ESI

Luminescent Iridium(III) Dipyrrinato Complexes: Synthesis, X-ray Structures, DFT and Photocytotoxicity Studies of Glycosylated Derivatives

[#]Neha Manav,[a] [#]Mohsin Y. Lone,[a] Md Kausar Raza,[b] Jaydeepsinh Chavda,[a] Shigeki Mori[c] and Iti Gupta*[a]

[a]Indian Institute of Technology Gandhinagar, Palaj Campus, Gandhinagar, Gujarat-382355, India.
[b]Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore-560012, India
[c]Advanced Research Support Center, Ehime University, Matsuyama 790-8577, Japan
[#]Equal Contribution, *Corresponding author, e-mail: iti@iitgn.ac.in

LIST OF CONTENTS

Figure S56 IR spectrum of compound **WS-Ir6.**

Figure S57 Comparison of absorption spectra of **Ir5**, **Ir6**, and, **WS-Ir6.**

Figure S58 MALDI-MS of compound **WS-Ir7.**

Figure S59 IR spectrum of compound **WS-Ir7.**

Figure S60 Comparison of absorption spectra of **Ir5**, **Ir7**, and, **WS-Ir7.**

Figure S61 Singlet oxygen generation studies: (a) **Rose Bengal**, (c) **Ir6**, and (e) **Ir7** in water.

Figure S62 Cell Viability plots in the presence of light on A549 and HaCaT cells for **Ir6** and **Ir7** in PBS.

Figure S63 Cell Viability plots in the (dark and light conditions) on A549 cell lines treated with water soluble iridium dipyrrinates (**WS-Ir6** and **WS-Ir7**) after 24 h incubation.

Figure S64 Confocal microscopic image of (a) **Ir6** (top) and (b) **Ir7** (bottom), showing red emission in HaCaT cells after 24-hour incubation in dark.

Figure S65 DFT-D3 based geometry optimized structure of iridium dipyrrinates **Ir1-Ir8.**

Table S3. Calculated electronic excitation energies and corresponding orbitals involved in the transition for **Ir1-Ir8** using CPCM-TD-BMK/6-311+ G (2d,p) level of approximation

Table S4 B3LYP/6-31G//B3LYP/LANL2DZ gas phase optimized coordinates of complexes **Ir1-Ir8.**

Table S1. X-ray crystal structure parameters of **Ir1** and **Ir4** complexes.

Complex	**Ir1**	**Ir4**
Empirical Formula	$C_{35}H_{25}IrN_4S$	$C_{42}H_{28}Cl_3IrN_6S_2$
Crystal System	Monoclinic	Triclinic
Space Group	P21/n (no. 14)	P-1 (no. 2)
R_1 (I >2.00σ(I))	0.0345	0.0605
${}_wR_2$ (All reflections)	0.0675	0.1351
GOF	0.976	0.974
Lattice Parameters	a = 14.5183(4) Å b =9.2894(3) Å c = 20.2339(6) Å β = 93.517(3)° V = 2723.73(14) Å^3	a = 9.3922(6) Å b =13.6988(11) Å c = 16.1785(6) Å β = 106.405(5)° V = 1826.3(2) Å^3
Z	4	2
T	-173.0°C	-173.0°C
D_{calc}	1.770 g/cm^3	1.781 g/cm^3
F_{000}	1424.0	964.0
$2\theta_{max}$	4.03 to 55.99°	4.60 to 51.99°
No. of Reflections Measured	Total: 49498 Unique: 6571 (Rint = 0.0835)	Total: 50381 Unique: 7164 (Rint = 0.1403)
CCDC number	2022646	2022648

Table S2. Selected bond distances, bond angles and dihedral angles observed in the crystals and the DFT optimized structures of **Ir1** and **Ir4**.

Complex	Dihedral Angles (°)	Bond Angles (°)	Bond Distances (Å)	
Ir1 (Crystal structure)	C26–C27–C32–S1 50.61(5) C28–C27–C32–C33 52.33(8)	N3–Ir–N4 85.8(1) N3-Ir-C18 175.6(1) N1–Ir–N2 173.8(1) N4-Ir-C7 172.3(1)	Ir-N1 2.044(3) Ir–N2 2.044(3) Ir-N3 2.126(3) Ir-N4 2.127(3)	Ir-C7 2.018(4) Ir-C18 2.010(4) C27-C32 1.483 S1-C32 1.742(5)
Ir1 (Optimized structure)	C26–C27–C32–S1 63.62 C28–C27–C32–C33 60.97	N3–Ir–N4 85.1 N3-Ir-C18 174.7 N1–Ir–N2 174.9 N4-Ir-C7 174.7	Ir-N1 2.077 Ir–N2 2.078 Ir-N3 2.192 Ir-N4 2.196	Ir-C7 2.028 Ir-C18 2.028 C27-C32 1.485 S1-C32 1.754
Ir4 (Crystal structure)	C26–C27–C32–S1 75.96(1) C28–C27–C32–C33 73.46(1)	N3–Ir–N4 87.2(3) N3-Ir-C18 175.0(3) N1–Ir–N2 174.2(3) N4-Ir-C7 176.6(3)	Ir-N1 2.036(6) Ir–N2 2.042(6) Ir-N3 2.115(7) Ir-N4 2.142(7)	Ir-C7 2.020(1) Ir-C18 2.019(9) C27-C32 1.487 (1) S1-C32 1.709(7)
Ir4 (Optimized structure)	C26–C27–C32–S1 62.37 C28–C27–C32–C33 60.47	N3–Ir–N4 85.10 N3-Ir-C18 174.5 N1–Ir–N2 174.7 N4-Ir-C7 174.9	Ir-N1 2.077 Ir–N2 2.076 Ir-N3 2.196 Ir-N4 2.195	Ir-C7 2.028 Ir-C18 2.028 C27-C32 1.484 S1-C32 1.748

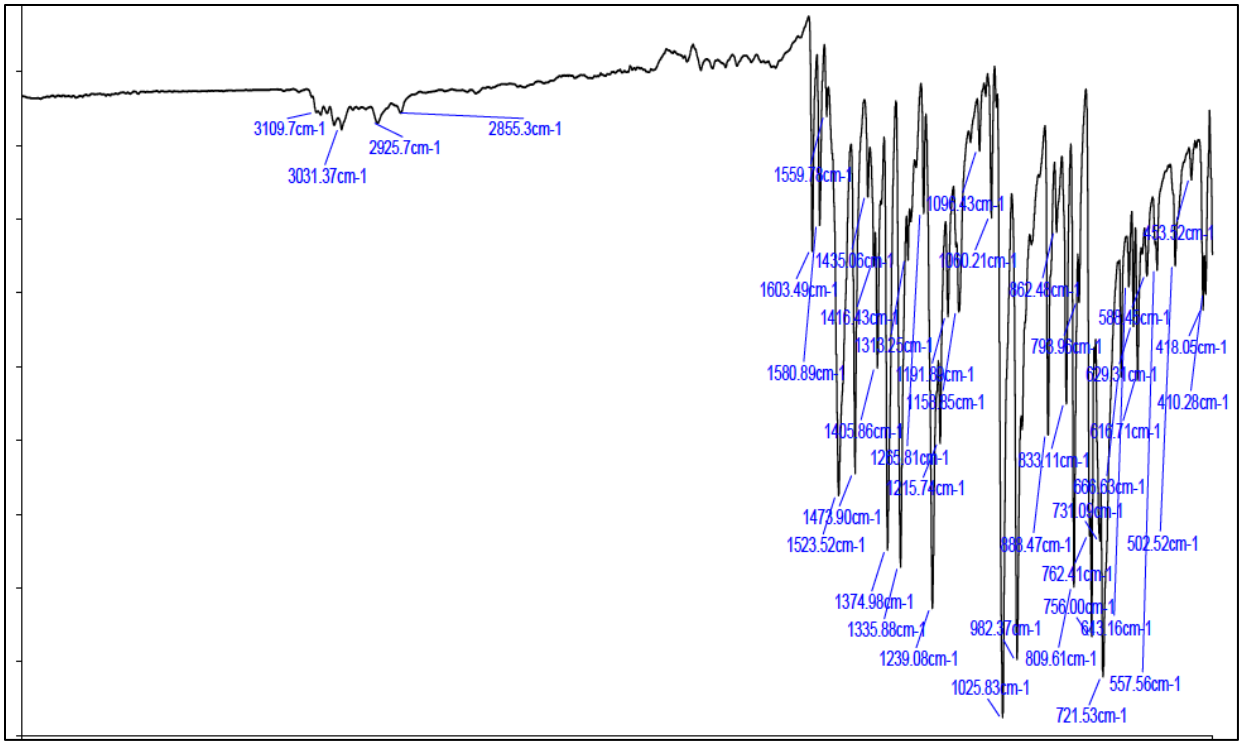


Figure S1 IR spectrum of compound **Ir1**.

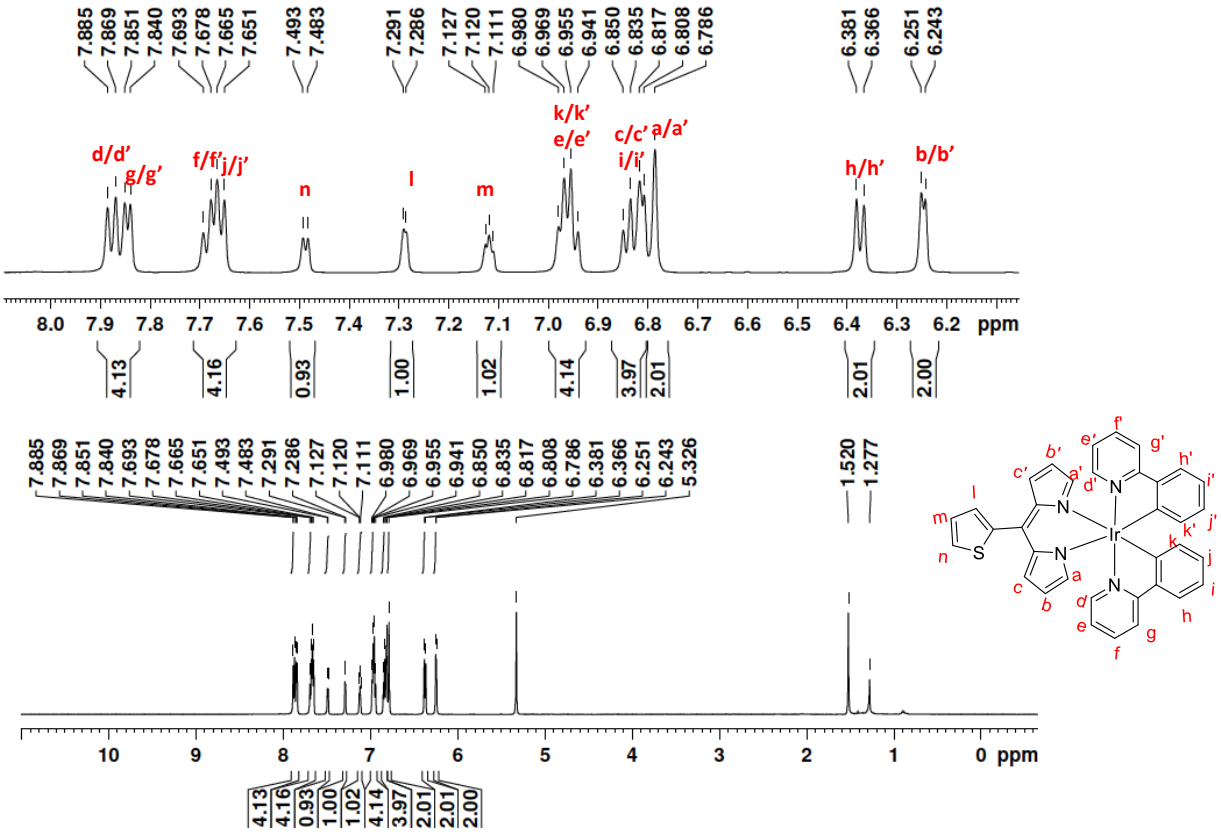


Figure S2 ^{1}H NMR of compound **Ir1** in CD_2Cl_2.

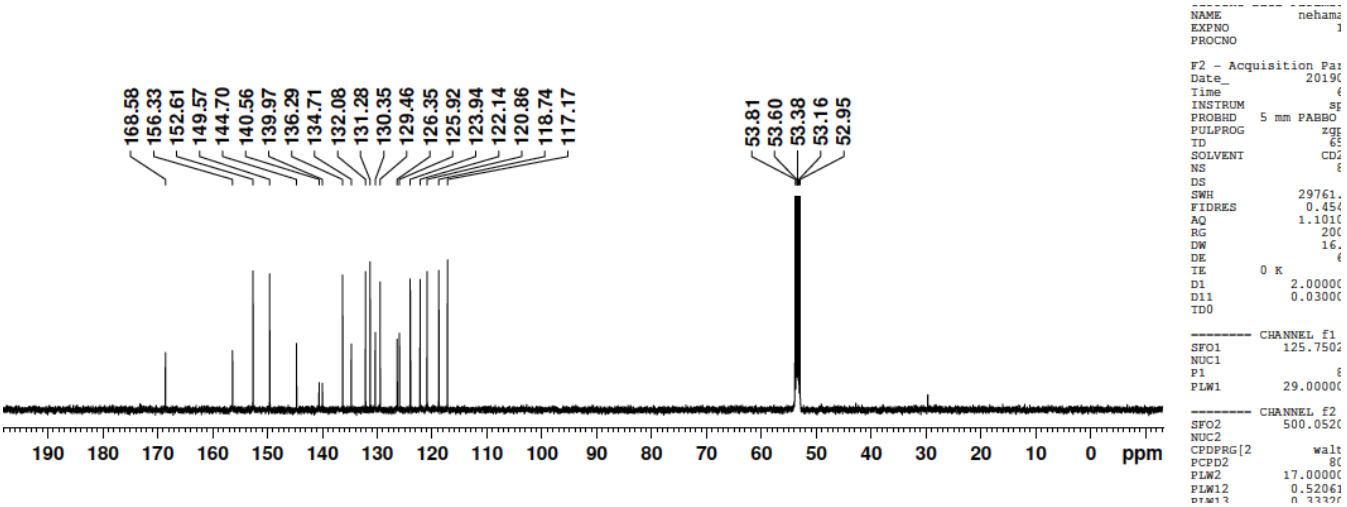


Figure S3 ^{13}C NMR of compound **Ir1** in CD_2Cl_2.

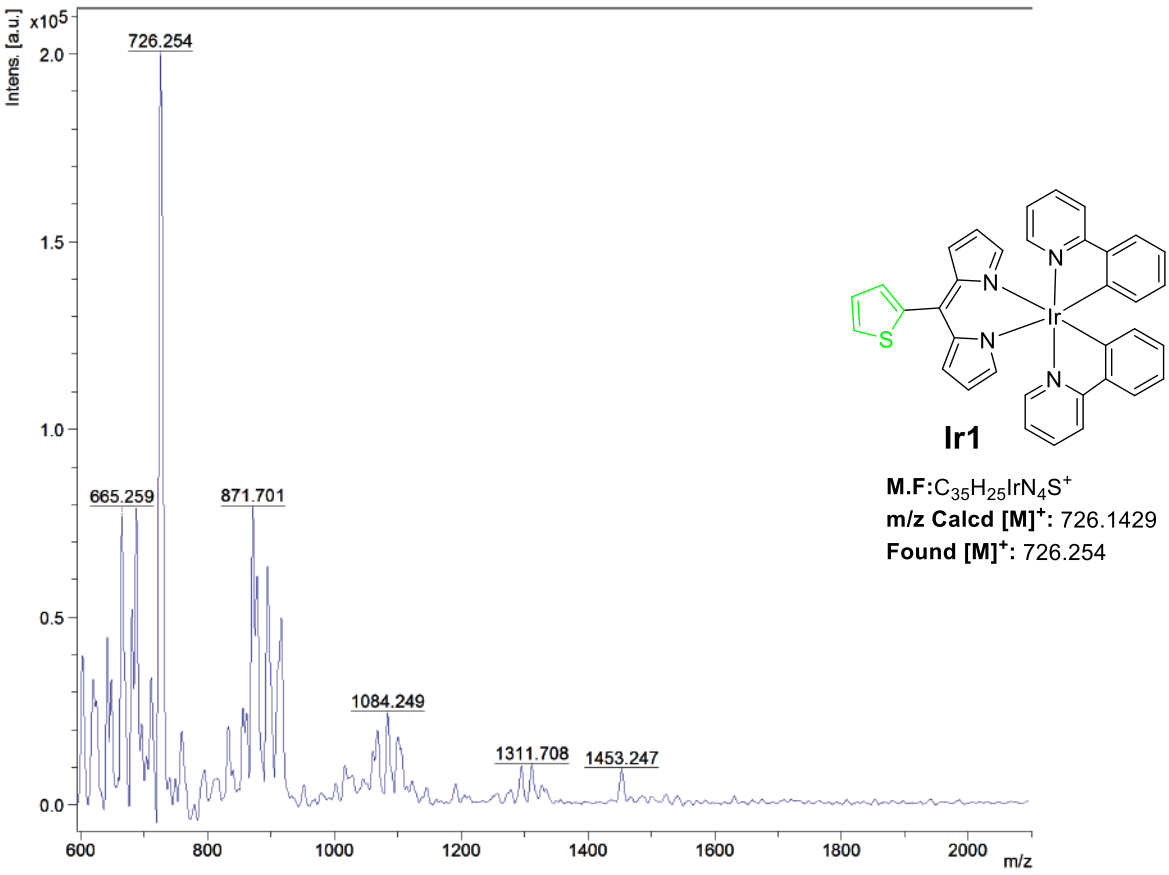


Figure S4 MALDI-MS of compound **Ir1**.

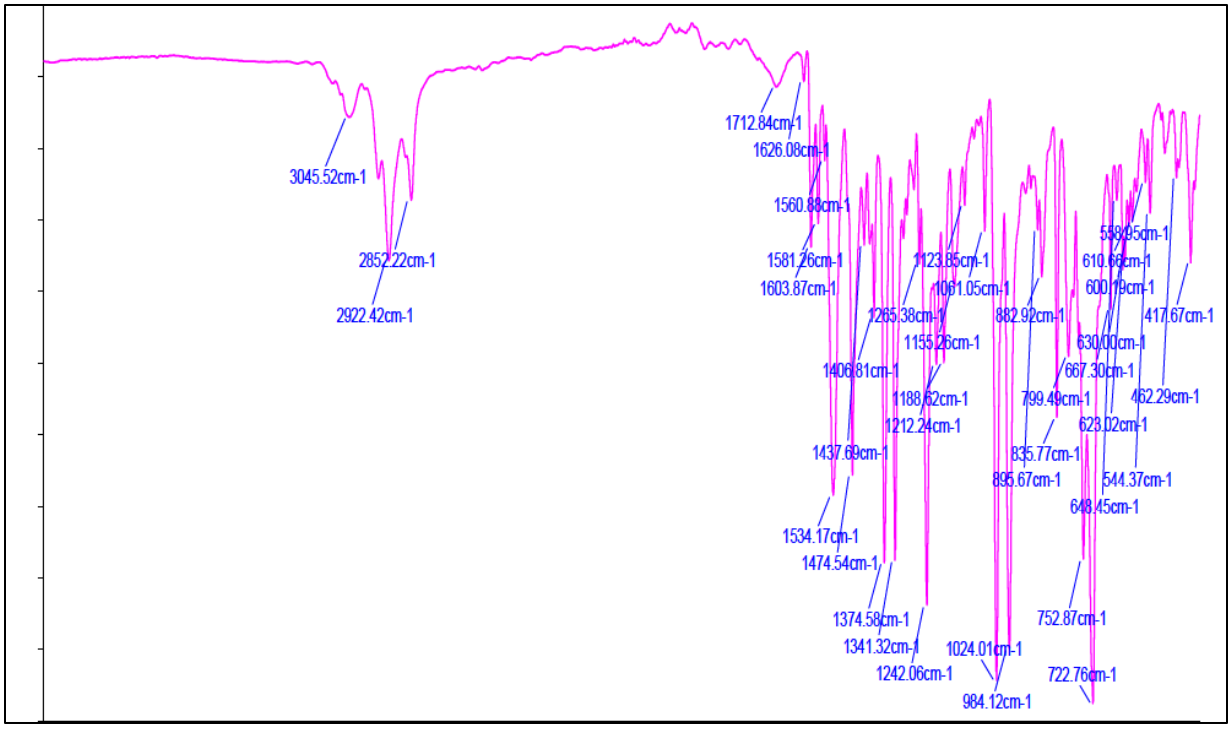


Figure S5 IR spectrum of compound **Ir2**.

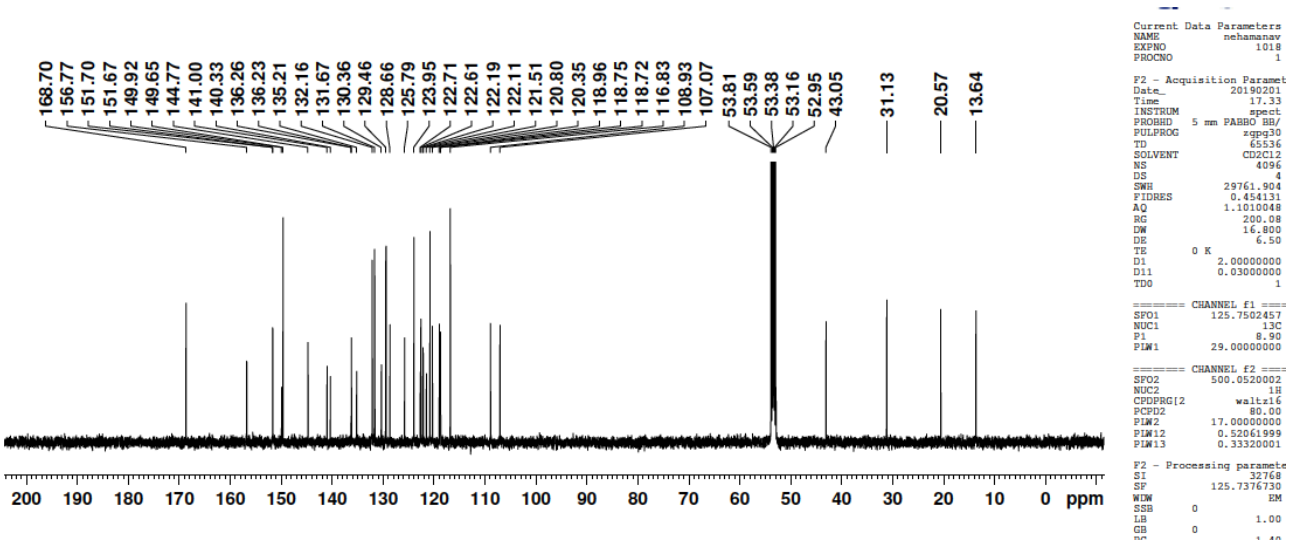


Figure S6 ^{13}C NMR of compound **Ir2** in CD_2Cl_2.

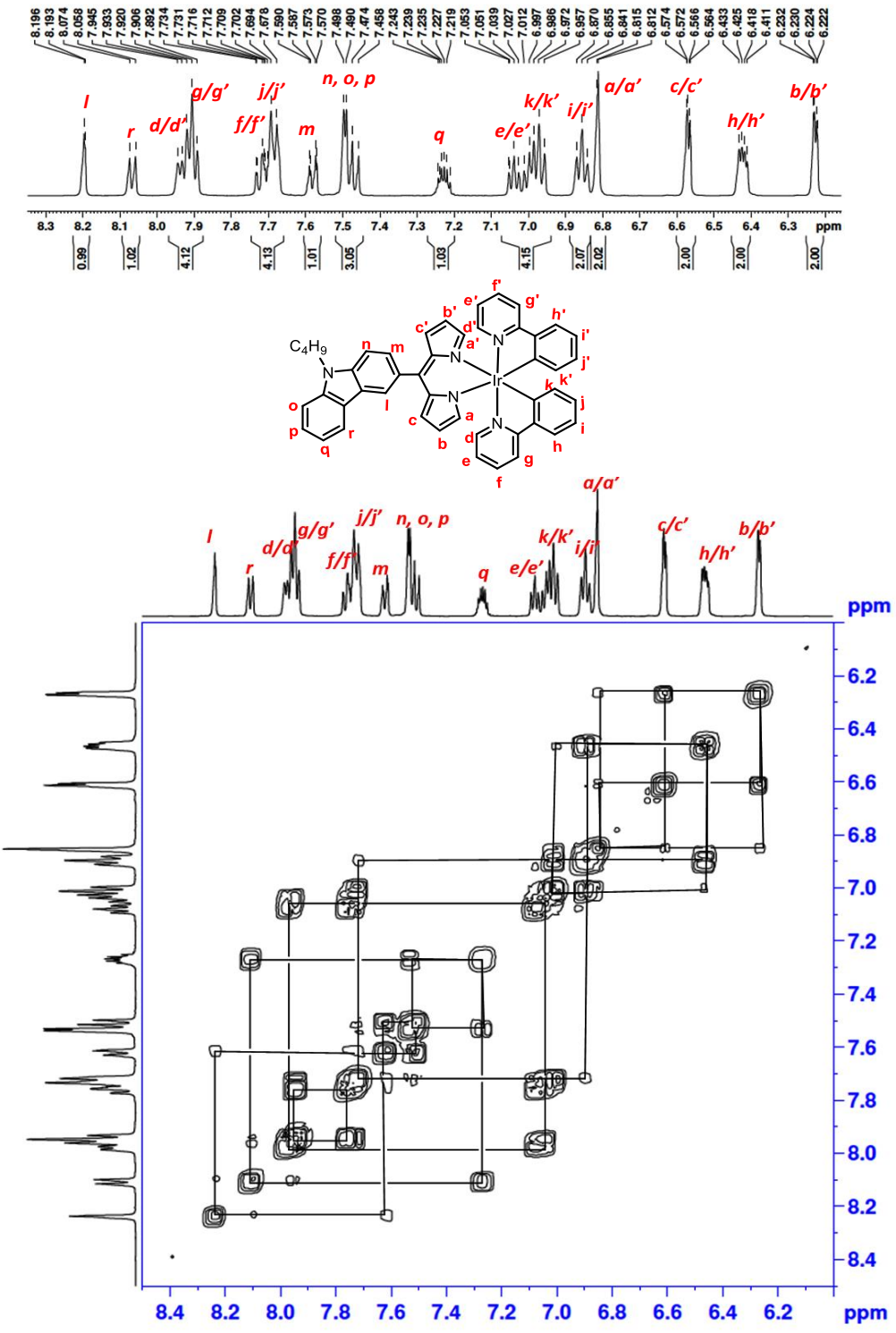


Figure S7. Partial ^{1}H NMR and ^{1}H-^{1}H COSY spectra of **Ir2,** recorded in CD_2Cl_2.

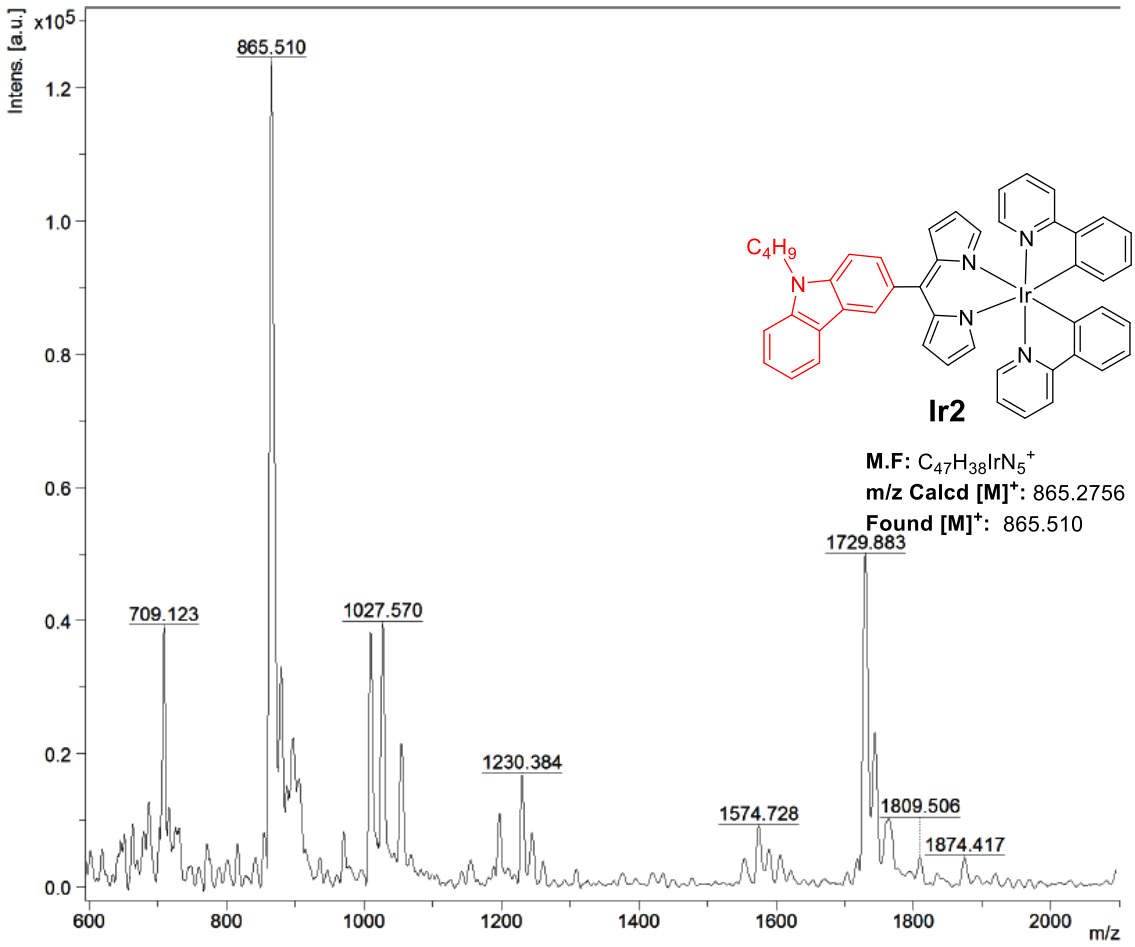


Figure S6 MALDI-MS of compound **Ir2**.

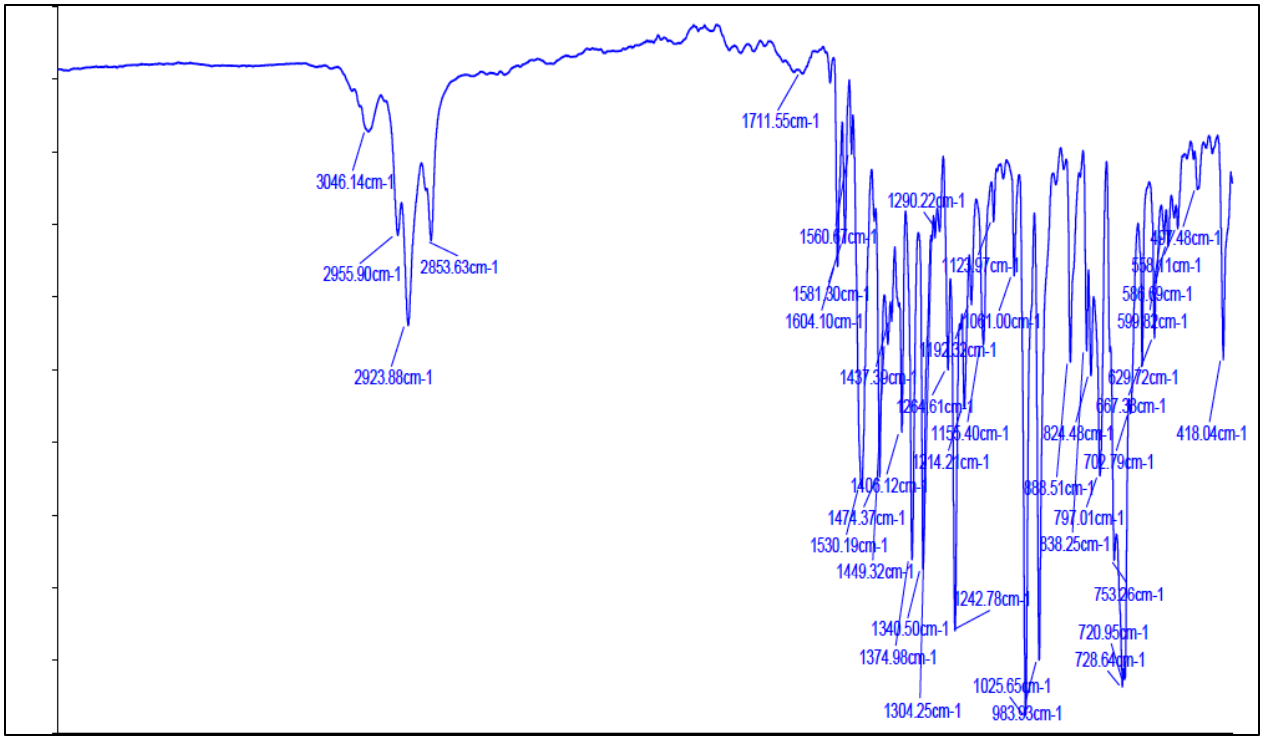


Figure S7 IR spectrum of compound **Ir3**.

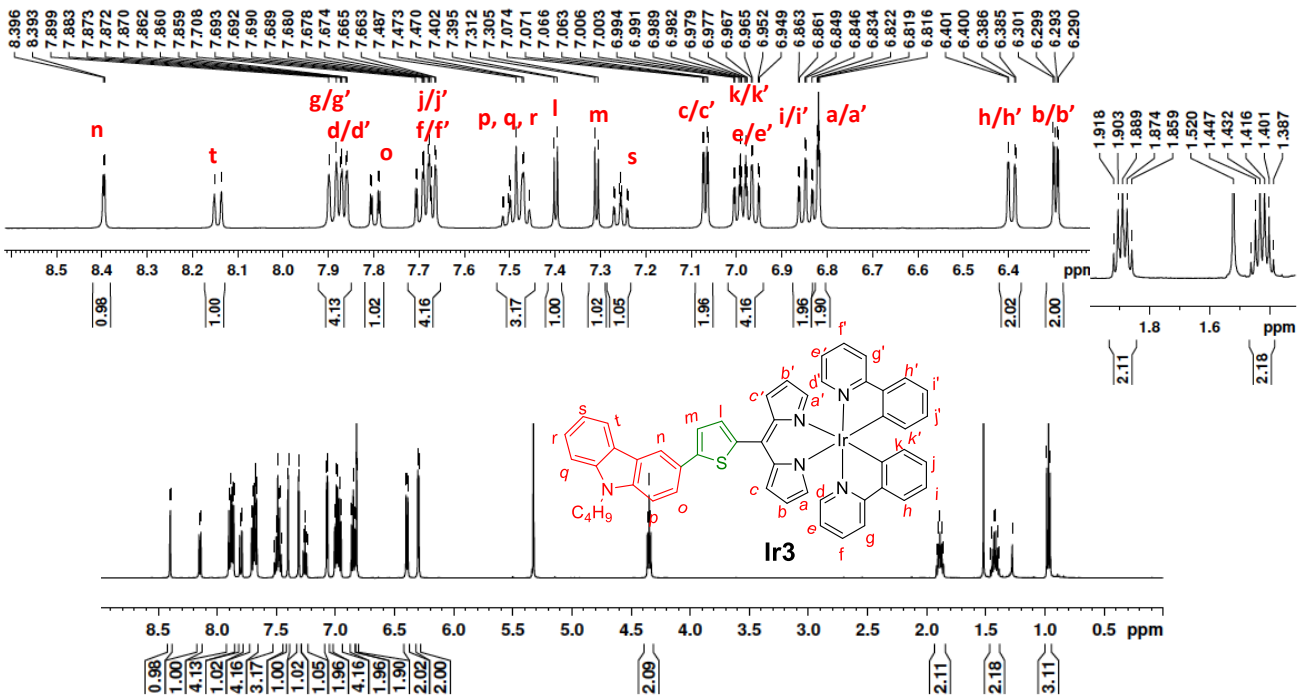


Figure S8 ^{1}H NMR of compound **Ir3** in CD_2Cl_2.

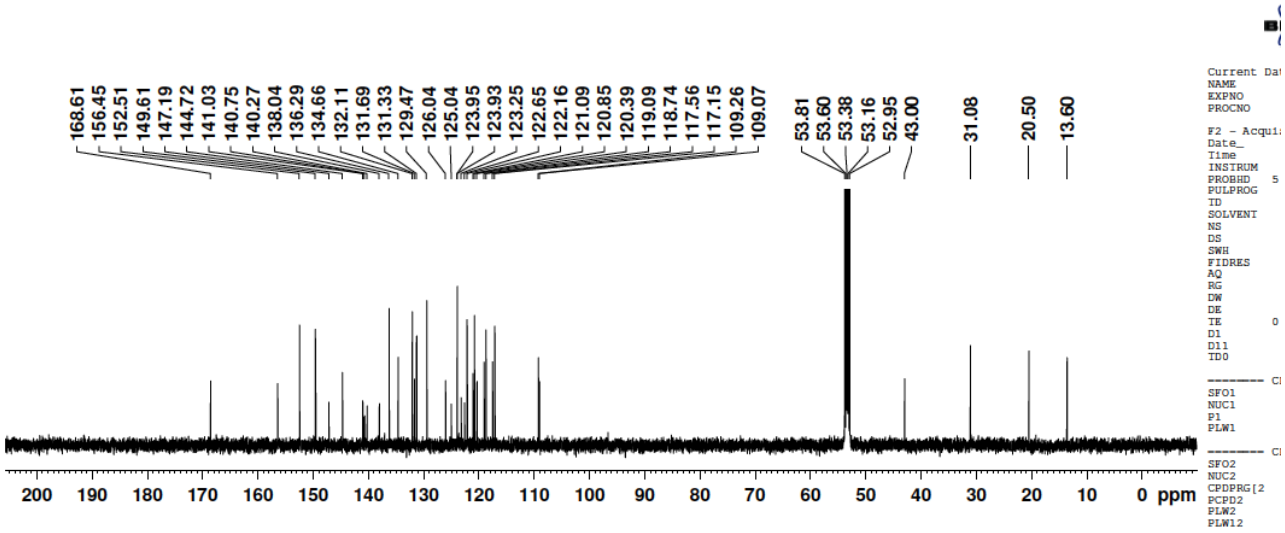


Figure S9 ^{13}C NMR of compound **Ir3** in CD_2Cl_2.

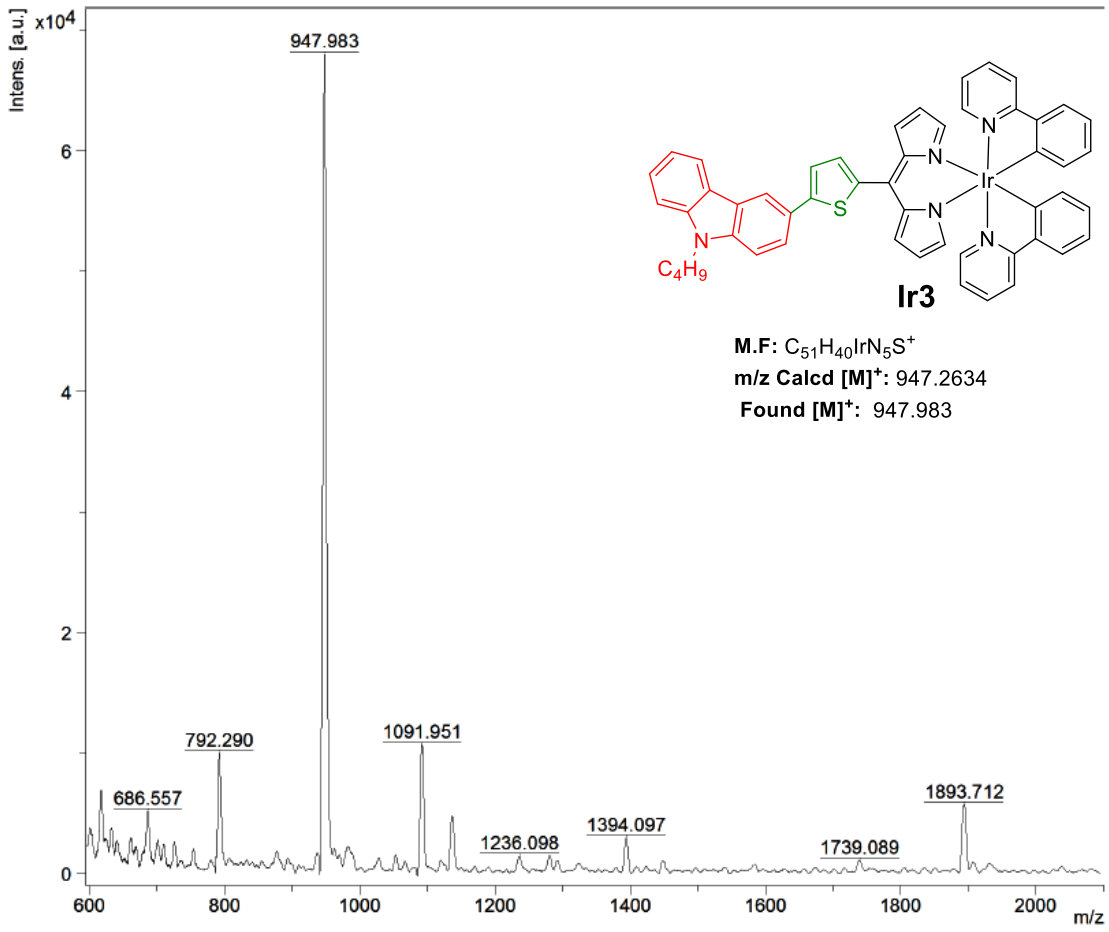


Figure S10 MALDI-MS of compound **Ir3**.

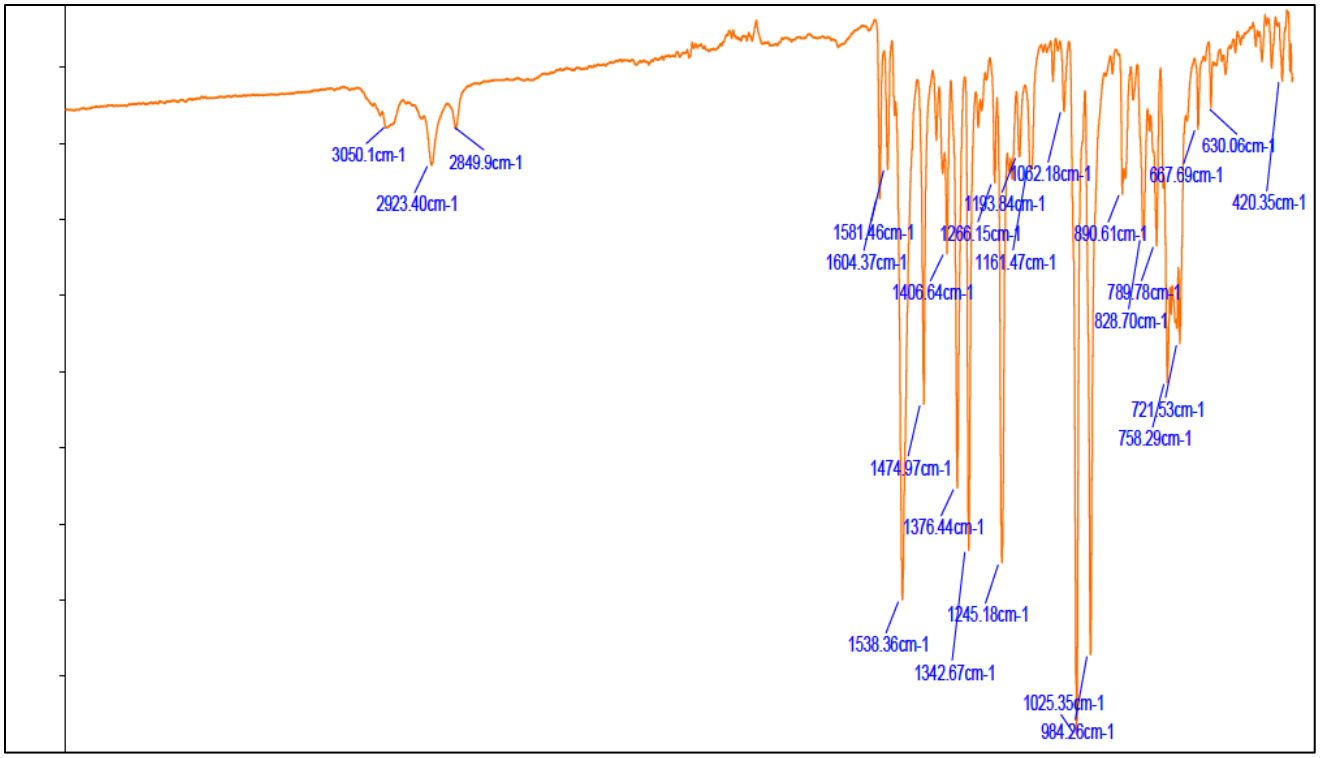


Figure S11 IR spectrum of compound **Ir4**.

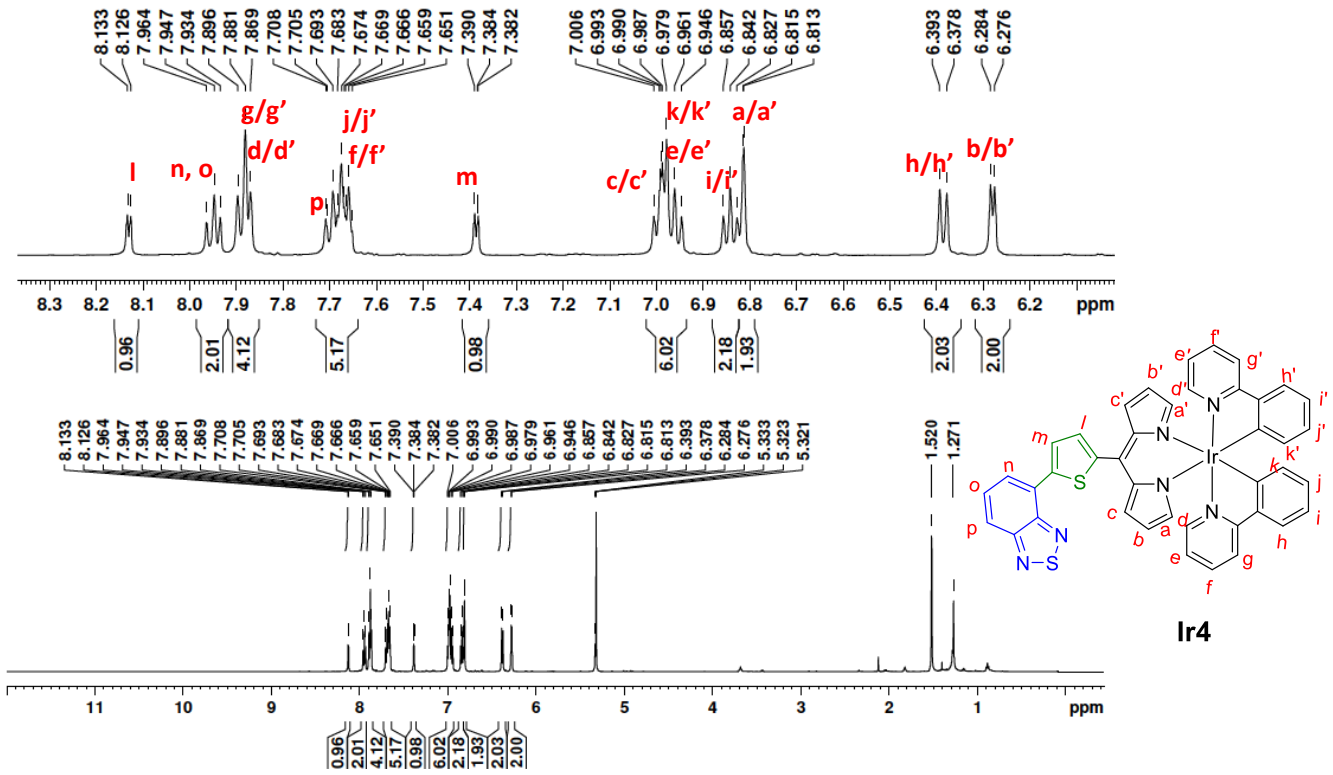


Figure S12 ^{1}H NMR of compound **Ir4** in CD_2Cl_2.

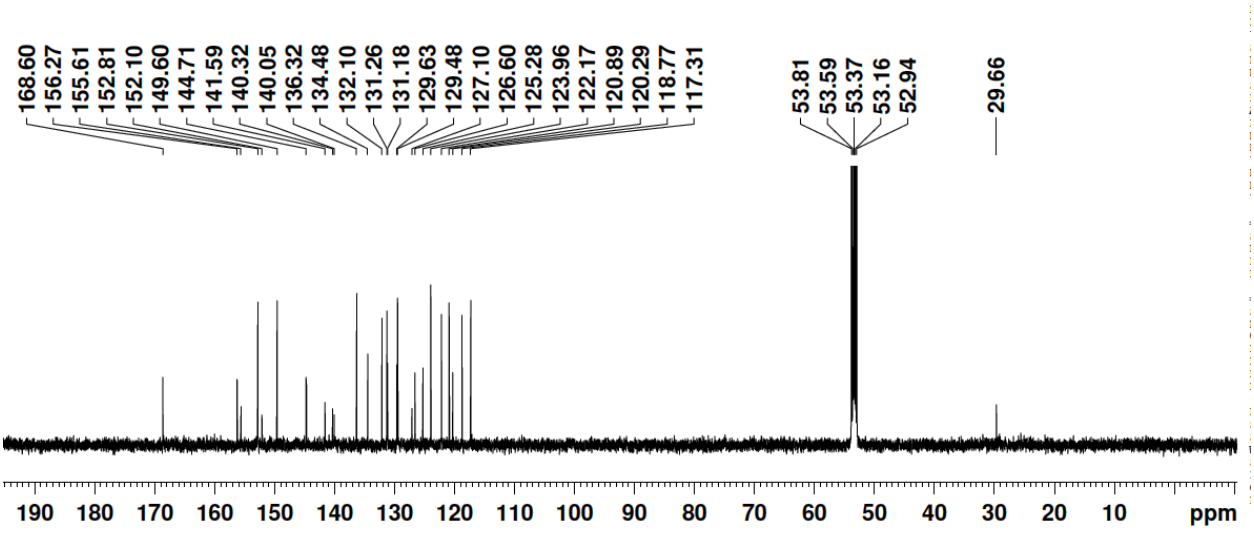


Figure S13 ^{13}C NMR of compound **Ir4** in CD_2Cl_2.

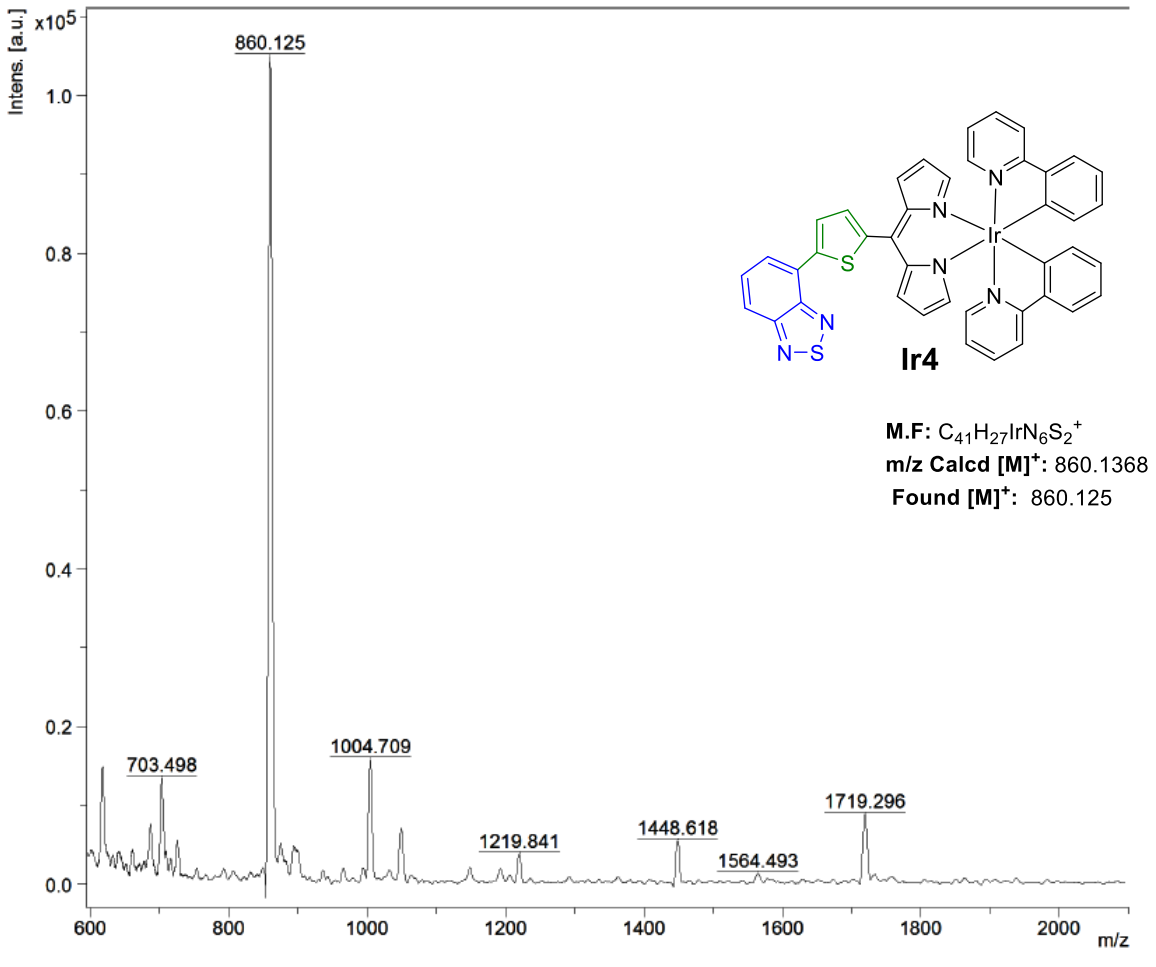


Figure S14 MALDI-MS of compound **Ir4**.

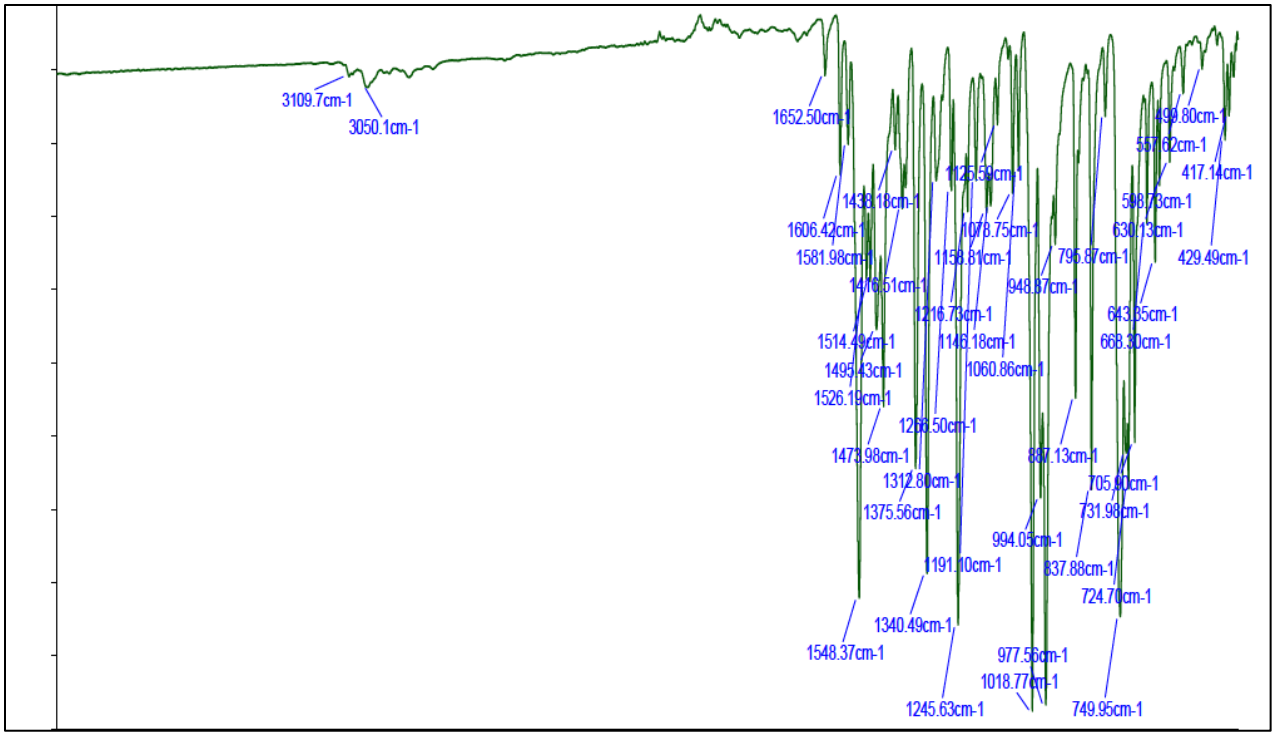


Figure S15 IR spectrum of compound **Ir5**.

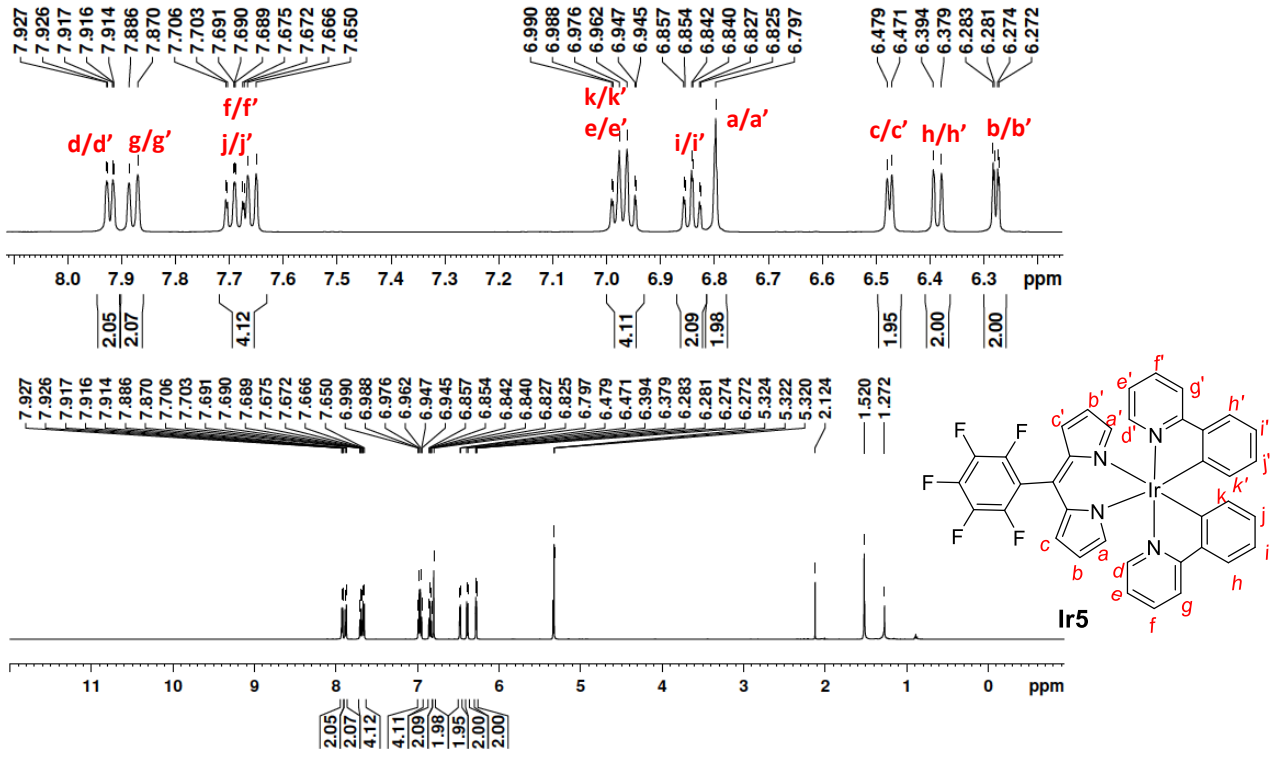


Figure S16 ^{1}H NMR of compound **Ir5** in CD_2Cl_2.

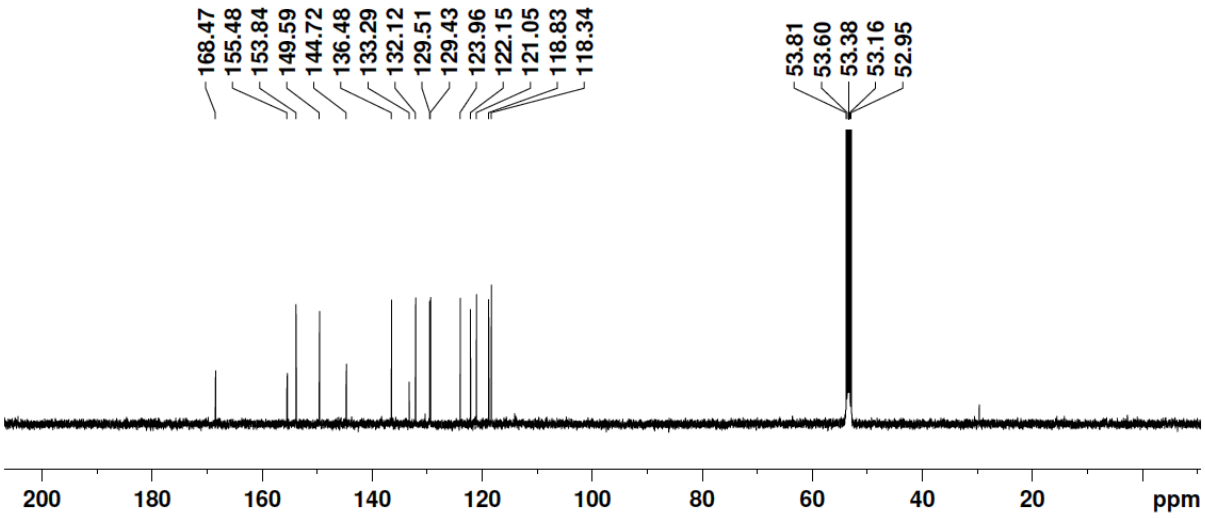


Figure S17 ^{13}C NMR of compound **Ir5** in CD_2Cl_2.

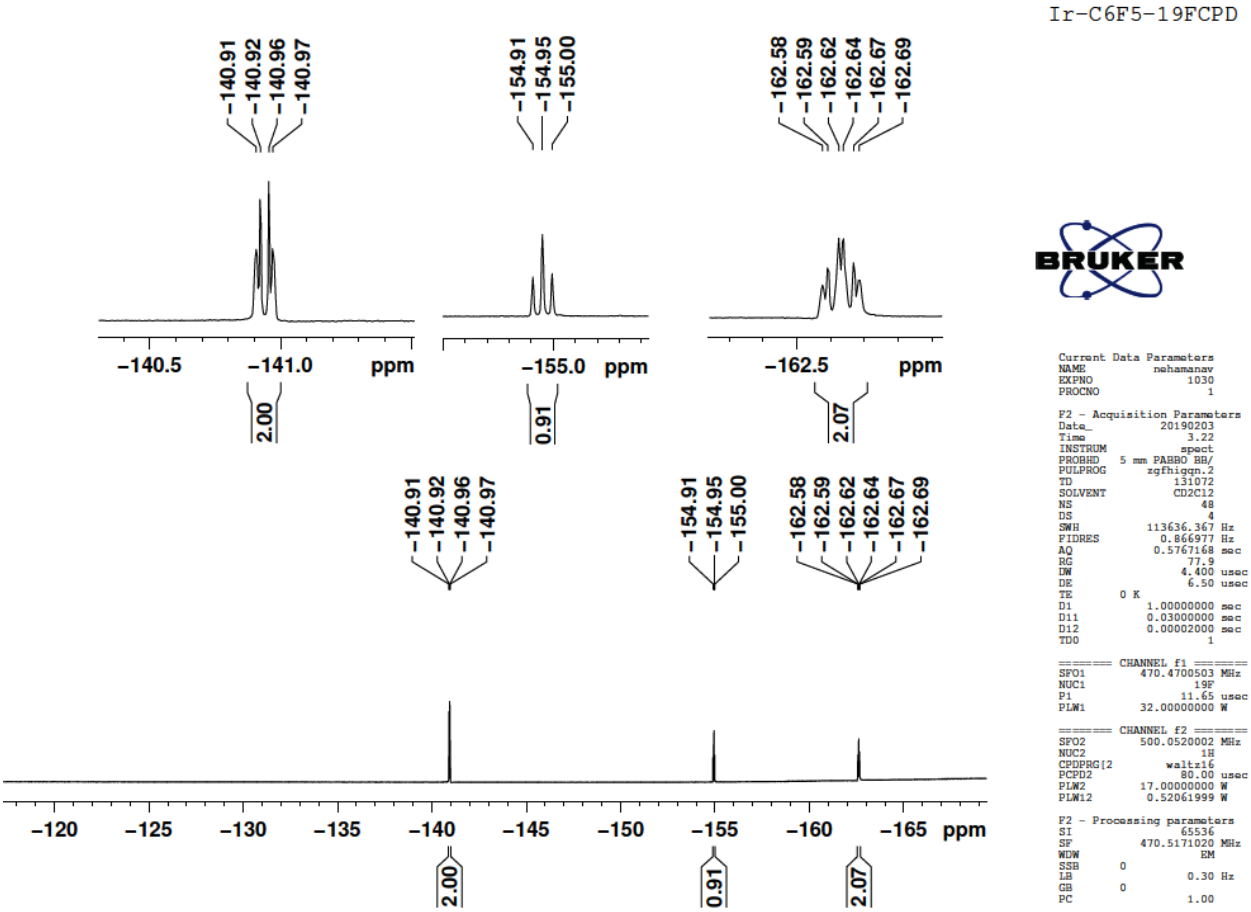


Figure S18 ^{19}F NMR of compound **Ir5** in CD_2Cl_2.

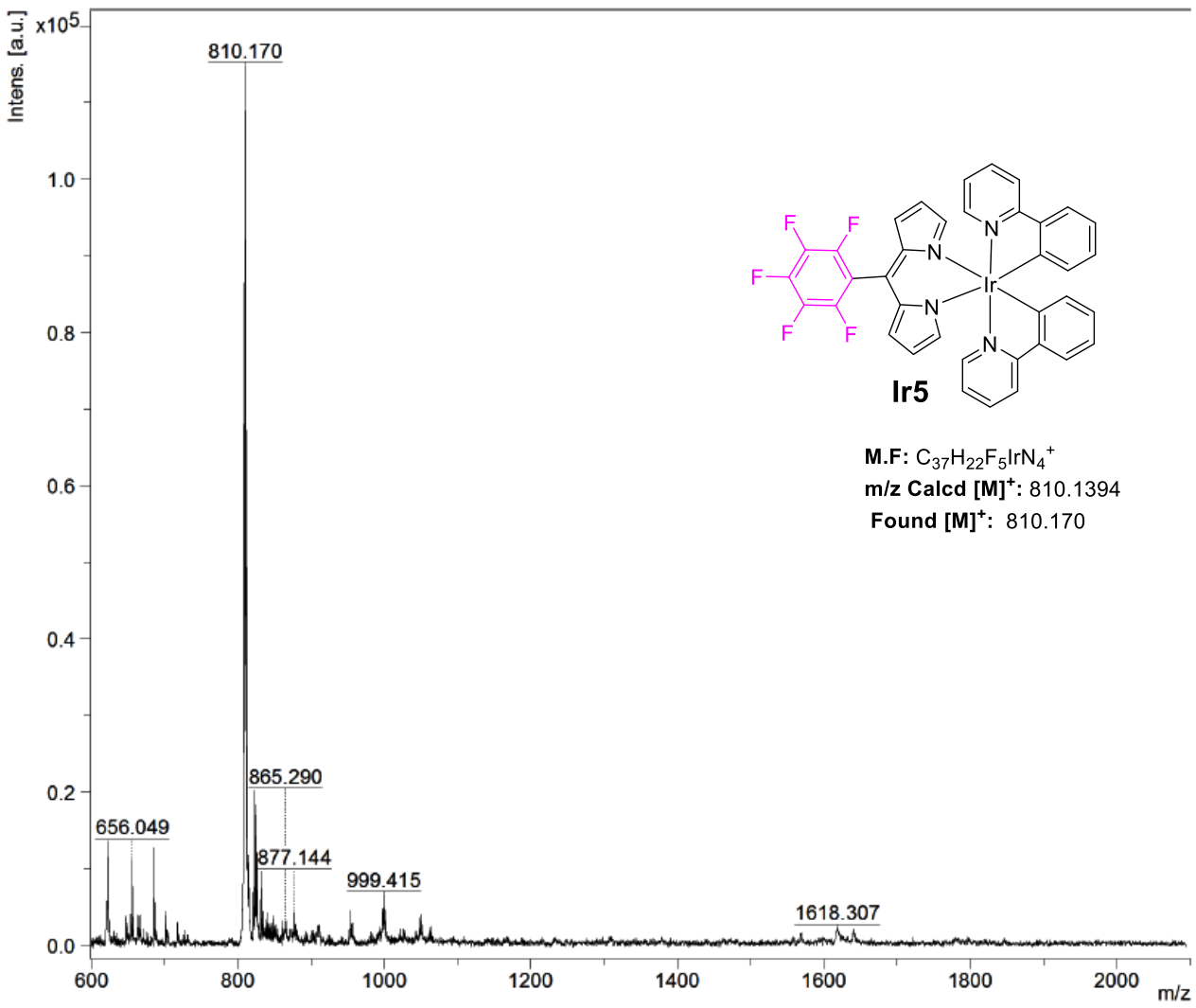


Figure S19 MALDI-MS of compound **Ir5**.

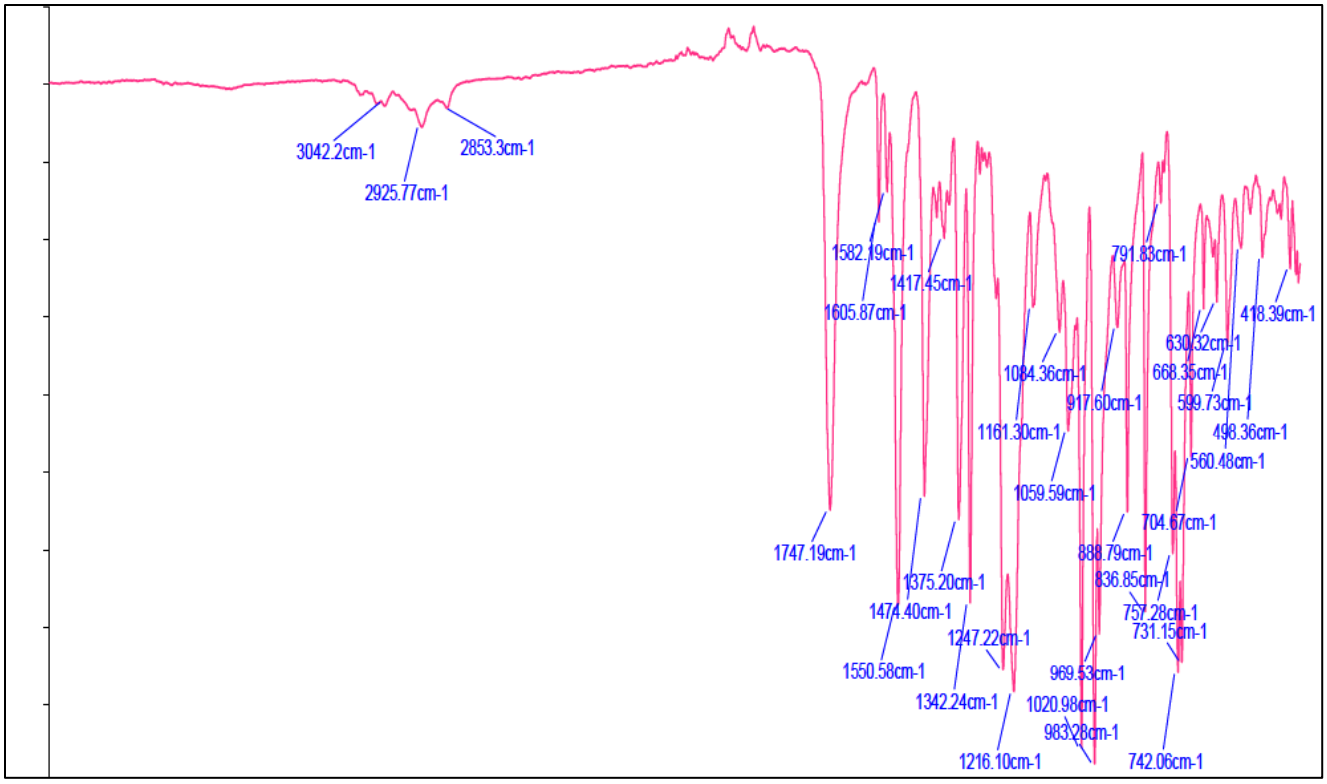


Figure S20 IR spectrum of compound **Ir6**.

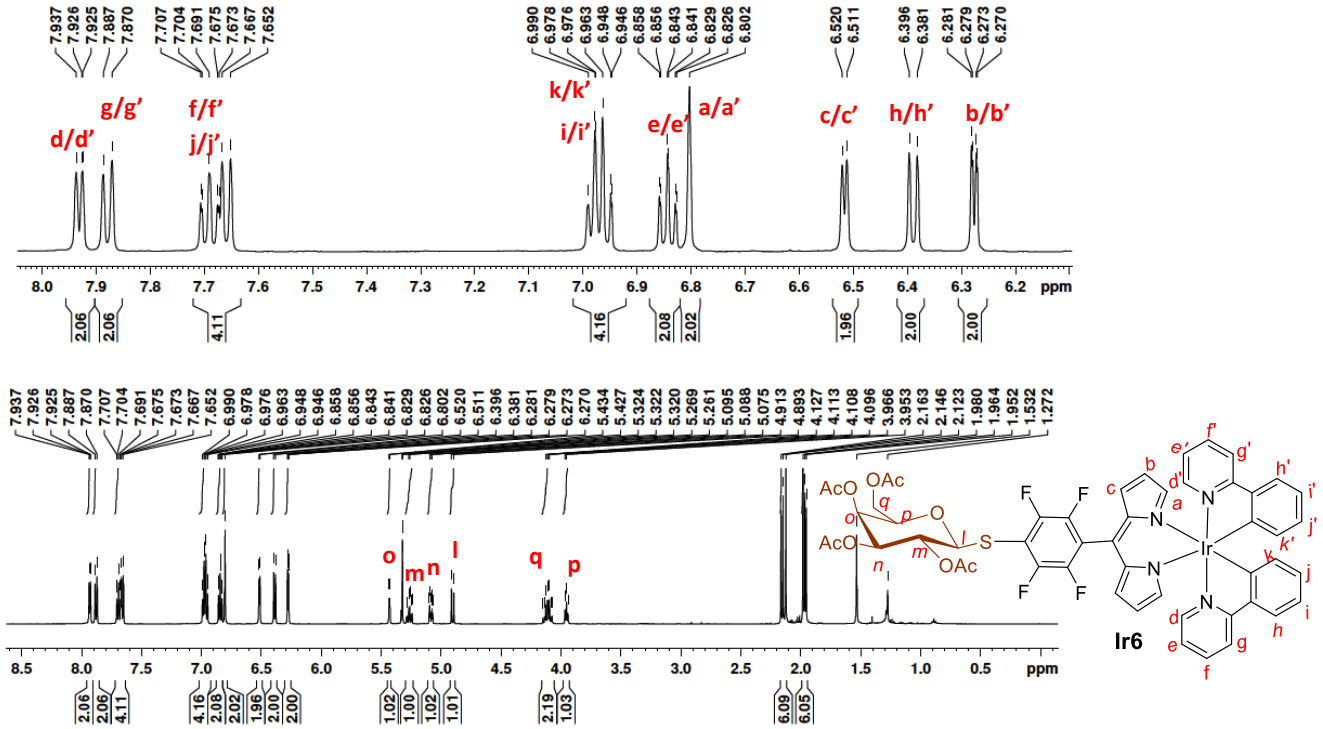


Figure S21 ^{1}H NMR of compound **Ir6** in CD_2Cl_2.

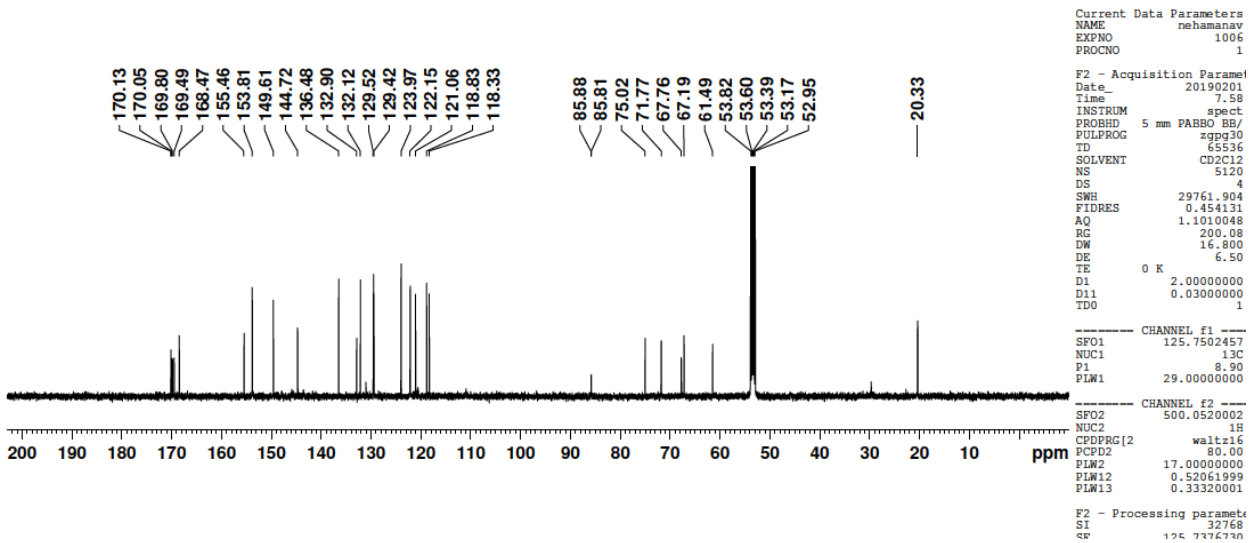
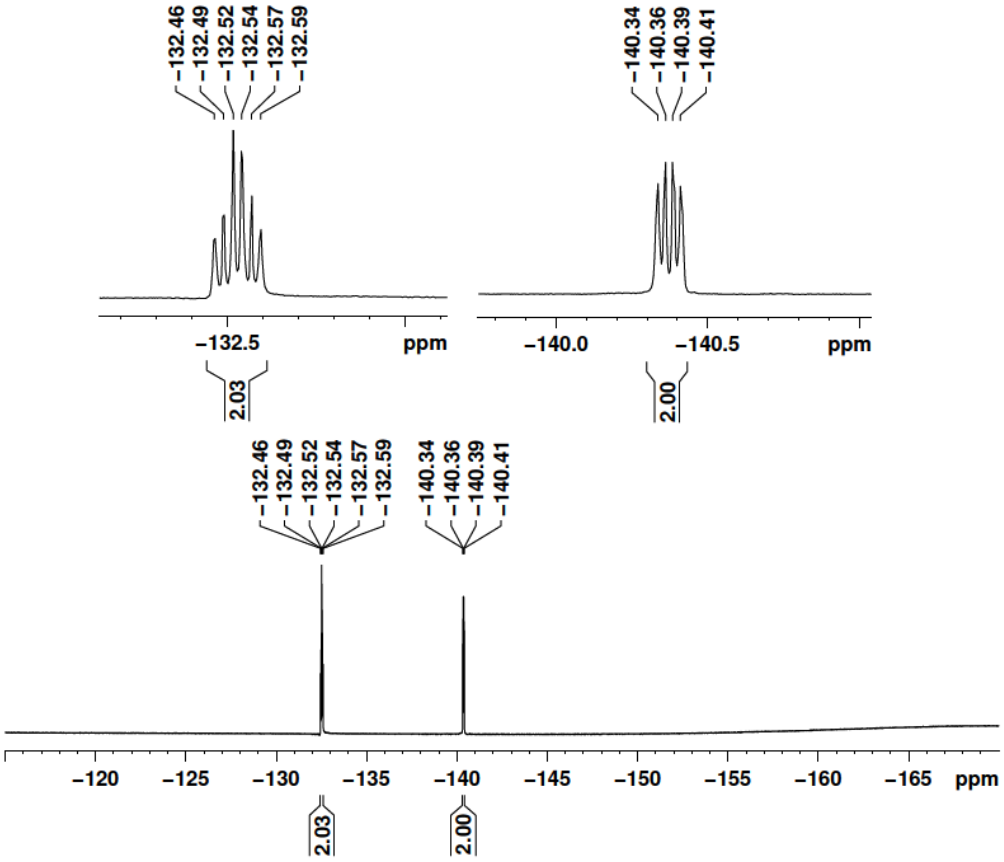


Figure S22 ^{13}C NMR of compound **Ir6** in CD_2Cl_2.



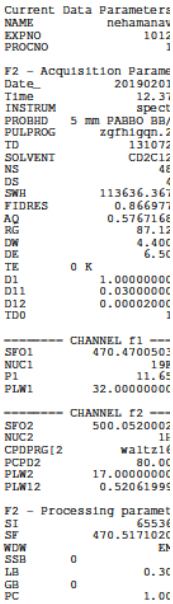


Figure S23 ^{19}F NMR of compound **Ir6** in CD_2Cl_2.

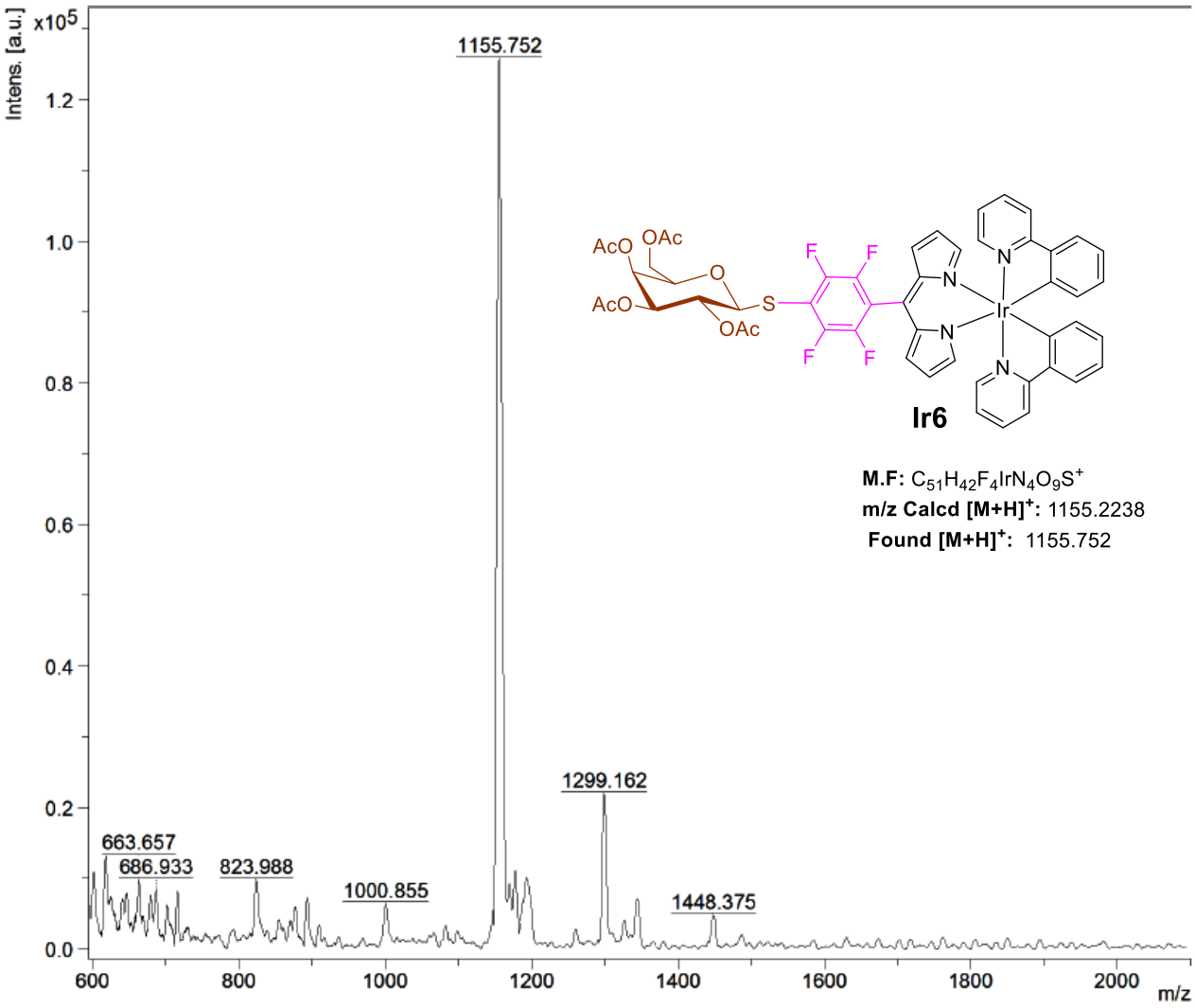


Figure S24 MALDI-MS of compound **Ir6**.

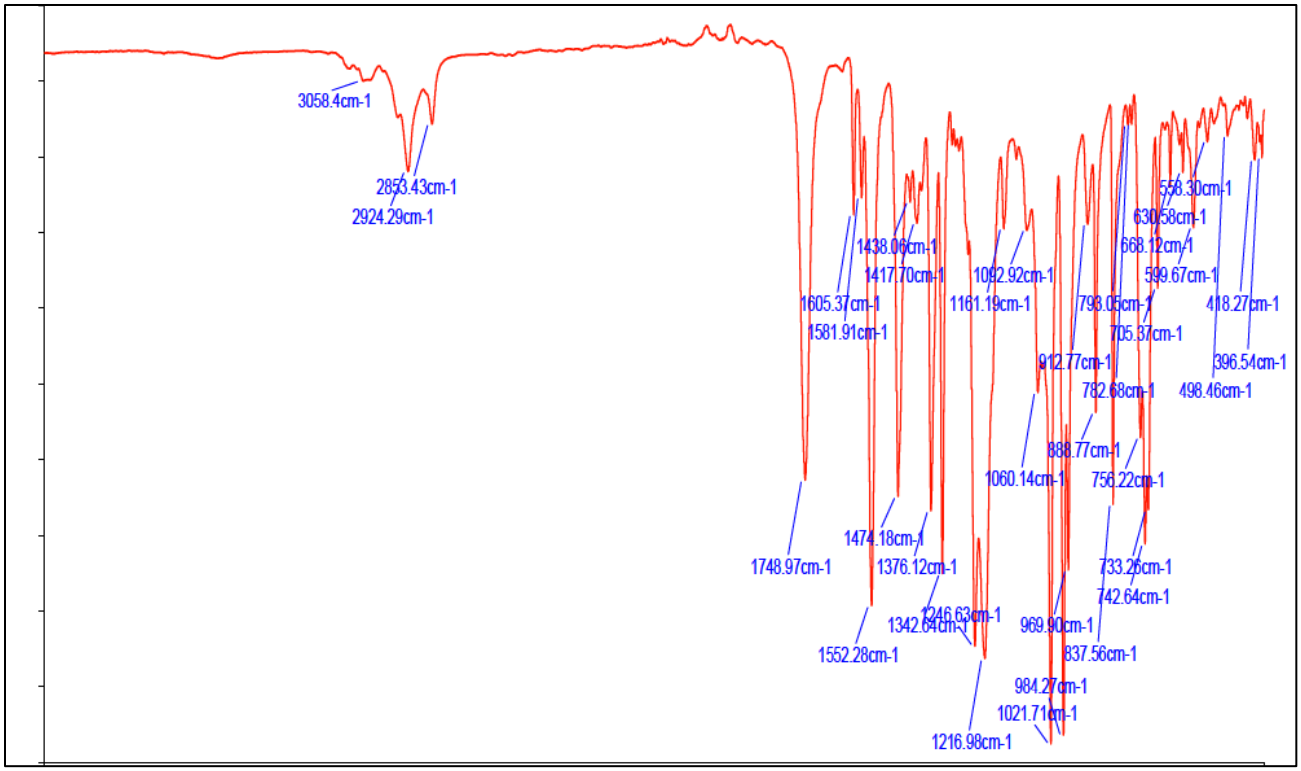


Figure S25 IR spectrum of compound **Ir7**.

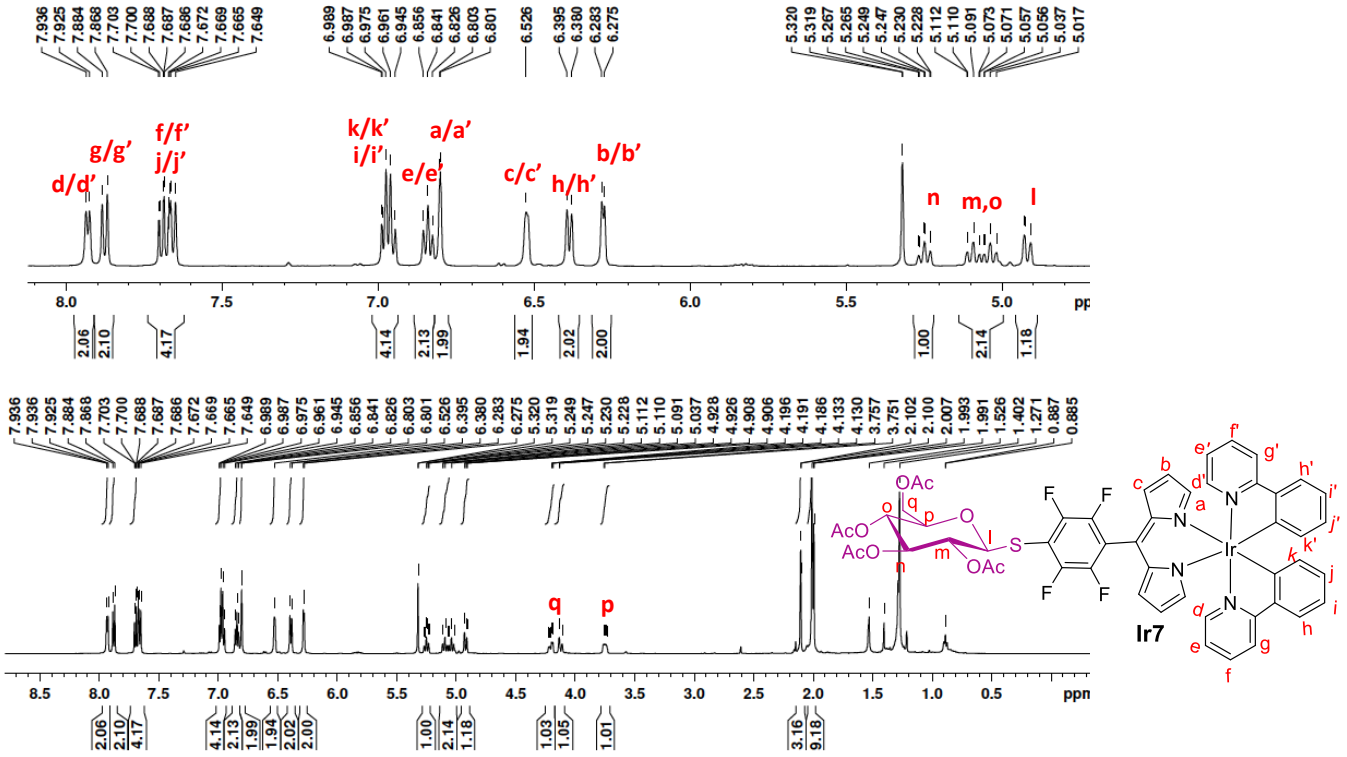


Figure S26 ^{1}H NMR of compound **Ir7** in CD_2Cl_2.

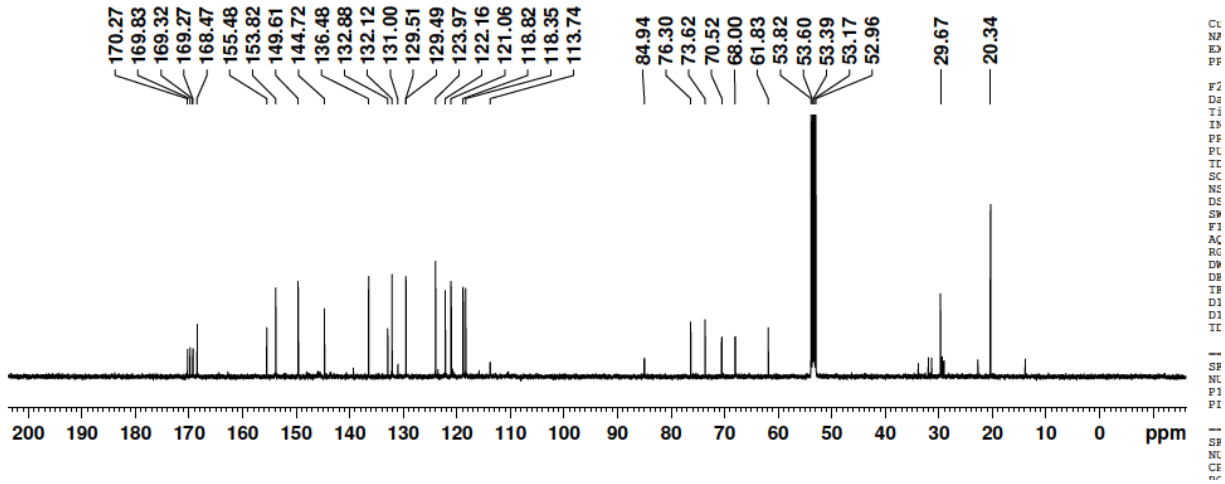


Figure S27 ^{13}C NMR of compound **Ir7** in CD_2Cl_2.

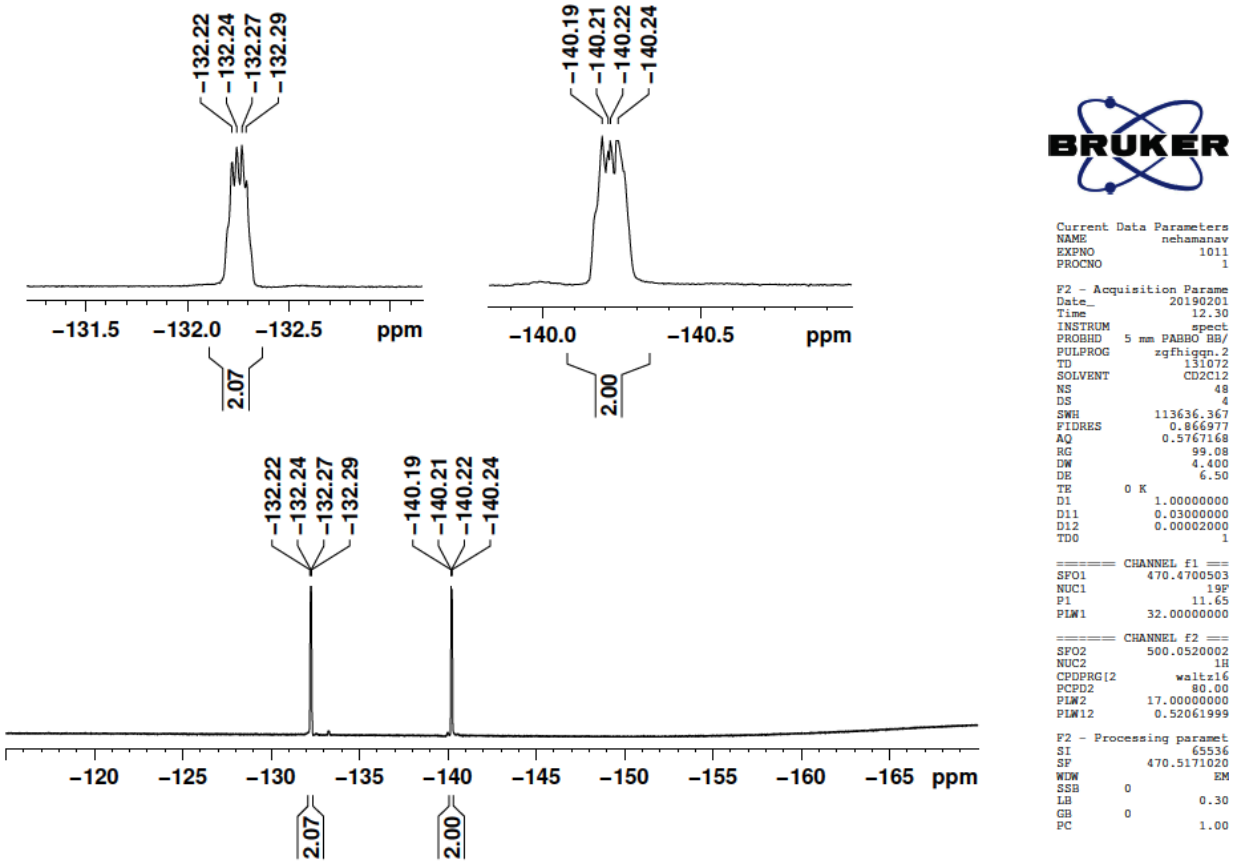


Figure S28 ^{19}F NMR of compound **Ir7** in CD_2Cl_2.

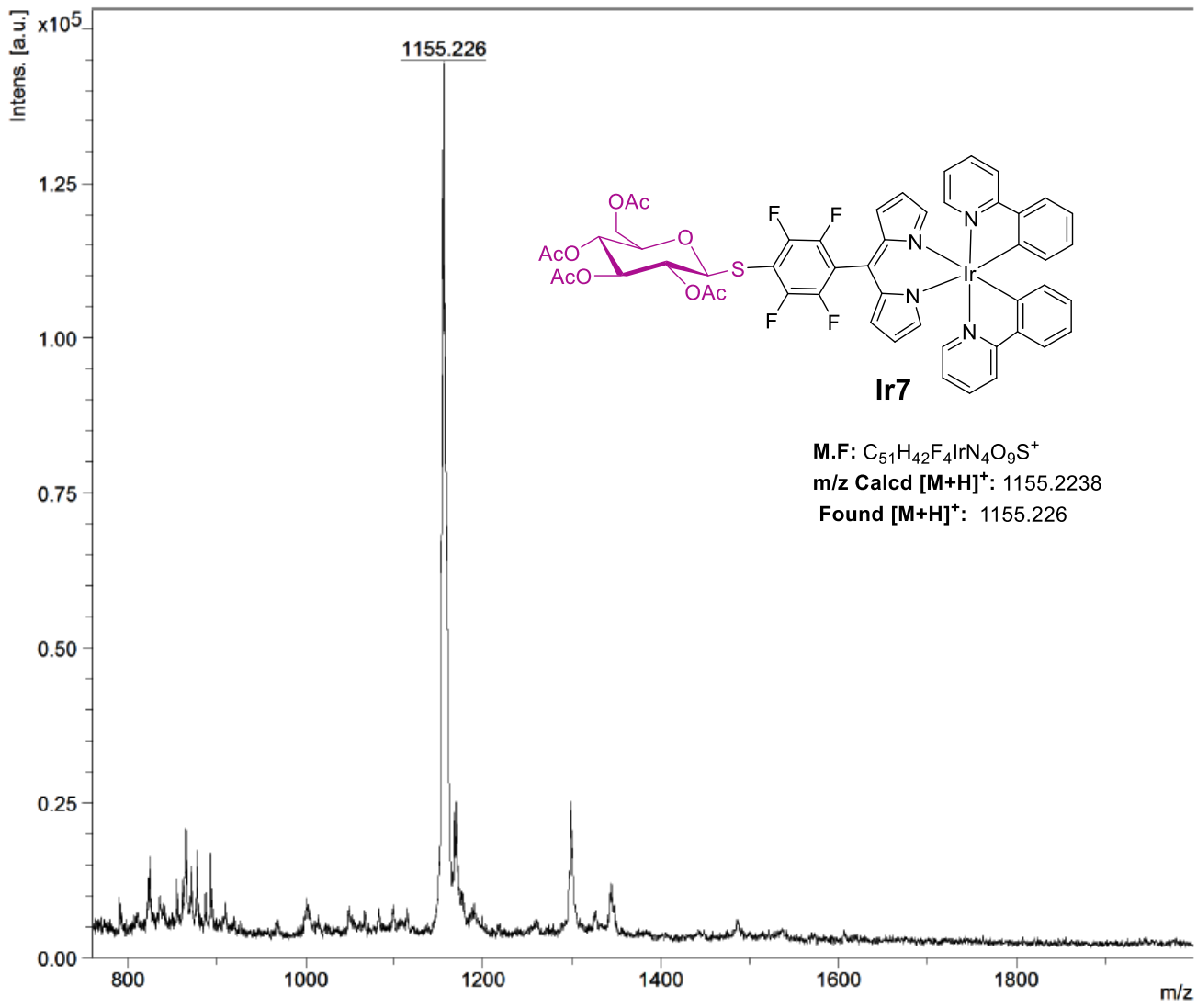


Figure S29 MALDI-MS of compound **Ir7**.

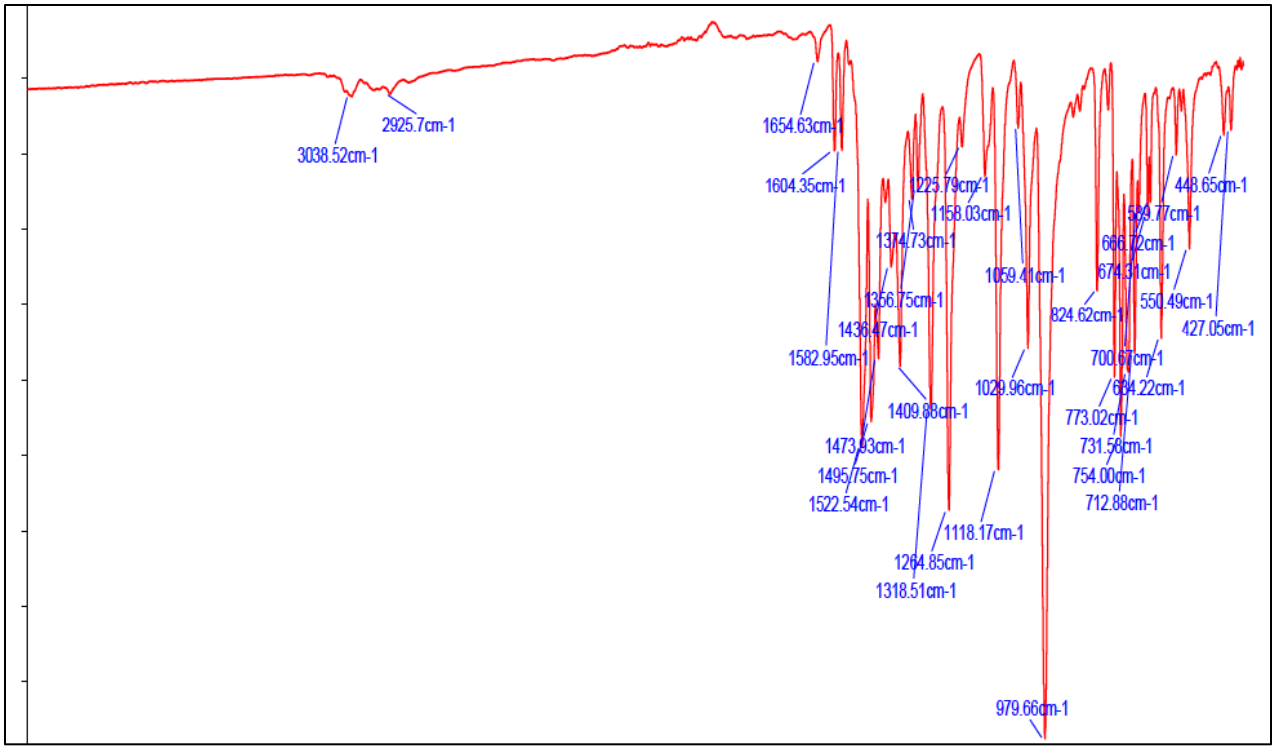


Figure S30 IR spectrum of compound **Ir8**.

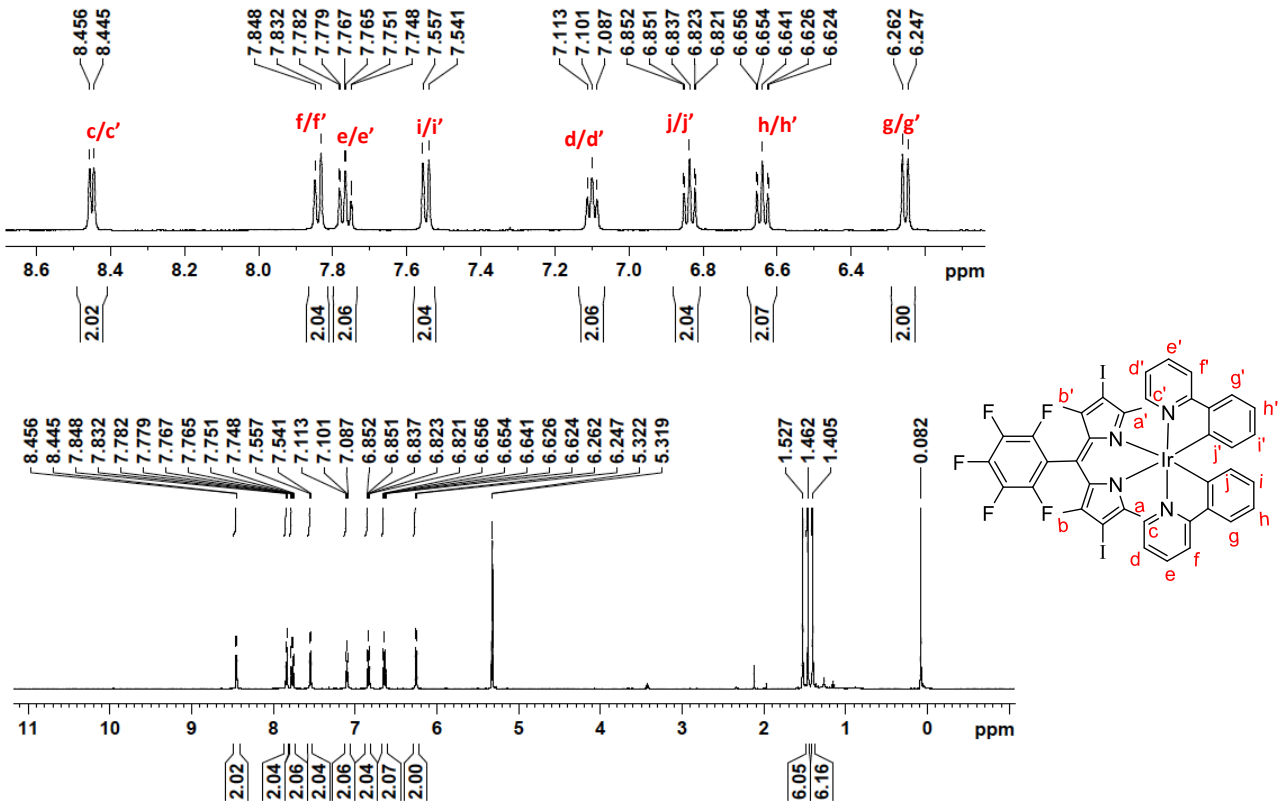


Figure S31 ^{1}H NMR of compound **Ir8** in CD_2Cl_2.

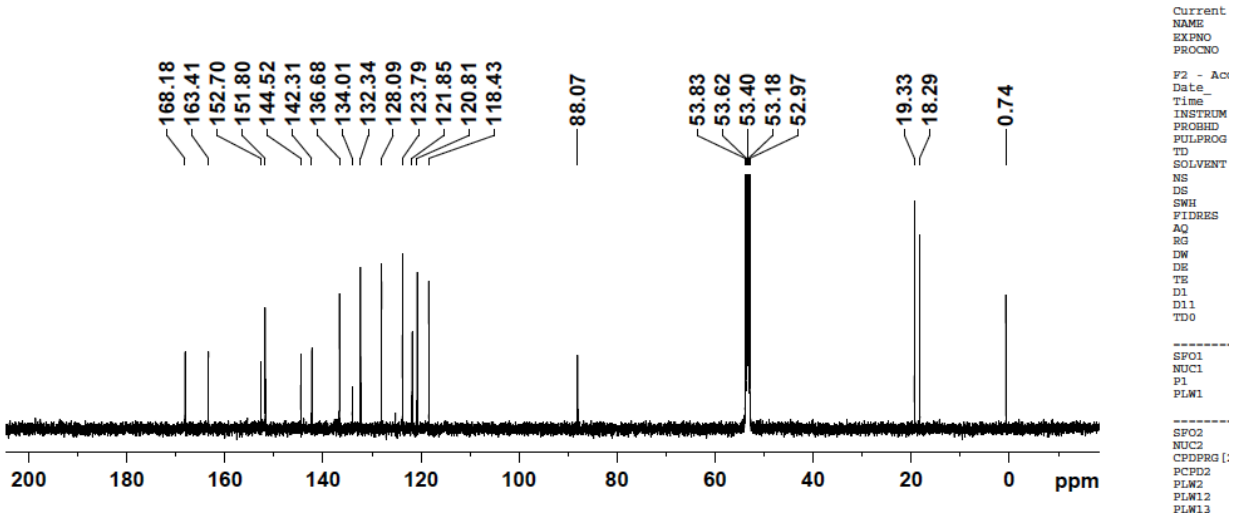


Figure S32 ^{13}C NMR of compound **Ir8** in CD_2Cl_2.

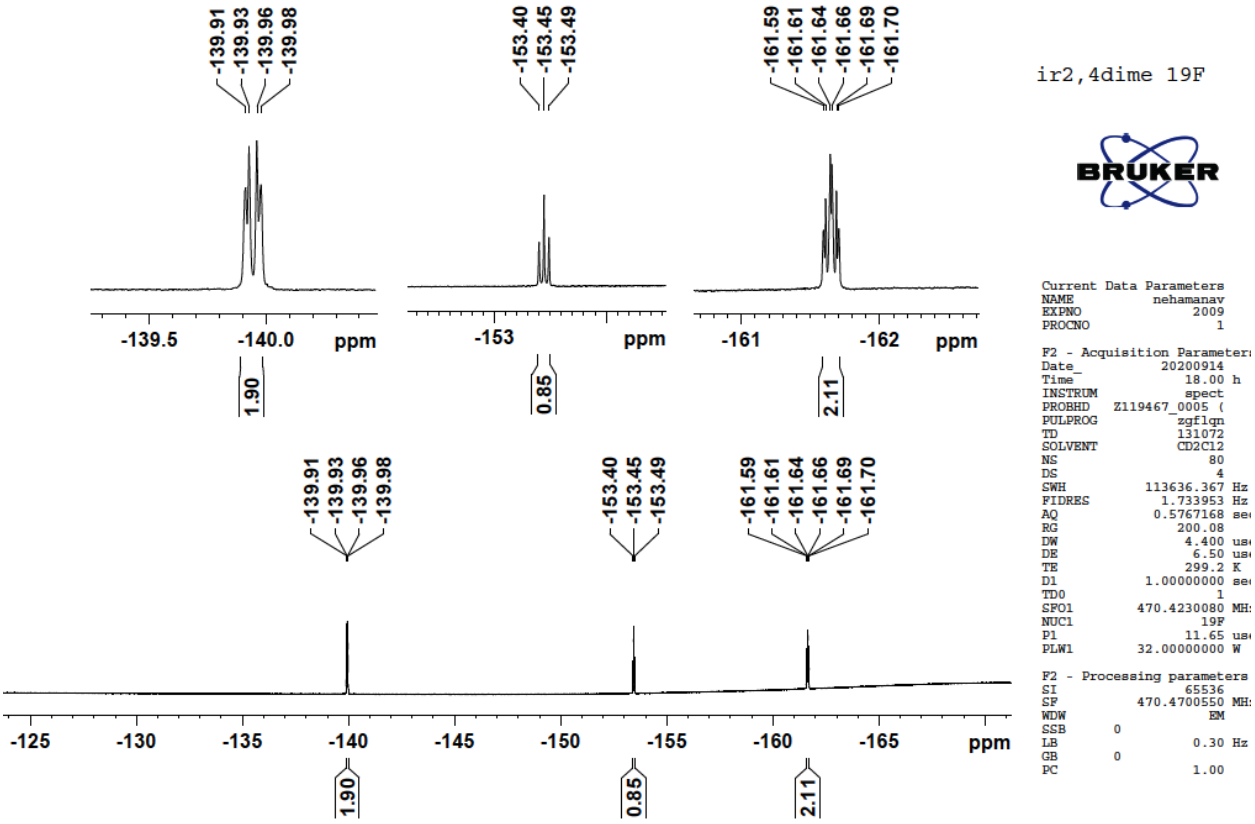


Figure S33 ^{19}F NMR of compound **Ir8** in CD_2Cl_2.

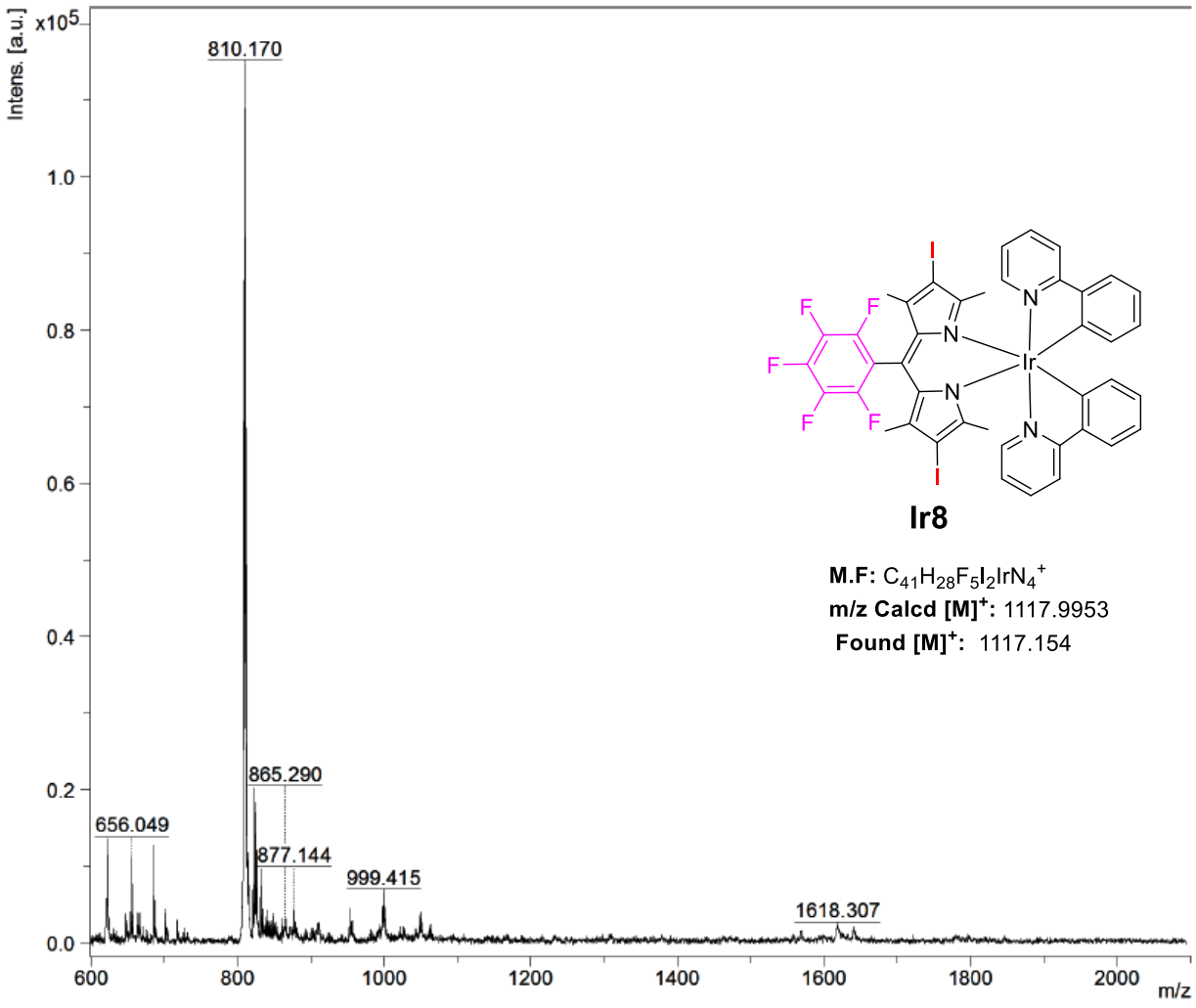


Figure S34 MALDI-MS of compound **Ir8**.

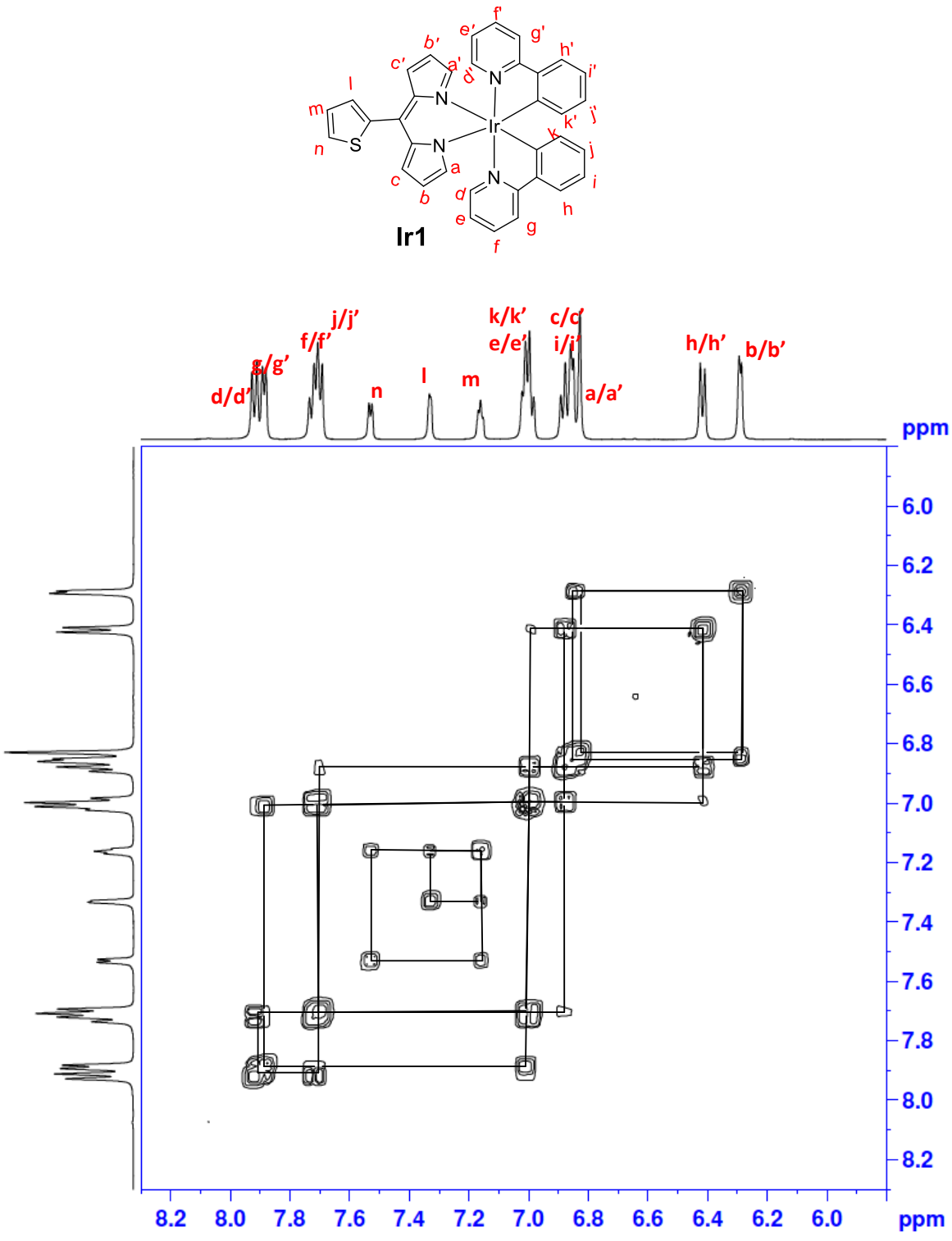


Figure S35 ^{1}H-^{1}H COSY of compound **Ir1** in CD_2Cl_2.

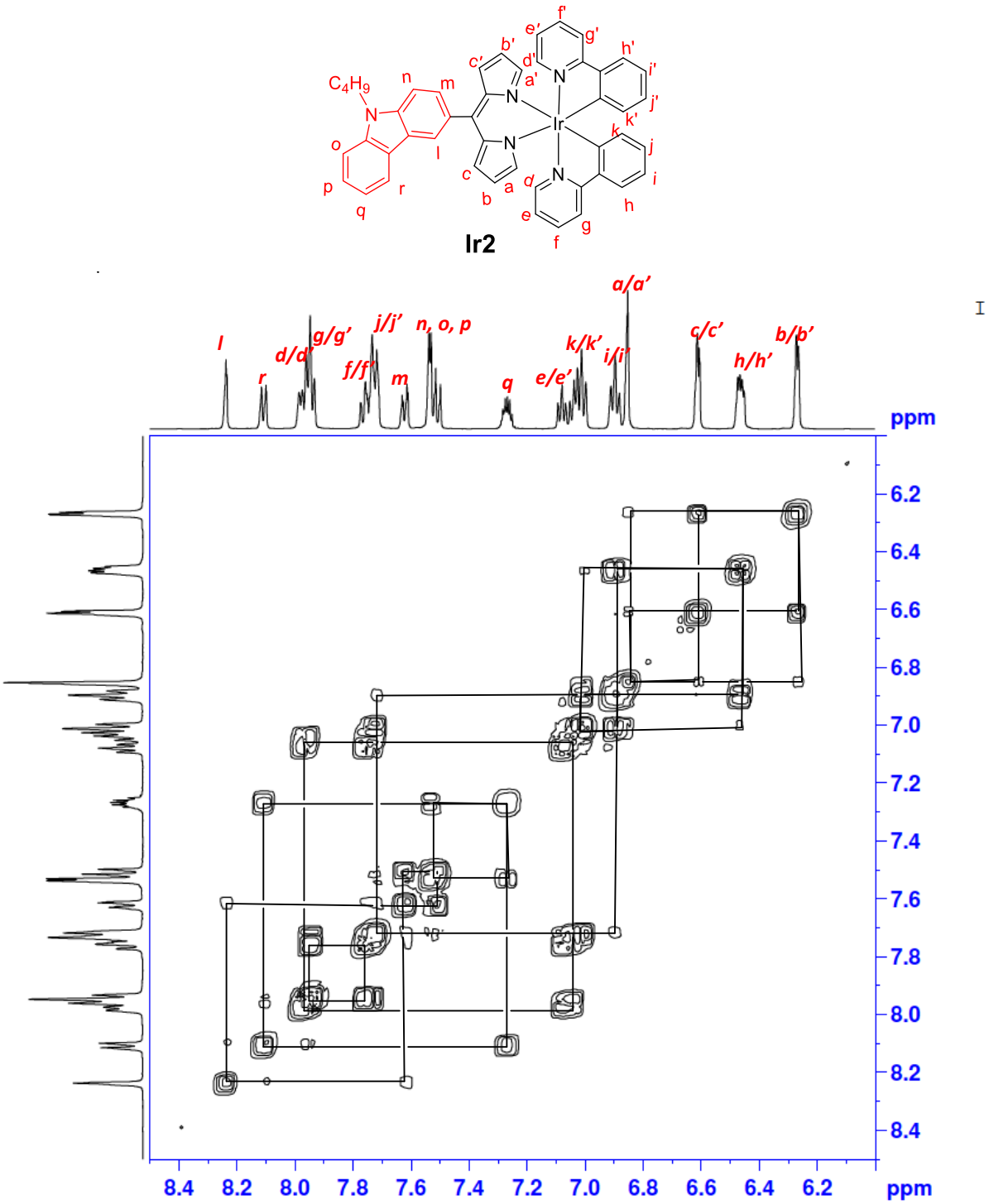


Figure S36 ^{1}H-^{1}H COSY of compound **Ir2** in CD_2Cl_2.

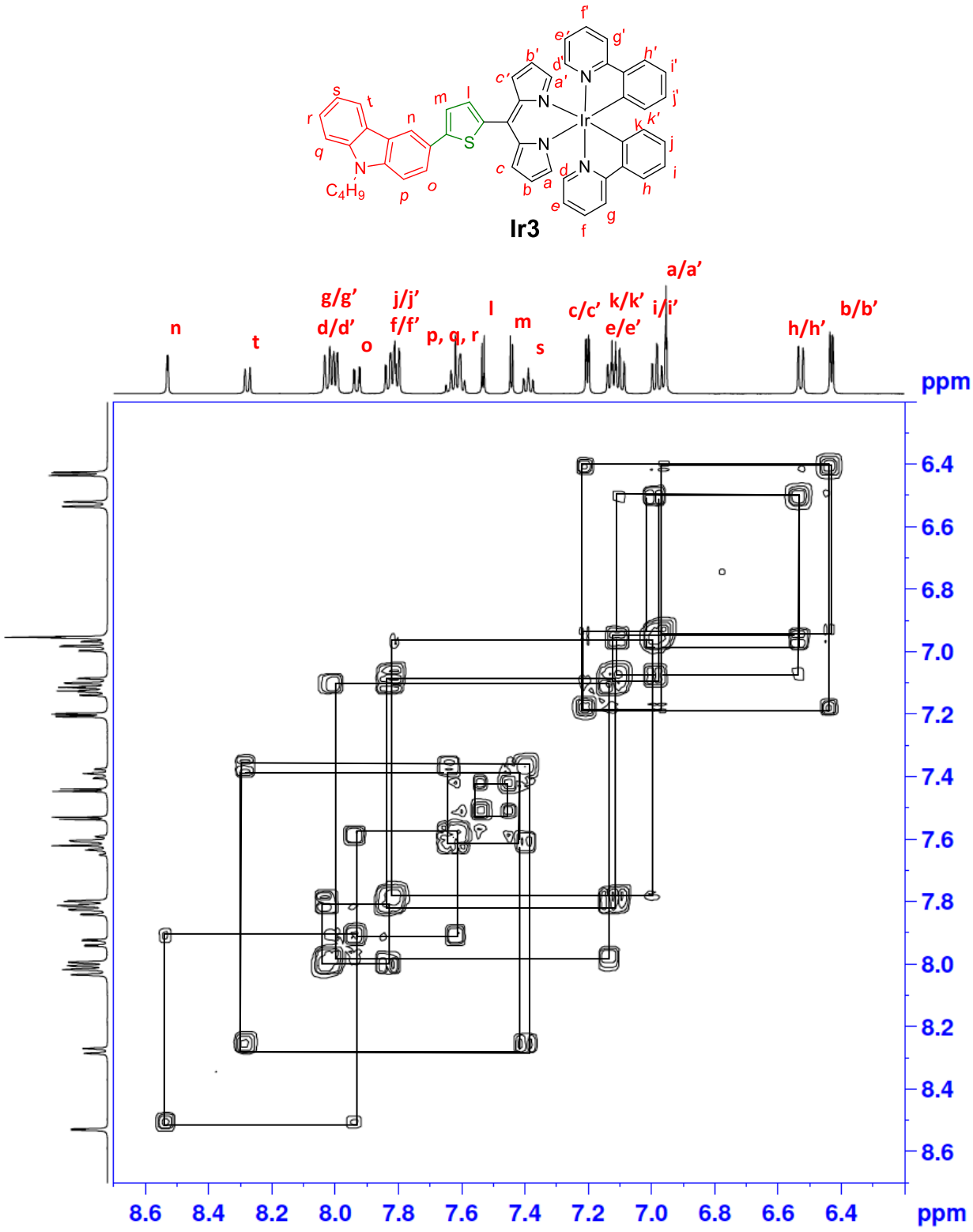


Figure S37 ^{1}H-^{1}H COSY of compound **Ir3** in CD_2Cl_2.

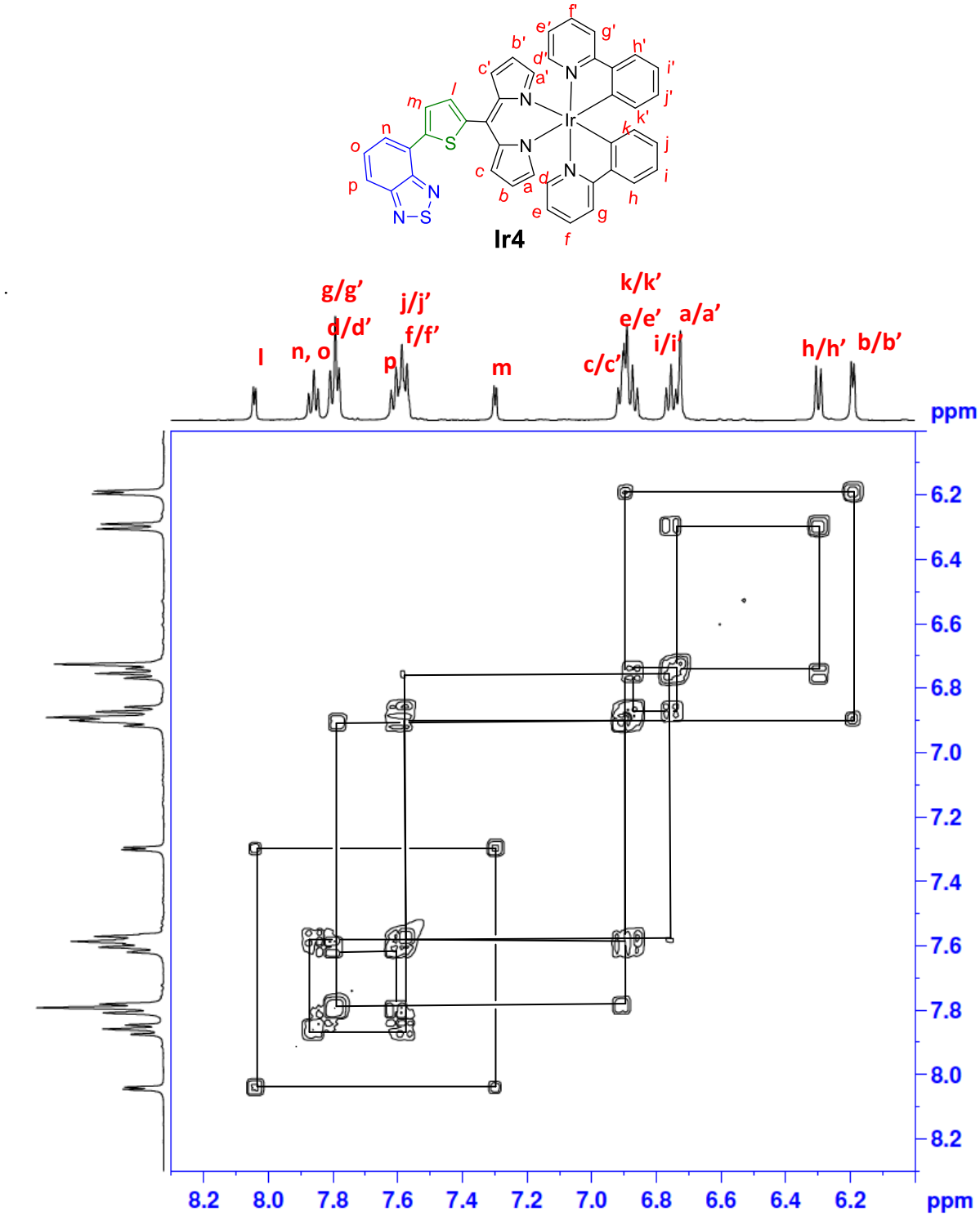


Figure S38 ^{1}H-^{1}H COSY of compound **Ir4** in CD_2Cl_2.

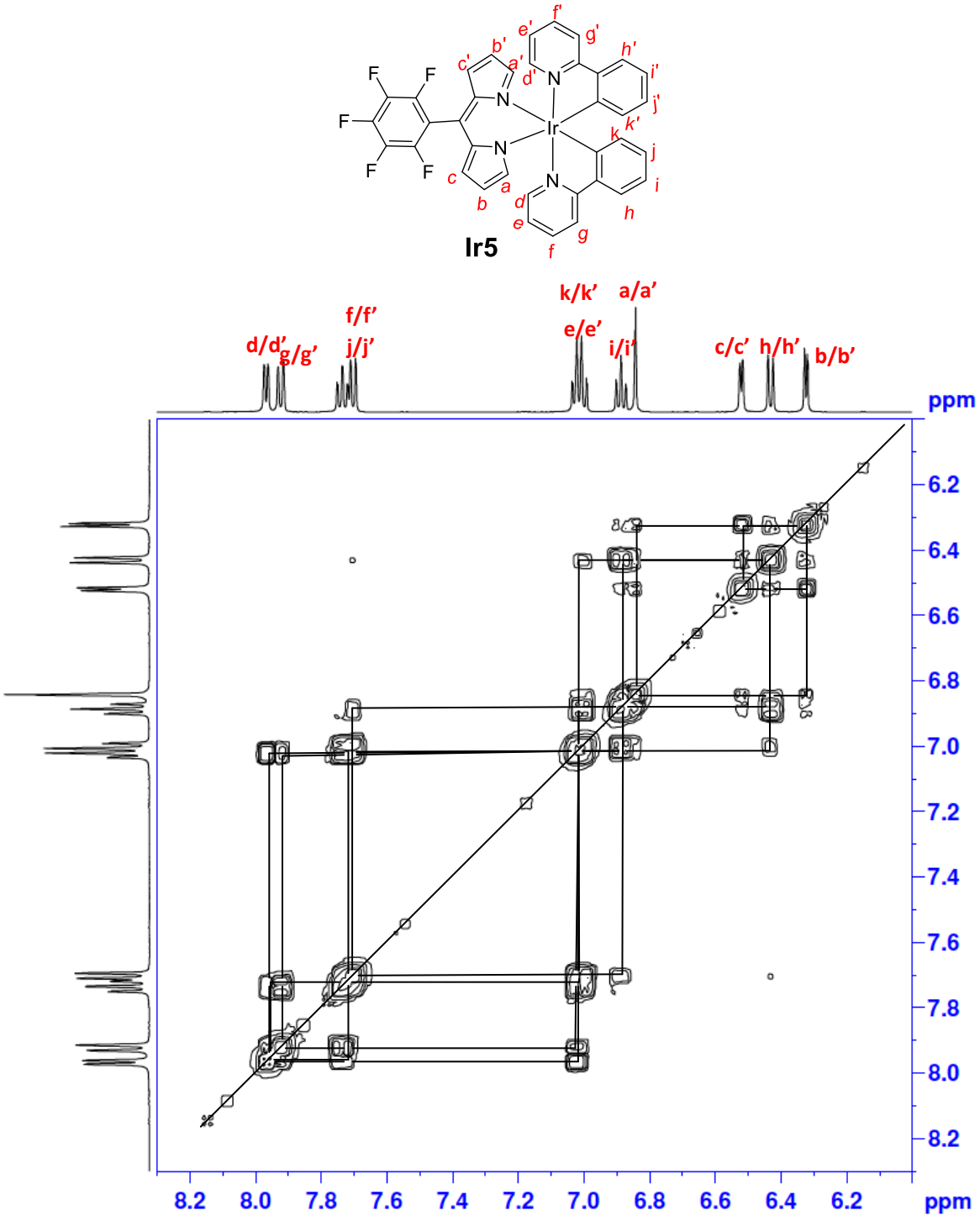


Figure S39 ^{1}H-^{1}H COSY of compound **Ir5** in CD_2Cl_2.

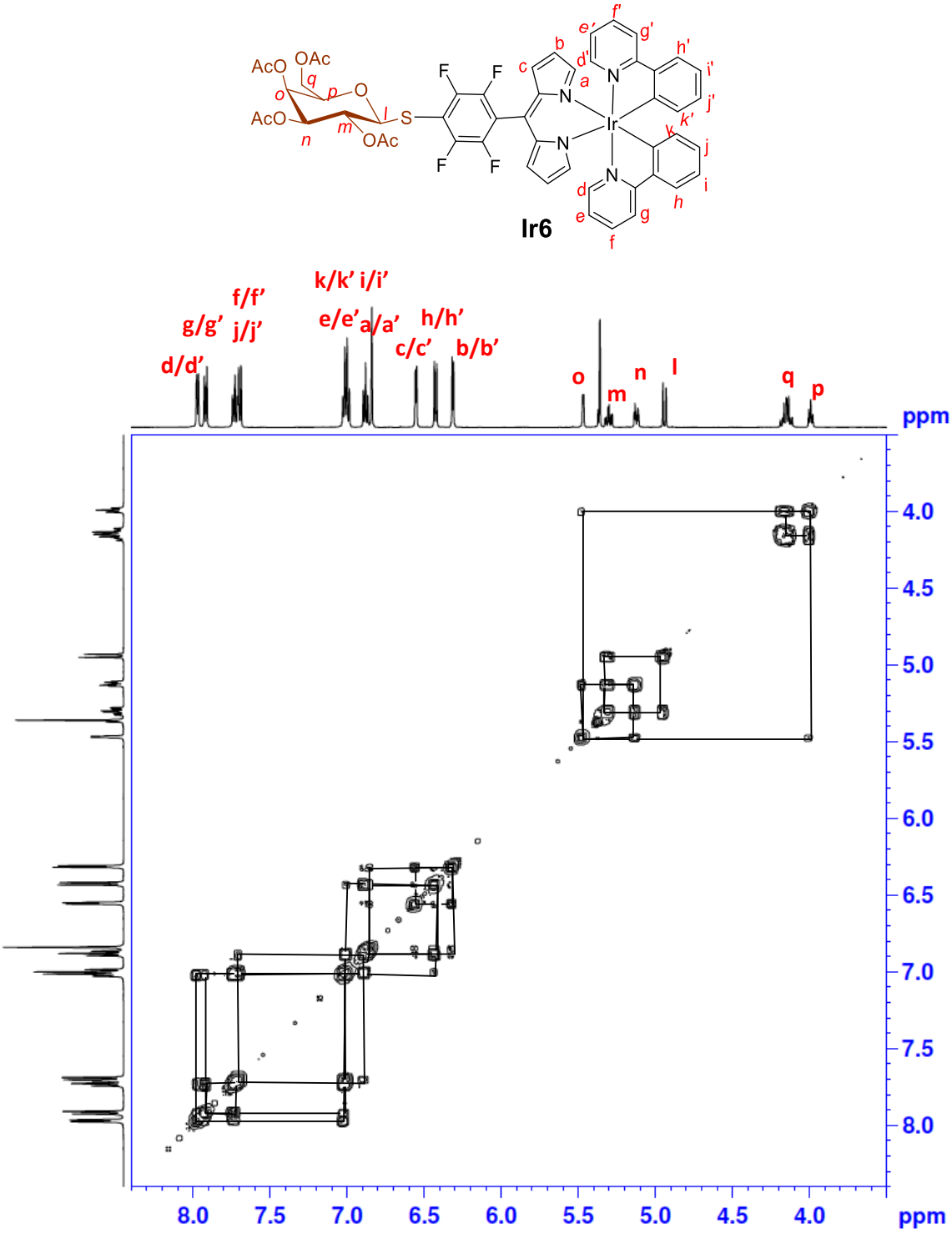


Figure S40 ^{1}H-^{1}H COSY of compound **Ir6** in CD_2Cl_2.

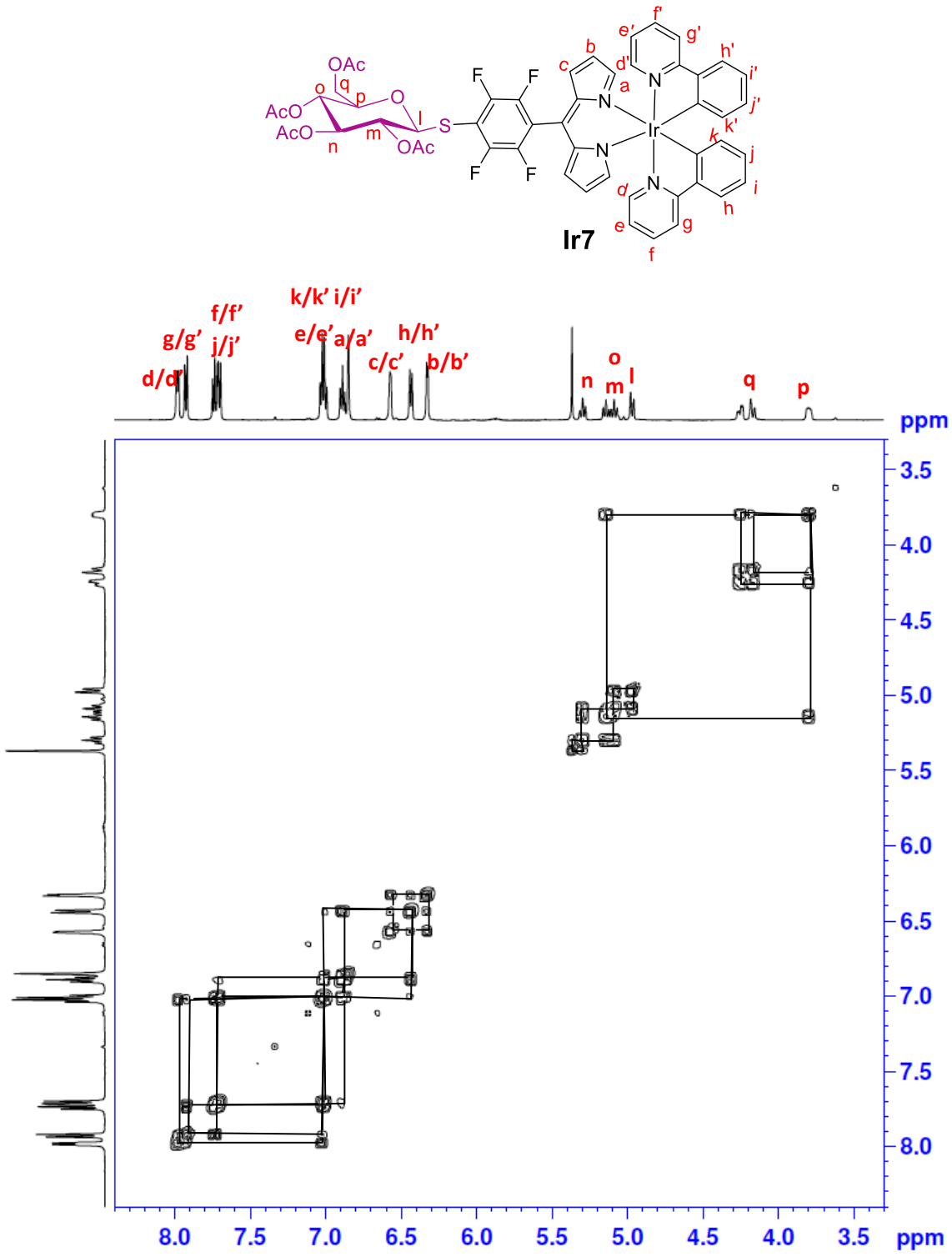


Figure S41 ^{1}H-^{1}H COSY of compound **Ir7** in CD_2Cl_2.

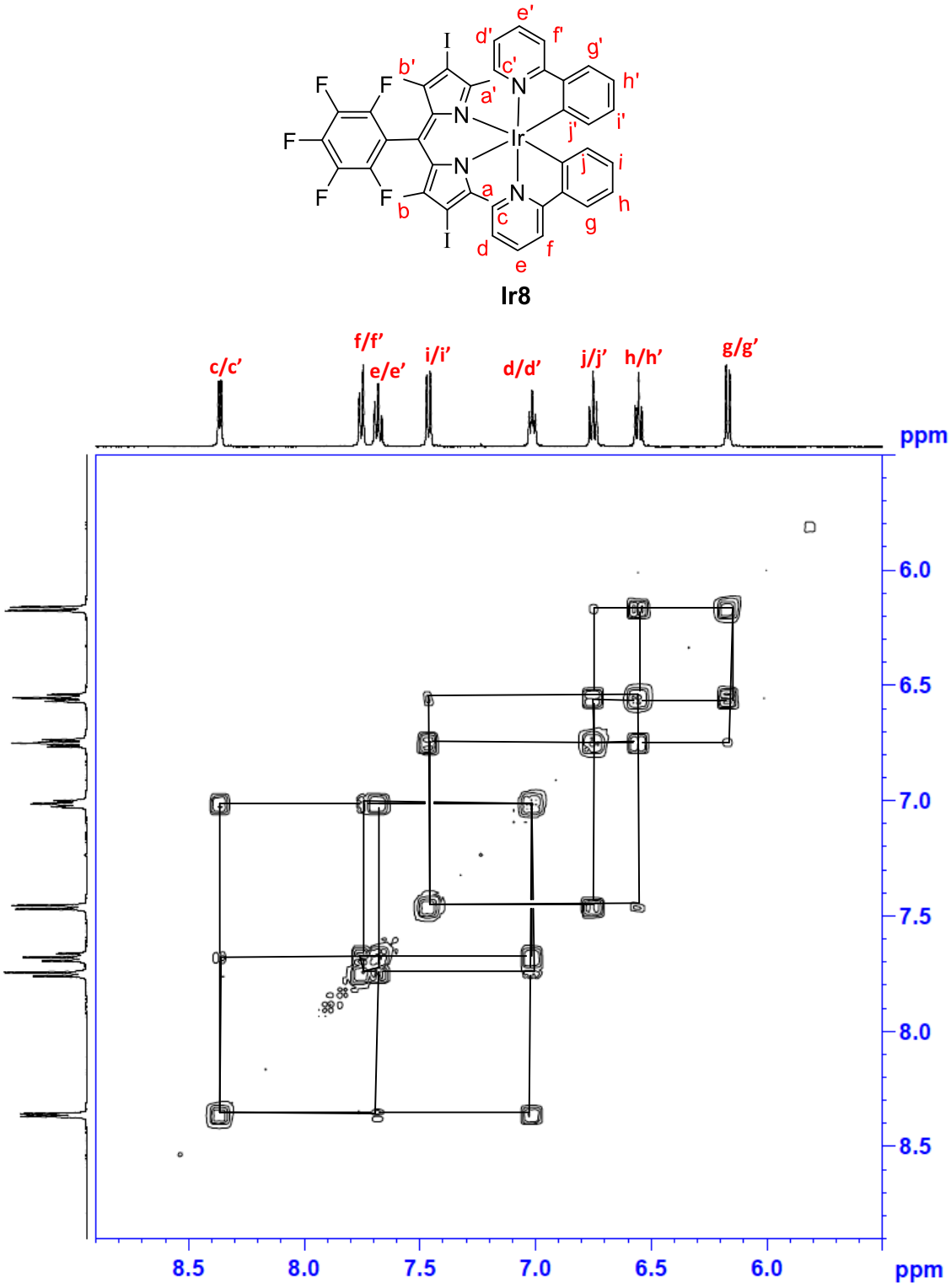


Figure S42 ^{1}H-^{1}H COSY of compound **Ir8** in CD_2Cl_2.

Singlet oxygen ($^1O_2$) quantum yield

Singlet oxygen generation quantum yields for iridium complexes (**Ir5-Ir7**) were calculated in DMSO and $CHCl_3$ solvents by using modified method[1,2] where 1,3-diphenylisobenzofuran (DPBF) was used as scavenger and Rose Bengal as standard/reference compound. All solutions were prepared in dark and saturated with oxygen. The samples containing iridium complex and DPBF were irradiated at 488 nm using OBIS Laser 488 (15 mW). The samples containing Rose Bengal and DPBF were irradiated at 532 nm using Oxxius Laser 532 (15 mW), white LED (3W). The DPBF absorbance was adjusted to 1.0 at 420 nm using 60 μM concentration and iridium complexes absorbance were adjusted to 0.2 at irradiation wavelength (488 nm). The concentration used for **Ir6** and **Ir7** is 8 μM in both solvents; while for **Ir5** it is 8 μM in DMSO and 6 μM in $CHCl_3$. Similarly absorbance for Rose Bengal was also adjusted to 0.2 at irradiation wavelength (532 nm) in DMSO. Since, Rose Bengal is poorly soluble in $CHCl_3$ hence Rose Bengal in DMSO solvent used as standard/reference.[3]

The photo-oxidation of DPBF sensitized by **Ir5-Ir7** was monitored by UV-vis spectrometer at various intervals and the obtained slope from absorption values at 420 nm were then used in below equation to calculate the singlet oxygen quantum yield.

The method is relative method[4] using Rose Bengal as a standard/reference.

The values of Φ_Δ of Rose Bengal in water (0.75), DMSO (0.16) and CHCl3 (0.76) were used in the following equation.[5]

$$\Phi_\Delta(S) = \Phi_\Delta(S_0) \times \{ \text{Slope}(S) / \text{Slope}(S_0)\},$$

where S is for sample and S_0 is for standard/reference.

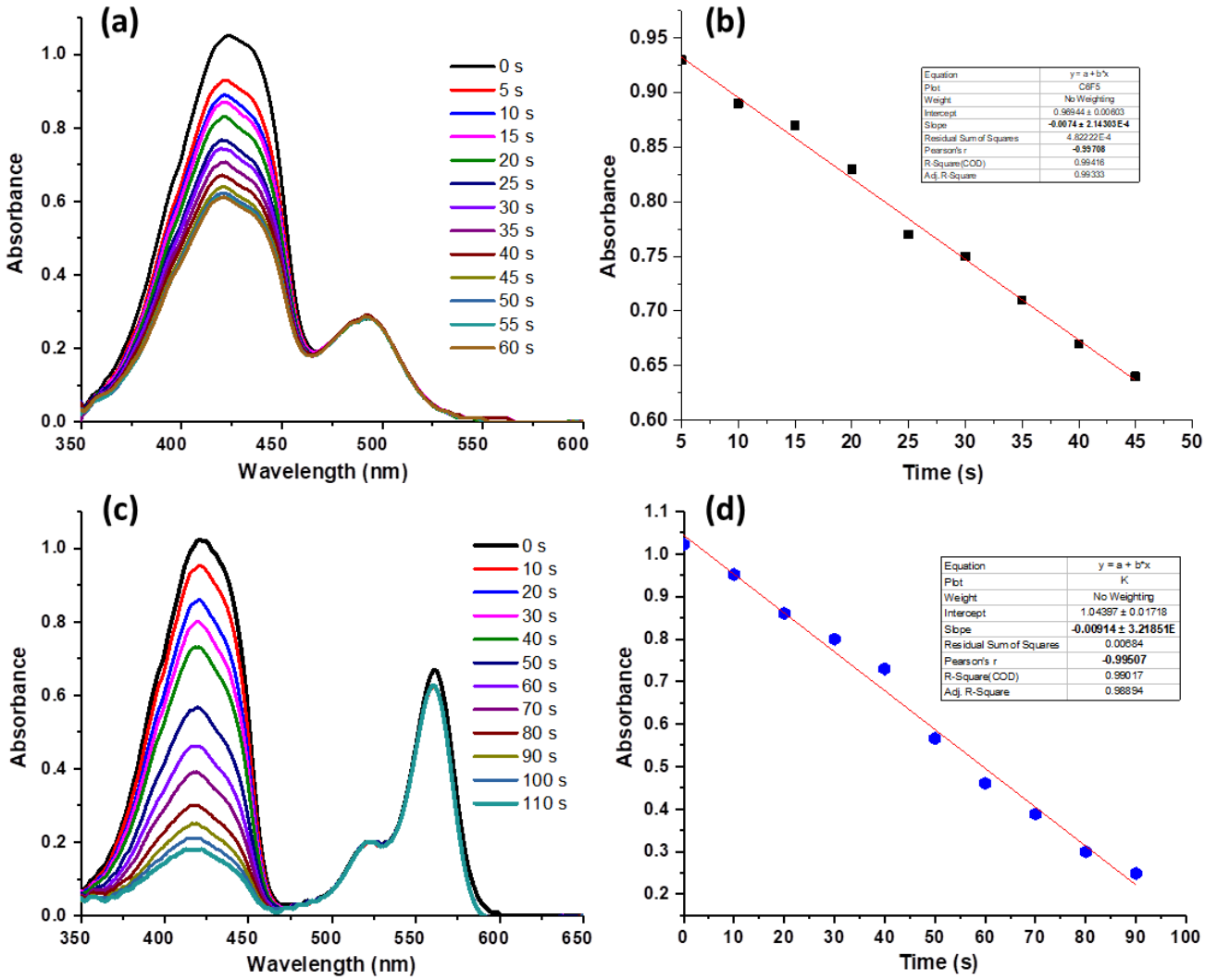


Figure S43 UV-vis spectral changes in DMSO upon photoirradiation of (a) **Ir5** (λ = 488 nm, 15 mW) and (c) Rose Bengal (λ =532 nm, 15 mW); the rate of decrease in absorption measured at 420 nm in (b) **Ir5** and (d) Rose Bengal. The concentration used for DPBF was 60 µM; Ir7 (8 µM) and Rose Bengal (8 µM).

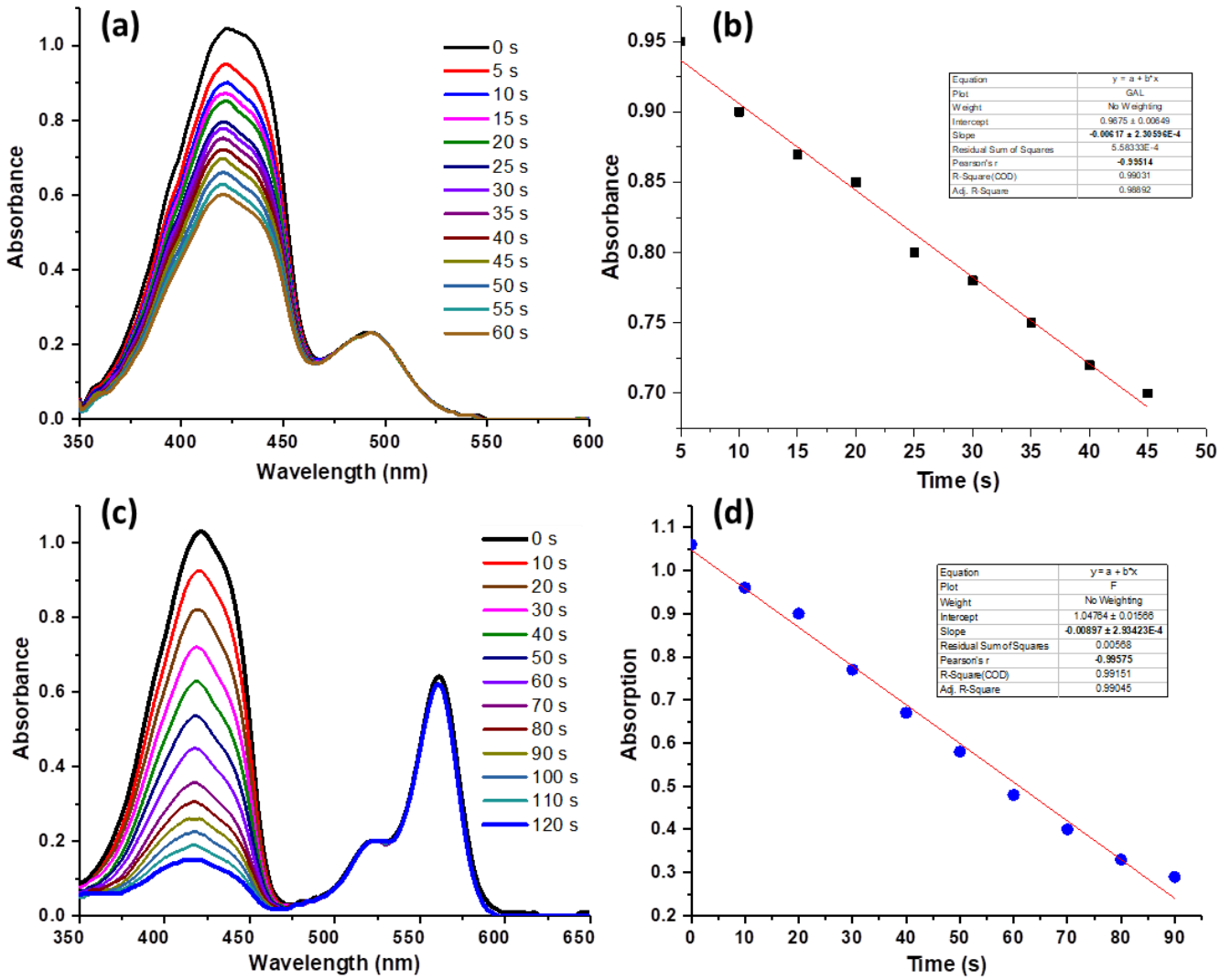


Figure S44 UV-vis spectral changes in DMSO upon photoirradiation of (a) **Ir6** (λ = 488 nm, 15 mW) and (c) Rose Bengal (λ =532 nm, 15 mW); the rate of decrease in absorption measured at 420 nm in (b) **Ir6** and (d) Rose Bengal. The concentration used for DPBF was 60 μM; **Ir6** (8 μM) and Rose Bengal (8 μM).

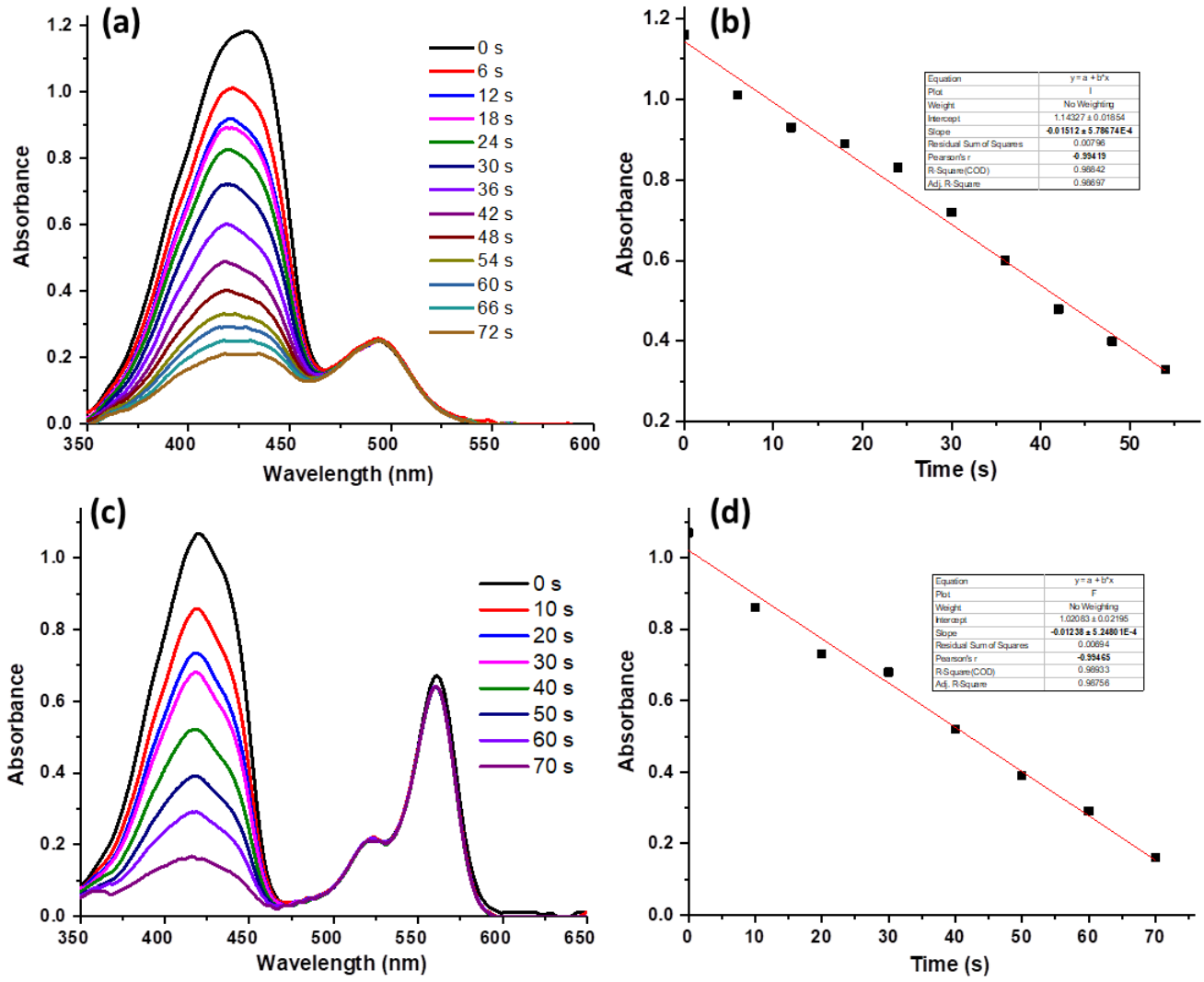


Figure S45 UV-vis spectral changes upon photoirradiation of (a) **Ir5** in $CHCl_3$ (λ = 488 nm, 15 mW) and (c) Rose Bengal in DMSO (λ =532 nm, 15 mW); the rate of decrease in absorption measured at 420 nm in (b) **Ir5** and (d) Rose Bengal. The concentration used for DPBF was 60 μM; **Ir5** (8 μM) and Rose Bengal (8 μM).

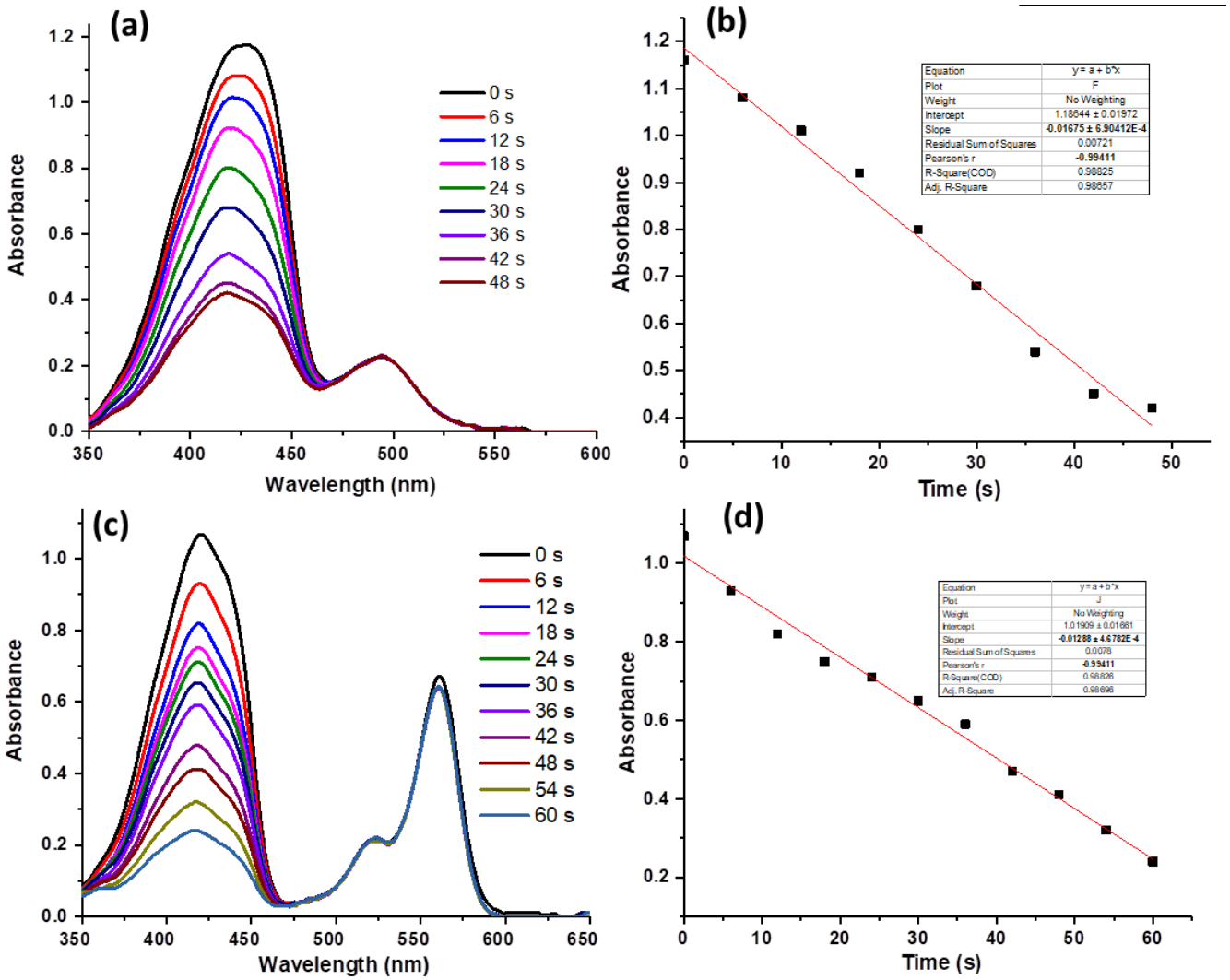


Figure S46 UV-vis spectral changes upon photoirradiation of (a) **Ir6** in $CHCl_3$ (λ = 488 nm, 15 mW) and (c) Rose Bengal in DMSO (λ =532 nm, 15 mW); the rate of decrease in absorption measured at 420 nm in (b) **Ir6** and (d) Rose Bengal. The concentration used for DPBF was 60 µM; **Ir6** (6 µM) and Rose Bengal (8 µM).

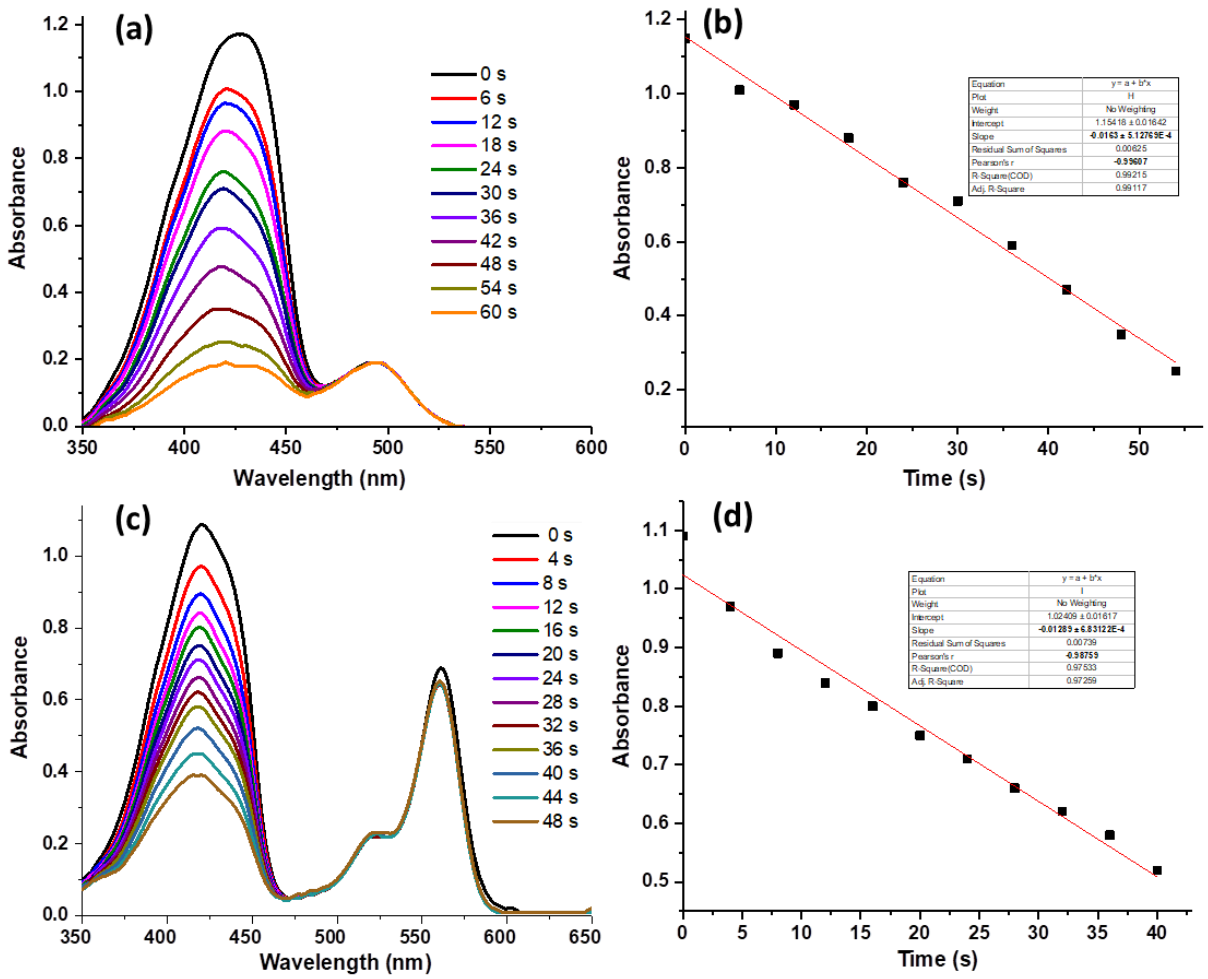


Figure S47 UV-vis spectral changes upon photoirradiation of (a) **Ir7** in $CHCl_3$ (λ = 488 nm, 15 mW) and (c) Rose Bengal in DMSO (λ =532 nm, 15 mW); the rate of decrease in absorption measured at 420 nm in (b) **Ir7** and (d) Rose Bengal. The concentration used for DPBF was 60 μM; **Ir7** (6 μM) and Rose Bengal (8 μM).

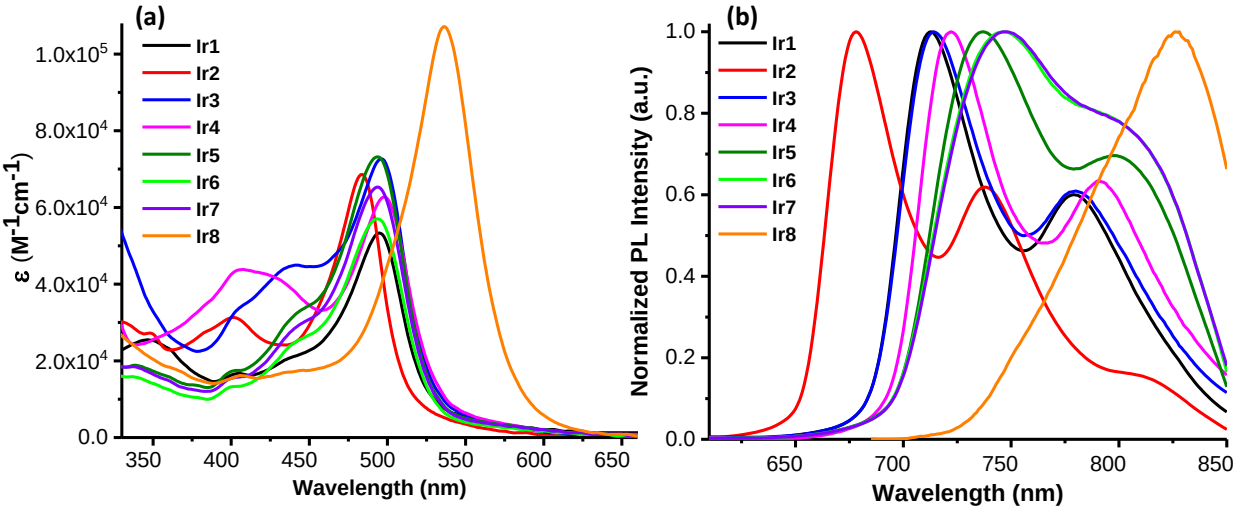


Figure S48 Absorption and emission spectra of **Ir1-Ir8** in toluene.

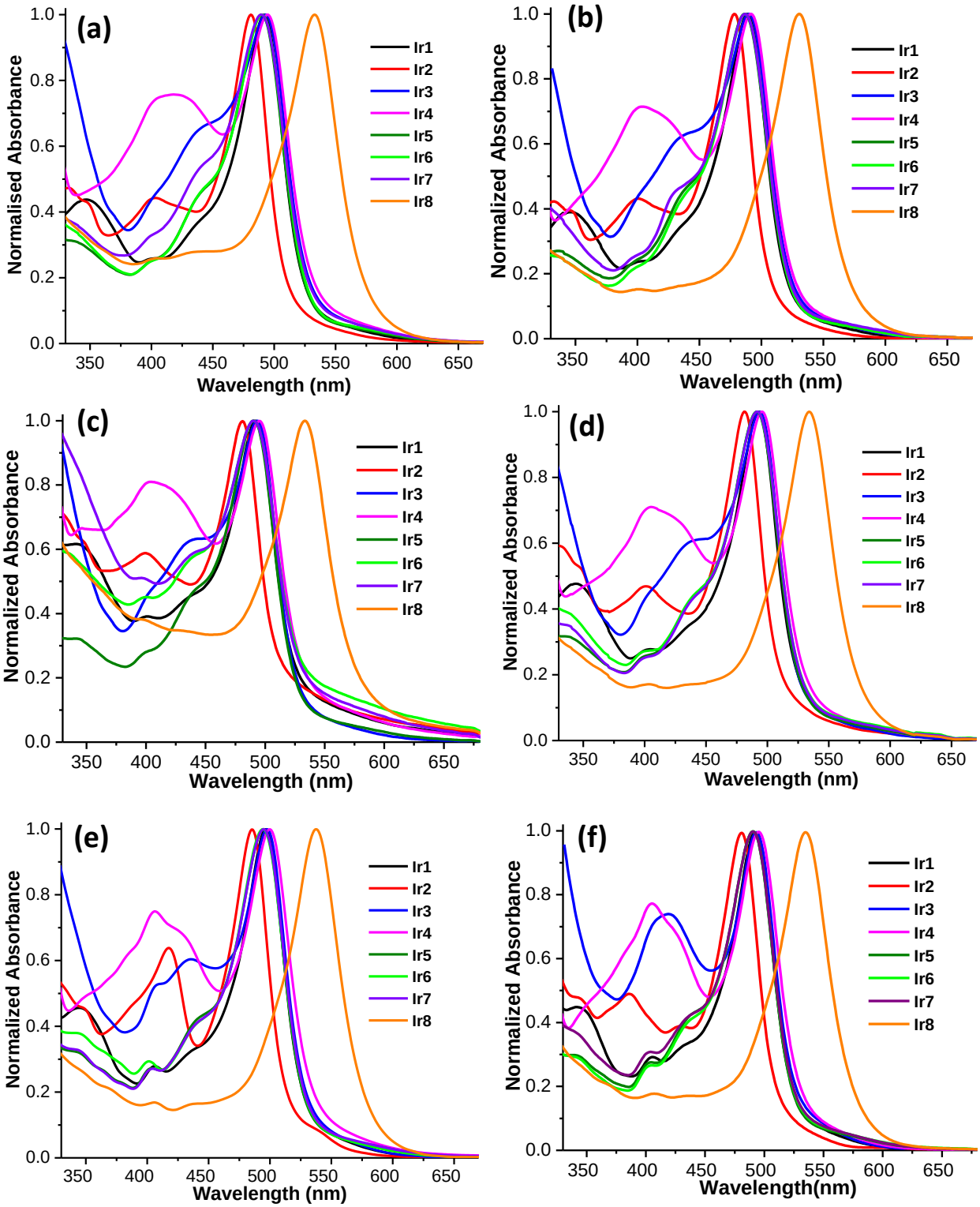


Figure S49 Solvatochromic absorption spectra of Iridium dipyrrinates (**Ir1**-**Ir8**) in solvent **(a)** DMF **(b)** ACN **(c)** THF **(d)** DCM **(e)** CCL_4 **(f)** Hexane.

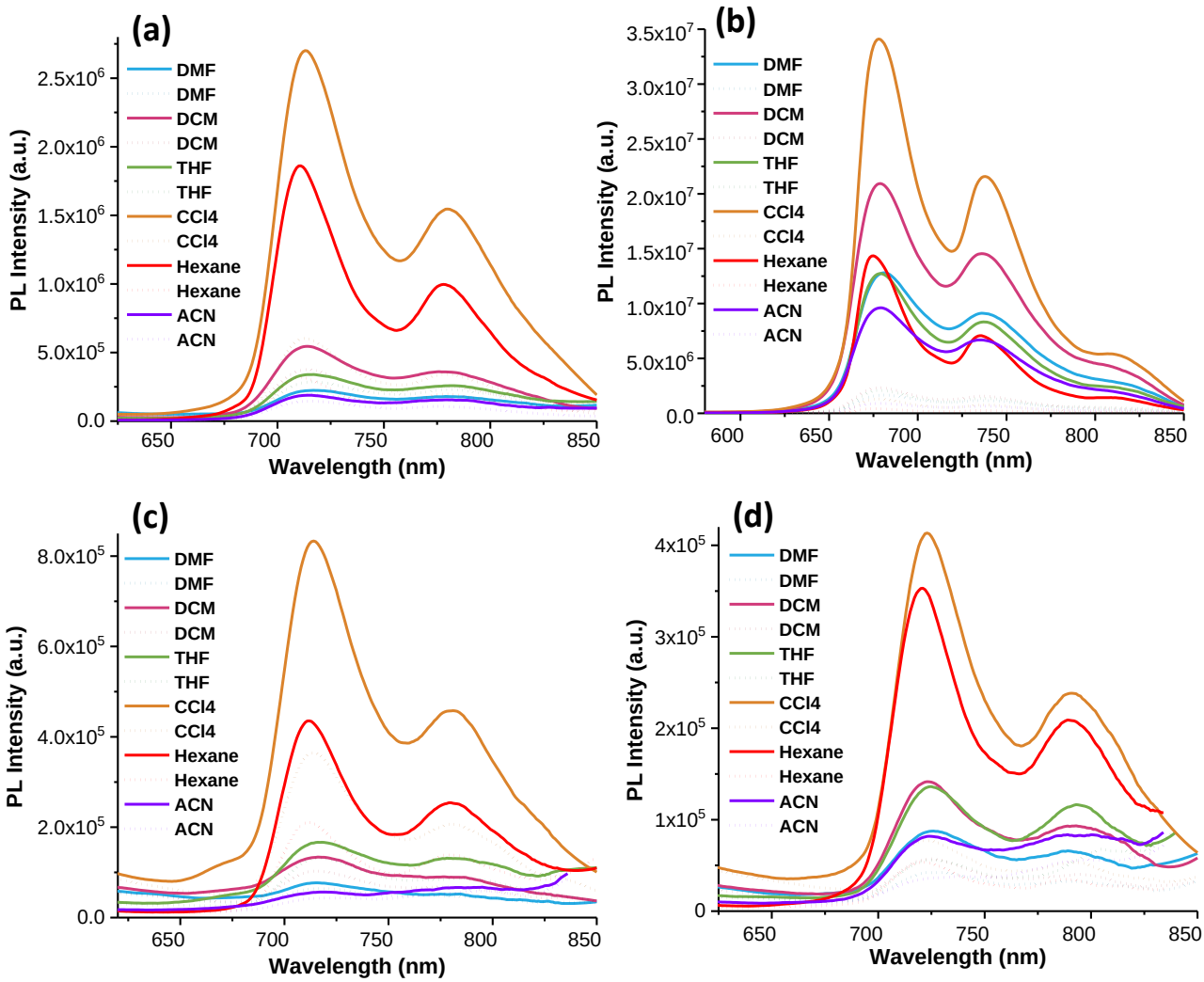


Figure S50 Emission spectra in deoxygenated (solid) and oxygenated (dashed) solvents of iridium dipyrrinates (a) **Ir1** (b) **Ir2** (c) **Ir3** (d) **Ir4.**

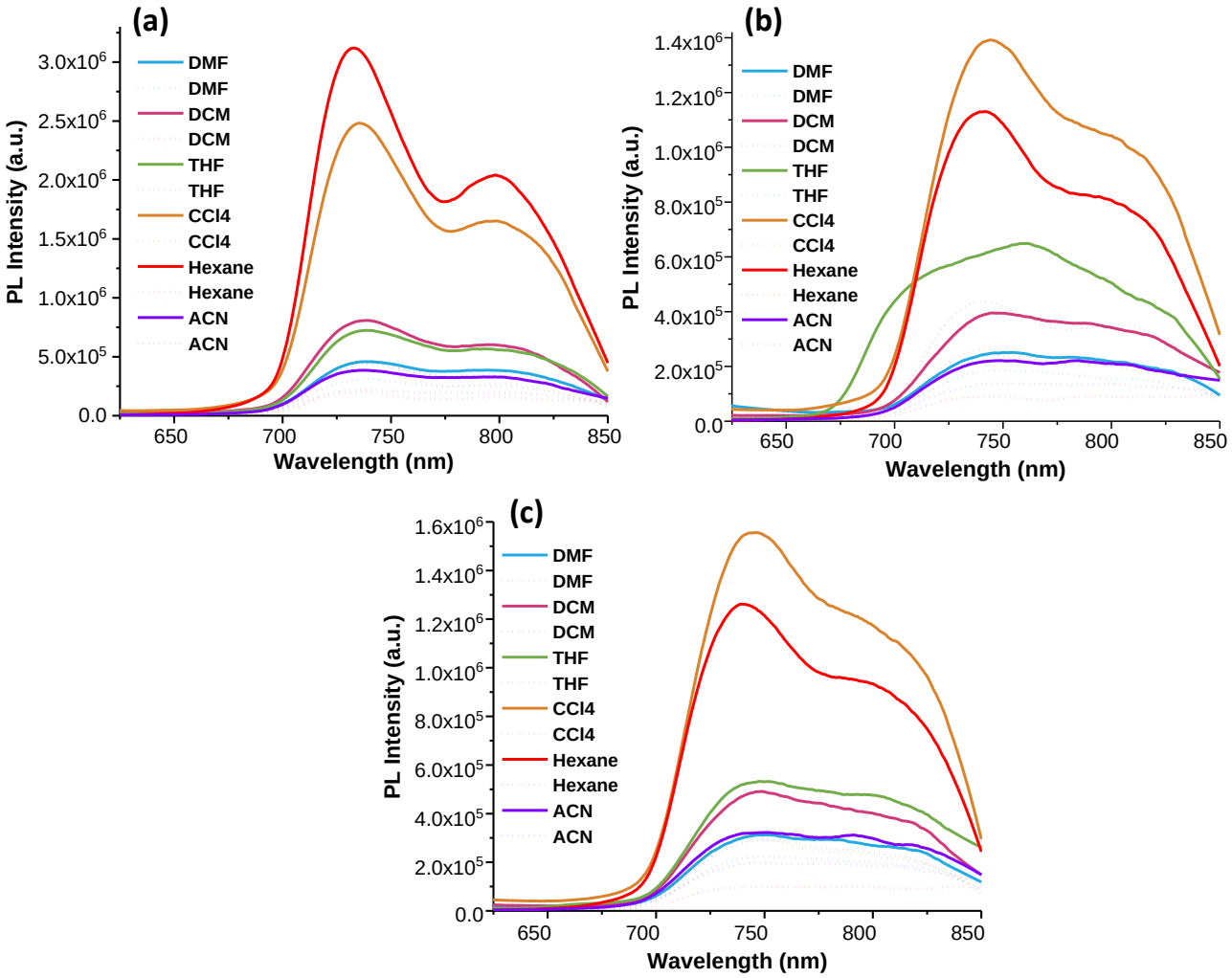


Figure S51 Emission spectra in deoxygenated (solid) and oxygenated (dashed) solvents of iridium dipyrrinates (a) **Ir5** (b) **Ir6** (c) **Ir7.**

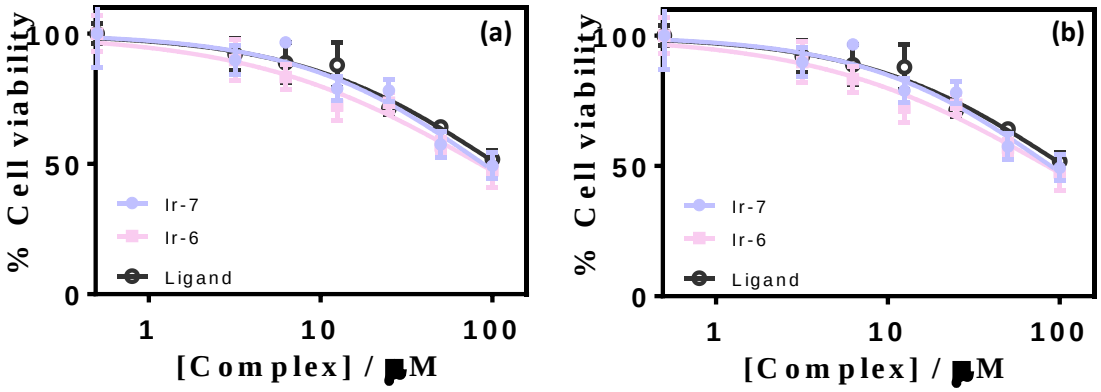


Figure S52 Cell Viability plots in the absence of light (Dark); (a) HaCaT and (b) A549 cell lines treated with iridium dipyrrinates **Ir6** and **Ir7** and ligand for 24 h incubation.

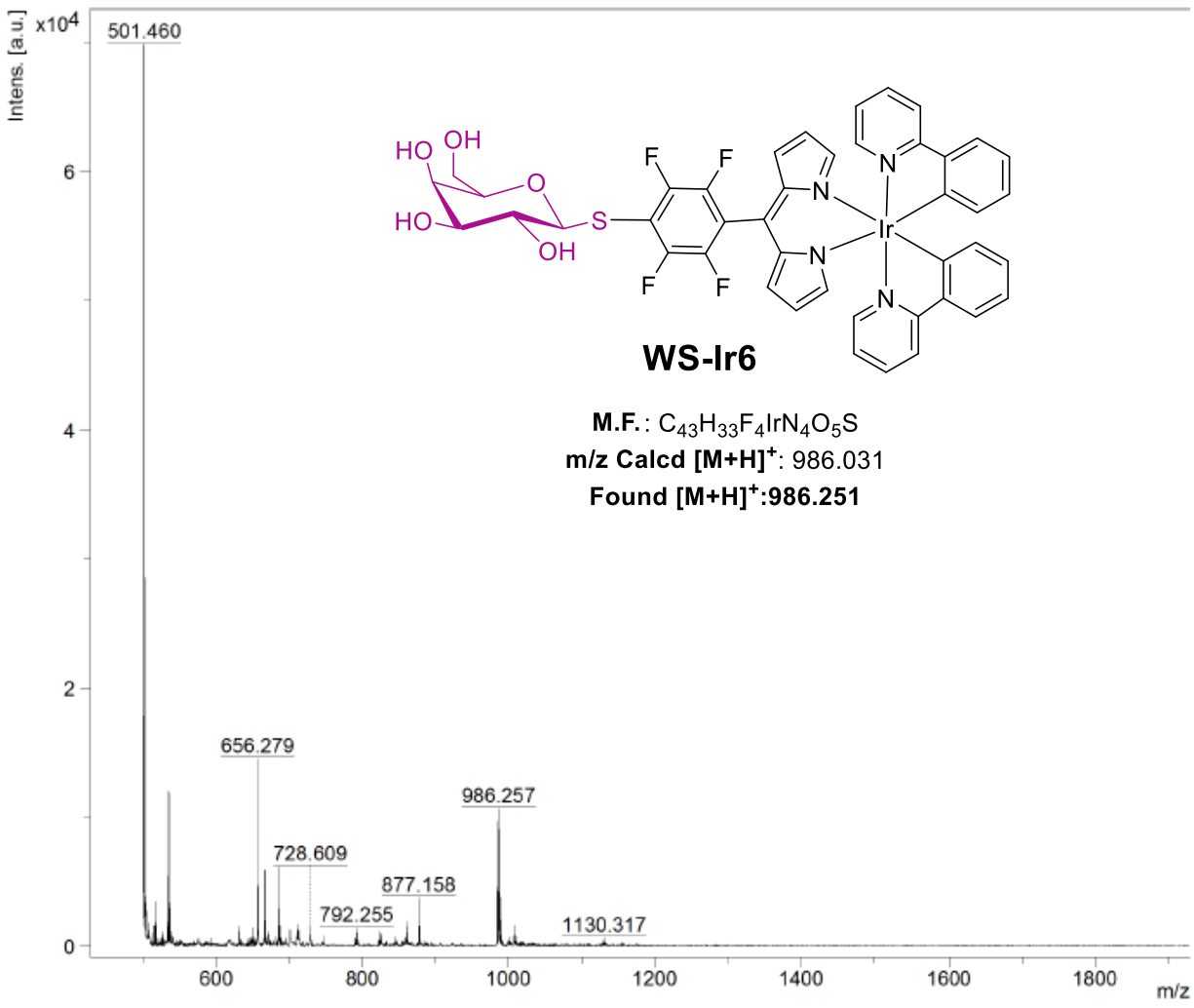


Figure S55 MALDI-MS of compound **WS-Ir6**

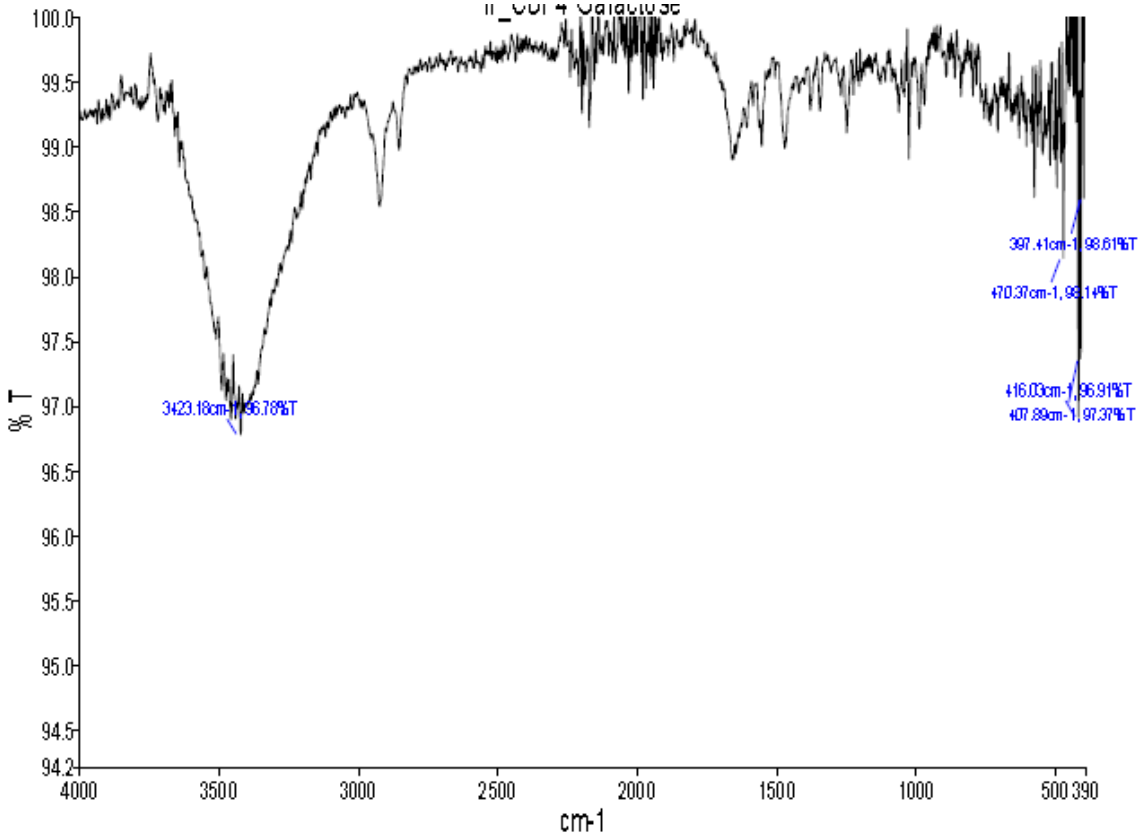


Figure S56 IR spectrum of compound **WS-Ir6**

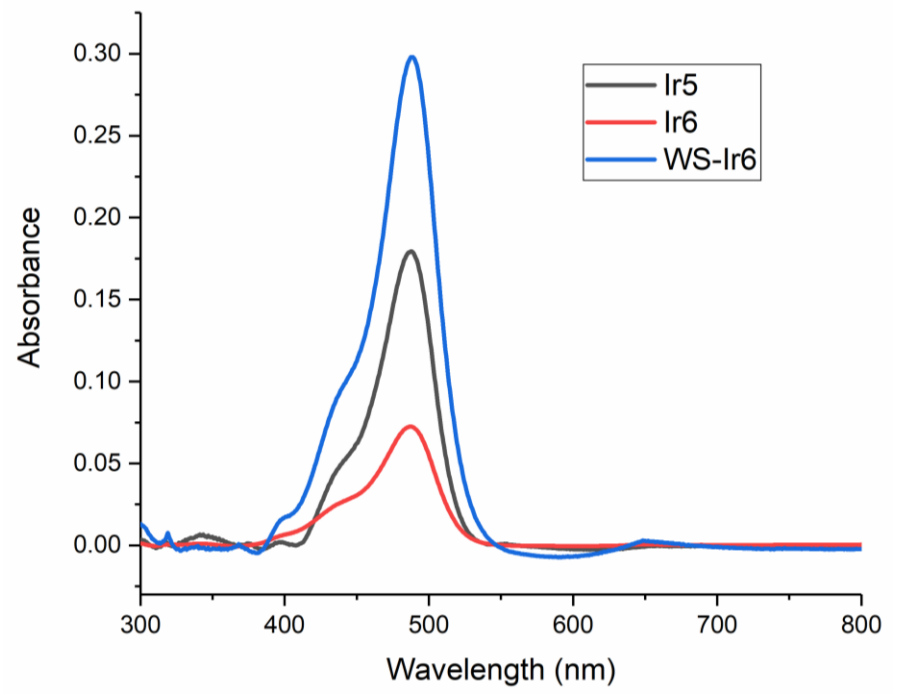


Figure S57 Comparison of absorption spectra of **Ir5, Ir6,** and, **WS-Ir6** in methanol**.**

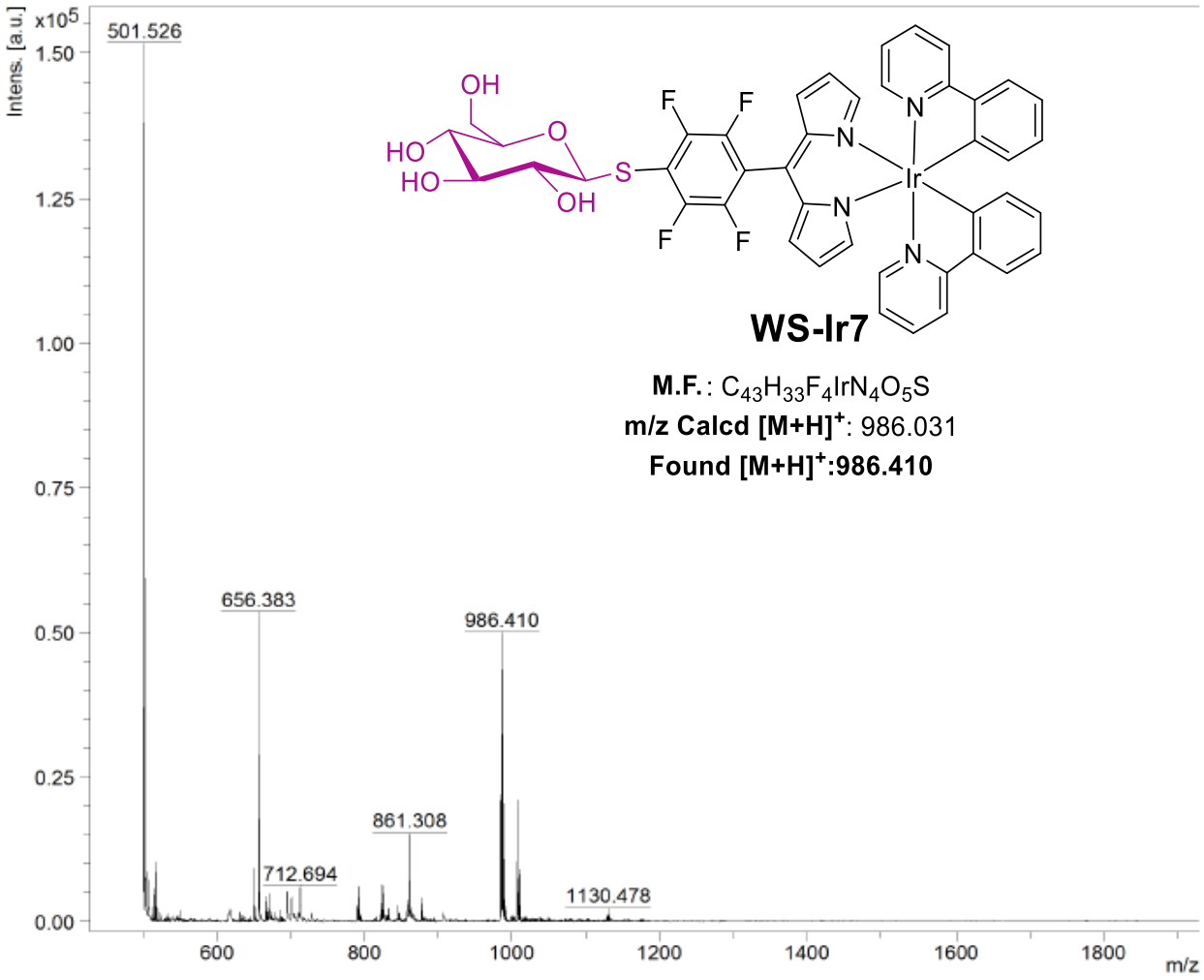


Figure S58 MALD-MS of compound **WS-Ir7.**

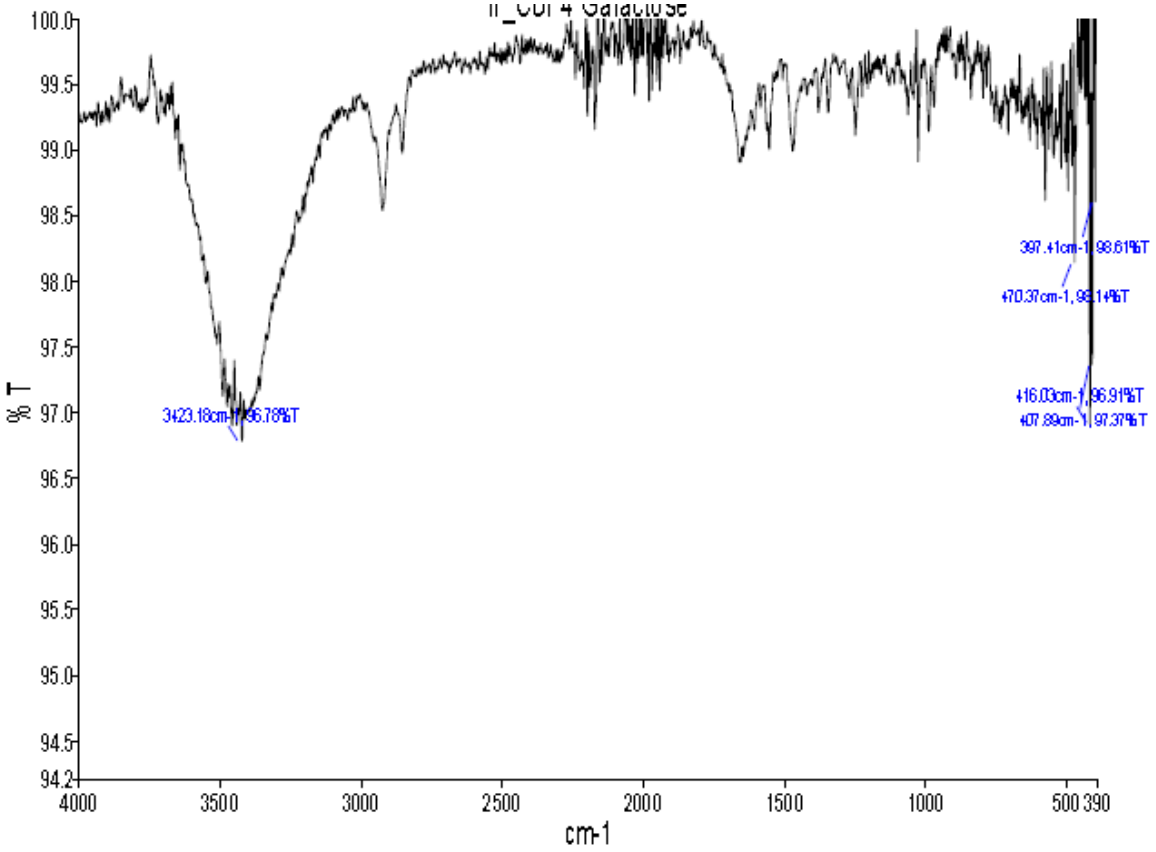


Figure S59 IR spectrum of compound **WS-Ir7.**

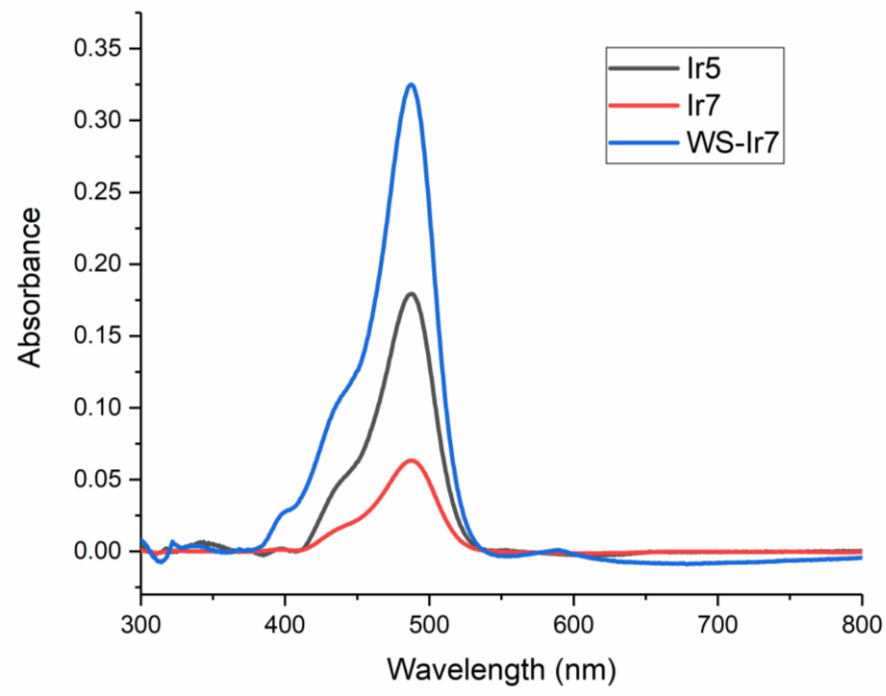


Figure S60 Comparison of absorption spectra of **Ir5**, **Ir7**, and **WS-Ir7** in methanol.

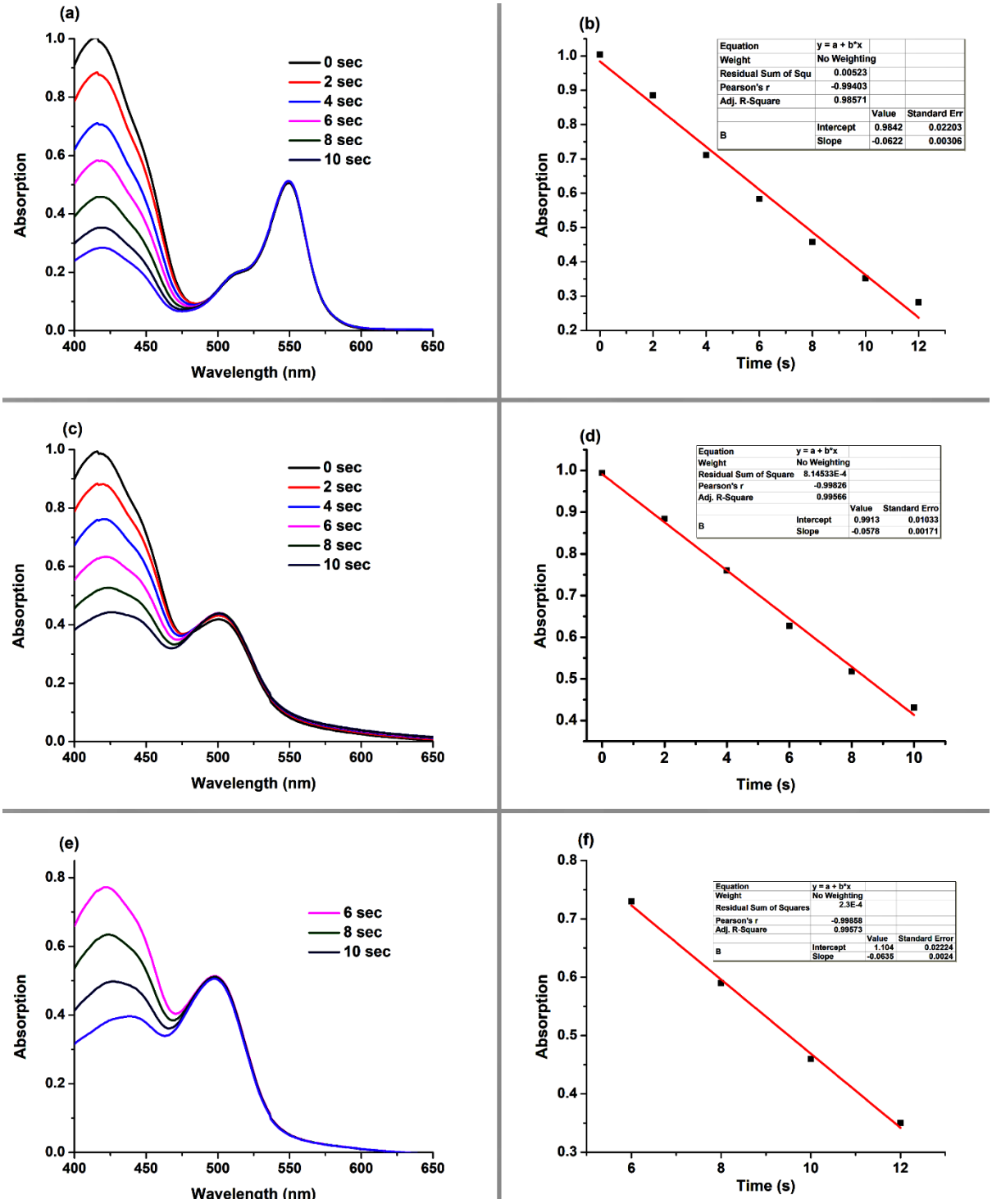


Figure S61 Changes in absorption spectra: (a) **Rose Bengal**, (c) **Ir6**, and (e) **Ir7** upon irradiation of light (LED light, 3W) in water**;** rate of decrease of absorbance at 410 nm: (b) Rose Bengal, (d) **Ir6**, and (f) **Ir7.**

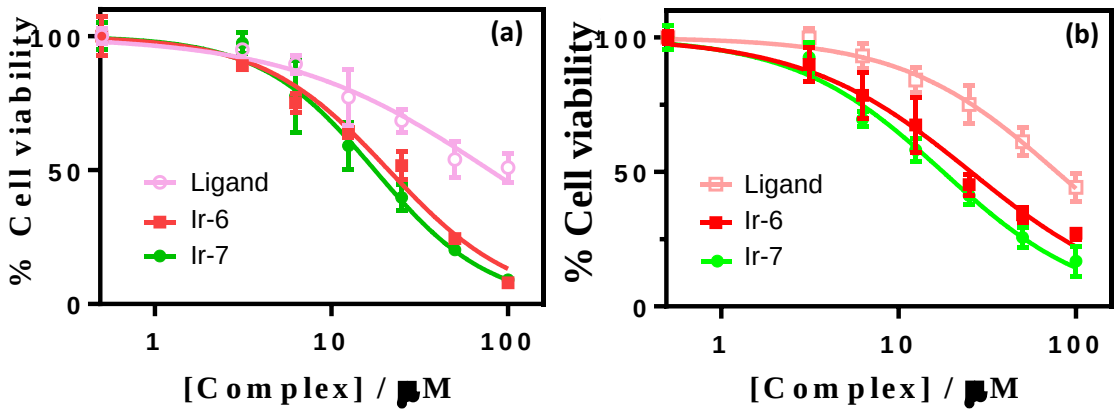


Figure S62 Cell Viability plots in the presence of light; (a) HaCaT and (b) A549 cell line treated with iridium dipyrrinates **Ir6** and **Ir7** and ligand for 24 h incubation, exposed to light (λ = 400-700 nm, 10 J cm^{-2} for 1 h)**.**

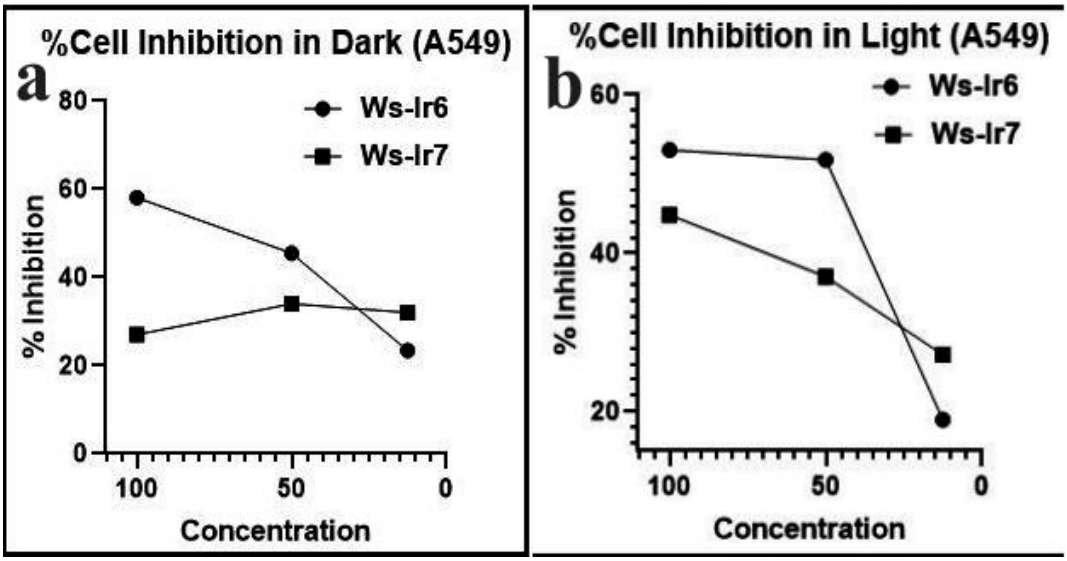


Figure S63 Cell Viability plots in the presence of light and dark conditions on A549 cell line, treated with water soluble iridium dipyrrinates (a) **WS-Ir6** and (b) **WS-Ir7** after 24 h incubation, exposed to light (λ = 400-700 nm, 10 J cm^{-2} for 1 h).

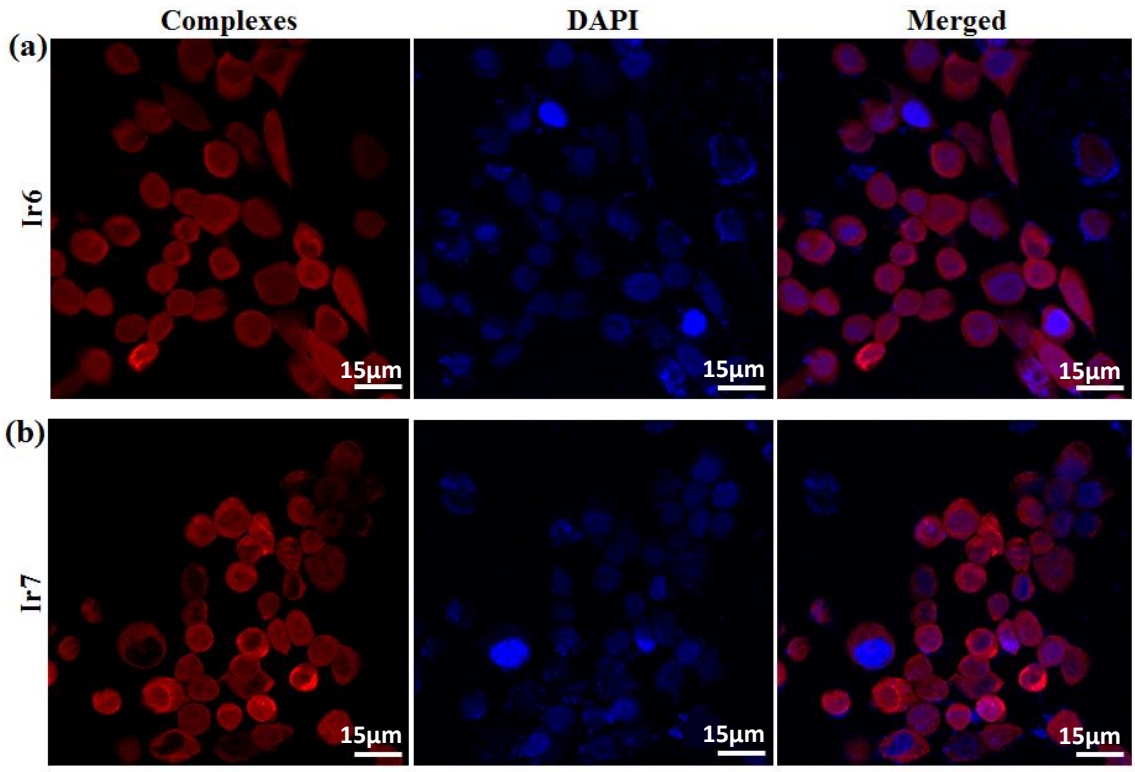
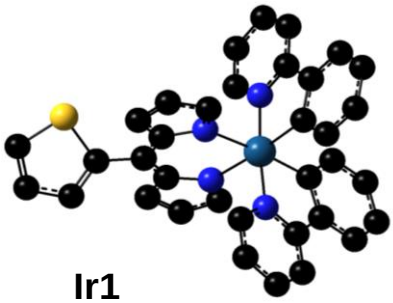
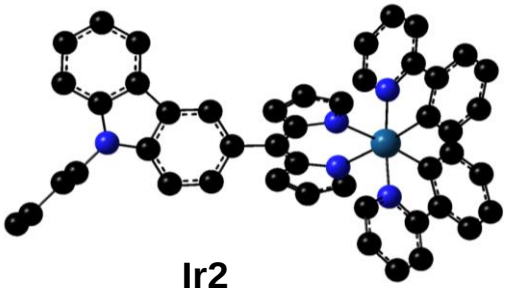


Figure S64 Confocal microscopic image of (a) **Ir6** (top) and (b) **Ir7** (bottom), showing red emission in HaCaT cell line at 24-hour incubation in dark; merged panels with DAPI showing preferable cytoplasmic distribution of iridium dipyrrinates. Scale bar 15 μm.



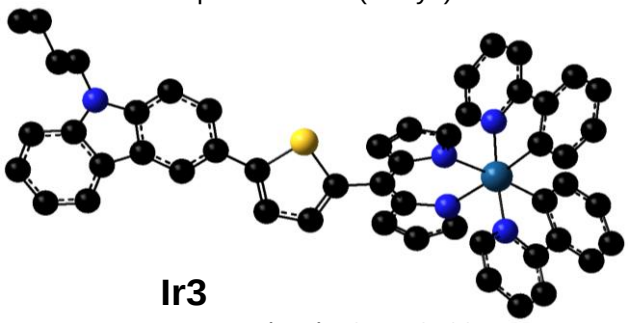
Ir1

Energy (a.u.): -2070.7434
Dipole Moment (Debye): 1.9670



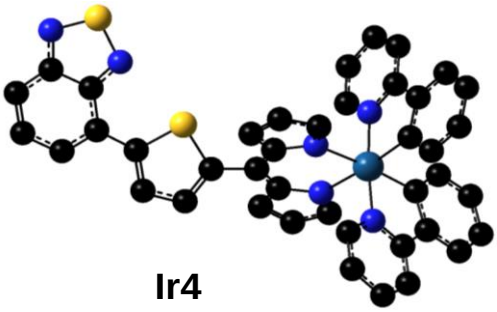
Ir2

Energy (a.u.): -2192.4636
Dipole Moment (Debye): 4.8277



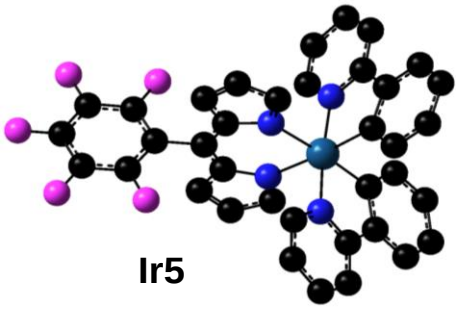
Ir3

Energy (a.u.): -2744.2722
Dipole Moment (Debye): 4.8936



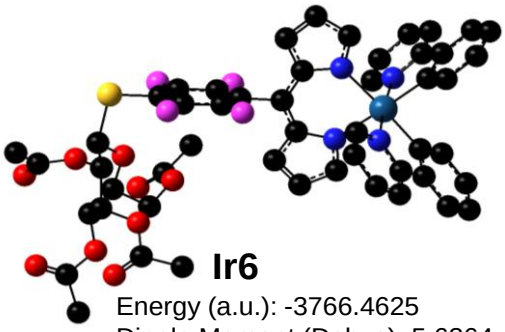
Ir4

Energy (a.u.): -2808.2641
Dipole Moment (Debye): 3.7802



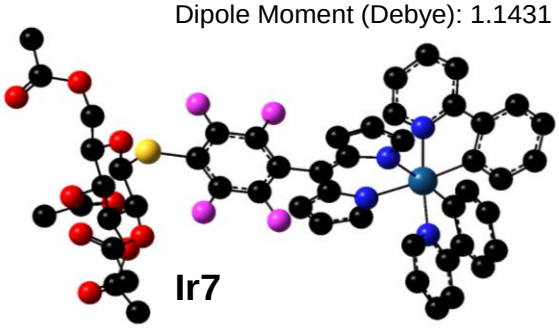
Ir5

Energy (a.u.): -2246.1178
Dipole Moment (Debye): 1.1431



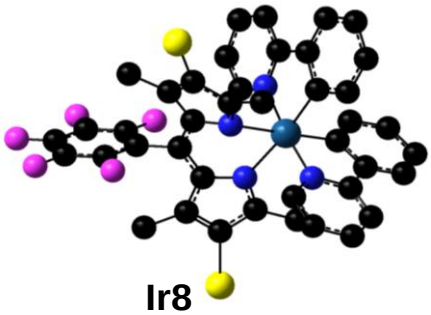
Ir6

Energy (a.u.): -3766.4625
Dipole Moment (Debye): 5.6364



Ir7

Energy (a.u.): -3766.4707
Dipole Moment (Debye): 3.3580



Ir8

Energy (a.u.): -2424.9190
Dipole Moment (Debye): 2.6422

Figure 65 DFT-D3 based geometry optimized structure of iridium dipyrrinates **Ir1-Ir8**.

Table S3. Calculated electronic excitation energies and corresponding orbitals involved in the transition for **Ir1-Ir8** using CPCM-TD-BMK/6-311+ G (2d,p) level of approximation.

Complexes	**Electronic Transition**	**Orbitals Contribution**	**Energy (nm)**	**Oscillatory strength *(f)***	**Experimental Absorption DMSO (nm)**
Ir1	$S_0 \rightarrow S_1$	HOMO-3→LUMO (10%) HOMO-1→LUMO (57%) HOMO→LUMO (7%) HOMO→LUMO+1 (22%)	407	0.35	495
Ir2	$S_0 \rightarrow S_1$	HOMO-5→LUMO (4%) HOMO-4→LUMO (20%) HOMO-2→LUMO (3%) HOMO-1→LUMO (48%) HOMO→LUMO (23%)	397	0.36	484
Ir3	$S_0 \rightarrow S_1$	HOMO-4→LUMO (14%) HOMO-2→LUMO (74%) HOMO-1→LUMO (3%) HOMO→LUMO (8%)	411	0.40	496
Ir4	$S_0 \rightarrow S_1$	HOMO-4→LUMO+1 (24%) HOMO-3→LUMO+1 (11%) HOMO-1→LUMO+1 (54%) HOMO→LUMO+1 (6%)	403	0.32	498
Ir5	$S_0 \rightarrow S_1$	HOMO-3→LUMO (11%) HOMO-1→LUMO (86%)	400	0.50	494
Ir6	$S_0 \rightarrow S_1$	HOMO-3→LUMO (9%) HOMO-1→LUMO (71%) HOMO→LUMO+1 (16%)	408	0.37	494
Ir7	$S_0 \rightarrow S_1$	HOMO-3→LUMO (10%) HOMO-1→LUMO (85%) HOMO→LUMO+1 (2%)	401	0.47	494
Ir8	$S_0 \rightarrow S_1$	HOMO-3→LUMO (13%) HOMO-1→LUMO (8%) HOMO→LUMO (77%)	476	0.49	536

Table S4 B3LYP/6-31G//B3LYP/ LANL2DZ gas phase optimized coordinates of complexes **Ir1-Ir8**.

Ir1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.687723	-0.117822	-0.219689

2	6	0	-2.982017	-1.785807	-0.320753
3	6	0	-1.654203	-1.999887	-2.234044
4	6	0	-3.942549	-2.671326	-0.814519
5	6	0	-3.052097	-1.138489	1.063543
6	6	0	-2.570585	-2.913800	-2.783774
7	1	0	-0.765589	-1.742722	-2.771716
8	6	0	-3.733236	-3.244767	-2.072125
9	1	0	-4.815530	-2.907700	-0.242734
10	6	0	-2.001760	-0.284827	1.316842
11	6	0	-4.055797	-1.355803	2.008932
12	1	0	-2.382625	-3.353643	-3.740953
13	1	0	-4.447334	-3.926709	-2.484361
14	6	0	-1.903767	0.394512	2.532913
15	6	0	-3.977505	-0.683961	3.241844
16	1	0	-4.868030	-2.020203	1.799862
17	6	0	-2.901050	0.190808	3.504041
18	1	0	-1.085720	1.057726	2.722411
19	1	0	-4.734926	-0.836008	3.982205
20	1	0	-2.843633	0.700278	4.443285
21	7	0	-1.898360	-1.448004	-1.036466
22	7	0	0.319480	0.029519	-1.888705
23	6	0	0.051832	1.260051	-2.670934
24	6	0	1.775812	0.117010	-1.634479
25	6	0	1.209362	1.740306	-3.177529
26	1	0	-0.912295	1.701996	-2.812542
27	6	0	2.344516	0.980008	-2.502043
28	1	0	1.310494	2.519537	-3.903797
29	1	0	3.392269	1.119250	-2.668595
30	7	0	0.369057	-1.694100	0.278673
31	6	0	1.828160	-1.430762	0.343437
32	6	0	0.062715	-2.209959	1.634187
33	6	0	2.363929	-2.079246	1.399507
34	6	0	1.204922	-2.585549	2.250273
35	1	0	-0.916118	-2.273128	2.061784
36	1	0	3.406147	-2.199342	1.609740
37	1	0	1.281913	-3.123880	3.171823
38	6	0	2.521065	-0.647782	-0.523367
39	6	0	0.187016	2.320598	0.906046
40	6	0	1.745703	0.602541	1.232461
41	6	0	0.932090	3.223919	1.666806
42	6	0	-1.106281	2.689044	0.162852
43	6	0	2.560886	1.469266	1.982196
44	1	0	2.056009	-0.405496	1.052177
45	6	0	2.141893	2.788330	2.217386
46	1	0	0.588825	4.225638	1.820188
47	6	0	-1.647990	1.634995	-0.541326

48	6	0	-1.701495	3.951136	0.146949
49	1	0	3.494991	1.124191	2.373679
50	1	0	2.740386	3.451388	2.806528
51	6	0	-2.750031	1.815030	-1.378193
52	6	0	-2.837053	4.149373	-0.659955
53	1	0	-1.299851	4.752265	0.731552
54	6	0	-3.350483	3.086229	-1.435832
55	1	0	-3.133448	1.002555	-1.959444
56	1	0	-3.311079	5.108265	-0.688196
57	1	0	-4.199381	3.247444	-2.066947
58	7	0	0.575251	1.043021	0.750804
59	6	0	4.049053	-0.512972	-0.386754
60	6	0	4.834878	0.246401	-1.195893
61	16	0	5.027813	-1.330736	0.842260
62	6	0	6.345960	0.020700	-0.922590
63	1	0	4.455968	0.912938	-1.942262
64	6	0	6.557419	-0.887693	0.066886
65	1	0	7.129963	0.513565	-1.458623
66	1	0	7.514413	-1.282981	0.336745

Ir2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	2.372093	-0.036900	0.024001
2	6	0	3.216692	2.735101	0.346001
3	6	0	1.600992	2.577100	-1.386099
4	6	0	3.294191	4.127701	0.165101
5	6	0	3.967392	1.942101	1.328101
6	6	0	1.650992	3.960500	-1.593999
7	1	0	0.932792	1.933900	-1.986899
8	6	0	2.507991	4.741700	-0.809799
9	1	0	3.966191	4.715401	0.790701
10	6	0	3.691793	0.544901	1.329701
11	6	0	4.900592	2.506601	2.216801
12	1	0	1.024691	4.416900	-2.359499
13	1	0	2.559191	5.821100	-0.959299
14	6	0	4.381493	-0.251199	2.262401
15	6	0	5.568292	1.690101	3.125901
16	1	0	5.100792	3.576701	2.195401
17	6	0	5.306493	0.310101	3.144601
18	1	0	4.204693	-1.328599	2.296801
19	1	0	6.291892	2.114702	3.816601

20	1	0	5.834293	-0.324999	3.855801
21	7	0	2.369592	1.953200	-0.438199
22	7	0	1.032893	-0.523500	-1.440599
23	6	0	1.346793	-0.903800	-2.704299
24	6	0	-0.401407	-0.504601	-1.365799
25	6	0	0.158693	-1.135100	-3.490299
26	6	0	-0.918307	-0.886901	-2.666999
27	1	0	0.153093	-1.441400	-4.516399
28	7	0	0.805093	0.340500	1.280701
29	6	0	-0.598807	0.215499	1.002501
30	6	0	0.906693	0.738400	2.573401
31	6	0	-1.322707	0.554899	2.214001
32	6	0	-0.395307	0.879099	3.180401
33	1	0	-0.569708	1.181999	4.192601
34	6	0	-1.144707	-0.169601	-0.227599
35	6	0	3.462794	-2.734299	-0.159899
36	6	0	1.611394	-2.708800	1.326001
37	6	0	3.619894	-4.117899	0.038401
38	6	0	4.282093	-1.881299	-1.030199
39	6	0	1.737094	-4.085300	1.547201
40	1	0	0.818394	-2.121200	1.822701
41	6	0	2.753294	-4.794900	0.896301
42	1	0	4.416494	-4.649299	-0.482699
43	6	0	3.903893	-0.509099	-1.078199
44	6	0	5.371994	-2.368099	-1.774999
45	1	0	1.046194	-4.591900	2.219601
46	1	0	2.865195	-5.867900	1.057901
47	6	0	4.656193	0.342401	-1.907999
48	6	0	6.097493	-1.498198	-2.584599
49	1	0	5.647894	-3.420099	-1.719799
50	6	0	5.736693	-0.141999	-2.647399
51	1	0	4.404592	1.403401	-1.972799
52	1	0	6.941793	-1.862598	-3.163799
53	1	0	6.310093	0.535402	-3.279999
54	7	0	2.456093	-2.023400	0.492101
55	1	0	-1.963107	-0.946701	-2.908499
56	1	0	2.368493	-1.010800	-3.055799
57	1	0	1.856993	0.919300	3.066201
58	1	0	-2.392907	0.538899	2.303301
59	6	0	-2.629407	-0.230101	-0.333999
60	6	0	-3.257207	-1.481502	-0.528899
61	6	0	-3.383107	0.946998	-0.239599
62	6	0	-4.639307	-1.593502	-0.633899
63	1	0	-2.637806	-2.378001	-0.594999
64	6	0	-4.769207	0.864898	-0.346699
65	1	0	-2.897008	1.910299	-0.087099

66	6	0	-5.397507	-0.416602	-0.549799
67	1	0	-5.113806	-2.559402	-0.776599
68	6	0	-5.830208	1.854098	-0.294499
69	6	0	-7.072608	1.150297	-0.468399
70	6	0	-5.841408	3.238798	-0.117999
71	6	0	-8.302408	1.821297	-0.455999
72	6	0	-7.067208	3.903697	-0.109699
73	1	0	-4.908008	3.782698	0.011001
74	6	0	-8.277008	3.202397	-0.275399
75	1	0	-9.238108	1.286996	-0.581299
76	1	0	-7.094709	4.982697	0.027701
77	1	0	-9.215508	3.756796	-0.260399
78	7	0	-6.792807	-0.227003	-0.671199
79	6	0	-7.800307	-1.301903	-0.715299
80	6	0	-8.189407	-1.772903	0.695701
81	1	0	-7.392906	-2.149203	-1.313399
82	1	0	-8.695207	-0.927803	-1.264299
83	6	0	-9.241606	-2.886604	0.634101
84	1	0	-7.290506	-2.125503	1.239701
85	1	0	-8.571707	-0.918103	1.288801
86	6	0	-9.634906	-3.360704	2.030801
87	1	0	-10.141806	-2.529404	0.095701
88	1	0	-8.855006	-3.742603	0.046101
89	1	0	-10.387706	-4.156104	1.981901
90	1	0	-8.774506	-3.758603	2.581701
91	1	0	-10.058106	-2.546904	2.631501

Ir3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	3.724731	-0.106809	0.141648
2	6	0	5.486624	-2.017514	1.457255
3	6	0	3.904688	-1.170309	2.961676
4	6	0	6.079329	-2.778181	2.472257
5	6	0	5.916778	-2.049915	0.033700
6	6	0	4.442813	-1.921427	4.002759
7	1	0	3.047381	-0.537555	3.124814
8	6	0	5.555875	-2.728061	3.760491
9	1	0	6.933258	-3.403725	2.251557
10	6	0	5.182514	-1.204428	-0.825792
11	6	0	6.969183	-2.853001	-0.436954
12	1	0	3.997625	-1.873720	4.988635

13	1	0	6.000116	-3.309977	4.558904
14	6	0	5.540851	-1.187058	-2.188386
15	6	0	7.302538	-2.819491	-1.789155
16	1	0	7.523505	-3.495353	0.238350
17	6	0	6.588519	-1.987026	-2.662273
18	1	0	5.006831	-0.553147	-2.883309
19	1	0	8.112572	-3.434736	-2.163948
20	1	0	6.853624	-1.966701	-3.714948
21	7	0	4.432418	-1.193709	1.719759
22	7	0	2.416553	0.882499	1.465465
23	6	0	2.836486	2.180439	1.791181
24	6	0	1.027843	1.081262	1.123038
25	6	0	1.792035	3.061246	1.923710
26	1	0	3.877187	2.423163	1.903371
27	6	0	0.630381	2.359412	1.517241
28	1	0	1.830811	4.076970	2.292881
29	1	0	-0.356781	2.768516	1.558048
30	7	0	2.189273	-1.563631	0.323921
31	6	0	0.781212	-1.260194	0.096971
32	6	0	2.385660	-2.683040	-0.479789
33	6	0	0.192095	-2.368989	-0.551055
34	6	0	1.215955	-3.245311	-0.933195
35	1	0	3.378654	-3.045015	-0.691338
36	1	0	-0.837847	-2.556079	-0.744607
37	1	0	1.098490	-4.184474	-1.454930
38	6	0	0.188124	0.009237	0.488974
39	6	0	4.207895	1.902336	-2.036817
40	6	0	2.256183	0.871384	-2.614538
41	6	0	4.189095	2.651100	-3.222938
42	6	0	5.282060	2.130027	-1.055347
43	6	0	2.162644	1.604783	-3.796127
44	1	0	1.476317	0.179155	-2.457011
45	6	0	3.151820	2.510895	-4.125988
46	1	0	4.990782	3.343144	-3.428476
47	6	0	5.206420	1.318308	0.073472
48	6	0	6.317055	3.073845	-1.218560
49	1	0	1.311712	1.448403	-4.447386
50	1	0	3.119026	3.078611	-5.048415
51	6	0	6.171067	1.509466	1.086849
52	6	0	7.263492	3.241434	-0.212213
53	1	0	6.392109	3.670332	-2.118399
54	6	0	7.184533	2.461845	0.948442
55	1	0	6.126256	0.911986	1.990754
56	1	0	8.059905	3.967579	-0.329675
57	1	0	7.915368	2.598790	1.739337
58	7	0	3.254827	0.942469	-1.703836

59	6	0	-1.283410	0.380602	0.322039
60	6	0	-1.838052	1.585415	0.712089
61	16	0	-2.604792	-0.597086	-0.364747
62	6	0	-3.277902	1.674521	0.617335
63	1	0	-1.271544	2.417487	1.070027
64	6	0	-3.846723	0.532256	0.136695
65	1	0	-3.826024	2.560252	0.904477
66	6	0	-5.299269	0.218631	0.036153
67	6	0	-5.723782	-1.018656	-0.485714
68	6	0	-6.252112	1.160474	0.464102
69	6	0	-7.078427	-1.338262	-0.591368
70	1	0	-4.987449	-1.748216	-0.815877
71	6	0	-7.603305	0.847502	0.361417
72	1	0	-5.941137	2.119106	0.869698
73	6	0	-8.011228	-0.396952	-0.164823
74	1	0	-7.386300	-2.299443	-0.997123
75	6	0	-8.804214	1.575769	0.703094
76	6	0	-9.916716	0.752313	0.374110
77	6	0	-8.985204	2.844703	1.253278
78	6	0	-11.213623	1.223180	0.605515
79	6	0	-10.282029	3.304574	1.480458
80	1	0	-8.127997	3.467861	1.501837
81	6	0	-11.378130	2.498816	1.158329
82	1	0	-12.088490	0.635327	0.371216
83	1	0	-10.437543	4.293216	1.909252
84	1	0	-12.387302	2.864977	1.338478
85	7	0	-9.421423	-0.492575	-0.172811
86	6	0	-10.082667	-1.709560	-0.681060
87	6	0	-11.602736	-1.704776	-0.707515
88	1	0	-9.738738	-2.546856	-0.051890
89	1	0	-9.705877	-1.866662	-1.704546
90	6	0	-12.156885	-3.022117	-1.257805
91	1	0	-11.993577	-1.546013	0.307997
92	1	0	-11.959080	-0.880365	-1.345181
93	6	0	-13.683075	-3.041978	-1.292668
94	1	0	-11.762777	-3.184309	-2.275906
95	1	0	-11.791853	-3.858139	-0.636220
96	1	0	-14.056605	-3.996515	-1.691255
97	1	0	-14.103008	-2.909184	-0.283873
98	1	0	-14.074423	-2.233562	-1.929076

Ir4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-2.222235	-0.077658	-0.026553
2	6	0	-3.089148	-2.861014	-0.394910
3	6	0	-1.547235	-2.243068	-2.058246
4	6	0	-3.179131	-4.142860	-0.956217
5	6	0	-3.807462	-2.392893	0.792634
6	6	0	-1.602233	-3.497726	-2.649319
7	1	0	-0.920049	-1.454046	-2.453376
8	6	0	-2.437574	-4.465950	-2.085498
9	1	0	-3.829873	-4.881163	-0.502713
10	6	0	-3.535751	-1.049823	1.174193
11	6	0	-4.695926	-3.200120	1.524882
12	1	0	-1.002507	-3.704670	-3.528603
13	1	0	-2.507030	-5.458605	-2.519533
14	6	0	-4.201313	-0.567852	2.315684
15	6	0	-5.333408	-2.690893	2.652492
16	1	0	-4.894816	-4.224569	1.221107
17	6	0	-5.082163	-1.370137	3.045472
18	1	0	-4.030640	0.454290	2.645008
19	1	0	-6.021531	-3.312998	3.218148
20	1	0	-5.577372	-0.966522	3.926245
21	7	0	-2.269484	-1.925880	-0.965200
22	7	0	-0.765433	0.833850	-1.374967
23	6	0	-1.016718	1.342633	-2.585797
24	6	0	0.599017	1.025544	-1.137569
25	6	0	0.147156	1.882039	-3.186742
26	1	0	-2.018004	1.299668	-2.995952
27	6	0	1.162785	1.697022	-2.274250
28	1	0	0.208273	2.325361	-4.172342
29	1	0	2.200203	1.978030	-2.377703
30	7	0	-0.480182	-0.721719	1.137746
31	6	0	0.822287	-0.210607	1.048337
32	6	0	-0.530592	-1.450216	2.257096
33	6	0	1.560337	-0.674296	2.187225
34	6	0	0.711679	-1.460718	2.937186
35	1	0	-1.454245	-1.926915	2.557885
36	1	0	2.585366	-0.424913	2.412936
37	1	0	0.930227	-1.980139	3.861341
38	6	0	1.315497	0.575951	-0.012989
39	6	0	-3.319629	2.606352	0.453170
40	6	0	-1.570337	2.143466	1.957016
41	6	0	-3.471767	3.876594	1.026768
42	6	0	-4.120168	2.054464	-0.645439
43	6	0	-1.684940	3.387662	2.559763

44	1	0	-0.829624	1.416363	2.280864
45	6	0	-2.656316	4.273270	2.081347
46	1	0	-4.231428	4.548002	0.645125
47	6	0	-3.779322	0.729041	-1.040062
48	6	0	-5.163854	2.758303	-1.272807
49	1	0	-1.026067	3.649189	3.380142
50	1	0	-2.776737	5.256244	2.525576
51	6	0	-4.542431	0.155285	-2.073859
52	6	0	-5.892111	2.162617	-2.298354
53	1	0	-5.415084	3.770559	-0.967669
54	6	0	-5.578787	0.856555	-2.695747
55	1	0	-4.323855	-0.856001	-2.406916
56	1	0	-6.697784	2.707772	-2.782318
57	1	0	-6.147067	0.385408	-3.495009
58	7	0	-2.359943	1.759819	0.936304
59	6	0	2.738288	1.000497	0.030562
60	6	0	3.196220	2.296256	0.116644
61	16	0	4.073020	-0.120578	-0.041301
62	6	0	4.606715	2.395136	0.125267
63	1	0	2.527293	3.146975	0.181387
64	6	0	5.257581	1.179610	0.017065
65	1	0	5.126239	3.342478	0.210098
66	6	0	6.703283	0.955886	-0.030461
67	6	0	7.294229	-0.359404	-0.017622
68	6	0	7.600196	2.011677	-0.083261
69	6	0	8.737033	-0.531656	-0.053103
70	6	0	9.013605	1.837404	-0.116857
71	1	0	7.225225	3.028939	-0.104014
72	6	0	9.600622	0.597110	-0.103120
73	1	0	9.634376	2.727407	-0.157079
74	1	0	10.676031	0.460998	-0.128856
75	7	0	9.122250	-1.813639	-0.008998
76	7	0	6.629087	-1.516012	0.050953
77	16	0	7.751928	-2.718750	0.038584

Ir5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-1.281607	-0.134076	-0.109992
2	6	0	-3.557230	-2.031057	0.009465

3	6	0	-1.889133	-2.491478	-1.668248
4	6	0	-4.366384	-3.050926	-0.350479
5	6	0	-3.819208	-1.098018	1.175168
6	6	0	-2.742698	-3.696864	-2.125701
7	1	0	-0.958355	-2.281600	-2.151737
8	6	0	-3.922972	-3.955669	-1.510112
9	1	0	-5.289102	-3.227526	0.161620
10	6	0	-2.724517	-0.069643	1.327754
11	6	0	-4.877045	-1.144334	2.011435
12	1	0	-2.405248	-4.323131	-2.924708
13	1	0	-4.534250	-4.776077	-1.825647
14	6	0	-2.745631	0.812682	2.351522
15	6	0	-4.935357	-0.133956	3.177431
16	1	0	-5.655131	-1.865298	1.871698
17	6	0	-3.931876	0.776288	3.342834
18	1	0	-1.956996	1.525693	2.472789
19	1	0	-5.761681	-0.147978	3.857117
20	1	0	-3.966726	1.467689	4.159502
21	7	0	-2.303606	-1.732307	-0.700597
22	7	0	-0.180835	-0.215046	-1.720919
23	6	0	-0.482277	0.870877	-2.685591
24	6	0	1.269260	-0.010751	-1.432102
25	6	0	0.666043	1.375729	-3.187001
26	1	0	-1.464418	1.208061	-2.942415
27	6	0	1.813171	0.797944	-2.367058
28	1	0	0.753080	2.066664	-3.999769
29	1	0	2.854408	1.006449	-2.497748
30	7	0	-0.085605	-1.328805	0.873384
31	6	0	1.364178	-1.351247	0.687454
32	6	0	-0.418627	-2.200475	1.783395
33	6	0	1.930821	-2.322562	1.720794
34	6	0	0.864716	-2.848643	2.365221
35	1	0	-1.418971	-2.426728	2.086360
36	1	0	2.962675	-2.547125	1.894910
37	1	0	0.899777	-3.585069	3.141215
38	6	0	2.042190	-0.636653	-0.244553
39	6	0	-0.646803	2.690885	0.369968
40	6	0	0.984989	1.104075	1.180800
41	6	0	-0.009398	3.772608	0.868230
42	6	0	-1.921550	2.746942	-0.473662
43	6	0	1.791647	2.289937	1.753422
44	1	0	1.352411	0.104908	1.283334
45	6	0	1.314046	3.552926	1.619466
46	1	0	-0.411413	4.756611	0.738789
47	6	0	-2.386839	1.371530	-0.904310
48	6	0	-2.586943	3.863845	-0.837630

49	1	0	2.721194	2.115753	2.254385
50	1	0	1.851554	4.382820	2.027980
51	6	0	-3.441364	1.219668	-1.733380
52	6	0	-3.817805	3.717629	-1.760995
53	1	0	-2.268044	4.827964	-0.498778
54	6	0	-4.208893	2.481491	-2.191659
55	1	0	-3.742092	0.247548	-2.063241
56	1	0	-4.363243	4.586620	-2.065833
57	1	0	-5.050169	2.385998	-2.846258
58	7	0	-0.142274	1.323662	0.580867
59	6	0	3.568071	-0.454574	-0.138094
60	6	0	4.096968	0.806580	0.171078
61	6	0	4.426093	-1.543599	-0.343011
62	6	0	5.483655	0.975998	0.283822
63	6	0	5.812871	-1.370981	-0.234787
64	6	0	6.340572	-0.112861	0.081089
65	9	0	5.994843	2.187496	0.589035
66	9	0	3.269990	1.856732	0.361681
67	9	0	7.675724	0.049520	0.189526
68	9	0	6.641552	-2.417592	-0.433885
69	9	0	3.917920	-2.757375	-0.644705

Ir6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-3.987966	-0.098255	0.042038
2	6	0	-5.394222	2.484708	-0.014488
3	6	0	-3.290331	2.706614	1.012136
4	6	0	-5.630678	3.853624	0.178088
5	6	0	-6.306918	1.538104	-0.661462
6	6	0	-3.477580	4.065726	1.223712
7	1	0	-2.386565	2.198021	1.322839
8	6	0	-4.674779	4.647951	0.798436
9	1	0	-6.562525	4.290456	-0.161839
10	6	0	-5.827320	0.202533	-0.760962
11	6	0	-7.568010	1.903689	-1.163871
12	1	0	-2.701212	4.646112	1.709559
13	1	0	-4.859332	5.707513	0.946768
14	6	0	-6.674137	-0.732729	-1.380754
15	6	0	-8.379455	0.951953	-1.775361
16	1	0	-7.923158	2.927639	-1.081671
17	6	0	-7.927149	-0.368956	-1.882596

18	1	0	-6.351726	-1.766361	-1.479756
19	1	0	-9.354015	1.234842	-2.163365
20	1	0	-8.556313	-1.117900	-2.358888
21	7	0	-4.219405	1.933214	0.416037
22	7	0	-1.974610	-0.250954	0.917681
23	6	0	-1.693646	-0.567647	2.186499
24	6	0	-0.747599	-0.072023	0.272699
25	6	0	-0.292911	-0.609684	2.422867
26	6	0	0.307450	-0.299620	1.219080
27	1	0	0.189081	-0.840003	3.364016
28	7	0	-2.951956	0.434151	-1.824298
29	6	0	-1.573524	0.520505	-2.041545
30	6	0	-3.538594	0.742566	-2.986335
31	6	0	-1.345240	0.899527	-3.406438
32	6	0	-2.585015	1.038665	-3.997339
33	1	0	-2.804354	1.316891	-5.019835
34	6	0	-0.585949	0.280947	-1.074744
35	6	0	-4.475275	-2.919352	0.719803
36	6	0	-3.383070	-2.742699	-1.354747
37	6	0	-4.464979	-4.317168	0.604288
38	6	0	-5.021148	-2.155060	1.844733
39	6	0	-3.347766	-4.121302	-1.513931
40	1	0	-2.972337	-2.071130	-2.097877
41	6	0	-3.903028	-4.922667	-0.512523
42	1	0	-4.895093	-4.924234	1.392459
43	6	0	-4.889695	-0.742376	1.741641
44	6	0	-5.628775	-2.755452	2.961312
45	1	0	-2.895374	-4.548419	-2.401941
46	1	0	-3.895865	-6.004749	-0.600559
47	6	0	-5.399809	0.022621	2.804977
48	6	0	-6.118873	-1.967157	3.998781
49	1	0	-5.722658	-3.836130	3.028638
50	6	0	-6.001482	-0.574230	3.916694
51	1	0	-5.322346	1.106565	2.772086
52	1	0	-6.588003	-2.431679	4.861621
53	1	0	-6.382233	0.048002	4.723820
54	7	0	-3.933699	-2.153310	-0.275001
55	6	0	0.833288	0.425633	-1.540401
56	6	0	1.518610	1.633195	-1.419575
57	6	0	1.522434	-0.644399	-2.109482
58	6	0	2.840118	1.769802	-1.837148
59	6	0	2.844162	-0.517197	-2.524115
60	6	0	3.541700	0.688997	-2.382631
61	9	0	0.899348	2.702580	-0.892460
62	9	0	3.416279	2.969256	-1.716499
63	9	0	3.447613	-1.598149	-3.045419

64	9	0	0.912146	-1.832226	-2.256145
65	1	0	1.367434	-0.236327	1.013017
66	1	0	-2.493534	-0.752661	2.891017
67	1	0	-4.617104	0.740449	-3.069343
68	1	0	-0.378907	1.048324	-3.868447
69	16	0	5.210430	0.888131	-2.977623
70	6	0	6.212059	0.495222	-1.464590
71	6	0	5.995958	-0.973685	-1.027174
72	6	0	6.036484	1.317887	0.909691
73	6	0	6.034201	-1.319076	0.478803
74	1	0	5.018794	-1.299119	-1.369675
75	6	0	6.148656	-0.127340	1.481541
76	1	0	6.965104	1.835355	1.183126
77	1	0	6.875012	-1.978312	0.668662
78	8	0	5.893418	1.465199	-0.507393
79	6	0	4.876390	2.087591	1.550870
80	1	0	3.914290	1.639565	1.298133
81	1	0	4.999587	2.127722	2.631978
82	8	0	4.851642	3.434466	1.042989
83	6	0	5.236834	4.429996	1.874876
84	8	0	5.617820	4.256305	3.016451
85	6	0	5.118622	5.767687	1.189032
86	1	0	5.721254	5.777502	0.275211
87	1	0	4.079369	5.946854	0.894245
88	1	0	5.452468	6.557301	1.862346
89	8	0	4.832256	-2.078159	0.730582
90	6	0	4.965625	-3.375197	1.115074
91	8	0	6.035040	-3.919111	1.300420
92	6	0	3.619407	-4.040095	1.244043
93	1	0	3.389746	-4.551525	0.301711
94	1	0	3.661247	-4.792888	2.033587
95	1	0	2.826604	-3.317349	1.444227
96	8	0	6.885878	-1.833960	-1.787643
97	6	0	8.225045	-1.865247	-1.540426
98	8	0	8.764256	-1.249550	-0.639547
99	6	0	8.925036	-2.842223	-2.446115
100	1	0	9.442986	-2.278228	-3.230493
101	1	0	9.680225	-3.387623	-1.875652
102	1	0	8.226921	-3.535859	-2.916656
103	1	0	7.230998	0.620757	-1.835691
104	1	0	7.117230	-0.220323	1.969502
105	8	0	5.154575	-0.280217	2.517424
106	6	0	5.581759	-0.532670	3.785711
107	8	0	6.749693	-0.646275	4.094587
108	6	0	4.422629	-0.638794	4.743289
109	1	0	4.422246	-1.640390	5.185274

110	1	0	4.569291	0.076590	5.558076
111	1	0	3.464828	-0.454329	4.256072

Ir7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-4.410253	-0.081763	0.164003
2	6	0	-5.905887	2.439913	-0.054480
3	6	0	-3.877226	2.775576	1.085730
4	6	0	-6.204603	3.803400	0.079672
5	6	0	-6.747388	1.436760	-0.712815
6	6	0	-4.129157	4.131508	1.244480
7	1	0	-2.972735	2.314620	1.462580
8	6	0	-5.318862	4.653666	0.729962
9	1	0	-7.130616	4.191847	-0.328003
10	6	0	-6.221043	0.114557	-0.726671
11	6	0	-7.987389	1.740113	-1.302130
12	1	0	-3.407081	4.755867	1.758702
13	1	0	-5.551270	5.709122	0.833212
14	6	0	-7.006937	-0.873749	-1.345724
15	6	0	-8.734024	0.737658	-1.914405
16	1	0	-8.375057	2.755343	-1.288099
17	6	0	-8.238981	-0.572320	-1.932497
18	1	0	-6.652242	-1.901336	-1.376310
19	1	0	-9.691822	0.971610	-2.370704
20	1	0	-8.818747	-1.361531	-2.406481
21	7	0	-4.736605	1.948388	0.459075
22	7	0	-2.434739	-0.123547	1.118532
23	6	0	-2.192061	-0.371271	2.410116
24	6	0	-1.187854	0.033213	0.504362
25	6	0	-0.799646	-0.387800	2.693294
26	6	0	-0.163202	-0.138011	1.494128
27	1	0	-0.349465	-0.563014	3.661641
28	7	0	-3.329868	0.423061	-1.679285
29	6	0	-1.945856	0.526816	-1.855366
30	6	0	-3.882743	0.686173	-2.868154
31	6	0	-1.680088	0.866161	-3.223587
32	6	0	-2.901947	0.967858	-3.857376
33	1	0	-3.095741	1.214186	-4.893165
34	6	0	-0.986181	0.327168	-0.852454
35	6	0	-4.792465	-2.893878	0.930301
36	6	0	-3.666242	-2.743348	-1.127830

37	6	0	-4.721621	-4.292757	0.864227
38	6	0	-5.405049	-2.115124	2.010485
39	6	0	-3.573902	-4.124015	-1.239321
40	1	0	-3.263886	-2.081930	-1.884626
41	6	0	-4.114317	-4.913083	-0.220529
42	1	0	-5.142530	-4.888804	1.665556
43	6	0	-5.345647	-0.702035	1.852472
44	6	0	-6.010662	-2.703443	3.134719
45	1	0	-3.089090	-4.562096	-2.104584
46	1	0	-4.061278	-5.996258	-0.270797
47	6	0	-5.931391	0.074454	2.868243
48	6	0	-6.573632	-1.903200	4.124651
49	1	0	-6.046148	-3.784165	3.244057
50	6	0	-6.532424	-0.510190	3.986203
51	1	0	-5.915986	1.158991	2.792242
52	1	0	-7.041147	-2.357528	4.993751
53	1	0	-6.972182	0.121507	4.755094
54	7	0	-4.259740	-2.139578	-0.079638
55	6	0	0.445289	0.444110	-1.289058
56	6	0	1.169331	1.624101	-1.127900
57	6	0	1.104520	-0.634689	-1.878252
58	6	0	2.497853	1.725186	-1.529097
59	6	0	2.432274	-0.540056	-2.284751
60	6	0	3.161412	0.643682	-2.116948
61	9	0	0.580982	2.698117	-0.575027
62	9	0	3.125542	2.894070	-1.348903
63	9	0	3.000721	-1.617419	-2.845744
64	9	0	0.455708	-1.796733	-2.061512
65	1	0	0.901468	-0.073057	1.315755
66	1	0	-3.009987	-0.529696	3.100519
67	1	0	-4.957421	0.666547	-2.990584
68	1	0	-0.700275	1.019976	-3.654967
69	16	0	4.831964	0.813568	-2.719805
70	6	0	5.838208	0.406214	-1.222431
71	6	0	5.740985	-1.044126	-0.745074
72	6	0	6.482264	1.364397	0.808660
73	6	0	6.530304	-1.261995	0.570714
74	1	0	4.693080	-1.245671	-0.522190
75	6	0	7.066451	0.010458	1.282241
76	1	0	7.289900	1.932856	0.329757
77	1	0	7.377824	-1.916414	0.378907
78	1	0	6.881358	-0.137309	2.347723
79	8	0	5.416072	1.190505	-0.128042
80	6	0	5.928464	2.162267	1.986727
81	1	0	5.090098	1.631640	2.443722
82	1	0	6.716445	2.325626	2.724403

83	8	0	5.397256	3.424456	1.550101
84	6	0	6.260034	4.471431	1.502823
85	8	0	7.427997	4.389096	1.825097
86	6	0	5.536104	5.739729	1.129706
87	1	0	5.068221	5.626848	0.146753
88	1	0	4.738895	5.944009	1.851788
89	1	0	6.239597	6.572628	1.112614
90	8	0	8.497293	0.113145	1.090592
91	6	0	9.287481	-0.582668	1.950750
92	8	0	8.848646	-1.282194	2.840372
93	6	0	10.743902	-0.332017	1.656796
94	1	0	11.362017	-0.898204	2.354048
95	1	0	10.972286	-0.630663	0.628834
96	1	0	10.966548	0.736022	1.746616
97	8	0	5.654397	-1.929193	1.502678
98	6	0	5.925583	-3.230899	1.804674
99	8	0	6.821745	-3.863299	1.288377
100	6	0	4.865959	-3.797126	2.714441
101	1	0	3.991904	-4.075826	2.114329
102	1	0	5.249258	-4.692828	3.205546
103	1	0	4.545751	-3.061197	3.455064
104	8	0	6.066304	-2.033451	-1.745424
105	6	0	7.302239	-2.073923	-2.307059
106	8	0	8.198569	-1.301264	-2.028555
107	6	0	7.389793	-3.168331	-3.338011
108	1	0	7.037908	-2.776793	-4.299645
109	1	0	8.430361	-3.476672	-3.452538
110	1	0	6.763803	-4.020871	-3.067513
111	1	0	6.859811	0.659227	-1.528044

Ir8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-1.703632	-0.044590	0.131487
2	6	0	-3.796221	-1.201590	-1.565723
3	6	0	-2.087787	-0.262185	-2.883777
4	6	0	-4.509507	-1.528476	-2.728094
5	6	0	-4.173694	-1.552918	-0.194637
6	6	0	-2.751593	-0.575520	-4.061469
7	1	0	-1.123031	0.230013	-2.882061
8	6	0	-3.993263	-1.211378	-3.978605
9	1	0	-5.462290	-2.038217	-2.646363
10	6	0	-3.232519	-1.185723	0.807708

11	6	0	-5.339016	-2.271520	0.123975
12	1	0	-2.301552	-0.324049	-5.015290
13	1	0	-4.546111	-1.466171	-4.877504
14	6	0	-3.520336	-1.575495	2.126777
15	6	0	-5.593895	-2.642011	1.440950
16	1	0	-6.049403	-2.546932	-0.651065
17	6	0	-4.677649	-2.292861	2.441305
18	1	0	-2.831677	-1.317714	2.927369
19	1	0	-6.494444	-3.197387	1.687413
20	1	0	-4.869569	-2.580467	3.472791
21	7	0	-2.599288	-0.542483	-1.668391
22	7	0	-0.108791	1.304866	-0.711709
23	6	0	-0.280095	2.569774	-1.112683
24	6	0	1.213463	1.185053	-0.241826
25	6	0	0.895109	3.321662	-0.821565
26	6	0	1.841700	2.497020	-0.245012
27	7	0	-0.112113	-1.610711	-0.195246
28	6	0	1.275219	-1.357070	-0.176447
29	6	0	-0.278546	-2.939060	-0.302141
30	6	0	1.992461	-2.611673	-0.297038
31	6	0	0.994607	-3.567673	-0.371309
32	6	0	1.842945	-0.062526	-0.079099
33	6	0	-1.629350	1.584237	2.586988
34	6	0	-0.085314	-0.176213	2.736991
35	6	0	-1.234304	2.037640	3.853558
36	6	0	-2.702532	2.159756	1.775131
37	6	0	0.332050	0.225767	3.998133
38	1	0	0.335462	-1.046959	2.253441
39	6	0	-0.249393	1.362573	4.562849
40	1	0	-1.710633	2.911031	4.282856
41	6	0	-2.966205	1.495008	0.548618
42	6	0	-3.475124	3.258833	2.195382
43	1	0	1.099540	-0.339852	4.513522
44	1	0	0.054861	1.713232	5.544338
45	6	0	-4.069426	1.951101	-0.193764
46	6	0	-4.539485	3.703525	1.419139
47	1	0	-3.256883	3.761675	3.133386
48	6	0	-4.840510	3.036689	0.224978
49	1	0	-4.328234	1.464736	-1.130056
50	1	0	-5.135712	4.551930	1.743216
51	1	0	-5.679622	3.369130	-0.382320
52	7	0	-1.027933	0.484992	2.037477
53	6	0	3.329017	-0.018227	0.139100
54	6	0	3.894638	-0.174175	1.404600
55	6	0	4.206916	0.176493	-0.927451
56	6	0	5.270562	-0.134125	1.610098

57	6	0	5.587434	0.210539	-0.753429
58	6	0	6.120728	0.056360	0.523477
59	9	0	5.780038	-0.274746	2.839610
60	9	0	3.103933	-0.361582	2.474958
61	9	0	7.442431	0.093438	0.707176
62	9	0	6.401642	0.388034	-1.800488
63	9	0	3.724219	0.316646	-2.172059
64	53	0	1.285528	-5.671555	-0.574270
65	53	0	1.122446	5.388222	-1.259028
66	6	0	3.458479	-2.908798	-0.449299
67	1	0	3.885724	-2.399199	-1.320629
68	1	0	4.056843	-2.631060	0.420147
69	1	0	3.598069	-3.980893	-0.603744
70	6	0	-1.593684	-3.646790	-0.345847
71	1	0	-2.095577	-3.631494	0.628170
72	1	0	-2.271498	-3.189409	-1.065039
73	1	0	-1.446279	-4.690808	-0.630554
74	6	0	3.168772	2.955846	0.288255
75	1	0	3.444523	2.438656	1.207381
76	1	0	3.987405	2.821115	-0.429902
77	1	0	3.117442	4.025189	0.513707
78	6	0	-1.494176	3.093186	-1.805599
79	1	0	-2.193846	2.293990	-2.040011
80	1	0	-2.021613	3.833400	-1.193614
81	1	0	-1.201233	3.593518	-2.736186

REFERENCES

[1] S. Mandal, D. K. Poria, R. Ghosh, P. S. Ray, P. Gupta, *Dalt. Trans.* **2014**, *43*, 17463–17474.

[2] S. Moromizato, Y. Hisamatsu, T. Suzuki, Y. Matsuo, R. Abe, S. Aoki, *Inorg. Chem.* **2012**, *51*, 12697–12706.

[3] N. Epelde-Elezcano, V. Martínez-Martínez, E. Peña-Cabrera, C. F. A. Gómez-Durán, I. L. Arbeloa, S. Lacombe, *RSC Adv.* **2016**, *6*, 41991–41998.

[4] L. V. Lutkus, S. S. Rickenbach, T. M. McCormick, *J. Photochem. Photobiol. A Chem.* **2019**, *378*, 131–135.

[5] R.W. Redmond, J.N. Gamlin, *J. Photochem. Photobiol.*, **1999**, 70, 393.