Electronic Supporting Information (ESI†)

for

Novel mitochondria targeted copper(II) complexes of ferrocenyl terpyridine and anticancer active 8-hydroxyquinolines showing remarkable cytotoxicity, DNA and protein binding affinity

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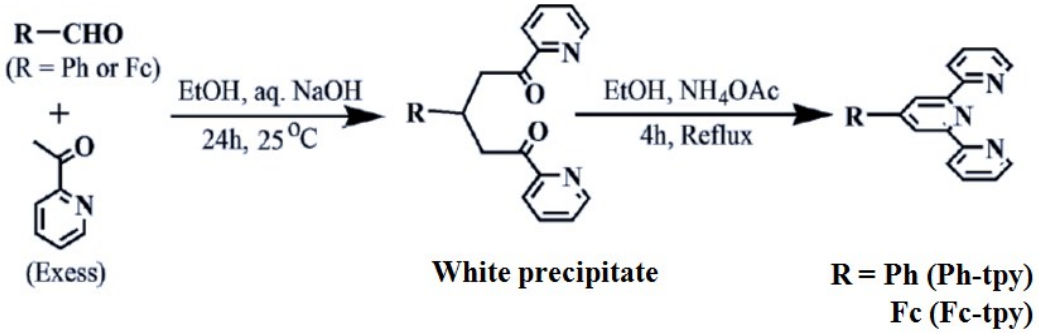

Fig. S1: Synthetic scheme for the preparation of Ph-tpy and Fc-tpy ligands.

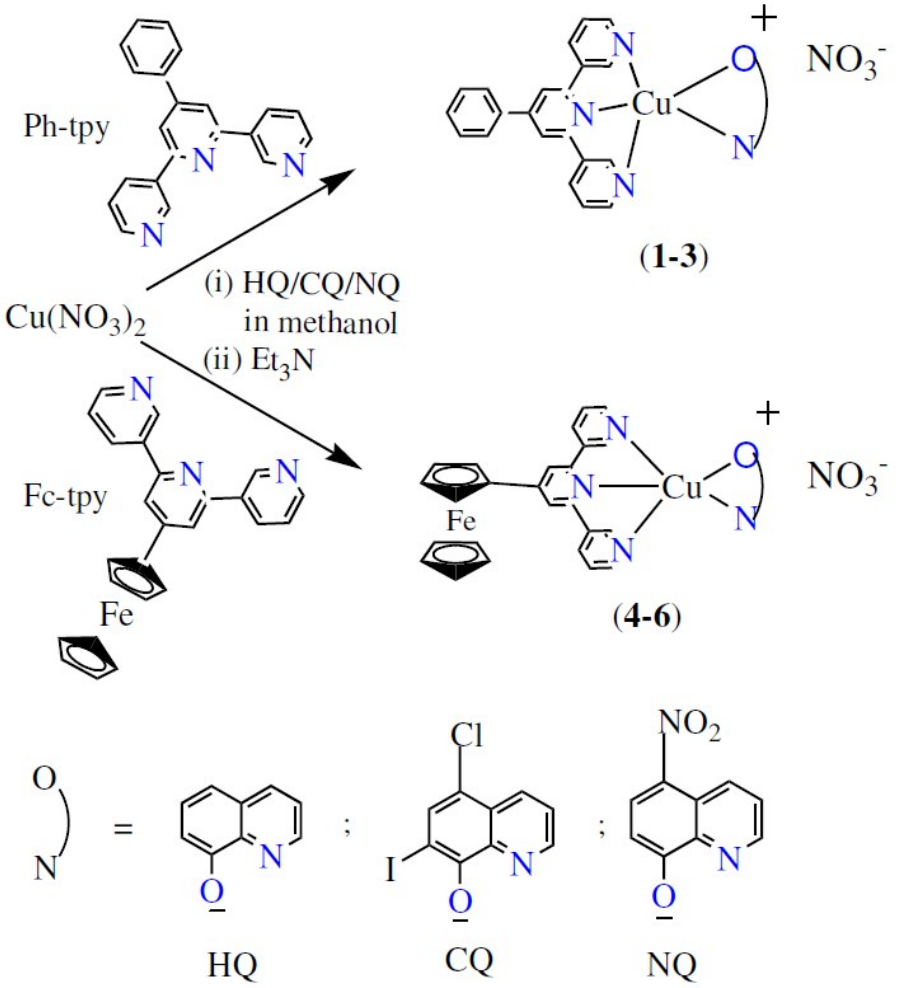

Fig. S2: Synthetic scheme for the preparation of the complexes **1-6**.

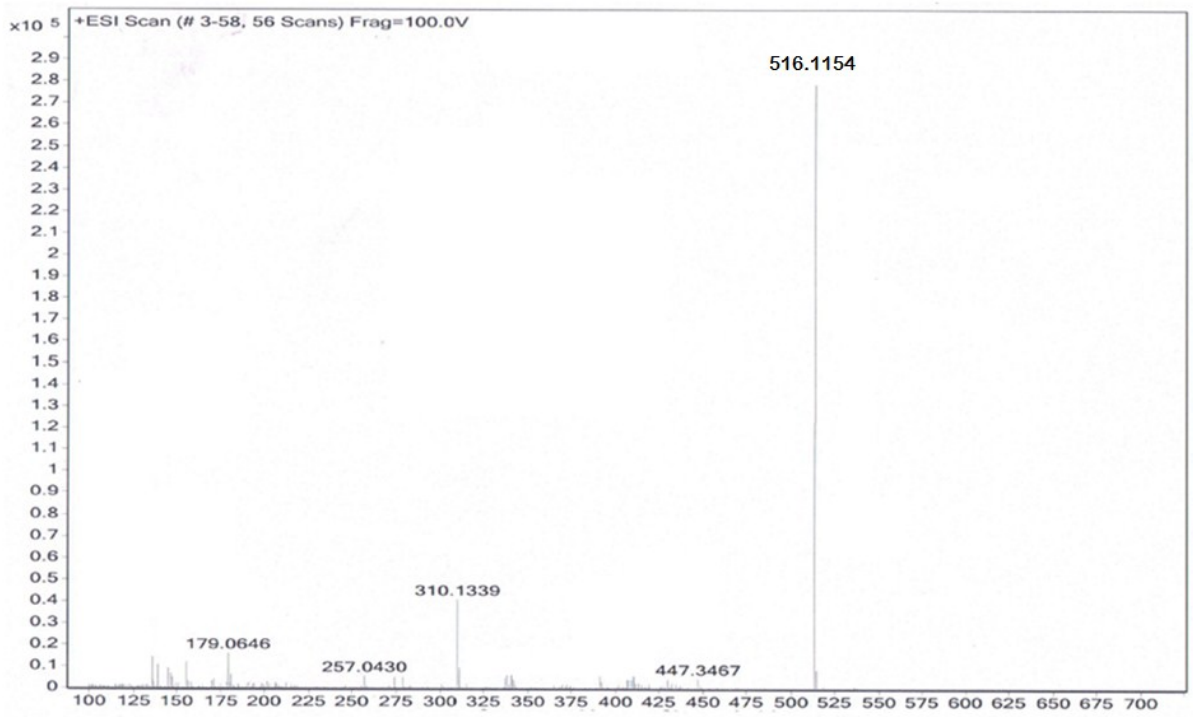

Fig. S3. The ESI-MS spectrum of complex [Cu(Ph-tpy)(HQ)]NO_3 (**1**) showing the prominent $[M–(NO_3^-)]^+$ peak at *m*/*z* = 516.1154. The peak at 310.1339 corresponds to M +1 species for the Ph-tpy ligand.

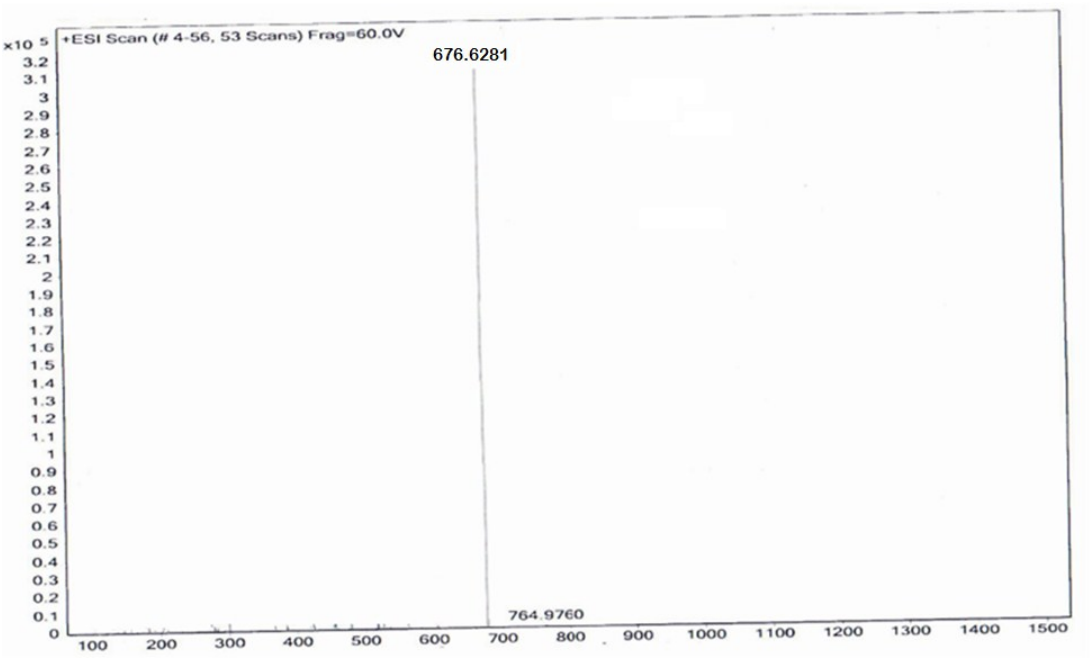

Fig. S4. The ESI-MS spectrum of the complex [Cu(Ph-tpy)(CQ)]NO_3 (**2**) showing the prominent $[M–(NO_3^-)]^+$ peak at m/z = 676.6281

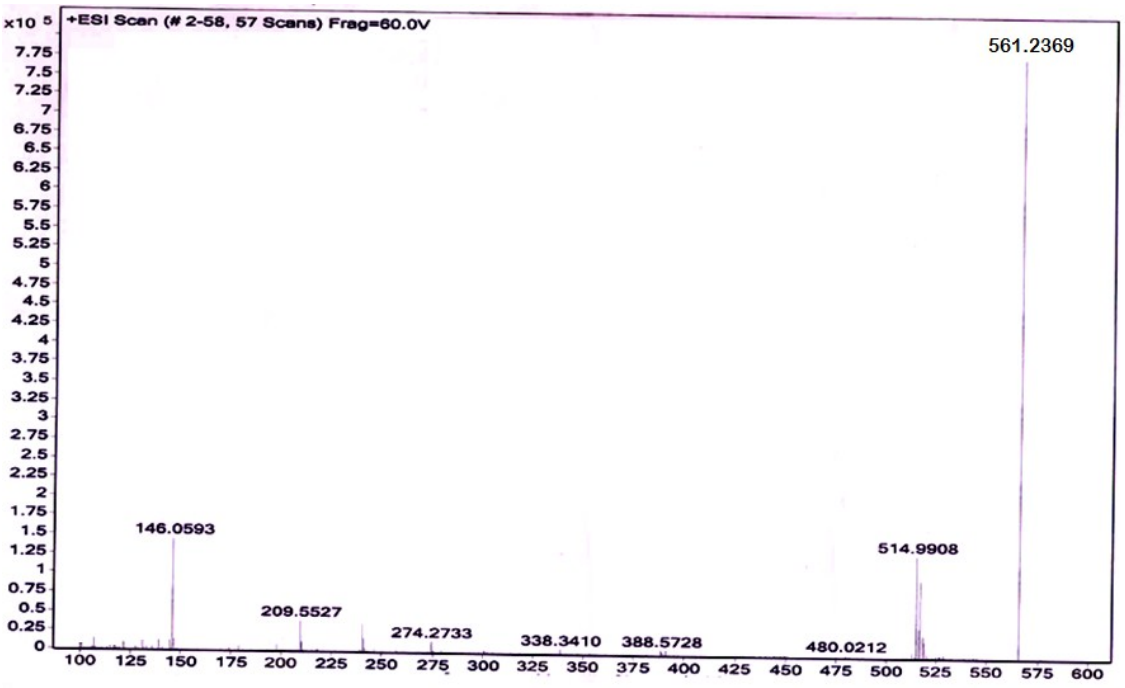

Fig. S5. The ESI-MS spectrum of the complex [Cu(Ph-tpy)(NQ)]NO_3 (**3**) showing the prominent $[M–(NO_3^-)]^+$ peak at m/z = 561.2369.

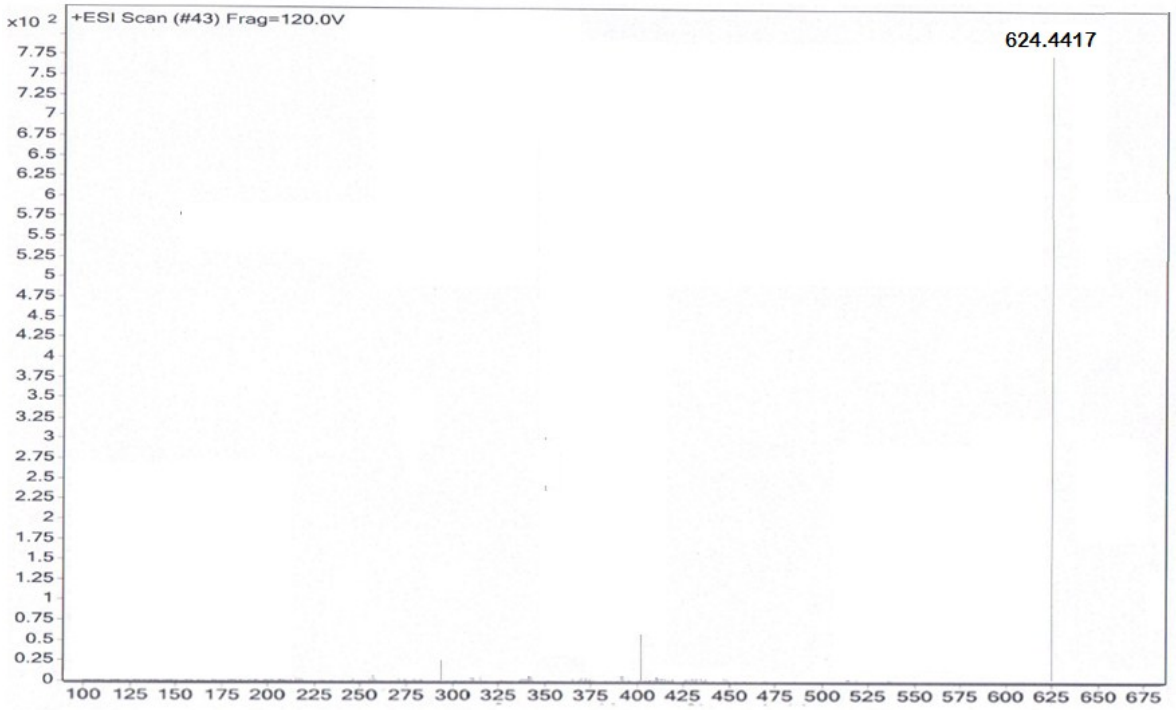

Fig. S6. The ESI-MS spectrum of the complex $[Cu(Fc\text{-}tpy)(HQ)]NO_3$ (**4**) showing the prominent $[M–(NO_3^-)]^+$ peak at m/z = 624.4417.

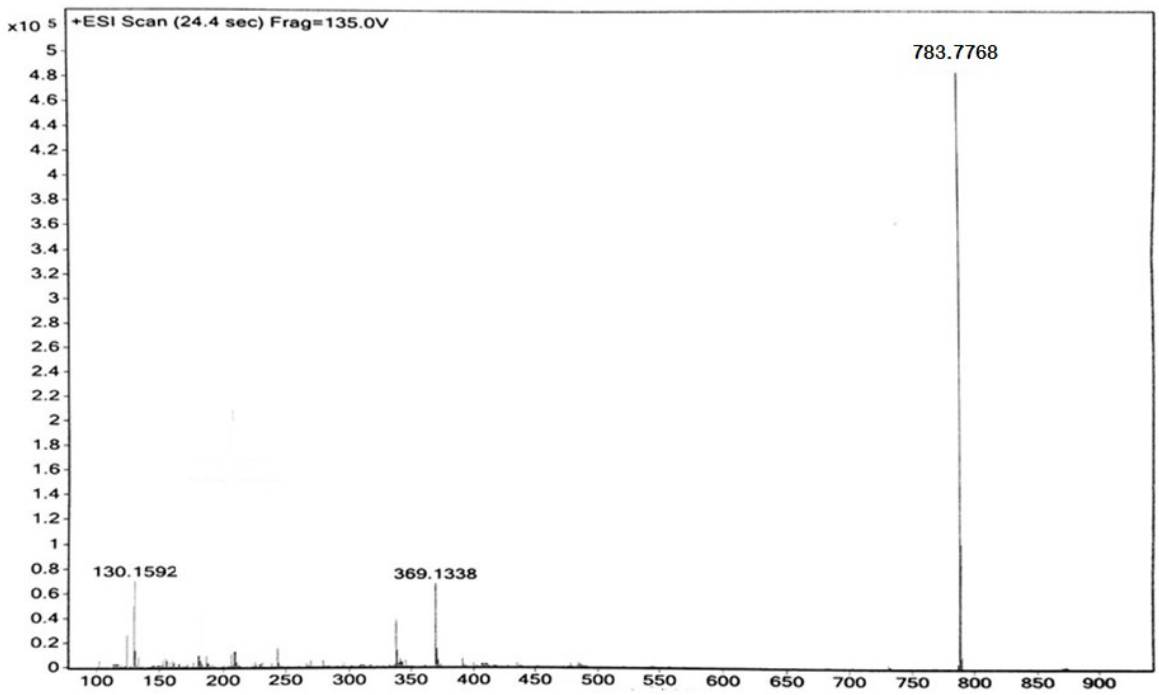

Fig. S7. The ESI-MS spectrum of the complex [Cu(Fc-tpy)(CQ)]NO_3 (**5**) showing the prominent $[M–(NO_3^-)]^+$ peak at m/z = 783.7768.

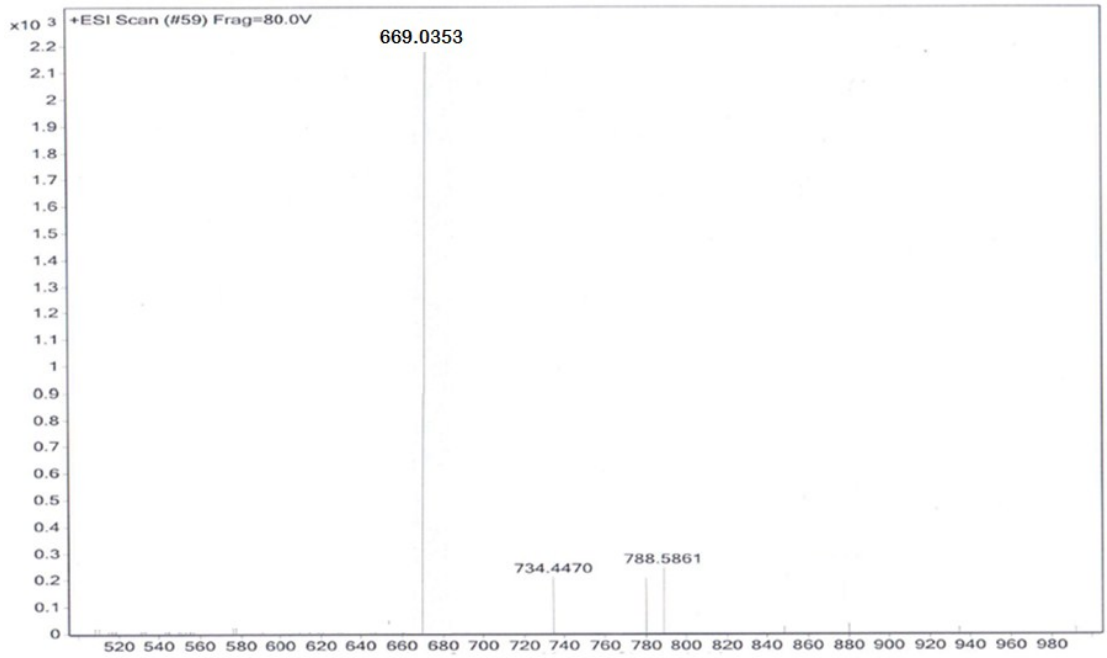

Fig. S8. The ESI-MS spectrum of the complex $[Cu(Fc\text{-}tpy)(NQ)]NO_3$ (**6**) showing the prominent $[M–(NO_3^-)]^+$ peak at m/z = 669.0353.

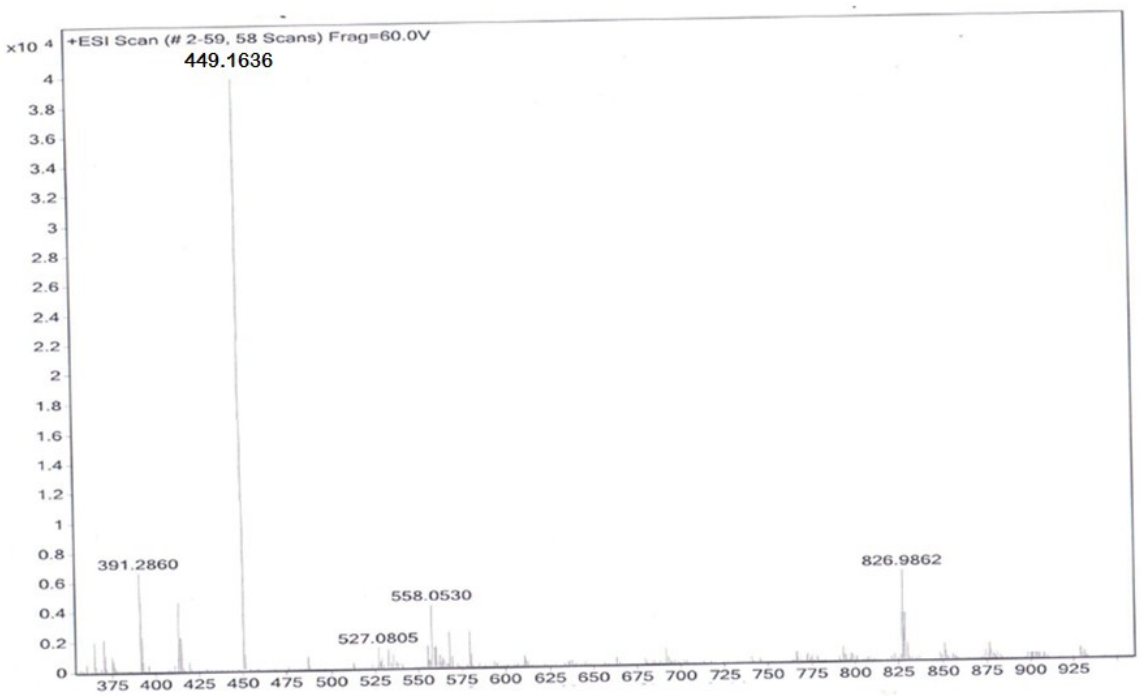

Fig. S9. The ESI-MS spectrum of the complex $[Cu(Fc\text{-}tpy)_2](ClO_4)_2$ (**7**) showing the prominent $[M–2(ClO_4^-)]^{2+}$ peak at m/z = 449.1636.

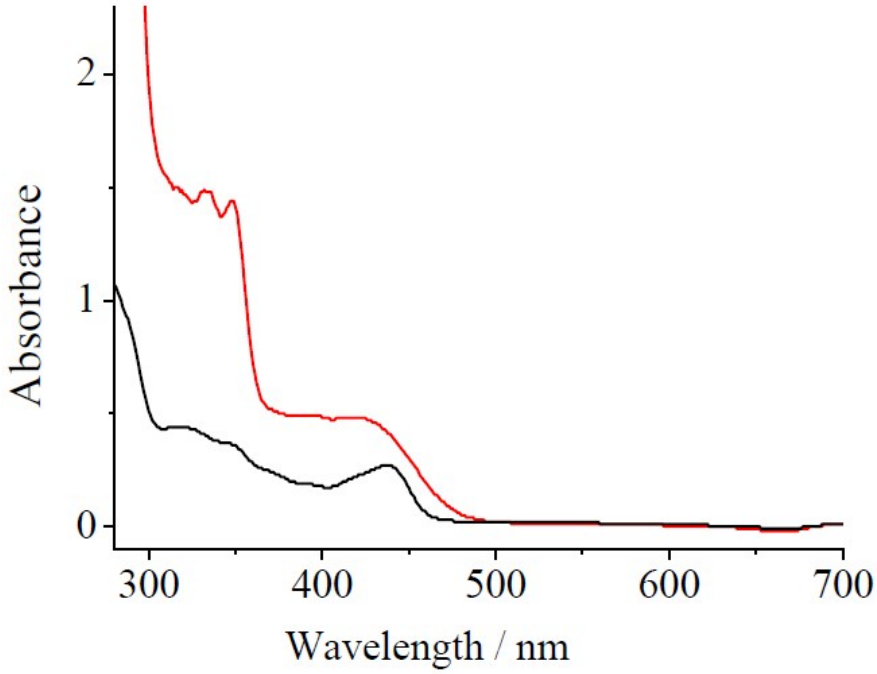

Fig. S10. The electronic absorption spectra of complexes **2** (red) and **3** (black) recorded in DMF.

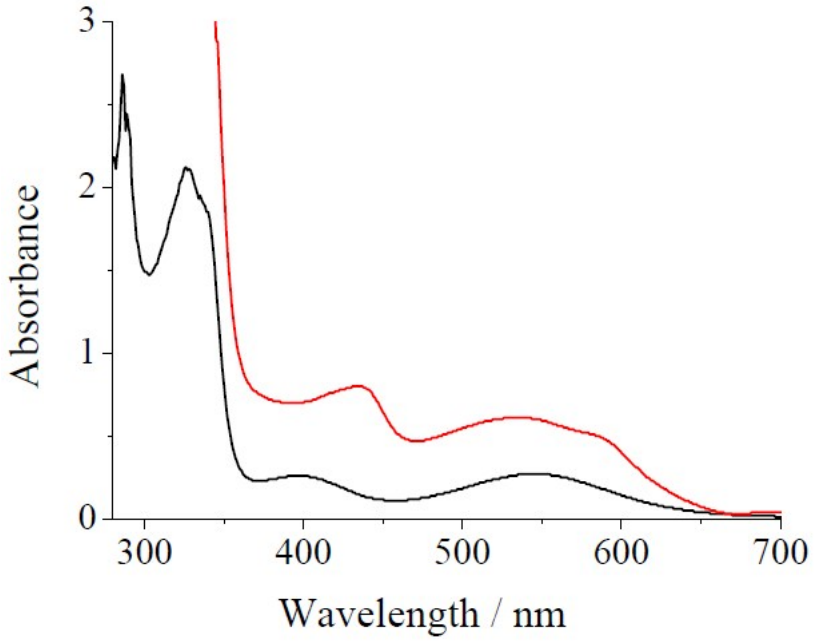

Fig. S11. The electronic absorption spectra of complexes **4** (black) and **6** (red) recorded in DMF.

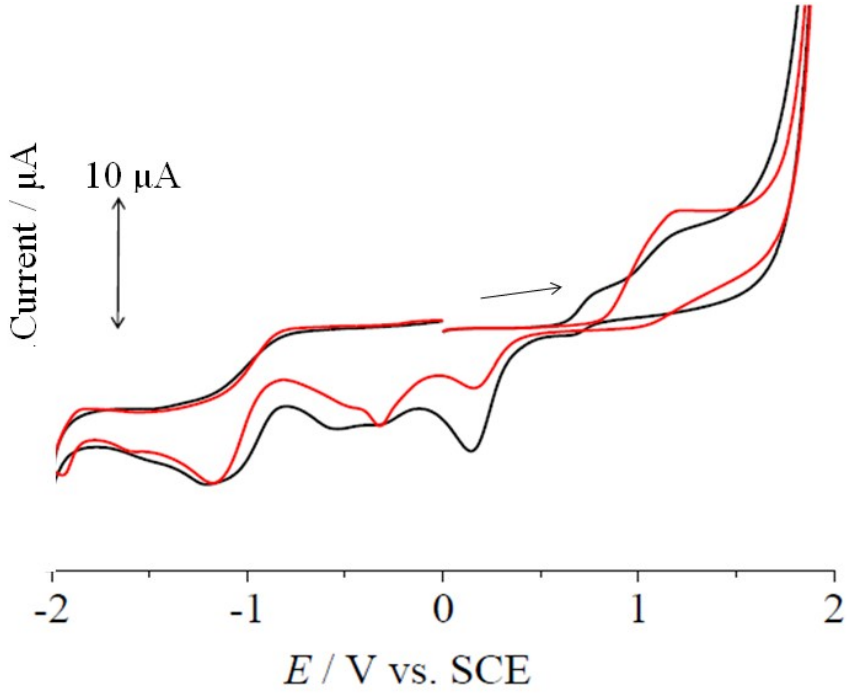

Fig. S12. Cyclic voltammograms of complexes **1** (red) and **4** (black) recorded in DMF in the presence of 0.1 M TBAP as supporting electrolyte.

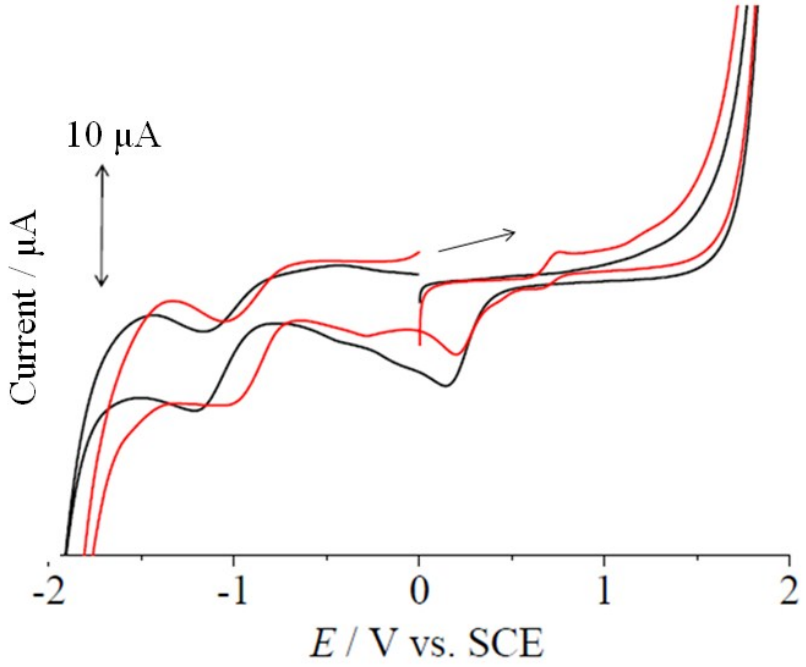

Fig. S13. Cyclic voltammograms of complexes **3** (black) and **6** (red curve) recorded in DMF in the presence of 0.1 M TBAP as supporting electrolyte.

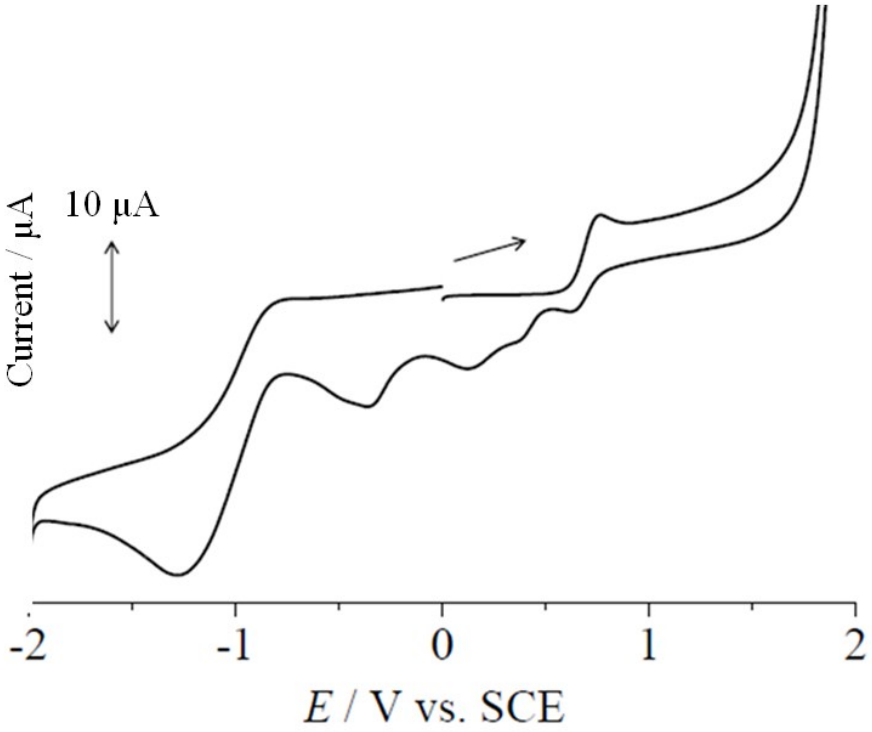

Fig. S14. Cyclic voltammograms of complex **7** recorded in DMF in the presence of 0.1 M TBAP as supporting electrolyte.

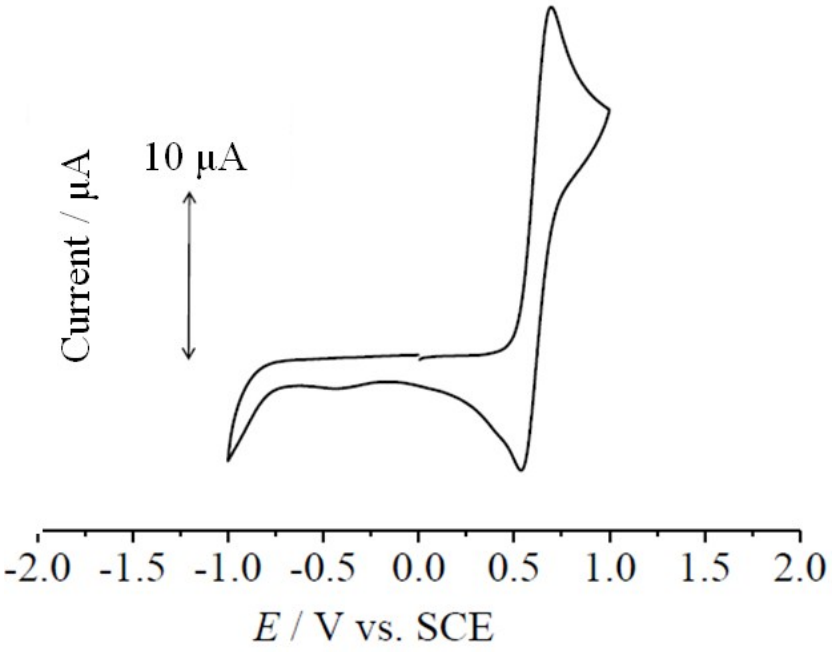

Fig. S15. Cyclic voltammograms of the free Fc-tpy ligand recorded in DMF in the presence of 0.1 M TBAP as supporting electrolyte.

Table S1. Selected bond distances (Å) and angles (°) for the complex [Fe(Fc-tpy)$_2$](NO_3)(PF_6).2H_2O (**7** as $NO_3^-PF_6^-$ salt) with estimated standard deviations (esd) in the parentheses.

Cu(1)-N(1A)	2.180(3)	N(2A)-Cu(1)-N(2B)	175.11(15)
Cu(1)-N(1B)	2.180(3)	N(2A)-Cu(1)-N(3B)	99.51(10)
Cu(1)-N(2A)	1.973(3)	N(1B)-Cu(1)-N(3A)	93.87(11)
Cu(1)-N(2B)	1.973(3)	N(2B)-Cu(1)-N(3A)	99.51(10)
Cu(1)-N(3A)	2.182(3)	N(3B)-Cu(1)-N(3A)	95.63(15)
Cu(1)-N(3B)	2.182(3)	N(1A)-Cu(1)-N(2A)	77.60(10)
N(1A)-Cu(1)-N(1B)	87.84(16)	N(1A)-Cu(1)-N(3A)	154.15(10)
N(1A)-Cu(1)-N(2B)	106.03(11)	N(2A)-Cu(1)-N(3A)	77.14(10)
N(1A)-Cu(1)-N(3B)	93.87(11)	N(1B)-Cu(1)-N(2B)	77.60(10)
N(2A)-Cu(1)-N(1B)	106.03(11)	N(1B)-Cu(1)-N(3B)	154.15(10)
		N(2B)-Cu(1)-N(3B)	77.14(10)

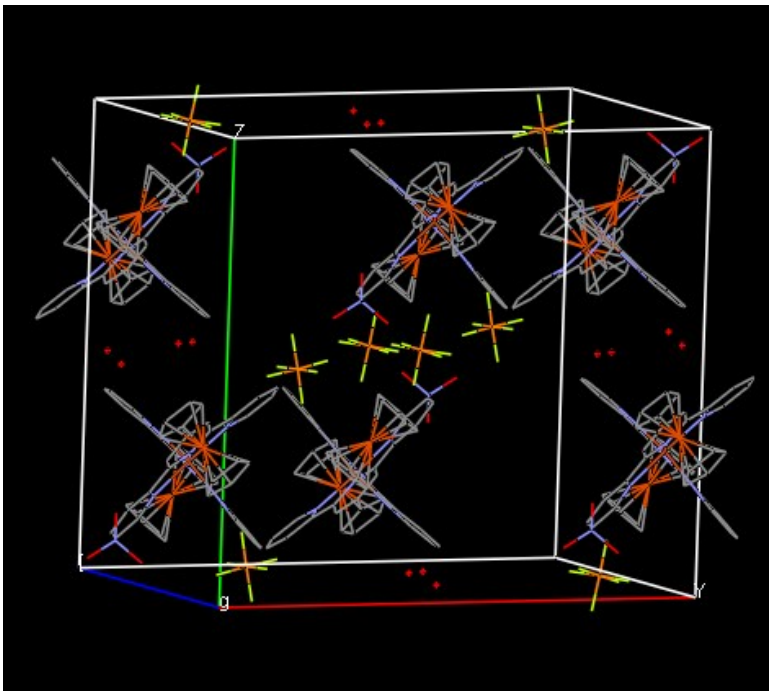

Fig. S16. The unit cell packing diagram for complex **7** (as $NO_3^-PF_6^-$ salt) in the solid state.

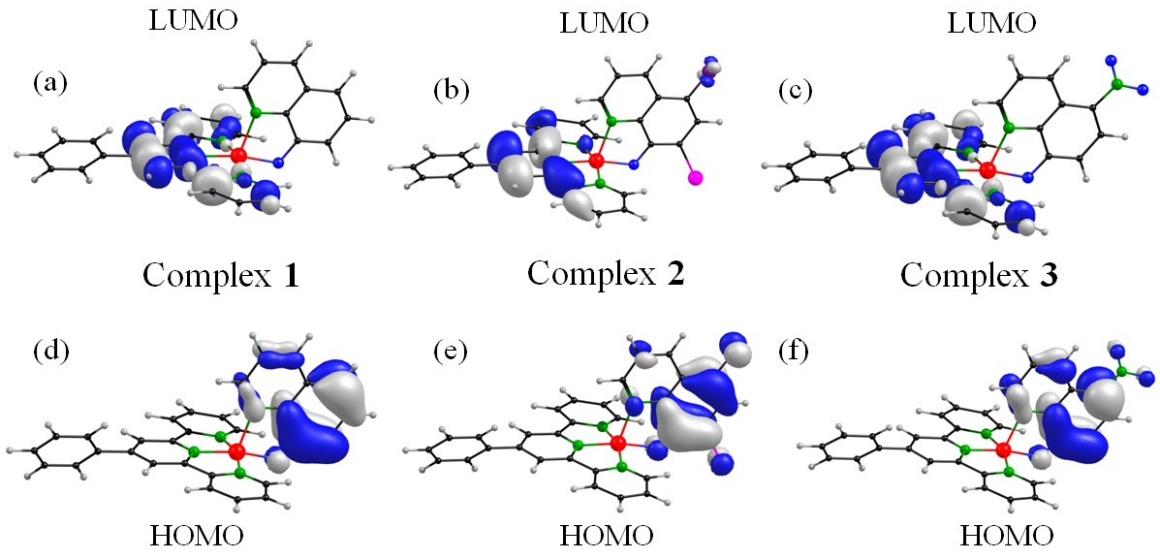

Fig. S17. The HOMOs and LUMOs of the complexes **1-3** corresponding to their DFT optimized structures.

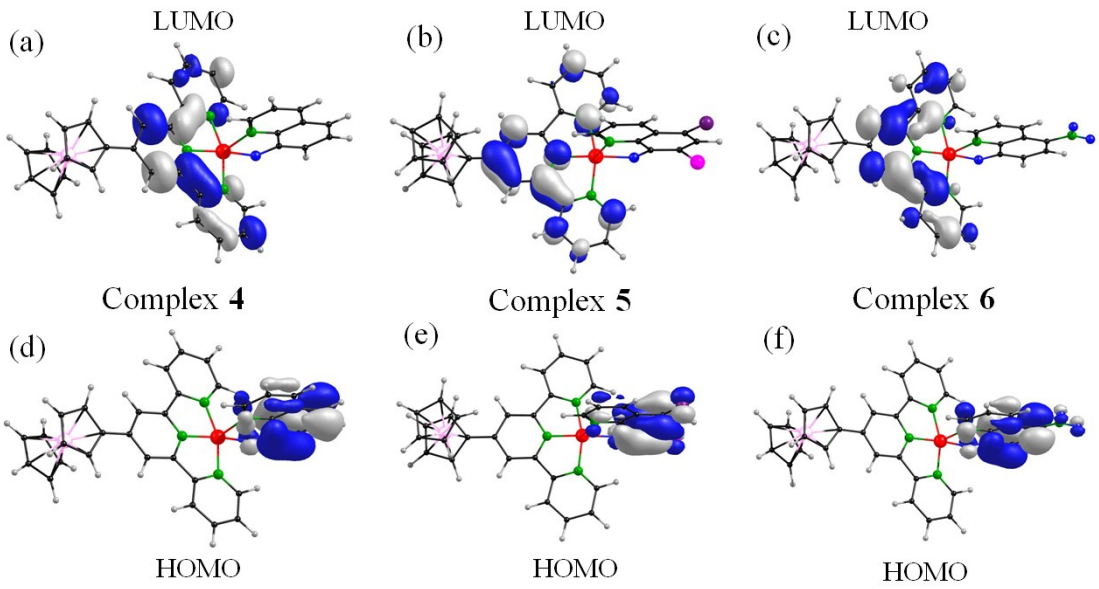

Fig. S18. The HOMOs and LUMOs of the complexes **4-6** corresponding to their DFT optimized structures.

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

Centre No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.053684	-4.632261	-0.981229
2	6	0	-0.917142	-3.660626	-0.667237
3	6	0	-0.544738	-2.318603	-0.677071
4	7	0	0.752526	-1.910206	-0.979804
5	6	0	1.669377	-2.859011	-1.283378
6	6	0	1.348146	-4.234580	-1.293599
7	6	0	-3.532526	-0.008604	0.062614
8	6	0	-2.844841	1.219731	-0.041925
9	6	0	-1.473685	1.202618	-0.313871
10	7	0	-0.808648	0.014846	-0.467688
11	6	0	-1.469188	-1.183329	-0.396277
12	6	0	-2.839416	-1.224434	-0.122700
13	6	0	-0.926607	3.694573	-0.393171
14	6	0	0.042048	4.689394	-0.632358
15	6	0	1.336653	4.319489	-0.976616
16	6	0	1.660590	2.947843	-1.072262
17	7	0	0.745961	1.976677	-0.841437
18	6	0	-0.551913	2.358067	-0.507677
19	6	0	5.099383	0.041111	-0.931791
20	6	0	3.744733	0.027480	-0.590771
21	6	0	3.372771	-0.021587	0.814293
22	6	0	4.385200	-0.054703	1.813541
23	6	0	5.746761	-0.039317	1.421612
24	6	0	6.080961	0.007601	0.076458
25	7	0	2.010508	-0.033301	1.103155

26	6	0	1.653888	-0.078042	2.391451
27	6	0	2.604316	-0.113770	3.463437
28	6	0	3.946965	-0.102356	3.180119
29	8	0	2.795951	0.057556	-1.495659
30	29	0	1.057035	0.030344	-0.819630
31	6	0	-4.979200	-0.022033	0.356695
32	6	0	-5.469216	-0.777173	1.434981
33	6	0	-6.838178	-0.783756	1.712522
34	6	0	-7.721070	-0.048221	0.914294
35	6	0	-7.233757	0.700086	-0.162737
36	6	0	-5.865197	0.719495	-0.442065
37	1	0	-0.219295	-5.692691	-0.979188
38	1	0	-1.937203	-3.964106	-0.425275
39	1	0	2.688882	-2.502496	-1.529472
40	1	0	2.119195	-4.968393	-1.546223
41	1	0	-3.383998	2.160042	0.094312
42	1	0	-3.378241	-2.173083	-0.065903
43	1	0	-1.946192	3.976434	-0.124523
44	1	0	-0.232589	5.745967	-0.547193
45	1	0	2.105950	5.072083	-1.173089
46	1	0	2.680616	2.613319	-1.345572
47	1	0	5.384717	0.077793	-1.980428
48	1	0	6.522633	-0.064485	2.183213
49	1	0	7.133124	0.019352	-0.219870
50	1	0	0.583992	-0.086927	2.623027
51	1	0	2.240067	-0.149365	4.489742
52	1	0	4.696522	-0.128668	3.973439
53	1	0	-4.786367	-1.347683	2.063452

54	1	0	-7.220142	-1.364421	2.554025
55	1	0	-8.791067	-0.058448	1.131847
56	1	0	-7.924633	1.269996	-0.786637
57	1	0	-5.492820	1.298780	-1.286417

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

Centre No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.100717	-4.530578	-1.268121
2	6	0	-2.095654	-3.588481	-0.937633
3	6	0	-1.722827	-2.258423	-0.763509
4	7	0	-0.401036	-1.835111	-0.896407
5	6	0	0.538521	-2.753393	-1.223456
6	6	0	0.216930	-4.115440	-1.416974
7	6	0	-4.759782	0.004869	-0.071756
8	6	0	-4.061058	1.229806	0.002242
9	6	0	-2.671463	1.222520	-0.147130
10	7	0	-2.001383	0.045140	-0.352048
11	6	0	-2.668189	-1.147476	-0.454894
12	6	0	-4.057246	-1.196931	-0.309382
13	6	0	-2.103338	3.705528	0.030085
14	6	0	-1.110296	4.703221	-0.041332
15	6	0	0.207714	4.344425	-0.295955
16	6	0	0.531733	2.980048	-0.467770
17	7	0	-0.405935	2.006294	-0.393323
18	6	0	-1.728326	2.377343	-0.153473
19	6	0	3.925381	0.022718	-0.167624
20	6	0	2.538209	0.001170	0.013056
21	6	0	2.023507	-0.172092	1.367617
22	6	0	2.913104	-0.313305	2.467842
23	6	0	4.310181	-0.280492	2.202347
24	6	0	4.806363	-0.116763	0.917362
25	7	0	0.638460	-0.188210	1.498505

26	6	0	0.137510	-0.345050	2.731352
27	6	0	0.959618	-0.493612	3.892216
28	6	0	2.328800	-0.478390	3.764662
29	8	0	1.694863	0.128284	-0.969687
30	29	0	-0.116699	0.068193	-0.511652
31	6	0	-6.226715	-0.018639	0.089812
32	6	0	-6.815146	-0.872742	1.037285
33	6	0	-8.203440	-0.888805	1.190004
34	6	0	-9.007855	-0.064048	0.395976
35	6	0	-8.422483	0.783077	-0.551238
36	6	0	-7.034352	0.812174	-0.704366
37	1	0	-1.374314	-5.581716	-1.408986
38	1	0	-3.134283	-3.905629	-0.826908
39	1	0	1.577304	-2.383150	-1.341035
40	1	0	1.007168	-4.824902	-1.681871
41	1	0	-4.607620	2.159385	0.178423
42	1	0	-4.603104	-2.139928	-0.391680
43	1	0	-3.141865	3.980090	0.224138
44	1	0	-1.385513	5.753742	0.100932
45	1	0	0.996474	5.100076	-0.365373
46	1	0	1.571044	2.655723	-0.678590
47	1	0	5.889905	-0.095876	0.745973
48	1	0	-0.952772	-0.357560	2.837087
49	1	0	0.484263	-0.617209	4.865917
50	1	0	2.978561	-0.590293	4.638168
51	1	0	-6.194257	-1.513391	1.662438
52	1	0	-8.662137	-1.546701	1.930379
53	1	0	-10.093212	-0.081827	0.515414

54	1	0	-9.052106	1.422717	-1.172537
55	1	0	-6.585434	1.468920	-1.448973
56	53	0	4.687751	0.267975	-2.097839
57	17	0	5.409036	-0.448191	3.508082

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

Centre No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.591927	-4.618519	-1.164998
2	6	0	-1.533422	-3.654211	-0.753388
3	6	0	-1.169518	-2.310548	-0.783909
4	7	0	0.093260	-1.891426	-1.200724
5	6	0	0.980994	-2.833826	-1.598582
6	6	0	0.665929	-4.210631	-1.592390
7	6	0	-4.082212	-0.019105	0.258319
8	6	0	-3.411204	1.212949	0.094426
9	6	0	-2.074272	1.204330	-0.311298
10	7	0	-1.423829	0.019430	-0.538866
11	6	0	-2.068992	-1.183067	-0.408955
12	6	0	-3.404648	-1.230870	-0.002017
13	6	0	-1.543152	3.697423	-0.432009
14	6	0	-0.603724	4.696521	-0.756026
15	6	0	0.654121	4.330989	-1.220207
16	6	0	0.971705	2.960879	-1.349972
17	7	0	0.086089	1.984916	-1.037470
18	6	0	-1.177286	2.362624	-0.584484
19	6	0	4.434894	0.071181	-1.581803
20	6	0	3.113619	0.050658	-1.104142
21	6	0	2.894611	-0.007526	0.342010
22	6	0	3.988580	-0.042256	1.244213
23	6	0	5.307666	-0.019318	0.700552
24	6	0	5.501291	0.036604	-0.691545
25	7	0	1.560176	-0.024872	0.739634

26	6	0	1.306174	-0.076777	2.049201
27	6	0	2.344851	-0.114657	3.035227
28	6	0	3.656702	-0.097920	2.642067
29	8	0	2.087257	0.081016	-1.886830
30	29	0	0.388813	0.044490	-1.057437
31	6	0	-5.491829	-0.040454	0.693229
32	6	0	-5.874651	-0.821701	1.796484
33	6	0	-7.209298	-0.835435	2.207904
34	6	0	-8.165504	-0.081444	1.518638
35	6	0	-7.785715	0.692728	0.416770
36	6	0	-6.451573	0.719751	0.004123
37	1	0	-0.858982	-5.681029	-1.147583
38	1	0	-2.526171	-3.965539	-0.421528
39	1	0	1.971515	-2.474711	-1.937496
40	1	0	1.413949	-4.938583	-1.922972
41	1	0	-3.938112	2.150301	0.290793
42	1	0	-3.932197	-2.182585	0.102019
43	1	0	-2.535076	3.975784	-0.069779
44	1	0	-0.872163	5.752662	-0.641796
45	1	0	1.400472	5.087068	-1.484846
46	1	0	1.962730	2.635495	-1.719952
47	1	0	6.532927	0.053200	-1.080183
48	1	0	0.258672	-0.090165	2.368605
49	1	0	2.072057	-0.156410	4.091451
50	1	0	4.473645	-0.126448	3.383279
51	1	0	-5.134450	-1.406390	2.341597
52	1	0	-7.507462	-1.436107	3.069358
53	1	0	-9.209055	-0.097435	1.840830

54	1	0	-8.534205	1.276991	-0.122030
55	1	0	-6.164367	1.319026	-0.859392
56	7	0	6.505308	-0.051888	1.540083
57	8	0	6.377105	-0.101245	2.755819
58	8	0	7.586025	-0.027676	0.970901
59	1	0	4.607304	0.114551	-2.657047

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

Centre No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.465194	4.179854	-2.559430
2	6	0	-0.344025	3.355405	-1.753764
3	6	0	0.263066	2.585661	-0.763972
4	7	0	1.639750	2.602053	-0.553226
5	6	0	2.400013	3.405059	-1.334866
6	6	0	1.839035	4.210371	-2.350162
7	6	0	-2.336298	0.606641	1.292581
8	6	0	-1.407847	-0.022106	2.170006
9	6	0	-0.048071	0.227308	2.016228
10	7	0	0.409294	1.055227	1.021465
11	6	0	-0.467999	1.689905	0.179474
12	6	0	-1.839850	1.479528	0.284500
13	6	0	0.951149	-1.148981	3.921920
14	6	0	2.106300	-1.527858	4.632961
15	6	0	3.345215	-1.028690	4.247938
16	6	0	3.422873	-0.153339	3.142656
17	7	0	2.324700	0.218900	2.443108
18	6	0	1.086788	-0.279652	2.841769
19	6	0	6.233322	1.455544	0.006320
20	6	0	4.867027	1.178730	0.099518
21	6	0	4.322630	0.064778	-0.662721
22	6	0	5.180419	-0.718459	-1.483305
23	6	0	6.559468	-0.400685	-1.546837
24	6	0	7.059498	0.664538	-0.813243
25	7	0	2.956156	-0.171535	-0.537229

26	6	0	2.440362	-1.191105	-1.230621
27	6	0	3.228553	-2.033360	-2.082170
28	6	0	4.574655	-1.801615	-2.206677
29	8	0	4.058332	1.885326	0.847816
30	29	0	2.267636	1.342071	0.825819
31	1	0	0.006880	4.791569	-3.342787
32	1	0	-1.423548	3.326984	-1.908259
33	1	0	3.489417	3.402817	-1.135580
34	1	0	2.489149	4.845418	-2.958251
35	1	0	-1.766651	-0.673667	2.968610
36	1	0	-2.531779	1.981532	-0.391796
37	1	0	-0.026487	-1.531667	4.219237
38	1	0	2.020258	-2.210441	5.484211
39	1	0	4.256775	-1.303209	4.785870
40	1	0	4.390411	0.267868	2.806693
41	1	0	6.647813	2.285770	0.572515
42	1	0	7.217513	-0.997637	-2.173250
43	1	0	8.124450	0.905001	-0.866158
44	1	0	1.366199	-1.380149	-1.134520
45	1	0	2.739171	-2.846419	-2.617147
46	1	0	5.203062	-2.423883	-2.846383
47	6	0	-3.746249	0.348756	1.412874
48	26	0	-5.049637	1.125380	2.727362
49	6	0	-4.357004	-0.717661	2.210334
50	6	0	-4.820693	1.010034	0.687831
51	6	0	-6.042006	0.368905	1.044041
52	6	0	-5.753044	-0.702981	1.966221
53	6	0	-5.125108	1.747330	4.669693

54	6	0	-4.630599	2.807395	3.816418
55	6	0	-5.644035	3.110800	2.857936
56	6	0	-6.756101	2.222911	3.094903
57	6	0	-6.445174	1.408620	4.239086
58	1	0	-3.808506	-1.510410	2.710365
59	1	0	-4.691228	1.751283	-0.092019
60	1	0	-7.009394	0.547958	0.585707
61	1	0	-6.472301	-1.438175	2.316912
62	1	0	-4.669348	1.442699	5.608428
63	1	0	-3.750378	3.408719	4.023805
64	1	0	-5.643531	3.950588	2.172602
65	1	0	-7.735422	2.311796	2.637378
66	1	0	-7.136328	0.752914	4.759656

Table S6. The DFT coordinates used for energy optimization of complex **5.**

Centre No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040703	-4.616052	-1.039533
2	6	0	-0.990556	-3.636479	-0.688806
3	6	0	-0.611988	-2.296649	-0.722578
4	7	0	0.675420	-1.900220	-1.080124
5	6	0	1.571658	-2.855871	-1.422968
6	6	0	1.240823	-4.228735	-1.412984
7	6	0	-3.564087	0.049568	0.113284
8	6	0	-2.851831	1.271802	-0.047850
9	6	0	-1.499907	1.235864	-0.374388
10	7	0	-0.847242	0.039902	-0.536233
11	6	0	-1.519455	-1.151363	-0.419181
12	6	0	-2.871269	-1.177642	-0.094202
13	6	0	-0.932749	3.720651	-0.560580
14	6	0	0.032526	4.696605	-0.877880
15	6	0	1.308313	4.302266	-1.263319
16	6	0	1.617769	2.925511	-1.319471
17	7	0	0.706499	1.973007	-1.009102
18	6	0	-0.574863	2.377015	-0.638541
19	6	0	5.050023	0.010766	-1.163565
20	6	0	3.700307	0.010565	-0.795070
21	6	0	3.379044	-0.018218	0.629960
22	6	0	4.411316	-0.046276	1.605870
23	6	0	5.758246	-0.044763	1.149526
24	6	0	6.071986	-0.016863	-0.200527
25	7	0	2.025209	-0.016102	0.949811

26	6	0	1.698102	-0.042604	2.247748
27	6	0	2.672766	-0.072207	3.295121
28	6	0	4.010721	-0.073993	2.980935
29	8	0	2.728773	0.034928	-1.655602
30	29	0	0.990008	0.032321	-0.951755
31	1	0	-0.319685	-5.674484	-1.018957
32	1	0	-2.000908	-3.930791	-0.399693
33	1	0	2.580997	-2.507610	-1.721130
34	1	0	1.994504	-4.968480	-1.698669
35	1	0	-3.366831	2.224065	0.080731
36	1	0	-3.398855	-2.127069	0.011895
37	1	0	-1.938877	4.020815	-0.263832
38	1	0	-0.230124	5.757931	-0.822421
39	1	0	2.073684	5.039378	-1.523690
40	1	0	2.621739	2.571580	-1.629428
41	1	0	7.121544	-0.016311	-0.520111
42	1	0	0.632204	-0.041269	2.501464
43	1	0	2.335349	-0.093054	4.331604
44	1	0	4.775110	-0.096287	3.763516
45	53	0	5.542690	0.053565	-3.193809
46	17	0	7.027590	-0.078310	2.303493
47	6	0	-4.963382	0.053071	0.442362
48	26	0	-5.838254	-0.230245	2.226548
49	6	0	-5.859898	-1.104946	0.388725
50	6	0	-5.782251	1.212903	0.765701
51	6	0	-7.127168	0.766742	0.909183
52	6	0	-7.175367	-0.654495	0.661011
53	6	0	-5.585570	-1.311924	3.938896

54	6	0	-4.807159	-0.092072	3.989796
55	6	0	-5.708189	1.010478	3.886665
56	6	0	-7.041611	0.479031	3.743651
57	6	0	-6.963851	-0.955527	3.814537
58	1	0	-5.592924	-2.078560	-0.011954
59	1	0	-5.449177	2.244042	0.744750
60	1	0	-7.997537	1.404156	1.029489
61	1	0	-8.083768	-1.246262	0.584620
62	1	0	-5.209465	-2.299731	4.193234
63	1	0	-3.764866	-0.035893	4.287569
64	1	0	-5.459394	2.054699	4.037263
65	1	0	-7.955795	1.059931	3.802390
66	1	0	-7.807071	-1.635160	3.892758

Table S7. The DFT coordinates used for energy optimization of complex **6.**

Centre No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.952236	-4.509950	-1.393445
2	6	0	-1.957739	-3.569043	-1.097834
3	6	0	-1.591262	-2.241328	-0.890485
4	7	0	-0.265127	-1.818579	-0.959633
5	6	0	0.686109	-2.737960	-1.252011
6	6	0	0.372287	-4.096106	-1.475599
7	6	0	-4.667982	0.004694	-0.252900
8	6	0	-3.949214	1.227417	-0.110872
9	6	0	-2.563544	1.221642	-0.215912
10	7	0	-1.878035	0.051970	-0.437054
11	6	0	-2.548521	-1.135015	-0.598278
12	6	0	-3.934623	-1.190650	-0.503777
13	6	0	-2.004825	3.696968	0.069687
14	6	0	-1.011973	4.695799	0.085242
15	6	0	0.317759	4.344979	-0.117727
16	6	0	0.649447	2.989042	-0.328438
17	7	0	-0.289452	2.012312	-0.340284
18	6	0	-1.620798	2.375515	-0.145853
19	6	0	4.065755	0.040028	-0.123082
20	6	0	2.669165	0.004488	0.038906
21	6	0	2.129485	-0.218278	1.382326
22	6	0	2.990510	-0.394169	2.495328
23	6	0	4.398776	-0.348124	2.268442
24	6	0	4.902060	-0.133191	0.971798
25	7	0	0.740160	-0.240836	1.465085

26	6	0	0.195326	-0.440321	2.667263
27	6	0	0.983535	-0.627751	3.848903
28	6	0	2.350502	-0.605274	3.765206
29	8	0	1.846825	0.158985	-0.941014
30	29	0	-0.002406	0.079080	-0.526214
31	1	0	-1.220384	-5.558899	-1.558164
32	1	0	-3.001258	-3.882981	-1.035274
33	1	0	1.729001	-2.373630	-1.313545
34	1	0	1.172248	-4.805417	-1.709031
35	1	0	-4.490143	2.160695	0.057161
36	1	0	-4.462212	-2.136970	-0.627646
37	1	0	-3.052729	3.962613	0.222347
38	1	0	-1.294046	5.740370	0.254651
39	1	0	1.108164	5.101793	-0.115754
40	1	0	1.696835	2.675490	-0.498052
41	1	0	5.994798	-0.102888	0.829859
42	1	0	-0.897622	-0.458974	2.738206
43	1	0	0.478351	-0.786494	4.803282
44	1	0	2.978137	-0.747204	4.661158
45	7	0	5.374374	-0.517327	3.343064
46	8	0	4.975868	-0.706565	4.484658
47	8	0	6.556724	-0.459829	3.038608
48	1	0	4.476574	0.205232	-1.118570
49	6	0	-6.097142	-0.022956	-0.123635
50	26	0	-7.474895	0.447891	-1.503011
51	6	0	-6.937750	1.078736	0.355706
52	6	0	-6.973868	-1.167058	-0.337895
53	6	0	-8.298171	-0.765407	-0.003947

54	6	0	-8.271525	0.609233	0.436889
55	6	0	-7.753516	1.746456	-3.051934
56	6	0	-7.028886	0.574502	-3.497407
57	6	0	-7.856814	-0.566575	-3.274339
58	6	0	-9.083084	-0.110555	-2.665674
59	6	0	-9.029331	1.323311	-2.566340
60	1	0	-6.563378	2.003684	0.784667
61	1	0	-6.647603	-2.176891	-0.558049
62	1	0	-9.162762	-1.419010	0.059596
63	1	0	-9.115022	1.145746	0.863911
64	1	0	-7.472399	2.772506	-3.276835
65	1	0	-6.126663	0.598079	-4.101565
66	1	0	-7.667791	-1.572452	-3.631712
67	1	0	-9.972845	-0.714871	-2.523903
68	1	0	-9.856155	1.973817	-2.296935

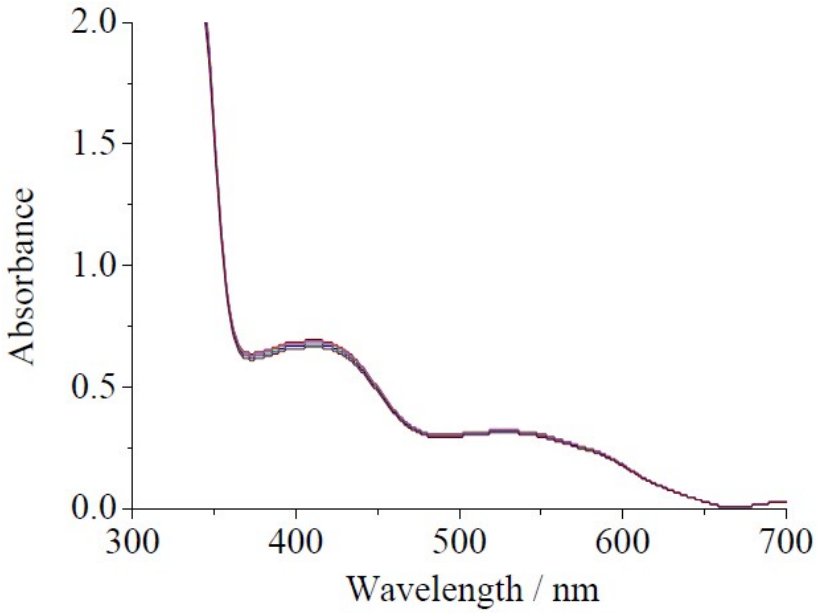

Fig. S19. Absorption spectral plots of complex **5** in DMSO–10% DMEM medium (1:99 v/v, pH = 7.4, 37 °C). The spectra were recorded after keeping the solution at 37 °C and recorded at different time intervals. The spectral data indicate the stability of the complex in the cellular medium up to 48 hours.

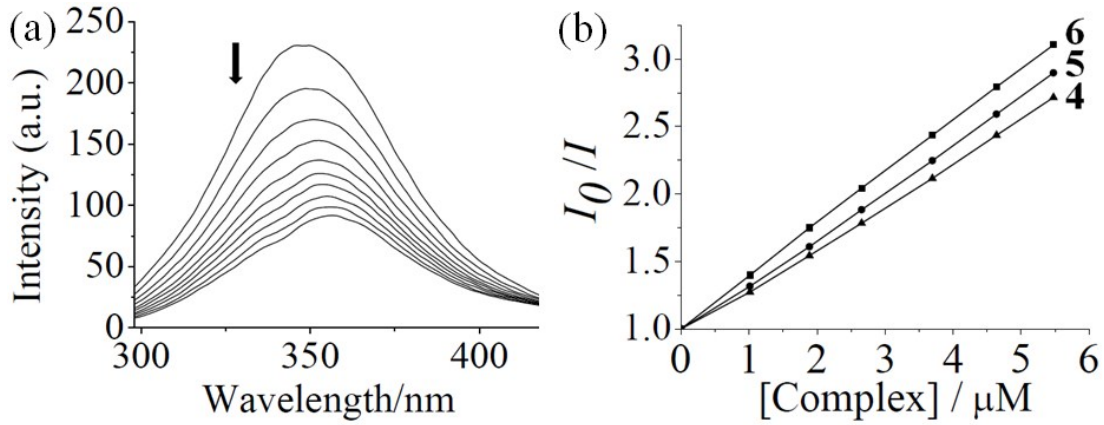

Fig. S20. Emission spectral traces of human serum albumin (2 μM) in the presence of complex **5**. The inset shows the plots of (I_0/I) vs [complex] for **4** (▲), **5** (●) and **6** (■).

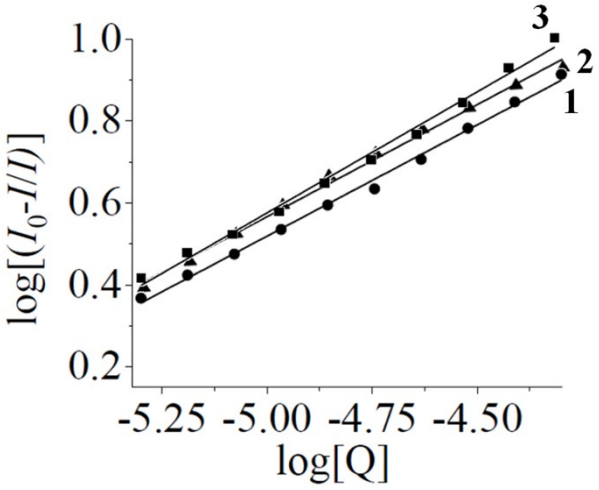

Fig. S21: Scatchard plots of log[(I_0-I)/I] against log[Q] for **1** (●), **2** (▲) and **3** (■) to determine the binding constant (K_{HSA}) for HSA–complex interaction.

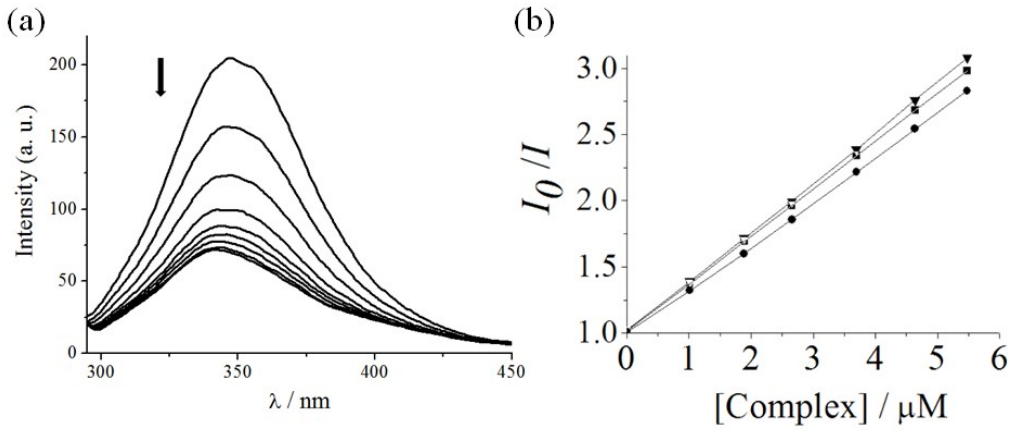

Fig. S22. Emission spectral traces of human serum albumin (2 μM) in the presence of complex **3**. The inset shows the plots of (I_0/I) vs [complex] for **1** (●), **2** (■)and **3** (▼).