Supporting information

Cytotoxicity of Pd(II) and Pt(II) complexes of 2',6'-di(thiazol-2-yl)-2,4'-bipyridine: Insights into the mode of cell death and cell cycle arrest

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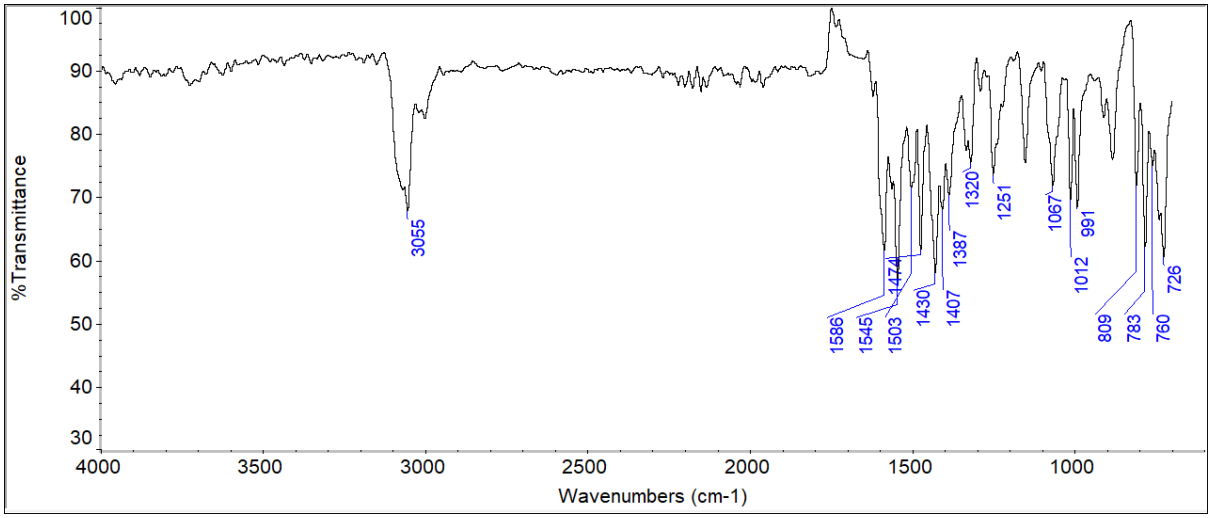

Fig. S1 AT IR spectrum of the ligand **1**.

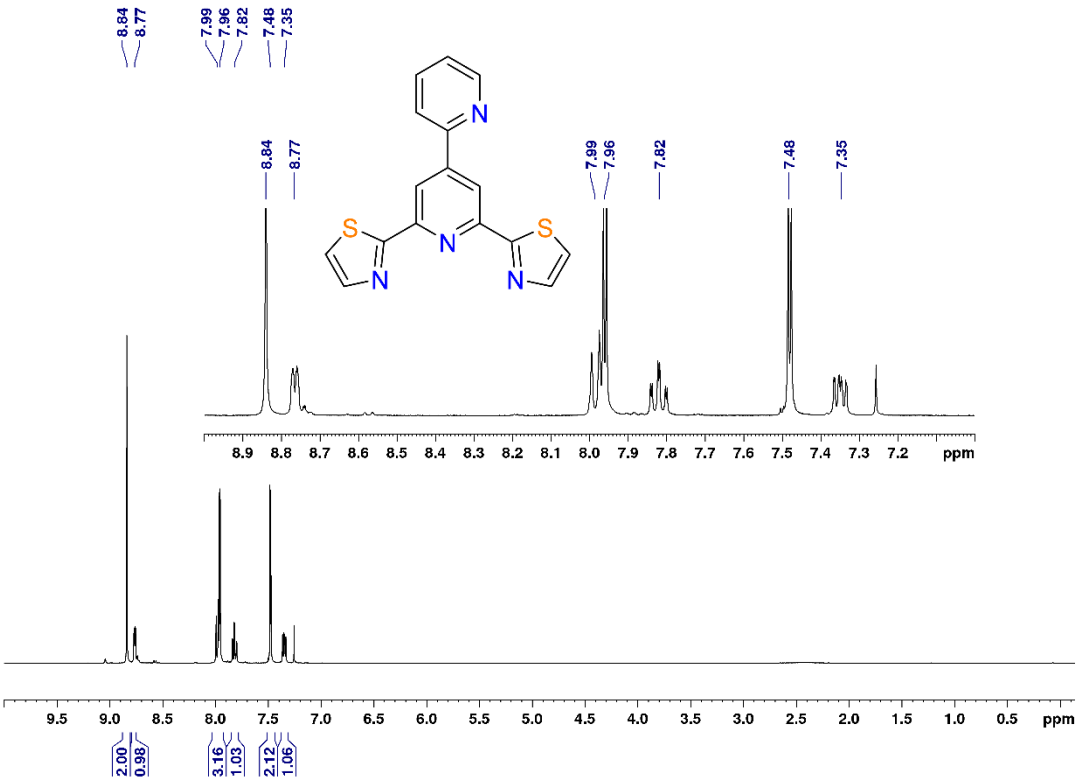

Fig. S2 ^{1}H NMR spectrum of **1** in $CDCl_3$.

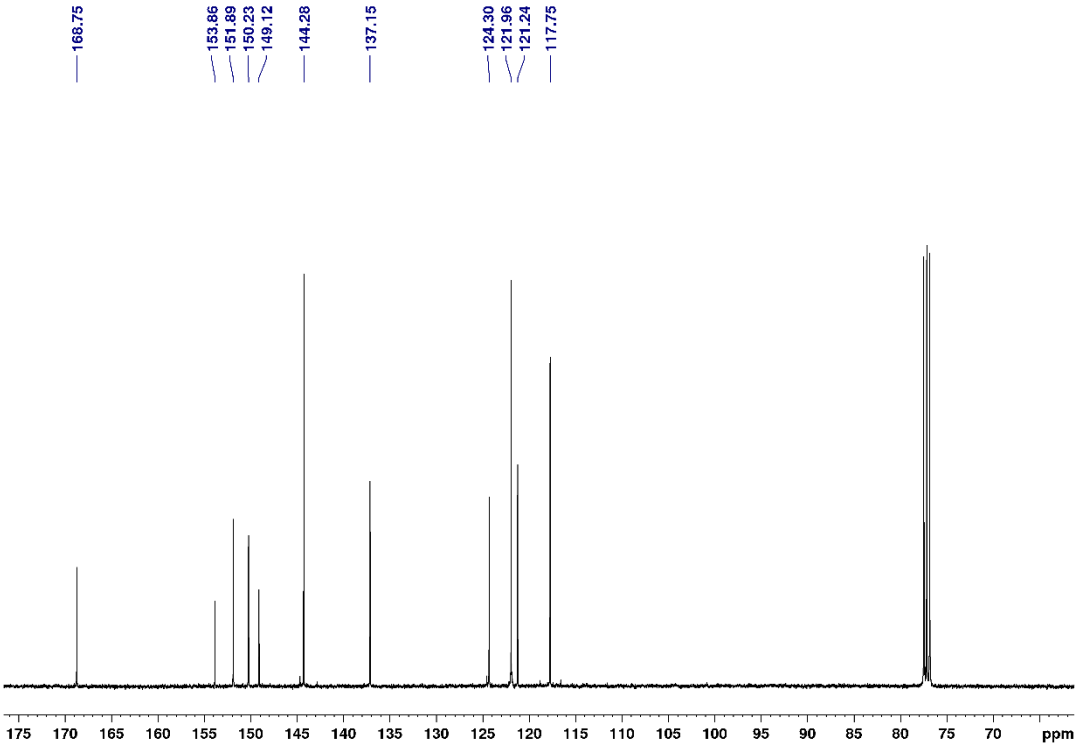

Fig. S3 ^{13}C NMR spectrum of **1** in $CDCl_3$.

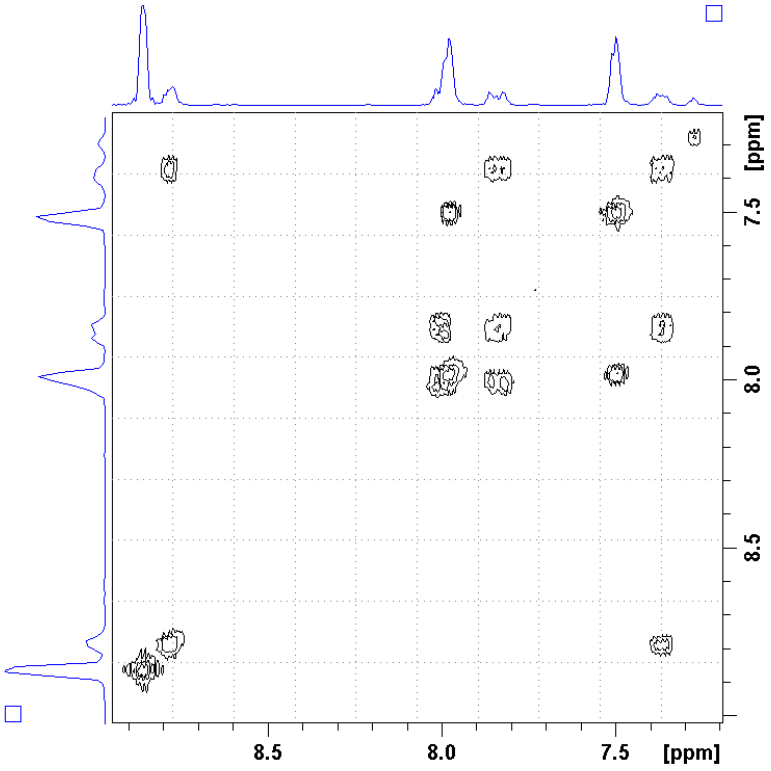

Fig. S4 {^{1}H, ^{1}H} COS90 spectrum of **1** in $CDCl_3$.

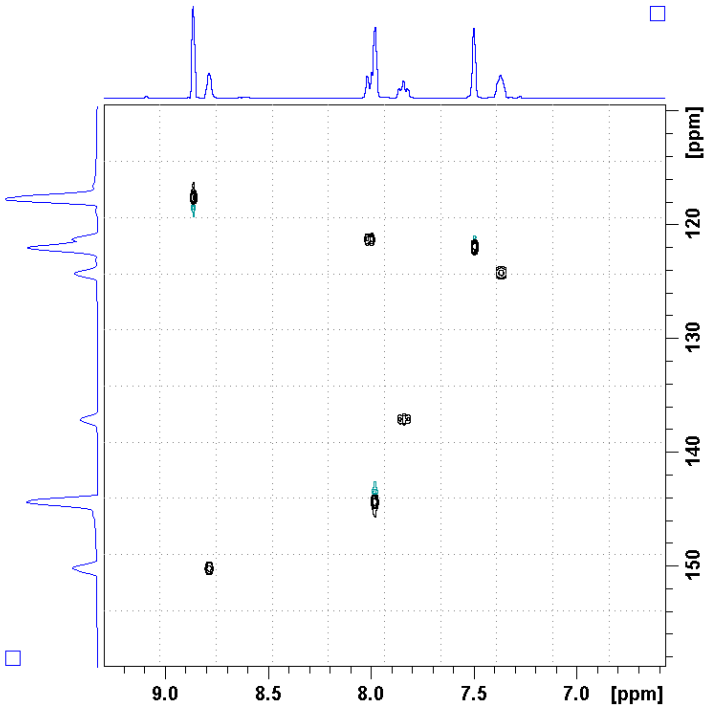

Fig. S5 {^{13}C, ^{1}H} HSQC spectrum of **1** in $CDCl_3$.

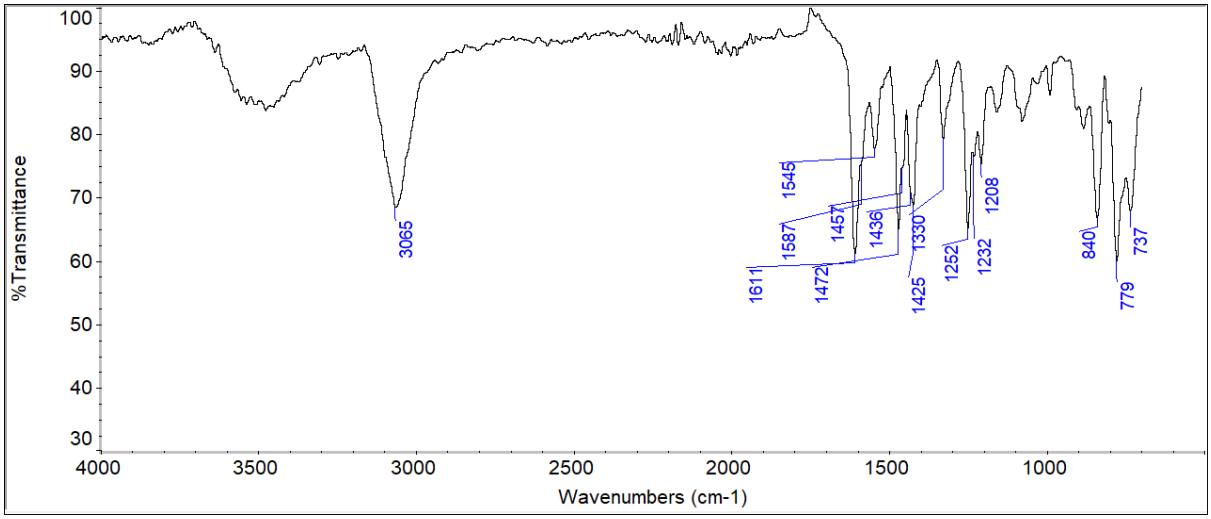

Fig. S6 AT IR spectrum of **2**.

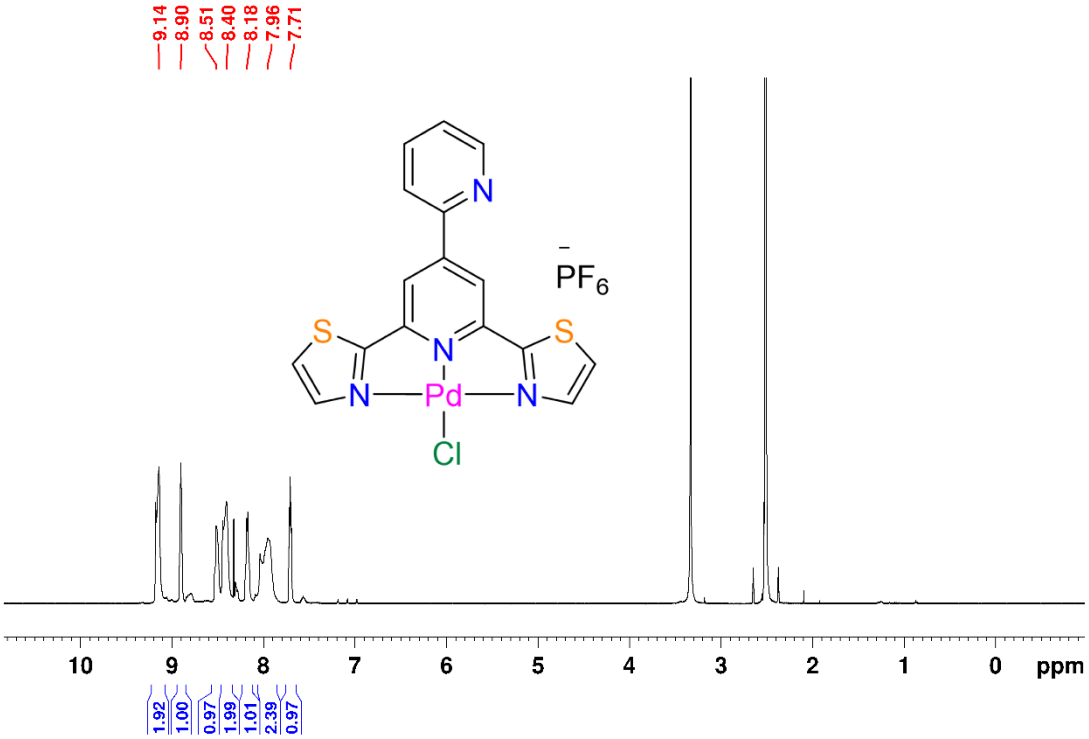

Fig. S7 ^{1}H NMR spectrum of **2** in DMSO-d_6.

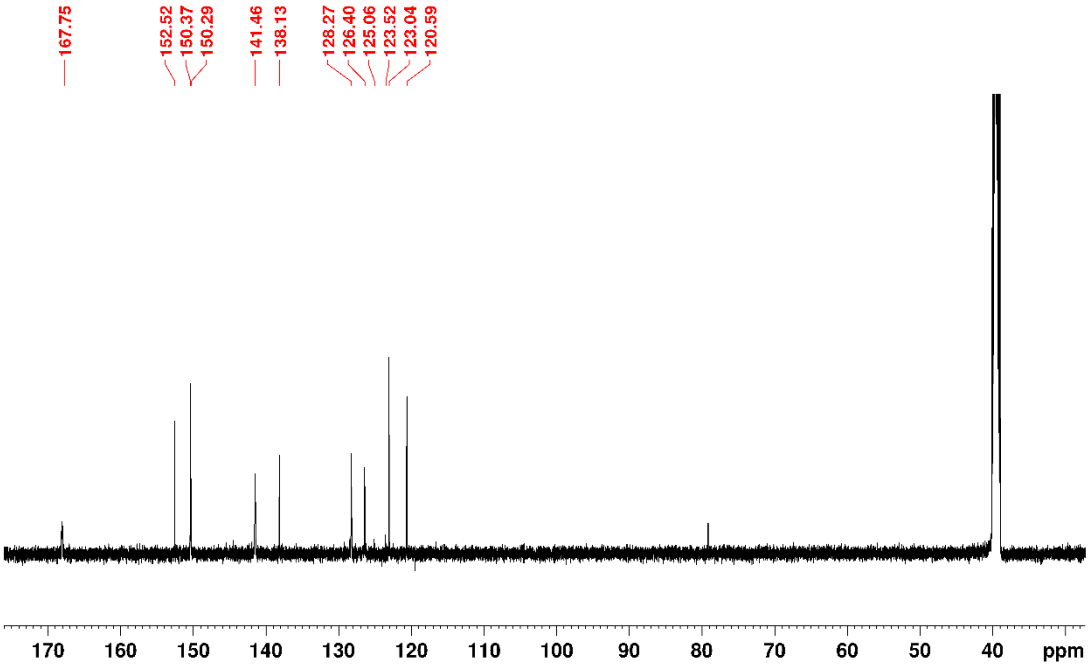

Fig. S8 ^{13}C NMR spectrum of **2** in DMSO-d_6.

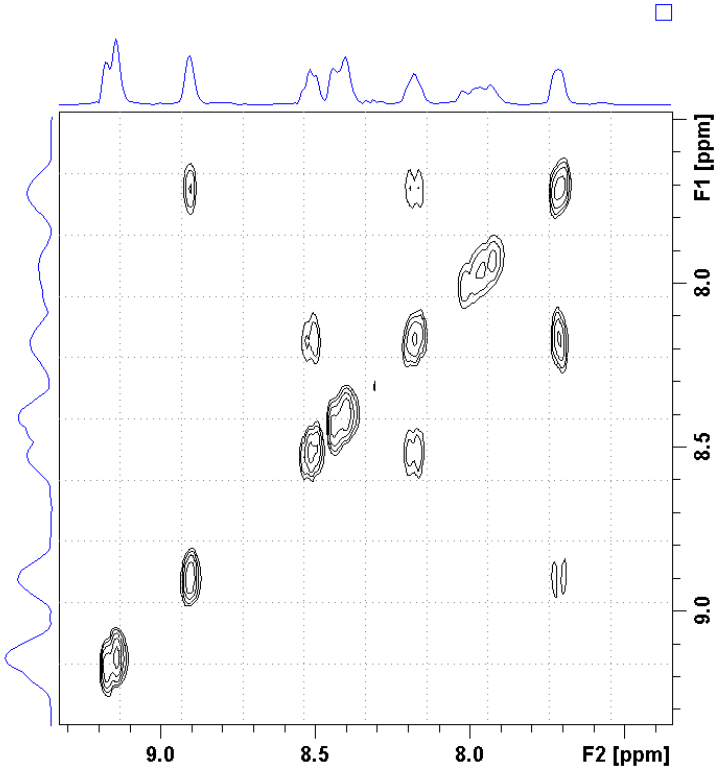

Fig. S9 {^{1}H, ^{1}H} COS90 spectrum of **2** in DMSO-d_6.

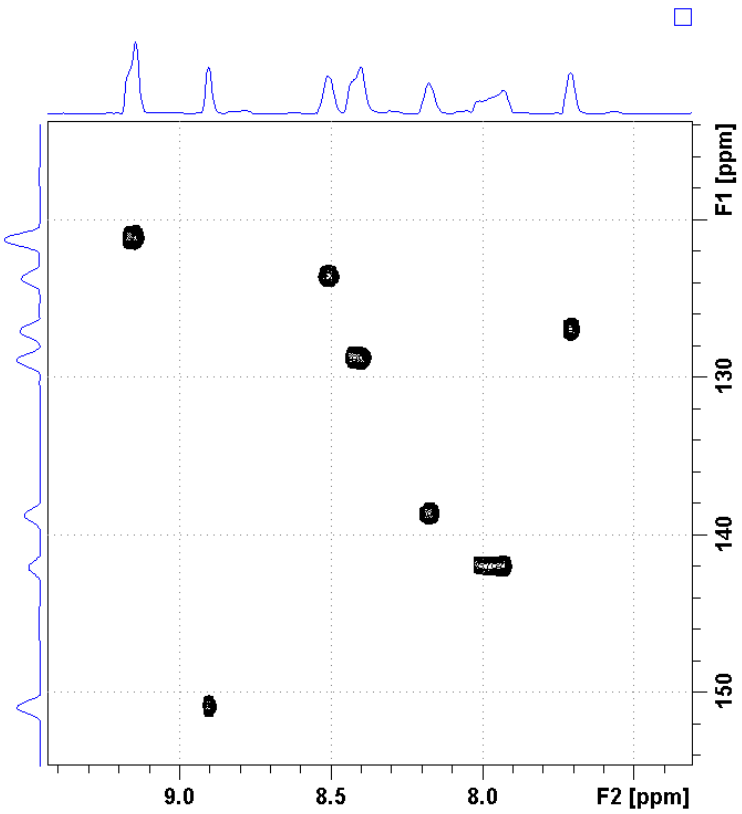

Fig. S10 {^{13}C, ^{1}H} HSQC spectrum of **2** in DMSO-d_6.

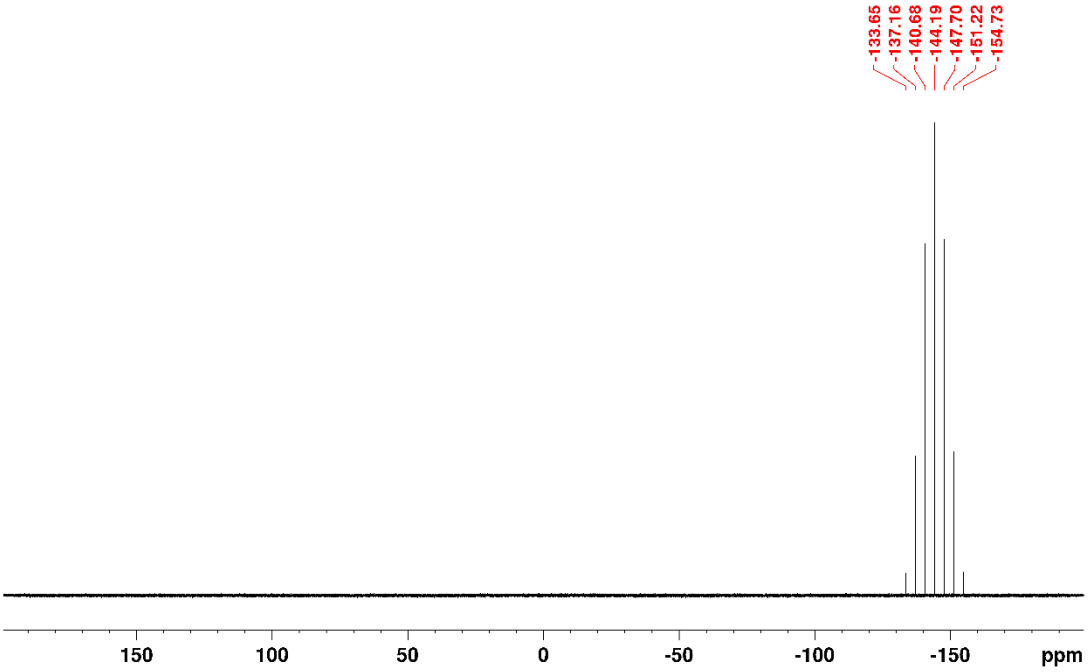

Fig. S11 ^{31}P spectrum of **2** in DMSO-d_6.

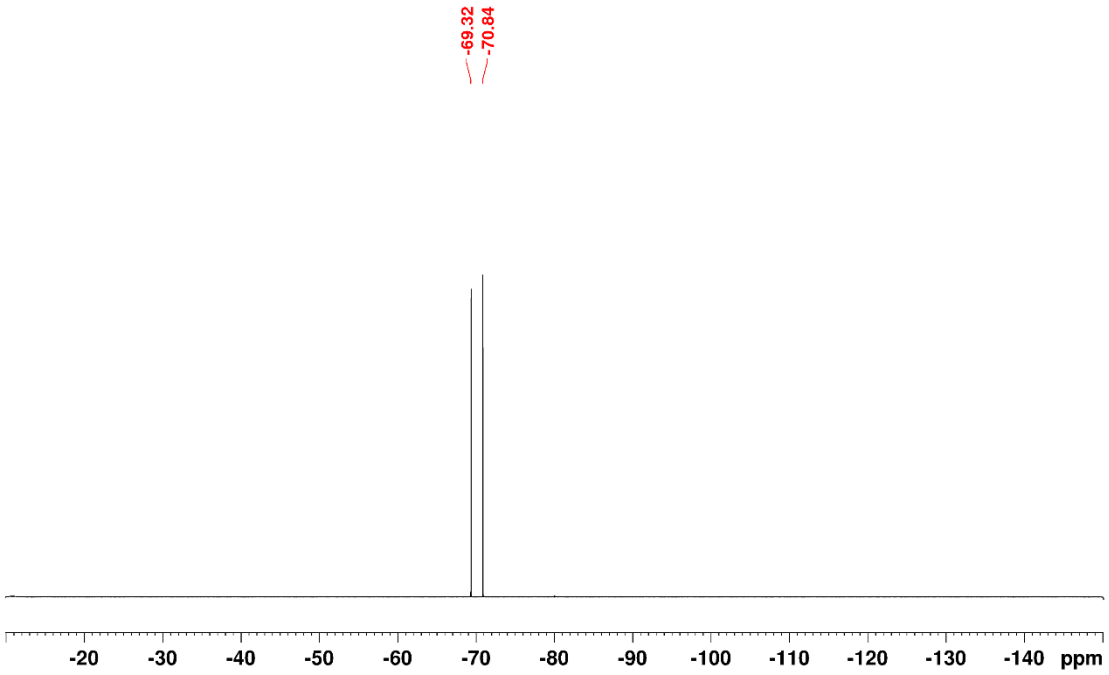

Fig. S12 ^{19}F spectrum of **2** in DMSO-d_6.

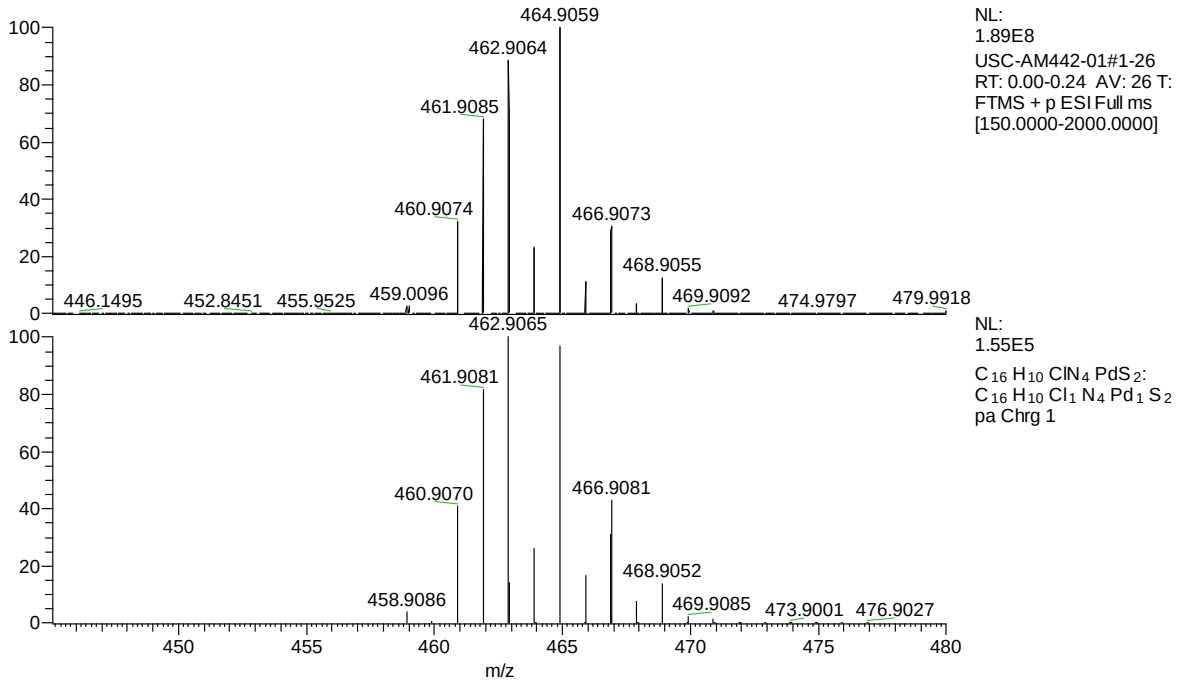

Fig. S13 Experimental (Up) and theoretical (down) ISOTOPIC pattern for the $[M–PF_6]^+$ ion of compound **2**.

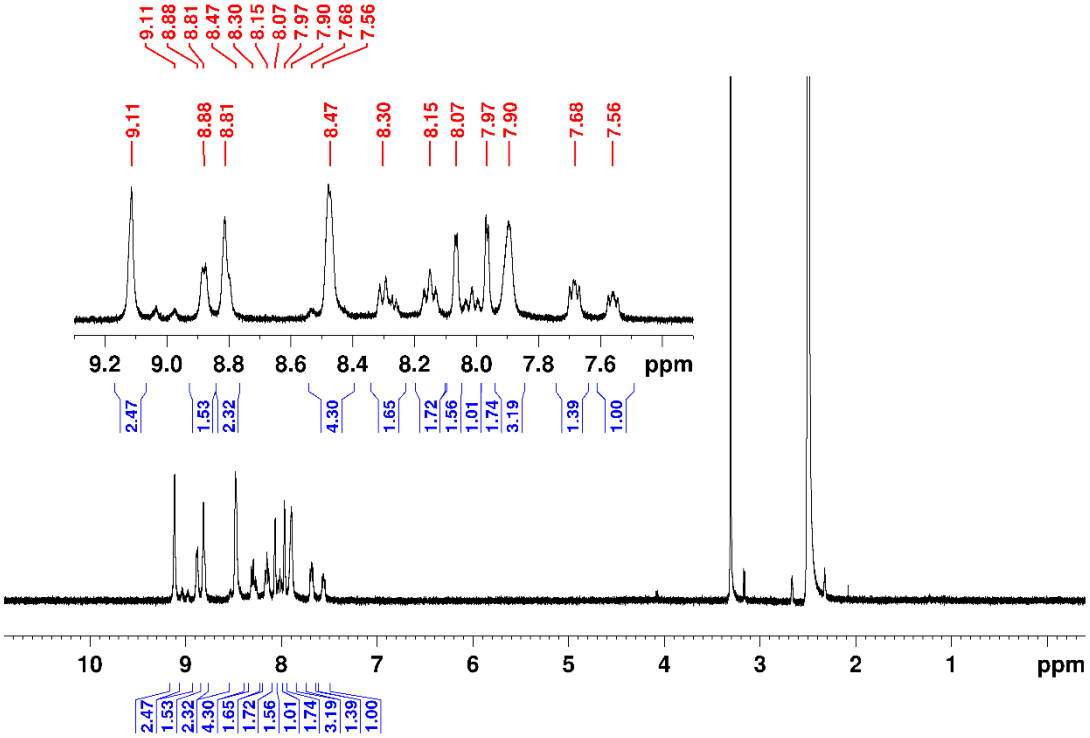

Fig. S14 ^{1}H NMR spectrum of **3** in DMSO-d_6 (It breaks up in DMSO).

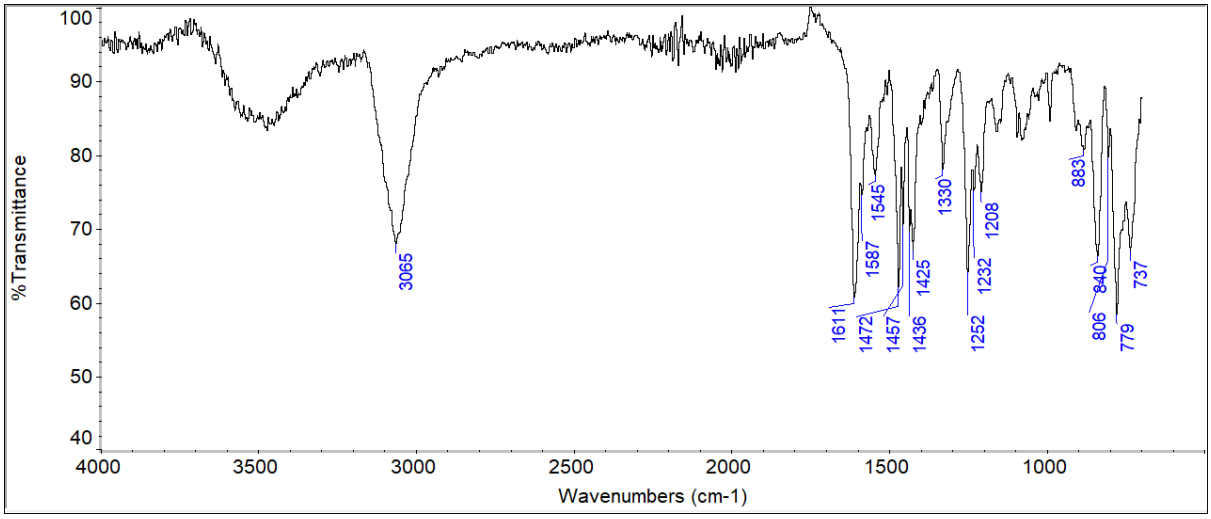

Fig. S15 AT IR spectrum of **3**.

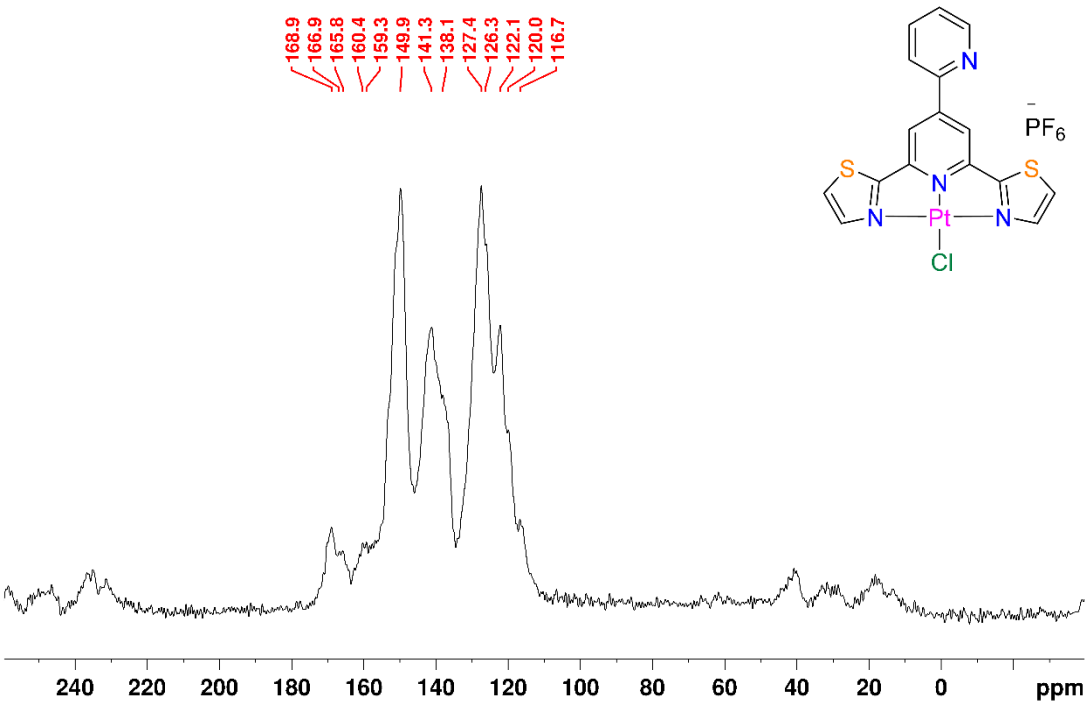

Fig. S16 Solid-state ^{13}C NMR spectrum of **3.**

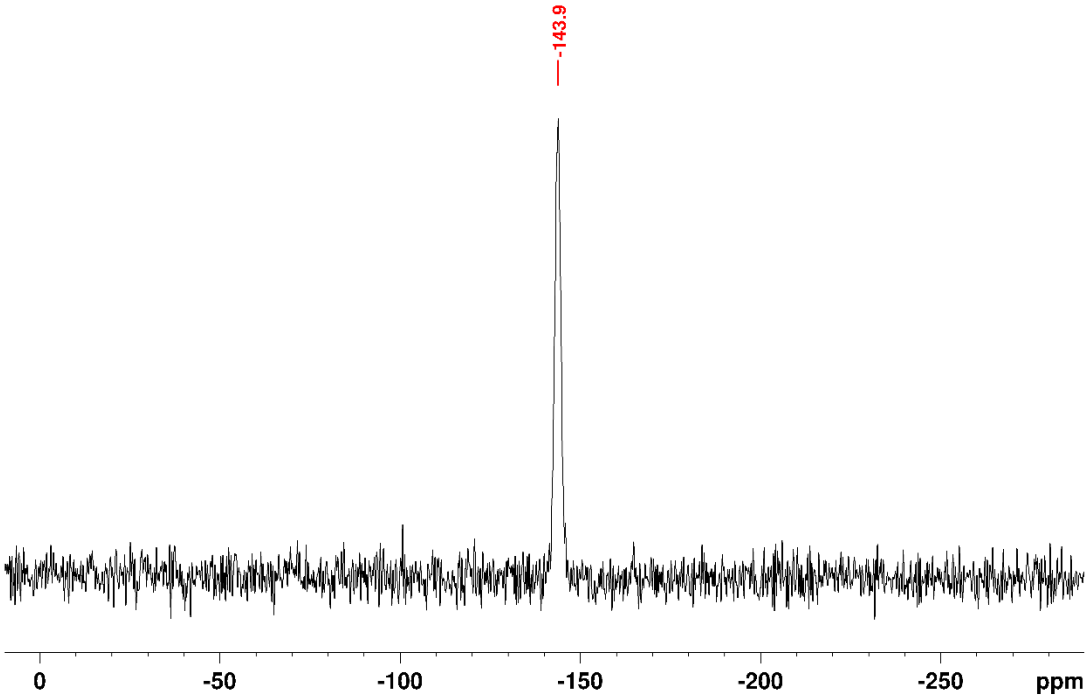

Fig. S17 Solid-state ^{31}P spectrum of **3.**

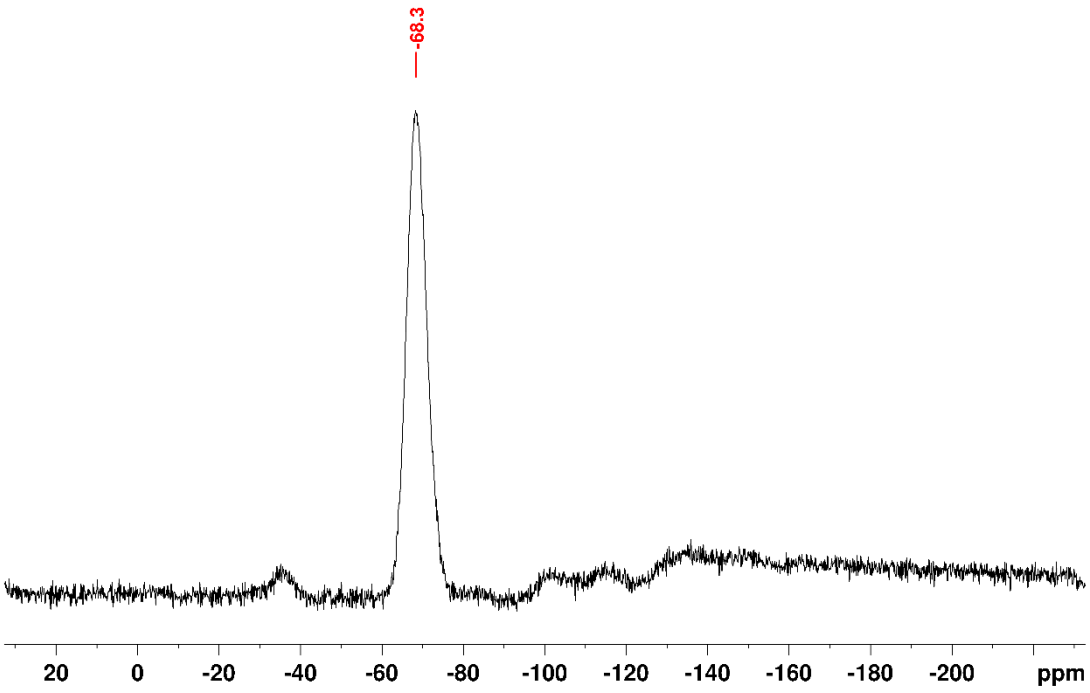

Fig. S18 Solid-state ^{19}F spectrum of **3.**

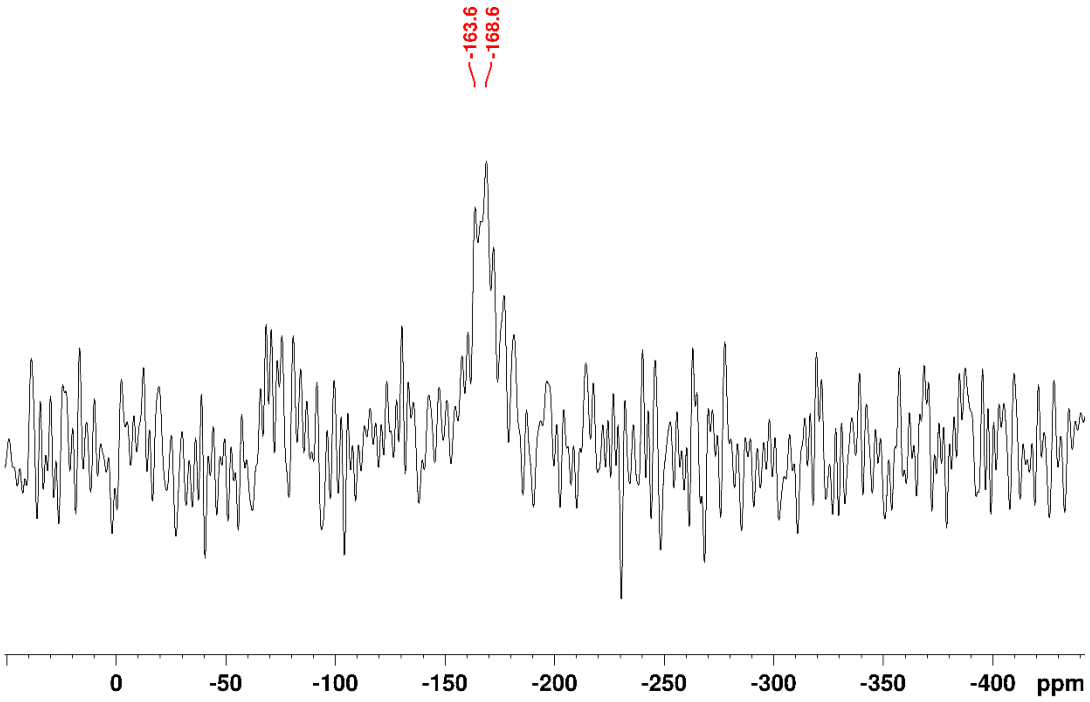

Fig. S19 Solid-state ^{15}N spectrum of **3.**

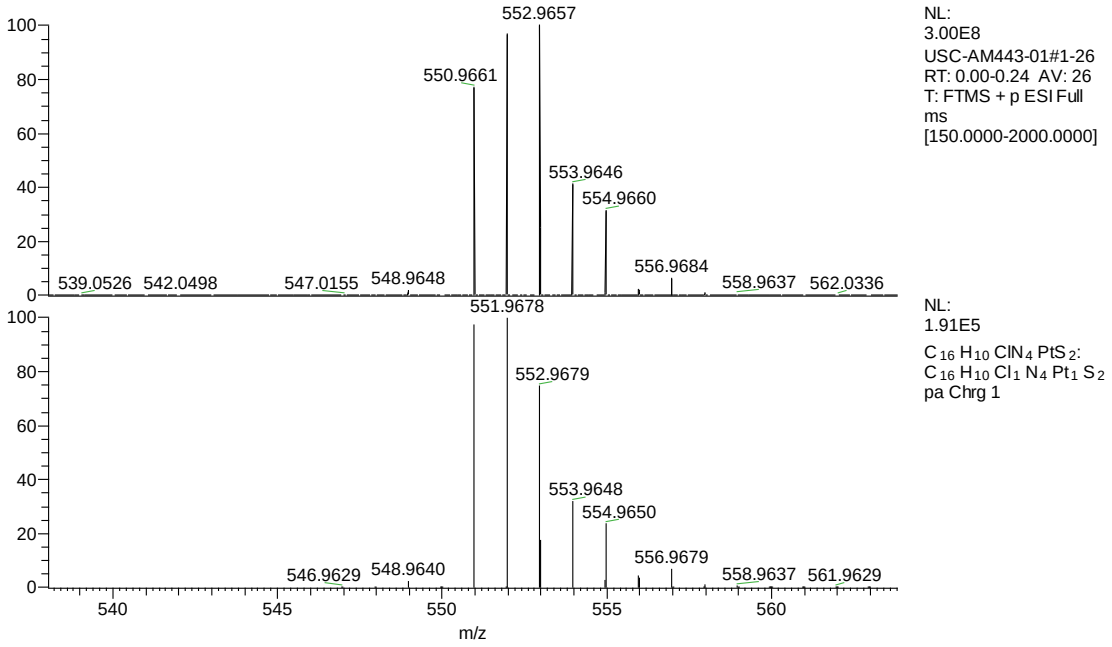

Fig. S20 Experimental (Up) and theoretical (down) ISOTOPIC pattern for the $[M–PF_6]^+$ ion of compound **3**.

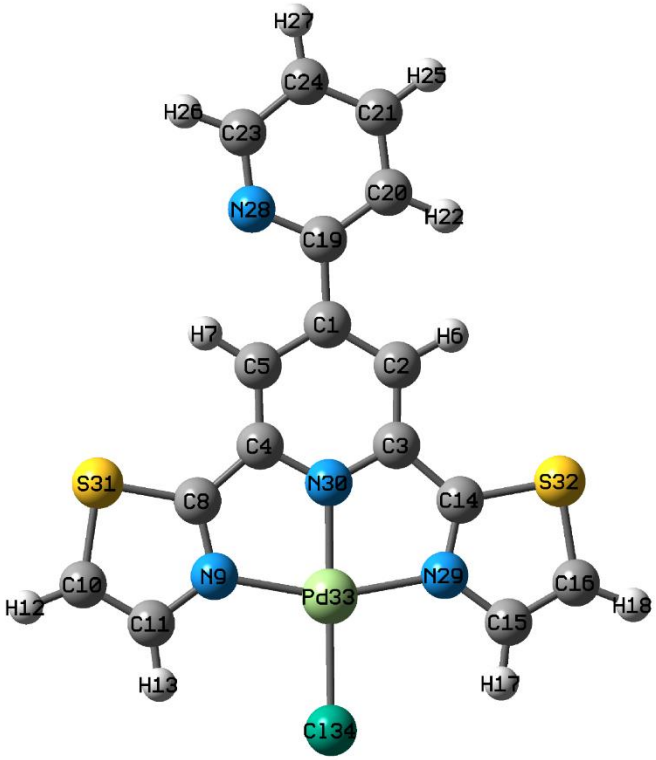

Fig. S21 Local minimum structure of **2** obtained at B3LYP/LANL2DZ level of theory.

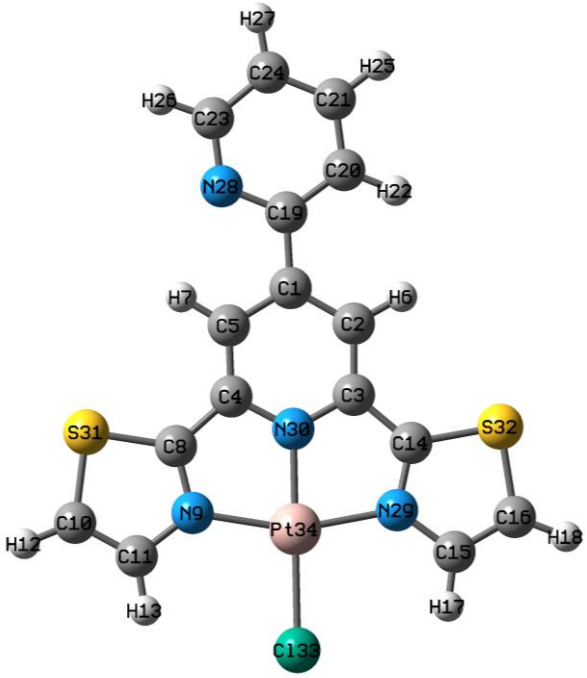

Fig. S22 Local minimum structure of **3** obtained at B3LYP/LANL2DZ level of theory.

Table S1 Atomic coordinates of the optimized structure of **2**.

Center number*	Atomic number	Atomic type	Coordinates (Å)		
			X	Y	Z
1	6	0	-2.616006	-0.140324	-0.000009
2	6	0	-1.848098	-1.334694	-0.000052
3	6	0	-0.44792	-1.248416	-0.000039
4	6	0	-0.547854	1.145461	-0.00001
5	6	0	-1.946185	1.114319	0.000002
6	1	0	-2.323902	-2.308393	-0.000163
7	1	0	-2.554714	2.012132	-0.000034
8	6	0	0.365452	2.293573	0.00004
9	7	0	1.694465	2.062906	0.000052
10	6	0	1.736734	4.375453	0.000069
11	6	0	2.471026	3.213084	0.000071
12	1	0	2.086983	5.396613	0.000075
13	1	0	3.548415	3.12323	0.0001
14	6	0	0.556525	-2.318498	-0.000082
15	6	0	2.730623	-3.061529	-0.000103
16	6	0	2.096826	-4.281157	-0.000085
17	1	0	3.797005	-2.883184	-0.000093
18	1	0	2.530441	-5.269774	-0.000238
19	6	0	-4.105544	-0.145541	-0.000007
20	6	0	-4.87606	-1.32842	0.000575
21	6	0	-6.279096	-1.228621	0.000534
22	1	0	-4.414258	-2.310108	0.001128
23	6	0	-6.034955	1.17892	-0.000509
24	6	0	-6.874756	0.044426	-0.000045
25	1	0	-6.891283	-2.125361	0.000969
26	1	0	-6.450864	2.182089	-0.00094
27	1	0	-7.953299	0.163504	-0.000112
28	7	0	-4.689396	1.088827	-0.000484
29	7	0	1.861359	-1.979243	-0.0001
30	7	0	0.150657	-0.026313	-0.000019
31	16	0	-0.026018	4.031938	0.000048
32	16	0	0.311178	-4.084936	-0.000076
33	46	0	2.139154	0.057076	0.000001
34	17	0	4.485763	0.150016	0.000087

Table S2 Atomic coordinates of the optimized structure of **3**.

Center number*	Atomic number	Atomic type	Coordinates (Å)		
			X	Y	Z
1	6	0	2.882238	0.138995	0.000047
2	6	0	2.117807	1.335091	0
3	6	0	0.718355	1.257638	-0.000014
4	6	0	0.8114	-1.144228	0.000019
5	6	0	2.208109	-1.113166	0.000034
6	1	0	2.597242	2.307049	-0.000046
7	1	0	2.814645	-2.0124	0.000027
8	6	0	-0.108026	-2.284383	0.000009
9	7	0	-1.438412	-2.033868	-0.000005
10	6	0	-1.511544	-4.344679	0.000019
11	6	0	-2.231161	-3.175423	-0.00002
12	1	0	-1.874504	-5.36133	0.000037
13	1	0	-3.307265	-3.071249	-0.000032
14	6	0	-0.284968	2.325073	-0.000059
15	6	0	-2.470232	3.051102	-0.000097
16	6	0	-1.844533	4.272697	-0.000085
17	1	0	-3.535253	2.864707	-0.000097
18	1	0	-2.284577	5.258407	-0.000081
19	6	0	4.371558	0.139049	0.000086
20	6	0	5.146462	1.319177	0.000447
21	6	0	6.549059	1.214612	0.000396
22	1	0	4.688071	2.302483	0.000796
23	6	0	6.296923	-1.191748	-0.000396
24	6	0	7.140652	-0.060391	-0.000029
25	1	0	7.164251	2.109323	0.00069
26	1	0	6.709382	-2.196375	-0.000697
27	1	0	8.218779	-0.183111	-0.000076
28	7	0	4.951556	-1.097213	-0.00033
29	7	0	-1.59187	1.973533	-0.000057
30	7	0	0.111096	0.033292	0.000003
31	16	0	0.256398	-4.025099	-0.000039
32	16	0	-0.056498	4.090309	-0.000142
33	17	0	-4.242763	-0.131293	0.000154
34	78	0	-1.862069	-0.043533	0.000004

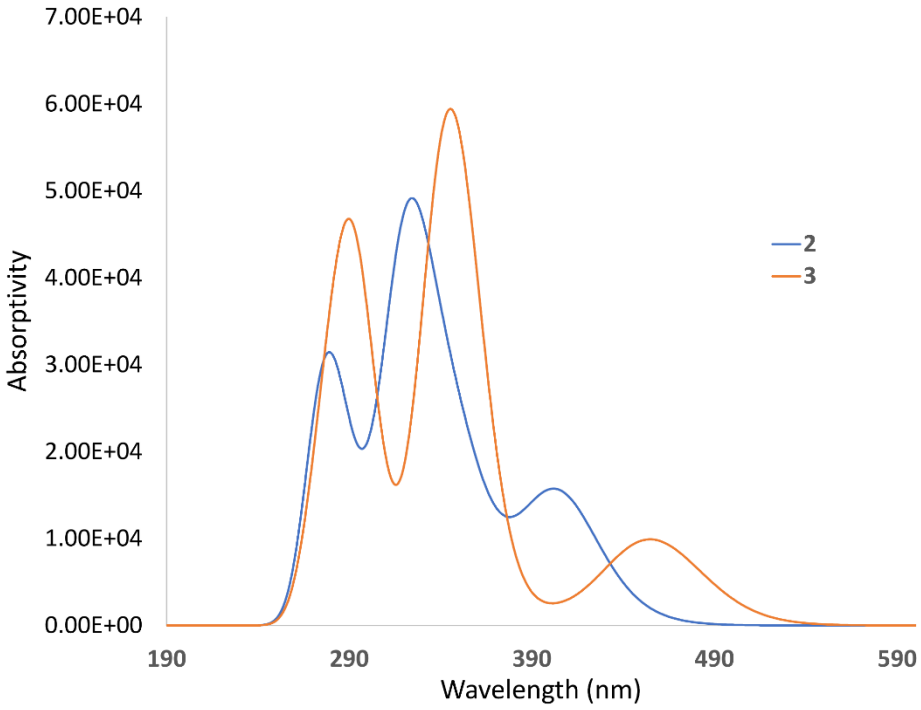

Fig. S23 Theoretical electronic spectra of **2** and **3** obtained at B3LYP/LANL2DZ level of theory.

Table S3 Computed excitation energies (eV), electronic transition configurations and oscillator strengths (*f*) of **2** and **3** at B3LYP/LANL2DZ level of theories (selected, $f > 0.001$) (Selected)			
Energy (cm^{-1})	Wavelength (nm)	*f*	Major contributions
✓ **2**			
24773	403	0.1265	HOMO→LUMO (74%)
28744	347	0.2406	HOMO−5→LUMO (97%)
31128	321	0.283	HOMO−1→LUMO+1 (86%)
32706	305	0.0942	HOMO−7→LUMO (88%)
35401	282	0.2079	HOMO−7→LUMO+1 (96%)
36564	273	0.215	HOMO→LUMO+3 (91%)
✓ **3**			
22002	454	0.123	HOMO→LUMO (89%)
24729	404	0.0181	HOMO→LUMO+1 (95%)
28544	350	0.3329	HOMO−5→LUMO (81%)
29277	341	0.4219	HOMO−6→LUMO (91%)
33816	295	0.2334	HOMO−6→LUMO+1 (68%)
34510	289	0.2899	HOMO−8→LUMO (29%), HOMO→LUMO+2 (67%)
35886	278	0.2171	HOMO−7→LUMO+1 (91%)
37185	268	0.072	HOMO−9→LUMO (91%)

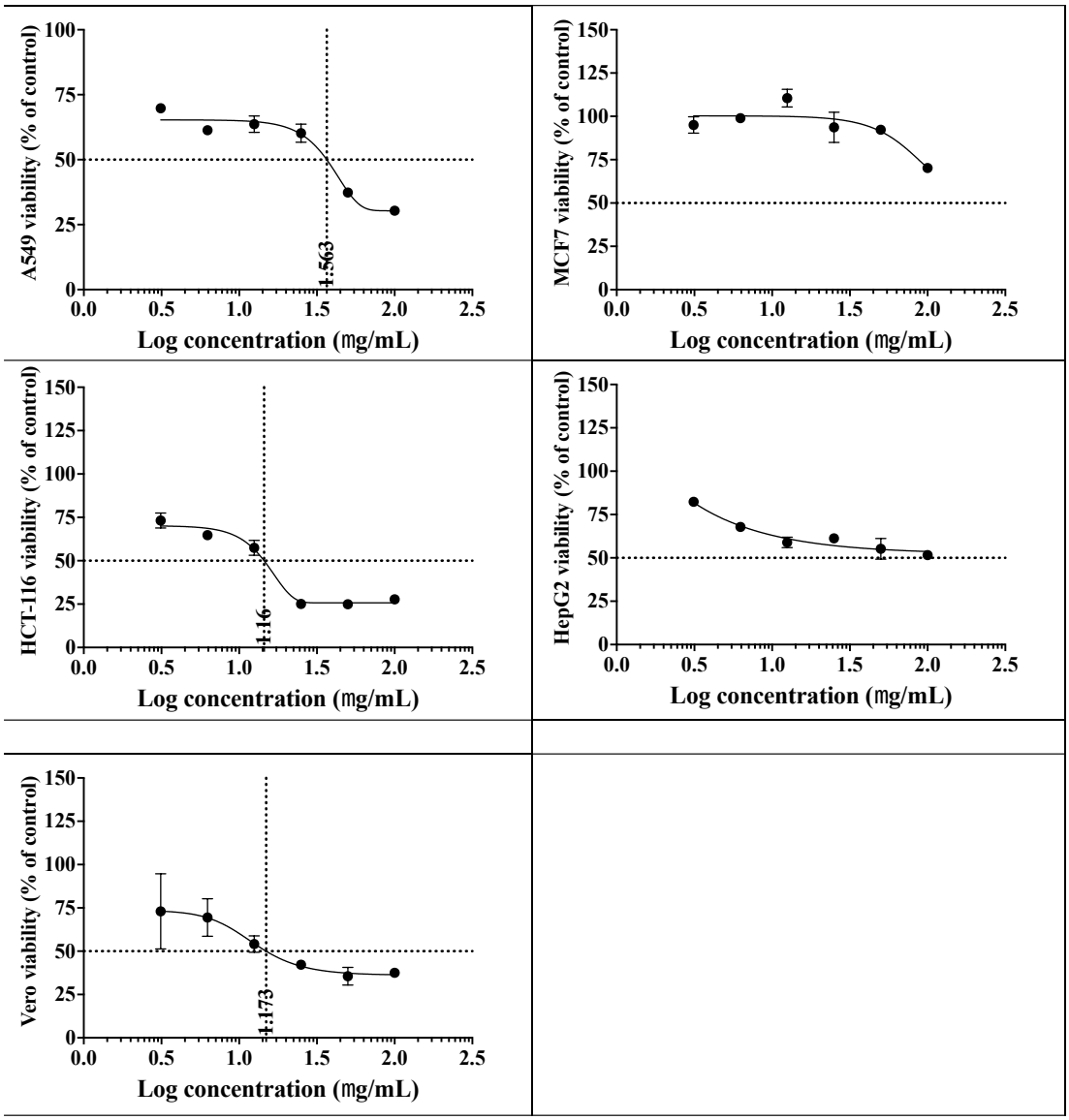

Fig. S24 The dose-response curves of **2** against MCF7, HepG2, A549, HCT116, and normal epithelial kidney of an African green monkey, Vero cell line, using MTT assay.

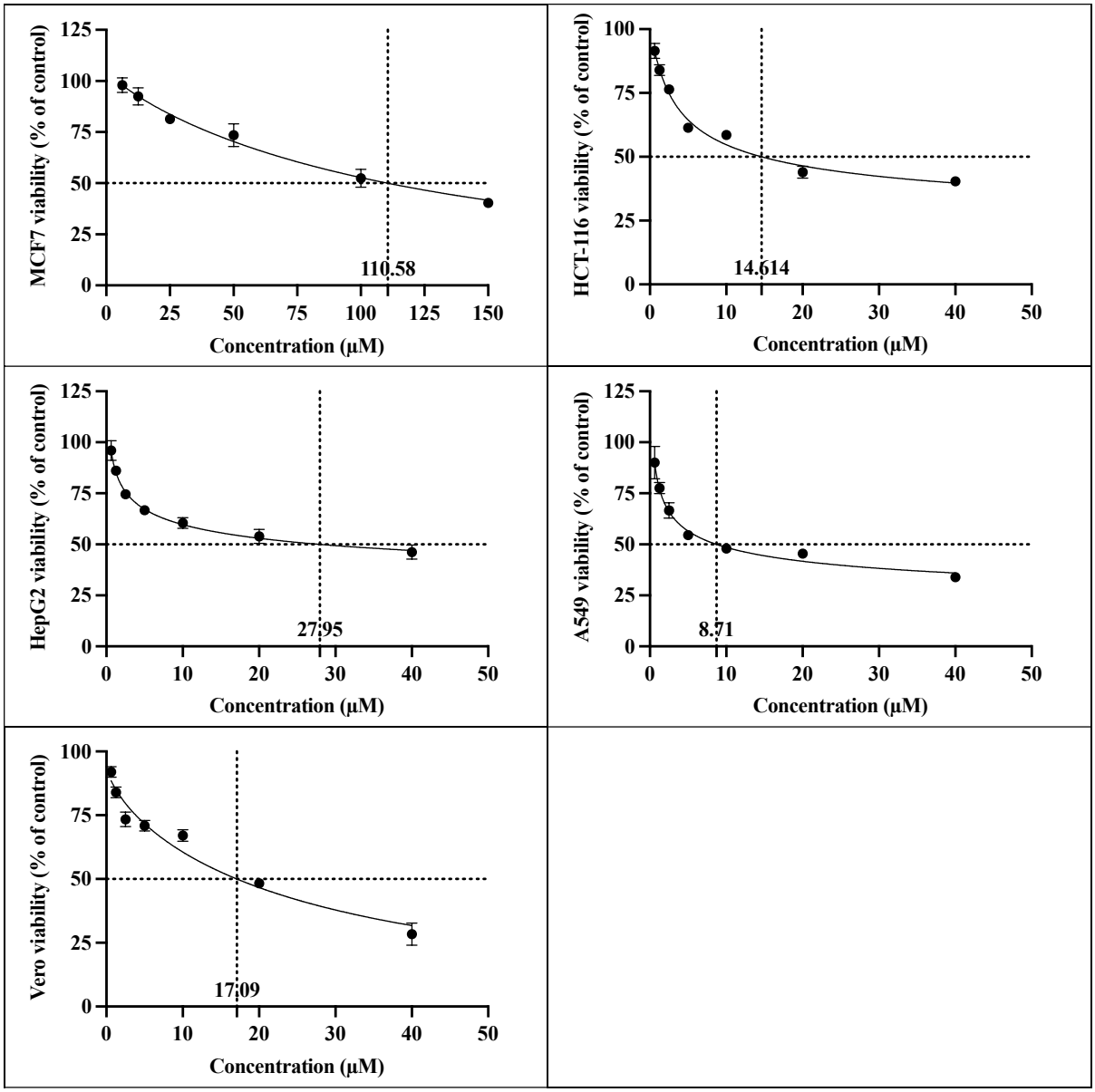

Fig. S25 The dose-response curves of cisplatin against MCF7, HepG2, A549, HCT116, and normal epithelial kidney of an African green monkey, Vero cell line, using MTT assay.

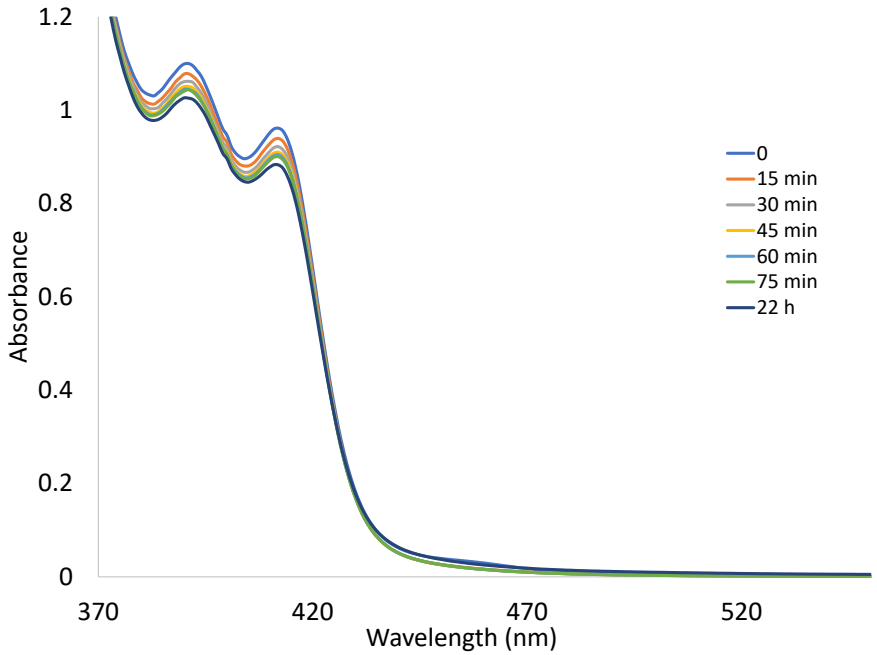

Fig. S26 UV/Vis spectral changes upon incubation of the aqueous DMSO solution of **2** for 22 h.