Dual-Functional 8-Hydroxyquinoline Fluorescent Probe for Simultaneous Detection of Solvent Microenvironments and Trace Water in Organic Media

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SUPPORTING INFORMATION

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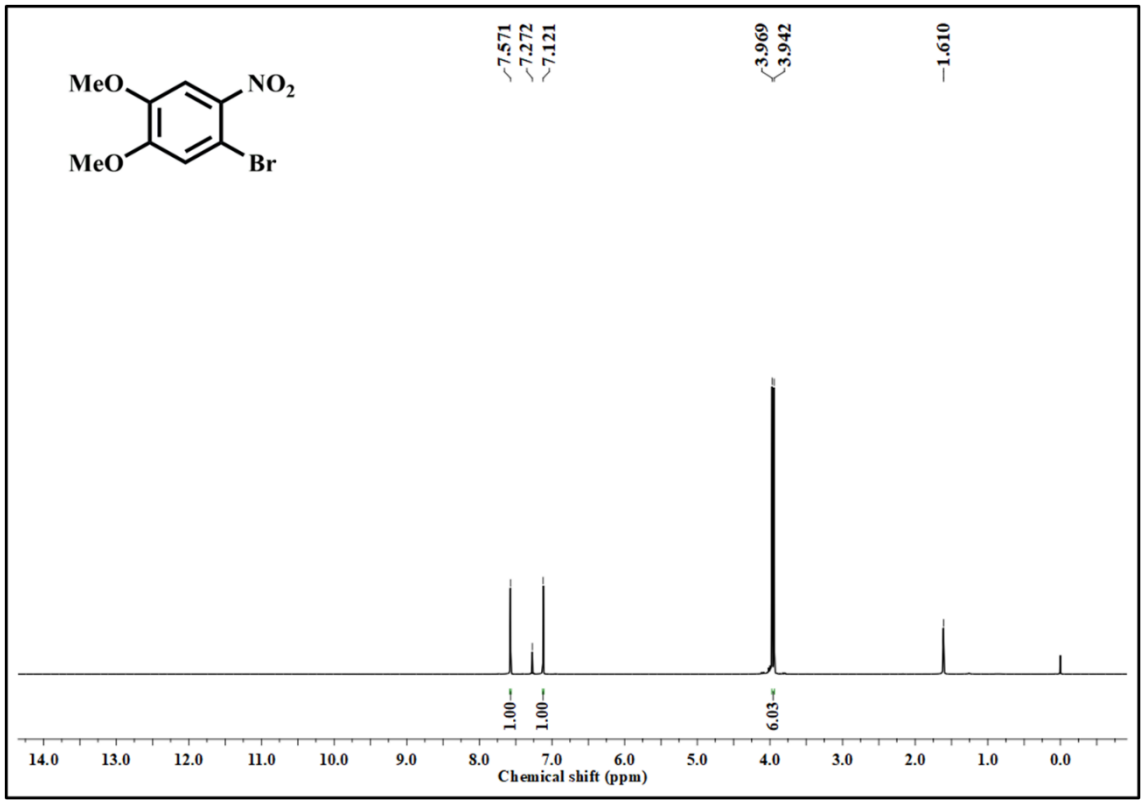


Fig. S1 ^{1}H-NMR spectrum of BDN

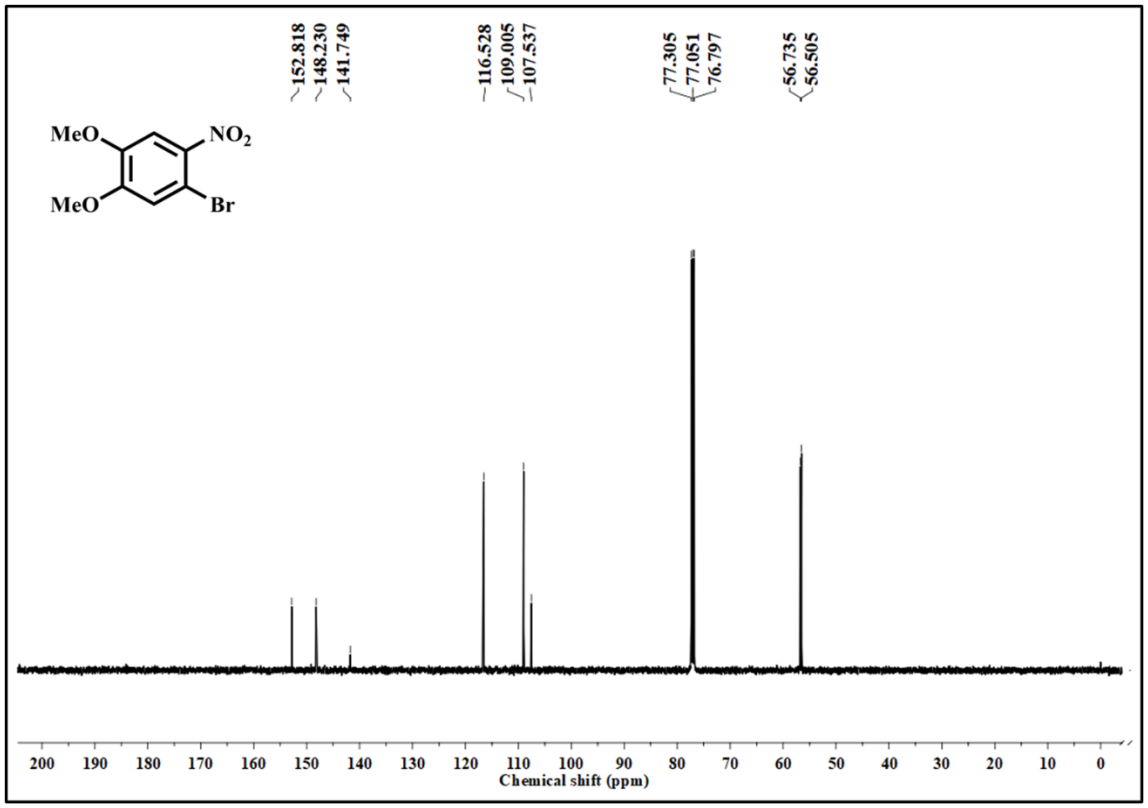


Fig. S2 ^{13}C-NMR spectrum of BDN

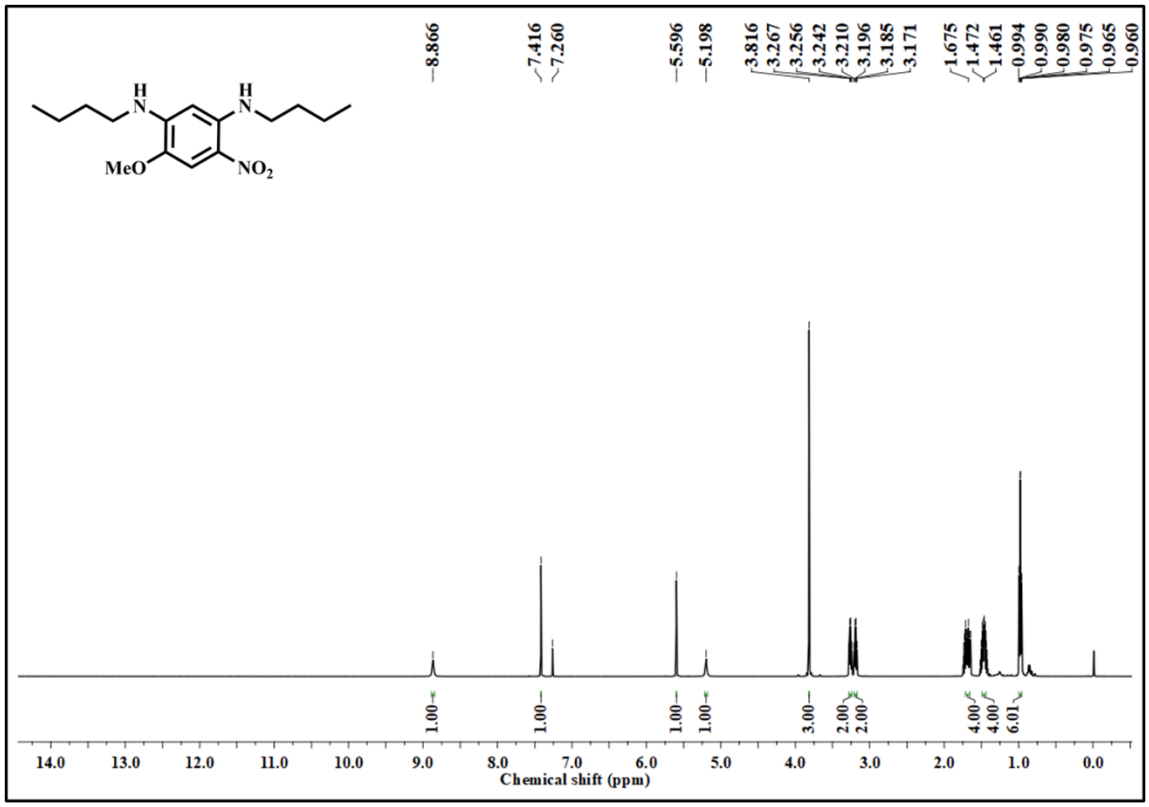


Fig. S3 ^{1}H-NMR spectrum of DBNA

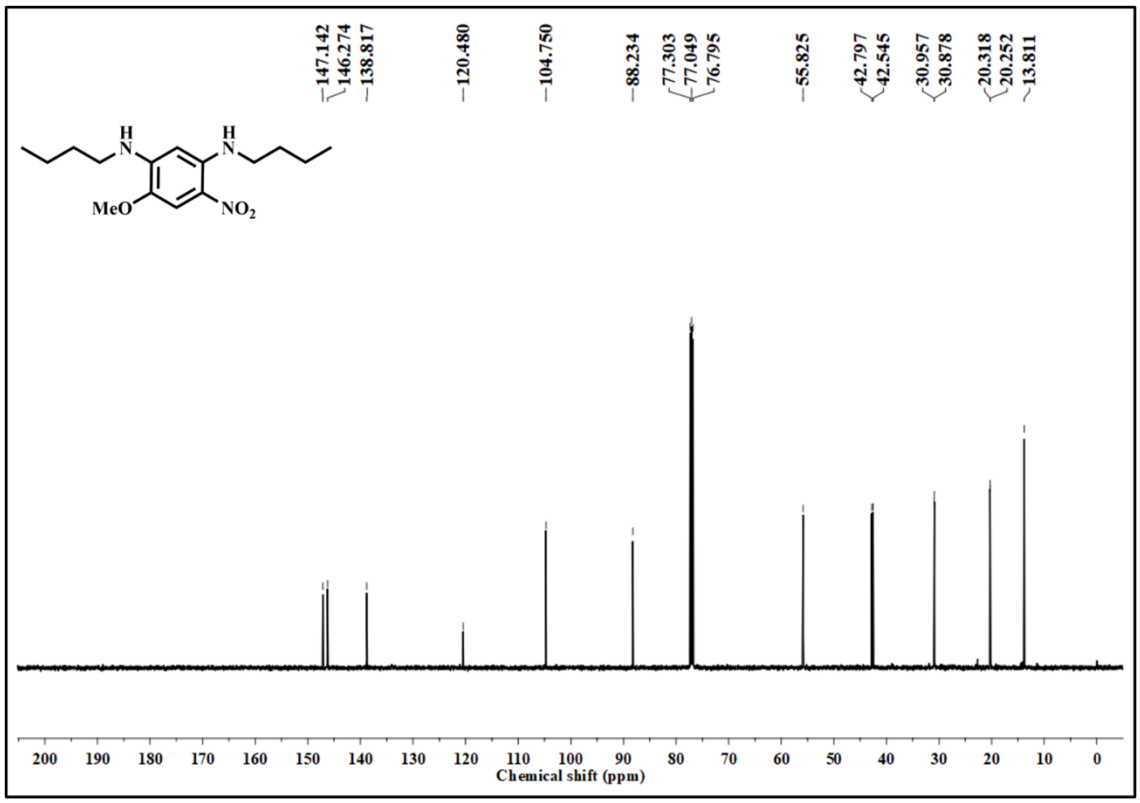


Fig. S4 ^{13}C-NMR spectrum of DBNA

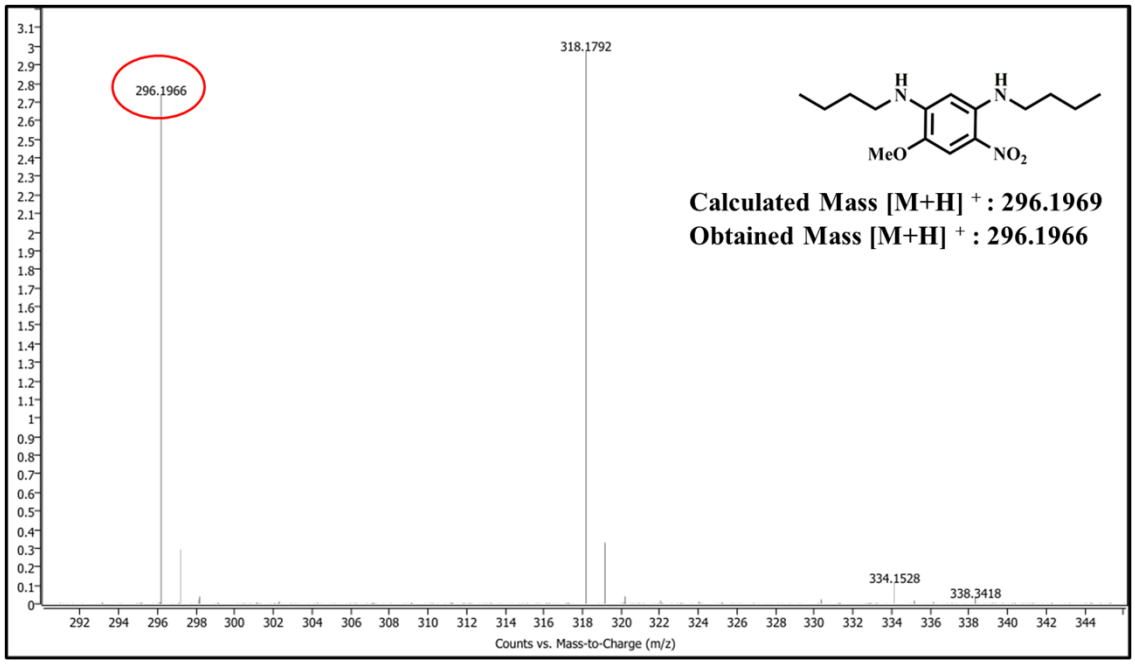


Fig. S5 HRMS spectrum of DBNA

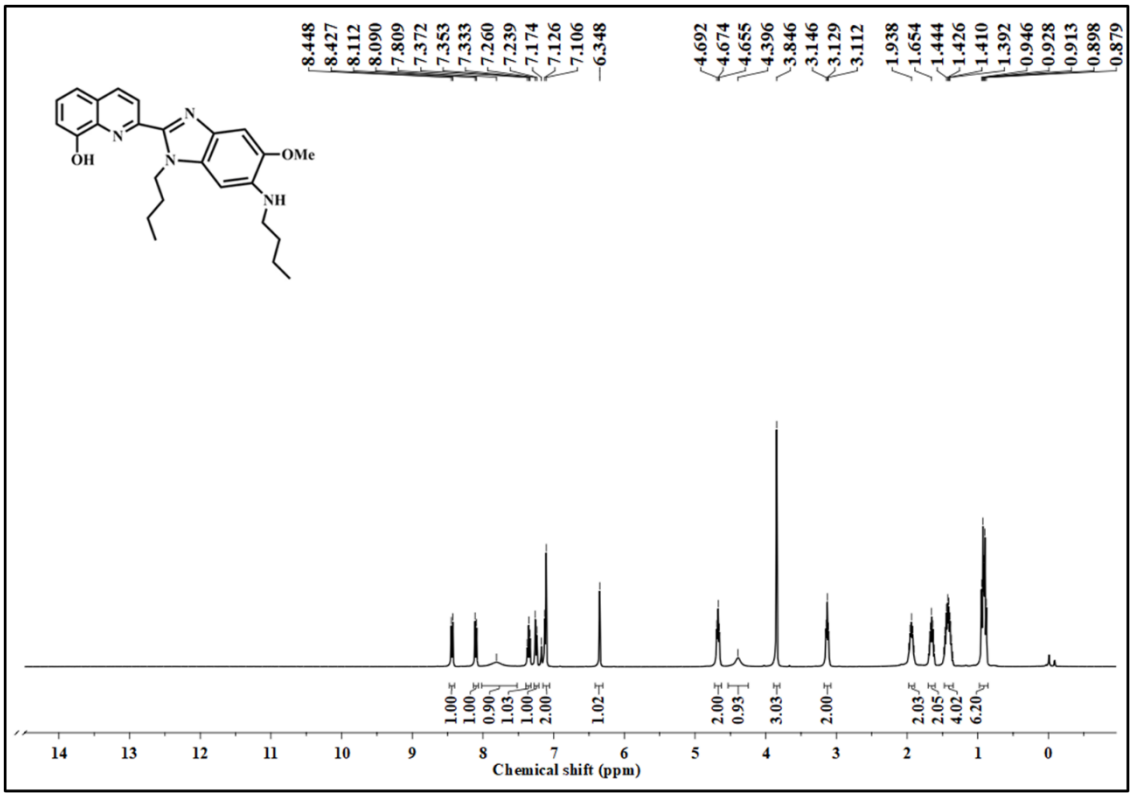


Fig. S6 ^{1}H NMR spectrum of DBIMHQ

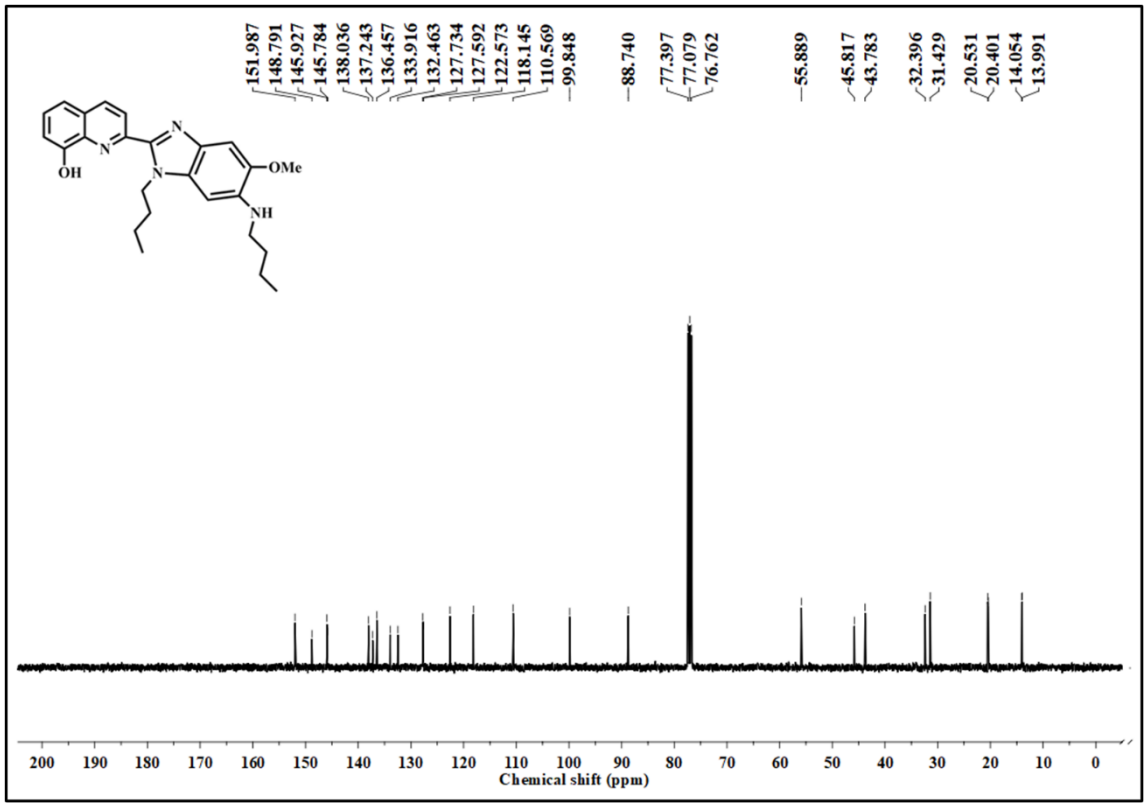


Fig. S7 ^{13}C NMR spectrum of DBIMHQ

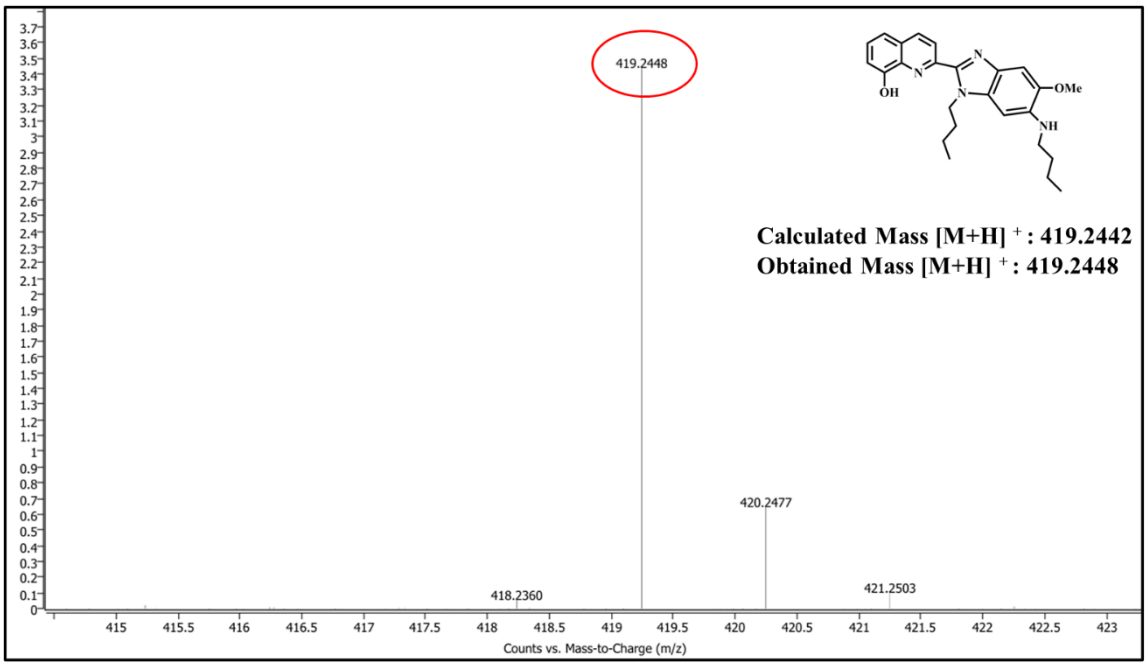


Fig. S8 HRMS spectrum of DBIMHQ

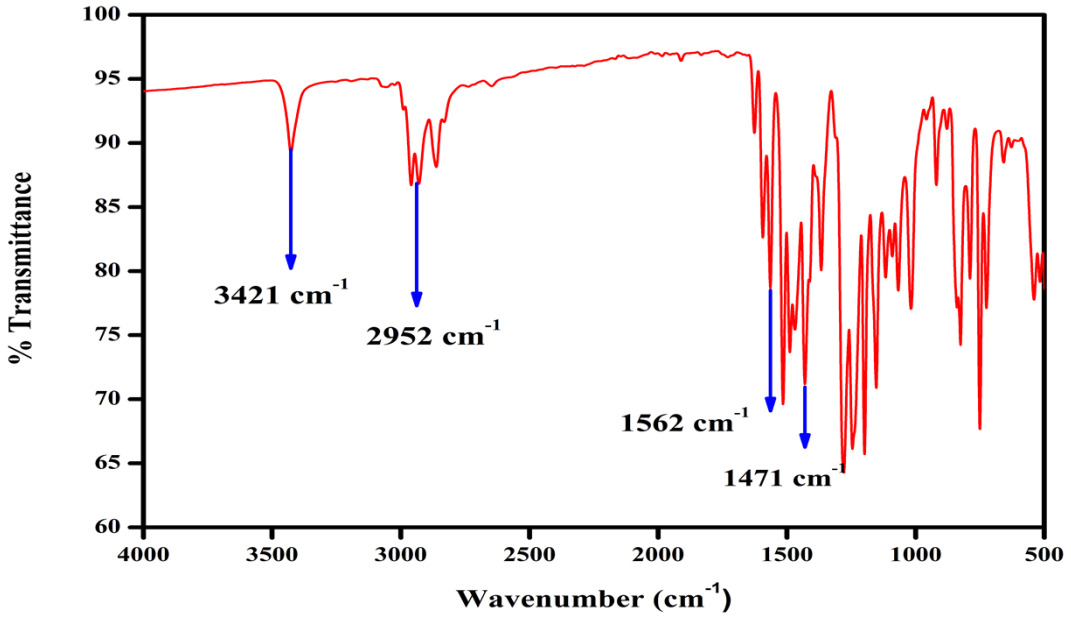


Fig. S9 FT-IR spectrum of DBIMHQ

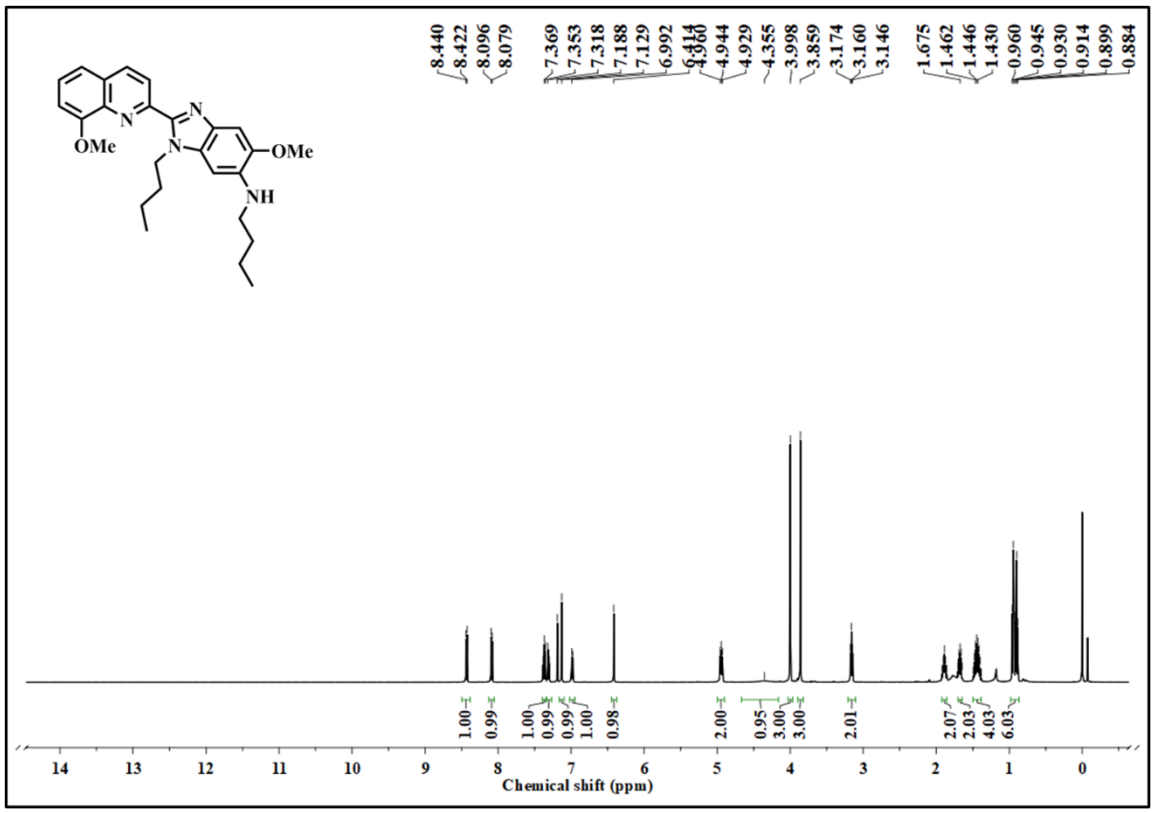
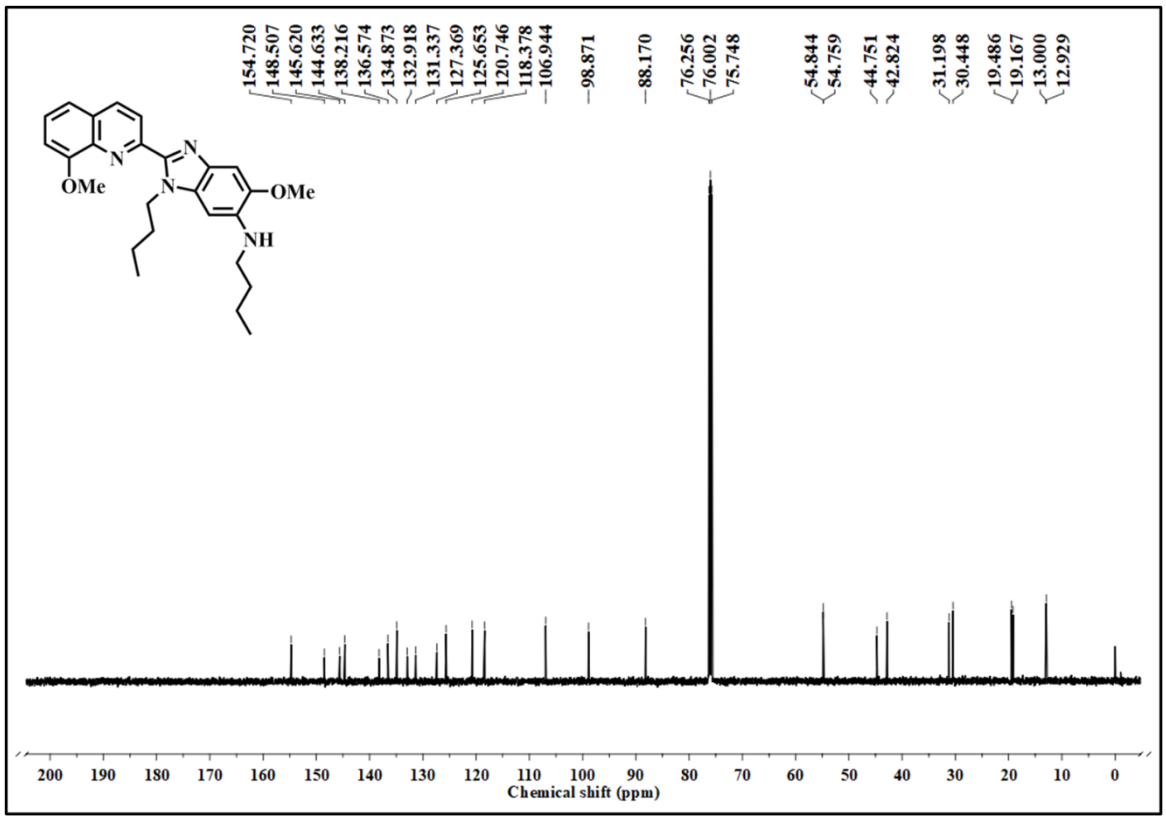


Fig. S10 ^{1}H NMR spectrum of DBIMMQ



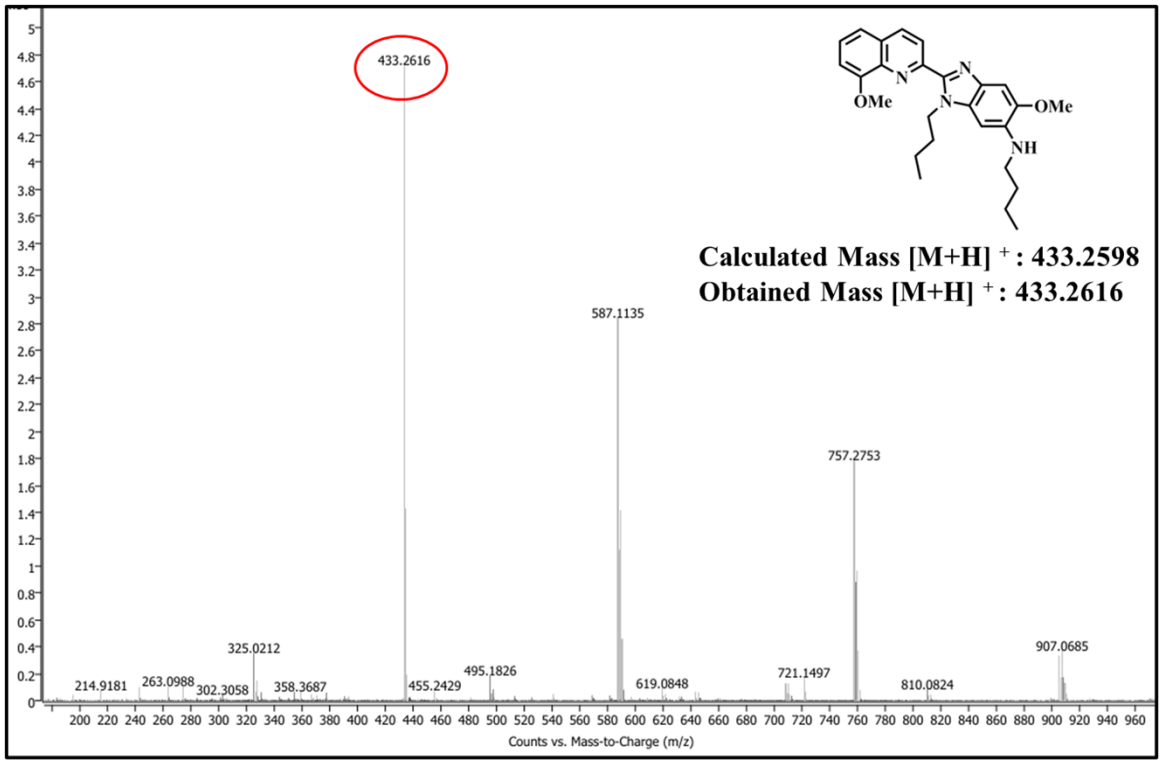


Fig. S11 ^{13}C NMR spectrum of DBIMMQ

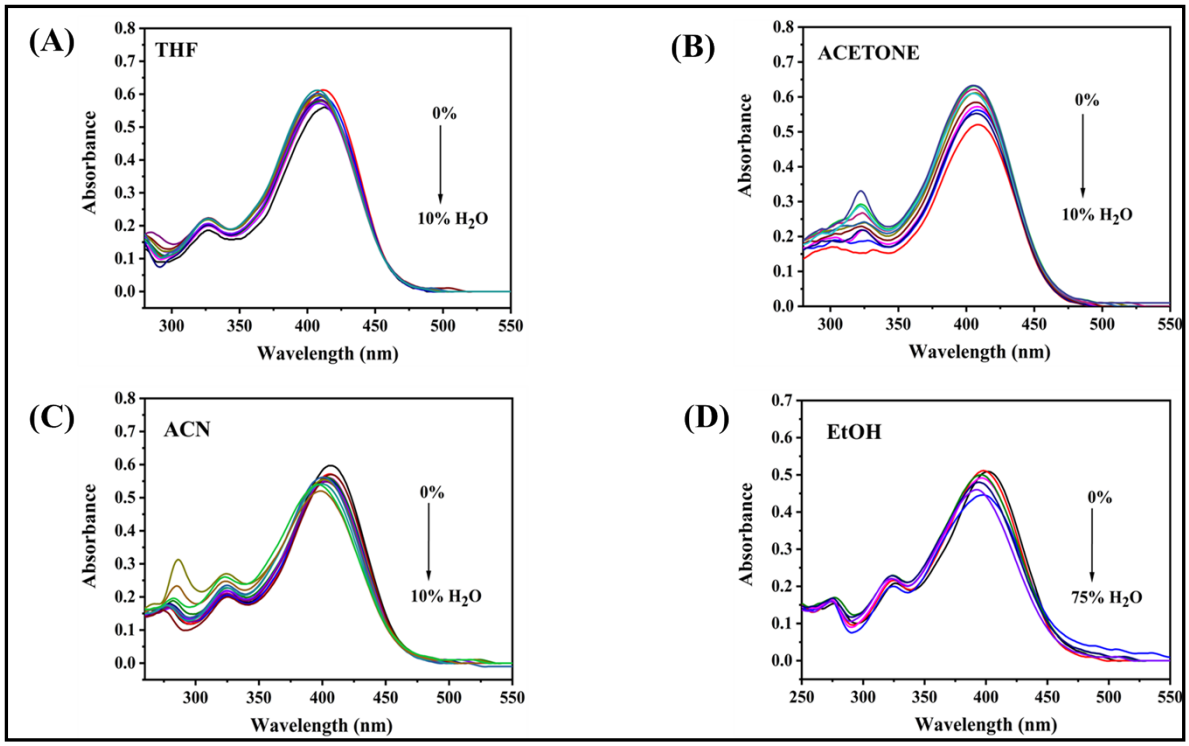
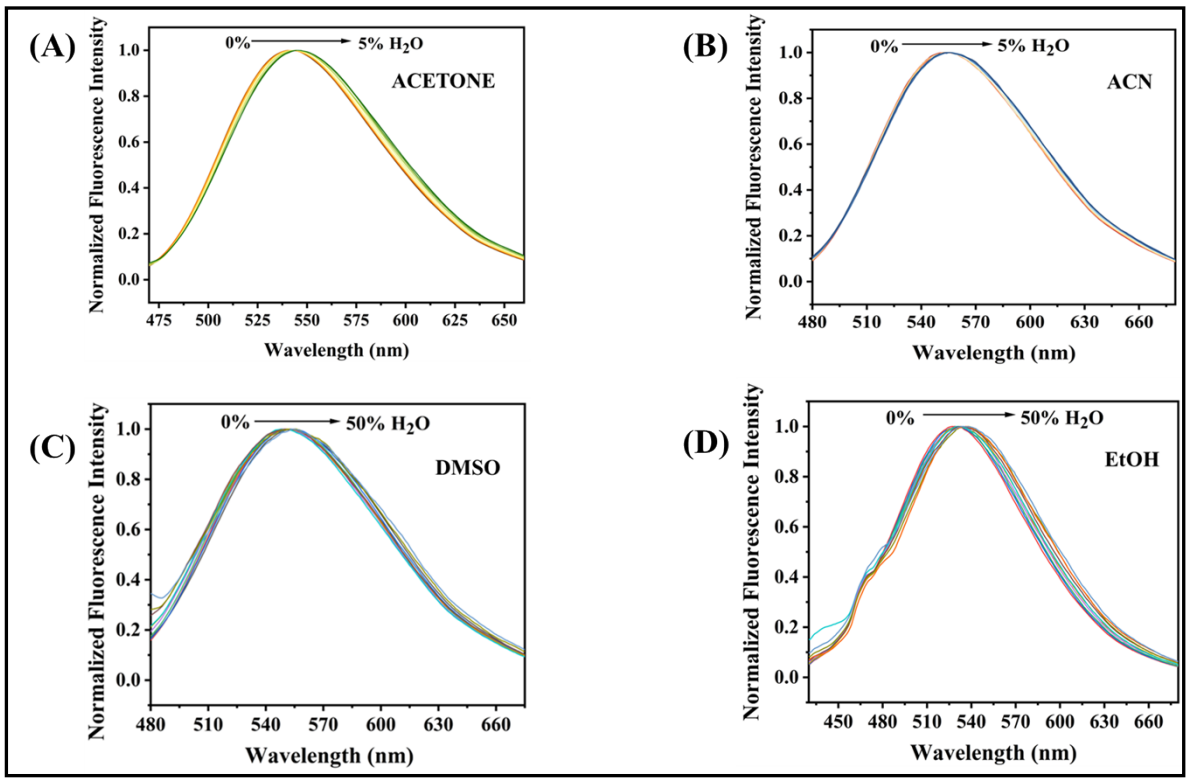


Fig. S12 HRMS spectrum of DBIMMQ

Fig. S13 UV-visible absorption spectra of DBIMHQ with increasing water content (A) THF,



(B) Acetone, (C) ACN, (D) EtOH.

Fig. S14 Normalized fluorescence emission spectra of DBIMHQ in (A) Acetone, (B) ACN, (C) DMSO, (D) EtOH

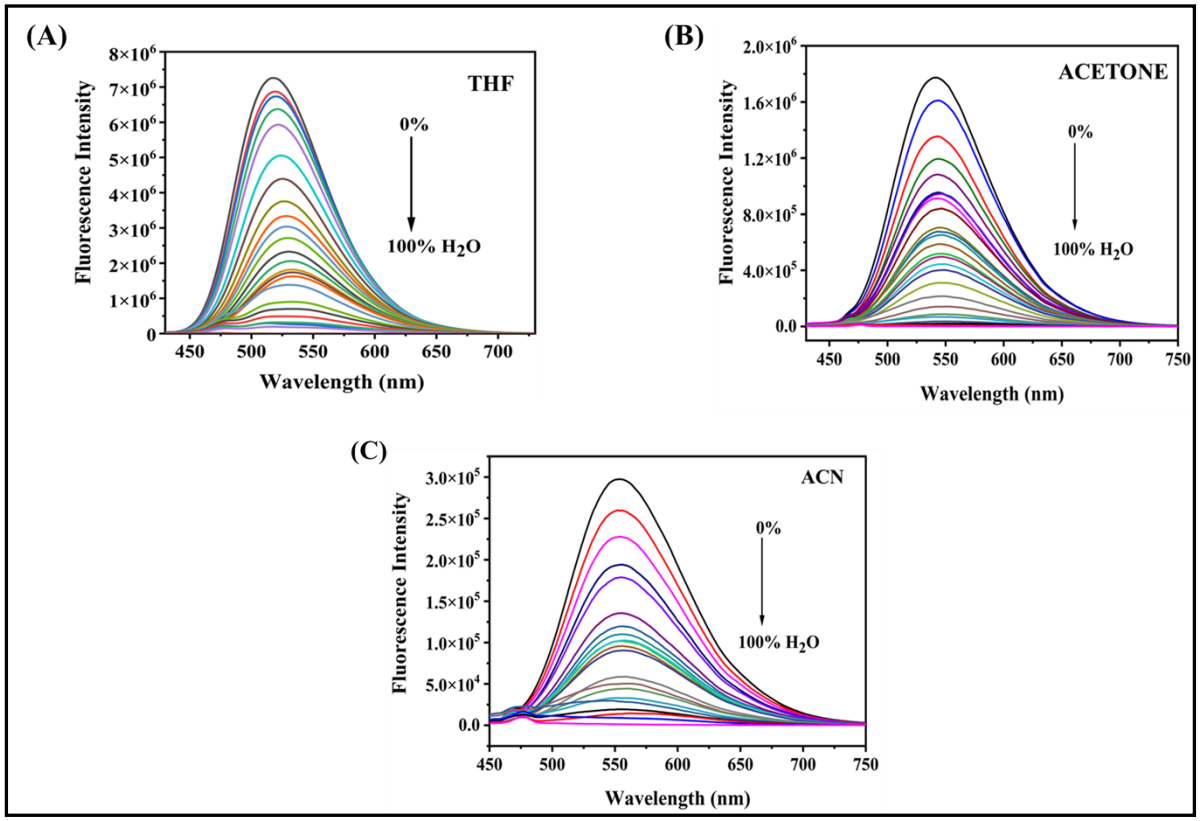


Fig. S15 Fluorescence emission spectra of DBIMHQ at higher water contents (A) THF, (B) Acetone, (C) ACN.

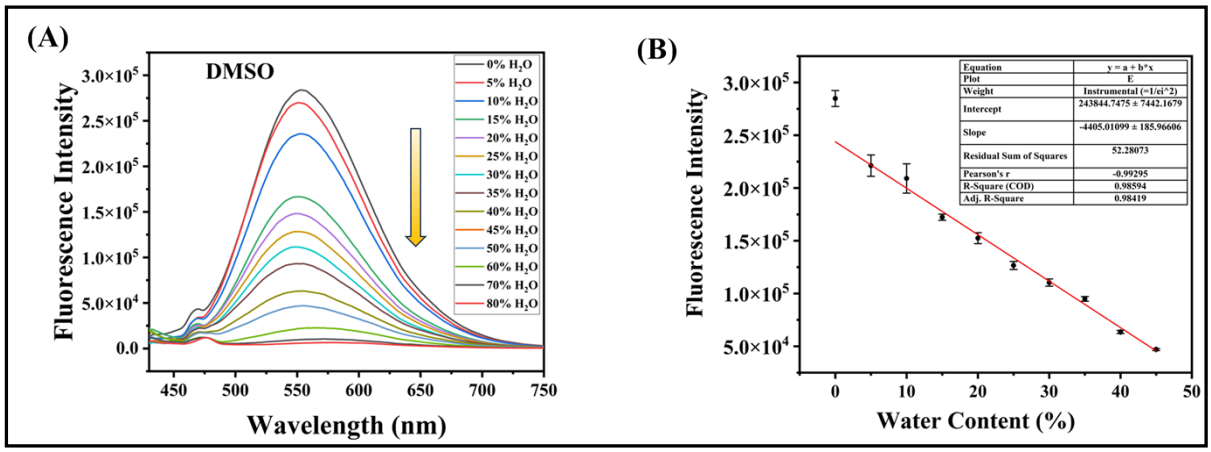


Fig. S16 (A) Fluorescence emission spectra of DBIMHQ in DMSO, (B) Plot of fluorescence intensity *vs* water content in DMSO.

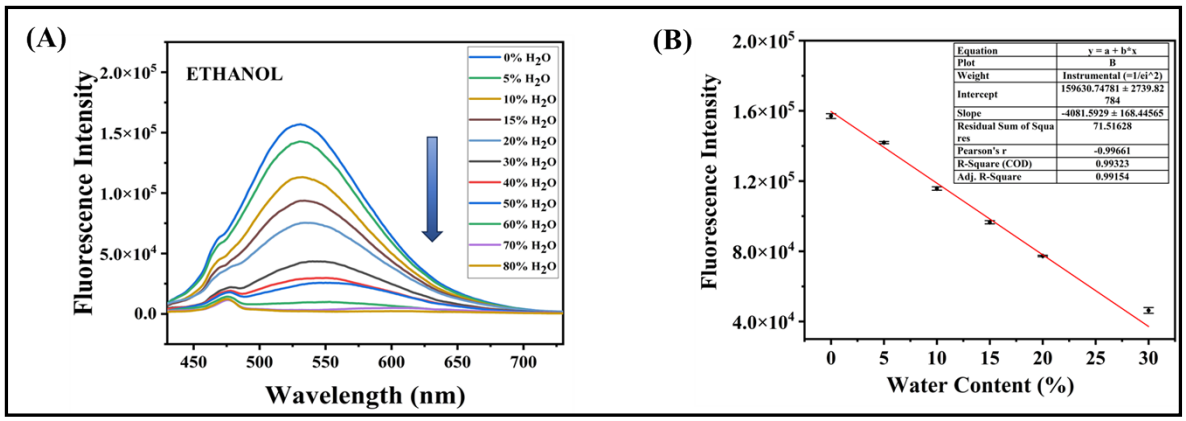


Fig. S17 (A) Fluorescence emission spectra of DBIMHQ in EtOH, (B) Plot of fluorescence intensity *vs* water content in EtOH.

Table S1. Relative Quantum yield calculation for DBIMHQ

Sample	Excitation Wavelength	QY_S	A_S	F_S	η_S	A_X	F_X	η_X	QY_X
DBIMHQ	410 nm	0.577	1.16×10^9	0.08	1.33	4.10×10^8	0.06	1.407	0.304

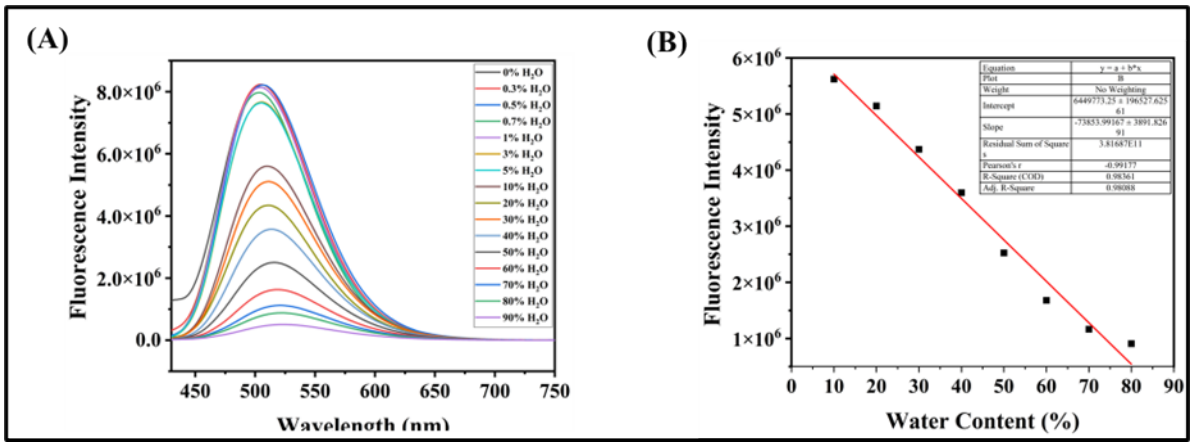
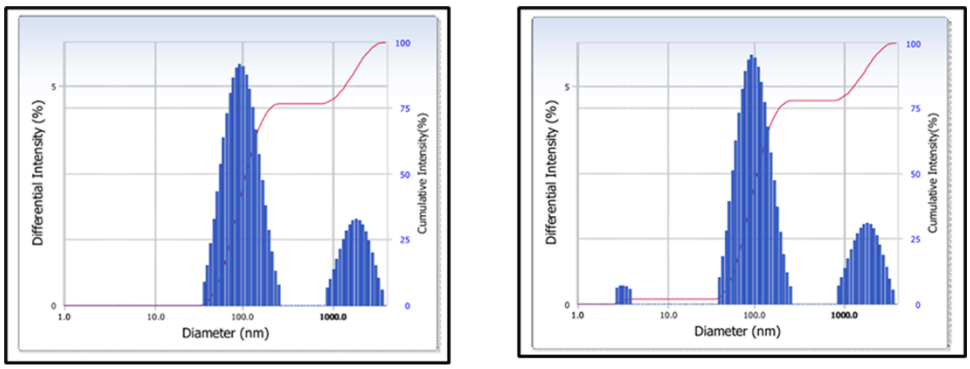


Fig. S18 (A)Fluorescence emission spectra of DBIMMQ in THF with increasing water content and (B) Plot of fluorescence intensity *vs* water content in THF.



(a) Zavg = 248.8 nm
PDI = 0.199

(b) Zavg = 253.7 nm
PDI = 0.191

Fig. S19 DLS-based particle size analysis of DBIMHQ (1µM) in (a) 10% H_2O-THF and (b) 50% H_2O-THF.

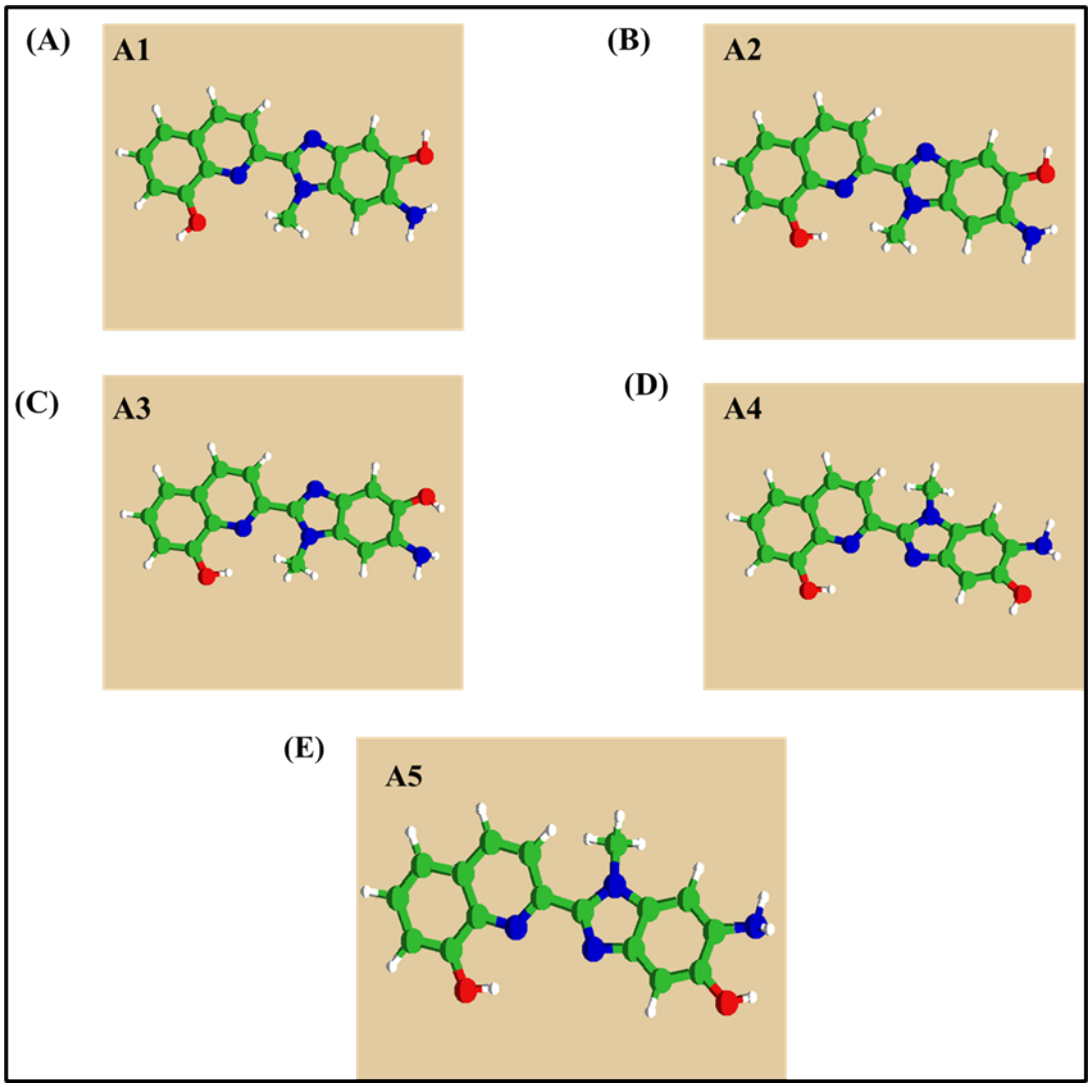


Fig. S20 DFT study for geometric optimisation and energy calculation.

Table S2. Relative energy of various conformers of DBIMHQ

Conformer	Electronic Energy (kcal/mol)
A1	4.10
A2	0
A3	1.14
A4	3.09
A5	4.10

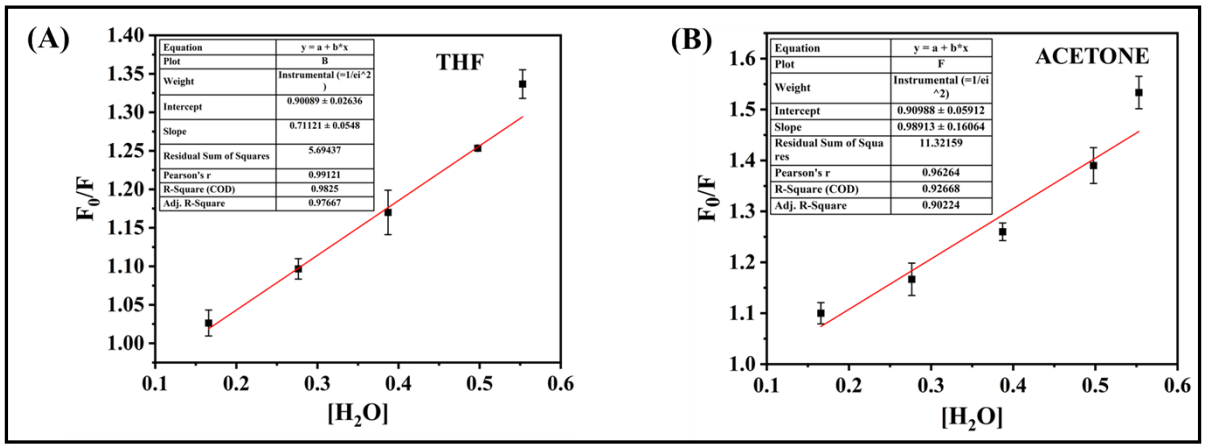


Fig. S21 (A) Stern-Volmer plot for fluorescence intensity in THF solvent with the addition of water, and (B) Stern-Volmer plot for fluorescence intensity in acetone solvent with the addition of water.

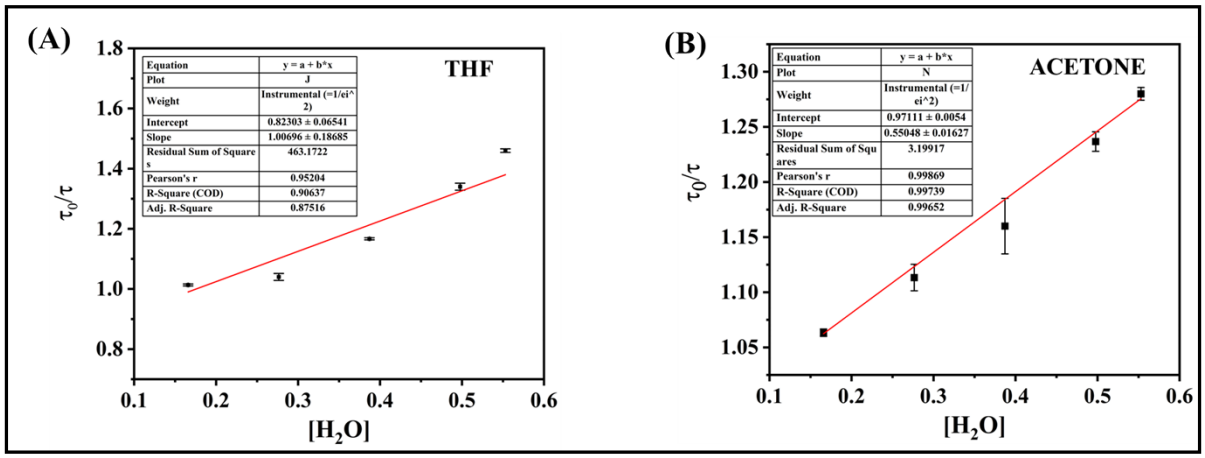


Fig. S22 (A) Stern-Volmer plot for lifetime in THF solvent with the addition of water, and (B) Stern-Volmer plot for lifetime in acetone solvent with the addition of water.

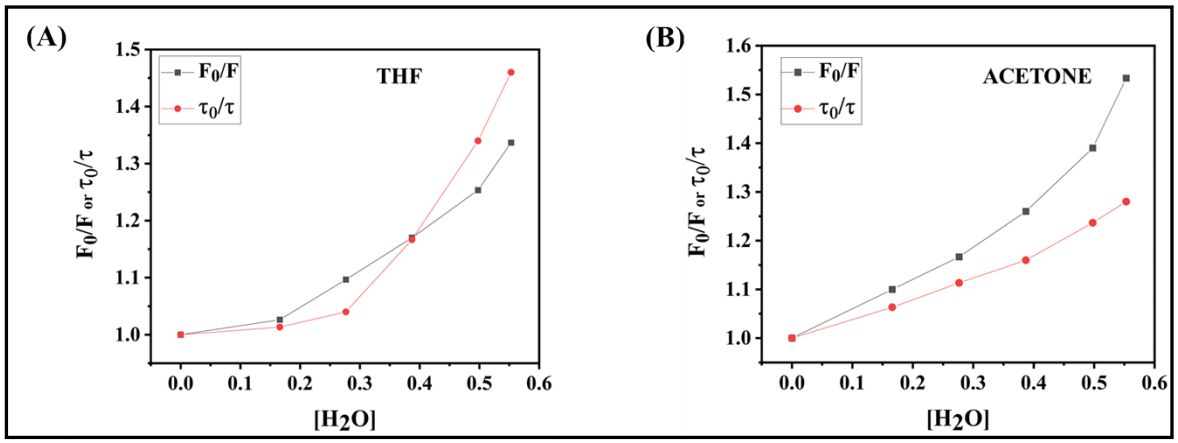


Fig. S23 (A) Stern-Volmer plot combining fluorescence intensity and lifetime measurements with increasing water concentration (A) THF solvent and (B) Acetone solvent.

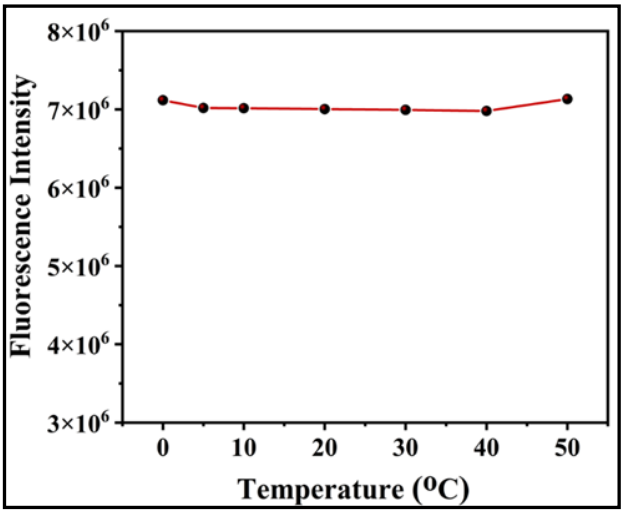


Fig. S24 Temperature sensitivity of DBIMHQ in pure THF solvent.

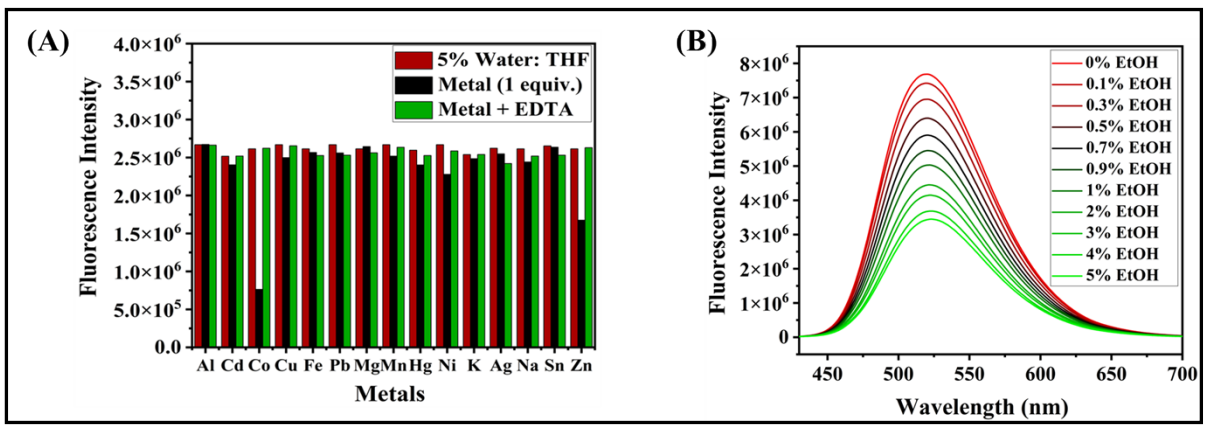


Fig. S25 Non-metal interference study for DBIMHQ (1µM) in THF with 5% water (A) EDTA masking control for metal ions and (B) Incremental addition of ethanol to THF solvent.

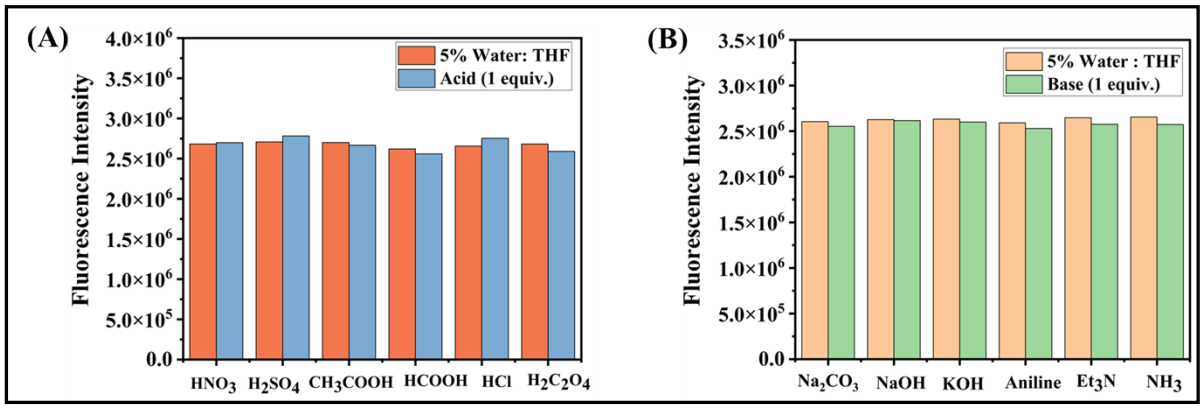


Fig. S26 Non-metal interference study for DBIMHQ (1µM) in THF with 5% water (A) Acid contaminants and (B) Base contaminants.

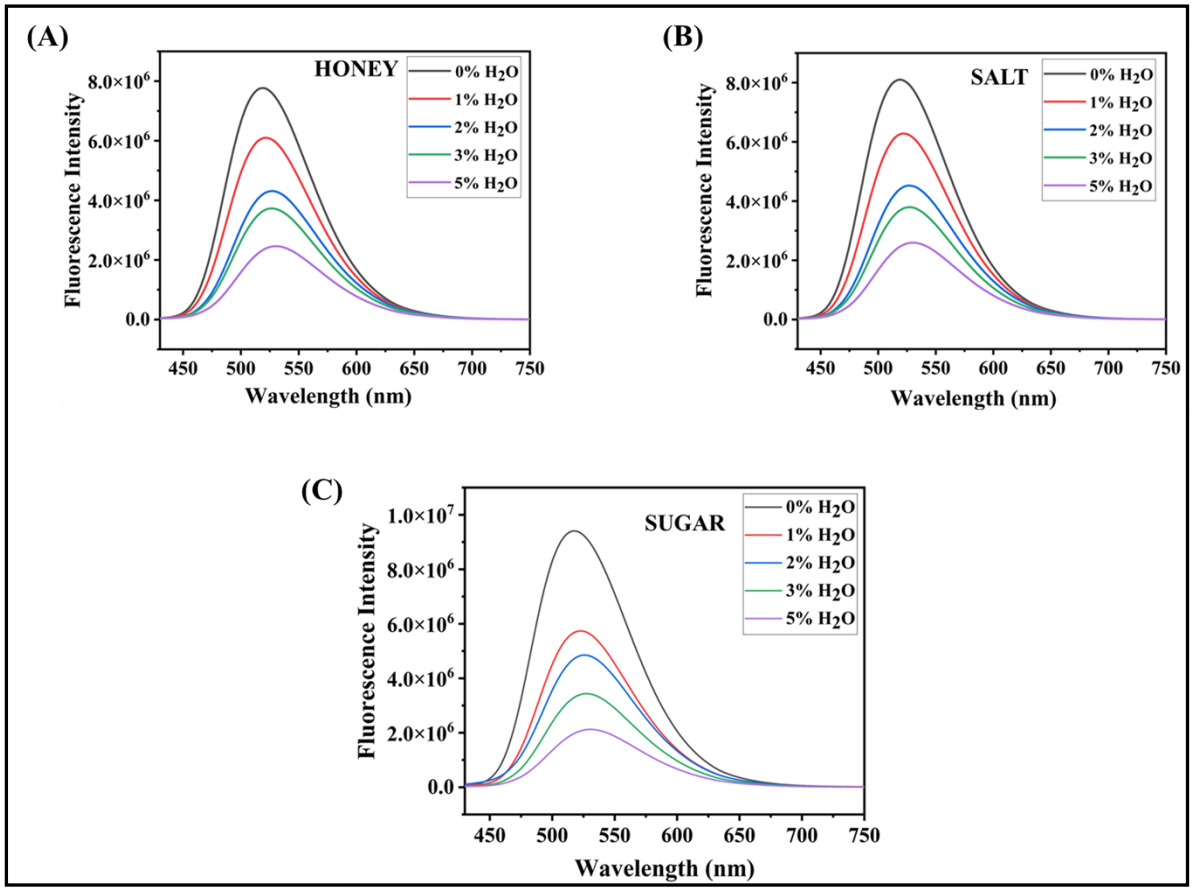


Fig. S27 Quantitative analysis of water in real samples (A) Honey, (B) Salt, and (C) Sugar.

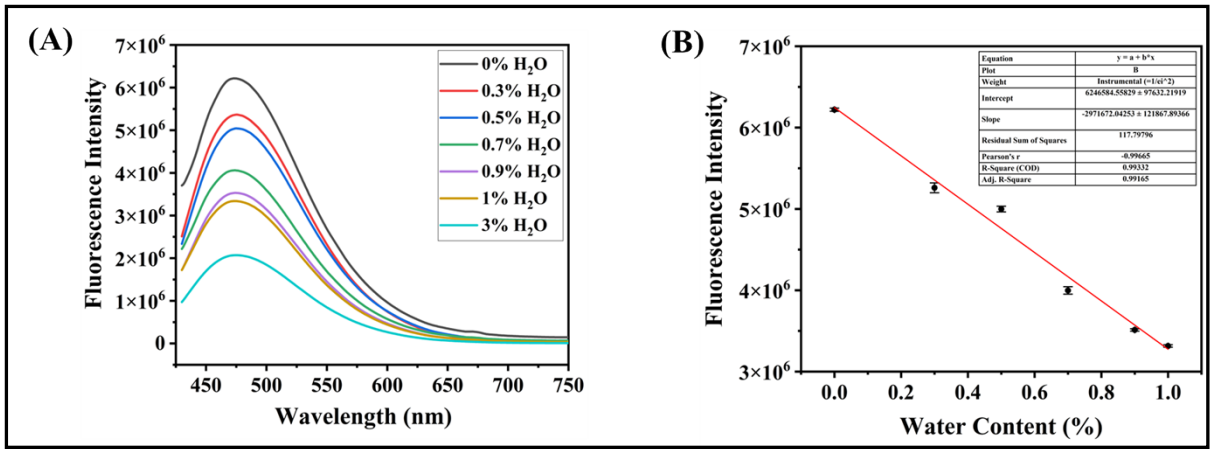


Fig. S28 (A) Fluorescence emission spectra of chitosan thin film in THF solvent with increasing water content and (B) Plot of fluorescence intensity *vs* water content in THF.

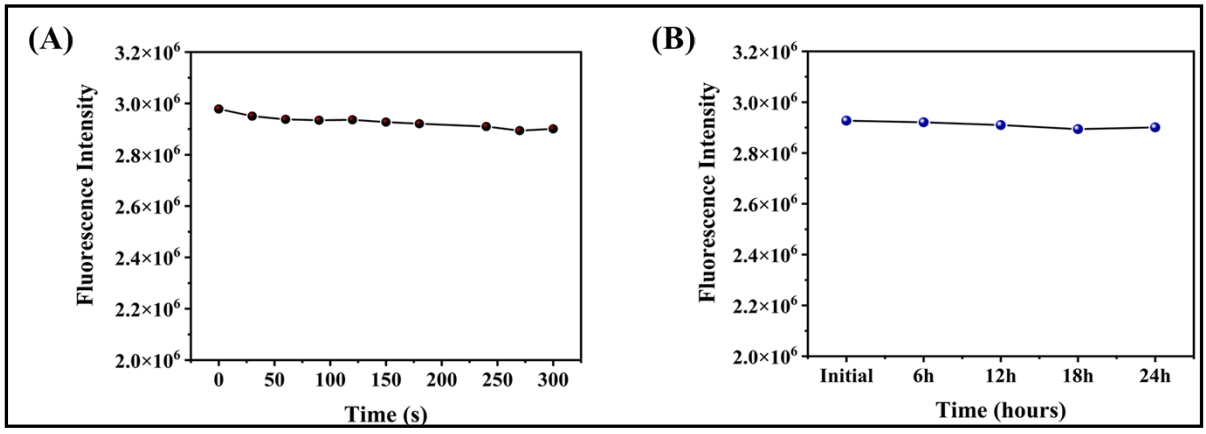


Fig. S29 (A) Response time analysis of chitosan thin film in THF: water mixture at various time intervals, and (B) Stability studies of chitosan thin film THF-water solvent mixture.

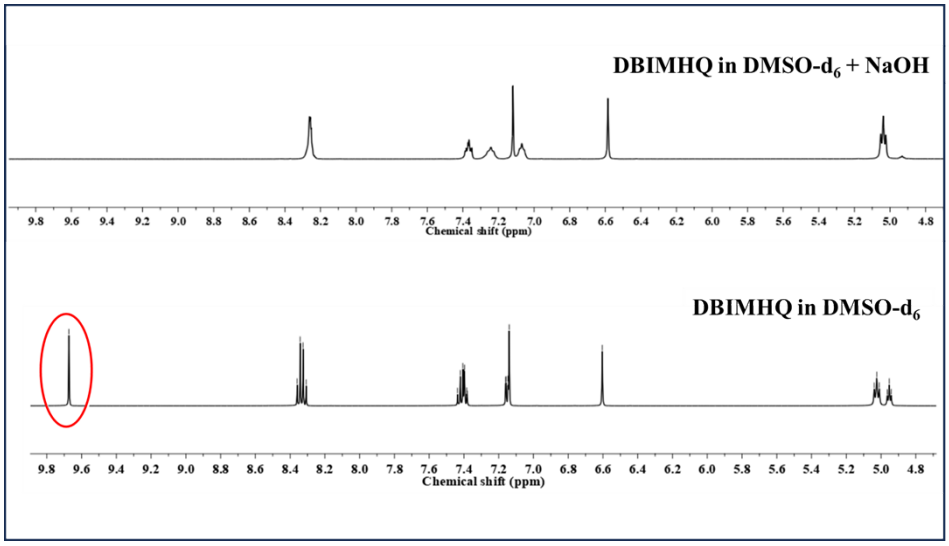
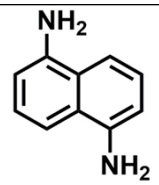
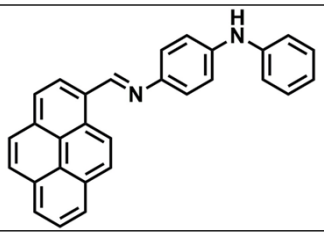
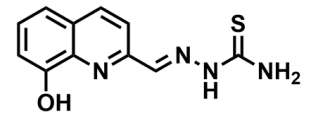
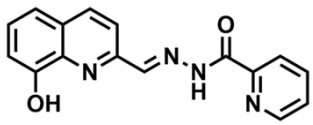
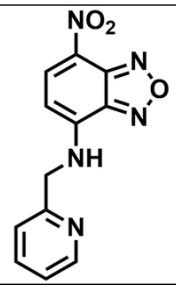
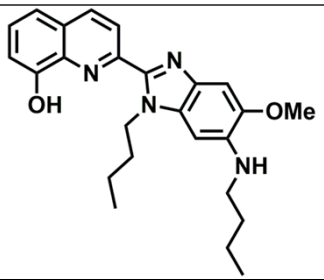


Fig. S30 ^{1}H NMR spectrum of DBIMHQ in the presence of NaOH.

Table S3. Comparison of previous reports with DBIMHQ

Sl. No.	Sensor	Solvent	LOD (%)	LOQ (%)	Response (s)	References
1		ACN THF	0.08 0.13	0.24 0.40	-	1
2		ACN Dioxane DMSO EtOH THF	0.06246 0.18329 0.17478 0.39660 0.47389	0.20823 0.61097 0.58262 1.32201 1.57965	-	2
3	 	DMSO DMF ACN EtOH DMSO DMF ACN EtOH	0.0220 0.0246 0.1404 0.1513 0.0274 0.0461 0.0221 0.0595	- -	<5s	3
4		ACN Dioxane Acetone DMSO THF	0.0019 0.007 0.0013 0.0068 0.0037	-	≤1.2s	4
5	Karl Fischer Titration	Acetone EtOH THF DMF	0.026 0.026 0.016 0.036	-	30s	5
6		THF Acetone ACN DMSO EtOH	0.0130 0.1743 0.1100 1.4271 1.6742	0.0435 0.5812 0.3668 4.7570 5.5807	30s	Present Work

References

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2. R. AbhijnaKrishna, N. Vijay and S. Velmathi, *New J. Chem.*, 2022, **46**, 17903–17911.
3. J. T. Wang, Y. Y. Pei, S. F. Ren, M. Y. Yan, W. Luo, B. Zhang and Q. F. Li, *Spectrochim. Acta A: Mol. Biomol. Spectrosc.*, 2020, **229**, 117956.
4. Z. Zhang, Q. Liu, W. Wang, R. Shi, T. Jiang, J. Li, P. Jiang, H. Yu and Y. Qi, *Spectrochim Acta A Mol Biomol Spectrosc.*, 2024, **323**, 124880.
5. N. Dantan, W. Frenzel, and S. Kuppers, Talanta, 2000, **52**, 101-109.