Electronic Supplementary Information (ESI)

Dark to Bright Fluorescence State by Inter-connecting Fluorophores:

Concentration Dependent Blue to NIR emission and Live Cell Imaging Application

Parthasarathy Gayathri,[a] Siva Bala Subramaniyan,[a] Anbazhagan Veerappan,[a] Anwarhussaini Syed,[b] Subbalakshmi Jayanty,[b] Mehboobali Pannipara,[c,d] Abdullah G. Al-Sehemi,[c,d] Dohyun Moon*[e] Savarimuthu Philip Anthony*[a]

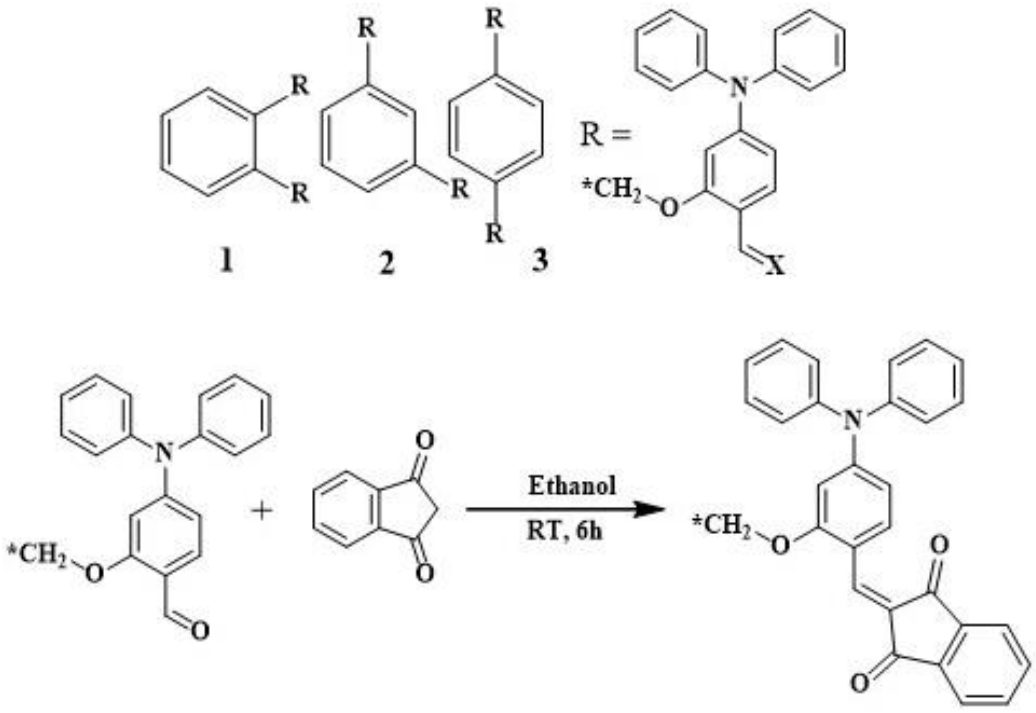
[a)]School of Chemical & Biotechnology, SASTRA Deemed University, Thanjavur-613401, Tamil Nadu, India. Fax: +914362264120; Tel: +914362264101; E-mail: philip@biotech.sastra.edu

[b)] Department of Chemistry, Birla Institute of Technology and Science, Pilani-Hyderabad Campus, Hyderabad - 500078, India

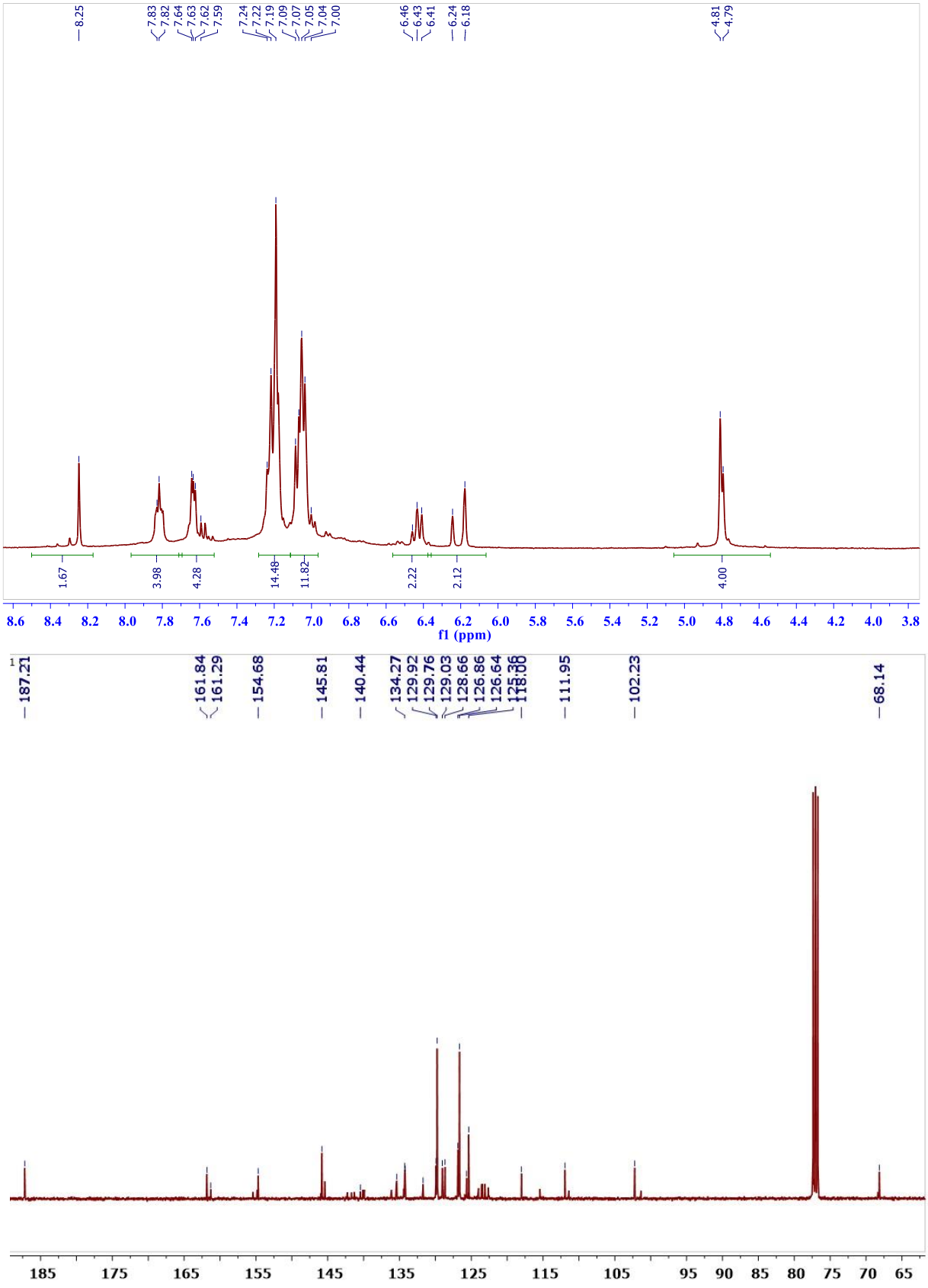
[b)]Department of chemistry, King Khalid University, Abha 61413, Saudi Arabia.

[c)]Research center for Advanced Materials Science, King Khalid University, Abha 61413, Saudi Arabia.

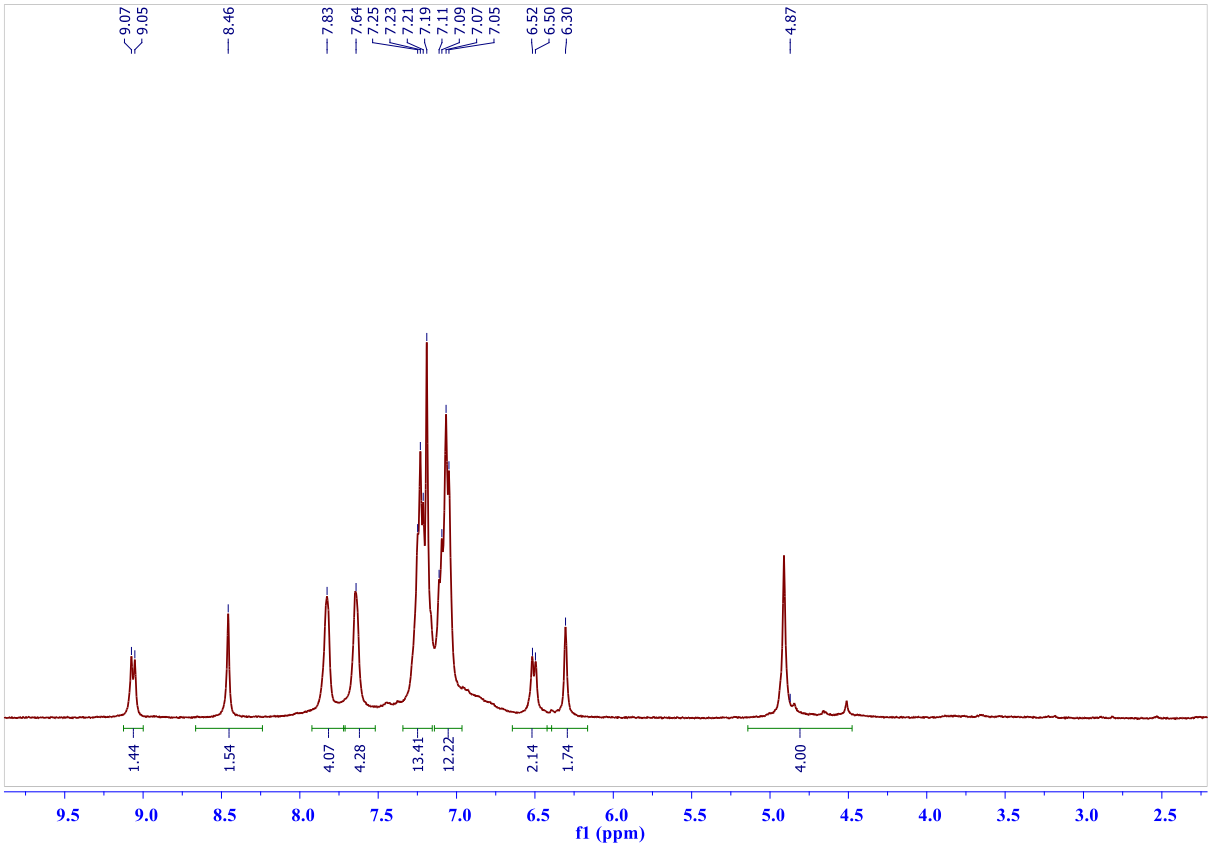
[b)]Beamline Department, Pohang Accelerator Laboratory, 80 Jigokro-127beongil, Nam-gu, Pohang, Gyeongbuk, Korea, Email: dmoon@postech.ac.kr

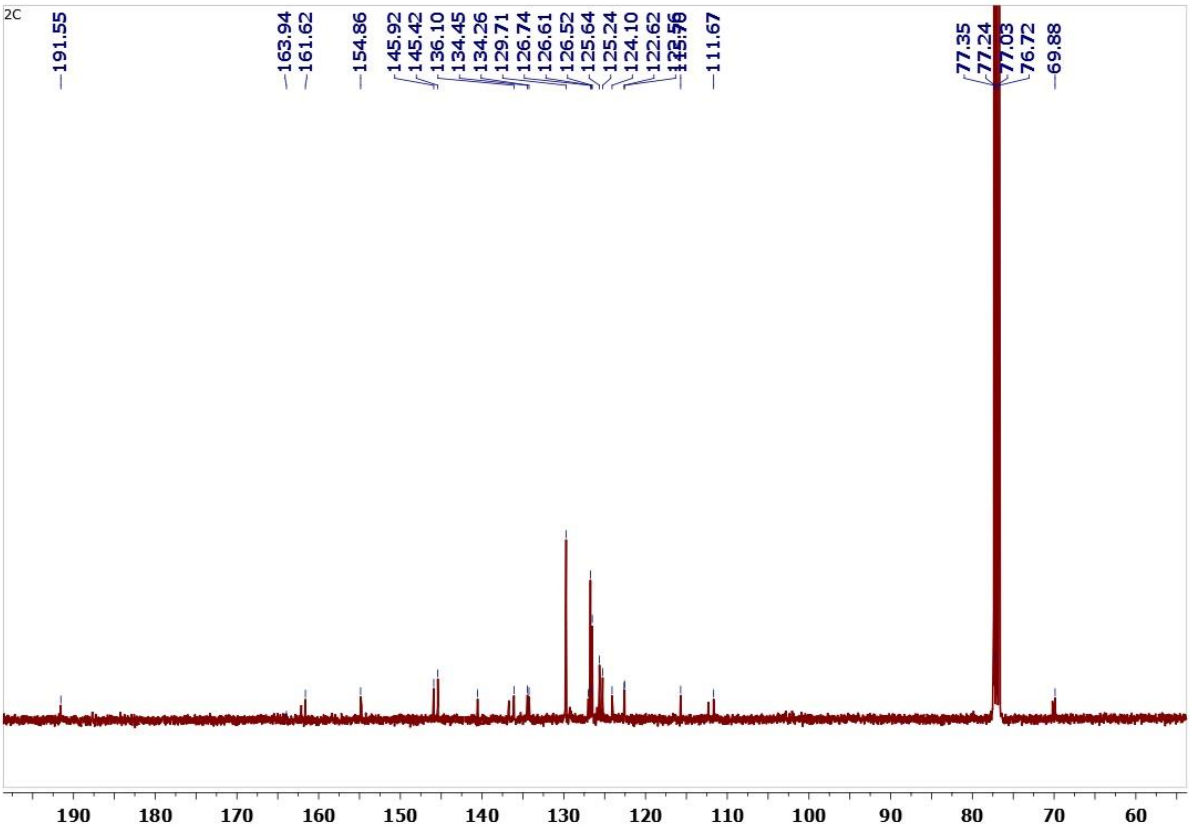


Scheme S1. Synthesis of isomers **1-3.**

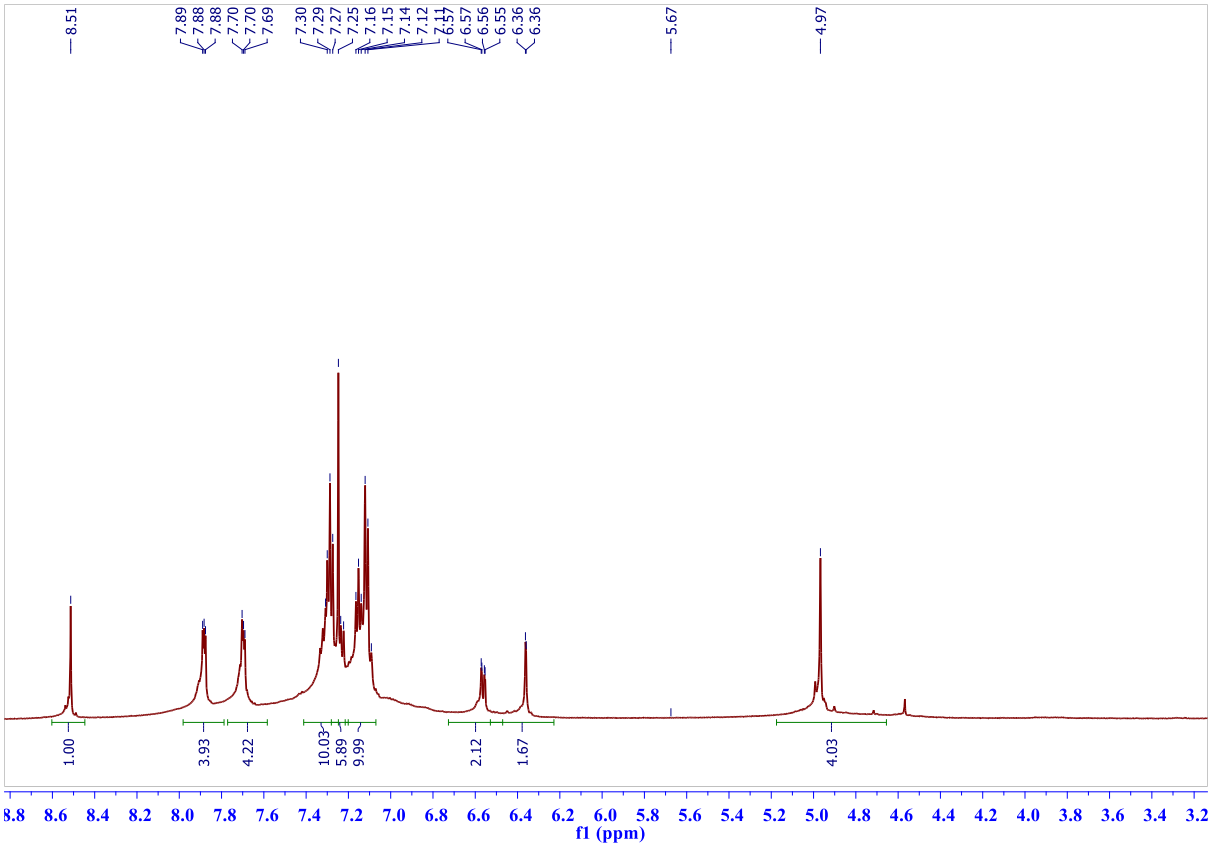


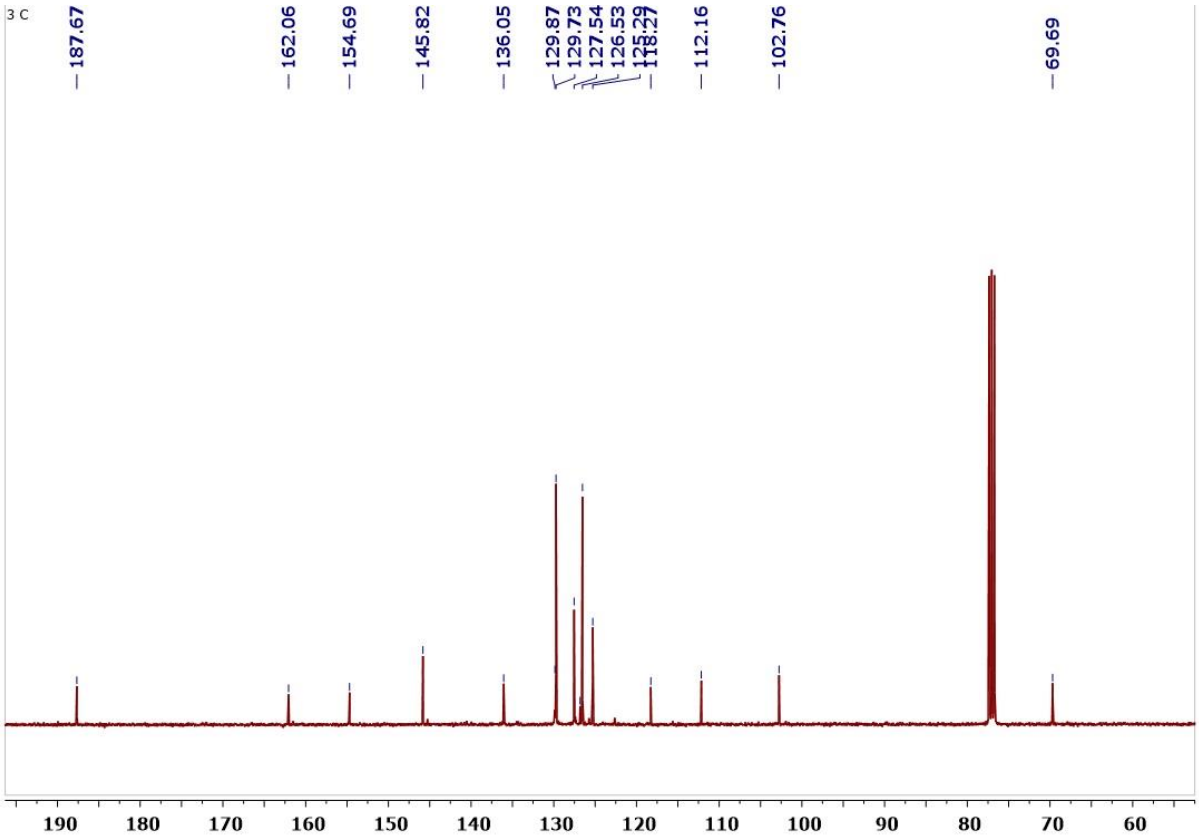
^{1}H and ^{13}C NMR of ***1.***



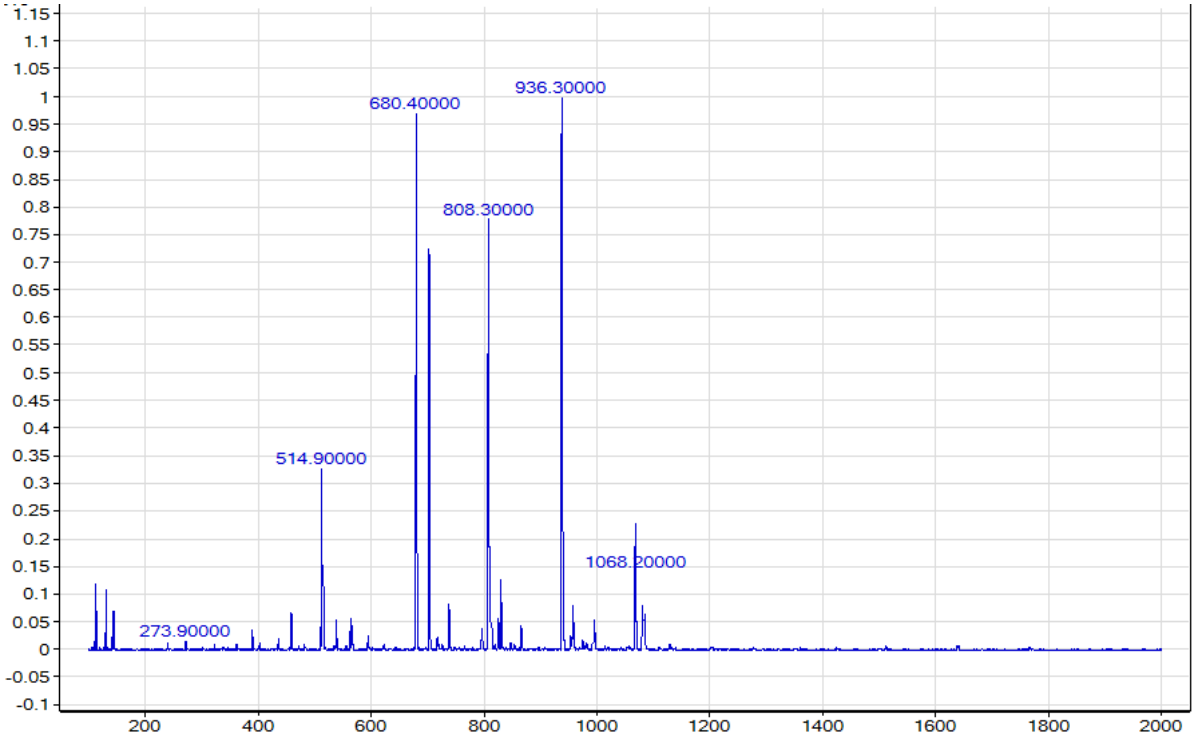


^{1}H and ^{13}C NMR of ***2.***

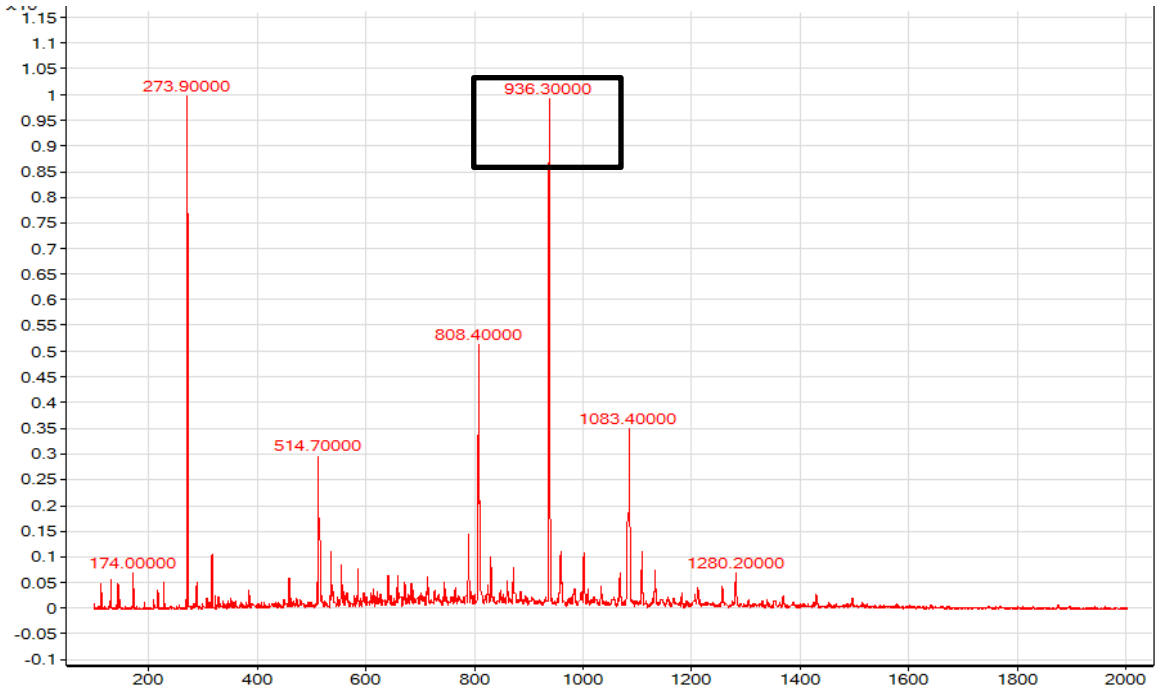




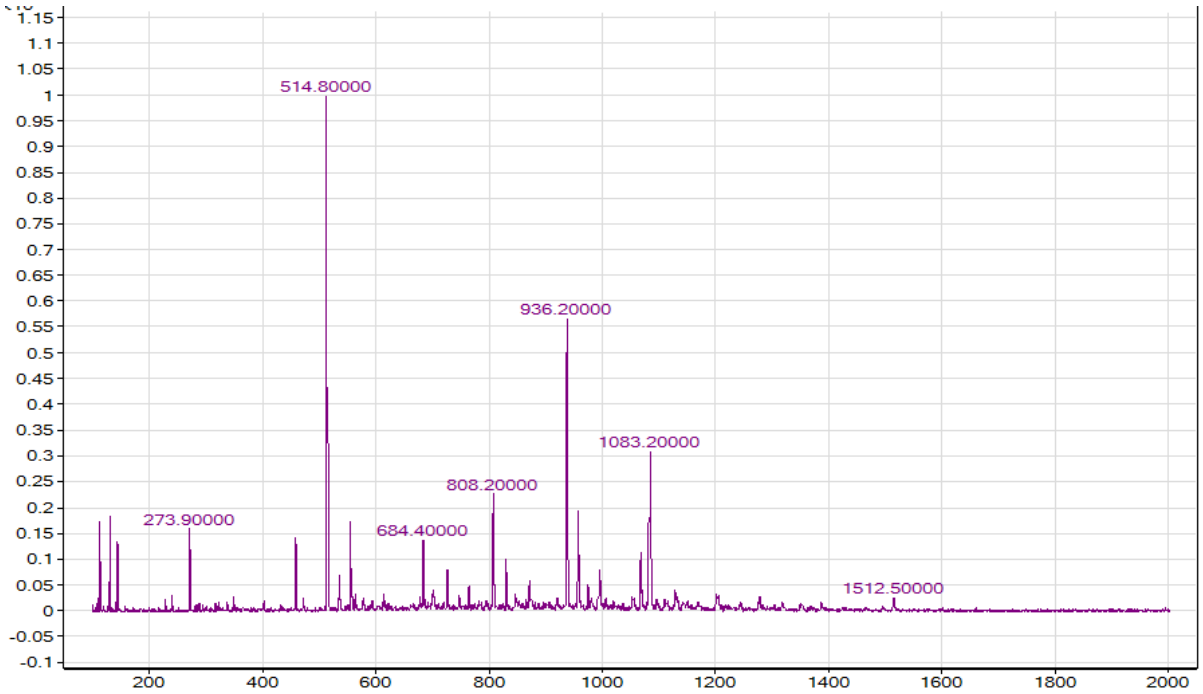
^{1}H and ^{13}C NMR of ***3.***



1: m/z calcd for $C_{64}H_{44}N_2O_6$ (M + H): 936.32, found: 936.30.



2: m/z calcd for $C_{64}H_{44}N_2O_6$ (M + H): 936.32, found: 936.30.



3: m/z calcd for $C_{64}H_{44}N_2O_6$ (M + H): 936.32, found: 936.20.

Table S1. **1-3** fluorescence efficiency in solution compared to fluorescein.

S.NO	Solvents	Quantum yield (Φ_F) compared to Fluorescein		
		1	**2**	**3**
1	CH_3CN	0.005	0.008	0.006
2	$CHCl_3$	0.047	0.078	0.074
3	DMF	0.016	0.029	0.021
4	DMSO	0.013	0.016	0.014
5	Ethyl acetate	0.021	0.037	0.028
6	Ethanol	0.005	0.004	0.003
7	Methanol	0.002	0.001	0.001
8	THF	0.021	0.045	0.060
9	Toluene	0.089	0.090	0.085

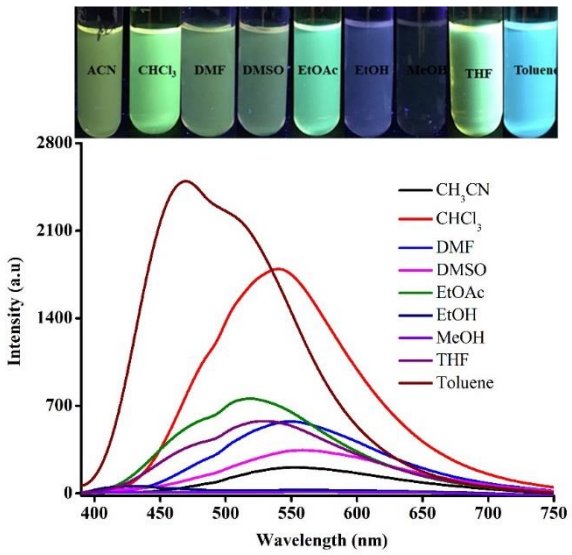


Figure S1. Digital images and fluorescence spectra of **3** in different solvents.

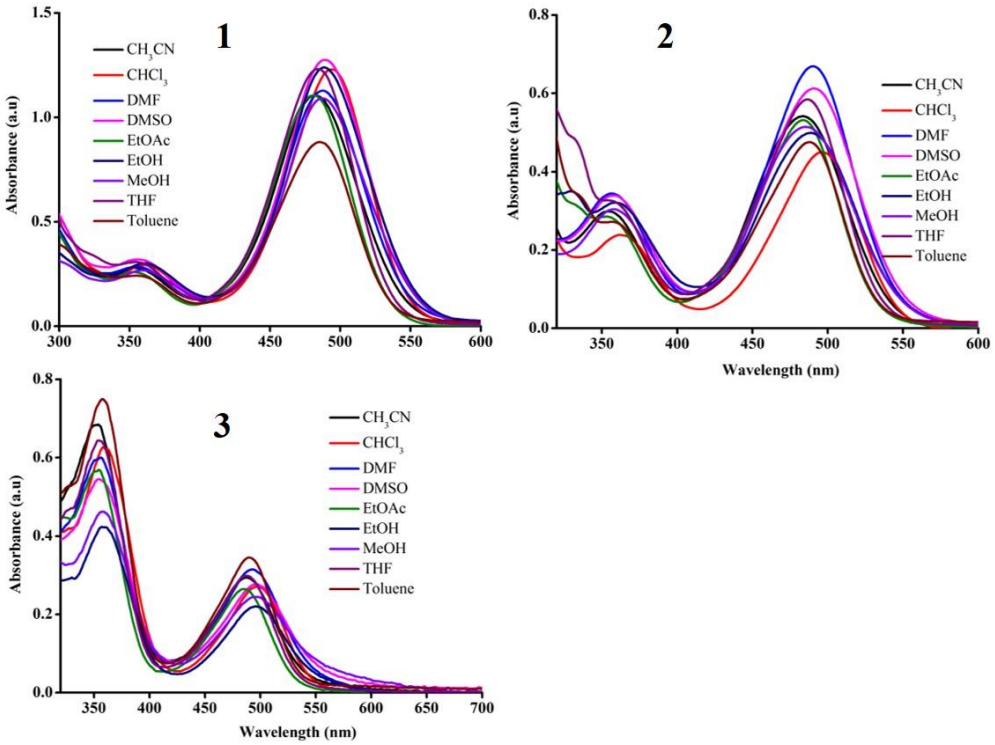


Figure S2. Absorption spectra of **1-3** in different solvents.

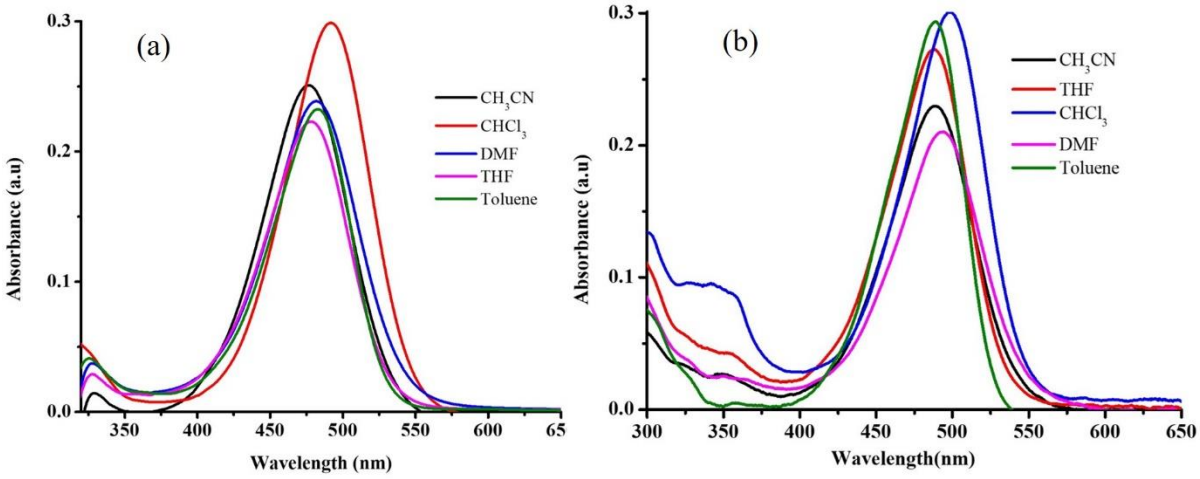


Figure S3. Absorption spectra of (a) TPA-indanedione and (b) 3-OCH_3TPA-indanedione**.**

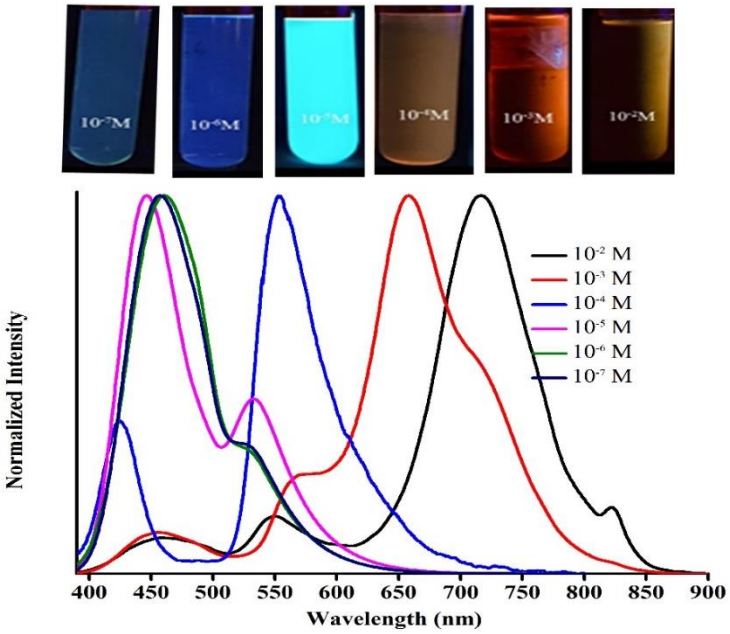


Figure S4. Concentration dependent fluorescence digital images and spectra of **2** (10^{-7} – 10^{-2} M) in $CHCl_3$. λexc = 365 nm (for digital images) and 370 nm (for spectra).

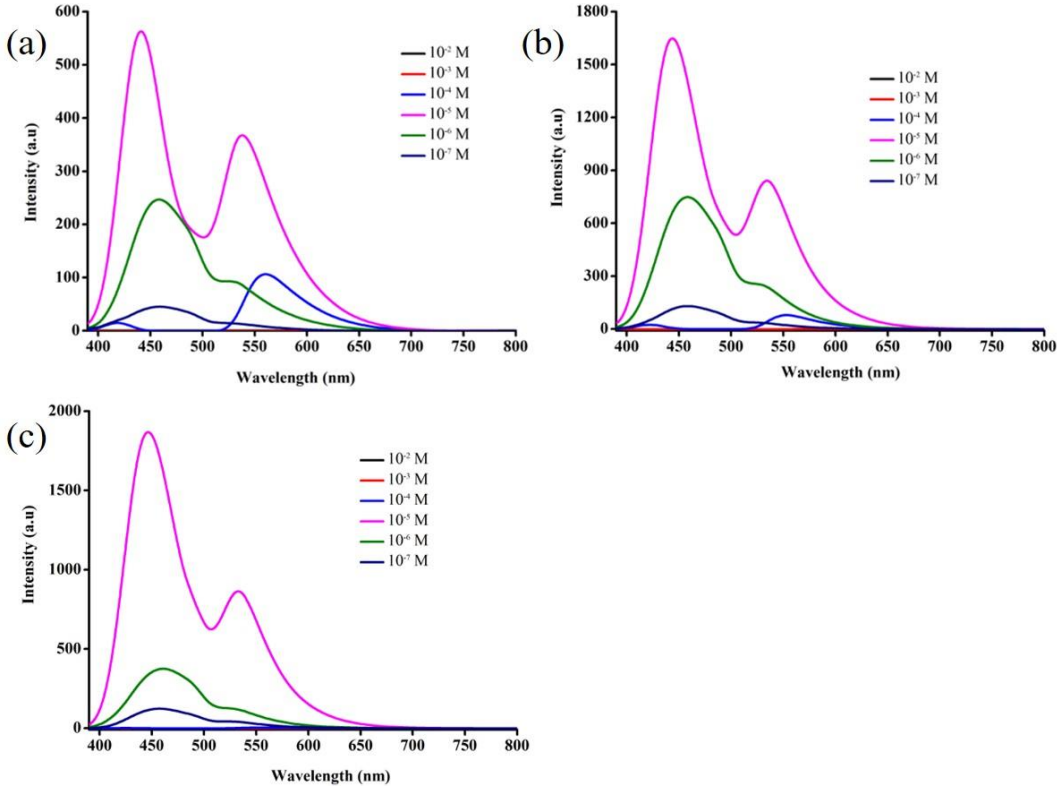


Figure S5. Concentration dependent fluorescence spectra of (a) **1**, (b) **2** and (c) **3** in $CHCl_3$.

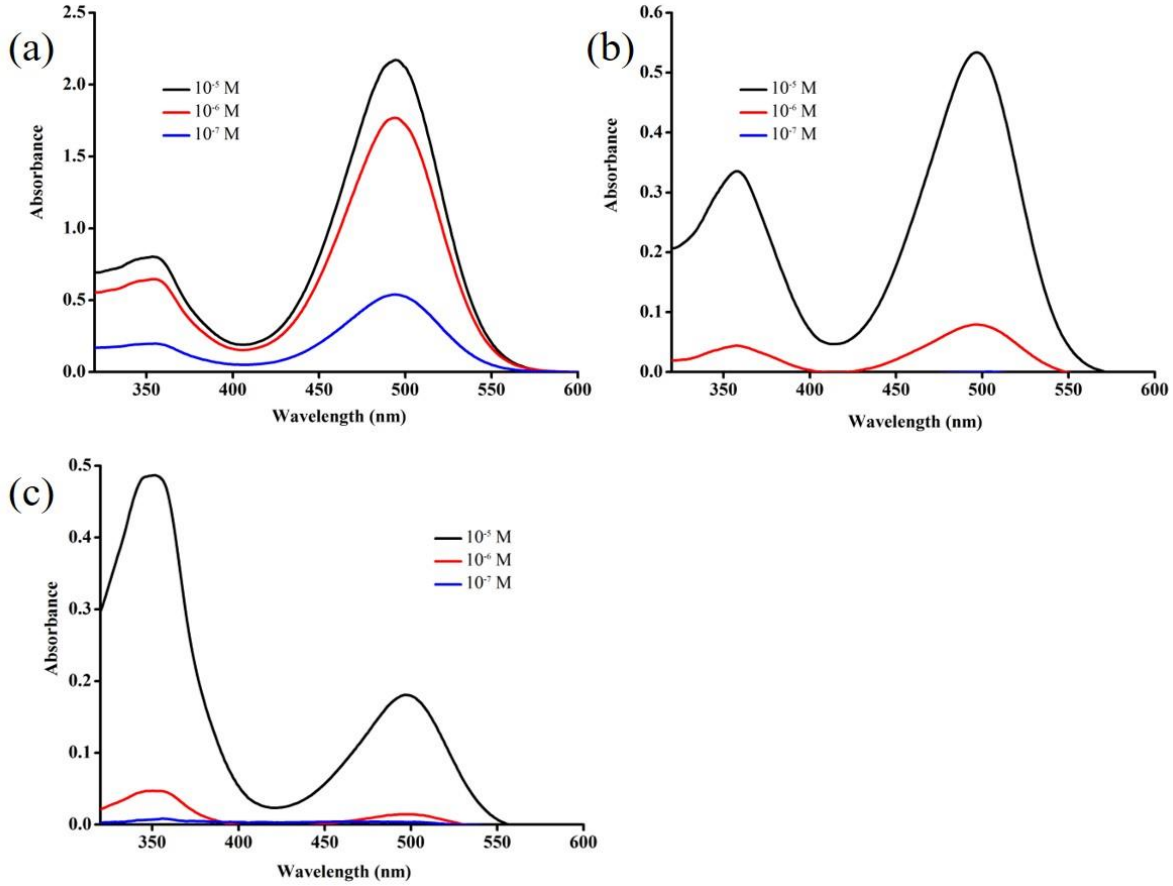


Figure S6. Concentration dependent absorption spectra of (a) **1**, (b) **2** and (c) **3** in $CHCl_3$.

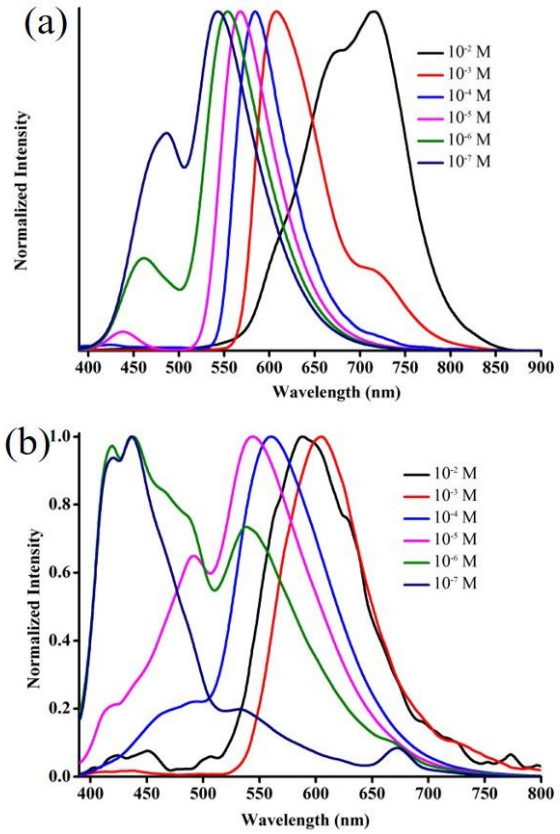


Figure S7. Concentration dependent fluorescence spectra of **1** in (a) THF and (b) DMSO.

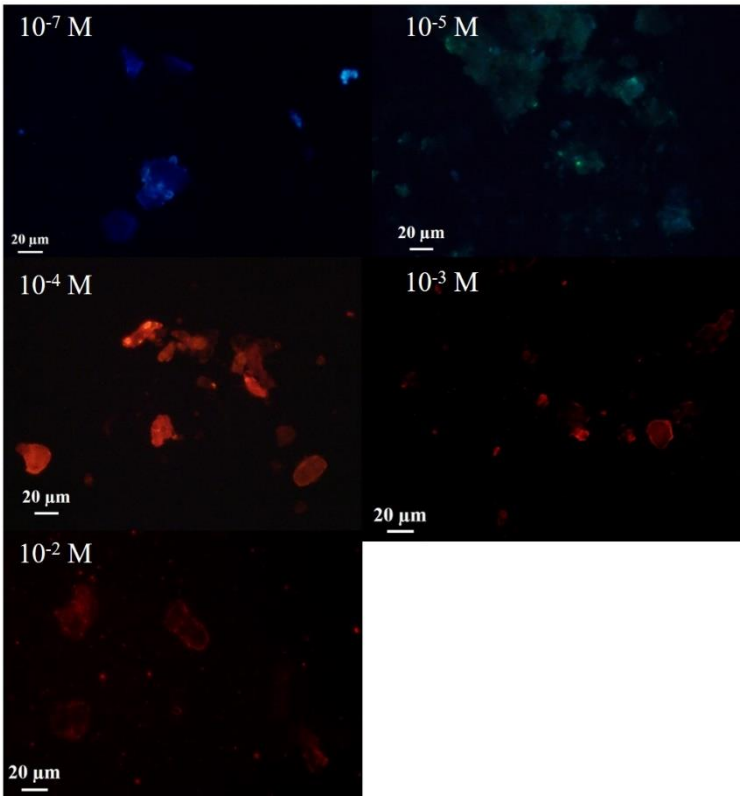


Figure S8. Confocal fluorescence microscopic images of **1**-PMMA composite thin films from different concentration.

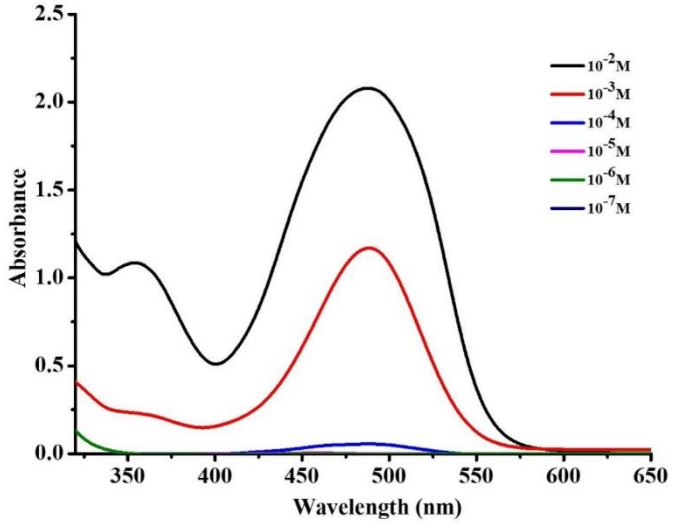


Figure S9. Concentration dependent absorption spectra of **1** in PMMA film.

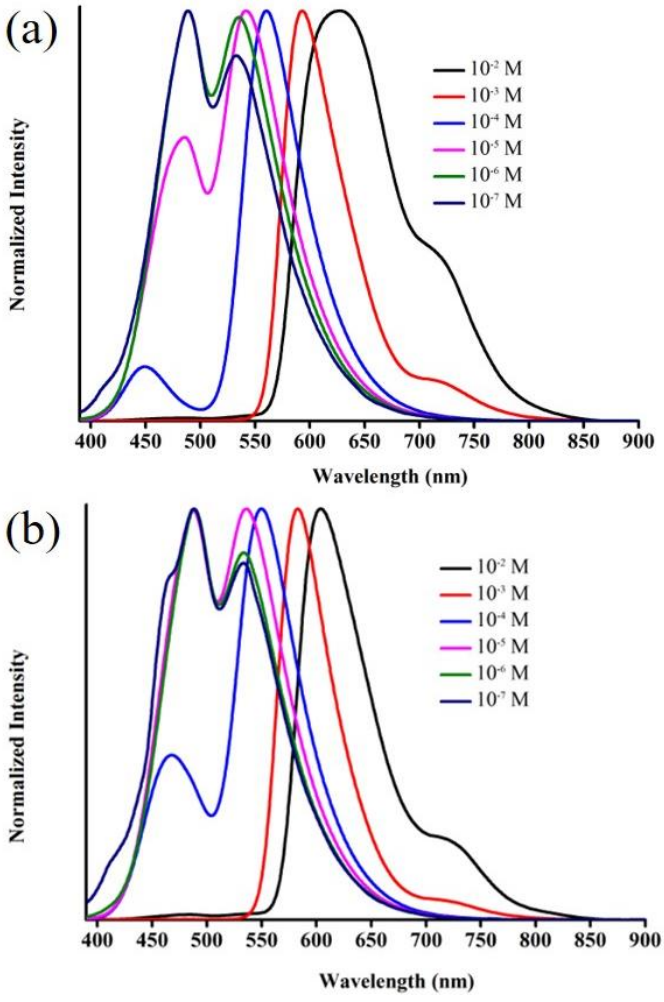


Figure S10. Concentration dependent fluorescence spectra of (a) **2** and (b) **3** in THF.

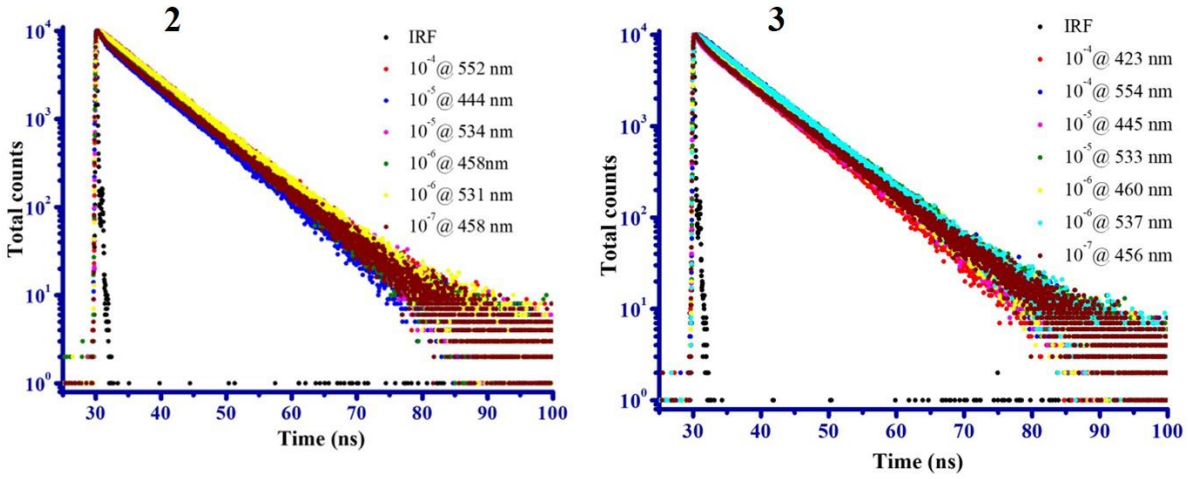


Fig. S11. Lifetime decay plot of **2** and **3** in $CHCl_3$ from 10^{-4} to 10^{-7} M.

Table S2. Fluorescence lifetime data of **2** in $CHCl_3$ at different concentration.

Conc.	λ_{em} (nm)	B_1 (%)	B_2 (%)	τ_1 (ns)	τ_2 (ns)	χ^2
10^{-4}	552	0.61	99.39	3.774 ± 0.065	7.240 ± 0.033	1.1
10^{-5}	444	5.83	94.17	0.97 ± 0.061	7.103 ± 0.02	1.02
10^{-5}	534	1.78	98.22	3.695 ± 0.082	7.226 ± 0.034	1.08
10-6	458	4.36	95.64	1.16 ± 0.091	7.354 ± 0.021	1.11
10^{-6}	531	1.12	98.88	3.919 ± 1.548	7.421 ± 0.038	1.17
10^{-7}	458	4.81	95.19	1.073 ± 0.080	7.353 ± 0.02	1.06

Table S3. Fluorescence lifetime data of **3** in $CHCl_3$ at different concentration.

Conc.	λ_{em} (nm)	B_1 (%)	B_2 (%)	τ_1 (ns)	τ_2 (ns)	χ^2
10^{-4}	423	4.57	95.43	1.009 ± 0.0822	7.298 ± 0.019	1.02
10^{-4}	554	2.7	97.3	3.803 ± 0.065	7.308 ± 0.034	1.14
10^{-5}	445	3.94	96.06	0.874 ± 0.069	7.558 ± 0.022	1.05
10^{-5}	533	0.82	99.18	3.966 ± 0.067	7.662 ± 0.035	1.07
10^{-6}	460	3.46	96.54	1.103 ± 0.114	7.554 ± 0.019	1.1
10^{-6}	537	10.13	89.87	6.670 ± 2.791	7.695 ± 0.189	1.13
10^{-7}	456	5.48	94.52	1.242 ± 0.072	7.691 ± 0.022	1.06

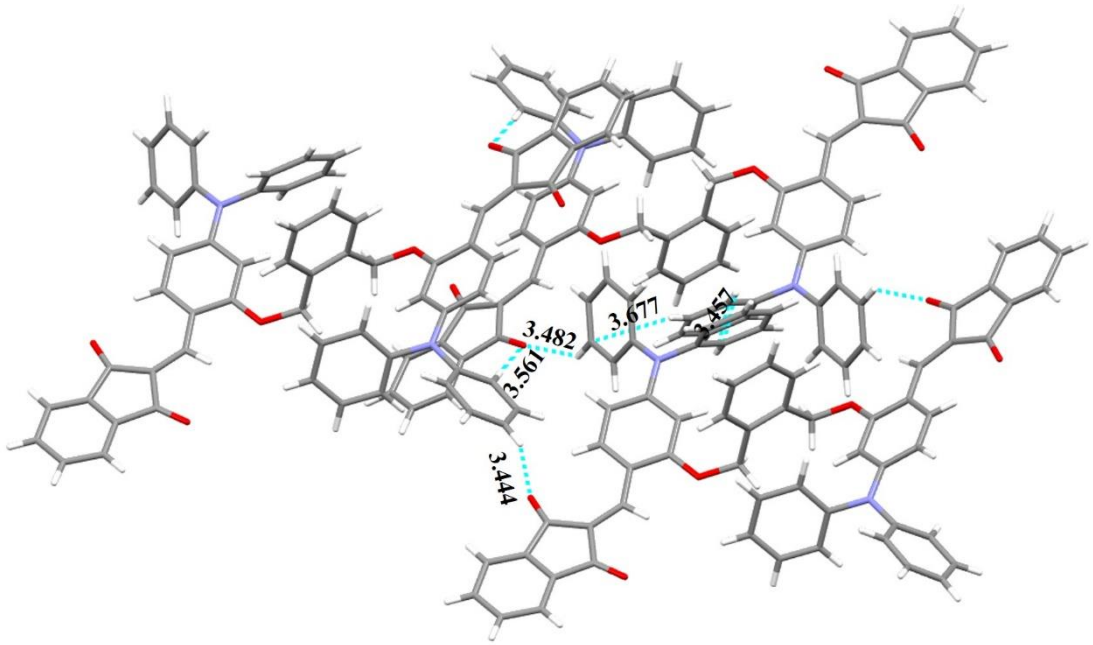


Fig. S12. Intermolecular interactions in the crystal lattice of **1**. C (grey), H (white), O (red) and N (blue). Dotted lines indicate the H-bonding and C-H…π interactions in Å.

Table S4. Solid state fluorescence data of 1-3 and corresponding single AIEgen.

1		**2**		**3**		**3-OMe-TPA**	
λ_{max} (nm)	**Φ_f (%)**	**λ_{max} (nm)**	**Φ_f (%)**	**λ_{max} (nm)**	**Φ_f (%)**	**λ_{max} (nm)**	**Φ_f (%)**
498,622, 708	2.3	434, 536	5.3	439, 594	4.0	611	19.4

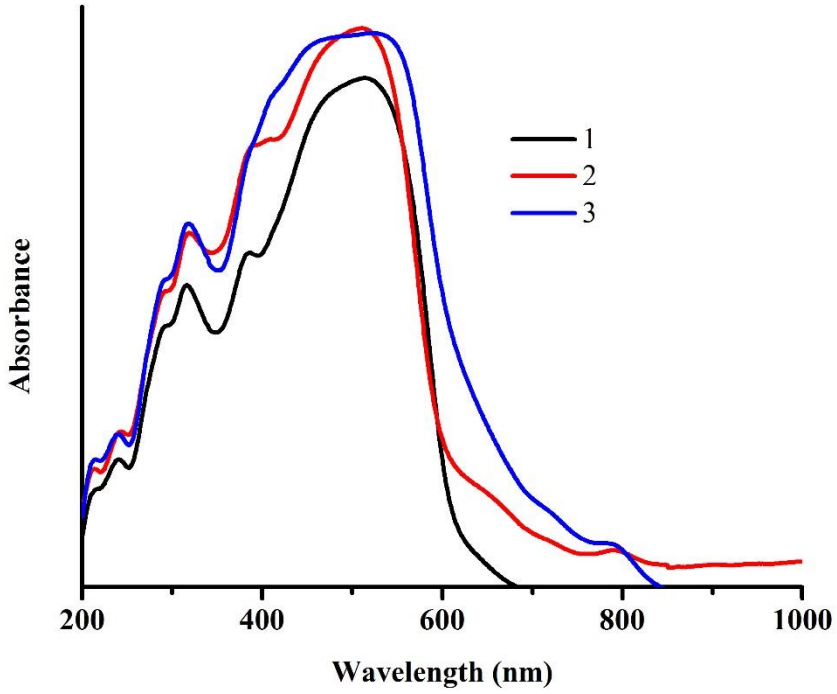


Figure S13. Solid state absorption spectra of **1-3**.

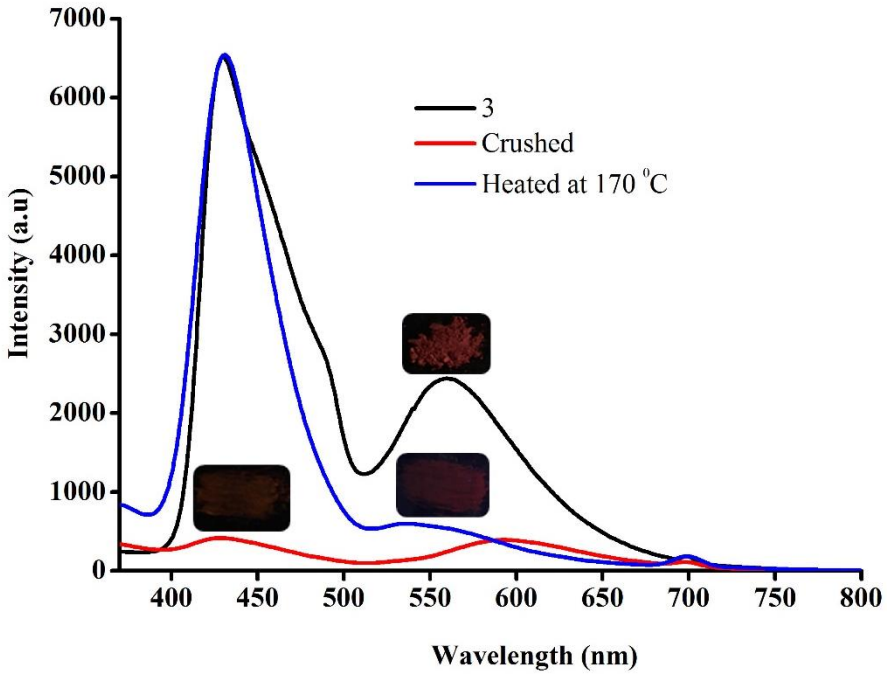


Figure S14. Mechanofluorochromism of **3**.

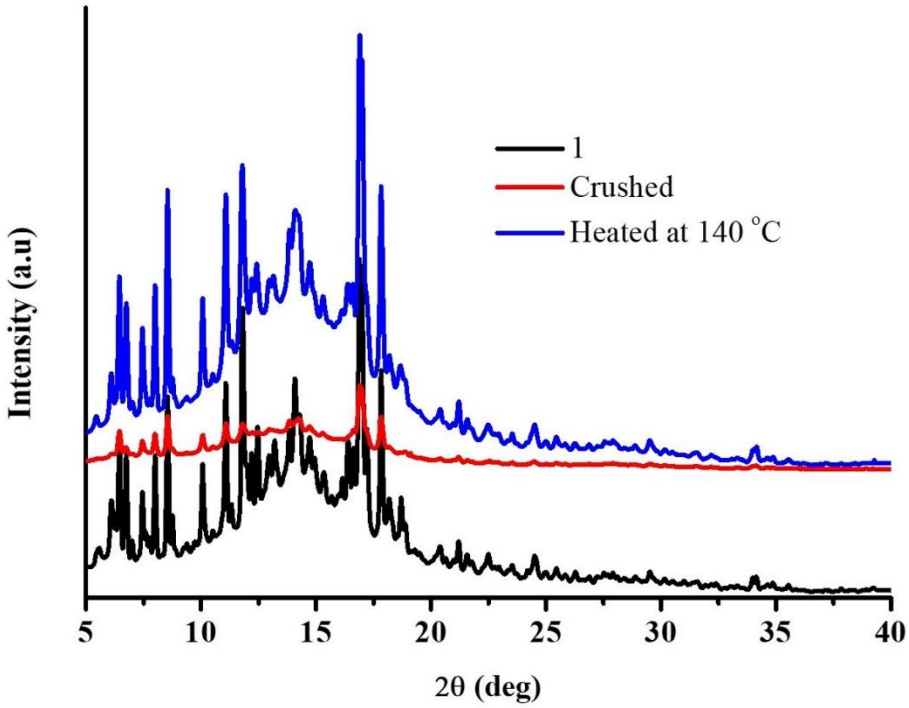


Figure S15. PXRD pattern of **1**.

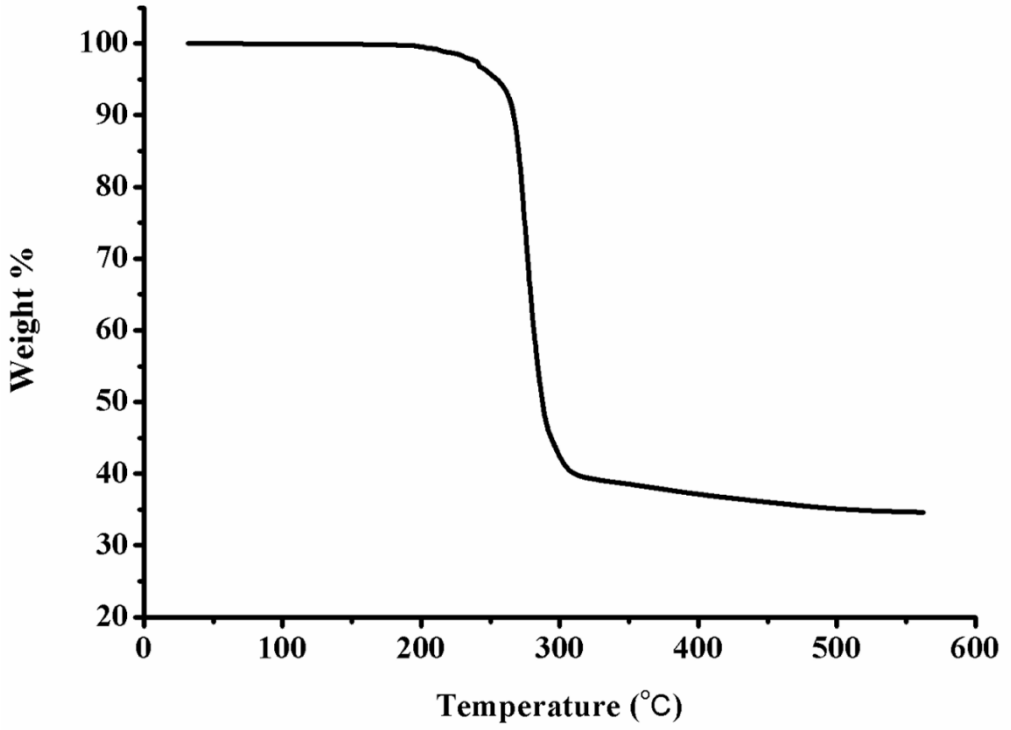


Figure S16. Thermogravimeric analysis of **1**.