Supporting Information

High efficiency green OLEDs based on homoleptic iridium complexes with steric phenylpyridazine ligands

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Contents:

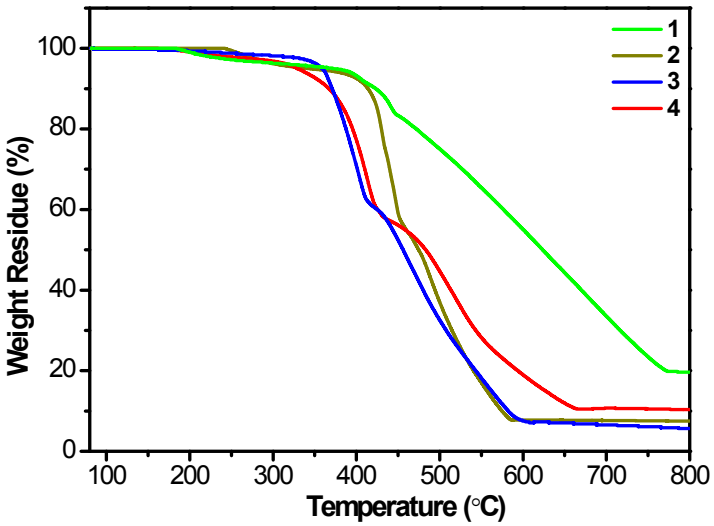


Fig S1. Thermal gravimetric spectra of iridium (III) complexes.

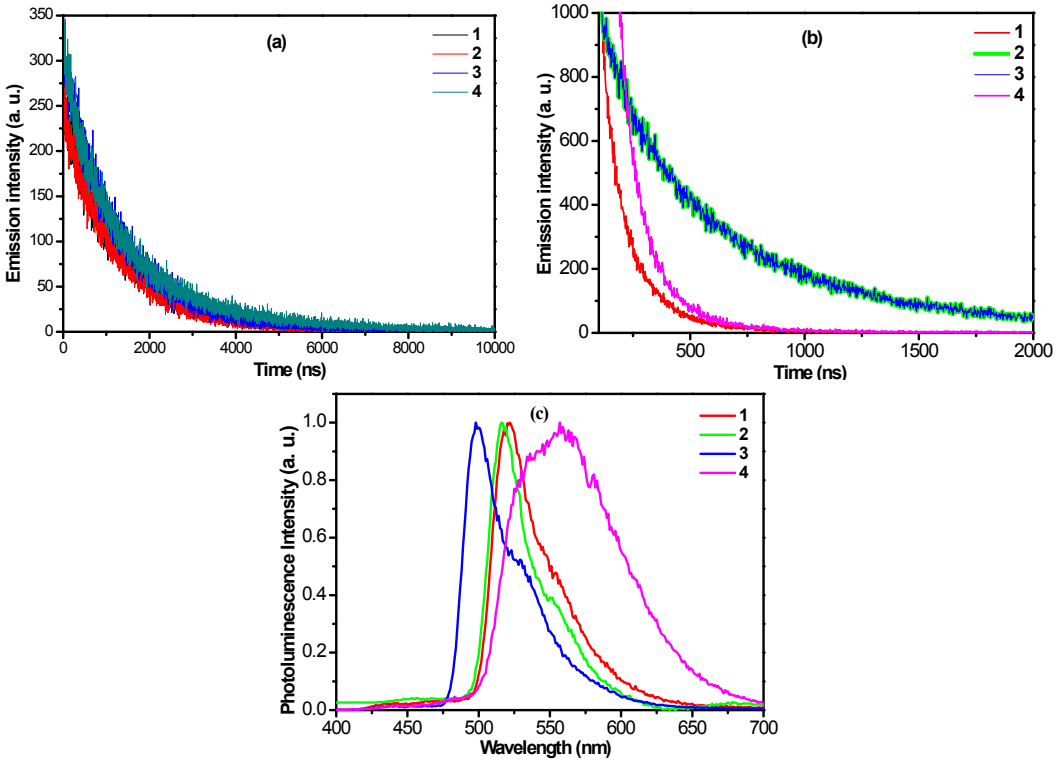


Fig. S2. Emission decay curves of irdium(III) complexes in PMMA (0.01 wt%) (**a**) and neat power (**b**). PL spectra of iridium complexes in PMMA (0.01 wt%) at temperatures of 77 K (c).

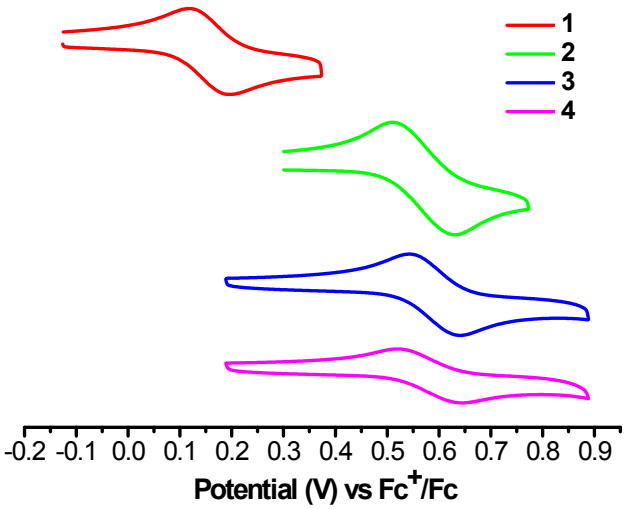


Fig S3. Cyclic voltammetry curves of iridium (III) complexes in CH_2Cl_2.

Table S1. Selected bond lengths of iridium complexes in the ground state S_0 and the lowest lying triplet state T_1.

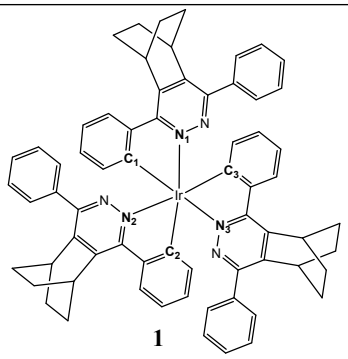
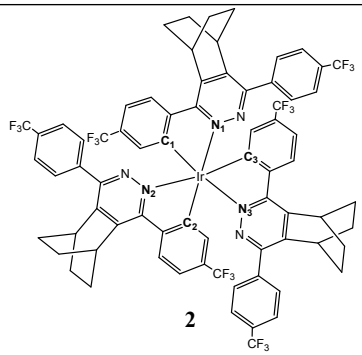
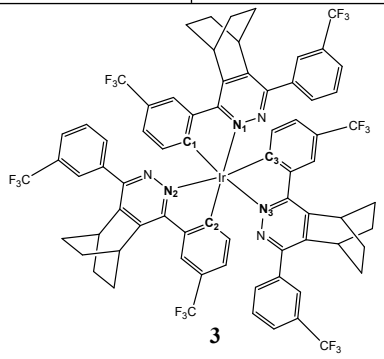
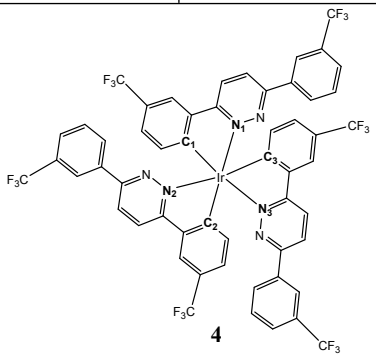
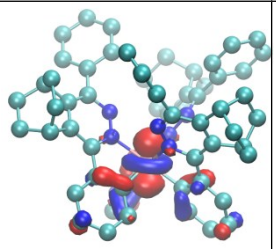
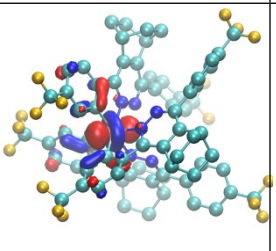
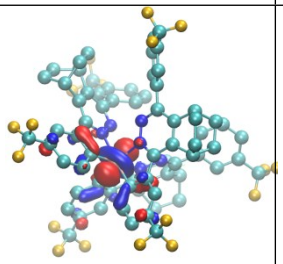
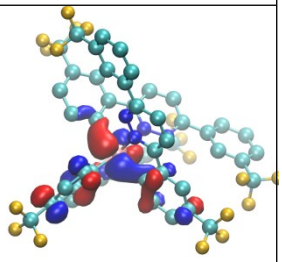
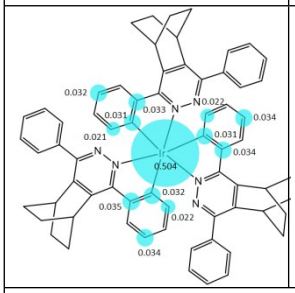
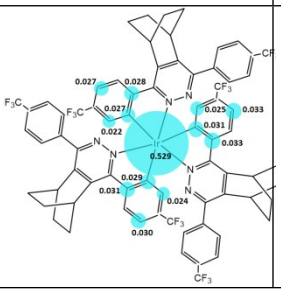
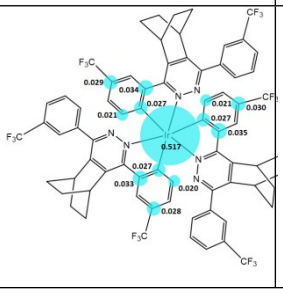
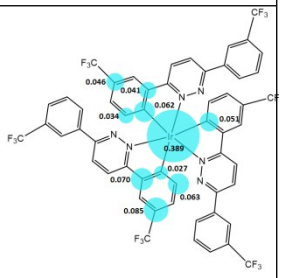
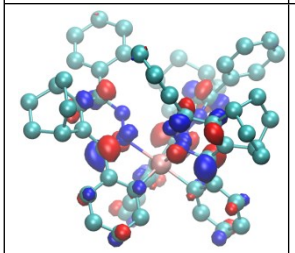
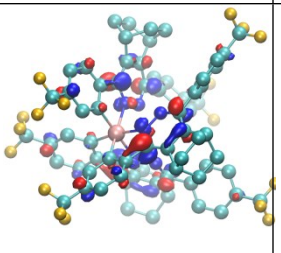
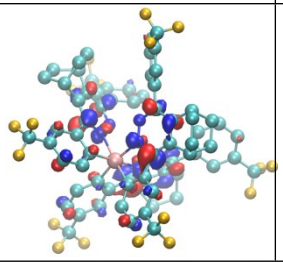
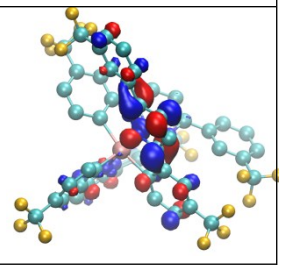
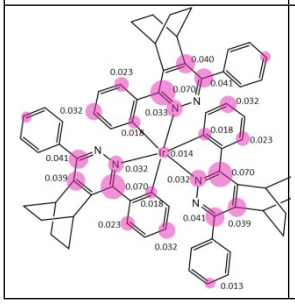
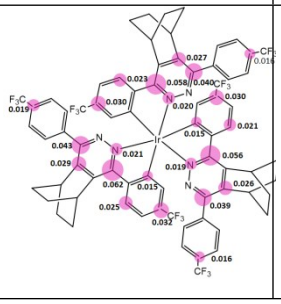
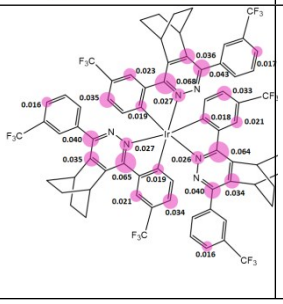
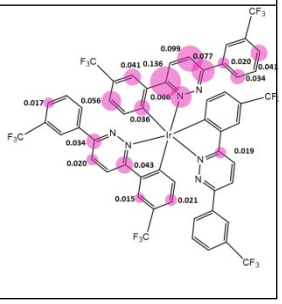
Iridium complex	 **1**		 **2**	
	S_0	T_1	S_0	T_1
Ir–C_1 (Å)	2.030	2.043	2.029	2.026
Ir–C_2 (Å)	2.030	2.021	2.029	1.987
Ir–C_3 (Å)	2.030	1.999	2.029	2.040
Ir–N_1 (Å)	2.163	2.186	2.160	2.187
Ir–N_2 (Å)	2.163	2.183	2.156	2.132
Ir–N_3 (Å)	2.162	2.119	2.159	2.171
Iridium complex	 **3**		 **4**	
	S_0	T_1	S_0	T_1
Ir–C_1 (Å)	2.025	2.001	2.009	1.988
Ir–C_2 (Å)	2.025	2.019	2.088	2.066
Ir–C_3 (Å)	2.025	2.041	2.105	2.100
Ir–N_1 (Å)	2.160	2.112	2.043	2.075
Ir–N_2 (Å)	2.161	2.181	2.073	2.056
Ir–N_3 (Å)	2.161	2.181	2.186	2.287

Table S2. Contour plots and individual atomic contributions for HOMOs and LUMOs.*

HOMO			
1	**2**	**3**	**4**
			
			
LUMO			
1	**2**	**3**	**4**
			
			

* Contour plots (Isovalue=0.04). The areas of the circles are proportional to the atomic contributions, and only contributions greater than 0.015 are shown. All the H atoms were omitted for clarity.

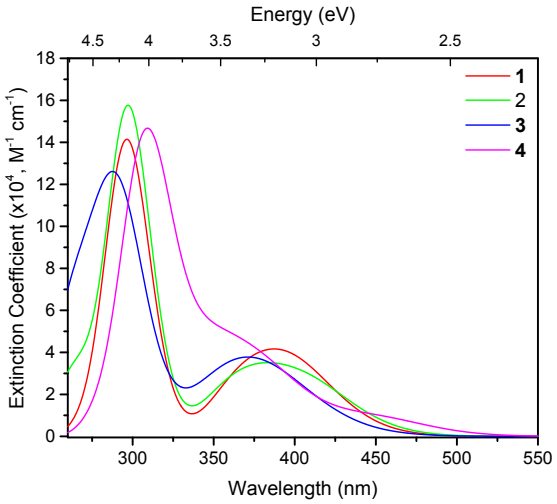


Fig. S4 Simulated UV-vis spectra for iridium complexes **1**, **2**, **3** and **4** at B3LYP/6-31g(d)/LANL2DZ level of theory with PCM in CH_2Cl_2 medium. The curves are plotted using Gaussian broadening function with a full width at half-maximum of 0.4 eV.

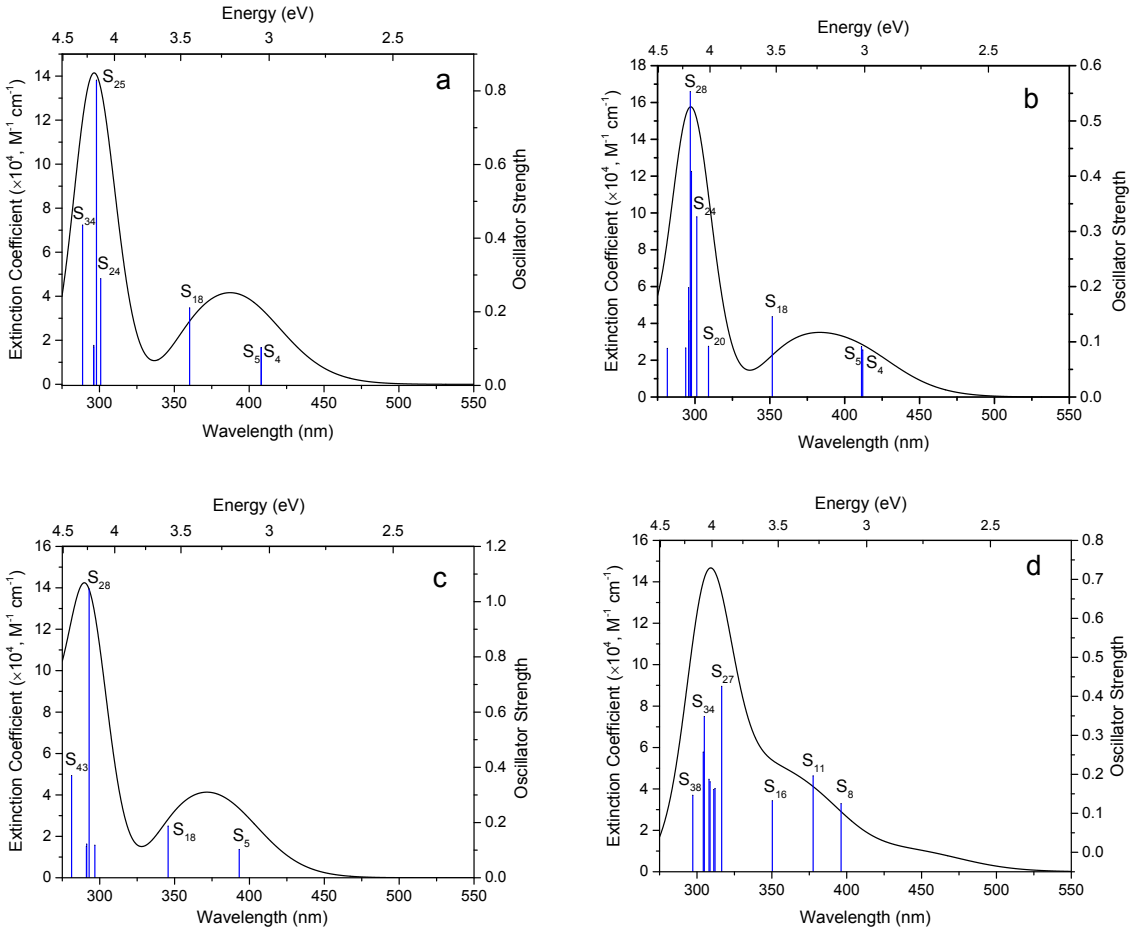


Fig. S5 Simulated UV-vis absorption spectra with transition oscillator strength for a) complex **1**, b) complex **2**, c) complex **3** and d) complex **4**.

Table S3. Contour plots and individual atomic contributions for transitions in the high energy region.*

Complex			
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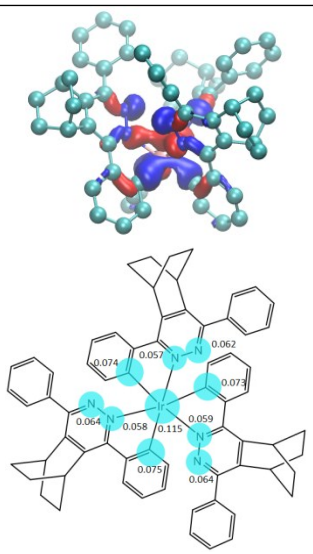
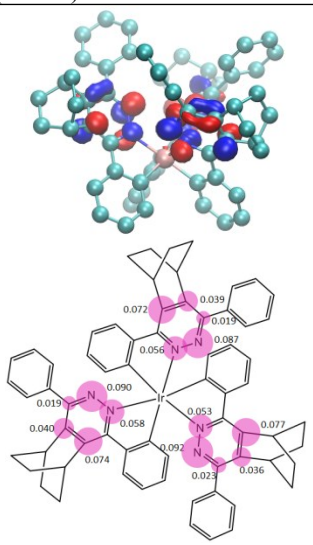
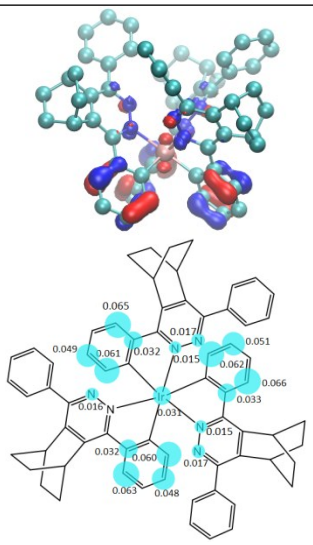
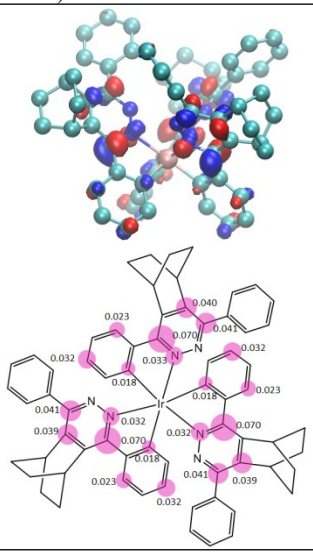
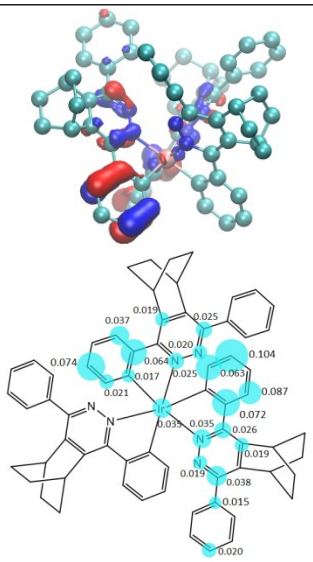
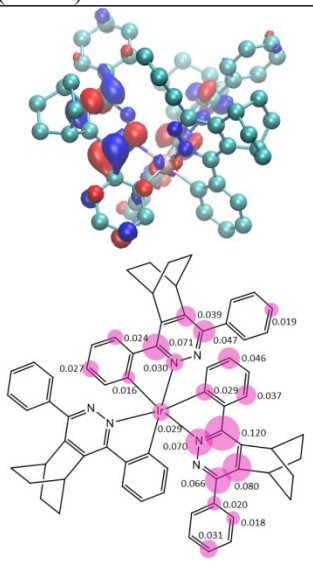
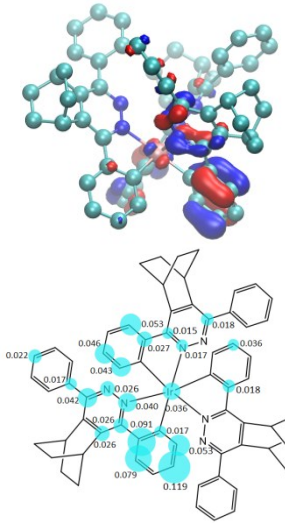
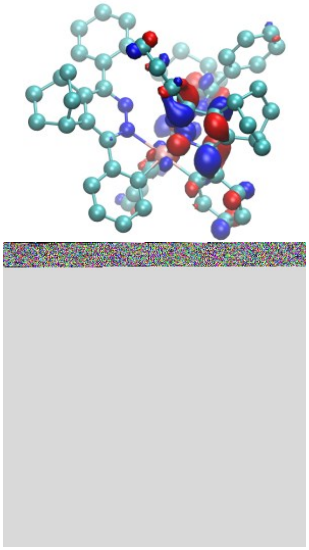
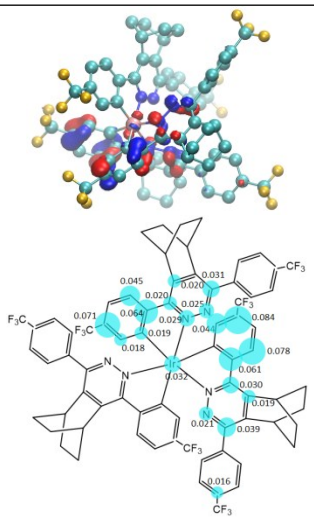
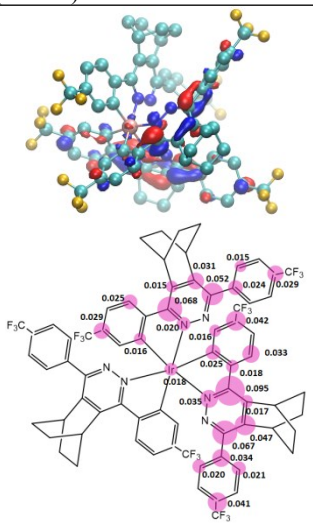
			
		HOMO−5→LUMO (18.6%)	
			
		HOMO−4→ LUMO+2 (19.3%)	
			

<table>
<tr><td></td><td></td><td colspan="2">HOMO−3→ LUMO+1 (17.3%)</td></tr>
<tr><td></td><td></td><td>  </td><td>  </td></tr>
<tr><td rowspan="4">2</td><td rowspan="4">S_{28}</td><td colspan="2">HOMO−4→ LUMO+2(33.1%)</td></tr>
<tr><td>  </td><td>  </td></tr>
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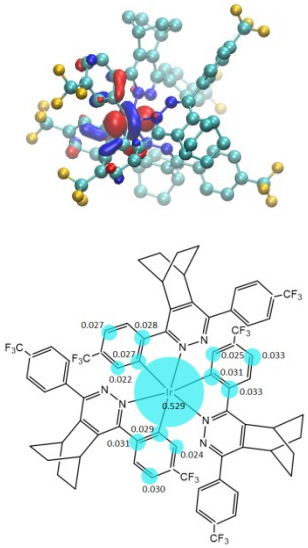
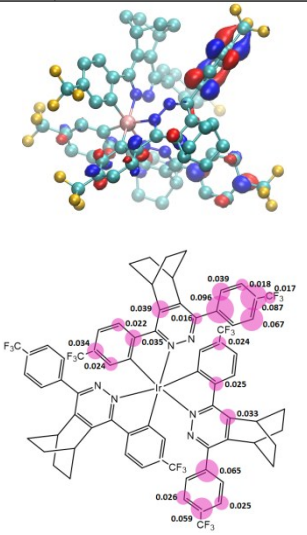
<tr><td>  </td><td>  </td></tr>
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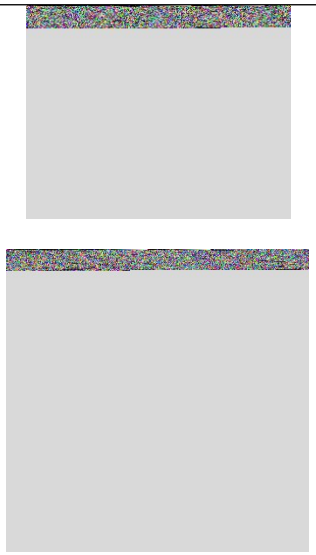
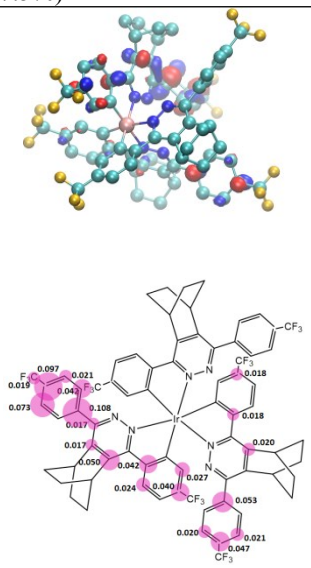
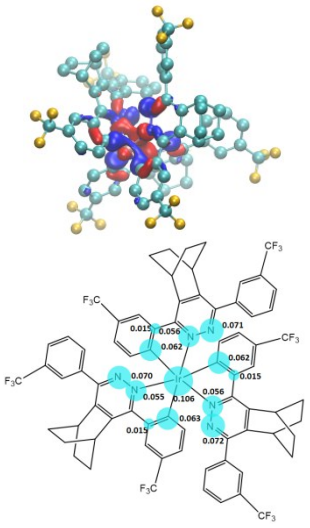
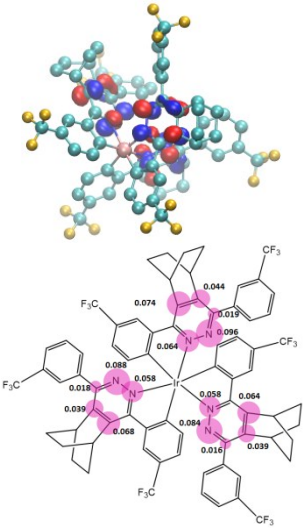
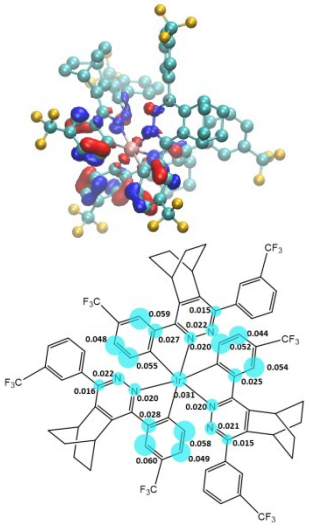
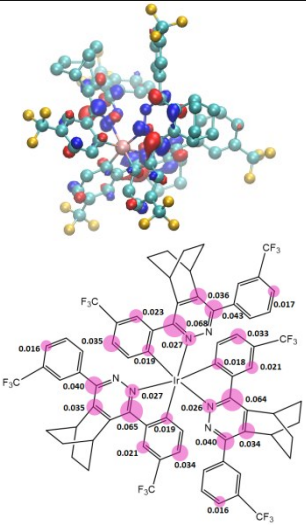
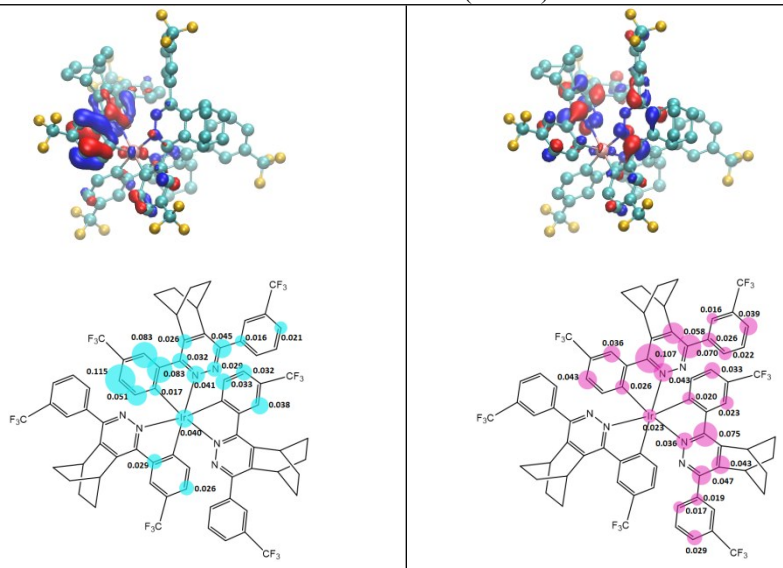
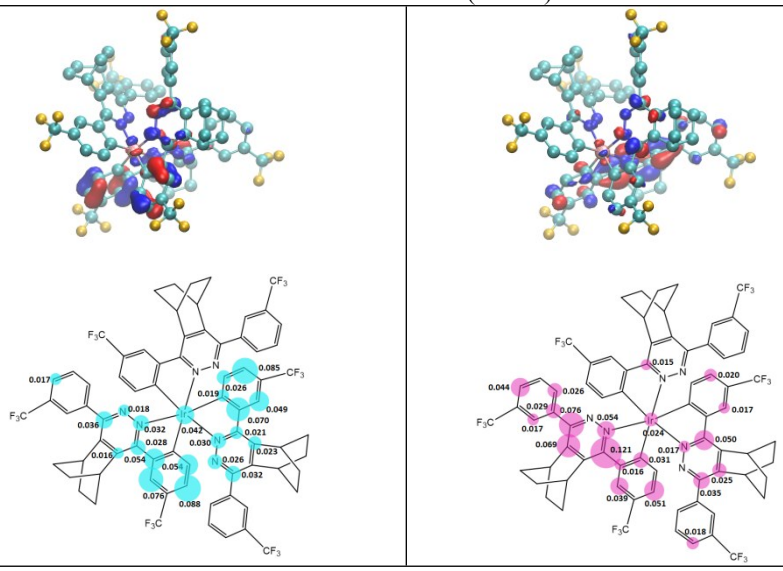
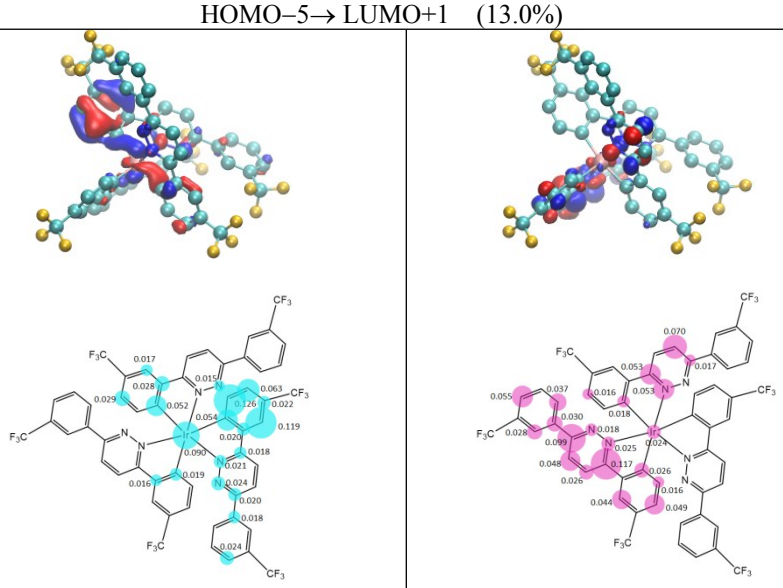
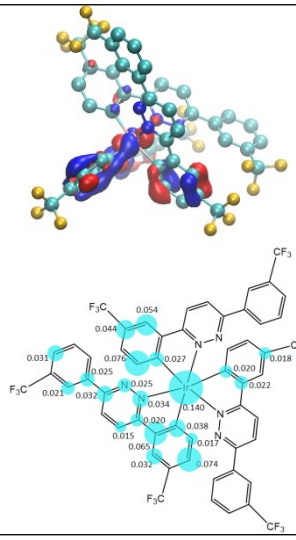
		HOMO→ LUMO+8(27.5%)	
			
3	S_{28}	HOMO−6→ LUMO+3(15.2%)	
			
		HOMO−5→ LUMO(14.3%)	
			

		HOMO−4→ LUMO+1(27.1%)
		
		HOMO−3→ LUMO+2 (23.3%)
		
4	S_{27}	HOMO−5→ LUMO+1 (13.0%)
		

		HOMO–4→ LUMO+1(71.3%)	
			

* Contour plots (Isovalue=0.04). The areas of the circles are proportional to the atomic contributions, and only contributions greater than 0.015 are shown. All the H atoms were omitted for clarity.

Table S4. Calculated PL wavelengths using different hybrid functionals.

Complex	PLwavelength (nm)		Exptl (nm)[a]
	M06-2X/6-31g(d)/Lanl2dz	CAM-B3LYP/6-31g (d)/Lanl2dz	
1	514	603	525
2	522	618	525
3	507	599	510
4	525	566	560

[a] Experimental results.

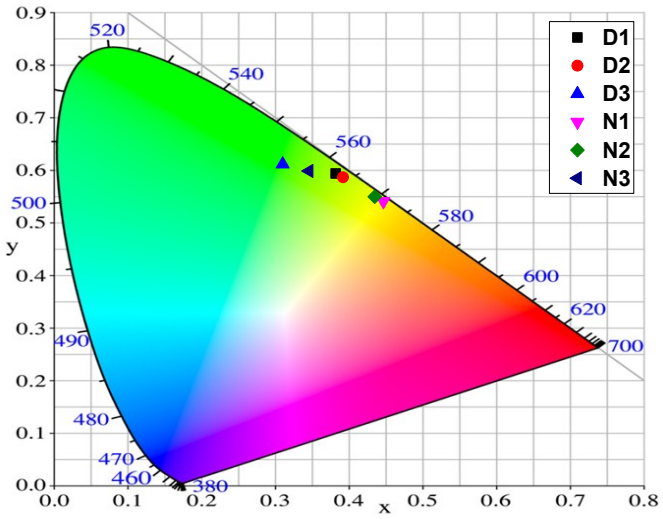


Fig. S6. CIE coordinates of EL devices of **D1**, **D2**, **D3**, **N1**, **N2** and **N3**.

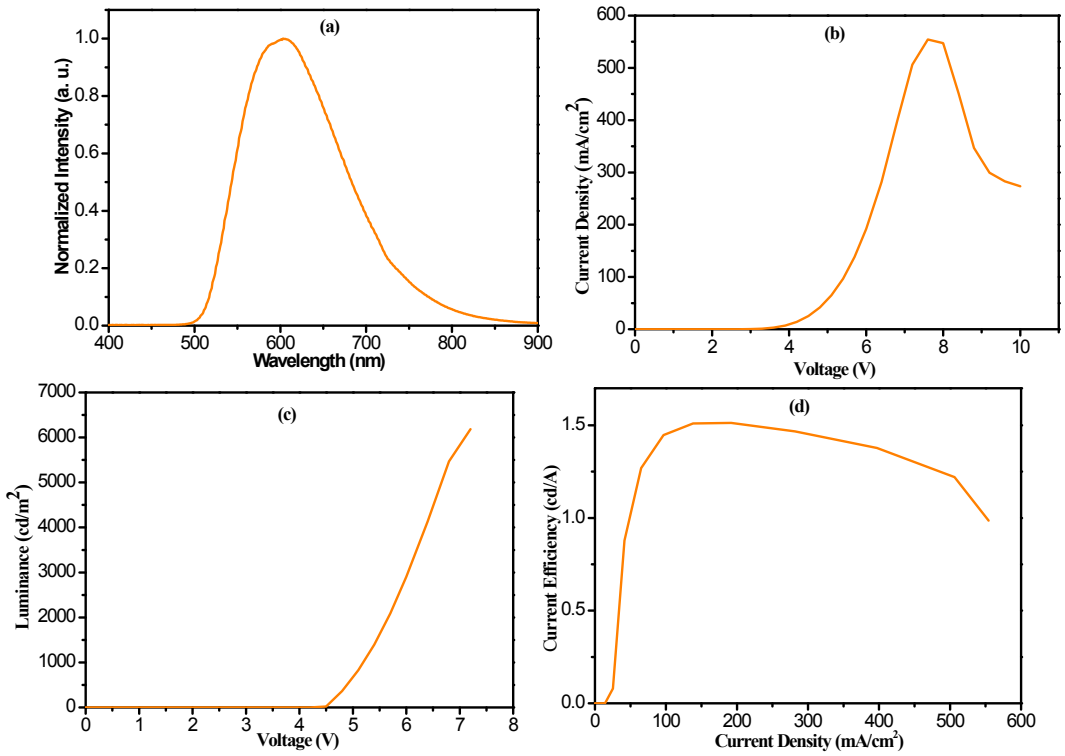
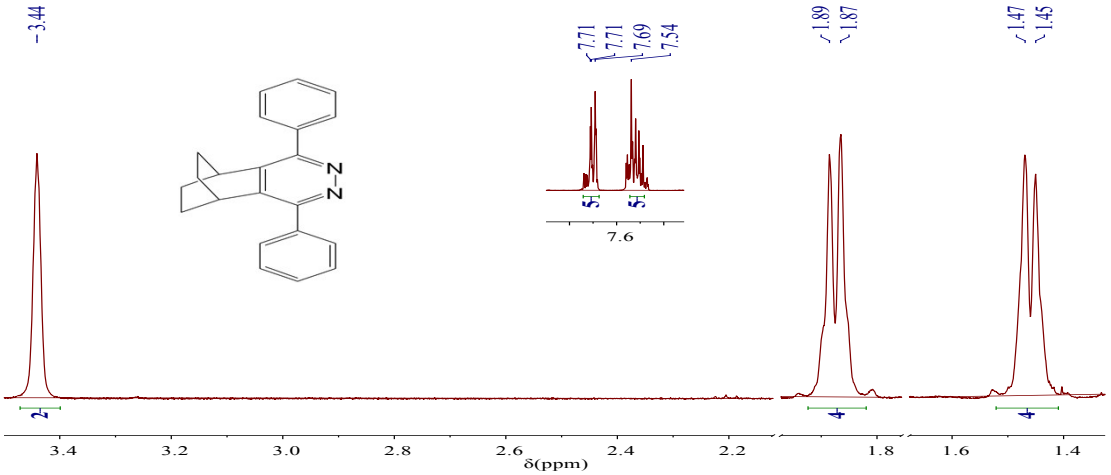


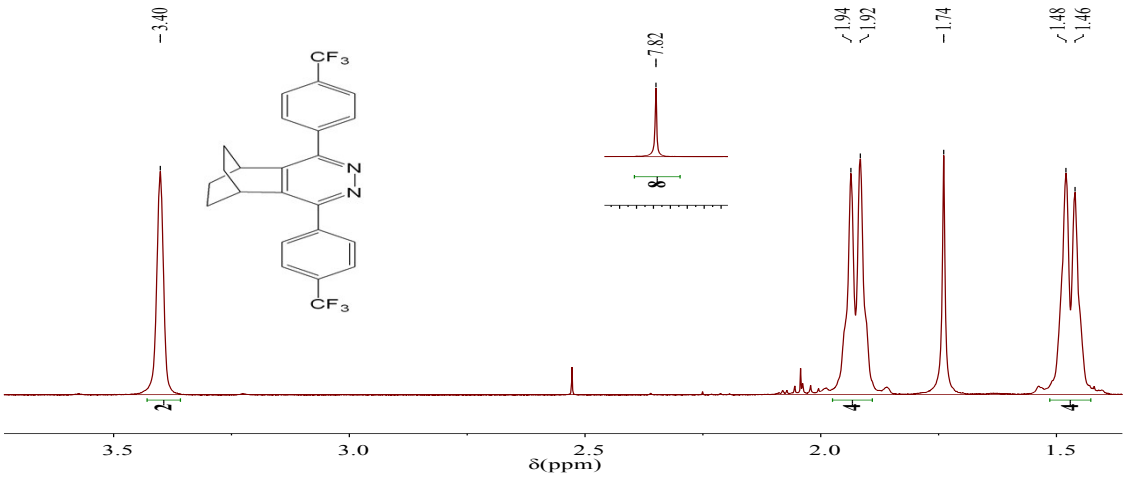
Fig. S7. The performance of non-doped OLEDs device based on complex **4**. (a) EL spectra of device. (b) Current density-voltage characteristics. (c) Luminance-voltage characteristics. (d) Luminance efficiencies vs. current density.

12, ^{1}H, ^{19}F & ^{13}C-NMR spectra

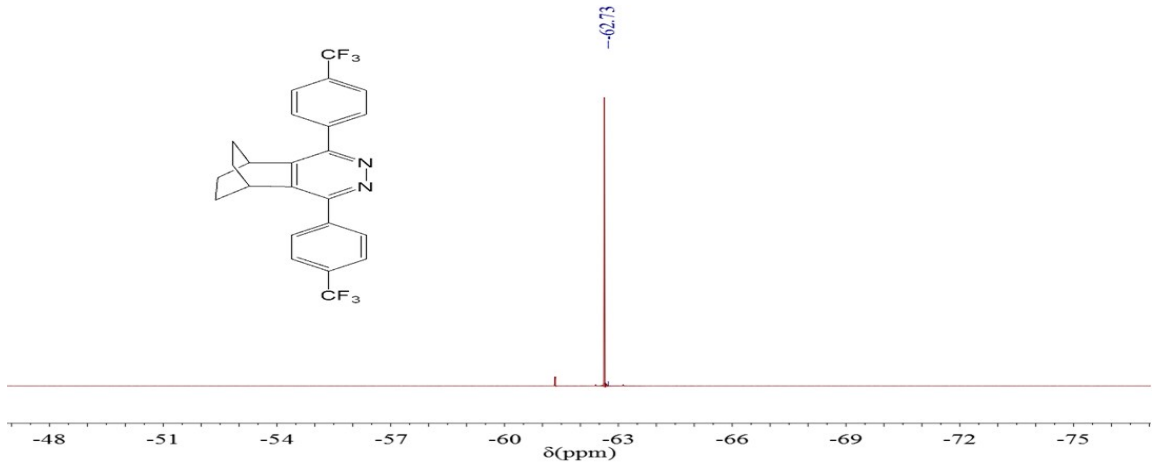
^{1}H-NMR Spectrum of **L1** in $CDCl_3$ (400 MHz):



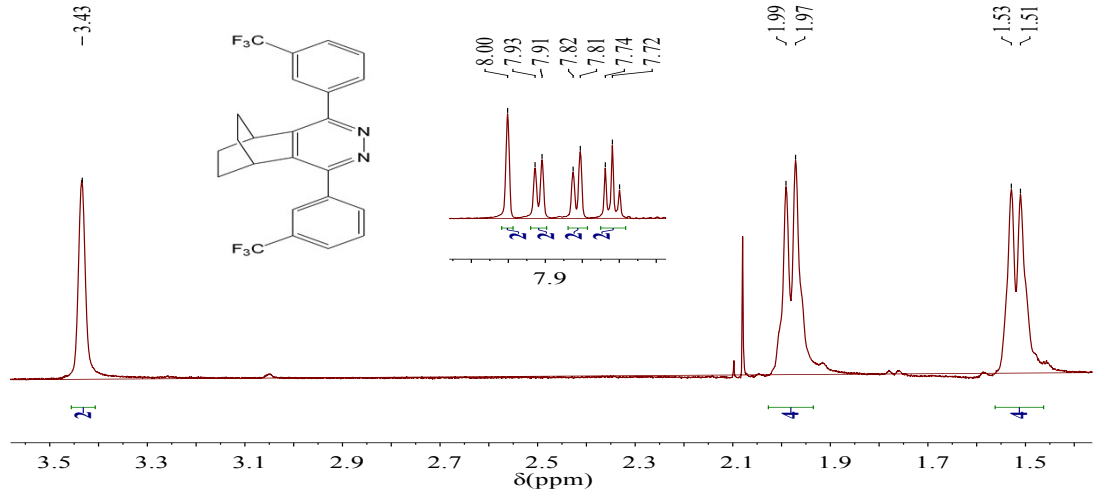
^{1}H-NMR Spectrum of **L2** in $CDCl_3$ (400 MHz):



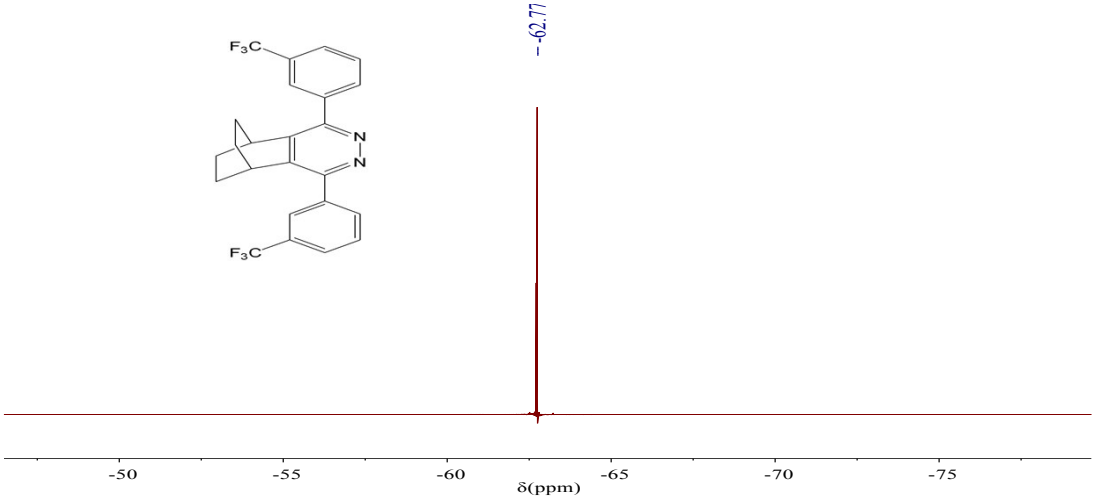
^{19}F-NMR Spectrum of **L2** in $CDCl_3$ (376 MHz):



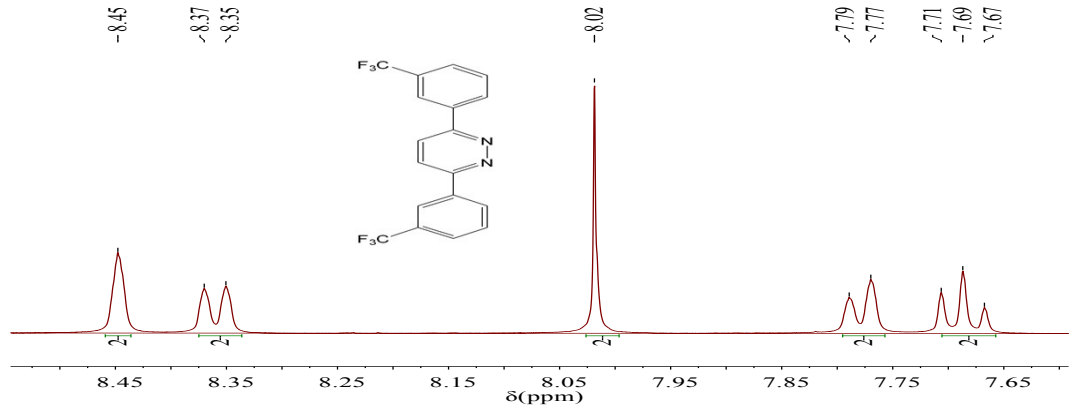
^{1}H-NMR Spectrum of **L3** in $CDCl_3$ (400 MHz):



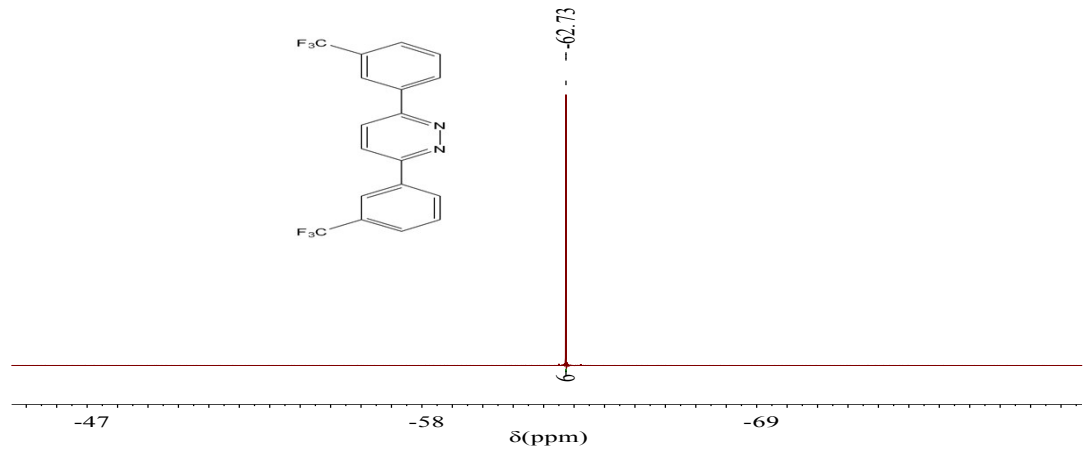
^{19}F-NMR Spectrum of **L3** in $CDCl_3$ (376 MHz):



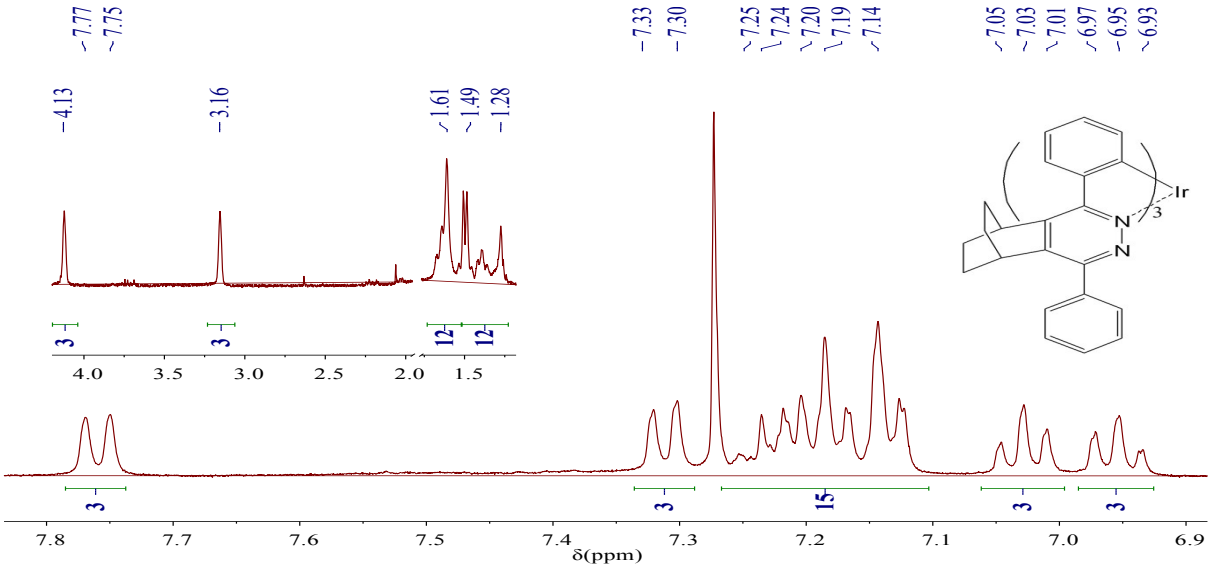
^{1}H-NMR Spectrum of **L4** in $CDCl_3$ (400 MHz):



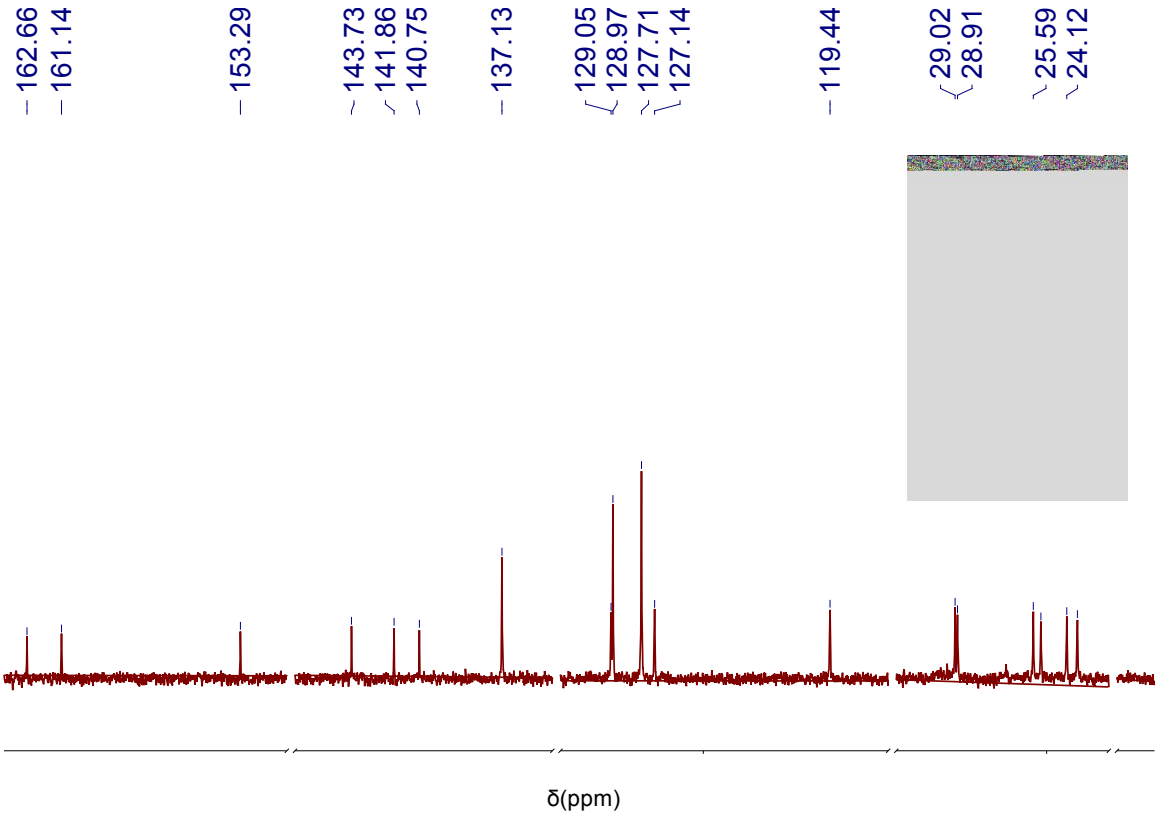
^{19}F-NMR Spectrum of **L4** in $CDCl_3$ (376 MHz):



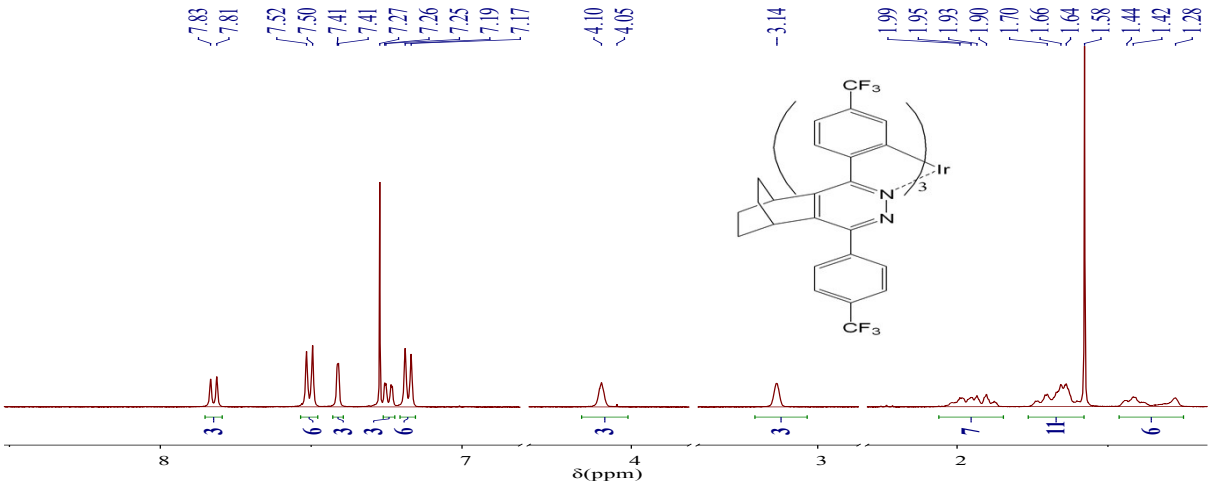
^{1}H-NMR Spectrum of complex **1** in $CDCl_3$ (400 MHz):



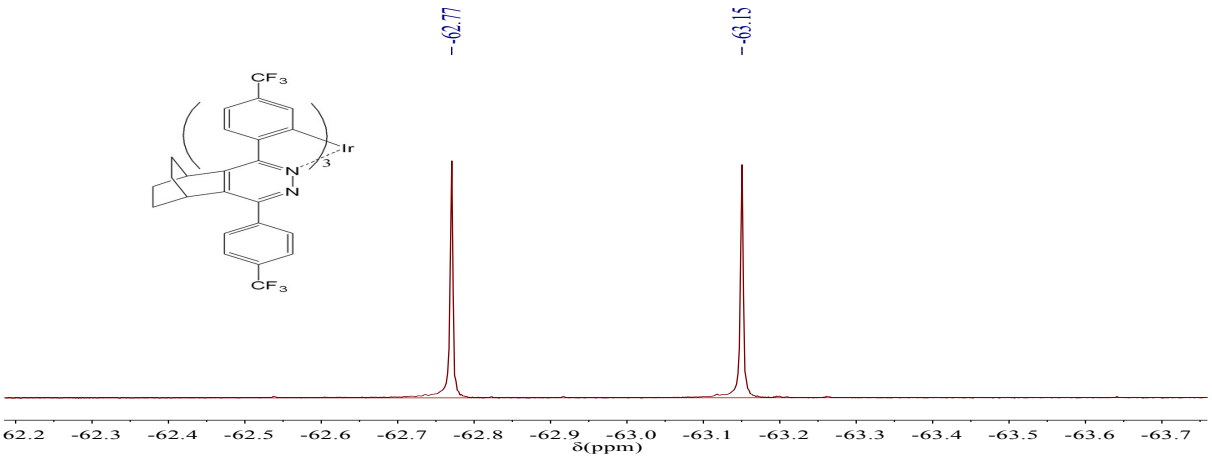
^{13}C-NMR Spectrum of complex **1** in $CDCl_3$ (100 MHz):



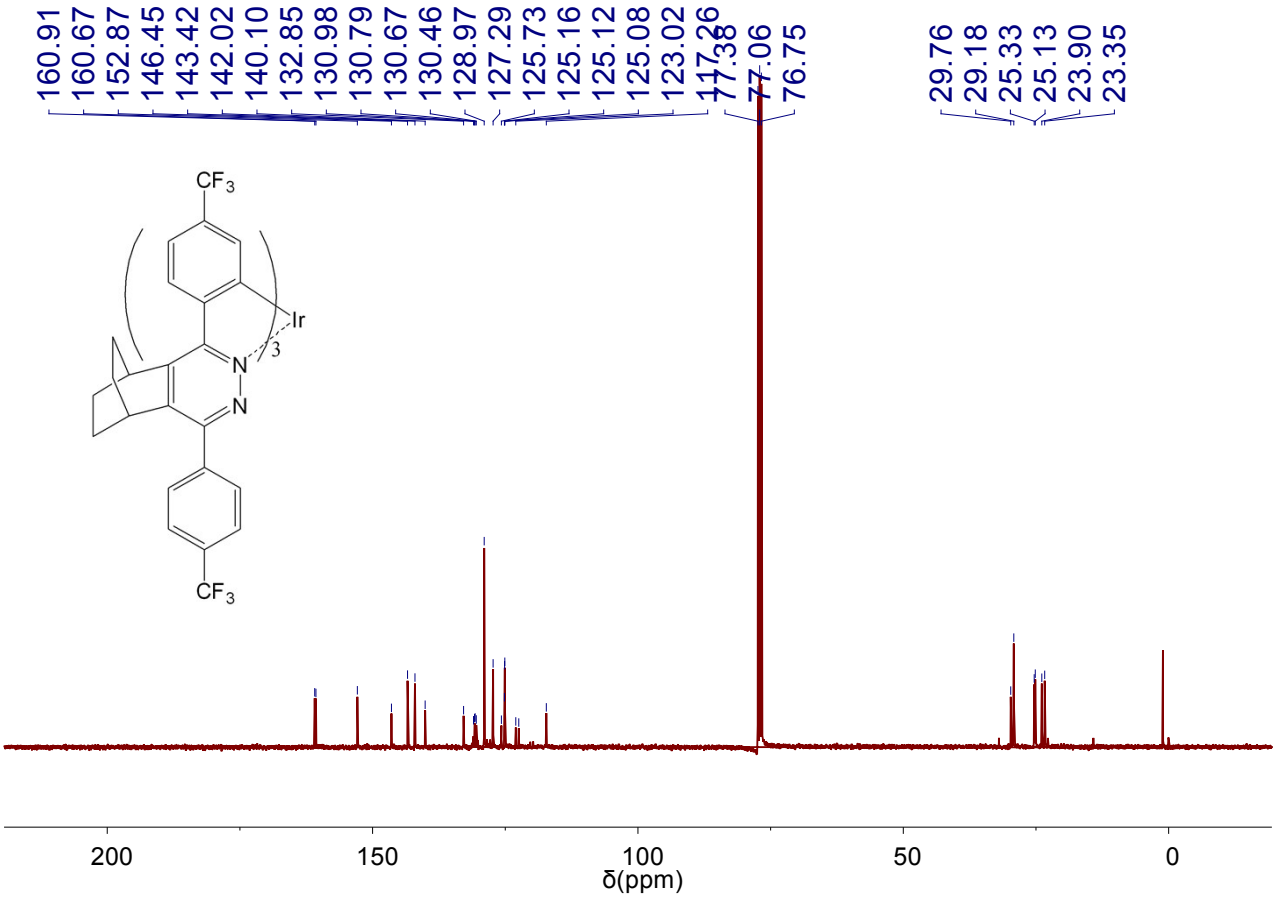
^{1}H-NMR Spectrum of complex **2** in $CDCl_3$ (400 MHz):



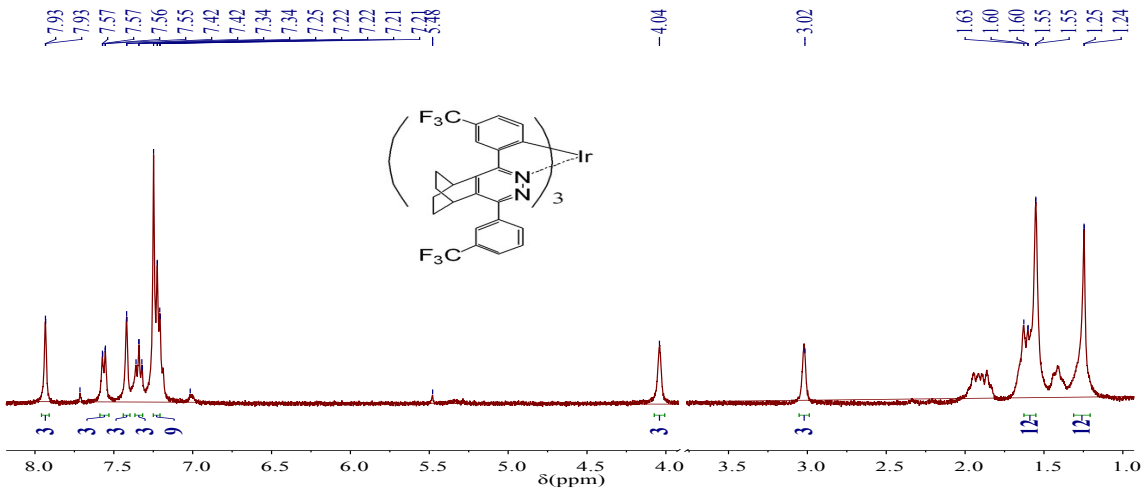
^{19}F-NMR Spectrum of complex **2** in $CDCl_3$ (376 MHz):



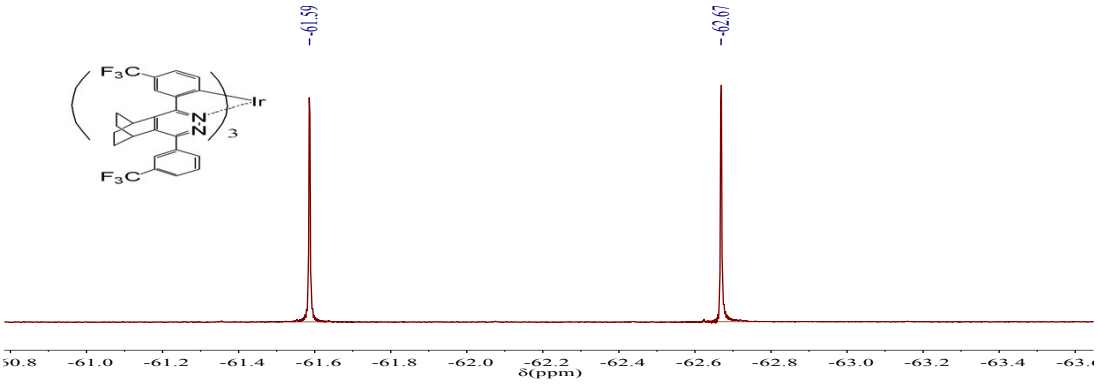
^{13}C-NMR Spectrum of complex **2** in $CDCl_3$ (100 MHz):



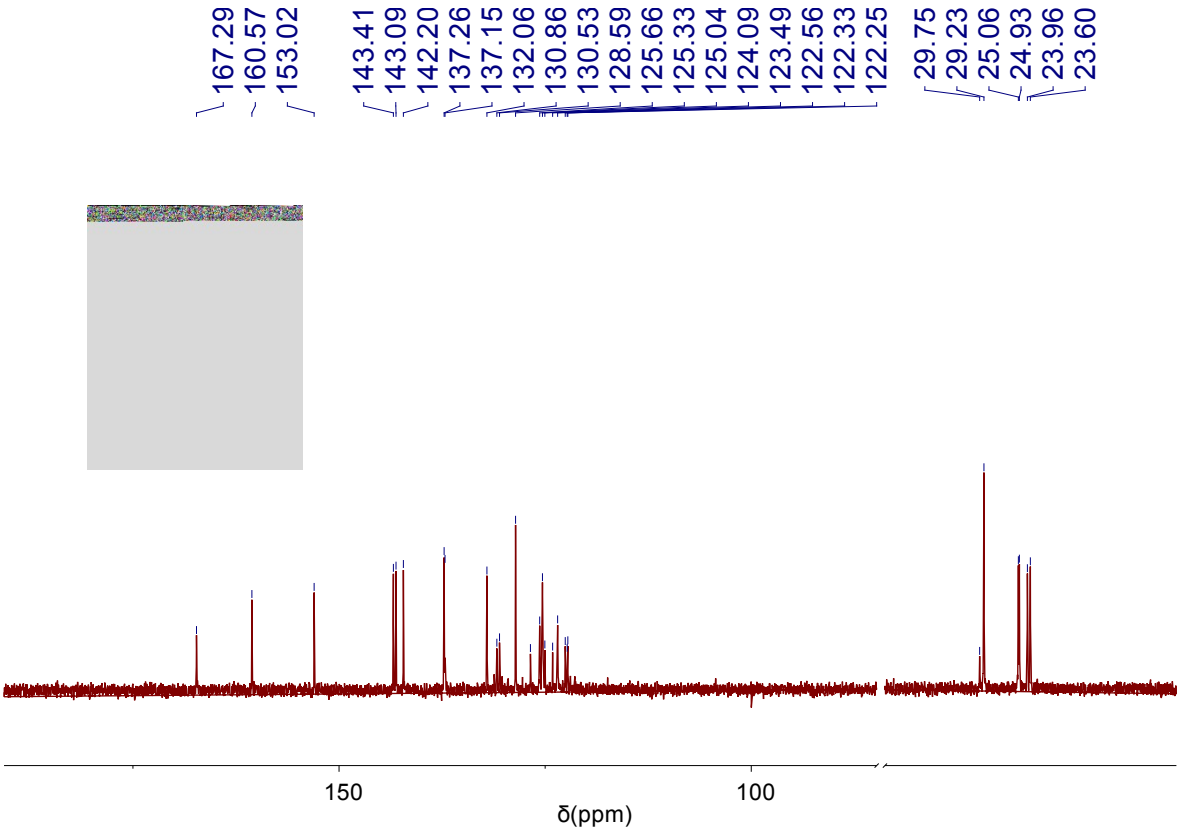
^{1}H-NMR Spectrum of complex **3** in $CDCl_3$ (400 MHz):



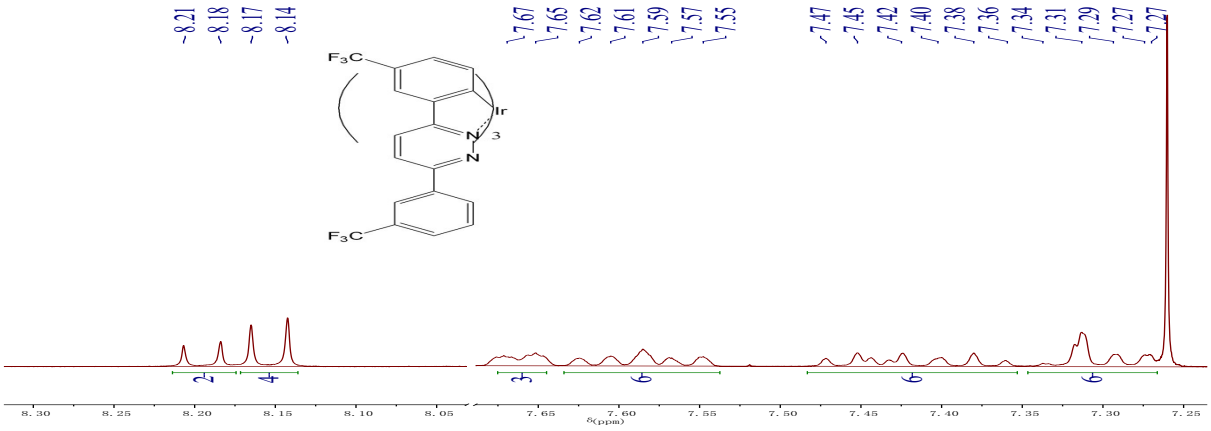
^{19}F-NMR Spectrum of complex **3** in $CDCl_3$ (376 MHz):



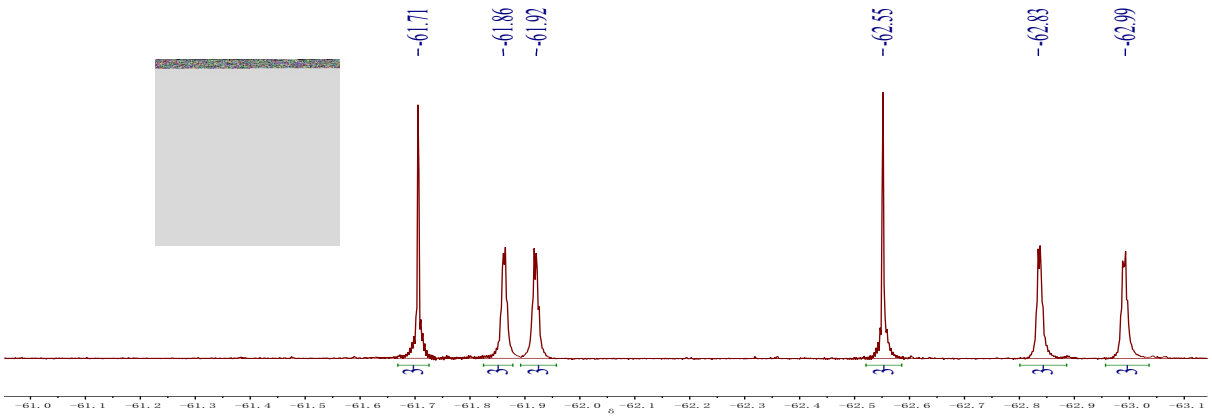
^{13}C-NMR Spectrum of complex **3** in $CDCl_3$ (100 MHz):



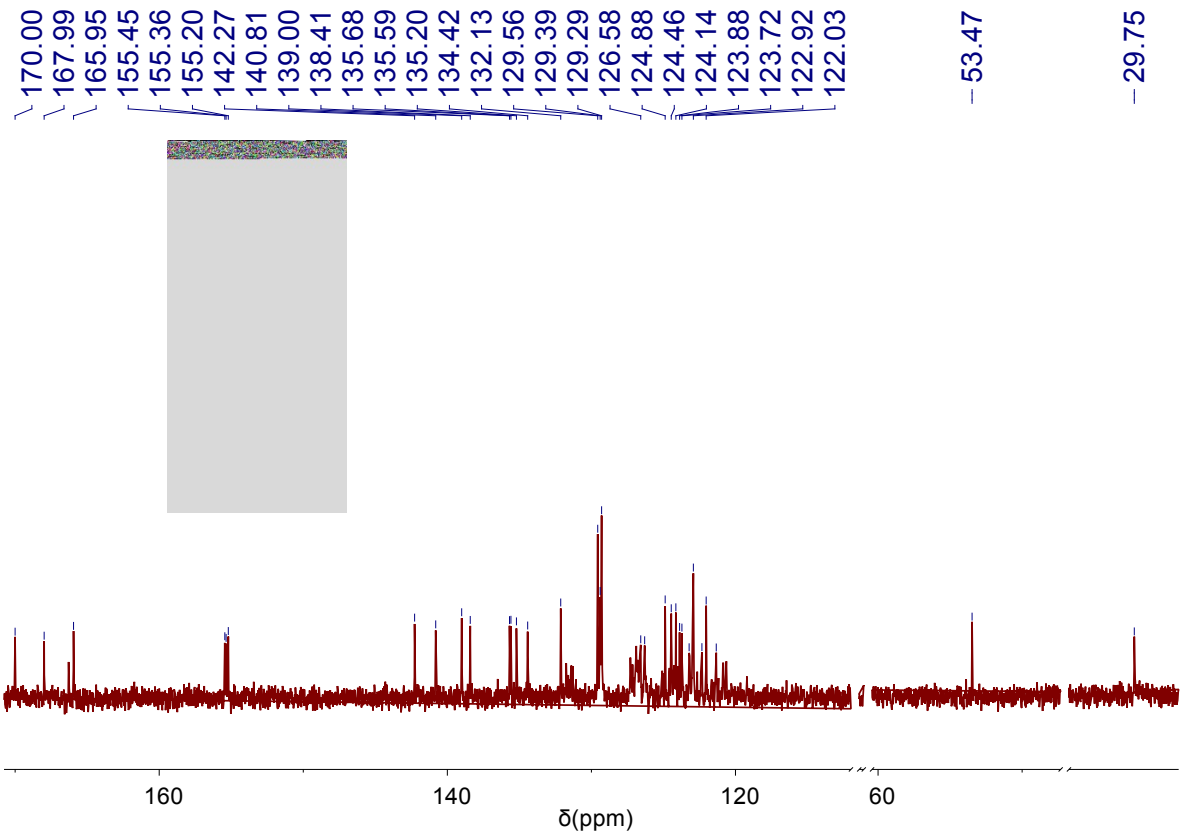
^{1}H-NMR Spectrum of complex **4** in $CDCl_3$ (400 MHz):



^{19}F-NMR Spectrum of complex **4** in $CDCl_3$ (376 MHz):

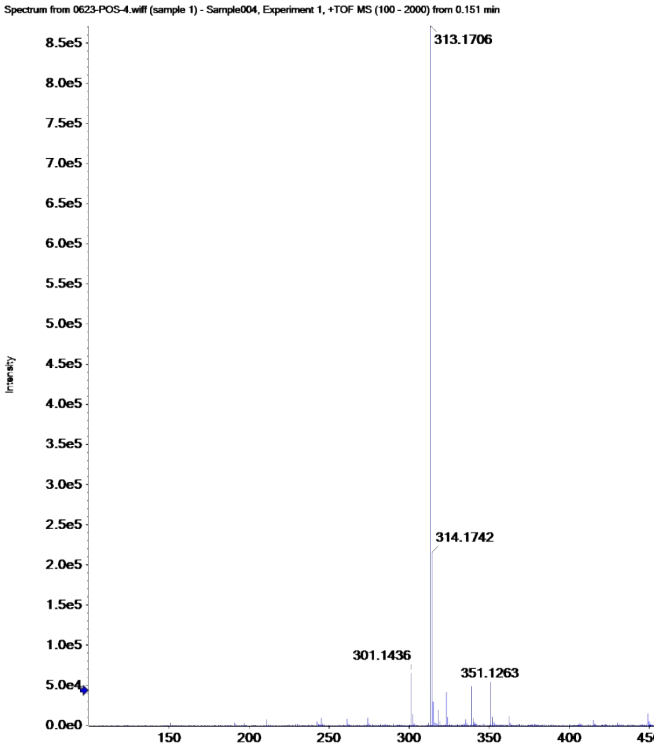


^{13}C-NMR Spectrum of complex **4** in $CDCl_3$ (100 MHz):

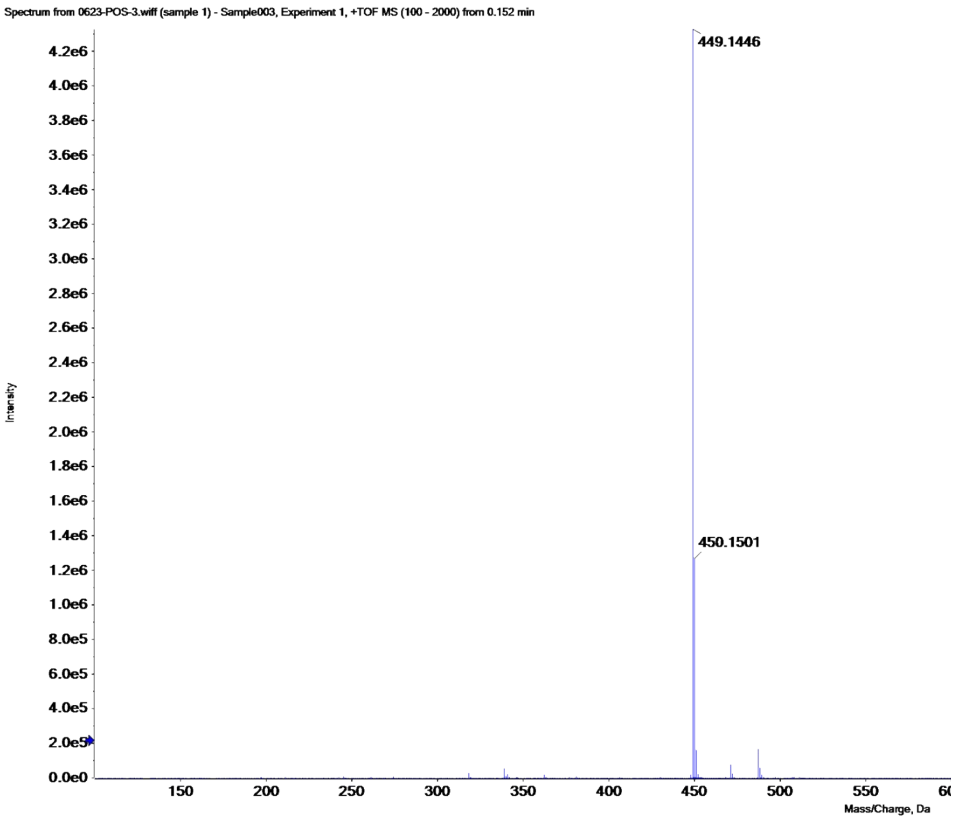


13. High resolution mass spectrometers (HRMS)

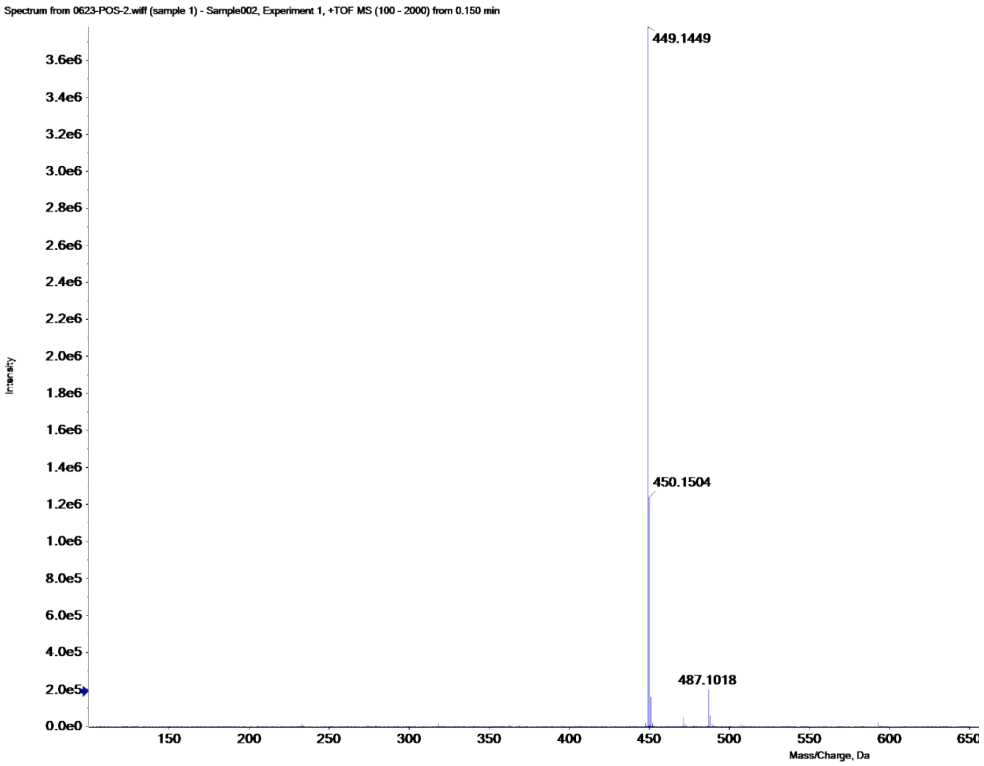
HRMS of **L1**:



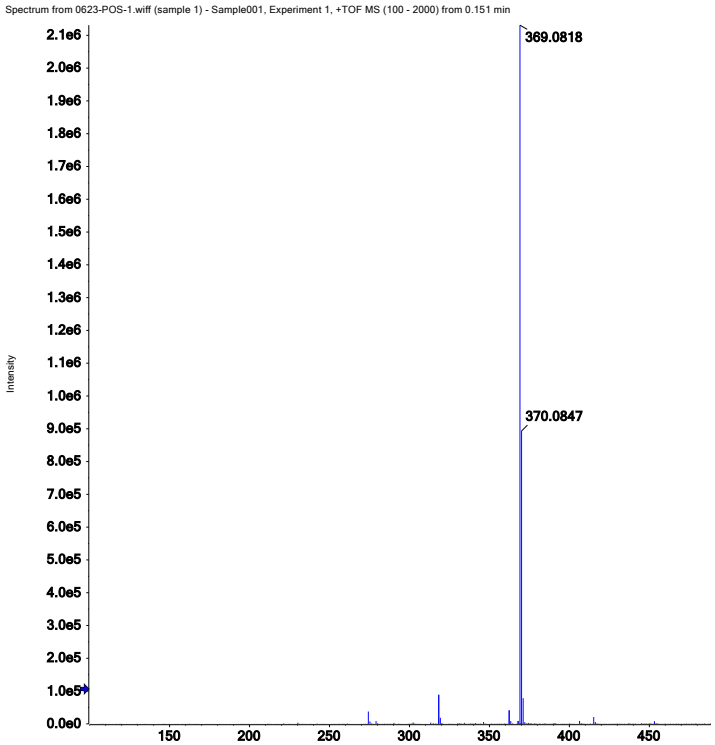
HRMS of **L2:**



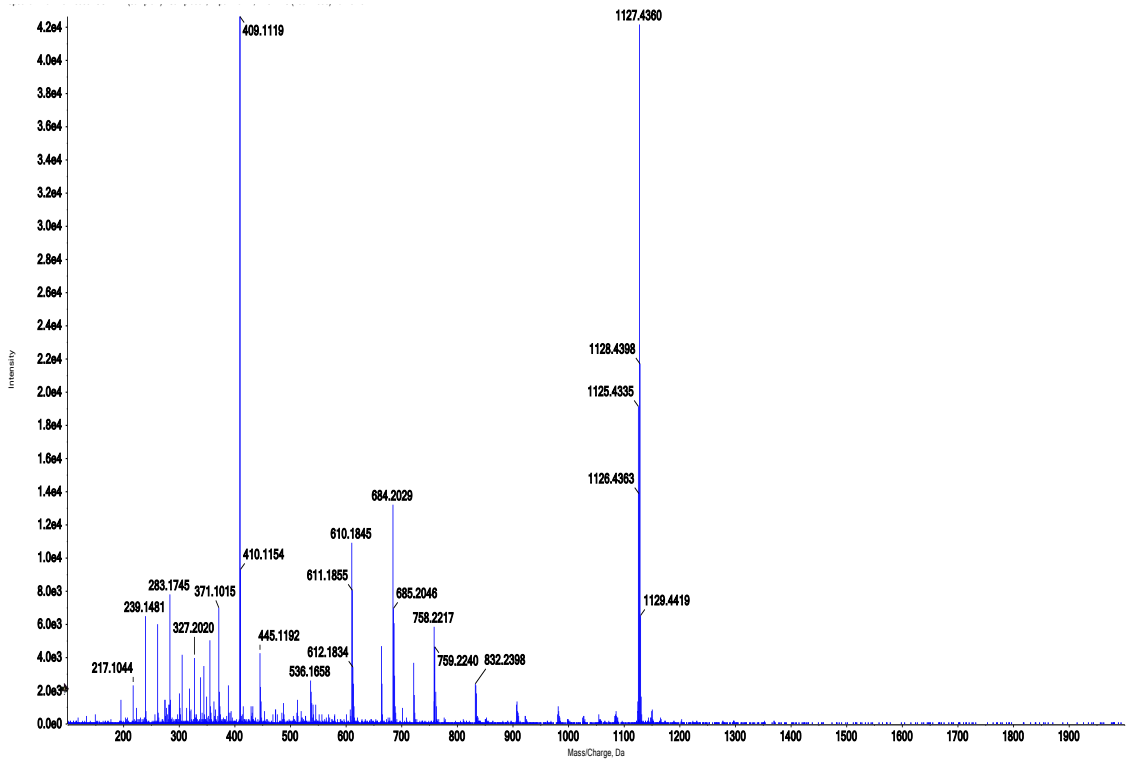
HRMS of **L3:**



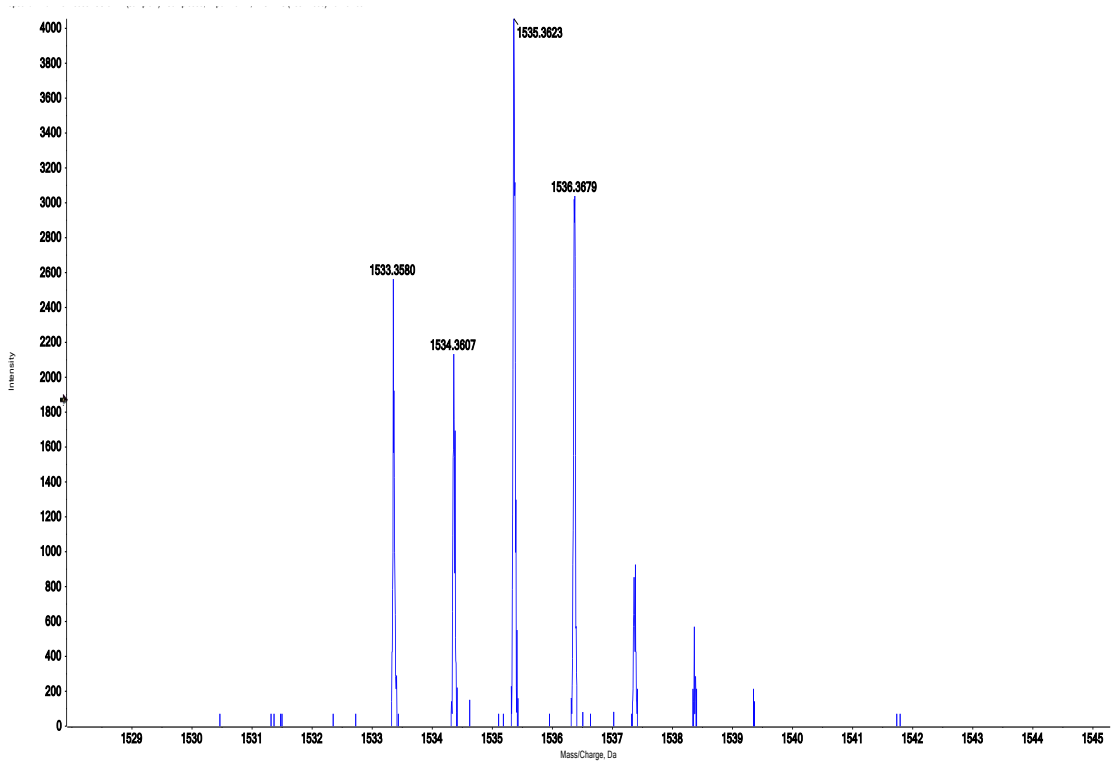
HRMS of **L4:**



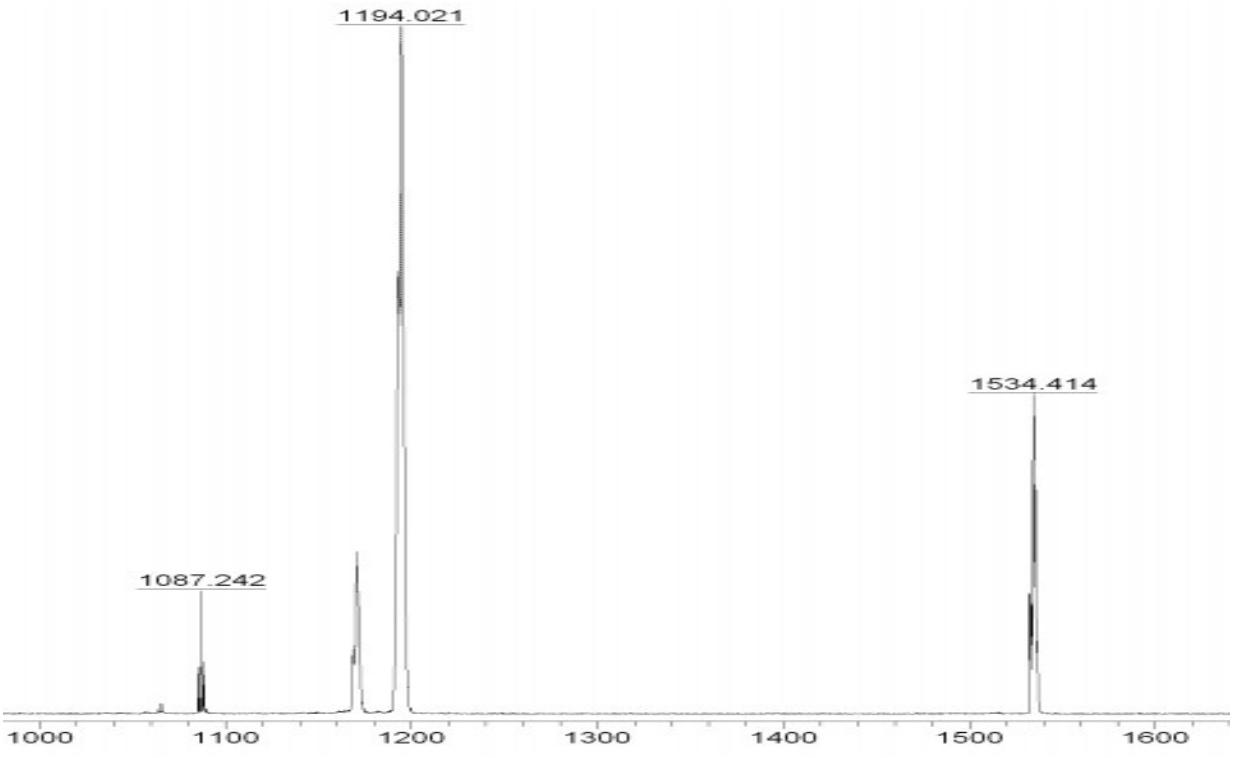
HRMS of complex **1:**



HRMS of complex **2:**



HRMS of complex **3:**



HRMS of complex **4:**