

## SUPPLEMENTARY INFORMATION

### **Synthesis and application of a new class of *D-π-A* type charge transfer probe containing imidazole – naphthalene units for detection of F<sup>-</sup> and CO<sub>2</sub>**

Ramesh C. Gupta, Rashid Ali, Syed S. Razi, Priyanka Srivastava, Sushil K. Dwivedi and

Arvind Misra\*

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi – 221 005 UP  
INDIA

[arvindmisra2003@yahoo.com](mailto:arvindmisra2003@yahoo.com); [amisra@bhu.ac.in](mailto:amisra@bhu.ac.in)

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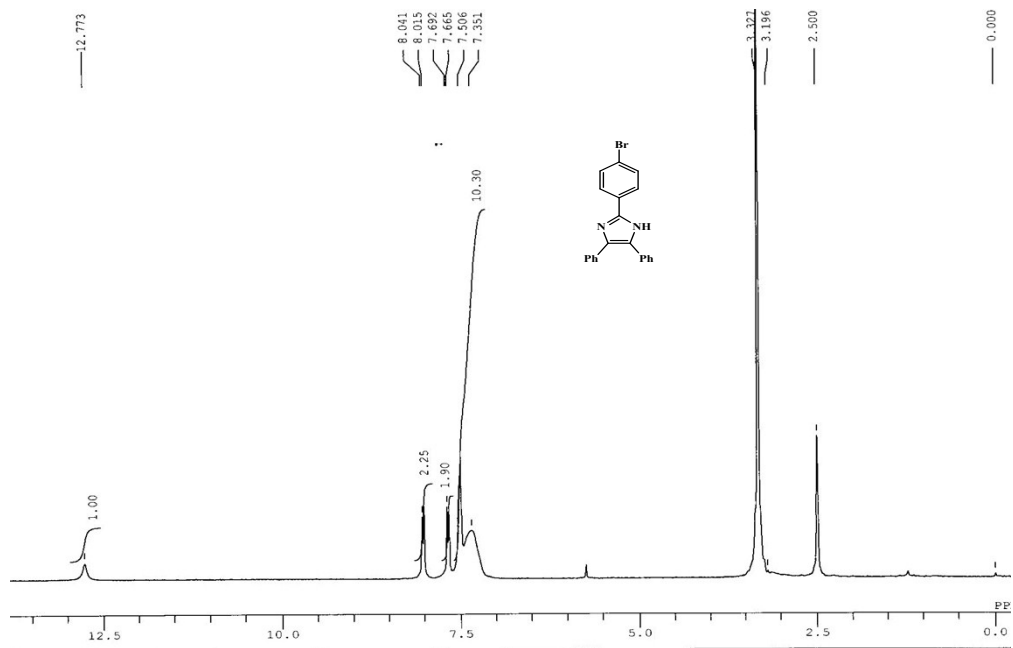
**Table-S14:** Photophysical properties of **4**

**Figure S15:** (a) Absorption and (b) Normalised Emission spectra of probe **3** in different solvents.

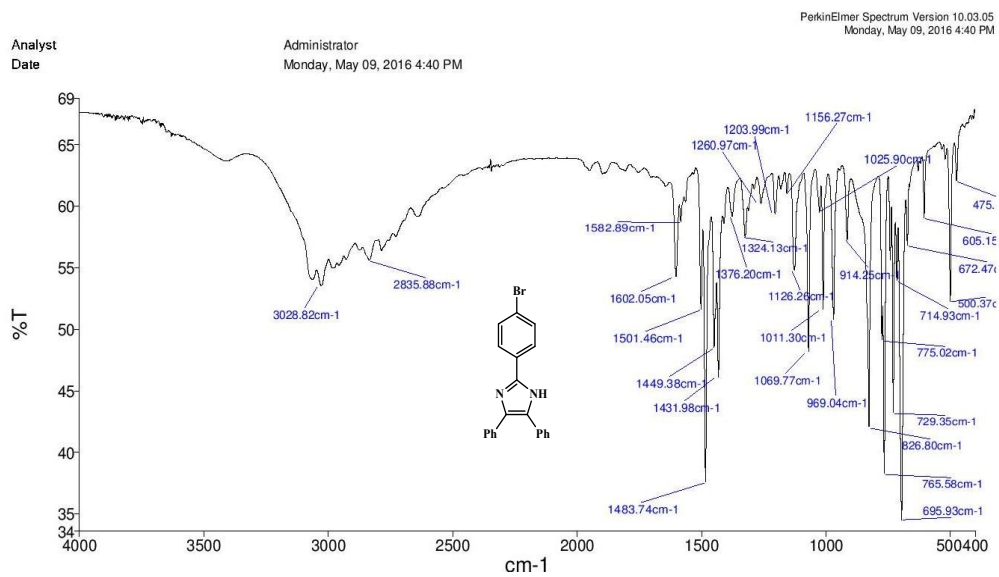
**Figure S16:** (a) Absorption and (b) Normalized Emission spectra of probe **4** in different solvents.

**Figure S17:** (a) Absorption (10 μM) and (b) emission spectra of **3** (10 μM) upon interaction with CN<sup>-</sup>, AcO<sup>-</sup> and F<sup>-</sup> anions (150.0 equiv) in DMSO.

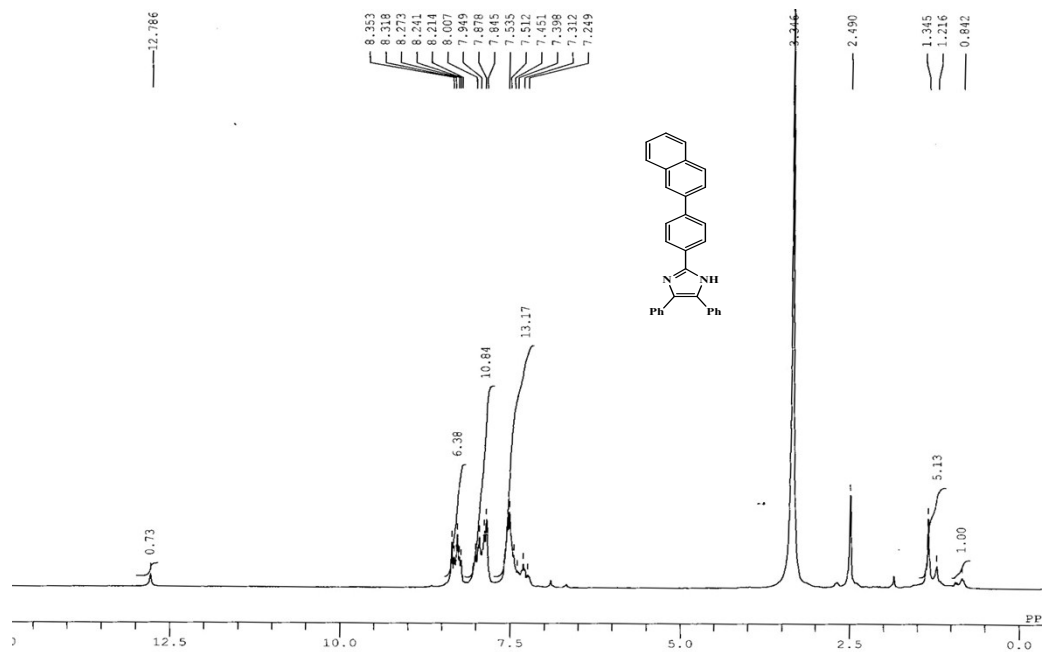
**Figure S18:** Fluorescence intensity change of **3**+F<sup>-</sup> system (10 μM, λ<sub>ex</sub> = 340 nm) upon bubbling with different concentration of CO<sub>2</sub> gas.



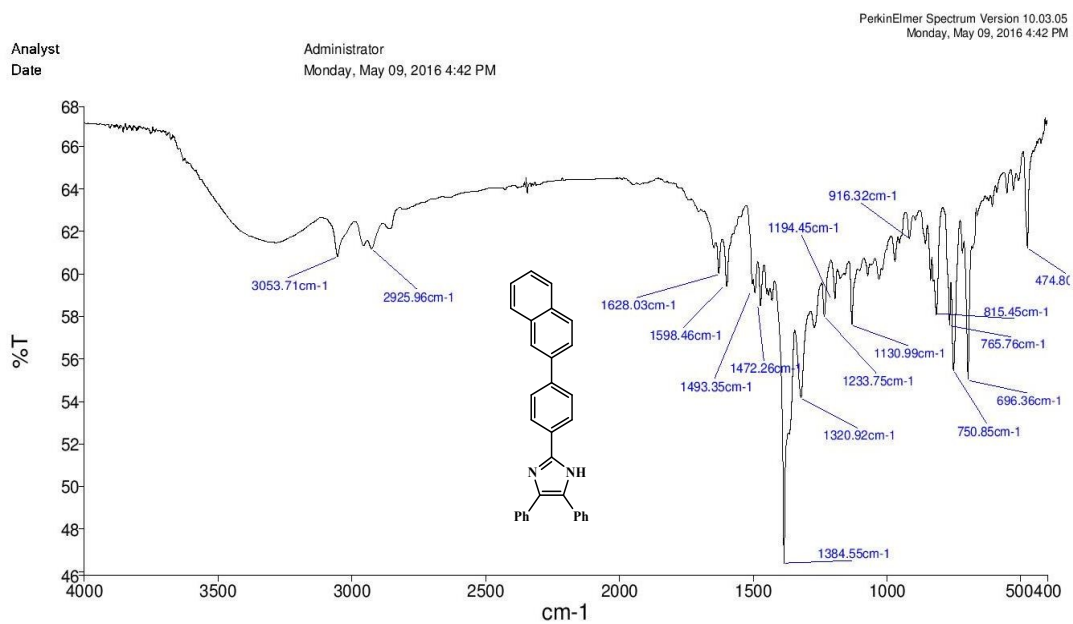
**Figure S1:** <sup>1</sup>H NMR spectrum of 1 in DMSO-*d*<sub>6</sub>.



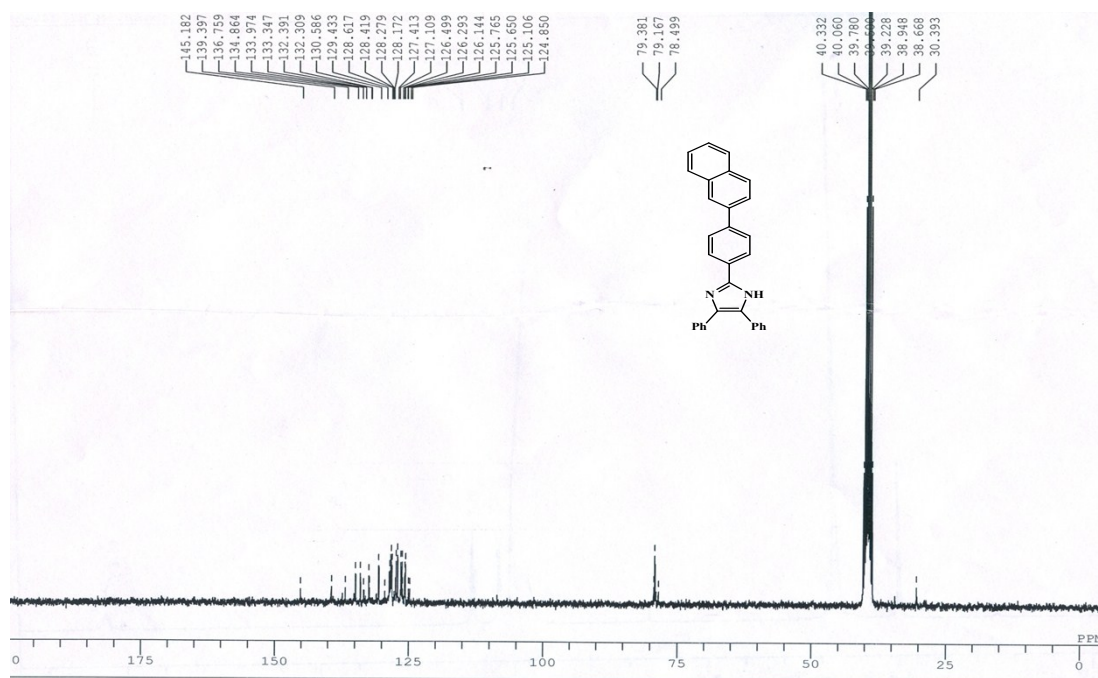
**Figure S2:** FT-IR spectrum of 1.



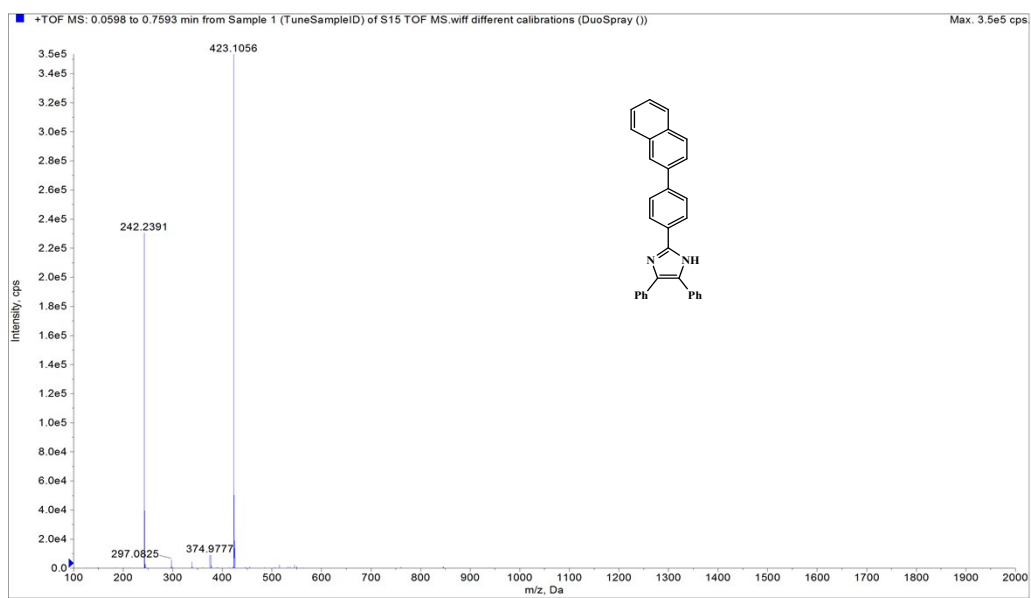
**Figure S3:** <sup>1</sup>H NMR spectrum of 3 in DMSO-*d*<sub>6</sub>.



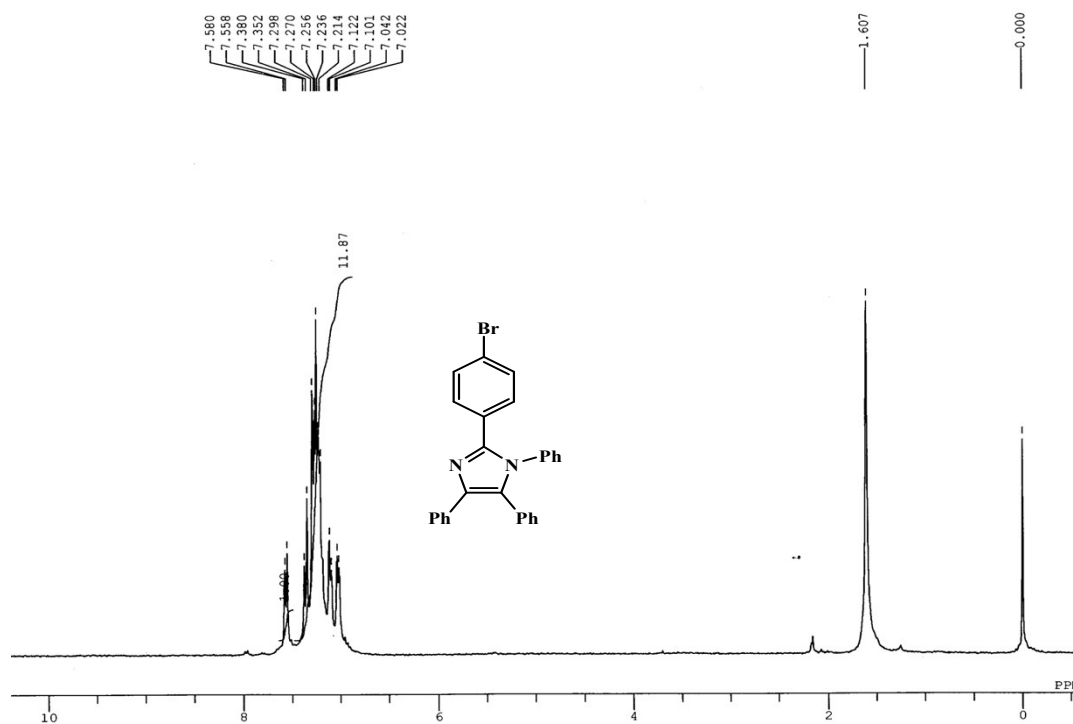
**Figure S4:** FT-IR spectrum of 3.



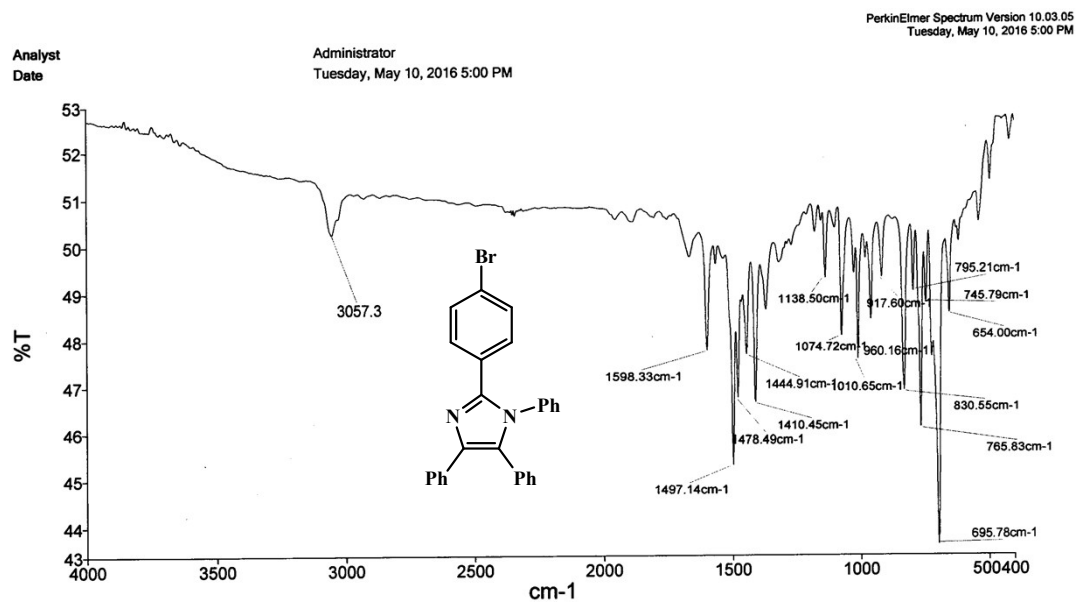
**Figure S5:**  $^{13}\text{C}$  NMR spectrum of **3** in  $\text{DMSO-}d_6$ .



**Figure S6:** ESI-MS spectrum of **3**.



**Figure S7:** <sup>1</sup>H NMR spectrum of **2** in DMSO-*d*<sub>6</sub>.



**Figure S8:** FT-IR spectrum of **2**.

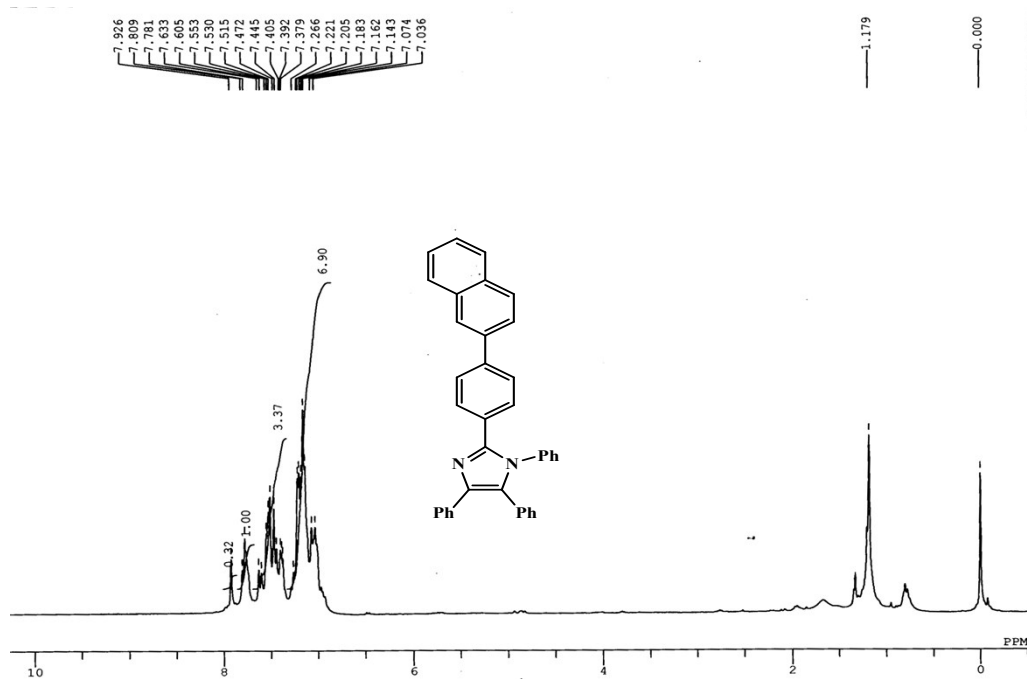


Figure S9: <sup>1</sup>H NMR spectrum of **4** in DMSO-*d*<sub>6</sub>.

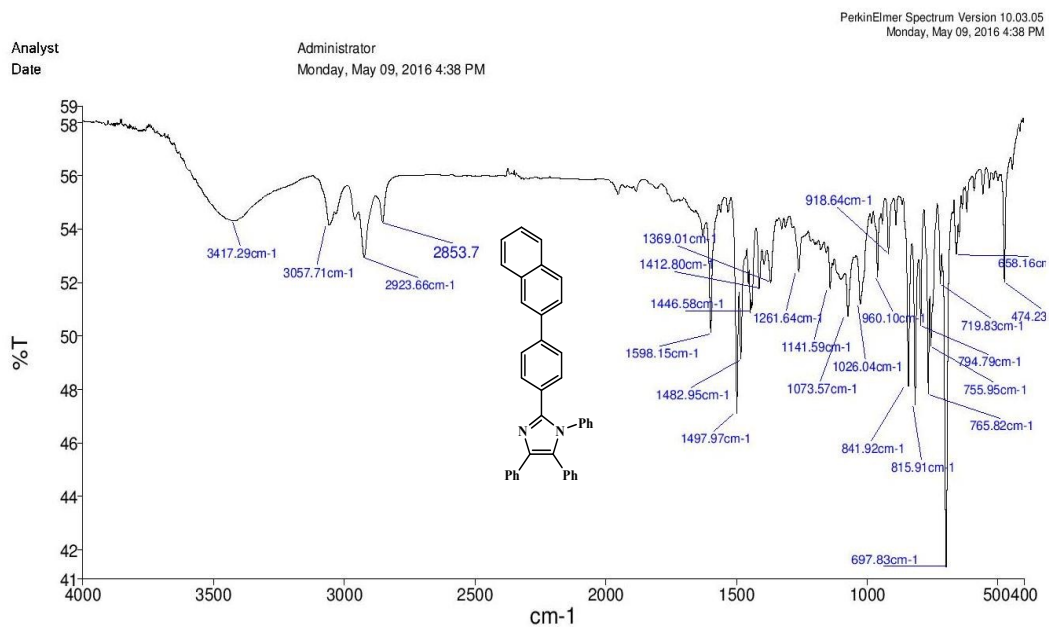


Figure S10: FT-IR spectrum of **4**.

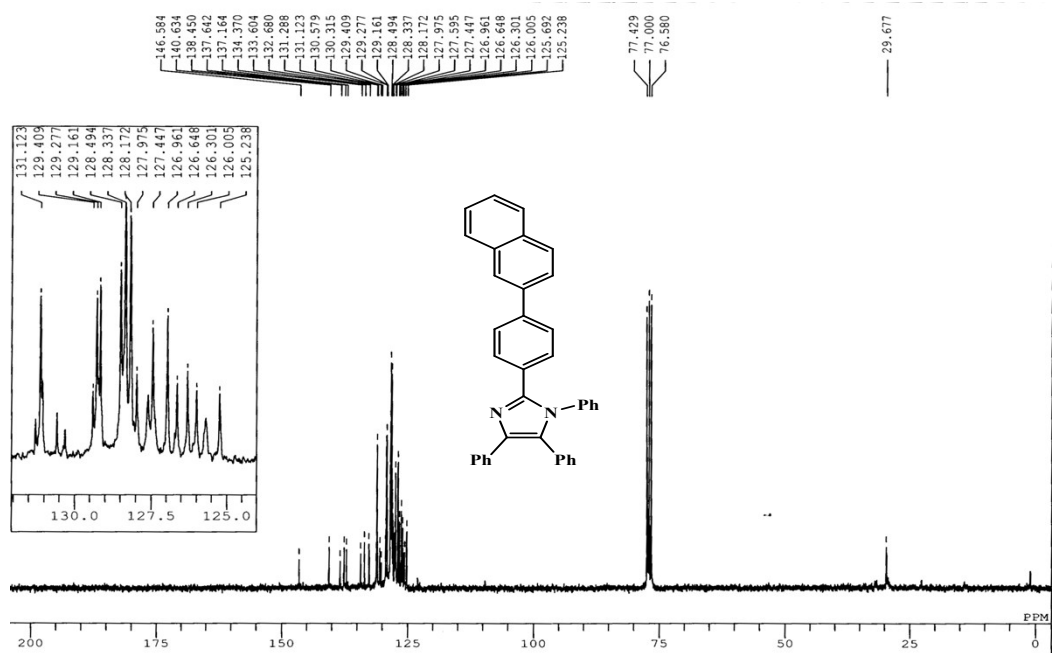


Figure S11: <sup>13</sup>C NMR spectrum of 4 in DMSO-*d*<sub>6</sub>.

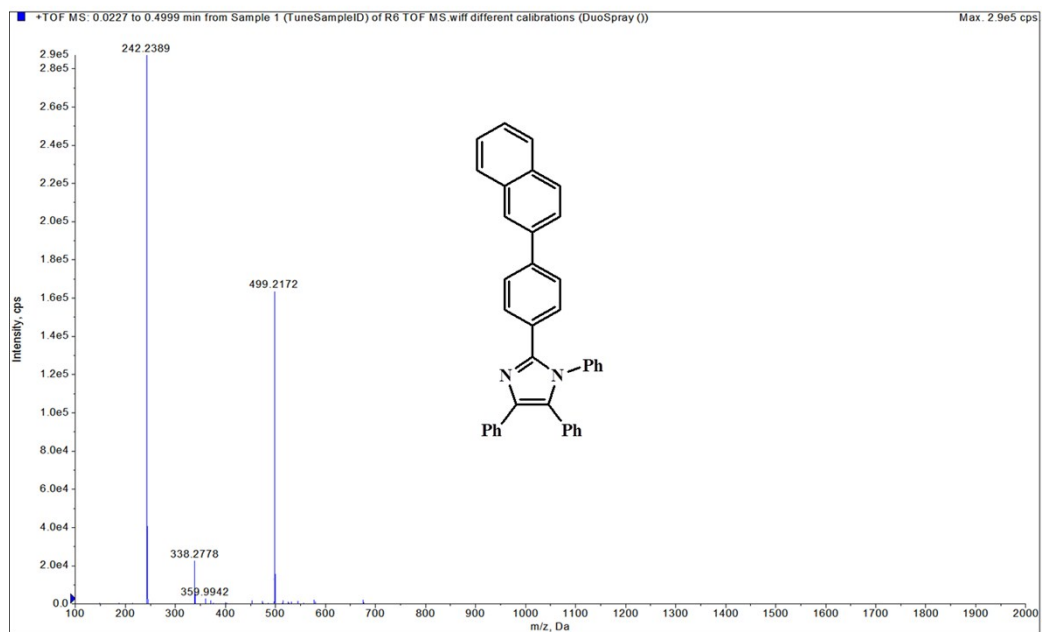


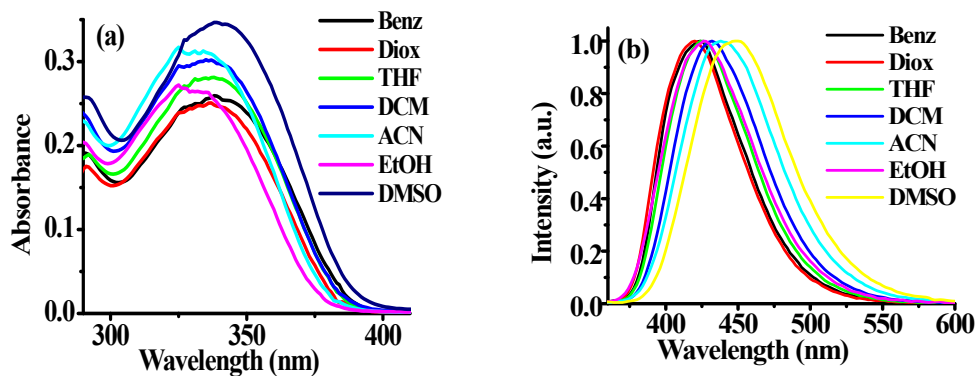
Figure S12: ESI-MS spectrum of 4.

**Table-S13: Photophysical properties of 3**

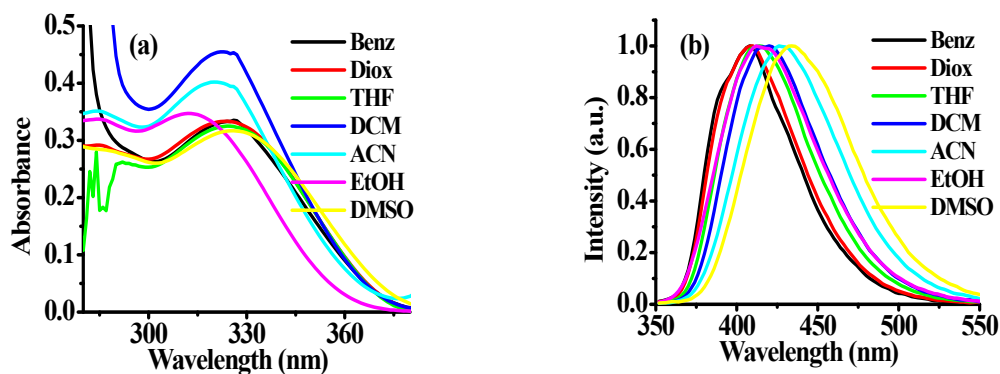
S.N	Entry	$\lambda_{\max}$ (nm)	Molar absorptivity $\epsilon = \text{M}^{-1}\text{cm}^{-1}$	$\lambda_{\text{em}}$ (nm)	Stoke's Shift $\Delta\bar{\nu}$ (nm)	Quantum yield $\Phi$
1.	Benzene	338	$2.59 \times 10^4$	423	85	0.644
2.	Dioxane	337	$2.50 \times 10^4$	420	83	0.650
3.	THF	338	$2.81 \times 10^4$	426	88	0.610
4.	DCM	335	$3.02 \times 10^4$	431	96	0.633
5.	ACN	325	$3.17 \times 10^4$	438	113	0.557
6.	EtOH	325	$2.72 \times 10^4$	426	101	0.604
7.	DMSO	340	$3.46 \times 10^4$	448	108	0.585

**Table-S14: Photophysical properties of 4**

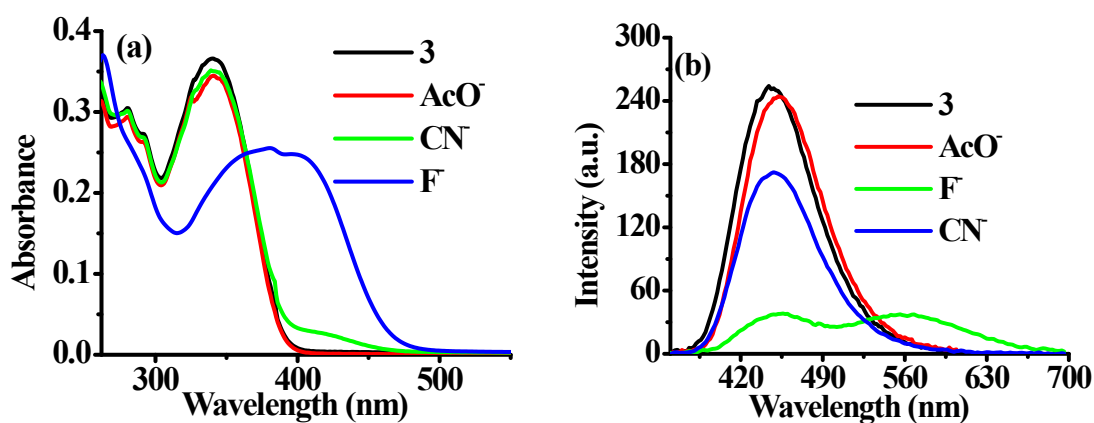
S.N	Entry	$\lambda_{\max}$ (nm)	Molar absorptivity $\epsilon = \text{M}^{-1}\text{cm}^{-1}$	$\lambda_{\text{em}}$ (nm)	Stoke's Shift $\Delta\bar{\nu}$ (nm)	Quantum yield $\Phi$
1.	Benzene	323	$3.33 \times 10^4$	408	85	0.573
2.	Dioxane	323	$3.33 \times 10^4$	410	87	0.714
3.	THF	324	$3.23 \times 10^4$	413	89	0.726
4.	DCM	322	$4.55 \times 10^4$	420	98	0.503
5.	ACN	321	$4.02 \times 10^4$	426	105	0.547
6.	EtOH	313	$3.46 \times 10^4$	411	98	0.686
7.	DMSO	326	$3.16 \times 10^4$	433	107	0.768

**Figure S15:** (a) Absorption and (b) Normalised Emission spectra of probe 3 in different solvents.

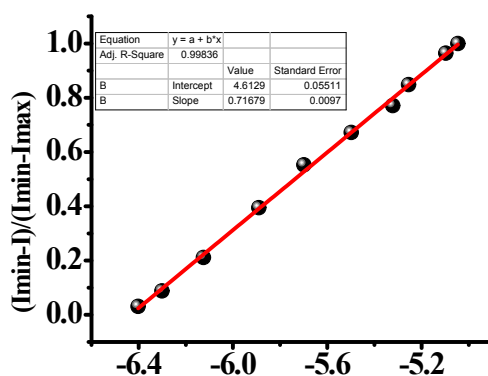




**Figure S16:** (a) Absorption and (b) Normalized Emission spectra of probe **4** in different solvents.



**Figure S17:** (a) Absorption (10  $\mu\text{M}$ ) and (b) emission spectra of **3** (10  $\mu\text{M}$ ) upon interaction with  $\text{CN}^-$ ,  $\text{AcO}^-$  and  $\text{F}^-$  anions (150.0 equiv) in DMSO.



**Figure S18:** Fluorescence intensity change  $\log [\text{CO}_2]$  of  $3+\text{F}^-$  system (10  $\mu\text{M}$ ,  $\lambda_{\text{ex}} = 340$  nm) upon bubbling with different concentration of  $\text{CO}_2$  gas.

**Calculation of limit of detection of CO<sub>2</sub>** : The detection limit of **3+F<sup>-</sup>** system for CO<sub>2</sub> was estimated from plot of normalized fluorescence change of **3+F<sup>-</sup>** system with CO<sub>2</sub> verses Log [CO<sub>2</sub>] using equation (4)<sup>1,2</sup> and found to be 3.67 x 10<sup>-7</sup> M.

$$\mathbf{10}^{-[\text{Slope} / \text{Intercept}]} \dots\dots\dots(4)$$

1. Shortreed, M.; Kopelman, R.; Kuhn, M.; Hoyland, B. *Anal. Chem.* **1996**, 68, 1414-1418.
2. Kim, M. H.; Jang, H. H.; Yi, S.; Chang S.-K.; Han, M. S. *Chem. Commun.* **2009**, 4838-4840.