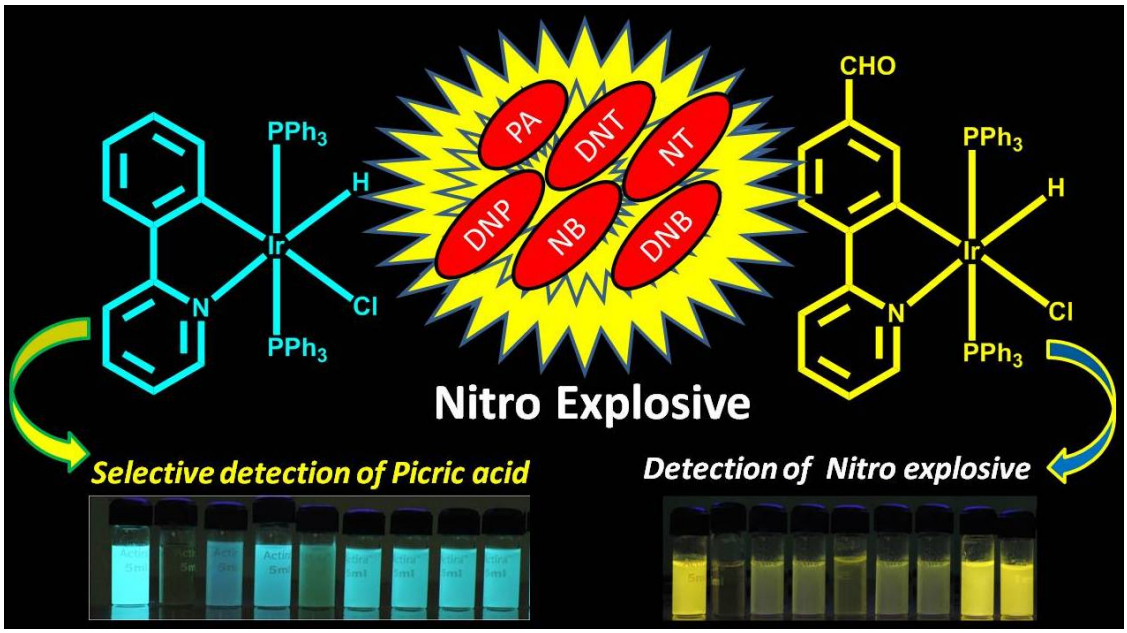
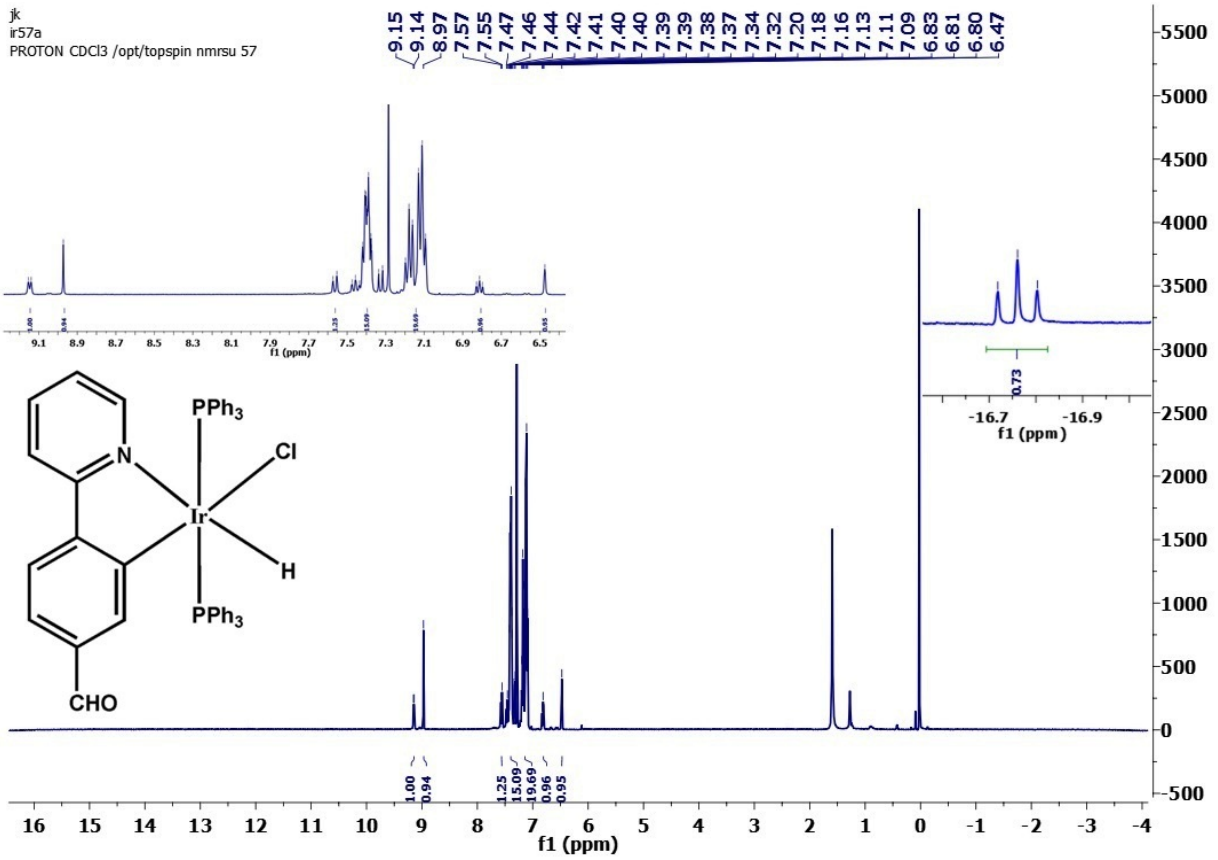
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.



Highly Sensitive Explosive Sensing by "Aggregation Induced Phosphorescence" Active Cyclometalated Iridium(III) Complexes

Parvej Alam,[a] Gurpreet Kaur,[b] Vishal kachwal,[a] Asish Gupta,[c] Angshuman Roy Chaudhury [b] and Inamur Rahaman Laskar*[a]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9.14
8.97
7.57
7.55
7.47
7.46
7.44
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.34
7.32
7.20
7.18
7.16
7.13
7.11
7.09
6.83
6.81
6.80
6.47
PPh3
Cl
N
Ir
H
PPh3
CHO
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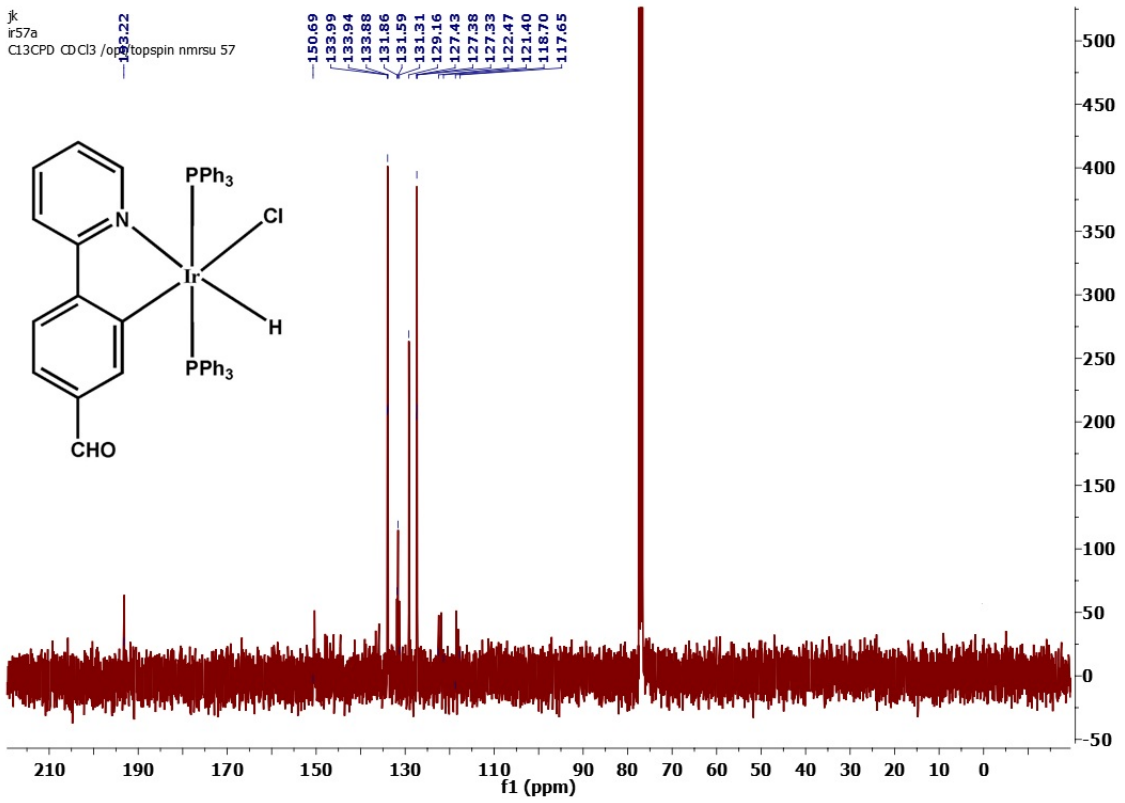
0.94
1.25
15.09
19.69
0.96
0.95
0.73
f1 (ppm)

a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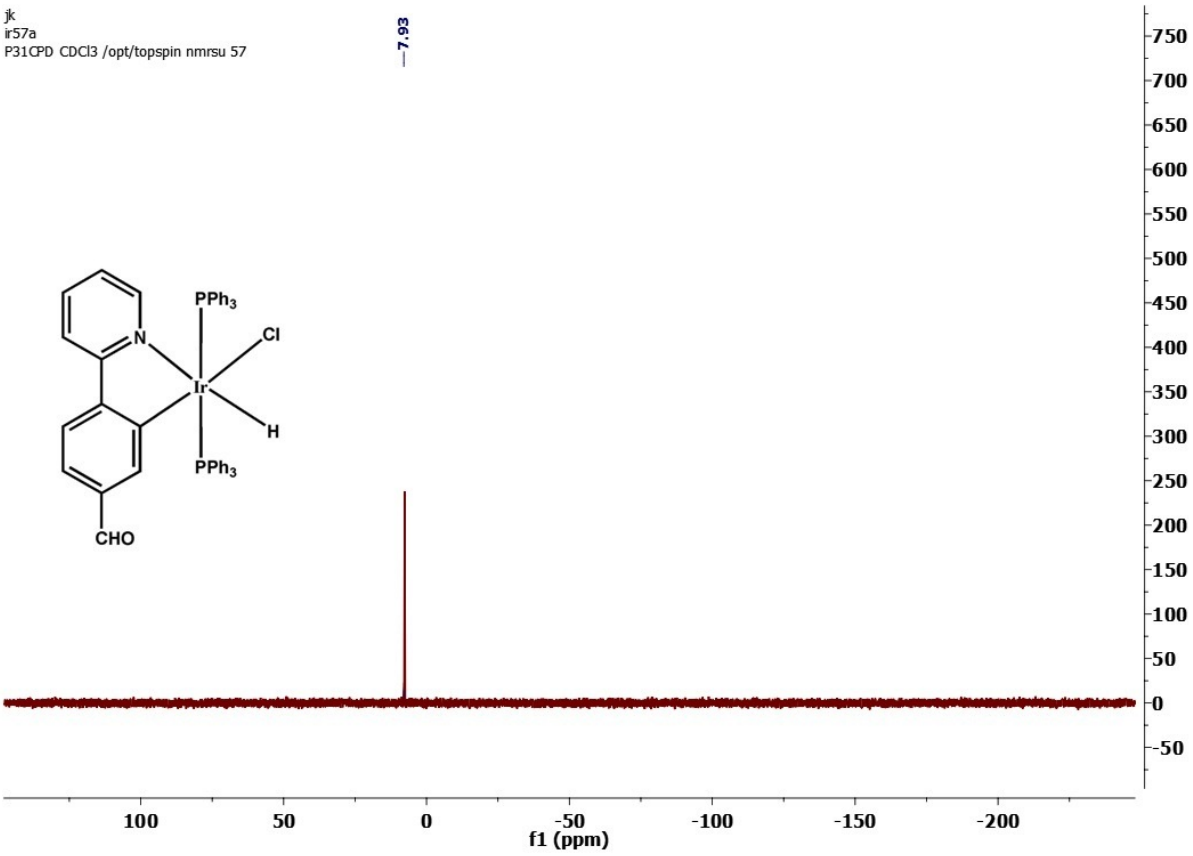
133.99
133.94
133.88
131.86
131.59
131.31
129.16
127.43
127.38
127.33
122.47
121.40
118.70
117.65
PPh3
Cl
N
Ir
H
PPh3
CHO
500
450
400
350
300
250
200
150
100
50
0
-50
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

b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650
600
550
500
450
400
350
300
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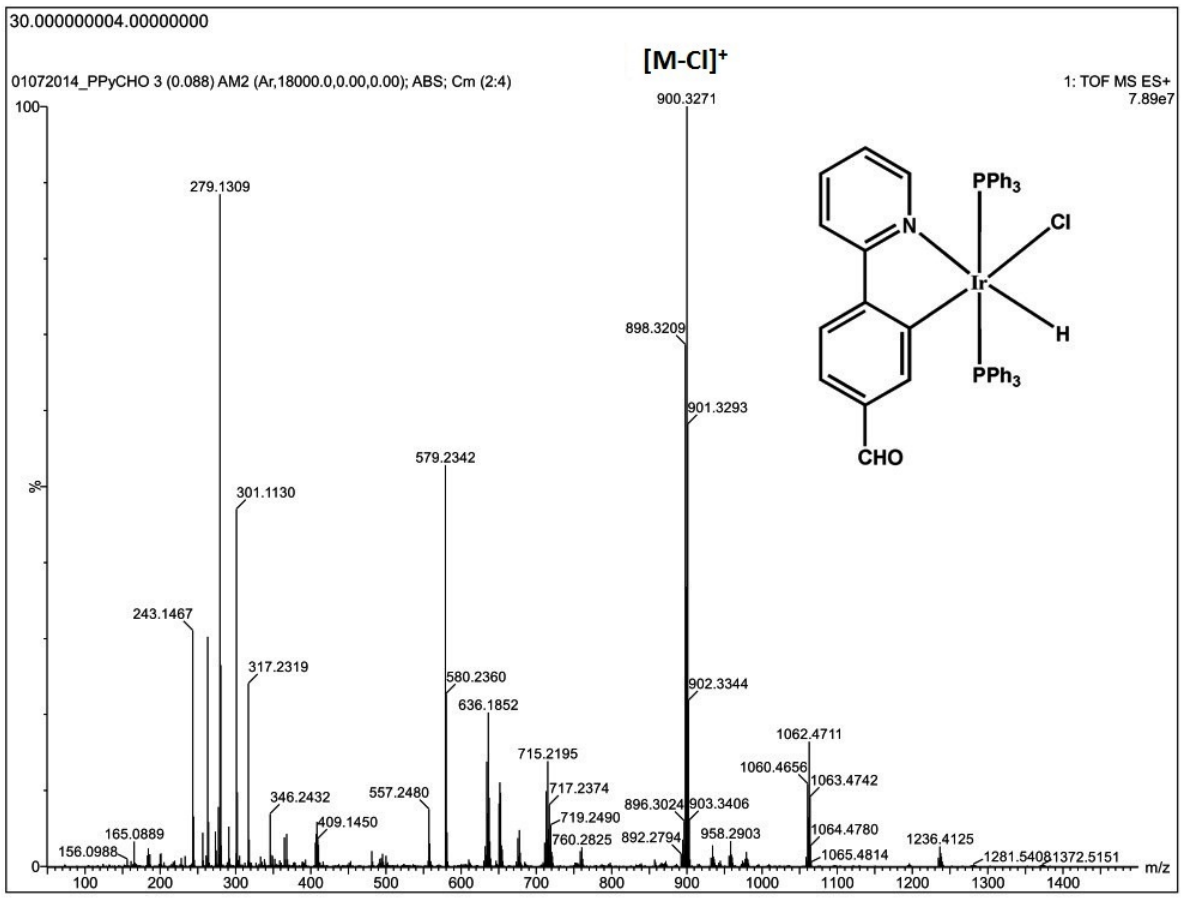
200
150
100
50
0
-50
100
50
0
-50
-100
-150
-200
f1 (ppm)

c



d

Fig. S1 (^{1}H, ^{31}P,^{13}C) NMR spectra and HRMS (a, b, c and d), respectively for **1**.

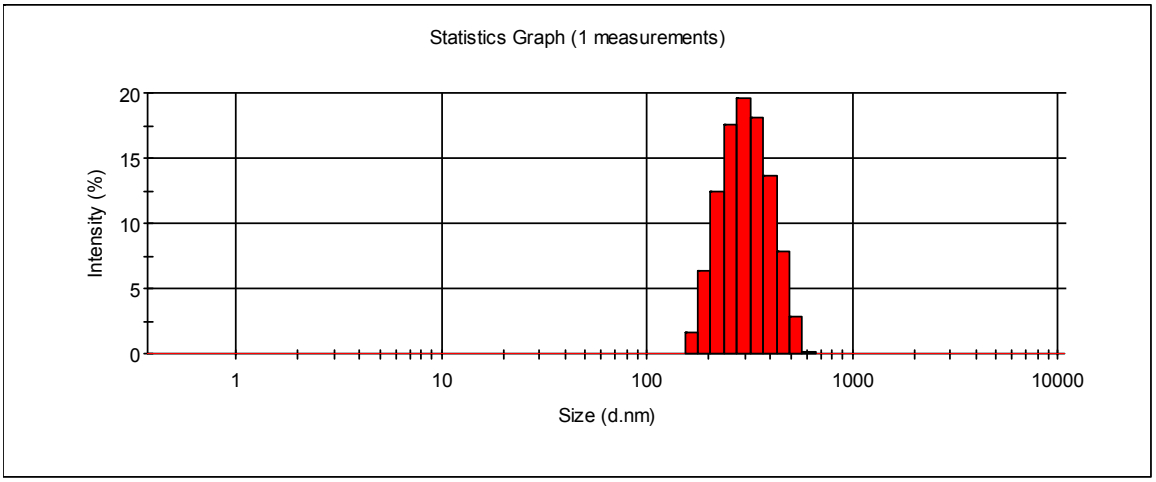
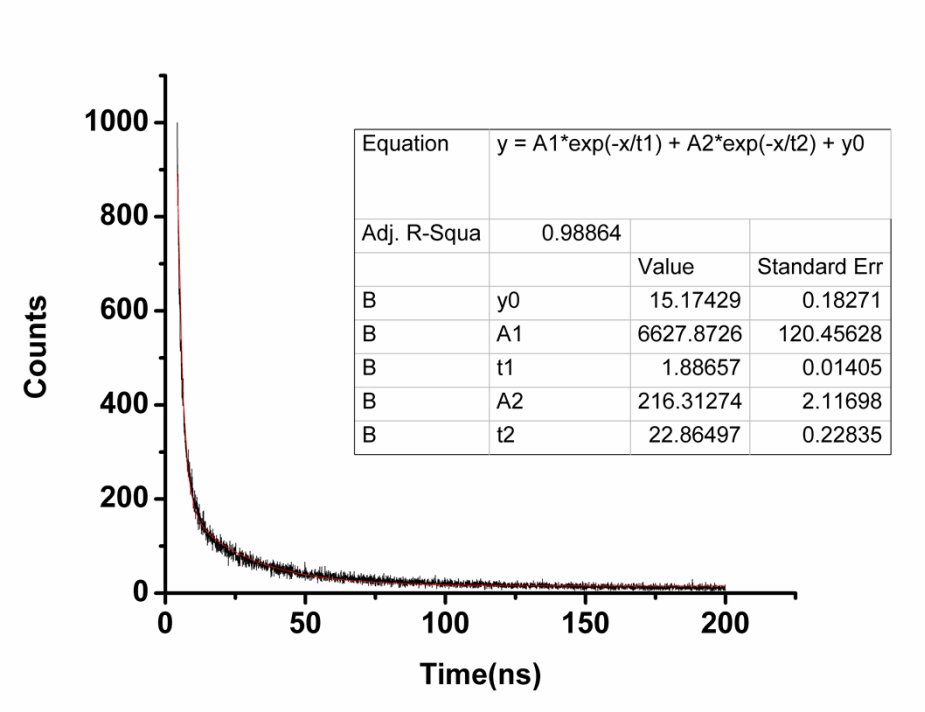
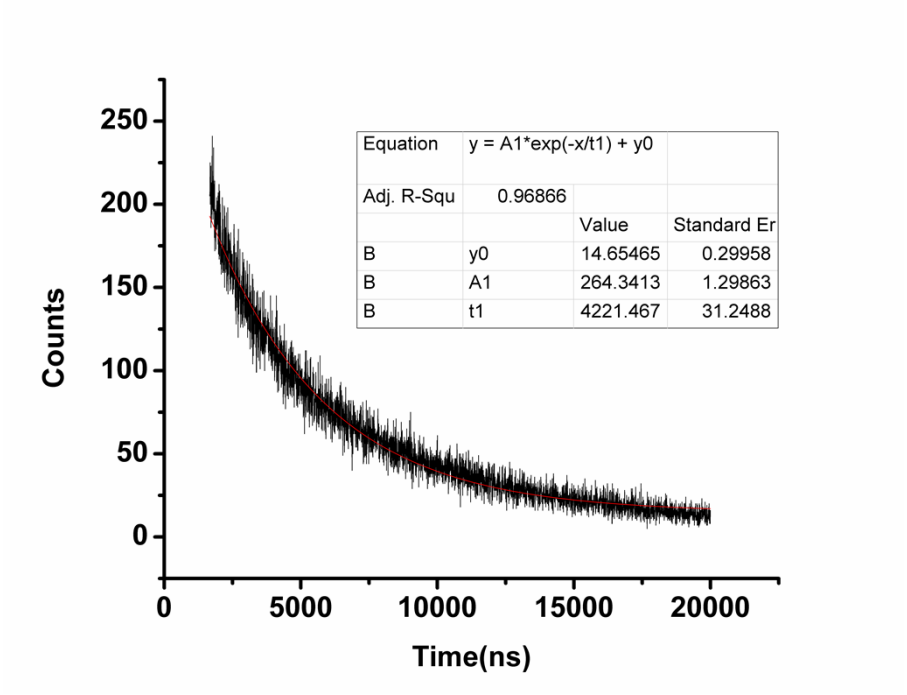


Fig. S2 Particle size distribution of nano-aggregates of **1** in a THF/water mixture with a 90% water fraction.

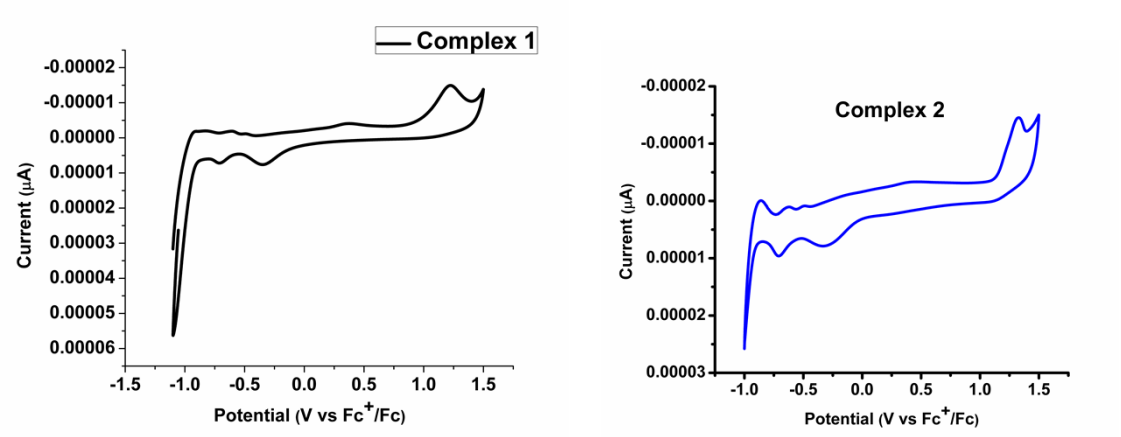


a



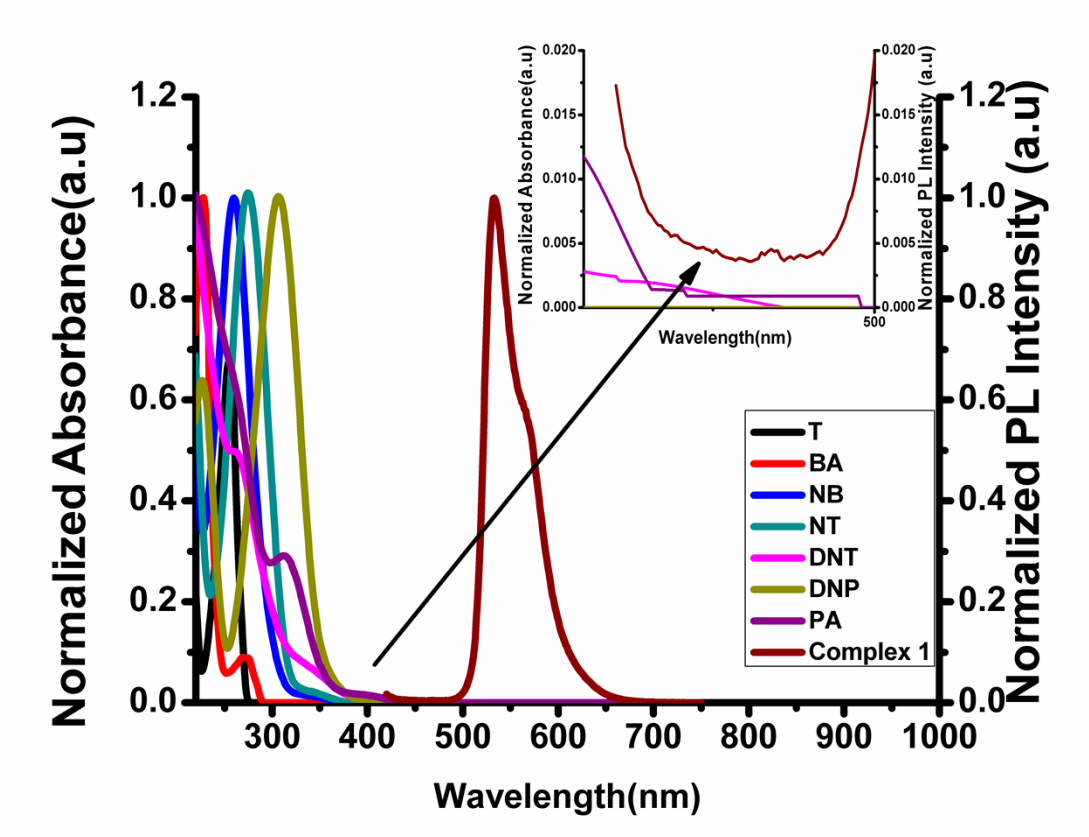
b

Fig. S3 Photoluminescence lifetime decay curves (a) in THF and (b) in f_w=90 % for **1** (the red line is the fitting curve).

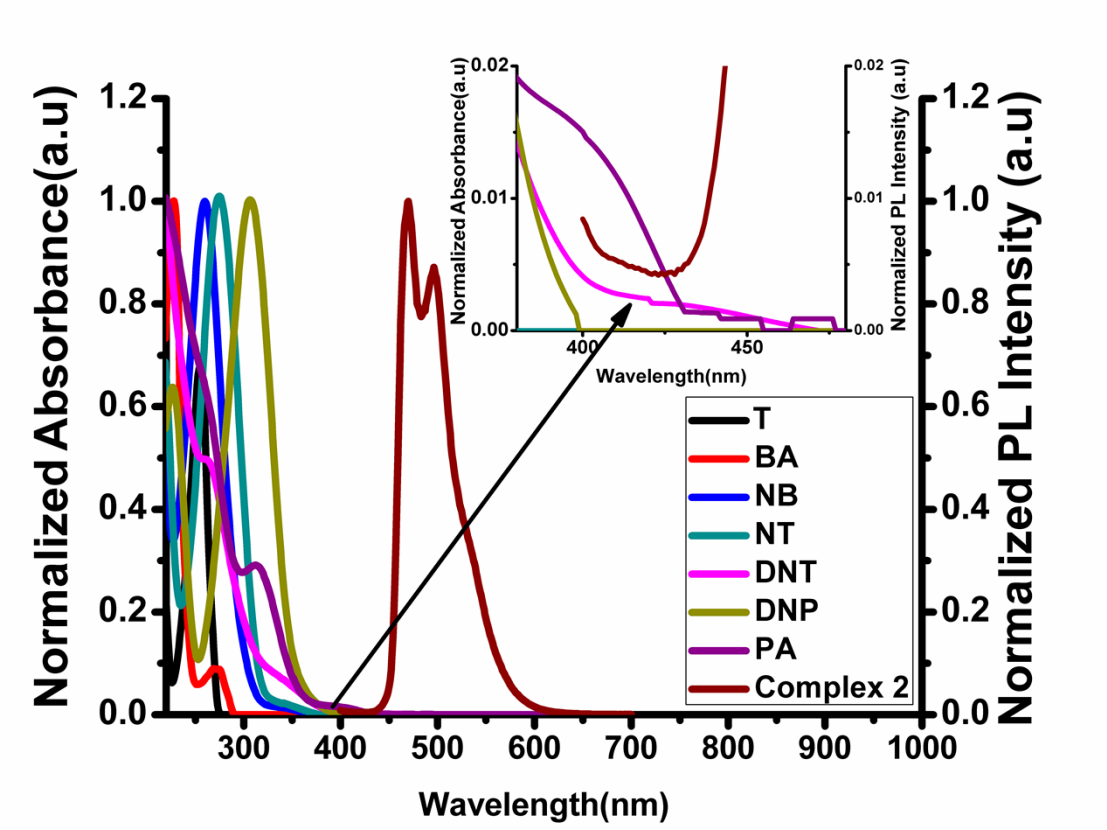


a b

Fig. S4 Cyclic voltammogram of **1** (a) and of **2** (b) respectively, recorded in CH_3CN (ACN) at a scan rate of 0.05 V s^{-1}



a



b

Fig. S5 (a) Absorption spectra of different aromatic compounds and emission spectra of **1** (b) Absorption spectra of different aromatic compounds and emission spectra of **2**, in THF. The spectral overlap between the emission of **1** and **2** and the absorption of aromatic compounds was shown in inset.

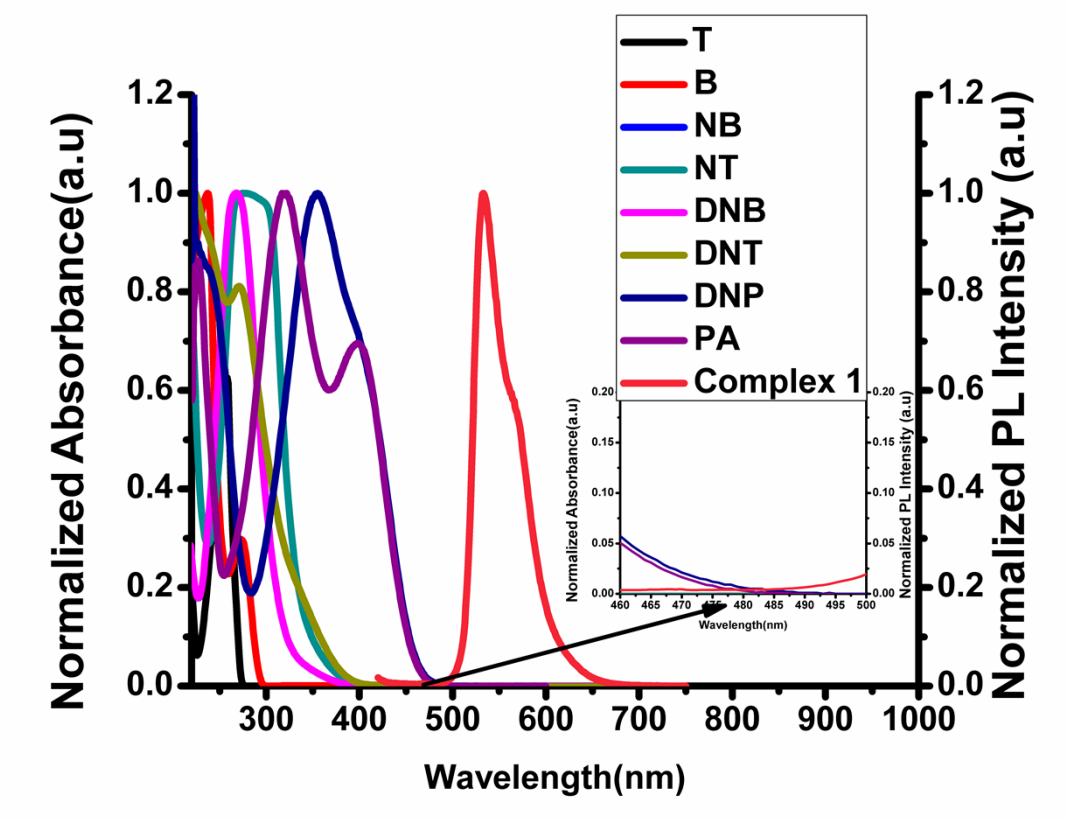


Fig. S6 Absorption spectra of different aromatic compounds and emission spectra of **1** in THF–water (v/v = 1: 9) mixtures. The spectral overlap between the emission of **1** and the absorption of aromatic compounds was shown in inset.

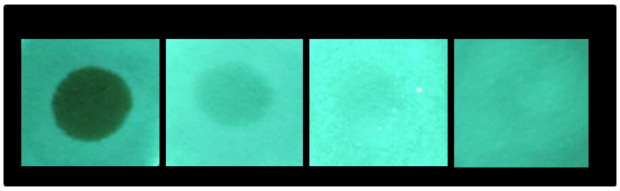


Fig. S7 Luminescent photographs of paper plates impregnated by **2** against different concentrations of PA: (a); 10^{-3}, (b); 10^{-6}, (c); 10^{-9},(d); 10^{-12}

Luminescence quenching titration study in THF: Water medium:

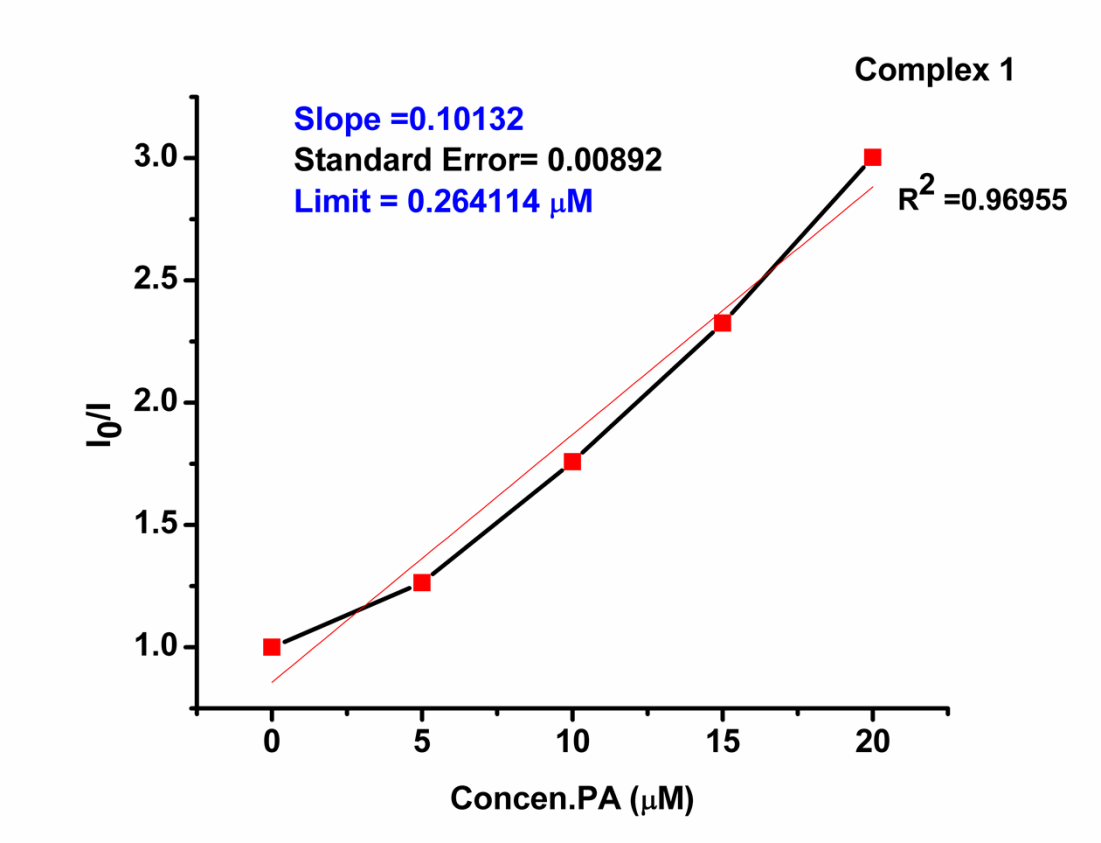
Luminescence quenching titration studies in THF : Water (1:9, v/v) were carried out with gradual increasing PA concentration (5μM, 10 μM and so on) in a micro quartz cuvette keeping the total volume 1.5 mL. For each addition, at least three fluorescence spectrums were recorded at 298K to obtain concordant value. The λ_{ex} was chosen 400 nm and 385 nm for **1** and **2**, respectively with 3 nm slit width.

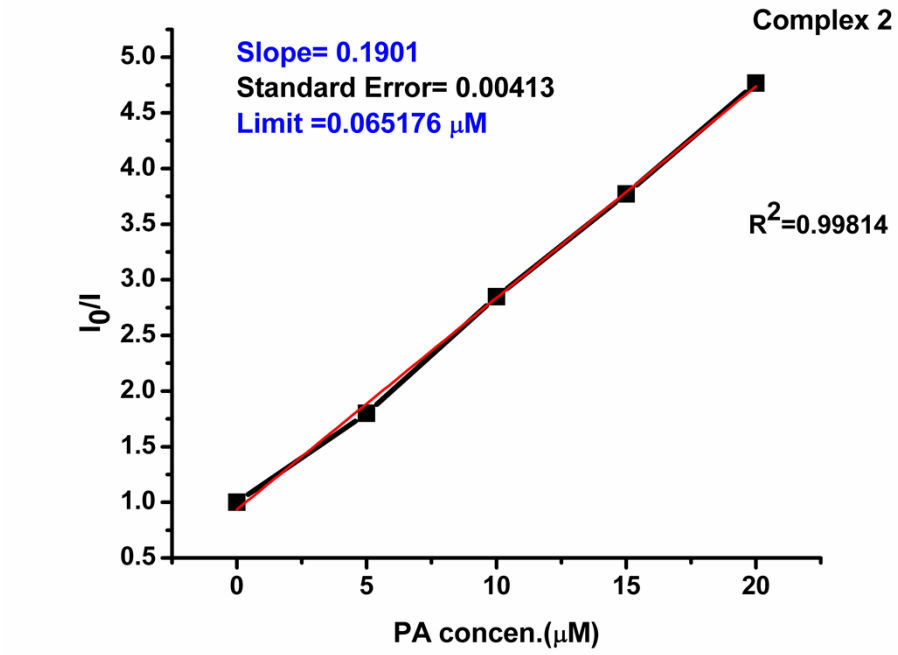
Detection limit calculations experimental procedure [1,2]

To determine the Signal/Noise ratio, the emission intensity of both complexes in THF : Water (1:9, v/v) without PA was measured by 10 times and the standard deviation of blank measurements was determined.

The detection limit is then calculated with the following equation.

Detection limit = 3σ/m; where σ is the standard deviation of blank measurements, m is the slope between the plot of PL intensity versus sample concentration.





References :

1. Mi-H. Yang, P. Thirupathi, and K.-H. Lee, Org. Lett., 2011, **13,** 5028. (b) D.En, Y.Guo, B.-T. Chen, B.Dong and M.-J. Peng, *RSC Adv*., 2014, **4**, 248; (c) L. N. Neupane, J. M.Kim, C. R.Lohani and K.-H. Lee, *J. Mater. Chem.,* 2012, **22**, 4003.

2. S. Kaur, V. Bhalla, V.Vij, M. Kumar, *J. Mater. Chem. C*, 2014, **2**, 3936.