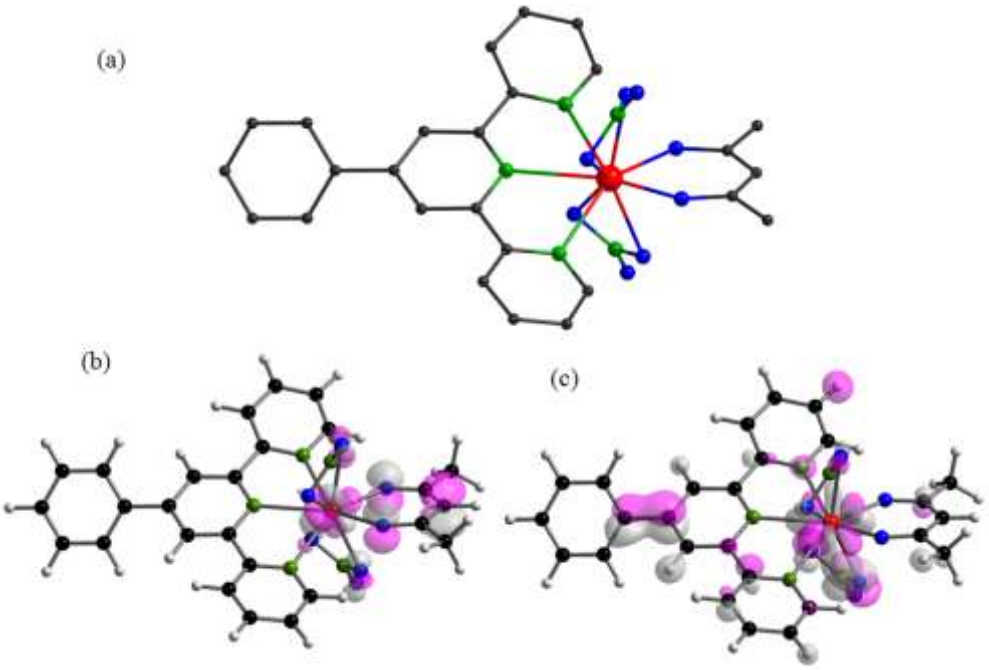

Fig. S11. The DFT optimized structure in (a), the HOMO in (b) and the LUMO in (c) for complex **1**.

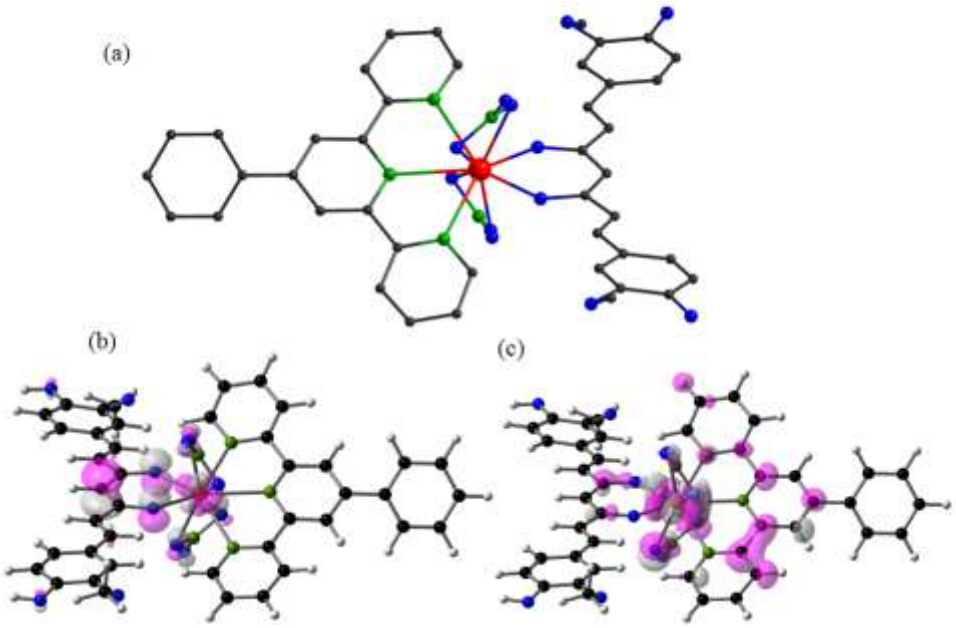

Fig. S12. The DFT optimized structure in (a), the HOMO in (b) and the LUMO in (c) for complex **2**.

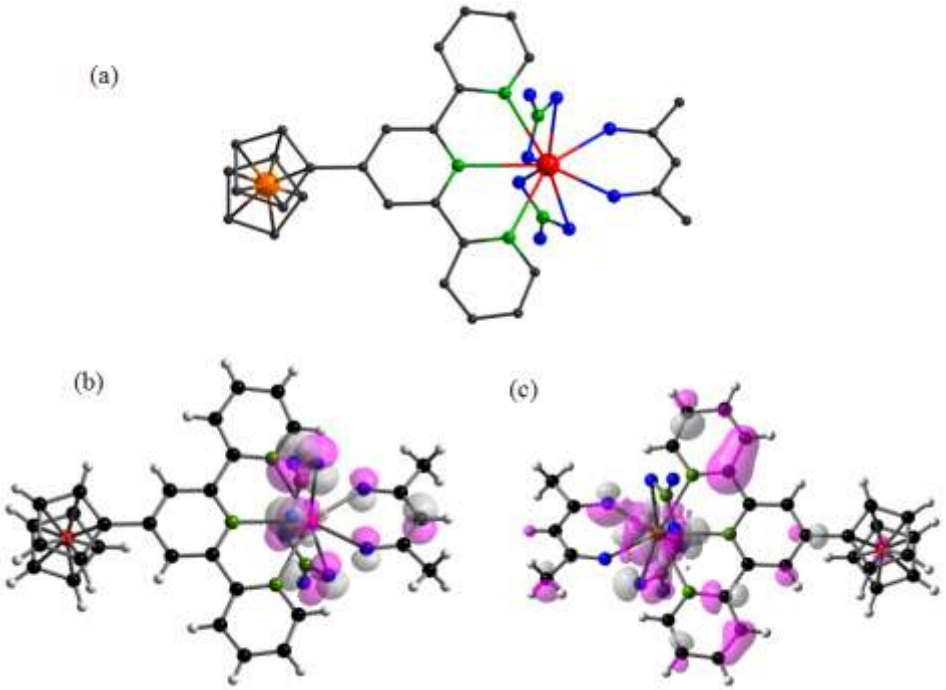

Fig. S13. The DFT optimized structure in (a), the HOMO in (b) and the LUMO in (c) for complex **3**.

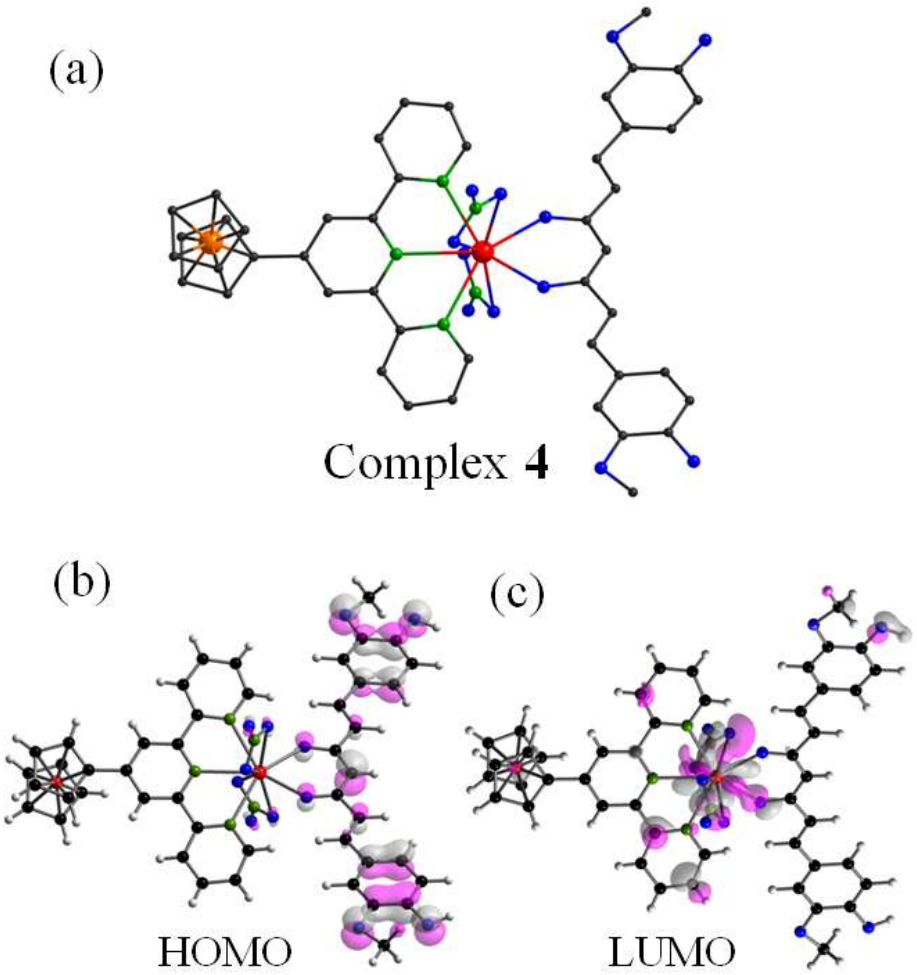

Fig. S14. The DFT optimized structure in (a), the HOMO in (b) and the LUMO in (c) for complex **4**.

Table S2: The DFT coordinates used for energy optimization of complex **1.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	-1.423248	-0.051063	-0.038388
2	8	0	-0.860582	-1.006584	2.014906
3	8	0	-3.291589	-1.145417	0.587437
4	8	0	-3.101560	1.351174	-0.572196
5	8	0	-1.811792	1.126473	1.961435
6	7	0	1.233630	0.004170	0.145517
7	6	0	-0.503014	4.736257	0.171642
8	1	0	-1.175096	5.604197	0.147732
9	7	0	-0.174027	-2.318321	-0.282972
10	8	0	-0.509036	0.366430	-2.139695
11	8	0	-2.310632	-1.116773	-1.928534
12	7	0	-0.238158	2.299660	-0.036799
13	7	0	-1.620929	-0.047600	2.678618
14	6	0	-4.591419	-0.946568	0.486037
15	6	0	1.126991	2.465314	0.198669
16	7	0	-1.587086	-0.268914	-2.756114
17	6	0	1.173677	-2.458268	0.048604
18	6	0	4.116465	0.031412	0.033433
19	6	0	5.626420	0.047837	-0.042513
20	6	0	-5.168466	2.551181	-1.134980
21	1	0	-4.535908	3.060926	-1.877784
22	1	0	-5.390891	3.259206	-0.318214
23	1	0	-6.117150	2.252891	-1.604761

24	6	0	1.746240	-3.722770	0.334193
25	1	0	2.805149	-3.799781	0.608916
26	6	0	1.954126	1.197455	0.160220
27	6	0	3.369175	1.231478	0.111426
28	1	0	3.889400	2.195558	0.098629
29	6	0	1.974799	-1.174154	0.075002
30	6	0	-0.418102	-4.754313	-0.050031
31	1	0	-1.075957	-5.632096	-0.097734
32	6	0	-0.937714	-3.470690	-0.319905
33	1	0	-1.993818	-3.307902	-0.582119
34	6	0	3.389072	-1.183350	0.014865
35	1	0	3.923136	-2.138001	-0.049019
36	6	0	-5.520223	-2.090297	0.993630
37	1	0	-4.932540	-2.821024	1.569244
38	1	0	-5.986701	-2.602348	0.135331
39	1	0	-6.320459	-1.680794	1.629379
40	6	0	6.373958	1.054215	0.622959
41	1	0	5.852679	1.817675	1.215147
42	8	0	-2.116777	-0.242615	3.866510
43	6	0	6.324692	-0.941356	-0.783115
44	1	0	5.763081	-1.717053	-1.320060
45	6	0	-4.423962	1.306063	-0.564916
46	6	0	0.943278	-4.877958	0.285821
47	1	0	1.377406	-5.862216	0.512425
48	6	0	8.460456	0.081938	-0.190135
49	1	0	9.557393	0.095480	-0.247729
50	6	0	-1.017931	3.441723	-0.047657
51	1	0	-2.081741	3.239895	-0.246491

52	6	0	1.694420	3.742031	0.438673
53	1	0	2.767430	3.841519	0.640415
54	6	0	7.778815	1.067566	0.552114
55	1	0	8.343868	1.847926	1.079719
56	6	0	0.873049	4.884551	0.426916
57	1	0	1.305515	5.877625	0.614351
58	6	0	-5.188477	0.224628	-0.058854
59	1	0	-6.279305	0.288305	-0.094613
60	8	0	-1.893388	-0.068998	-4.005427
61	6	0	7.729233	-0.920799	-0.858578
62	1	0	8.254867	-1.687485	-1.443825

Table S3: The DFT coordinates used for energy optimization of complex **2.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	-0.019955	0.282764	-0.008320
2	8	0	-1.675892	1.215580	-1.364701
3	8	0	-1.585067	-1.318860	-0.083178
4	8	0	1.158702	-1.614739	-0.195908
5	8	0	-0.017410	-0.118594	-2.332317
6	7	0	0.374800	2.928255	-0.102518
7	6	0	4.156595	0.622070	-2.504689
8	1	0	4.798662	-0.154638	-2.940718
9	7	0	-1.672707	1.788073	1.328883
10	8	0	1.516544	0.889820	1.634987
11	8	0	-0.209507	-0.607573	2.157963
12	7	0	2.177901	1.170469	-1.149539
13	7	0	-1.313452	0.370664	-2.411041
14	6	0	-1.601966	-2.646248	-0.123183
15	6	0	2.462638	2.521973	-1.346354
16	7	0	1.046157	-0.114912	2.480946
17	6	0	-1.735519	3.169923	1.149120
18	6	0	0.874036	5.768034	0.009081
19	6	0	1.138774	7.255381	0.071836
20	6	0	-2.875358	3.922068	1.528499
21	1	0	-2.903960	5.005139	1.359376
22	6	0	1.511057	3.493729	-0.679606
23	6	0	1.771653	4.885431	-0.638650

24	1	0	2.689337	5.280272	-1.087857
25	6	0	-0.508152	3.802959	0.528509
26	6	0	-3.932142	1.875542	2.296663
27	1	0	-4.774668	1.330896	2.742929
28	6	0	-2.774854	1.174877	1.896222
29	1	0	-2.677073	0.085547	2.015873
30	6	0	-0.279814	5.198302	0.599255
31	1	0	-1.003253	5.841313	1.112578
32	6	0	1.811018	7.915674	-0.989611
33	1	0	2.128119	7.344366	-1.871865
34	8	0	-2.130498	0.063287	-3.377390
35	6	0	0.718520	8.020501	1.191059
36	1	0	0.212756	7.525268	2.030401
37	6	0	0.888786	-2.917279	-0.163830
38	6	0	-3.981434	3.268994	2.104074
39	1	0	-4.872293	3.843719	2.394955
40	6	0	1.632514	10.048485	0.184595
41	1	0	1.823482	11.129378	0.228253
42	6	0	3.033133	0.255141	-1.735137
43	1	0	2.756789	-0.792454	-1.542863
44	6	0	3.573682	2.945669	-2.118720
45	1	0	3.768611	4.013828	-2.269420
46	6	0	2.051845	9.300470	-0.934081
47	1	0	2.565460	9.798201	-1.767796
48	6	0	4.425801	1.989413	-2.701054
49	1	0	5.288323	2.311263	-3.301689
50	6	0	-0.428995	-3.458748	-0.160355
51	1	0	-0.547359	-4.546027	-0.166648

52	8	0	1.742530	-0.559434	3.487359
53	6	0	0.967189	9.403956	1.247081
54	1	0	0.643482	9.980614	2.124173
55	6	0	-2.944918	-3.333773	-0.120442
56	1	0	-2.929865	-4.431464	-0.110707
57	6	0	2.049458	-3.881261	-0.122523
58	1	0	1.796001	-4.946272	-0.205521
59	6	0	-4.105819	-2.631055	-0.137284
60	1	0	-4.022147	-1.531737	-0.158749
61	6	0	3.330747	-3.464088	0.038082
62	1	0	3.497935	-2.379309	0.138268
63	6	0	4.550856	-4.312472	0.111932
64	6	0	5.809792	-3.689256	0.323979
65	6	0	4.518384	-5.729041	-0.006633
66	6	0	7.018201	-4.419617	0.410711
67	1	0	5.866019	-2.597738	0.433606
68	6	0	5.700572	-6.476827	0.064614
69	1	0	3.563997	-6.247262	-0.160912
70	6	0	6.962169	-5.853919	0.252191
71	1	0	5.667034	-7.570686	-0.041406
72	6	0	-5.489975	-3.176009	-0.136224
73	6	0	-6.584482	-2.271747	-0.187613
74	6	0	-5.775234	-4.568530	-0.096445
75	6	0	-7.931669	-2.703180	-0.190258
76	1	0	-6.396033	-1.190562	-0.233052
77	6	0	-7.099728	-5.023896	-0.086899
78	1	0	-4.956321	-5.297697	-0.066134
79	6	0	-8.194756	-4.120983	-0.113012

80	1	0	-7.310848	-6.102009	-0.041754
81	8	0	8.199913	-3.629324	0.533738
82	8	0	-8.905040	-1.660321	-0.152305
83	8	0	8.167439	-6.602777	0.269285
84	1	0	7.840791	-7.571939	0.200561
85	8	0	-9.537091	-4.576646	-0.046574
86	1	0	-9.437808	-5.596759	-0.060270
87	6	0	9.215664	-4.287088	1.389414
88	1	0	8.929093	-4.226615	2.460686
89	1	0	9.352731	-5.351035	1.107718
90	1	0	10.153500	-3.721440	1.236407
91	6	0	-10.116397	-2.008953	-0.931744
92	1	0	-9.918581	-1.938818	-2.022323
93	1	0	-10.471180	-3.031694	-0.690372
94	1	0	-10.880551	-1.258397	-0.656716

Table S4: The DFT coordinates used for energy optimization of complex **3.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	2.414771	0.007187	0.023602
2	8	0	2.165652	-0.600781	-2.457075
3	8	0	4.401112	-1.188283	-0.286560
4	8	0	4.129766	1.333909	0.905540
5	8	0	2.981826	1.323025	-2.100822
6	7	0	-0.182099	-0.019767	-0.422622
7	6	0	1.369926	4.655292	-0.054366
8	1	0	1.902723	5.409481	0.056001
9	7	0	1.284897	-2.289677	-0.287397
10	8	0	1.242132	0.300399	2.244481
11	8	0	2.711187	-1.226757	2.253265
12	7	0	1.161707	2.292507	-0.025592
13	7	0	2.547875	0.505121	-2.924726
14	6	0	5.619573	-1.015341	0.019937
15	6	0	-0.130711	2.390840	-0.364954
16	7	0	1.848796	-0.597946	2.879891
17	6	0	-0.037543	-2.431010	-0.447951
18	6	0	-2.939833	-0.063189	-0.881856
19	6	0	6.075758	2.340863	1.757920
20	1	0	5.435925	3.022762	1.976290
21	1	0	6.742309	2.703731	1.170649
22	1	0	6.494893	2.026964	2.562511
23	6	0	-0.606401	-3.691338	-0.515817

24	1	0	-1.527255	-3.784492	-0.615214
25	6	0	-0.890846	1.128713	-0.507963
26	6	0	-2.257927	1.126025	-0.724783
27	1	0	-2.721010	1.931546	-0.764747
28	6	0	-0.845686	-1.182178	-0.554187
29	6	0	1.537788	-4.656357	-0.302602
30	1	0	2.099549	-5.395646	-0.254723
31	6	0	2.038986	-3.390812	-0.241114
32	1	0	2.959695	-3.287717	-0.162493
33	6	0	-2.208275	-1.234810	-0.798179
34	1	0	-2.631573	-2.057013	-0.904854
35	6	0	6.561441	-2.102999	-0.386401
36	1	0	6.071640	-2.802410	-0.825968
37	1	0	6.996387	-2.457252	0.392290
38	1	0	7.220037	-1.747393	-0.987446
39	8	0	2.474662	0.747677	-4.112470
40	6	0	5.377768	1.197918	1.079201
41	6	0	0.196938	-4.805603	-0.435542
42	1	0	-0.177732	-5.656208	-0.472418
43	6	0	1.873808	3.407652	0.130670
44	1	0	2.765340	3.326622	0.380901
45	6	0	-0.701386	3.637374	-0.570645
46	1	0	-1.595304	3.708605	-0.817950
47	6	0	0.060784	4.764279	-0.407417
48	1	0	-0.317159	5.604043	-0.538523
49	6	0	6.108918	0.097109	0.673636
50	1	0	7.019061	0.106826	0.858254
51	8	0	1.597606	-0.842770	4.036625

52	6	0	-4.452211	-0.098406	-1.170079
53	26	0	-5.939807	-0.059731	0.207217
54	6	0	-5.258125	-1.305557	-1.231397
55	6	0	-5.245559	1.025913	-1.410050
56	6	0	-6.584302	0.584593	-1.647039
57	6	0	-6.598301	-0.828623	-1.557287
58	6	0	-5.991998	-0.966954	2.053833
59	6	0	-5.145191	0.177785	2.085029
60	6	0	-5.931152	1.303009	1.734372
61	6	0	-7.252042	0.861072	1.470643
62	6	0	-7.289763	-0.547874	1.665015
63	1	0	-4.927940	-2.314181	-1.095177
64	1	0	-4.946247	1.927344	-1.414978
65	1	0	-7.331521	1.140279	-1.830832
66	1	0	-7.361647	-1.379515	-1.688815
67	1	0	-5.732487	-1.857859	2.258912
68	1	0	-4.220306	0.184767	2.300790
69	1	0	-5.624946	2.200733	1.684843
70	1	0	-7.982089	1.408544	1.210336
71	1	0	-8.047979	-1.108091	1.554105

Table S5: The DFT coordinates used for energy optimization of complex **4.**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	60	0	-0.489379	-0.051449	0.190361
2	8	0	-0.284099	-1.649826	2.187481
3	8	0	-2.576969	-1.099226	0.067774
4	8	0	-2.077839	1.658230	0.008672
5	8	0	-0.918897	0.309232	2.690677
6	7	0	2.096094	-0.475440	0.471672
7	6	0	0.985764	4.043718	2.128460
8	1	0	0.525174	4.817216	2.361723
9	7	0	0.422614	-2.355946	-0.521310
10	8	0	0.692908	1.036413	-1.762102
11	8	0	-0.912481	-0.222880	-2.334212
12	7	0	0.972061	1.896334	1.120743
13	7	0	-0.558623	-0.809135	3.085082
14	6	0	-3.775652	-0.714772	-0.086668
15	6	0	2.269918	1.738093	1.413504
16	7	0	0.001337	0.535145	-2.683661
17	6	0	1.726944	-2.659952	-0.491275
18	6	0	4.840259	-0.933057	0.750998
19	6	0	2.175888	-3.877703	-0.973109
20	1	0	3.084554	-4.079490	-0.961318
21	6	0	2.909557	0.471786	0.990952

22	6	0	4.271611	0.266495	1.127311
23	1	0	4.808176	0.941908	1.474907
24	6	0	2.648865	-1.638620	0.083971
25	6	0	-0.050288	-4.486905	-1.470385
26	1	0	-0.678951	-5.090831	-1.793603
27	6	0	-0.431345	-3.272662	-0.983564
28	1	0	-1.338819	-3.070473	-0.972355
29	6	0	4.001932	-1.900064	0.224708
30	1	0	4.347126	-2.724633	-0.035108
31	8	0	-0.456319	-1.086827	4.262941
32	6	0	-3.334054	1.710083	-0.150689
33	6	0	1.271476	-4.788179	-1.469551
34	1	0	1.565205	-5.605588	-1.802465
35	6	0	0.366432	3.030900	1.468636
36	1	0	-0.530177	3.134769	1.246567
37	6	0	2.955763	2.735834	2.088749
38	1	0	3.853815	2.624095	2.304017
39	6	0	2.301345	3.888087	2.437333
40	1	0	2.756862	4.563872	2.885722
41	6	0	-4.162580	0.604773	-0.202481
42	1	0	-5.068863	0.765300	-0.326659
43	8	0	0.221974	0.771102	-3.848441
44	6	0	-4.843904	-1.823387	-0.124203
45	1	0	-5.876304	-1.565418	-0.236016
46	6	0	-3.941224	3.120249	-0.270592
47	1	0	-4.997750	3.237190	-0.392978
48	6	0	-4.480876	-3.124576	-0.016104
49	1	0	-3.448476	-3.382545	0.095710

50	6	0	-3.141992	4.213591	-0.221631
51	1	0	-2.085467	4.096649	-0.099245
52	6	0	-3.749162	5.623757	-0.341534
53	6	0	-2.921896	6.746031	-0.290508
54	6	0	-5.126088	5.779044	-0.501253
55	6	0	-3.471593	8.023290	-0.398508
56	1	0	-1.836481	6.623298	-0.163809
57	6	0	-5.676000	7.056588	-0.610289
58	1	0	-5.778229	4.894619	-0.541668
59	6	0	-4.849048	8.178655	-0.558809
60	1	0	-6.761634	7.178703	-0.736626
61	6	0	-5.549128	-4.233191	-0.053639
62	6	0	-5.170035	-5.571206	0.058065
63	6	0	-6.895655	-3.899681	-0.199194
64	6	0	-6.137253	-6.575455	0.023533
65	1	0	-4.108306	-5.833853	0.172034
66	6	0	-7.863385	-4.904062	-0.232765
67	1	0	-7.194632	-2.845158	-0.287069
68	6	0	-7.484413	-6.241803	-0.121570
69	1	0	-8.925025	-4.640781	-0.347126
70	8	0	-2.623843	9.173681	-0.345401
71	8	0	-5.748716	-7.946958	0.137199
72	8	0	-5.412348	9.488358	-0.669589
73	1	0	-6.314414	9.423043	-0.991478
74	8	0	-8.475878	-7.271682	-0.156865
75	1	0	-9.338666	-6.892280	0.025481
76	6	0	-3.411414	10.355230	-0.514434
77	1	0	-3.925910	10.309891	-1.451525

78	1	0	-4.124003	10.425658	0.280649
79	1	0	-2.773631	11.214236	-0.498907
80	6	0	-6.913366	-8.776419	0.115244
81	1	0	-7.563283	-8.500041	0.919062
82	1	0	-7.424242	-8.649335	-0.816290
83	1	0	-6.624026	-9.800527	0.226531
84	6	0	6.344336	-1.209411	0.932603
85	26	0	7.807522	-0.834521	-0.420144
86	6	0	7.018161	-2.432853	0.533075
87	6	0	7.256098	-0.319504	1.505172
88	6	0	8.543630	-0.940323	1.507481
89	6	0	8.406019	-2.228384	0.935300
90	6	0	7.736242	-1.042503	-2.466466
91	6	0	7.015562	0.116112	-2.058162
92	6	0	7.921678	0.969019	-1.381162
93	6	0	9.191781	0.340003	-1.353100
94	6	0	9.076694	-0.909889	-2.023067
95	1	0	6.604863	-3.244091	-0.029044
96	1	0	7.054410	0.547799	1.835771
97	1	0	9.348269	-0.556804	1.833632
98	1	0	9.108301	-2.860206	0.830042
99	1	0	7.380555	-1.777400	-2.952806
100	1	0	6.093634	0.285296	-2.211264
101	1	0	7.713387	1.817986	-1.009688
102	1	0	9.979581	0.690841	-0.957198
103	1	0	9.772587	-1.542743	-2.150607

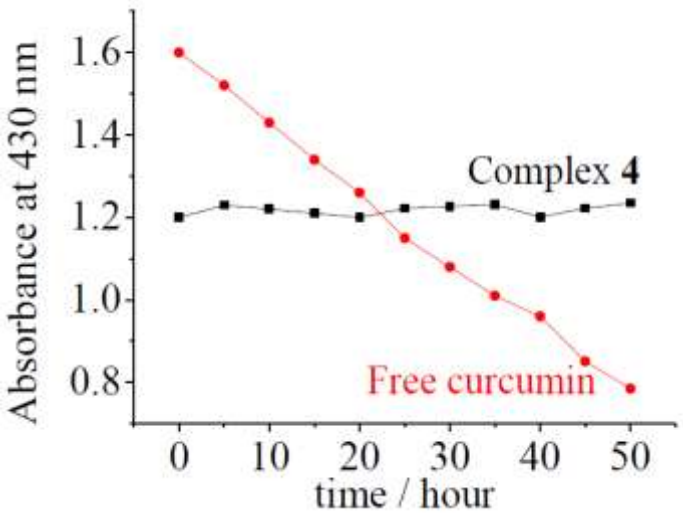

Fig. S15. Absorption spectral plots of complex **4** in DMSO–10% DMEM medium (1:99 v/v, pH = 7.4, 37 °C). The spectra were recorded after keeping the solution at 37 °C and recorded at different time intervals. The spectral data indicate the stability of the complex in the cellular medium up to 48 hours. The band at 430 nm characteristic of the curcumin moiety in the complex was monitored.

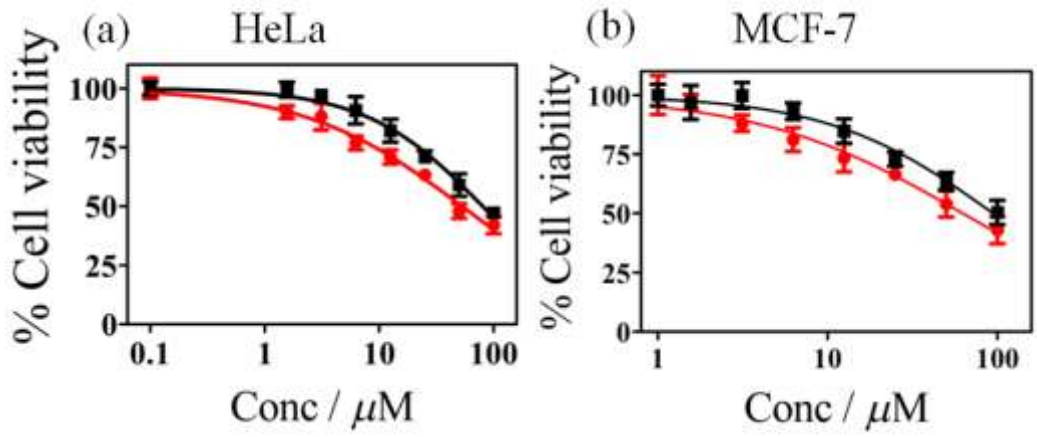

Fig. S16. Diagrams showing the cytotoxicity of complex **1** in (a) HeLa and (b) MCF-7 cells upon photo–irradiation with visible light (400–700 nm, 10 J cm^{-2}, red bars) and in dark (black bars) as determined from MTT assay.

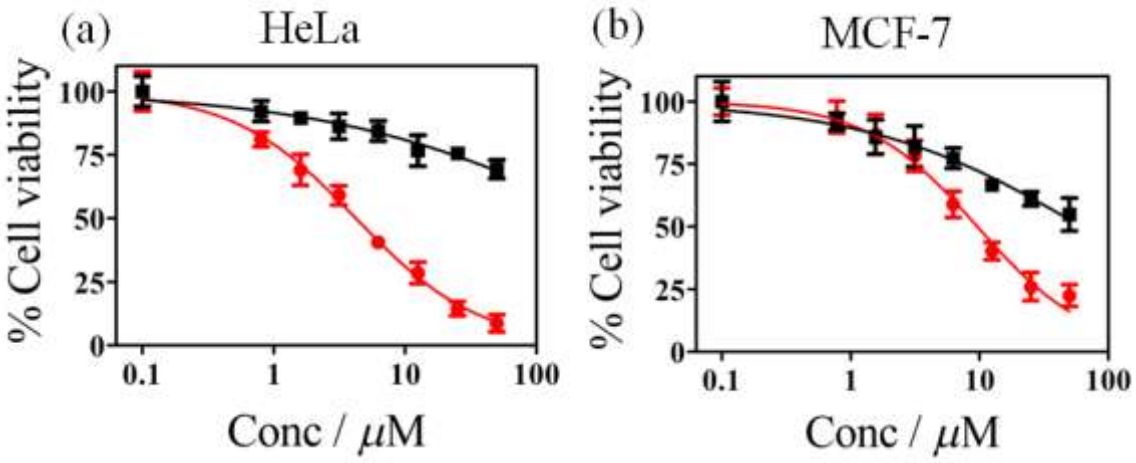

Fig. S17. Diagrams showing the cytotoxicity of complex **2** in (a) HeLa and (b) MCF-7 cells upon photo–irradiation with visible light (400–700 nm, 10 J cm^{-2}, red bars) and in dark (black bars) as determined from MTT assay.

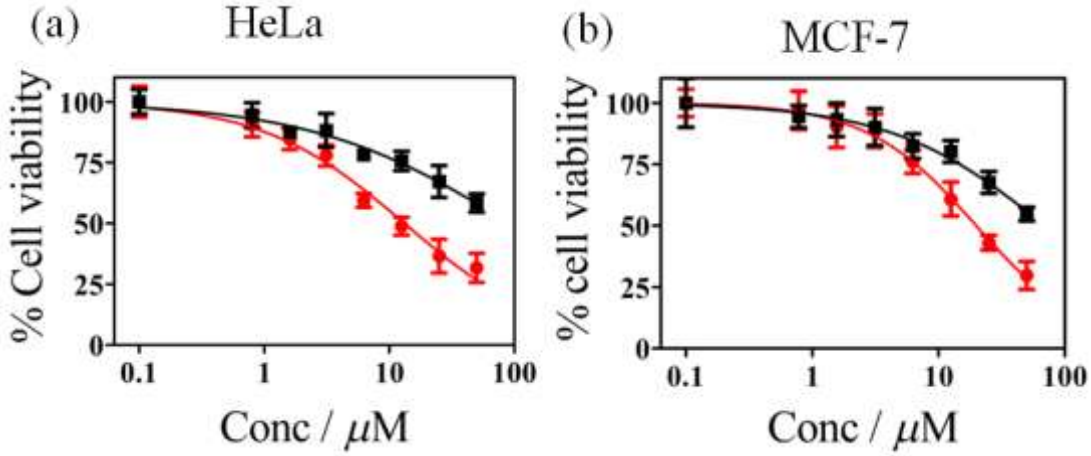

Fig. S18. Diagrams showing the cytotoxicity of complex **3** in (a) HeLa and (b) MCF-7 cells upon photo–irradiation with visible light (400–700 nm, 10 J cm^{-2}, red bars) and in dark (black bars) as determined from MTT assay.

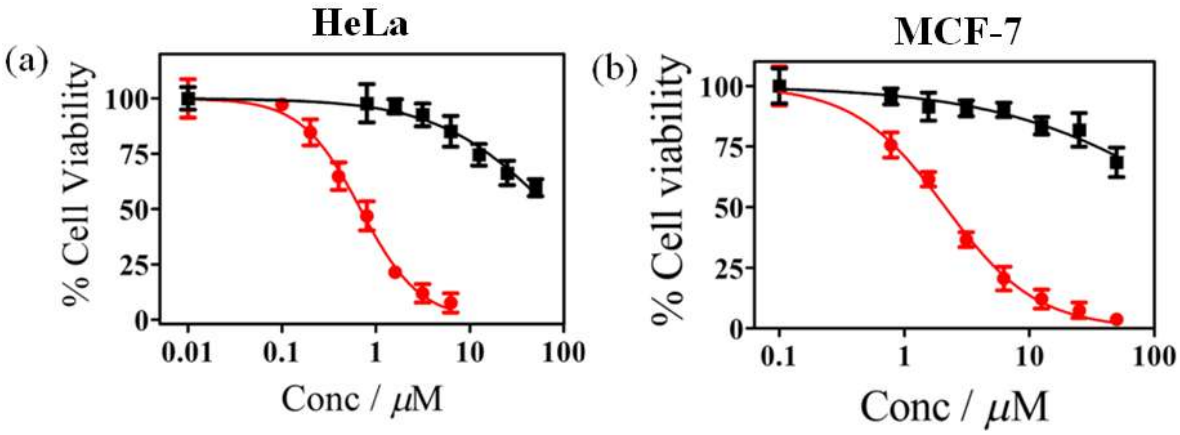

Fig. S19. Diagrams showing the cytotoxicity of complex **4** in (a) HeLa and (b) MCF-7 cells upon photo–irradiation with visible light (400–700 nm, 10 J cm^{-2}, red bars) and in dark (black bars) as determined from MTT assay.

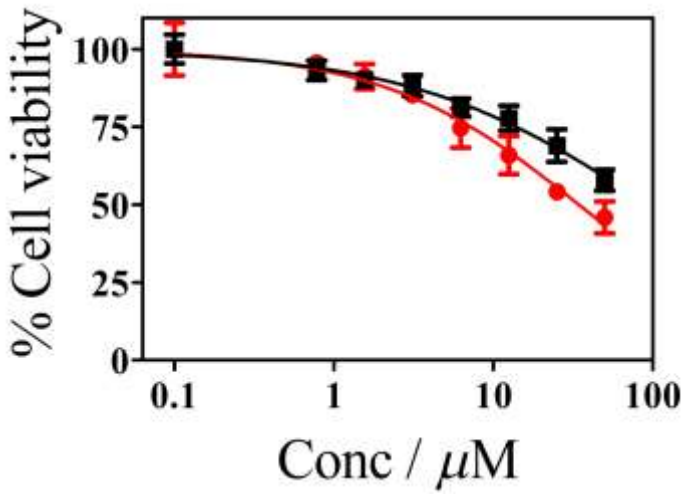

Fig. S20. Diagrams showing the cytotoxicity of complex **4** in MCF-10A epithelial cells upon photo–irradiation with visible light (400–700 nm, 10 J cm^{-2}, red bars) and in dark (black bars) as determined from MTT assay.

Table S6. Photo-induced SC DNA (0.2 μg, 33.3 μM) cleavage data[a] at 454 nm

Sl. No.	Reaction condition	[Complex]/ μM	*t*/ h	%NC
1.	DNA control	-	2	2
2.	DNA + Hcurc (in dark)	10	-	23
3.	DNA + Hcurc (in light)	10	2	45
4.	DNA + complex **4** (dark)	10	-	7
5.	DNA + complex **1**	10	2	13
6.	DNA + complex **2**	10	2	76
7.	DNA + complex **3**	10	2	25
8.	DNA + complex **4**	10	2	85

[a] Exposure time, *t*. SC and NC are supercoiled and nicked circular forms of pUC19 DNA. Additional pUC19 DNA cleavage data for the ligands (10 μM) and metal salt (10 μM) giving %NC for 2 h photo-exposure time: Ph-tpy, 4%; Fc-tpy, 18%; $Nd(NO_3)_3$, 15%.

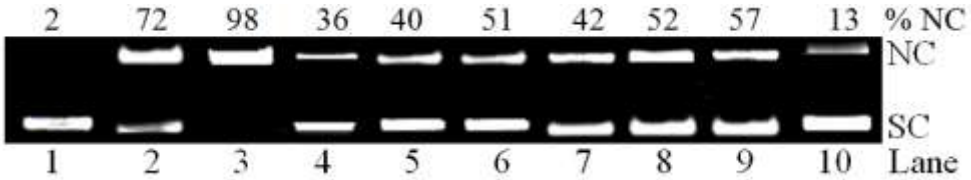

Fig. S21. Gel electrophoresis diagram showing the cleavage of SC pUC19 DNA (0.2 μg, 30 μM) by complex **2** in the presence of various additives in Tris-HCl buffer containing 10% DMF. The complex concentration and exposure time are 10 μM and 2 h, respectively. The additive concentrations/quantities are: sodium azide, 0.5 mM; KI, 0.5 mM; TEMP, 0.5 mM; DABCO, 0.5 mM; D_2O, 16 μL; DMSO, 4 μL; catalase, 4 units; SOD, 4 units.

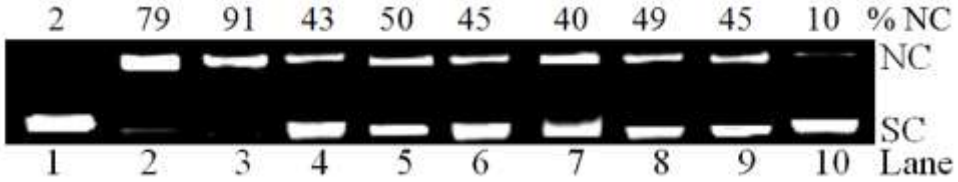

Fig. S22. Gel electrophoresis diagram showing the cleavage of SC pUC19 DNA (0.2 μg, 30 μM) by complex **4** in the presence of various additives in Tris-HCl buffer containing 10% DMF. The complex concentration and exposure time are 10 μM and 2 h, respectively. The additive concentrations/quantities are: sodium azide, 0.5 mM; KI, 0.5 mM; TEMP, 0.5 mM; DABCO, 0.5 mM; D_2O, 16 μL; DMSO, 4 μL; catalase, 4 units; SOD, 4 units.