A novel pyrene-2-(pyridin-2-ylmethylsulfanyl)ethylamine based turn-on dual sensor for Al^{3+}: experimental and computational studies†

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transition, vertical excitation energies, and oscillator strength in methanol, **Table. ST3**

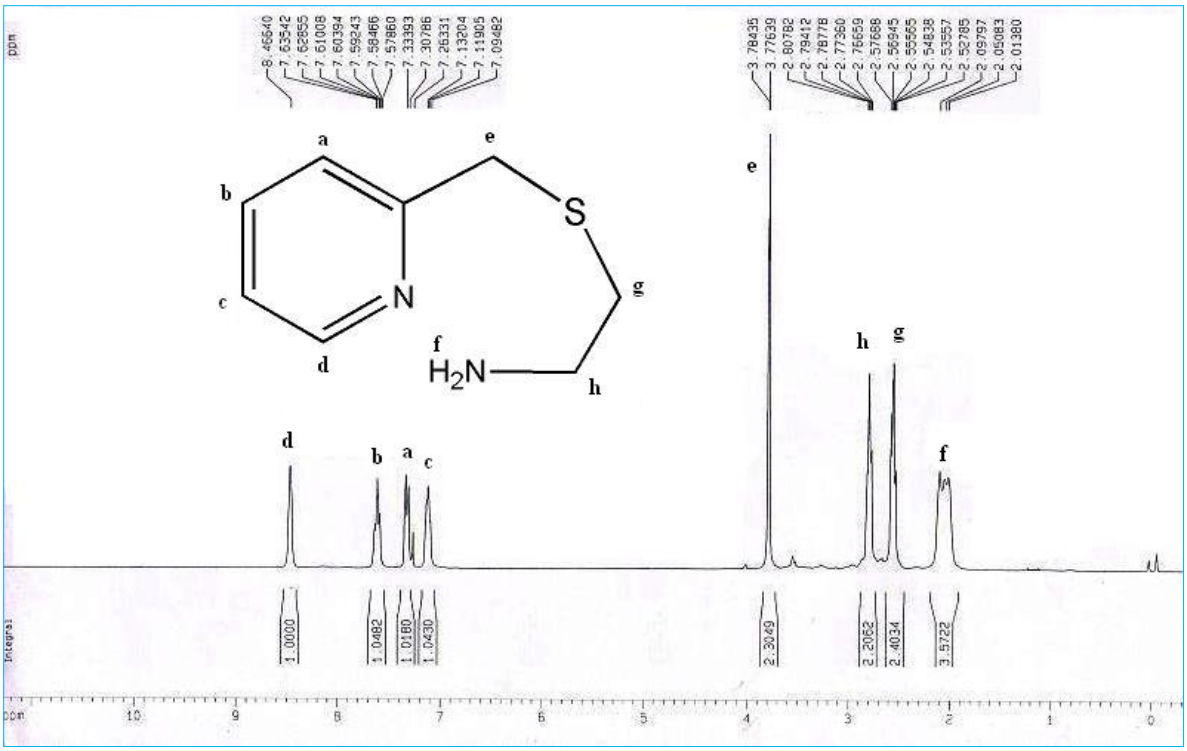


Fig. S1 ^{1}H NMR spectrum of **P** in $CDCl_3$ in Bruker 300 MHz instrument.

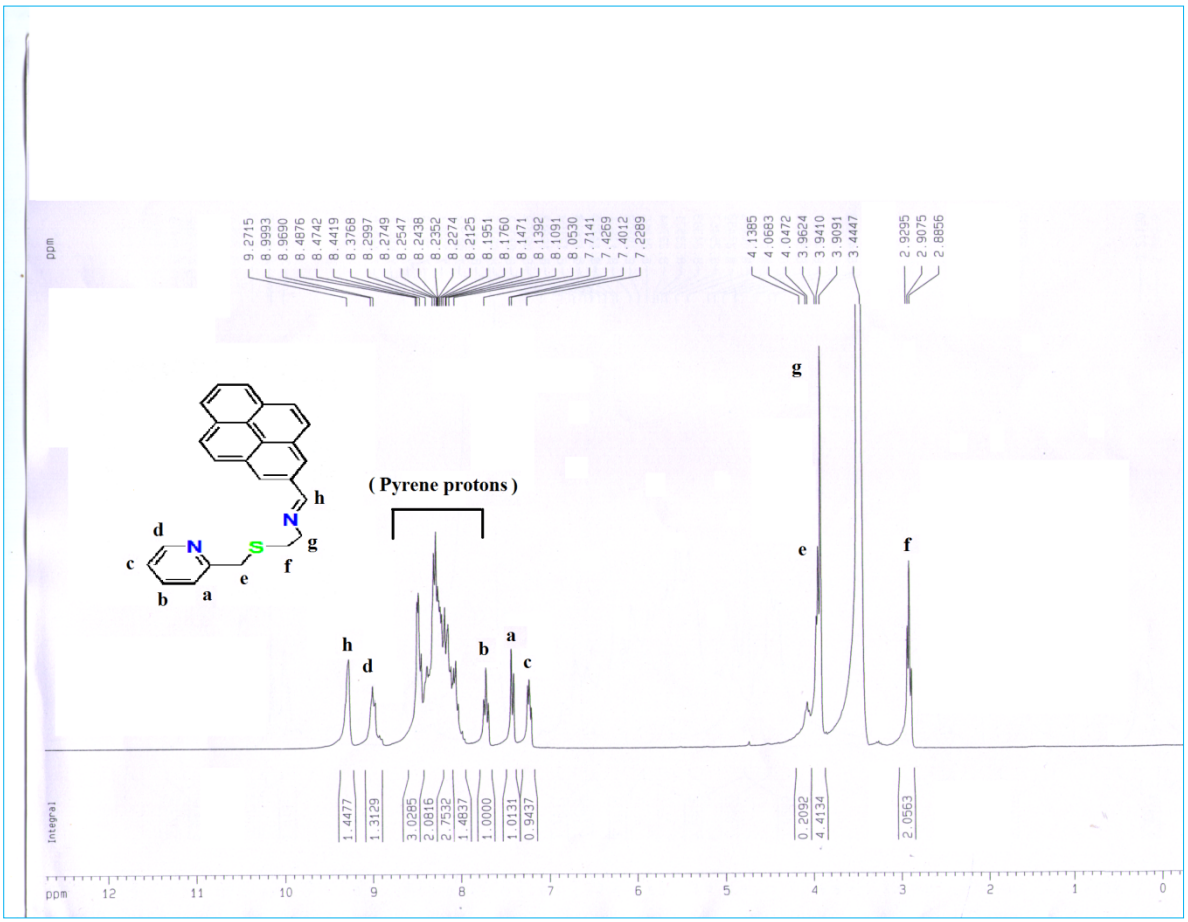


Fig.S2 ^{1}H NMR spectrum of **PP** in $DMSOd_6$ in Bruker 300 MHz instrument.

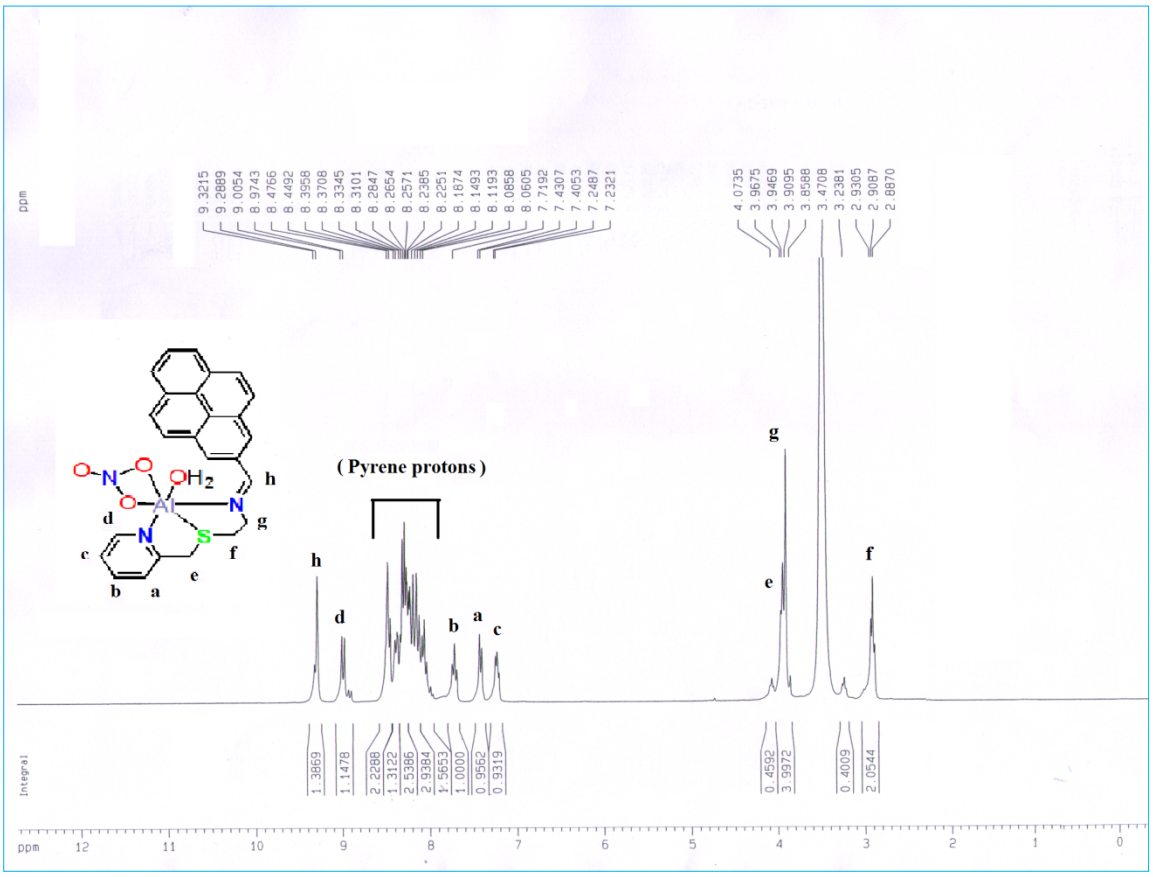


Fig.S3 ^{1}H NMR spectrum of **PP+ Al^{3+}** in DMSO-$d_6$in Bruker 300 MHz instrument.

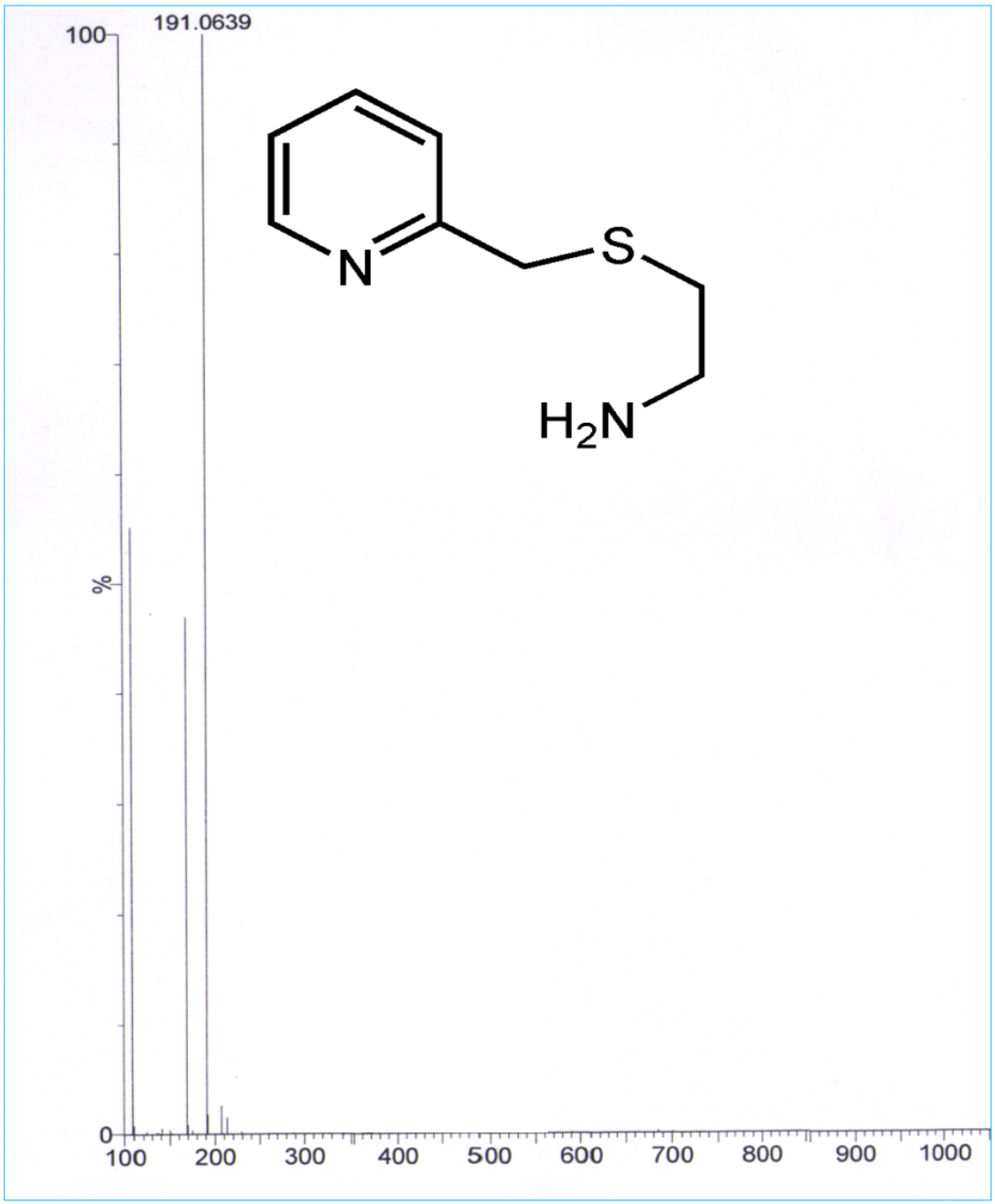


Fig. S4 Mass spectrum of **P** in CH_3OH.

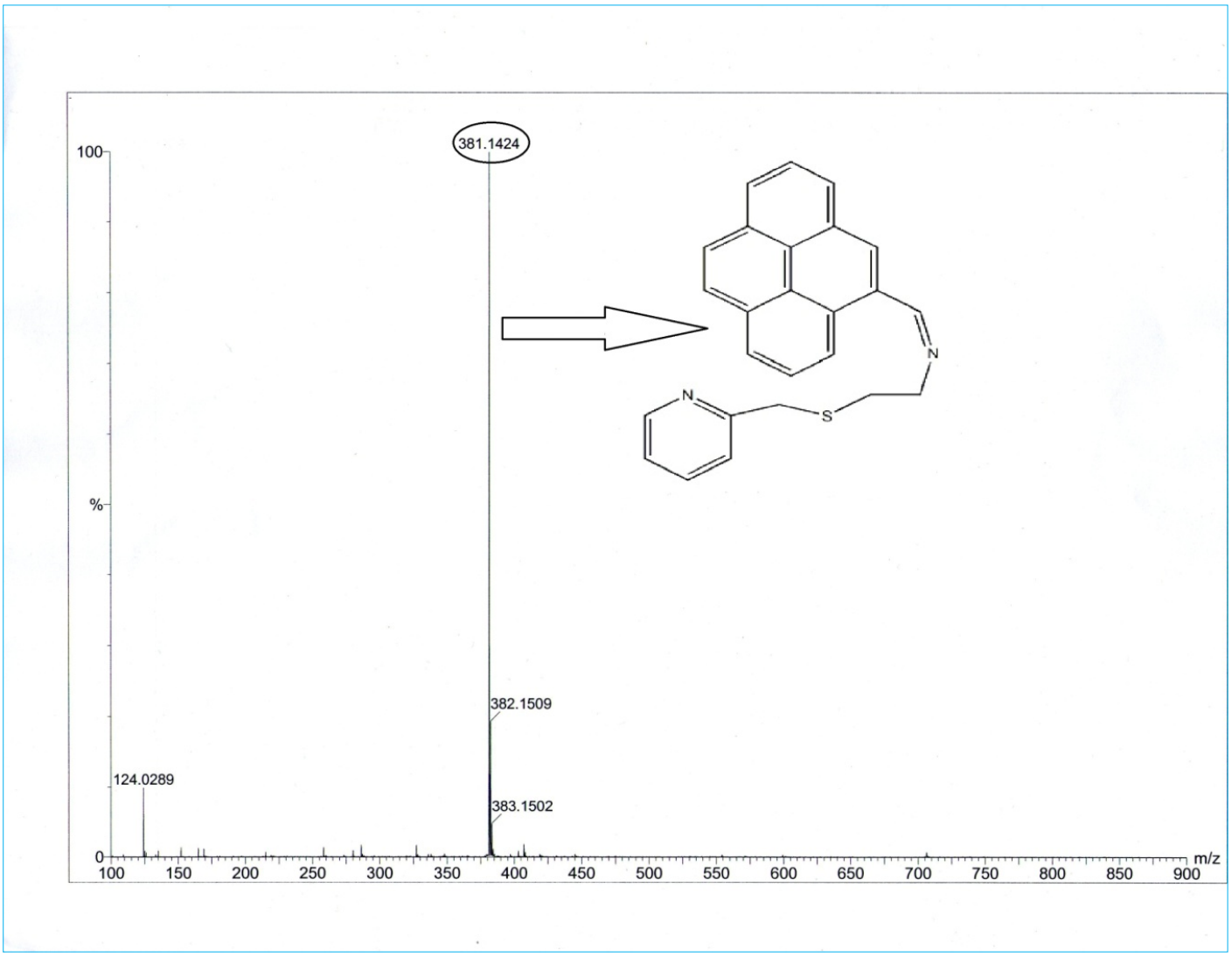


Fig.S5 Mass spectrum of **PP** in CH_3OH.

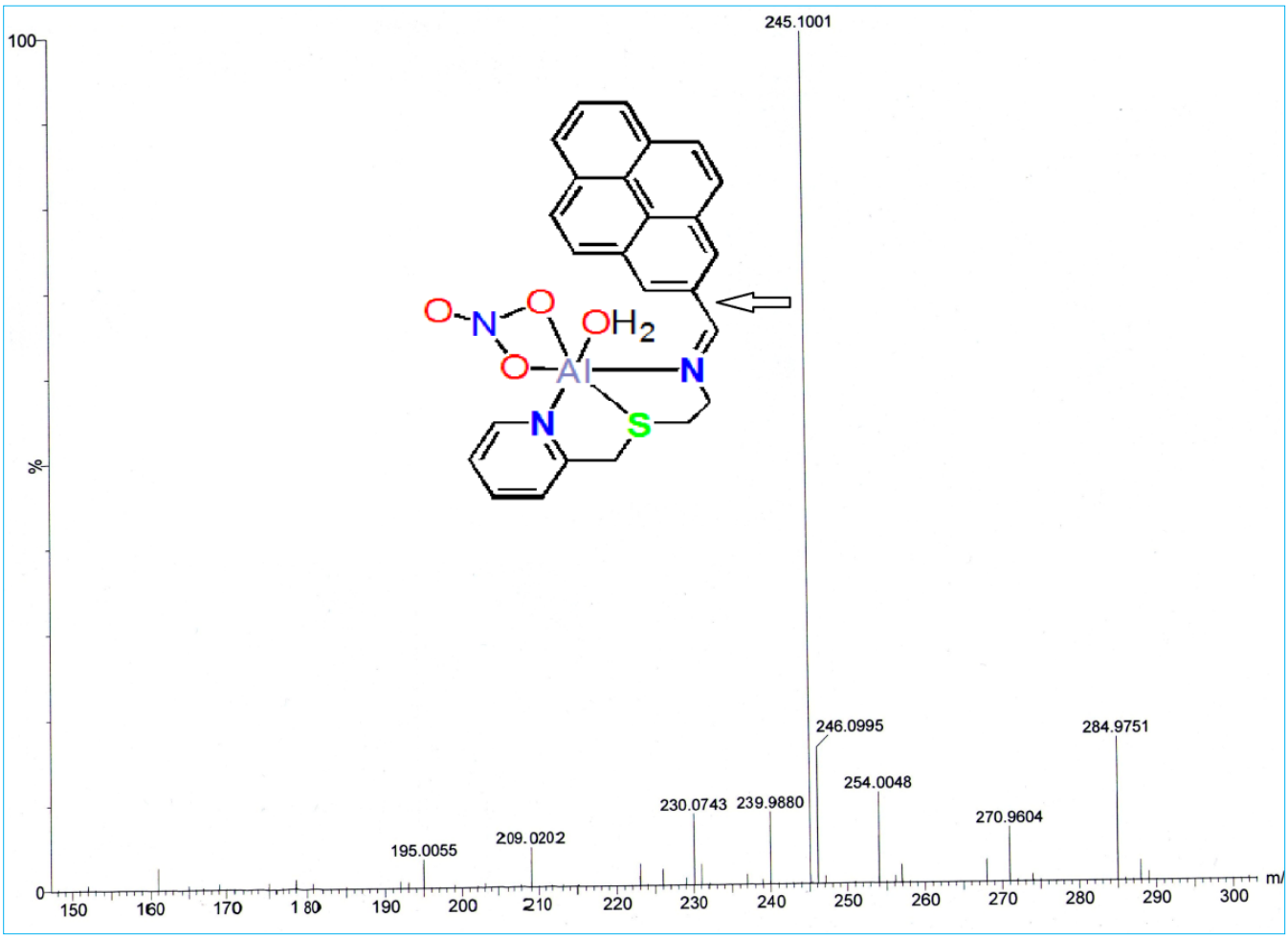


Fig.S6 Mass spectrum of **PP+Al^{3+}** in CH_3OH.

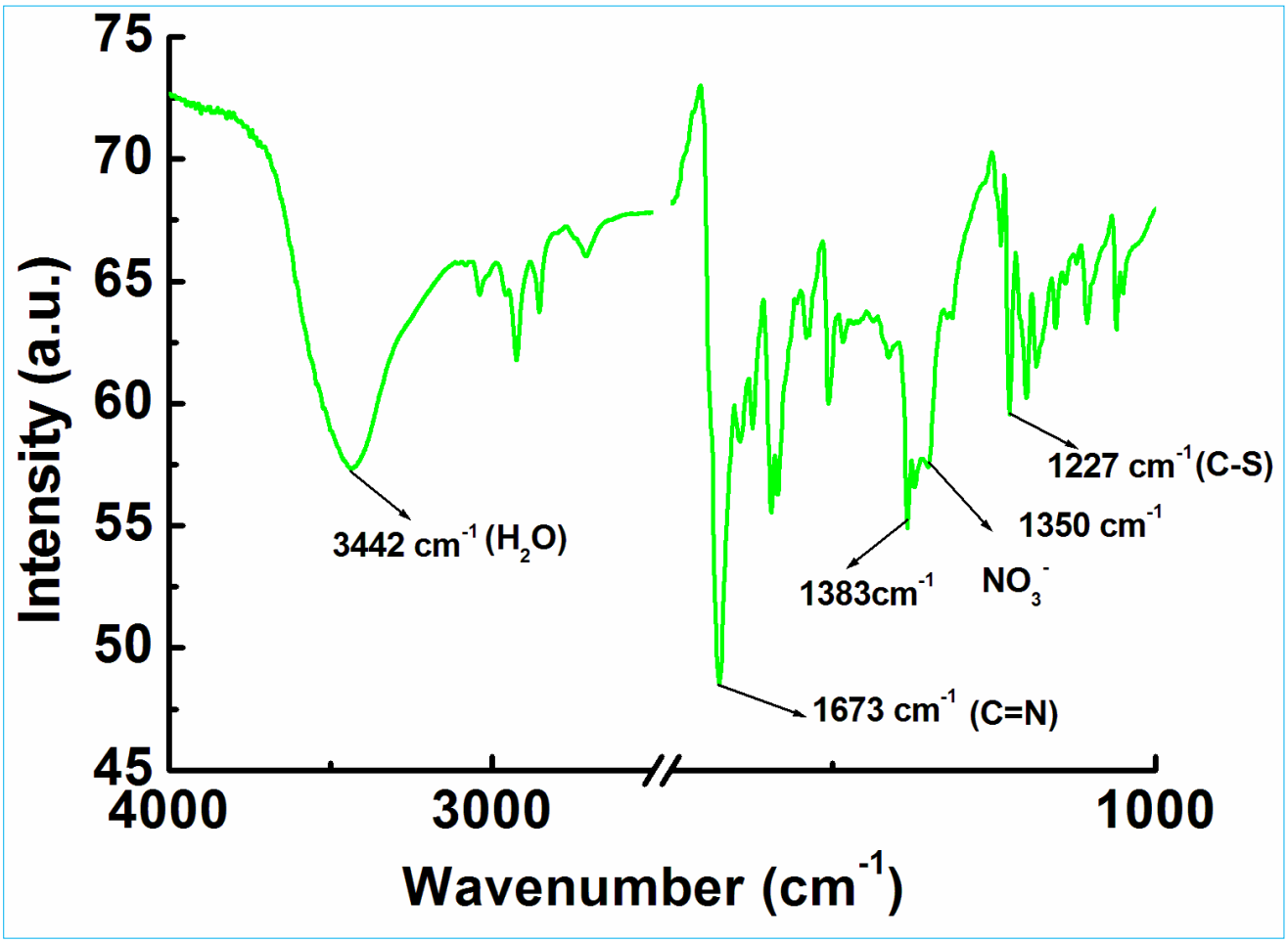


Fig. S7 IR spectrum of Al-**PP** complex.

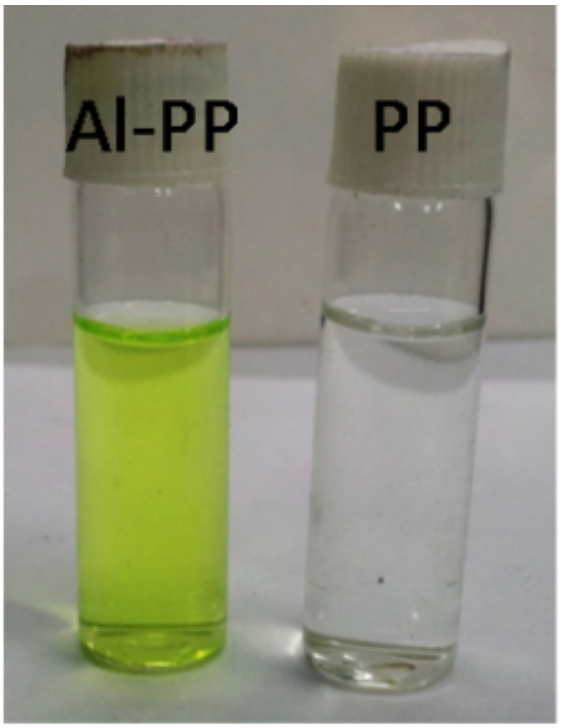
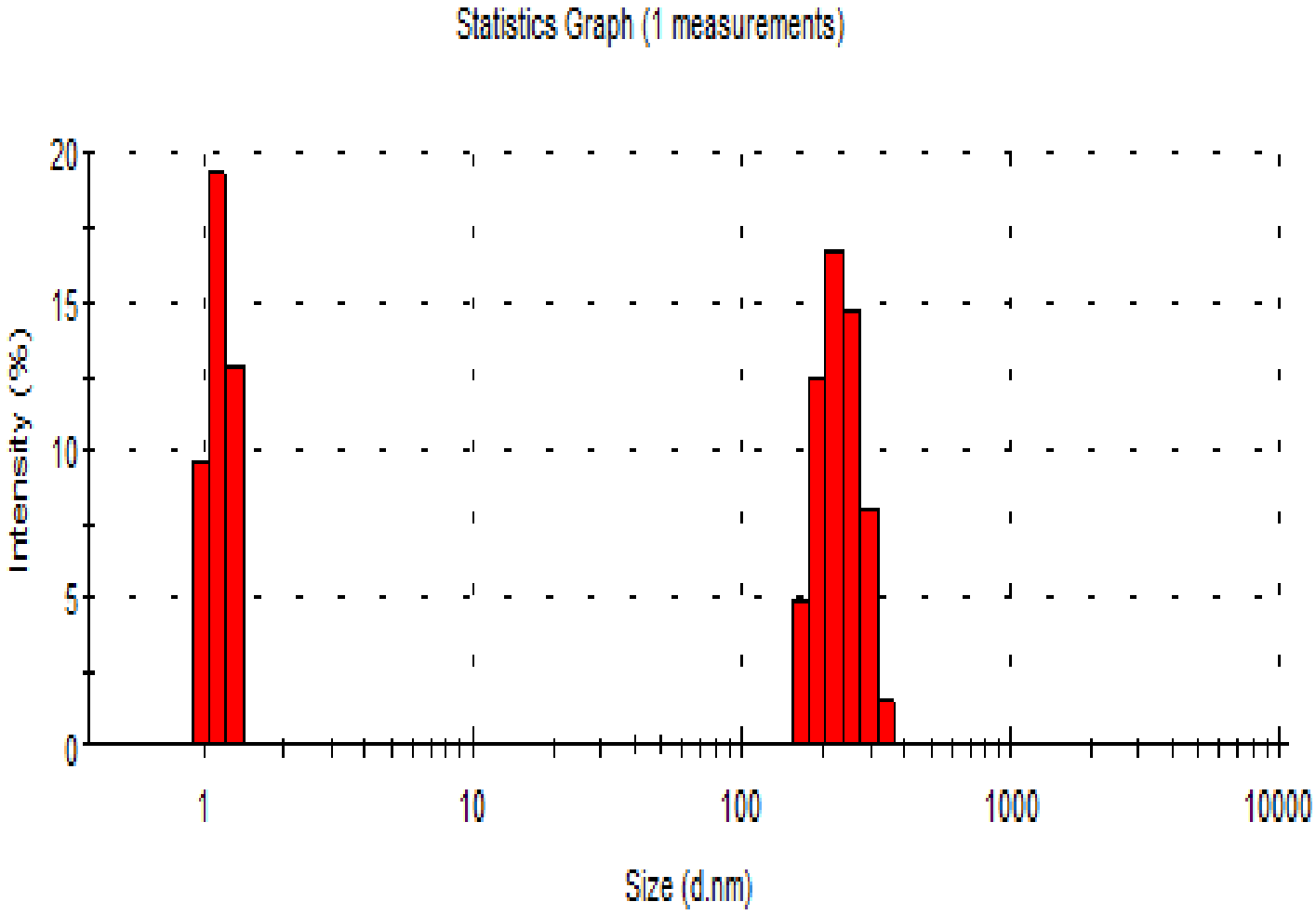
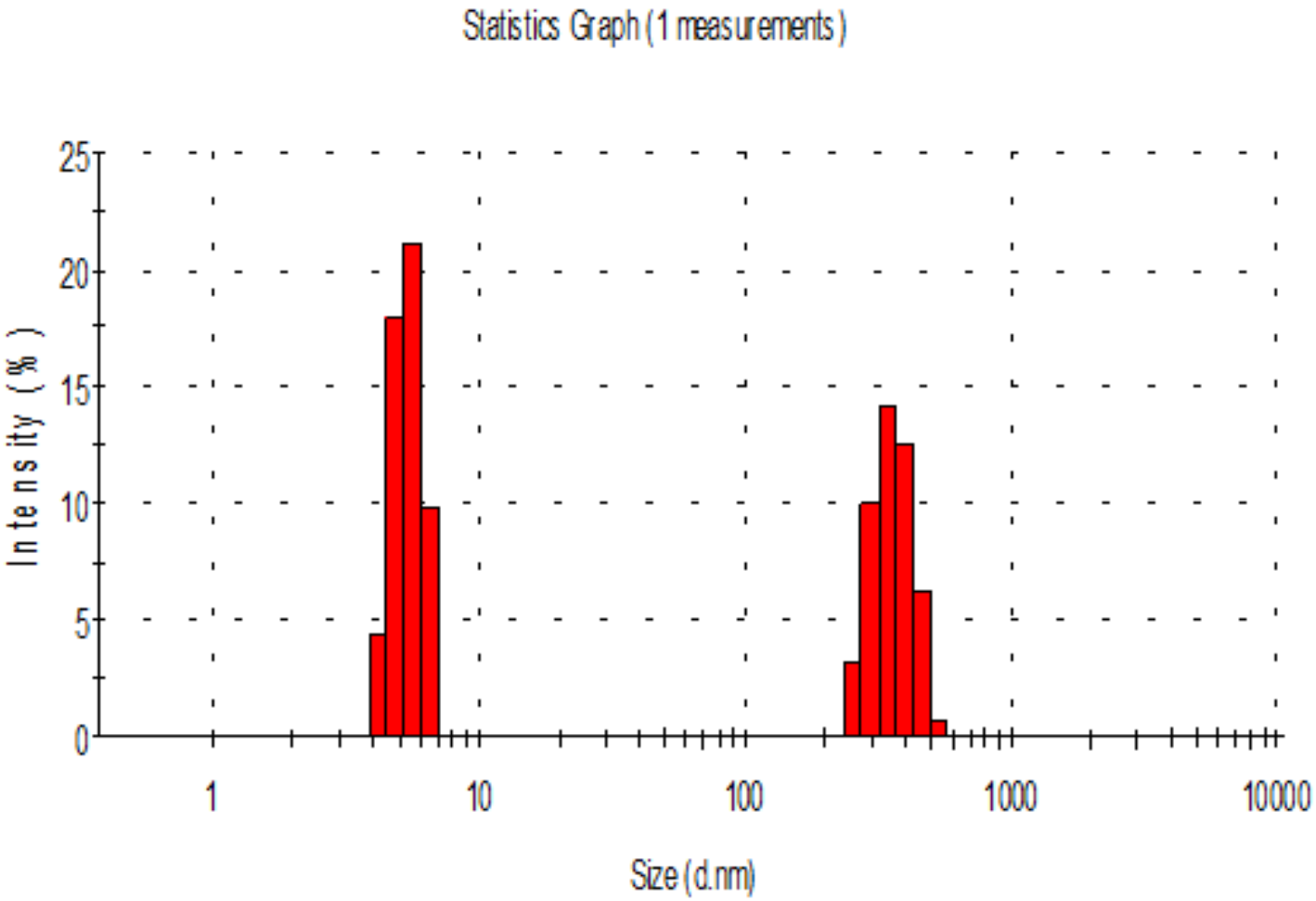


Fig. S8 Naked eye images of PP (20 μM) in presence of equimolar amount of Al^{3+} in aqueous-methanol solution at pH 7.2 (HEPES buffer).



Dynamic light scattering (DLS) plot of PP



Dynamic light scattering (DLS) plot of PP+ Al^{3+}

Fig.S9 Dynamic light scattering (DLS) plot.

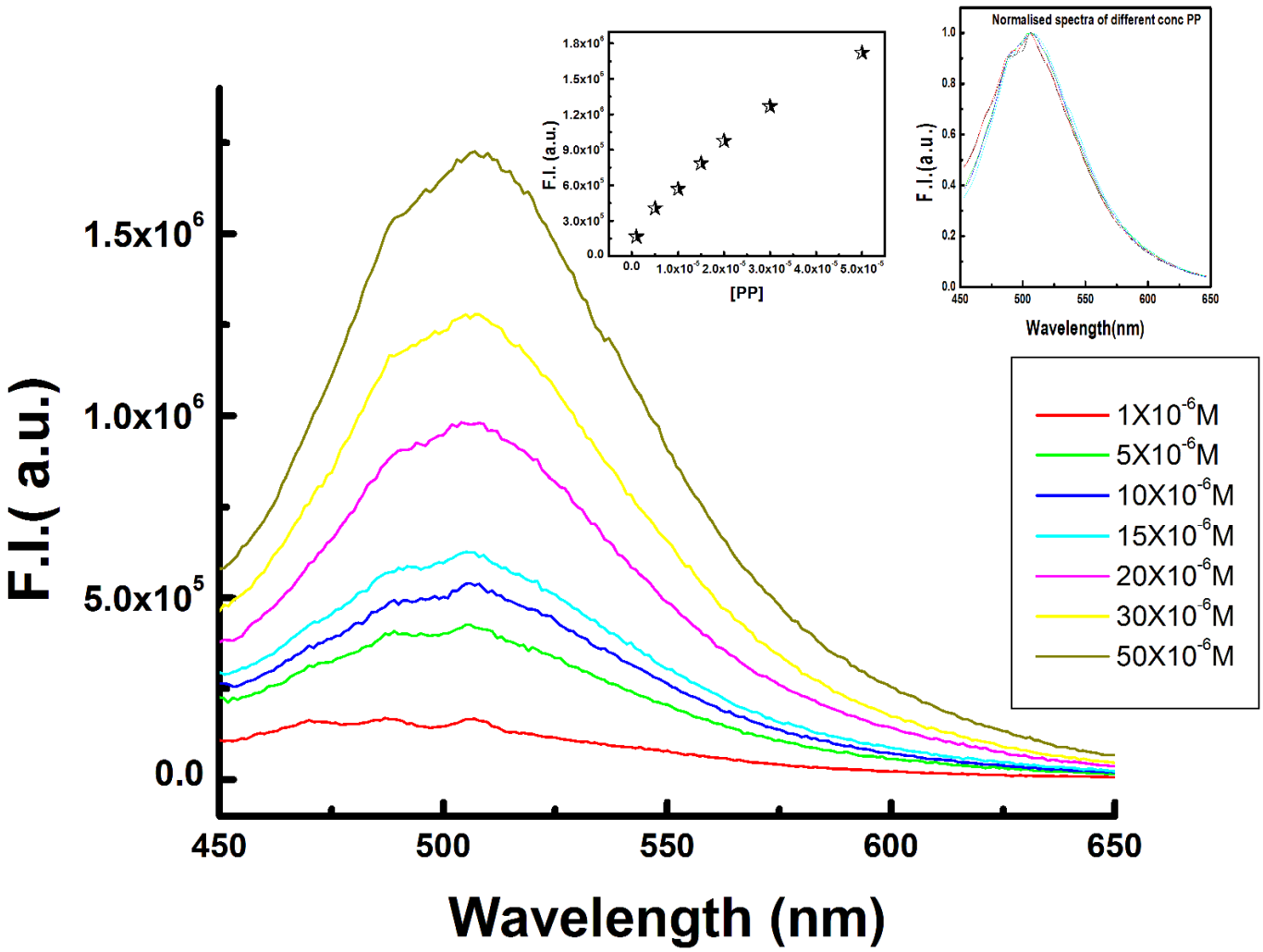


Fig. S10 Emission spectra of PP in different concentrations at λ_{ex}= 440nm (inset normalised spectra).

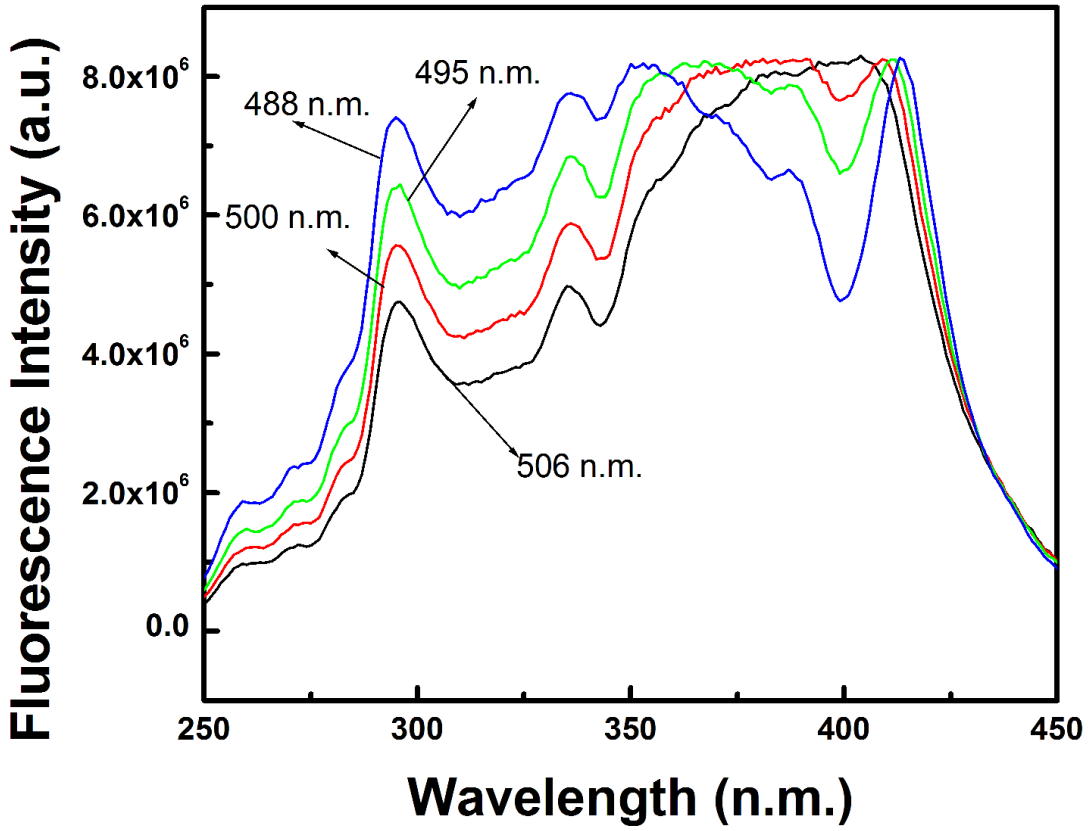
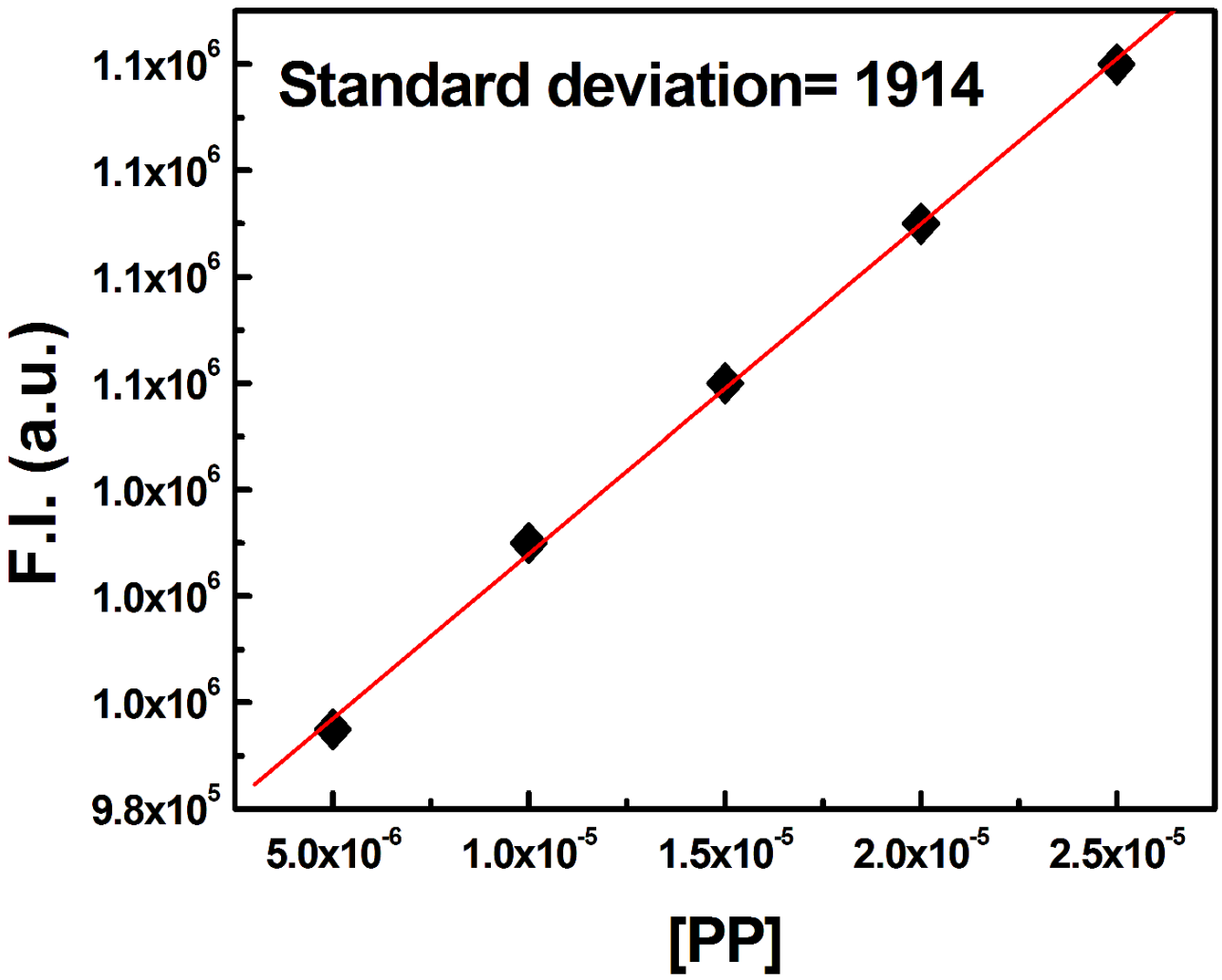
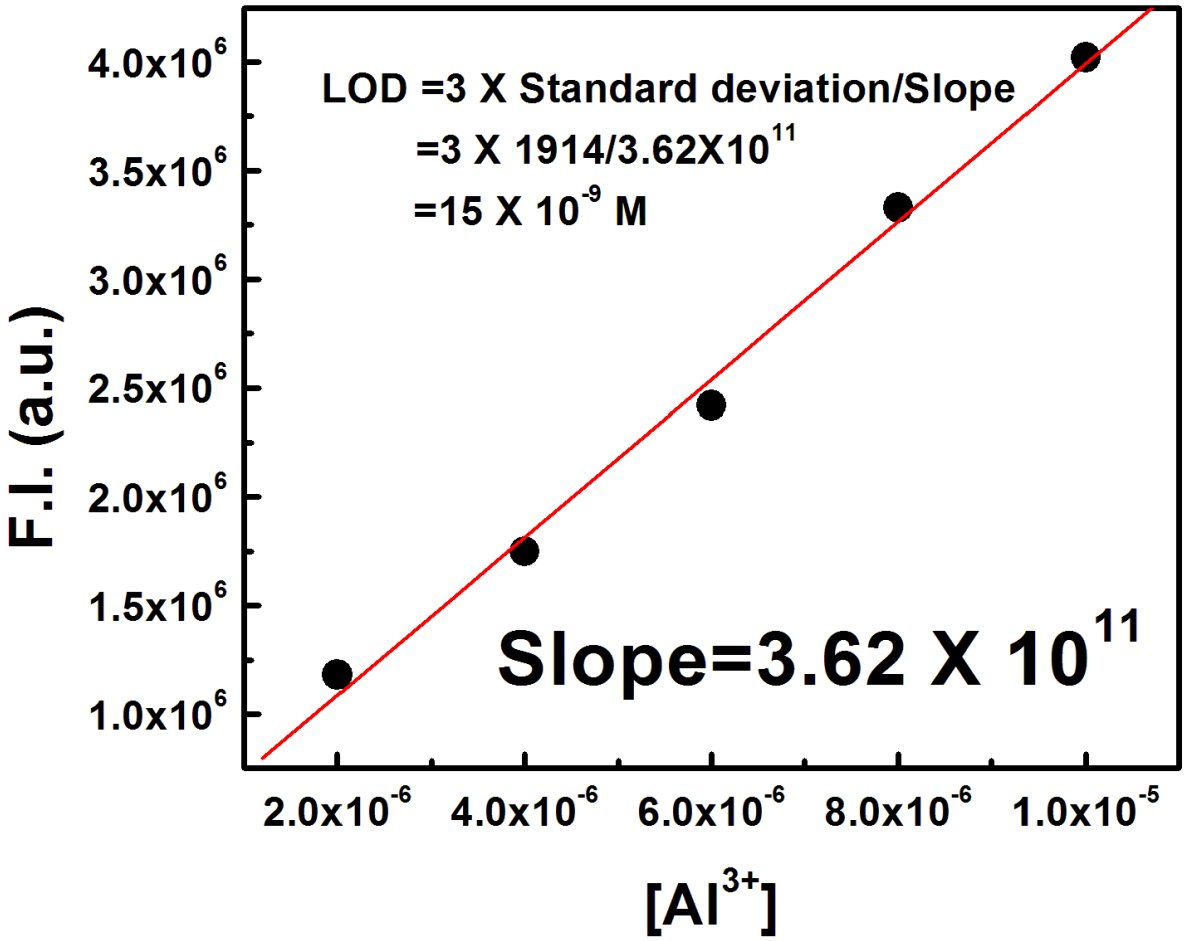


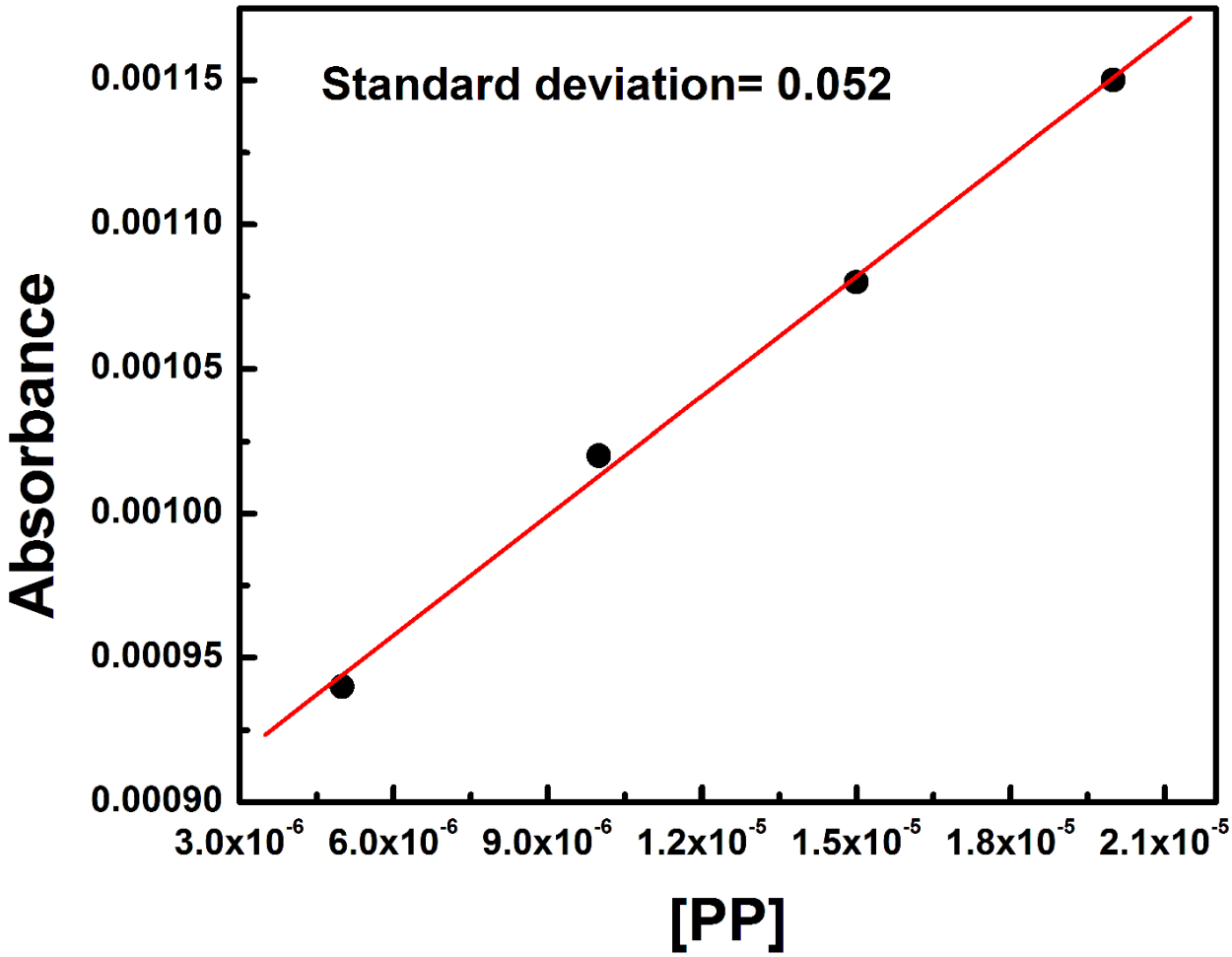
Fig.S11 Excitation spectra of PP in 506, 500, 495 and 488nm emission.

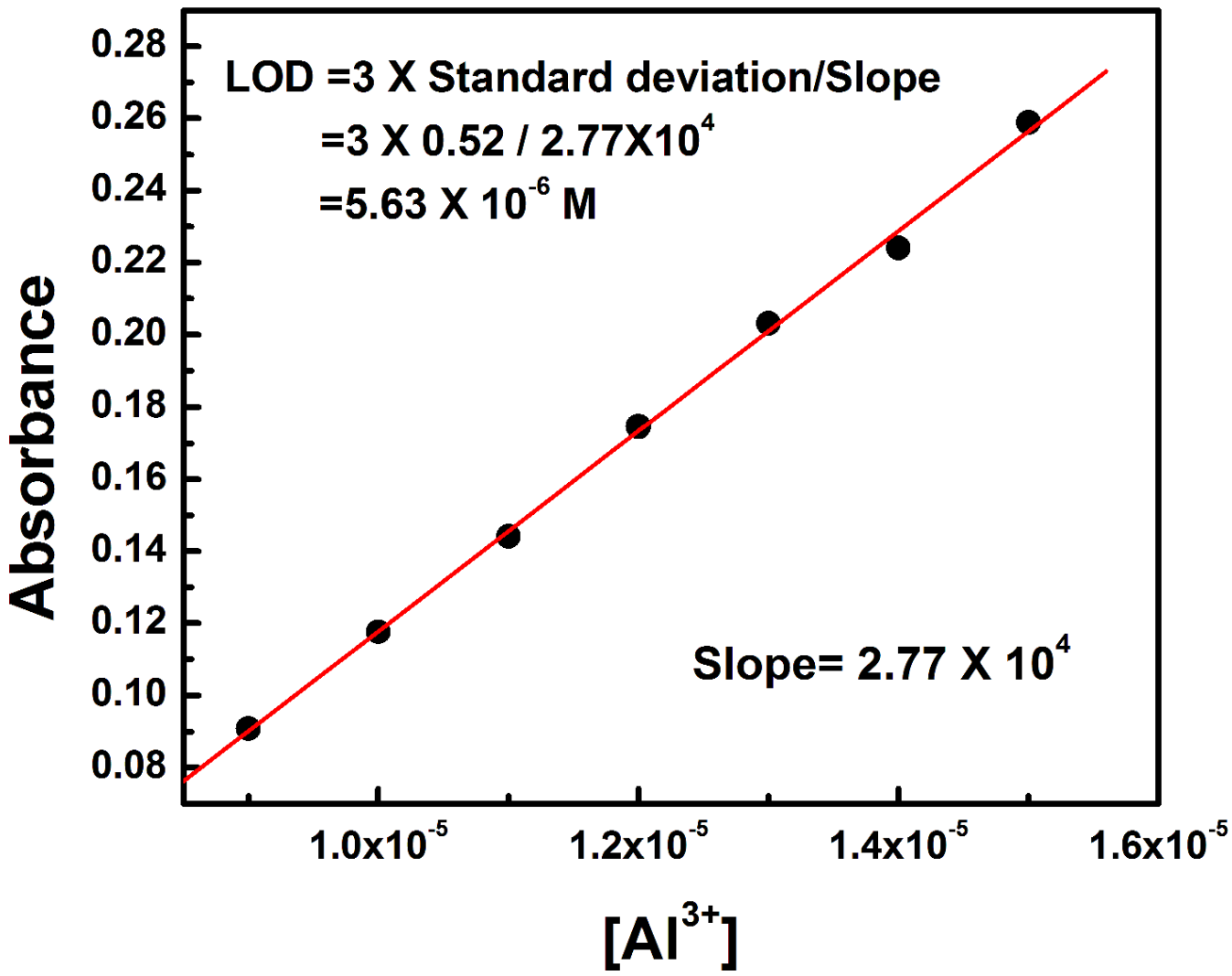

Standard deviation= 1914
F.I. (a.u.)
1.1x10^6
1.1x10^6
1.1x10^6
1.1x10^6
1.0x10^6
1.0x10^6
1.0x10^6
9.8x10^5
5.0x10^-6
1.0x10^-5
1.5x10^-5
2.0x10^-5
2.5x10^-5
[PP]



Limit of detection (LOD) plot using fluorescence technique.

Limit of quantification= 10 x Standard deviation of blank/Slope
= 10X 1914 / $3.62X10^{11}$
= 5.28 X 10^{-8} M


Standard deviation= 0.052
Absorbance
0.00115
0.00110
0.00105
0.00100
0.00095
0.00090
3.0x10-6
6.0x10-6
9.0x10-6
1.2x10-5
1.5x10-5
1.8x10-5
2.1x10-5
[PP]



Limit of detection (LOD) plot using UV-VIS technique.

Limit of quantification= 10X Standard deviation of blank / Slope
= 10X .52 / 2.77X10^4
= 1.87X 10^{-4} M

Fig. S12 Limit of detection and limit of quantification plots using fluorescence and UV-VIS techniques.

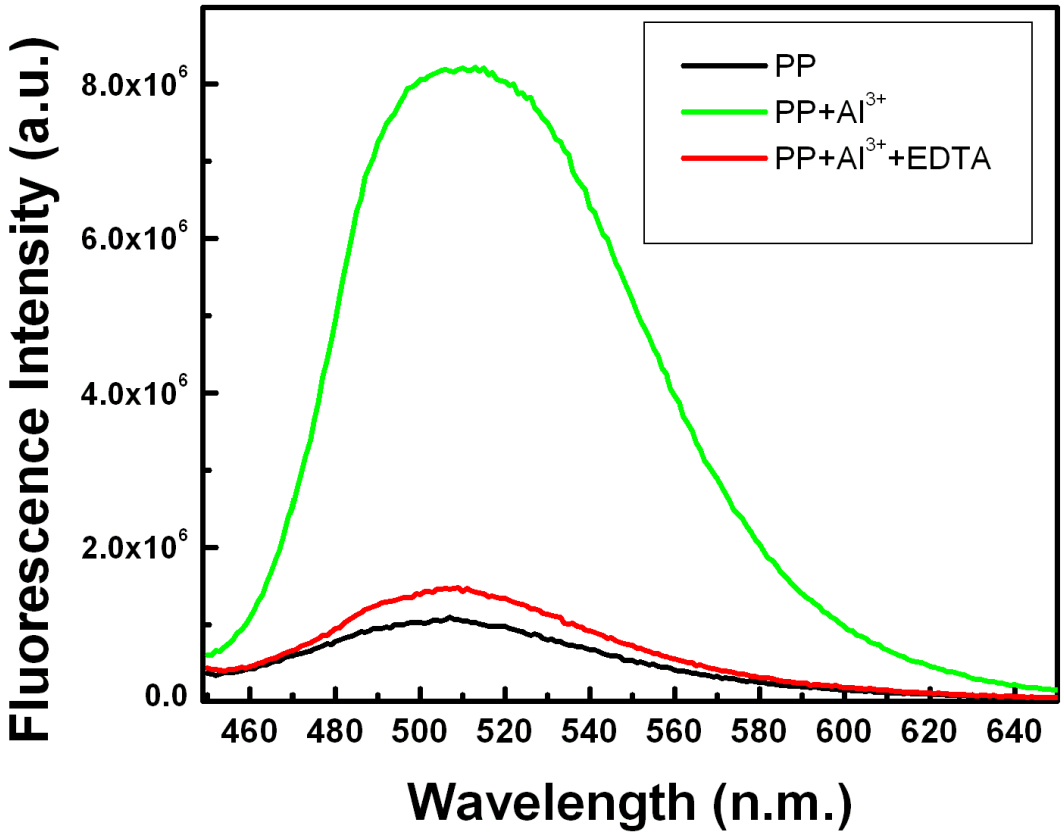


Fig.S13 Reversibility plot with EDTA.

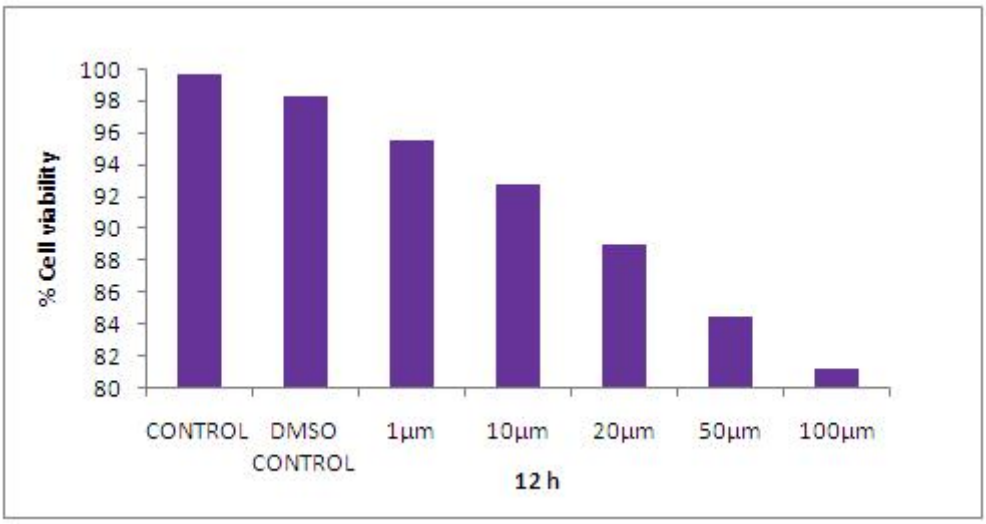


Fig.14 Cytotoxicity test of the ligand PP**.**

Table S1 Dynamic light scattering (DLS) data of PP and PP+Al^{3+}

		Size (d.nm)	% of Intensity	Width (n. nm)
PP				
	Peak 1	1.137	41.8	42.32
	PEAK 2	231.5	58.2	0.1206
PP+ Al^{3+}				
	Peak 1	5.402	53.3	0.6838
	Peak 2	358.9	46.7	61.47

Table S2 Selected parameters for the vertical excitation (UV-VIS absorptions) of L; electronic excitation energies (eV) and oscillator strength (f), configurations of the low-lying excited states of L; calculation of the $S_0 \rightarrow S_n$ energy gaps on optimized ground- state geometries (UV-vis absorption).

Electronic transition	Composition	Excitation energy	Oscillator strength (*f*)	CI	Assignment	λ_{exp} (nm)
$S_0 \rightarrow S_2$	HOMO–2 → LUMO+1	3.9974eV (339nm)	0.3895	0.15137	ILCT	343
	HOMO → LUMO			0.64857	ILCT	
	HOMO→ LUMO+1			-0.18792	ILCT	
$S_0 \rightarrow S_7$	HOMO-2→LUMO	4.2529 eV (291 nm)	0.1511	0.58459	ILCT	286/275
	HOMO→ LUMO + 1			0.26132	ILCT	
	HOMO→ LUMO + 4			0.21850	ILCT	
$S_0 \rightarrow S_{11}$	HOMO–2→ LUMO+1	4.6548eV (266 nm)	1.2965	0.64553	ILCT	263/260
	HOMO-1→ LUMO + 3			-0.12244	ILCT	
	HOMO→ LUMO			-0.14788	ILCT	
$S_0 \rightarrow S_{17}$	HOMO–7→LUMO +1	5.0265 eV (246 nm)	0.1124	0.10092	ILCT	243/233
	HOMO-2→ LUMO			0.16606	ILCT	
	HOMO→ LUMO+5			0.61462	ILCT	

Table S3 Main calculated optical transition for the complex 1 with composition in terms of molecular orbital contribution of the transition, vertical excitation energies, and oscillator strength in methanol.

Electronic transition	Composition	Excitation energy	Oscillator strength (*f*)	CI	Transition assigned	λ_{exp} (nm)
$S_0 \rightarrow S_6$	HOMO – 2 → LUMO+1	3.1468eV (394 nm)	0.3069	-0.11396	MLCT/ILCT	390
	HOMO – 1 → LUMO+1			0.65506	MLCT/ILCT	
	HOMO → LUMO + 3			-0.23348	ILCT	
$S_0 \rightarrow S_8$	HOMO – 2→ LUMO + 1	3.4719eV (357 nm)	0.0405	0.69131	MLCT/ILCT	360
	HOMO – 1→ LUMO + 1			0.11297	MLCT/ILCT	
$S_0 \rightarrow S_{11}$	HOMO – 4→ LUMO + 1	3.7093eV (334nm)	1.3617	0.14673	MLCT/ILCT	343
	HOMO – 1→ LUMO + 1			0.23355	MLCT/ILCT	
	HOMO → LUMO + 3			0.62749	ILCT	