Supporting Information for

Imidazole-2-thiohydantoin Conjugates for Trace Water Detection in Organic Solvents and Visual Colour Recognition for Real Time Monitoring

Bhagwat Giri Goswami[a,b] , Amutha Selvaganesan[a], Kommineni Kalyani[c], K.K.R. Datta [a*] Venkatramaiah Nutalapati [a,d*]

[a]*Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, SRM Nagar, Kattankulathur, 603203, India.*

[b]*Department of Chemistry, SSSTSRGDC Nainidanda Pauri Garhwal 246277, Uttarakhand, India*

[c]*Department of Chemistry, RVR&JC College of Engineering, Guntur, Andhra Pradesh 522019, India*

[d]*Centre for Interdisciplinary Research (CIDR), SRM University-AP, Amaravati, Andhra Pradesh 522 240, India*

To whom correspondence should be addressed
Dr. Venkatramaiah Nutalapati, E-mail: nvenkat83@gmail.com/venkatramaiah.n@srmap.edu.in

Table of Contents

1. Structural Characterization

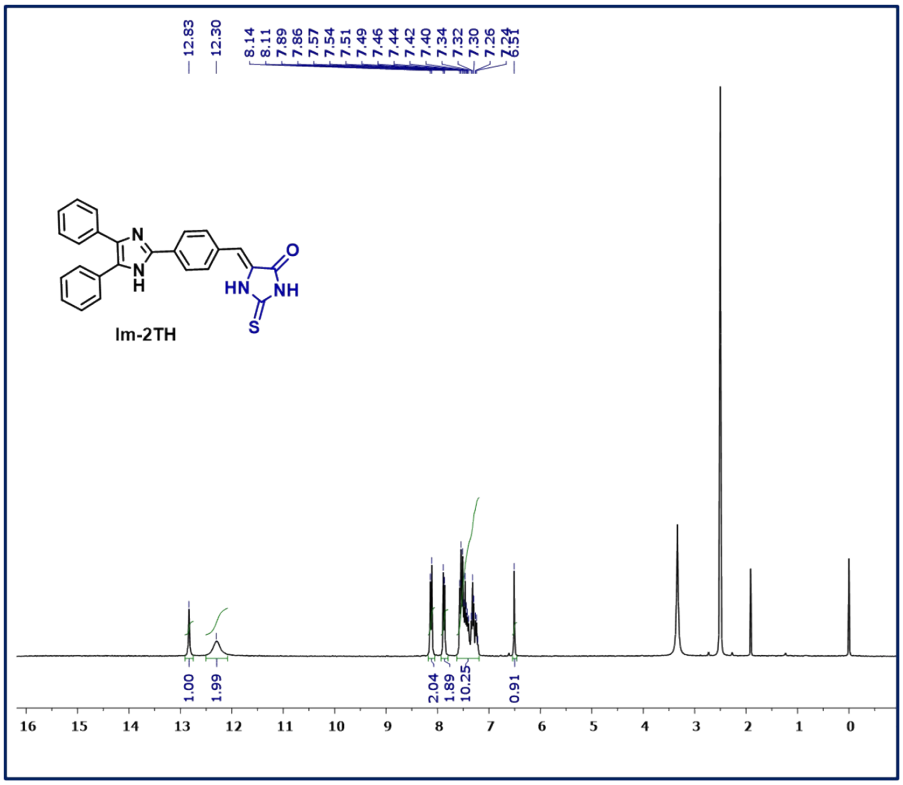


Fig. S1 ^{1}H NMR (500MHz) of **Im-2TH** in DMSO-d_6.

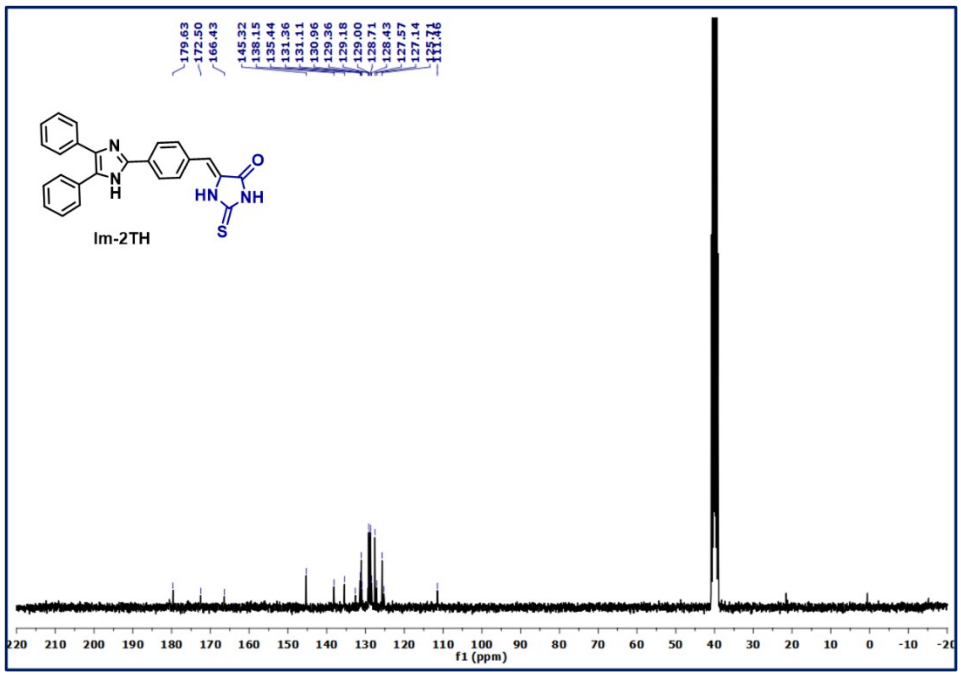


Fig. S2 ^{13}C NMR (125 MHz) of **Im-2TH** in DMSO-d_6.

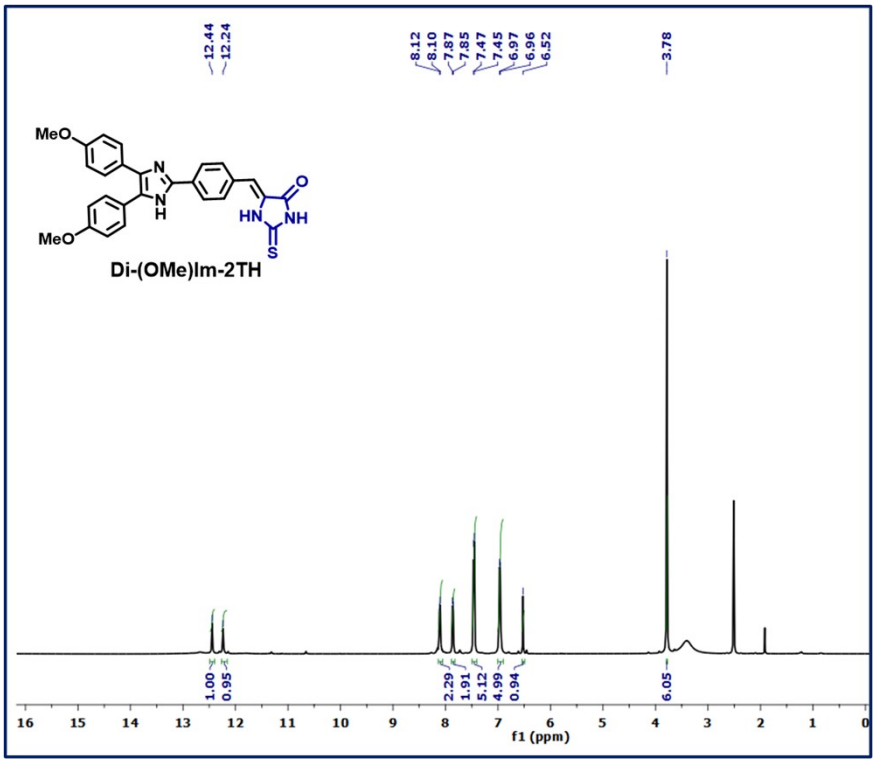


Fig. S3 ^{1}H NMR (500MHz) of **Di-OMeIm-2TH** in DMSO-$d_{6.}$

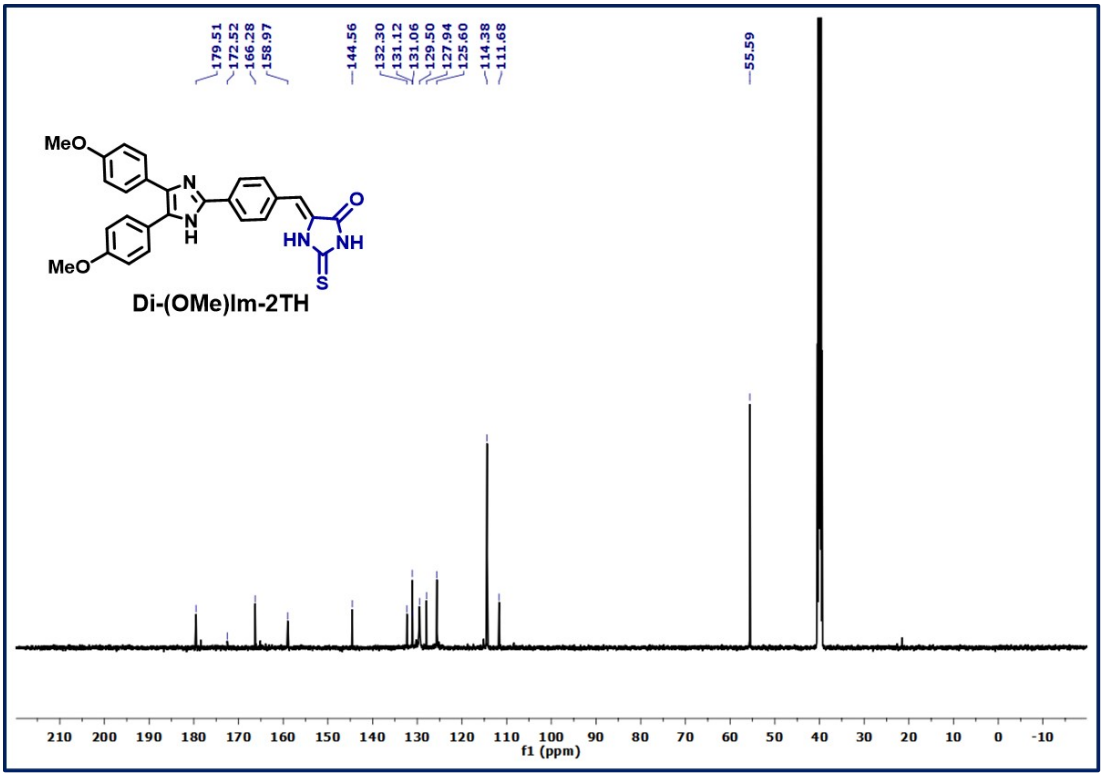


Fig. S4 ^{13}C NMR (125 MHz) of **Di-OMeIm-2TH** in DMSO-$d_{6.}$

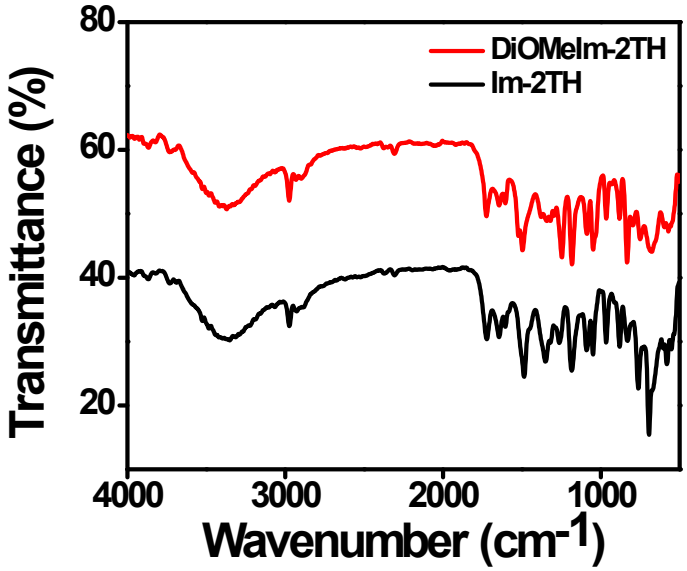


Fig. S5 FTIR spectra of **Im-2TH** and **DiOMeIm-2TH.**

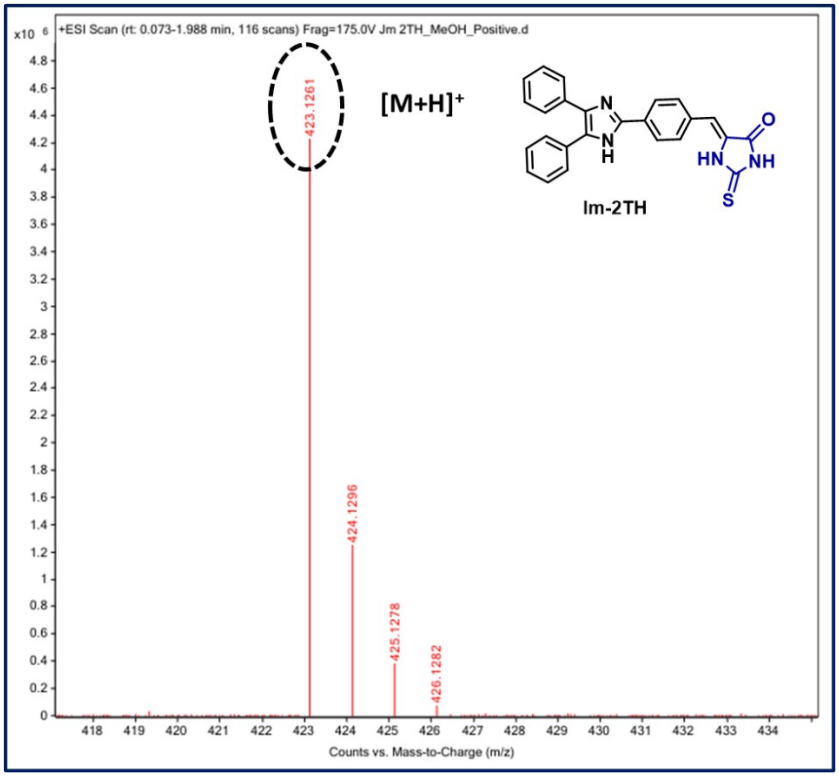


Fig. S6 Mass spectrum of **Im-2TH.**

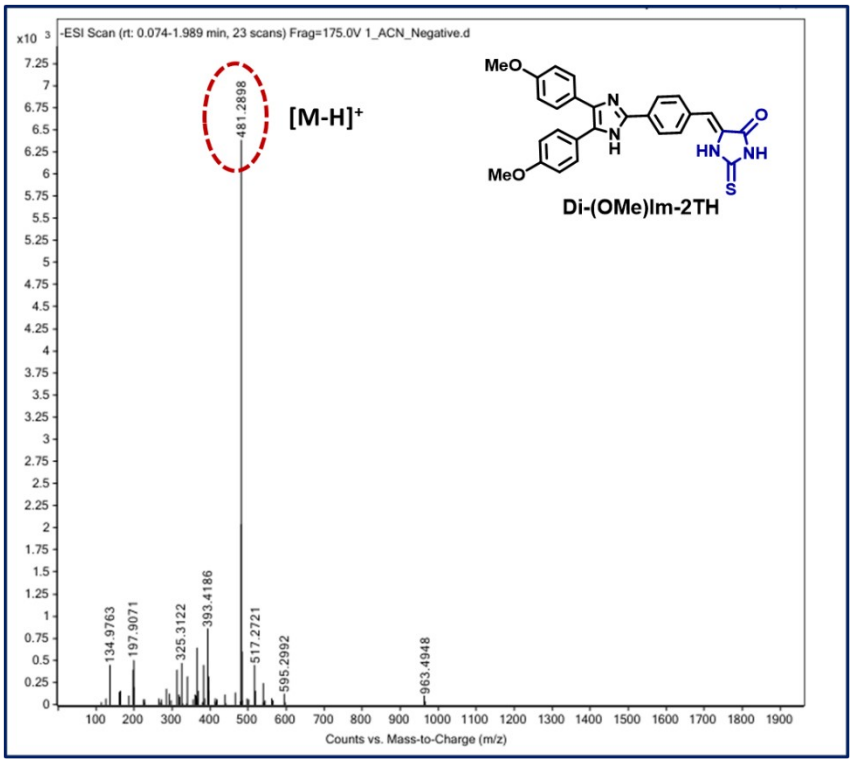


Fig. S7 Mass spectrum of **Di-OMeIm-2TH.**

2. Thermal Properties

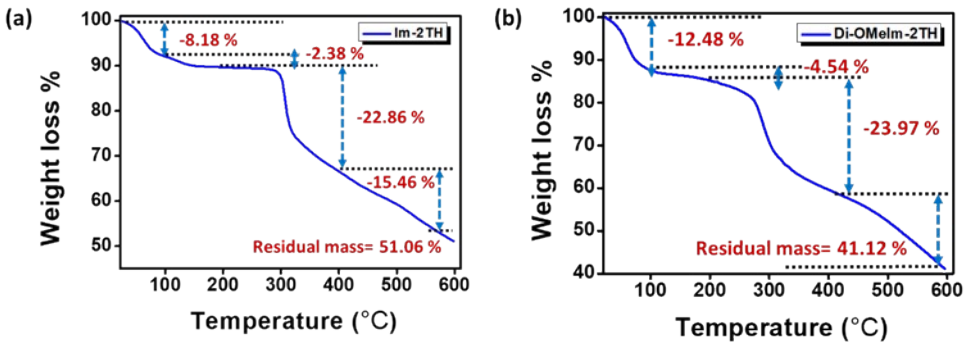


Fig S8. TGA profile of (a) **Im-2TH** and **Di-OMeIm-2TH.**

3. Photophysical Properties

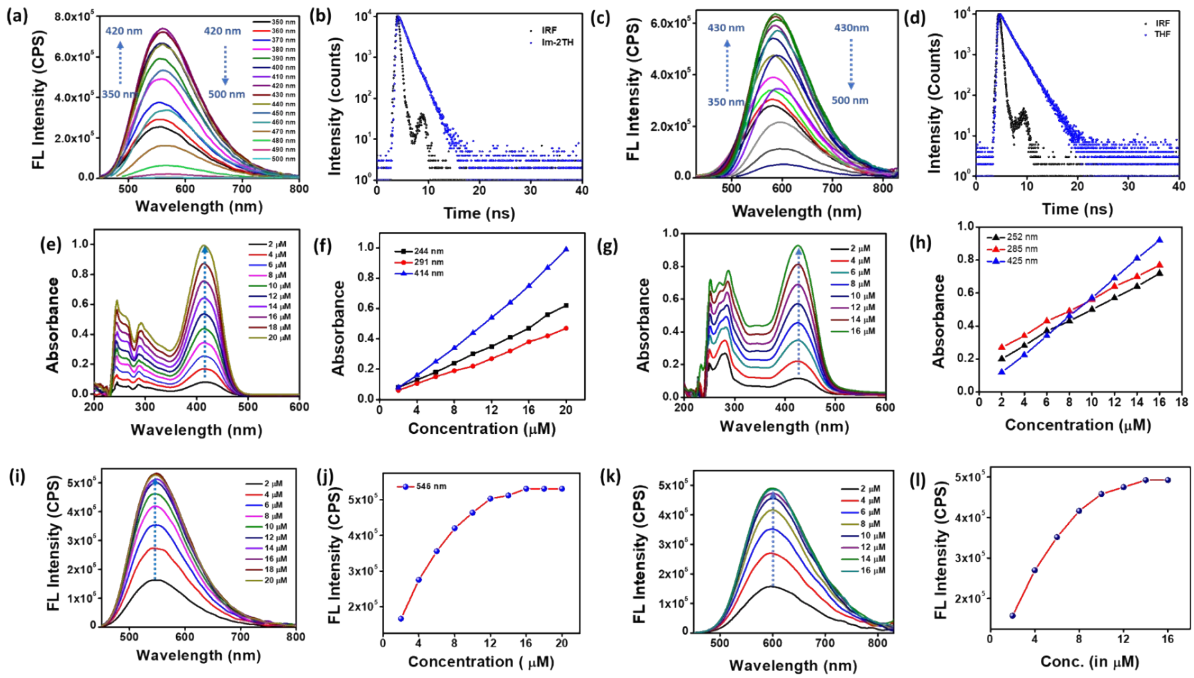


Fig. S9 Excitation dependent emission spectra and fluorescence lifetime decay of **Im-2TH** (a, b) and **Di-OMeIm-2TH** in THF **(c, d)**. Concentration-dependent absorption spectra of **Im-2TH** (10 μM) in THF and variation in absorption intensity at 244, 291 and 414 nm **(e, f)**. Concentration-dependent emission spectra of **Im-2TH** (10 μM) in THF and variation in emission intensity at 550 nm **(g, h).** Concentration-dependent absorption spectra of **Di-OMeIm-2TH** (10 μM) in THF and variation in absorption intensity at 252, 285 and 425 nm **(i, j).** Concentration-dependent emission spectra of **Di-OMeIm-2TH** (10 μM) in THF and variation in emission intensity at 585 nm (k, l).

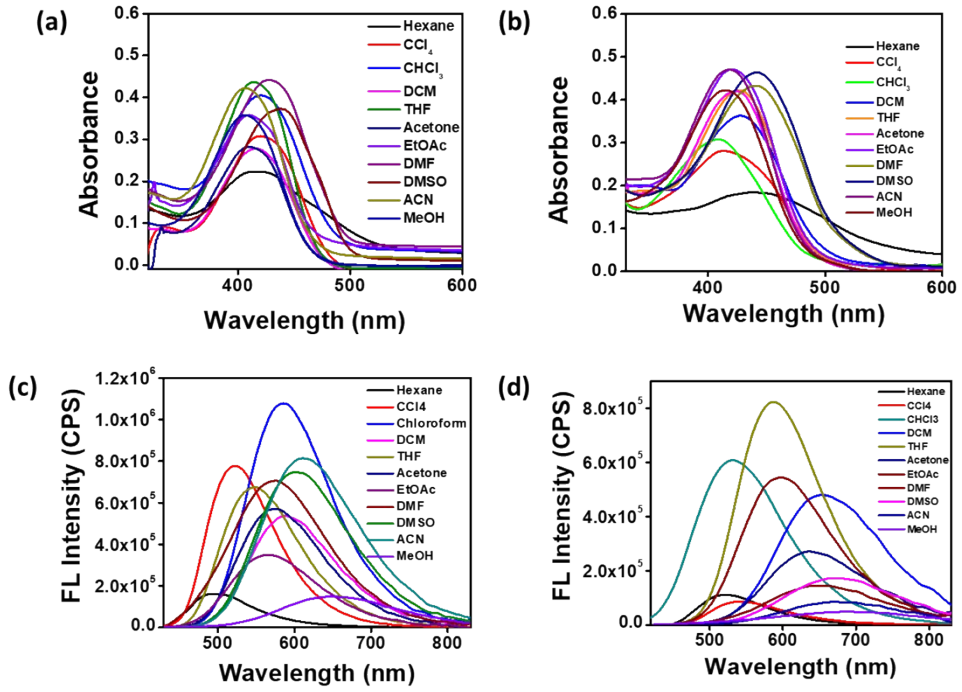


Fig. S10 Absorption spectra **(a, b) and** emission spectra **(c, d)** of **Im-2TH and DiOMeIm-2TH** in different solvents.

4. Lippert Mataga Plot

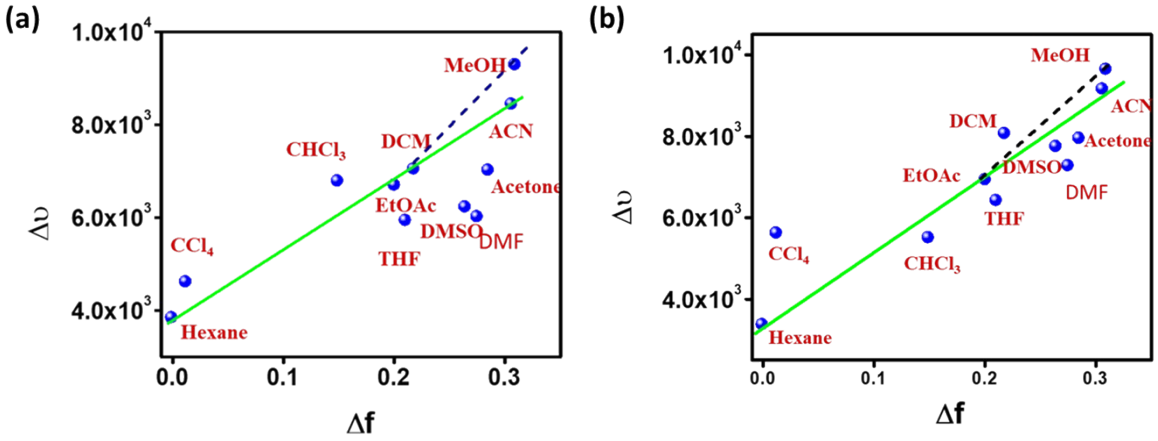
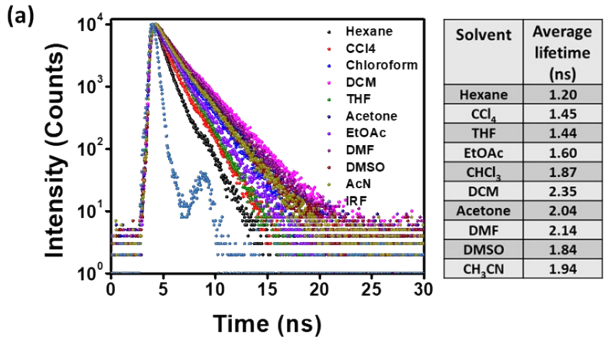
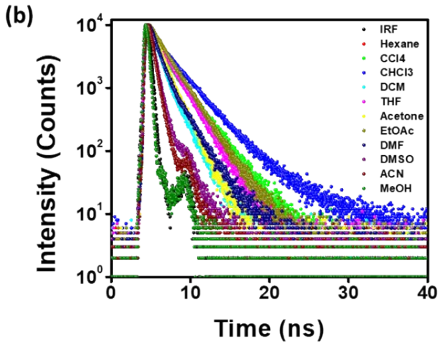


Fig. S11 Lippert-Matanga plot of **Im-2TH (a) and Di-OMeIm-2TH (b)** in various solvent with different polarities.

5. Fluorescence lifetime decay profile in different solvents



Solvent	Average lifetime (ns)
Hexane	1.20
CCl_4	1.45
THF	1.44
EtOAc	1.60
$CHCl_3$	1.87
DCM	2.35
Acetone	2.04
DMF	2.14
DMSO	1.84
CH_3CN	1.94



Solvent	Average lifetime
Hexane	2.20
CCl_4	2.56
$CHCl_3$	4.21
DCM	1.59
THF	2.02
Acetone	1.56
EtOAc	2.18
DMF	1.87
DMSO	1.34
CH_3CN	1.09

Fig. S12 Fluorescence lifetime decay of **Im-2TH (a)** and **DiOMeIm-2TH (b)** in different solvents.

6. Role of Viscosity

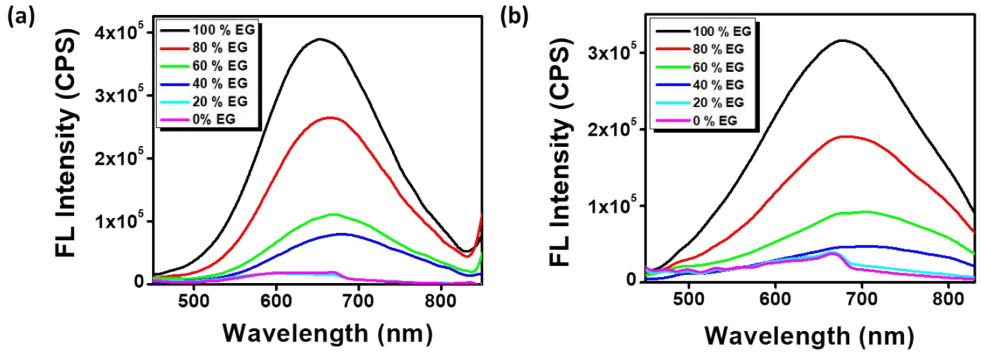
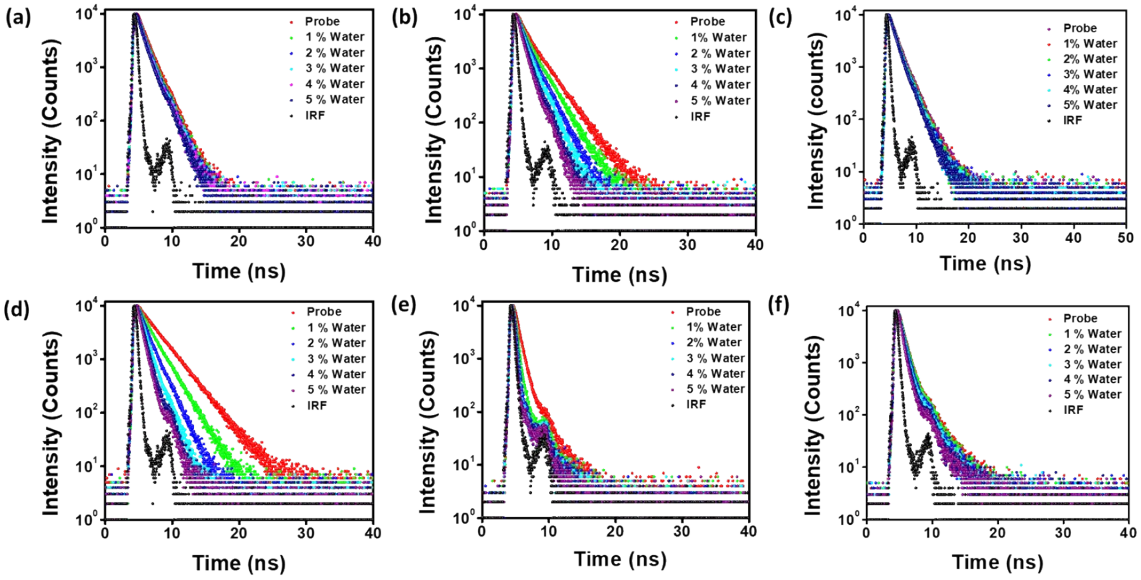


Fig. S13 Change in the fluorescence spectra of **Im-2TH (a) and Di-OMeIm-2TH** (b) in different viscosity regions.

7. Fluorescence lifetime of probes in different solvent with increasing water fraction



Water fraction (% v/v)	Average lifetime of Im-2TH (in ns)		
	THF	ACN	DMSO
0	1.49	2.35	1.75
1	1.42	1.97	1.73
2	1.43	1.65	1.69
3	1.41	1.44	1.66
4	1.41	1.25	1.63
5	1.35	1.14	1.60

Water fraction (% v/v)	Average lifetime of Di-OMeIm-2TH (in ns)		
	THF	ACN	DMSO
0	2.73	1.35	1.60
1	2.01	1.46	1.52
2	1.54	1.83	1.50
3	1.25	1.87	1.47
4	1.10	1.85	1.46
5	1.05	1.66	1.49

Fig. S14 A plot of fluorescence lifetime changes against varied concentrations of H_2O (0-5 %) in (a) THF (b) ACN and (c) DMSO for of **Im-2TH** (10 μM) and **Di-OMeIm-2TH** (10 μM) with varied concentrations of H_2O (0- 5 %) in (d) THF (e) ACN & (f) DMSO.

8. LOD calculations on **Im-2TH** and **Di-OMeIm-2TH** in different solvents

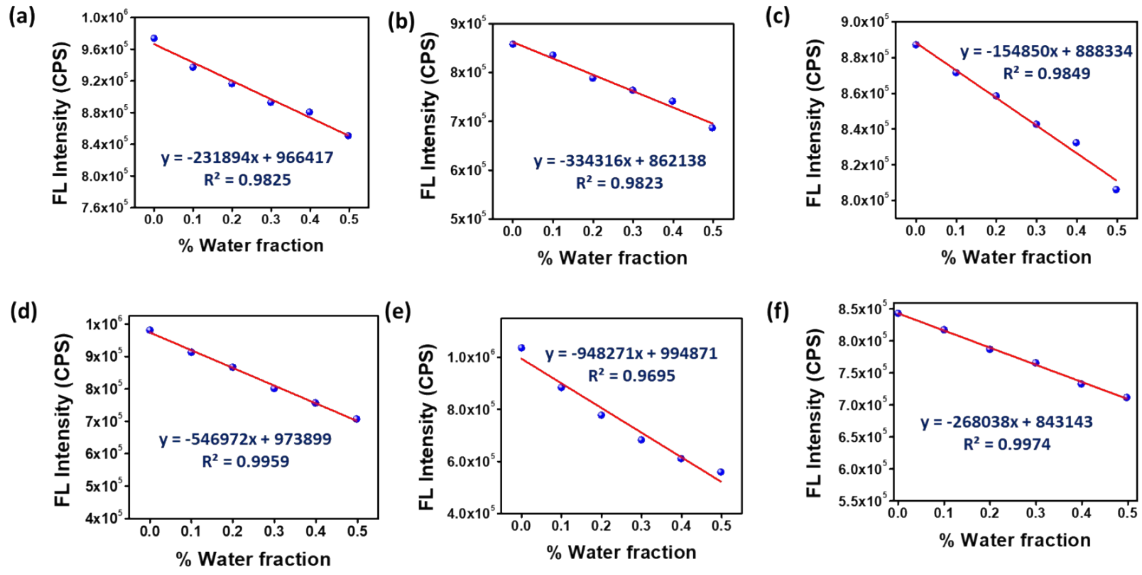
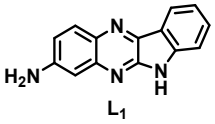
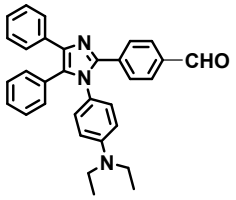
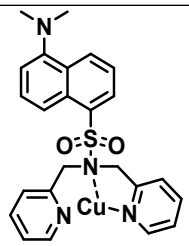
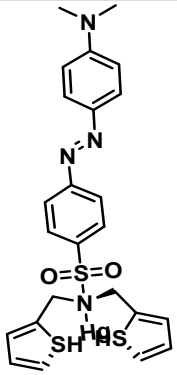
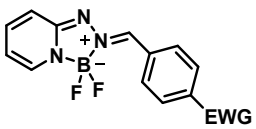
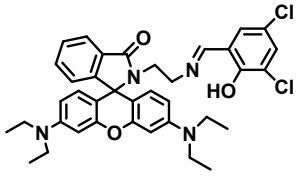
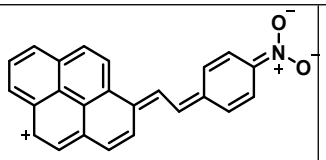
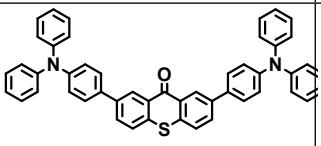
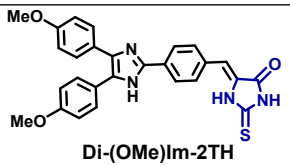


Fig. S15 A plot of fluorescence intensity changes against varied concentrations of H_2O (0-0.49 %) in (a) THF (b) ACN and (c) DMSO for of **Im-2TH** (10 μM) and **Di-OMeIm-2TH** (10 μM) with varied concentrations of H_2O (0-0.49 %) in (d) THF (e) ACN & (f) DMSO.

9. Table S1: Details about the reported fluorescent sensor for trace water detection.

Sr. No	Probe	LOD	Solvent used	Sensing mode	Self-Assembly	RGB Analysis	Ref.
1.	 L_1	0.018%, 0.027%, 0.012%, and 0.43%	CH_3CN, THF, DMF, and CH_3OH	*Turn-off*	Yes, but not in a detailed manner.	Yes, in coated surfaces	1
2.		0.03 (wt. %)	THF	*Turn-off*	Yes	No	2
3		0.00302, 0.033, 0.052, and 0.448 (wt. %)	THF, CH_3OH, acetone, and CH_3CN	*Turn-On*	No	No	3
4		0.0041% w/w, 0.0144% w/w and 0.1008% w/w).	THF, acetone and CH_3CN	*Turn-off*	No	No	4
5		0.028%, 0.013%, 0.021%, and 0.045%	THF, CH_3CN, acetone, and DMF	*Turn-off*	No	No	5
6		0.0464 v/v, 0.0298 v/v, and 0.0017 v/v	THF, CH_3CN and MeOH	*Turn-On*	No	No	6

7		**0.007%, 0.033%, and 0.036% (v/v)**	**THF, DMF, and CH3CN**	***Turn-off***	**No**	**No**	**7**
8		**35 ppm, 36 ppm and 60 ppm**	**Dioxane, THF, DMF**	***Turn-off***	**No**	**No**	**8**
9	 Di-(OMe)Im-2TH	**0.060 ppm, 0.034 ppm, and 0.124 ppm**	**THF, ACN, DMSO**	**Turn-off**	**Yes**	**Yes**	**Present work**

10. AIEE Study of Im-2TH

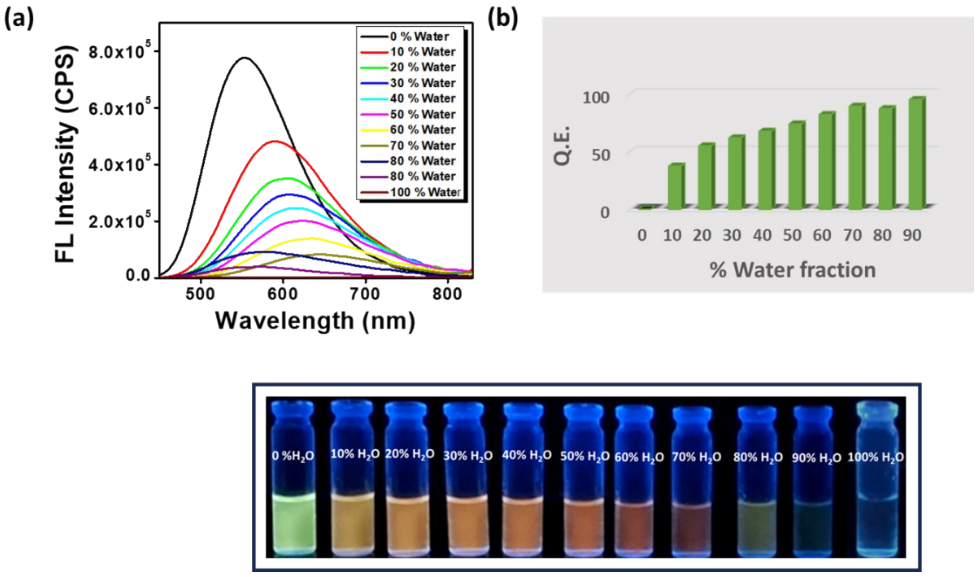


Fig. S16 Variation in emission spectra of **Im-2TH** with at different f_w in THF-Water ratio **(a)**. Quenching efficiency of **Im-2TH** at different water fraction **(b)**. Photograph of **Im-2TH** at different water fraction under the illumination of 365 nm light **(c)**.

11. AIEE Study of Di-OMeIm-2TH

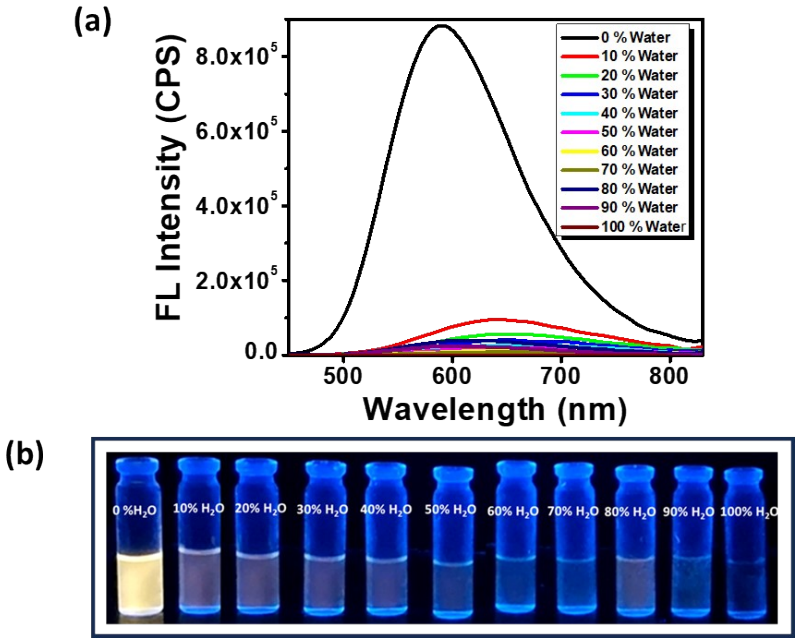


Fig. S17 Variation in emission spectra of **Di-OMeIm-2TH** with at different f_w in THF-Water ratio **(a)**. Photograph of **Di-OMeIm-2TH** at different water fraction under the illumination of 365 nm light **(b)**.

12. HR-SEM Analysis of Im-2TH in ACN & ACN-water

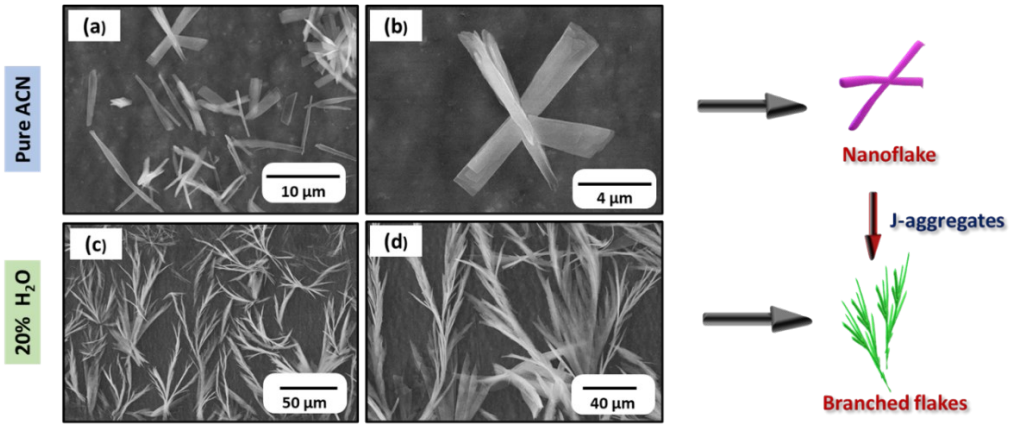


Fig. S18 HR-SEM images of different self-assembled structures formed by **Im-2TH** in different water fractions **(a, b)** f_w=0 %, **(c, d)** f_w=20 %.

13. HR-SEM Analysis of Di-OMeIm-2TH in THF & THF-water

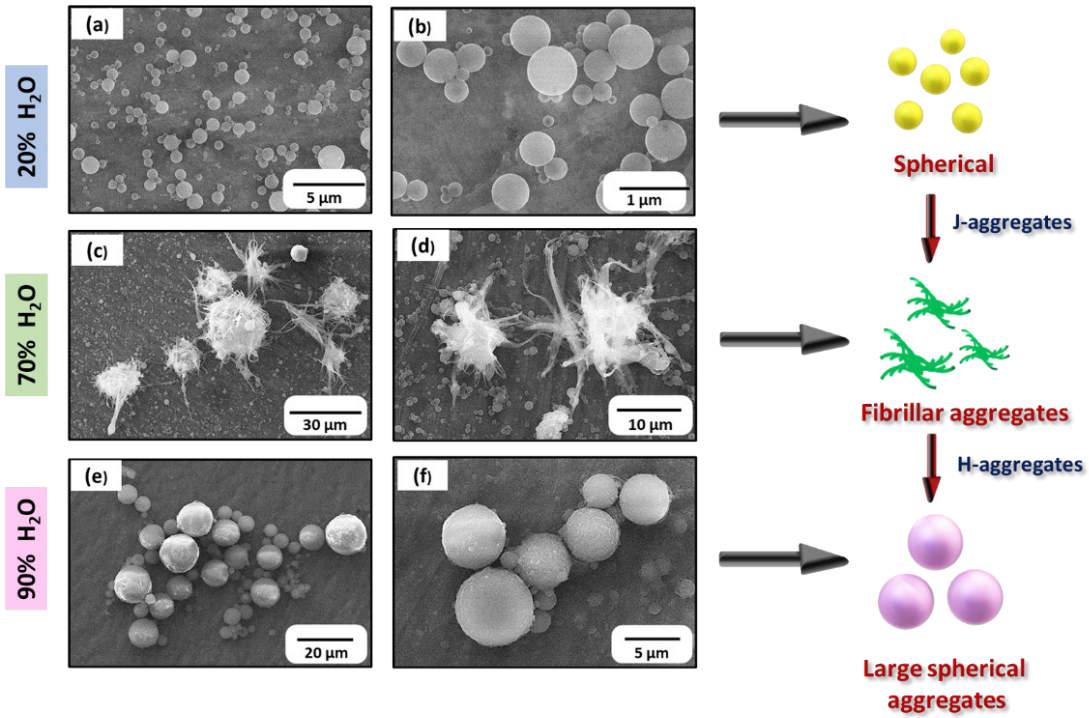


Fig. S19 HR-SEM images of different self-assembled structures formed by **Di-OMeIm-2TH** in different water fractions **(a, b)** f_w=20%, **(c, d)** f_w=70% & **(e, f)** f_w=90%.

14. HR-SEM Analysis of Di-OMeIm-2TH in ACN & ACN-water

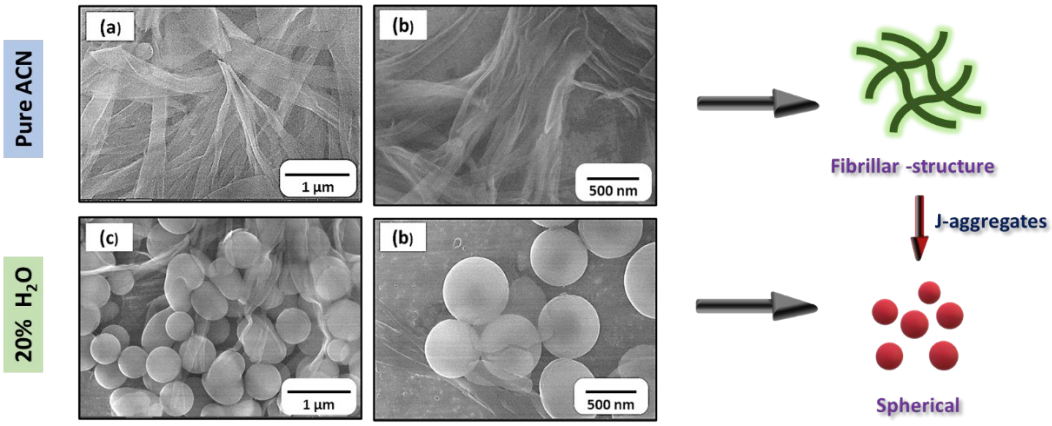


Fig. S20 HR-SEM images of different self-assembled structures formed by **Di-OMeIm-2TH** in different water fractions (a, b) f_w=0 %, (c, d) f_w=20 %.

15. Emission Spectra of Di-OMeIm-2TH with real samples

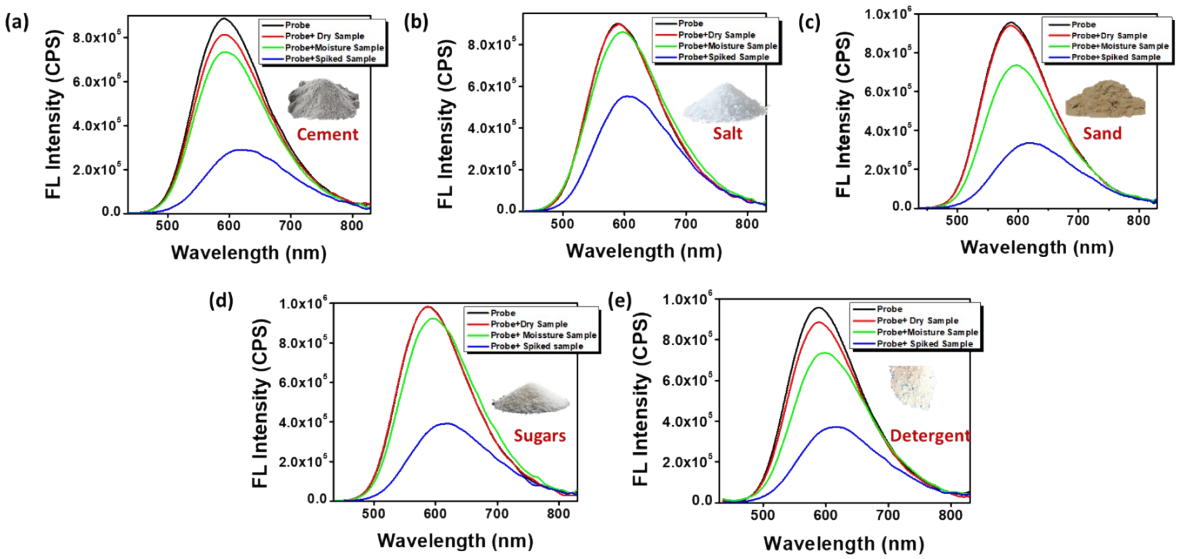


Fig. S21 Variation in the emission intensity of **Di-OMeIm-2TH** (10 µm, THF) in the presence of different commercial products (a) cement (b) Salt (c) sand (d) sugar and (e) detergent.

16. RGB Color array in DMSO

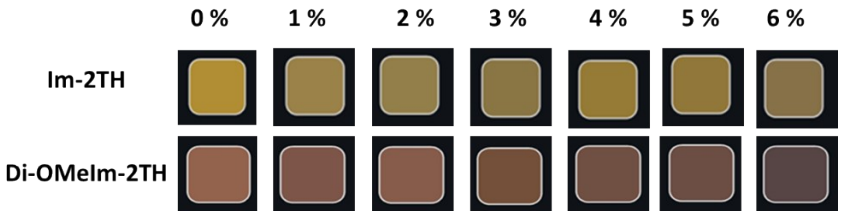


Fig. S22 RGB Color array for **Im-2TH** and **Di-OMeIm-2TH** in DMSO on addition of 0-6% trace water.

17. Im-2TH based Test strips for water sensing

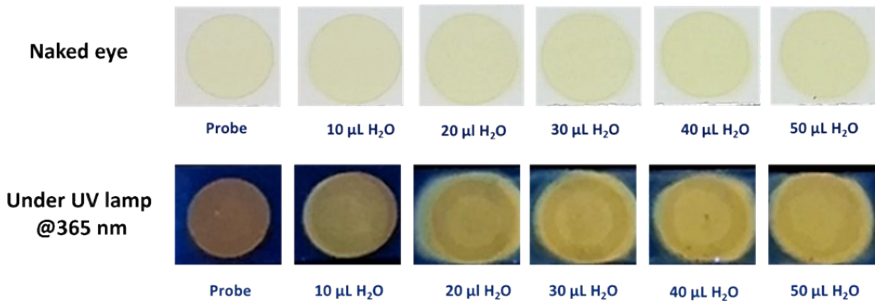


Fig. S23 Im-2TH coated test strips for water detection

18. References

1 M. Basak and G. Das, Amine-incorporated quinoxaline based fluorescent sensor for detection of trace water: Solvent influenced self-assembly, *Spectrochim Acta A Mol Biomol Spectrosc*, 2022, **280**, 121521.

2 M. M. Zafar, R. Yadav, A. Singh, N. Tyagi, A. Samanta and R. K. Mishra, Tetrasubstituted imidazole-based multifunctional fluorophores: trace water detection and lipid droplet (LD) imaging studies, *Chemical Communications*, 2025, **61**, 9091–9094.

3 P. Kumar, R. Kaushik, A. Ghosh and A. D. Jose, Detection of moisture by fluorescent OFF-ON sensor in organic solvents and raw food products, *Anal Chem*, 2016, **88**, 11314–11318.

4 P. Kumar and D. A. Jose, Naked eye detection of moisture in organic solvents and development of alginate polymer beads and test cassettes as a portable kit, *Anal Chim Acta*, 2020, **1136**, 178–186.

5 J. Nootem, C. Sattayanon, S. Namuangruk, P. Rashatasakhon, W. Wattanathana, G. Tumcharern and K. Chansaenpak, Solvatochromic triazaborolopyridinium probes toward ultra-sensitive trace water detection in organic solvents, *Dyes and Pigments*, 2020, **181**, 108554

6 G. Men, G. Zhang, C. Liang, H. Liu, B. Yang, Y. Pan, Z. Wang and S. Jiang, A dual channel optical detector for trace water chemodosimetry and imaging of live cells, *Analyst*, 2013, **138**, 2847–2857.

7 M. Noikham, C. Sriwiphasathit, K. Siriwong and T. Vilaivan, Solvatochromic fluorescent styryl pyrene probes for the quantitative determination of water content in organic solvents, *Dyes and Pigments*, 2023**, 208**, 110847

8 L. Ding, Z. Zhang, X. Li and J. Su, Highly sensitive determination of low-level water content in organic solvents using novel solvatochromic dyes based on thioxanthone, *Chemical Communications*, 2013, **49**, 7319–7321.