Supporting Information

Structural Isomerism Induces pH Dependent AIE Coupled ESIPT: An In-Depth Spectroscopic Exploration With Application In Amine Vapor Sensing

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1. NMR spectra of 3BTHMB in $CDCl_3$

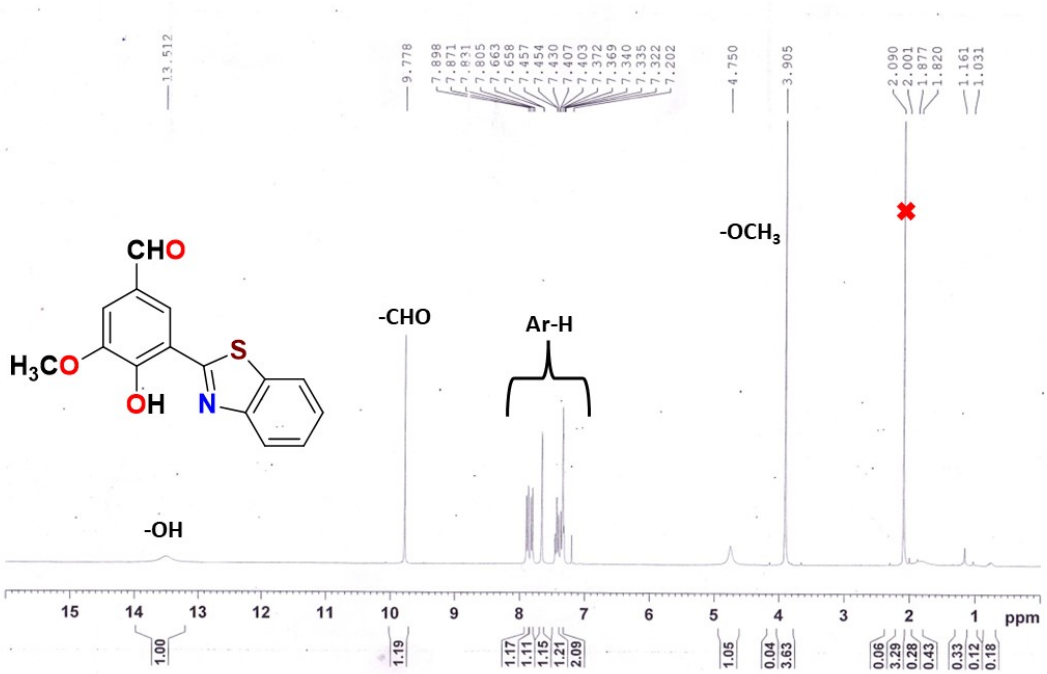


Figure S1: ^{1}H NMR spectrum of **3BTHMB** in $CDCl_3$. (× signifies peak for acetone).

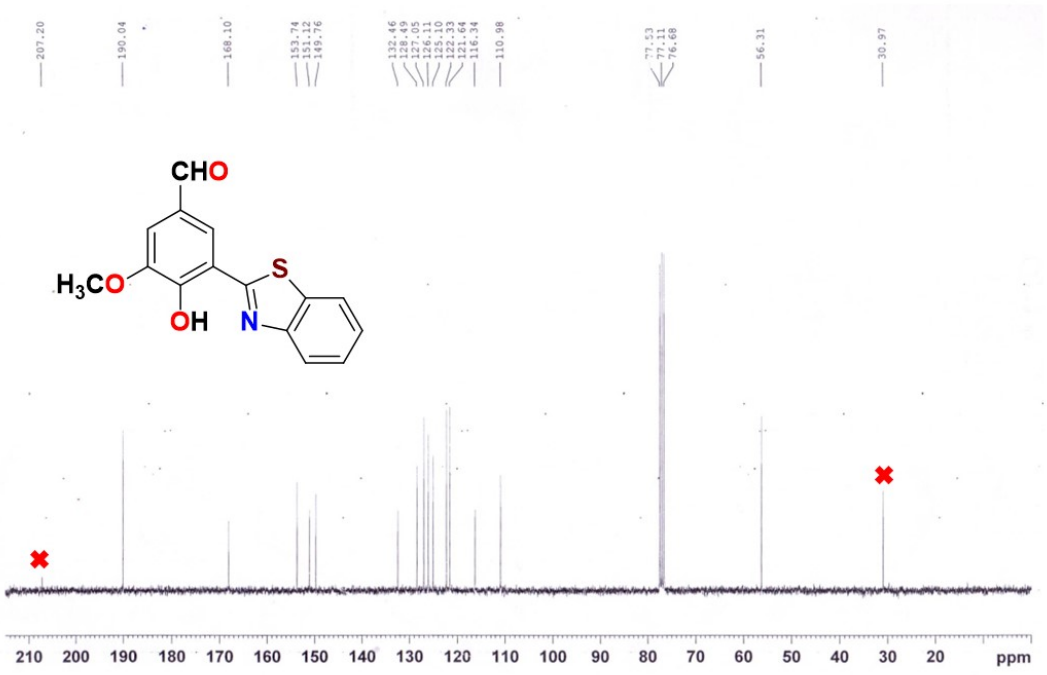


Figure S2: ^{13}C NMR spectrum of **3BTHMB** in $CDCl_3$. (× signifies peak for acetone).

2. ESI-MS of 3BTHMB

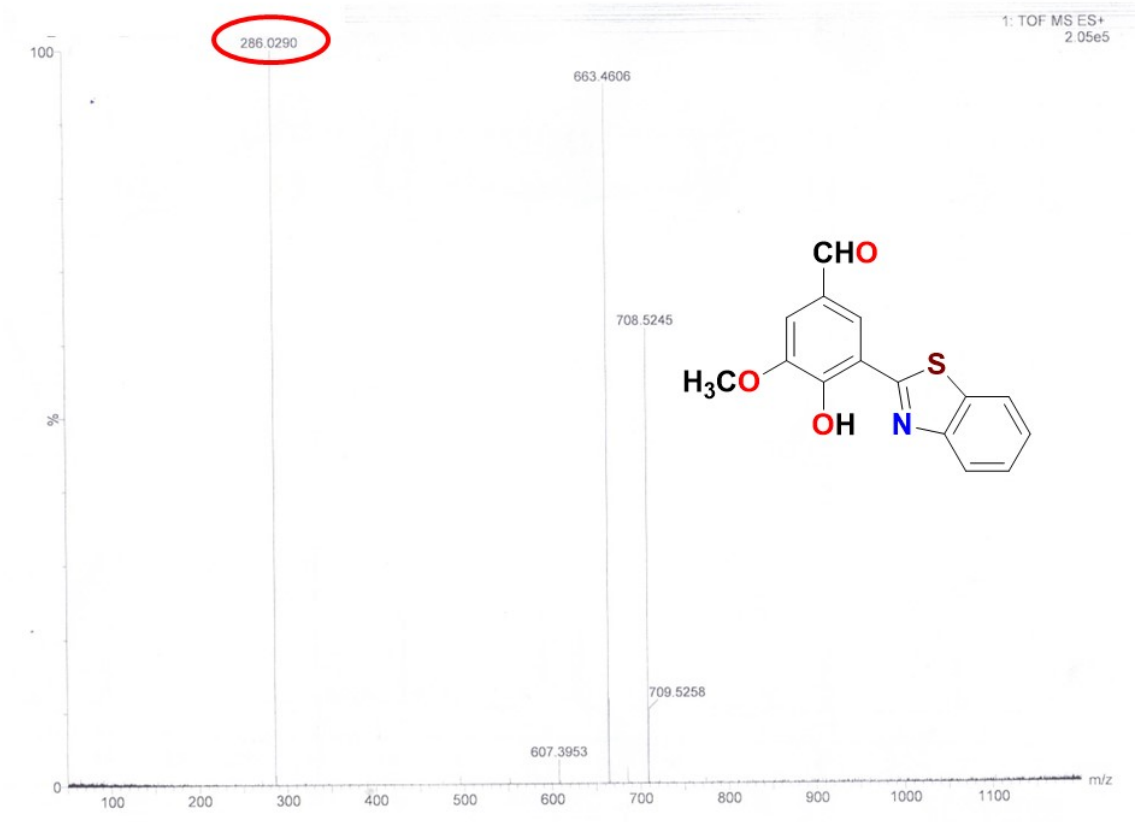


Figure S3: ESI-MS of **3BTHMB**.

3. Table for crystallographic parameters of 3BTHMB.

Table S1: Crystallographic parameters of 3BTHMB

Parameters	**3BTHMB**
Formula	C10 H10 O5
Formula Weight	210.05
Crystal System	monoclinic
Space group	P $2_{1/c}$
a [Å]	7.267(8)
b [Å]	18.18(2)
c [Å]	7.017(8)
α [º]	90
β [º]	94.884(14)
γ[º]	90
V [Å^3]	923.7(18)
h, k, l (max.)	8,20,7
Z	4
D(calc) [g/cm^{-3}]	1.500
F(000)	440
Temperature (K)	296
θ Min-Max [º]	2.2, 23.8
No. of unique data	1396
R(int)	0.068
Observed data [I > 2.0 σ(I)]	675
R1, wR2	0.0583, 0.1321
GOF on F^2	1.140

4. ORTEP diagram of 3BTHMB.

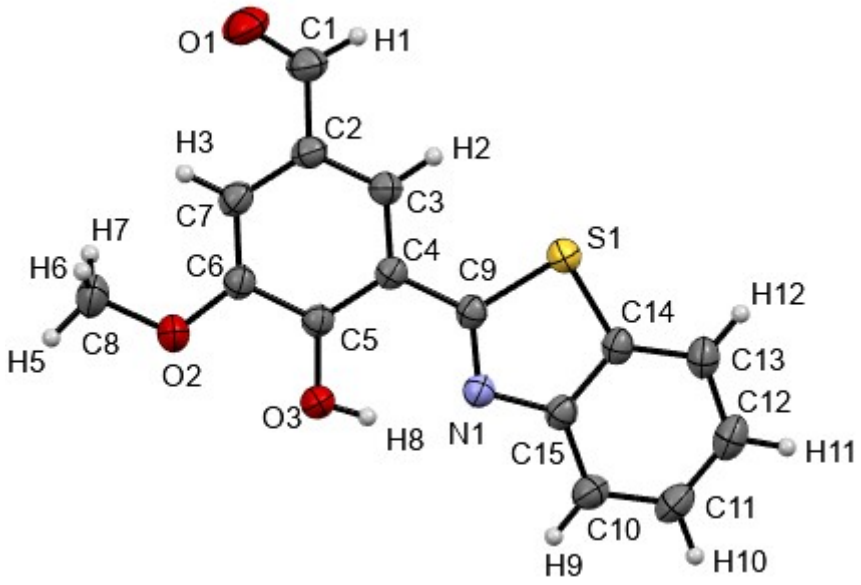
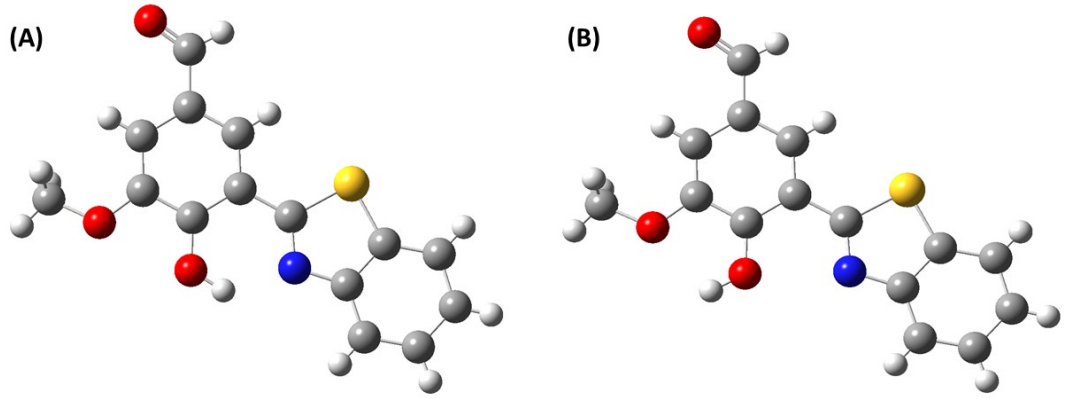
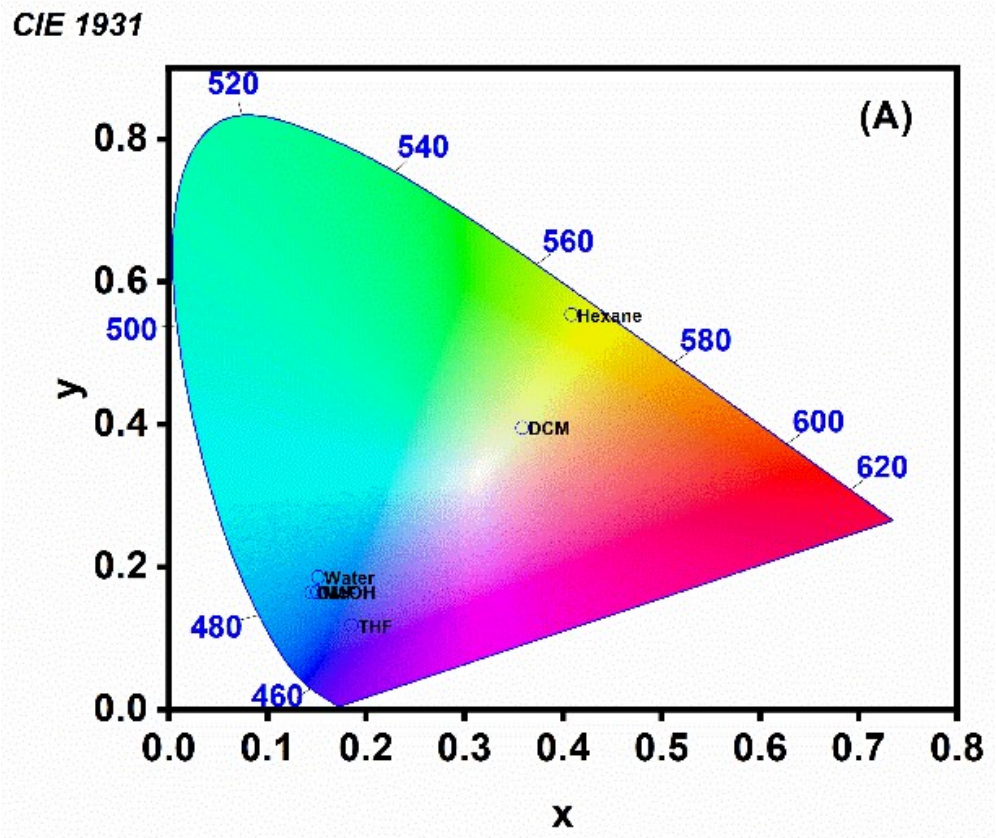


Figure S4. ORTEP diagram of **3BTHMB** with thermal ellipsoids at 30% probability.

5. Various types of Hydrogen bonded forms possible in 3BTHMB.



Scheme S1. 3BTHMB with (A) OH atom bonded to N atom, (B) OH atom bonded to OCH_3 group.



6. CIE diagram of 3BTHMB in various solvents, acid effect.

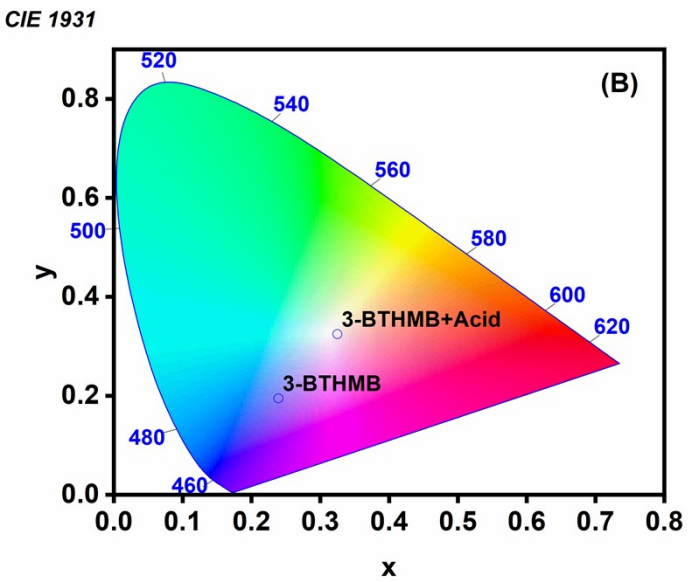


Figure S5. CIE coordinates in (A) various solvents and

(B) in presence of acid in THF

7. Lifetime emission decays of 3BTHMB in various solvents (10 μM) for the entire spectral range.

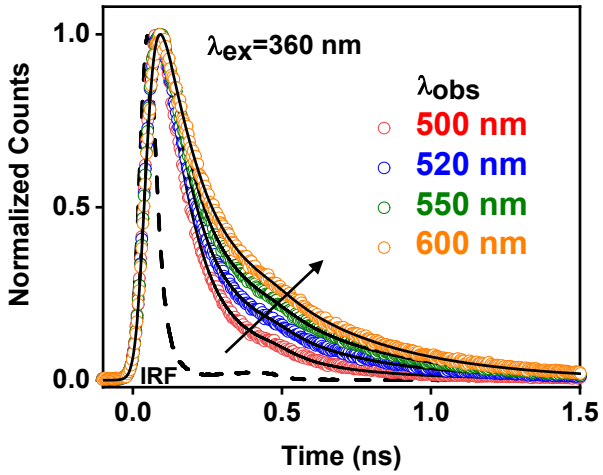


Figure S6: Lifetime emission decays of **3BTHMB** in hexane (10 μM). The excitation and monitoring wavelengths are provided in the insets.

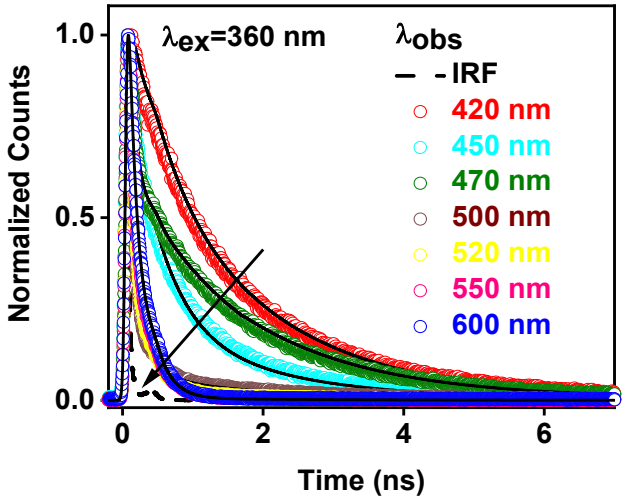


Figure S7: Lifetime emission decays of **3BTHMB** in DCM (10 μM). The excitation and monitoring wavelengths are provided in the insets.

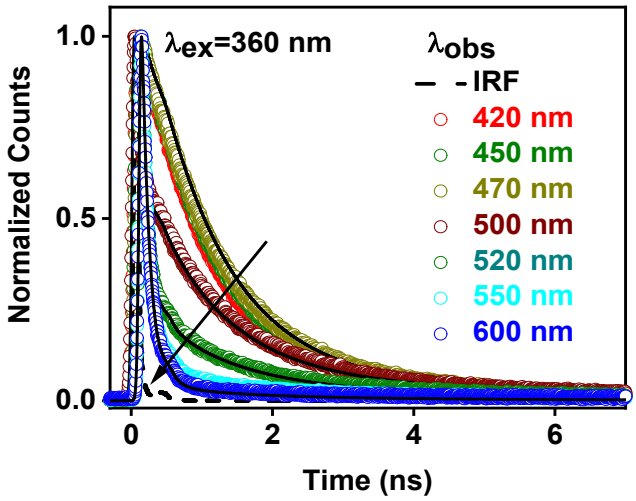


Figure S8: Lifetime emission decays of **3BTHMB** in THF (10 μM). The excitation and monitoring wavelengths are provided in the insets.

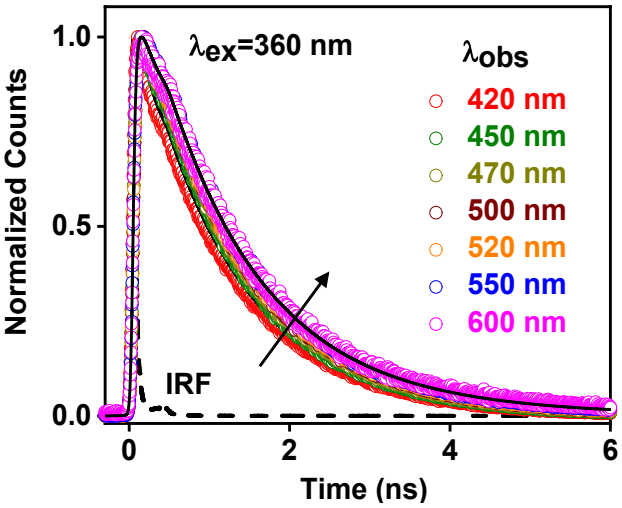


Figure S9: Lifetime emission decays of **3BTHMB** in DMF (10 μM). The excitation and monitoring wavelengths are provided in the insets.

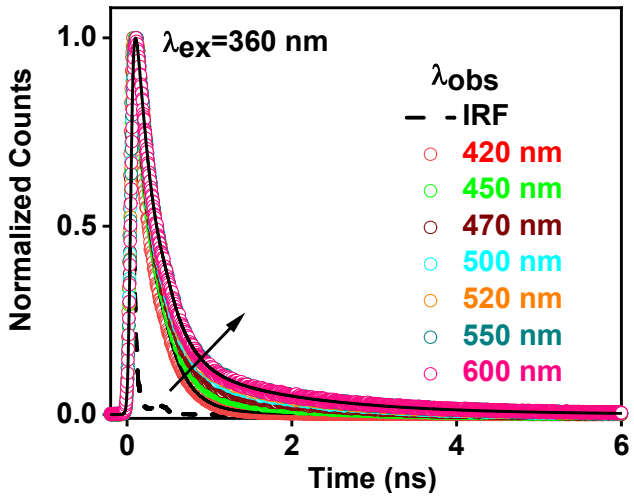


Figure S10: Lifetime emission decays of **3BTHMB** in MeOH (10 μM). The excitation and monitoring wavelengths are provided in the insets.

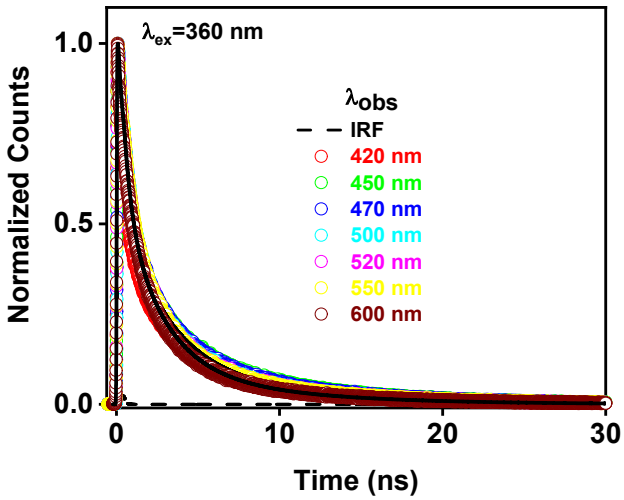


Figure S11: Lifetime emission decays of **3BTHMB** in water at pH 7.4 (10 μM). The excitation and monitoring wavelengths are provided in the insets.

8. Table for Excited state lifetime parameters of 3BTHMB in various solvents.

(In the subsequent tables (S2-S7), data is presented upon normalisation to 100. α_i's and c_i's denotes the amplitudes and contributions to the excited state population. The error in estimation of the lifetimes is around 10%.)

Table S2: Hexane

λobs (nm)	τ_1(ns)	α_1	c_1	τ_2(ns)	α_2	c_2
500		94	80		6	20
520		83	55		17	45
550		72	39		28	61
	0.10			**0.60**		
600		62	29		38	71

Table S3: DCM

λobs (nm)	τ_1(ns)	α_1	c_1	τ_2(ns)	α_2	c_2	τ_3(ns)	α_3	c_3
420		21	4		58	40		21	56
450		4	1		37	14		59	85
470		41	5		11	6		48	89
500	**0.12**	88	38	**0.50**	8	15	**1.8**	4	47
520		93	66		5	13		2	21
550		94	79		5	17		1	4
600		97	85		2	14		1	1

Table S4: THF

λobs (nm)	τ_1 (ns)	α_1	c_1	τ_2 (ns)	α_2	c_2	τ_3 (ns)	α_3	c_3
420		17	2		79	44		4	13
450		11	1		84	45		5	21
470		10	1		80	47		10	29
500	**0.10**	39	4	**0.88**	50	25	**3.3**	11	42
520		74	14		20	18		6	45
550		93	41		5	16		2	35
600		97	69		2	22		1	18

Table S5: DMF

λobs (nm)	τ_1 (ns)	α_1	c_1	τ_2 (ns)	α_2	c_2
420		97	94		3	6
450		94	89		6	11
470		91	85		9	15
500	**1.2**	87	78	**4.0**	13	22
520		85	77		15	23
550		84	75		16	25
600		83	74		17	26

Table S6: MeOH

λobs (nm)	τ_1 (ns)	α_1	c_1	τ_2 (ns)	α_2	c_2
420		99	95		1	5
450		95	75		5	25
470		93	65		7	35
500	**0.23**	90	58	**1.5**	10	42
520		88	55		12	45
550		88	54		12	46
600		88	54		12	46

Table S7: Water at pH 7.4

λobs (nm)	τ_1 (ns)	α_1	c_1	τ_2 (ns)	α_2	c_2	τ_3 (ns)	α_3	c_3
420		50	11		36	41		14	48
450		49	11		36	40		15	49
470		50	12		37	44		13	44
500	**0.34**	52	13	**1.9**	37	47	**6.4**	11	40
520		53	14		36	47		11	39
550		53	14		37	49		10	37
600		47	10		43	50		10	40

9. pK_a calculation for 3BTHMB

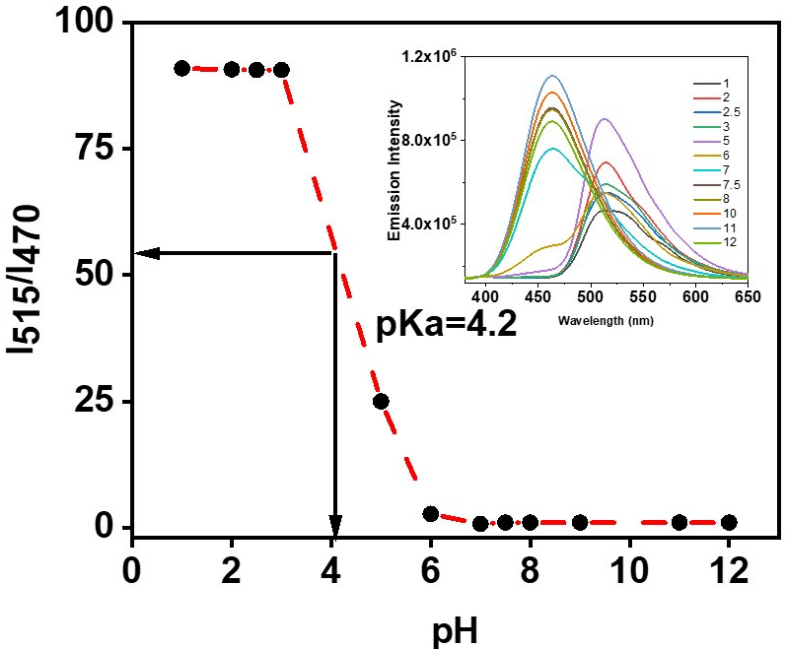
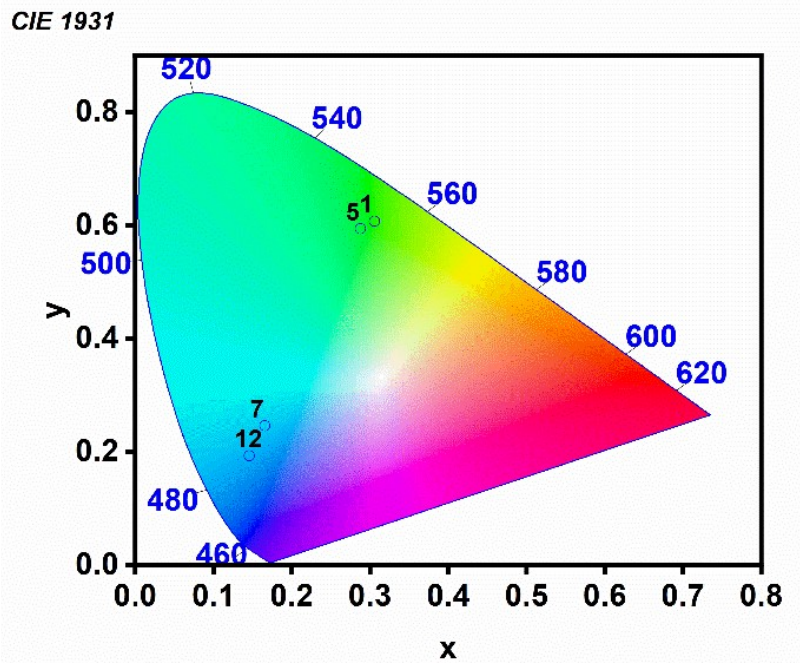


Figure S12: Plot of emission intensity ratio vs. pH to obtain pK_a **of 3BTHMB**, (inset) Emission spectra in various pH solutions.

10. Table for Excited state lifetime parameters of 3BTHMB at pH 4.2

Table S8: Data is presented upon normalisation to 100. α_i' s and c_i's denotes the amplitudes and contributions to the excited state population. The error in estimation of the lifetimes is around 10%

λobs (nm)	τ_1 (ns)	α_1	c_1	τ_2 (ns)	α_2	c_2	τ_3 (ns)	α_3	c_3
420		78	17		18	44		4	39
450		77	16		19	45		4	39
470		73	13		22	47		5	40
500	**0.14**	65	6	**1.50**	22	25	**7.4**	13	69
520		62	5		20	18		18	77
550		62	4		19	16		19	80
600		72	8		17	22		11	70



11. CIE coordinates in at 4 pH values.

Figure S13. CIE coordinates in at 4 pH values.

12. Emission spectra corresponding to amine vapor detection and subsequent regeneration.

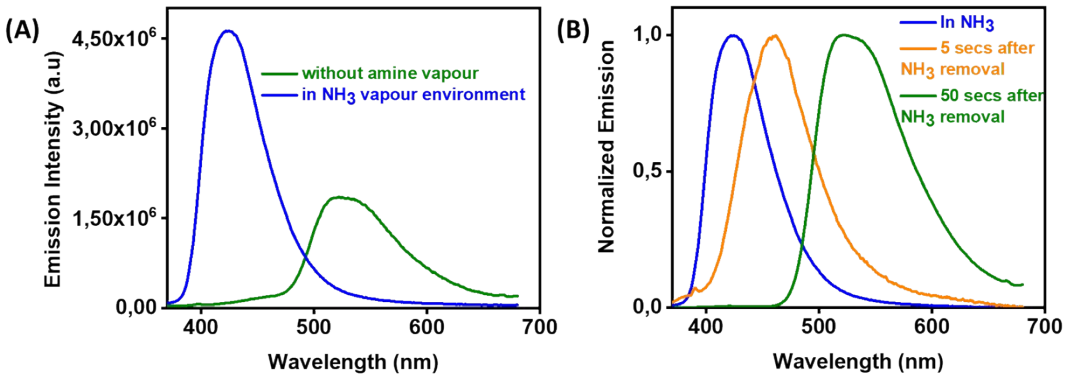


Figure S14. (A) Emission spectra of filter paper impregnated with **3BTHMB** (green curve) and upon exposure to NH_3 vapour (blue curve). (B) Regeneration of the emission spectra of **3BTHMB** upon removal of NH_3 source.

The experimental procedure for obtaining the above spectra (S14 A and B) are as follows: The emission spectrum of a filter paper coated with **3BTHMB** was recorded. Following this, a 5 mL vial containing ammonia was introduced inside the fluorimeter and an emission spectrum was recorded after a few seconds to ensure there is enough vapour interacting with **3BTHMB** coated on filter paper. For recording the recovery experiments, the vial was removed, and stopwatch was started. After 5 secs, a shifted emission spectrum was observed. After 50 secs, the recorded emission spectrum was practically similar to the one observed for **3BTHMB** without NH_3 vapour. It is to be mentioned that the background scattering from the filter paper needed to be subtracted from the emission spectra recorded. For doing so, emission spectrum of a blank filter paper was recorded using the same parameters employed for the emission experiments (Ex: 360 nm. Start: 375 nm, End: 700 nm, Slits: 2,2)