Supporting Informations

For

Flanking-donor controlled diversity in mechanical-force-induced reversible fluorochromism and enhanced emission for carboxylic acid and ester-linked solid-state emitters

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Contents:

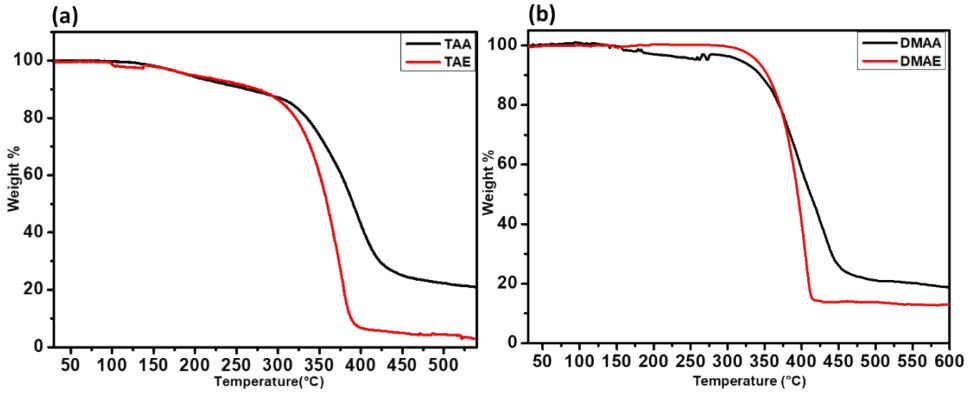


Figure S1: TGA thermogram for (a) **TAA/ TAE** and (b) **DMAA/DMAE**

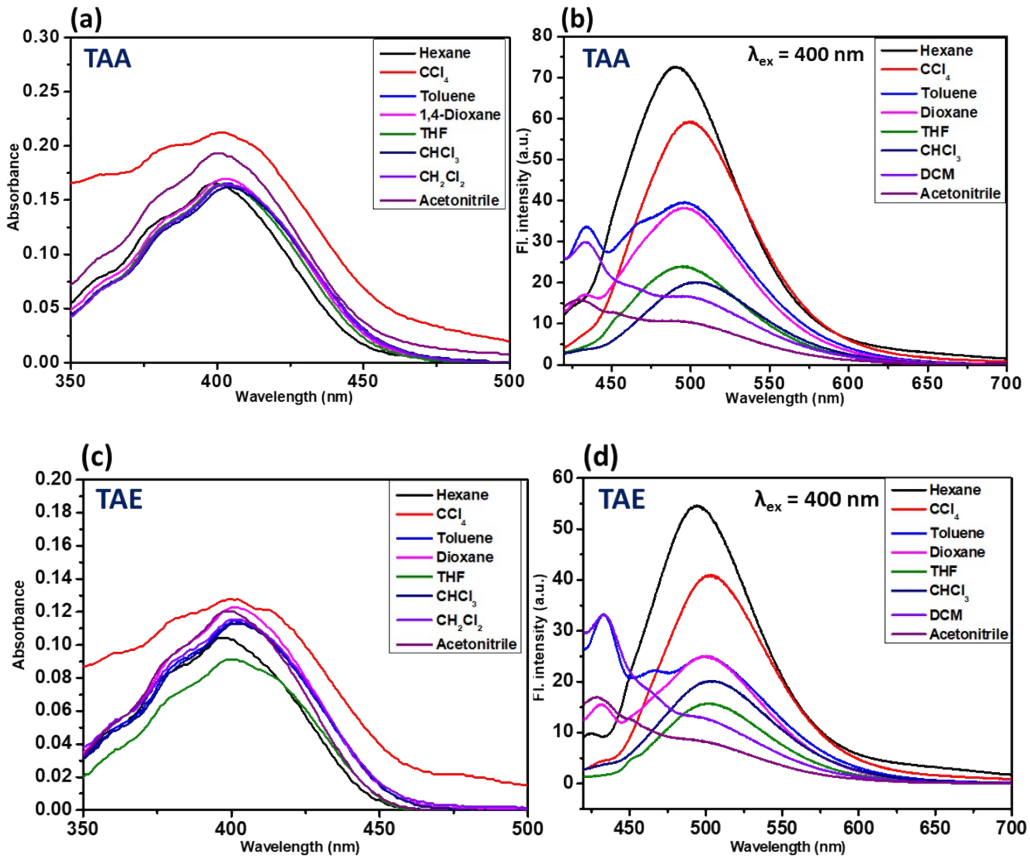


Figure S2: Absorbance and emission spectra of TAA/TAE in various solvents.

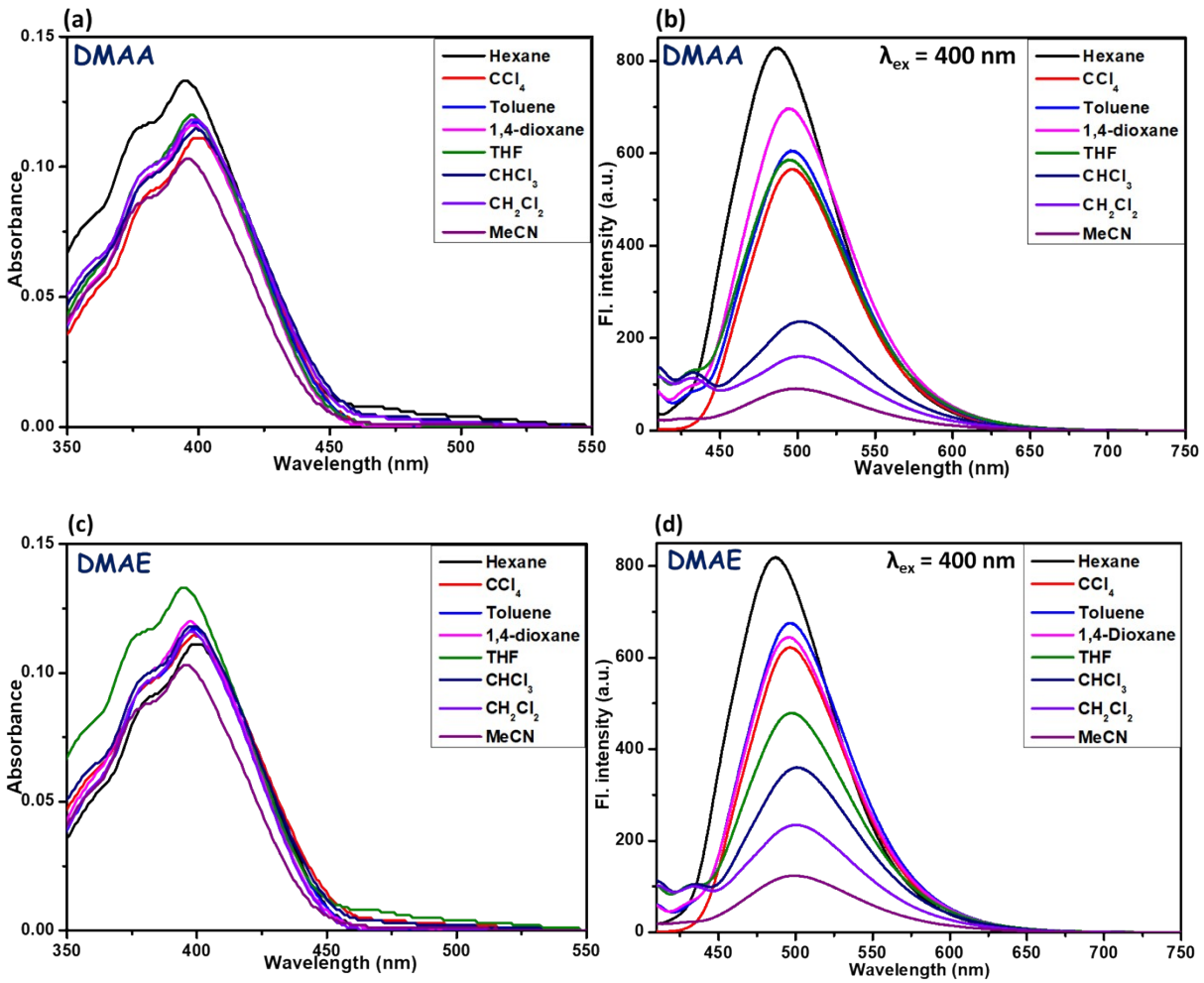


Figure S3: Absorbance and emission spectra of DMAA/DMAE in various solvents.

Table S1: Absorbance and emission values of all the compounds with various solvents

Solvents	**$\lambda_{abs.}$ / λ_{em} (nm) for TAA**	**$\lambda_{abs.}$ / λ_{em} (nm) for TAE**	**$\lambda_{abs.}$ / λ_{em} (nm) for DMAA**	**$\lambda_{abs.}$ / λ_{em} (nm) for DMAE**
Hexane	400/ 490	396/ 494	395/ 487.4	395/ 486.6
CCl_4	403/ 499	401/ 502	400/ 496.2	400/ 496.4
Toluene	404/ 433; 493	401/ 433; 499	399/ 497.2	399/ 496.2
1,4-Dioxane	403/ 432; 494	401/ 431; 499	398/ 495.4	398/ 496.2
THF	403/ 495	400/ 503	398/ 495.2	398/ 498.2

$CHCl_3$	404/ 503	401/ 503	399/ 502	399/ 501
CH_2Cl_2	400/ 435; 498	401/ 433; 494	399/ 502.4	399/ 500.4
MeCN	403/ 429; 491	398/ 429; 494	396/ 498.8	397/ 499.8

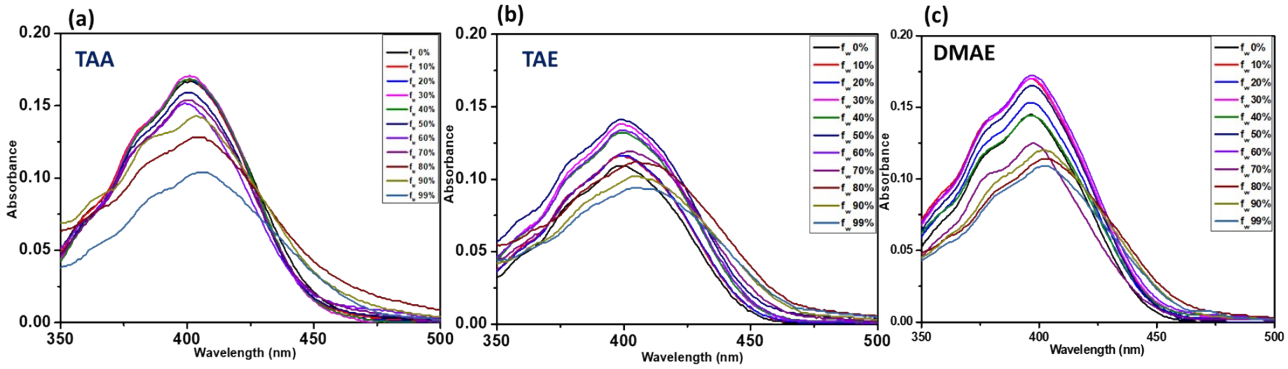


Figure S4: Absorption spectra of (a) **TAA** (b) **TAE** [λ_{ex} = 400 nm] and (c) **DMAE** [λ_{ex} = 396 nm] upon water addition with 10 μM probe in acetonitrile.

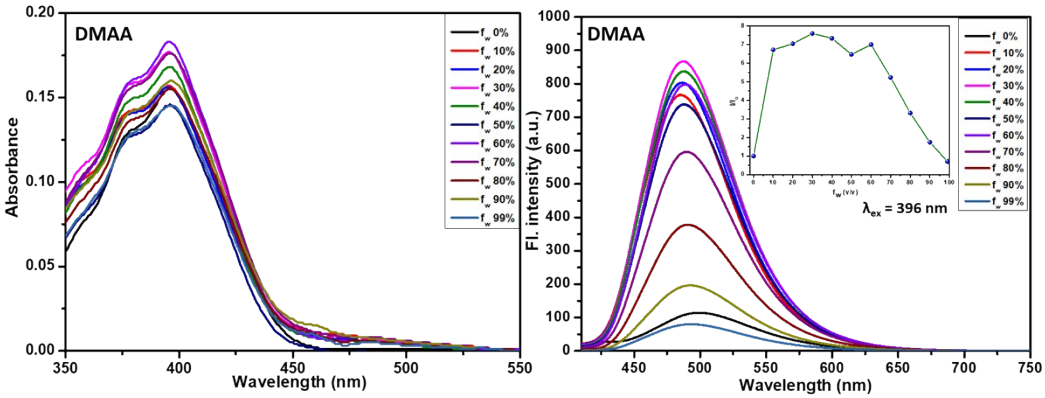


Figure S5: Absorption and Emission spectra of **DMAA** [λ_{ex} = 396 nm] upon water addition with 10 μM probe in acetonitrile.

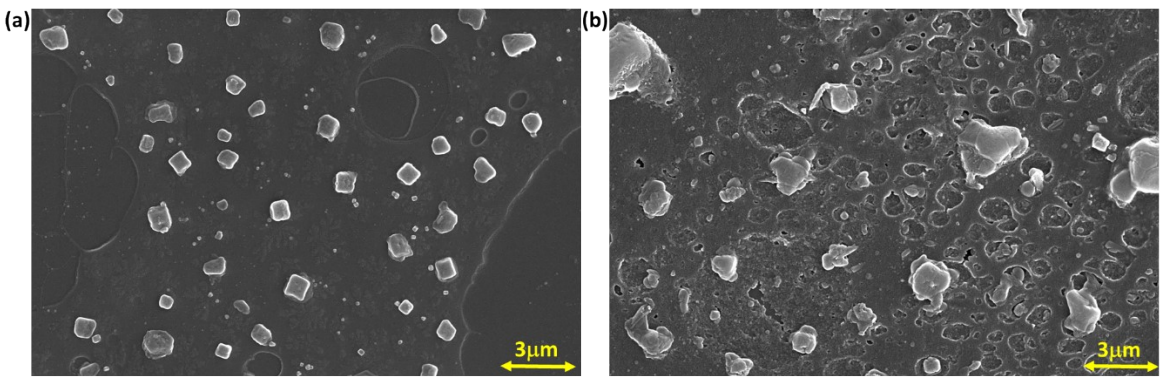


Figure S6: FE-SEM images of TAE at (a) f_w. = 80% (Aggregated State) and (b) f_w. = 90% (decreased emission state) [drop casted on silicon wafer].

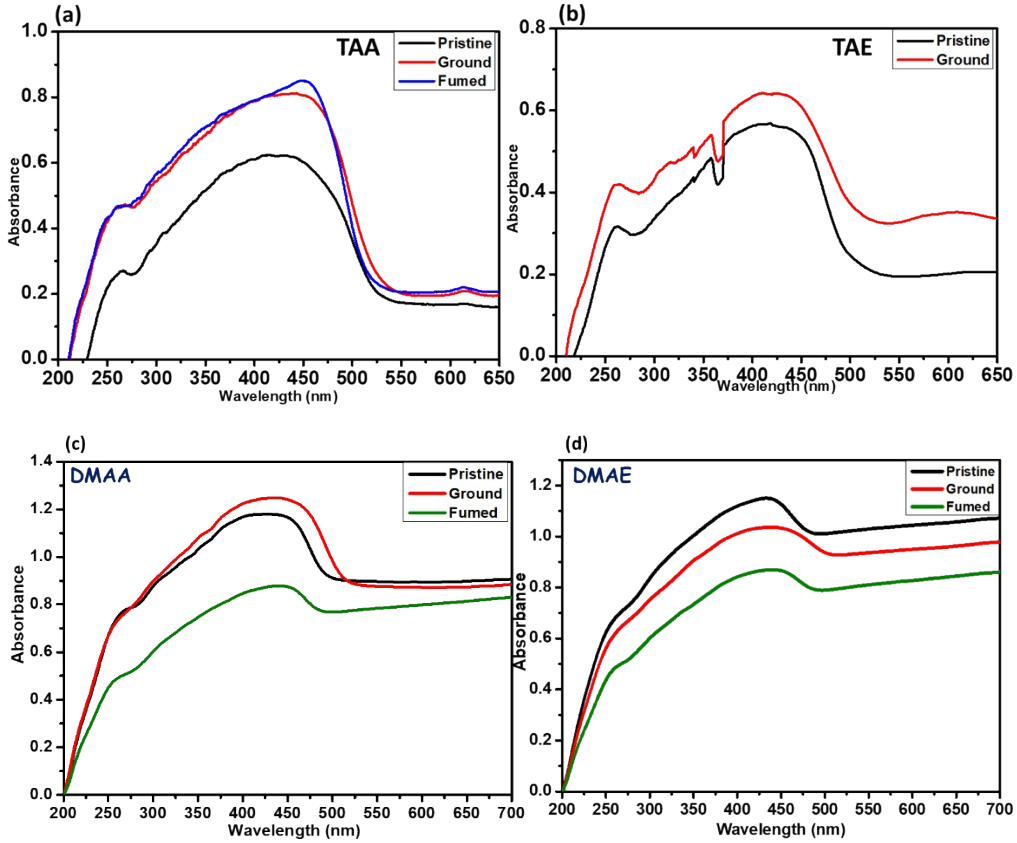


Figure S7: Solid-state absorption spectra of (a) **TAA**, (b) **TAE**, (c) **DMAA** and (d) **DMAE** before and after grinding

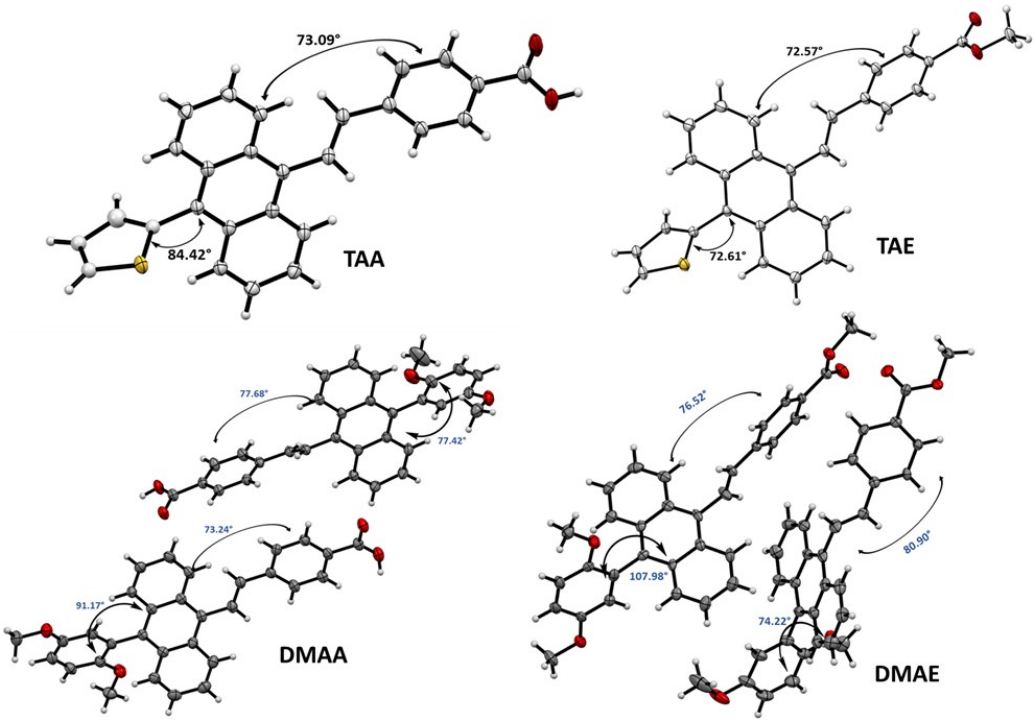


Figure S8: ORTEP diagram of **TAA**, **TAE**, **DMAA** and **DMAE** with 50% probability level

Table S2: List of various intermolecular interactions (Å) of **TAA**/**TAE**

Compounds	C···H	H···H	O···H	O···O
TAE (9 interactions) (5 C-H···π interactions)	2.872 (C-H···π) 2.781 (C-H···π) 2.869 (C-H···π) 2.827 2.775 (C-H···π) 2.897 (C-H···π)	2.375	2.474 (C-H···O) 2.542 (C-H···O)	
TAA (8 interactions) (4 C-H···π interactions)	2.859 (C-H···π) 2.792 (C-H···π) 2.625 2.880 (C-H···π) 2.830 (C-H···π)	2.371	1.733 (O-H···O)	2.614

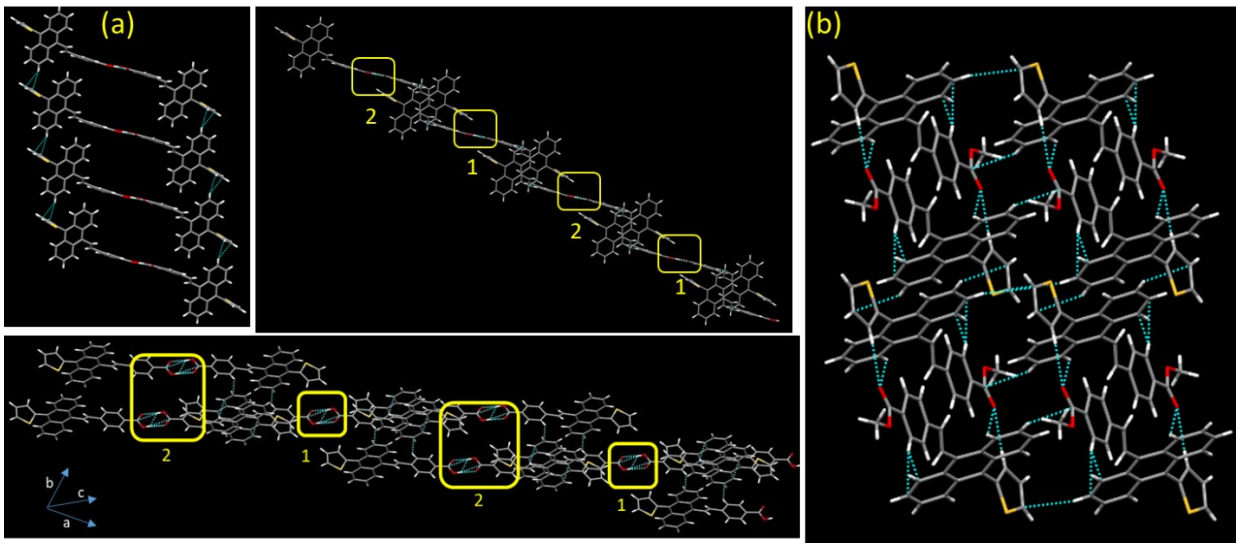


Figure S9: The packing pattern of **(a) TAA (b) TAE** ***(a-axis view)***

Table S3: List of various intermolecular interactions (Å) of **DMAA/DMAE**

Compounds	C···H	C···C	C···O	H···H	O···H	O···O
DMAE (22 interactions) (7 C-H···π interactions) **Eight interactions are from DMB (bold)**	2.841 (C-H···π) 2.892 (C-H···π) **2.853 (C-H···π)** **2.817 (C-H···π)** 2.898 (C-H···π) 2.802 (C-H···π) 2.828 (C-H···π)	**3.349** (not π···π) **3.390** (not π···π)	3.201 3.178 3.204 3.211	2.354	**2.701** **2.684** 2.594 2.668 2.713 **2.507** 2.649 **2.621**	
DMAA (21 interactions) (9 C-H···π interactions) **Nine interactions are from DMB (bold)**	2.894 (C-H···π) **2.899 (C-H···π)** **2.900 (C-H···π)** 2.549 **2.829 (C-H···π)** **2.845 (C-H···π)** **2.824 (C-H···π)** **2.778 (C-H···π)** **2.762 (C-H···π)** 2.865 (C-H···π)	3.326 (π···π) 3.373 (not π···π) 3.342 (π···π)		2.163 2.373 **2.342**	1.769 (O-H···O) **2.456 (C-H···O)**	2.590 2.618

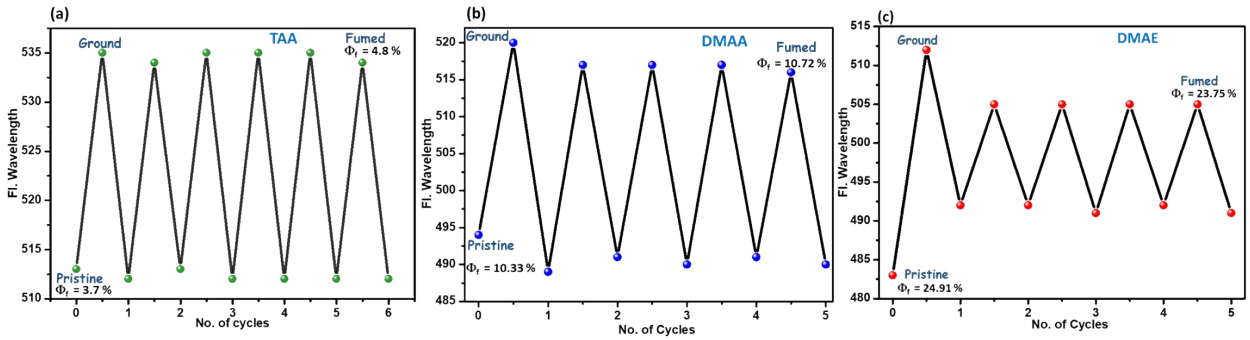


Figure S10: The plot of change in maximum emission wavelength with multiple grinding/fuming process.

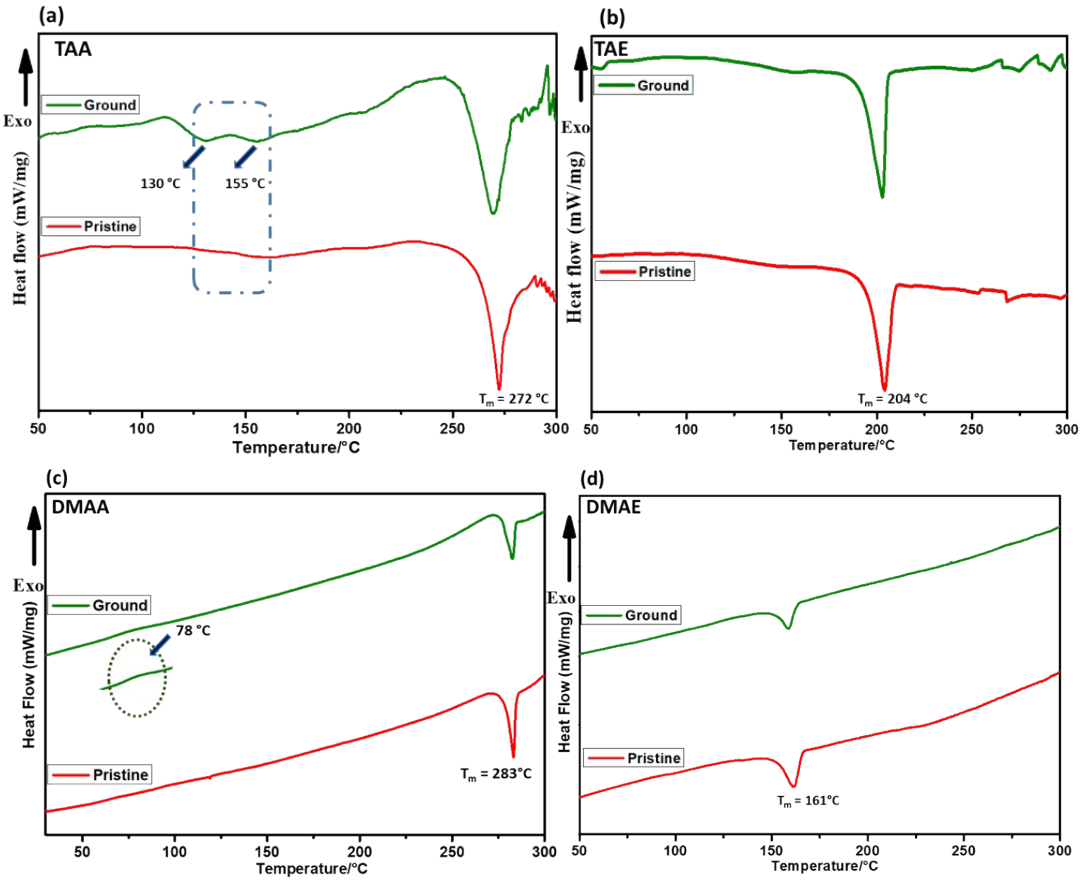


Figure S11: DSC analysis of (a) **TAA** (b) **TAE** (c) **DMAA** (d) **DMA**

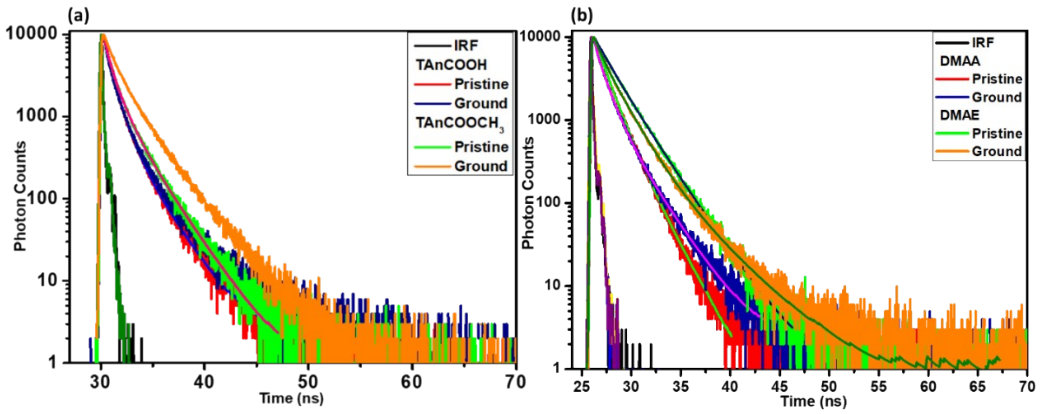


Figure S12: Lifetime plot for (a) **TAA**; **TAE** (b) **DMAA**; **DMAE**

Compounds	States	α_1	α_2	α_3	τ_1	τ_2	τ_3	$\langle\tau\rangle$	χ^2
TAA	Pristine	0.37	0.56	0.06	0.88	0.27	2.26	0.63	1.02
	Ground	0.34	0.62	0.03	1.04	0.30	2.74	0.64	1.06

TAE	Pristine	0.32	0.11	0.57	0.96	2.31	0.28	0.73	1.16
	Ground	0.38	0.40	0.21	1.29	0.35	2.74	0.77	1.04
DMAA	Pristine	0.25	0.63	0.12	0.26	1.2	2.12	1.07	1.05
	Ground	0.36	0.09	0.54	1.06	2.48	0.22	0.75	1.04
DMAE	Pristine	0.28	0.39	0.31	1.55	2.52	0.23	1.52	1.06
	Ground	0.37	0.57	0.05	0.44	1.82	3.99	1.43	1.01

Table S4: Lifetime Parameters (τ; ns) measurement of excited state. λ_{ex}= 405 nm

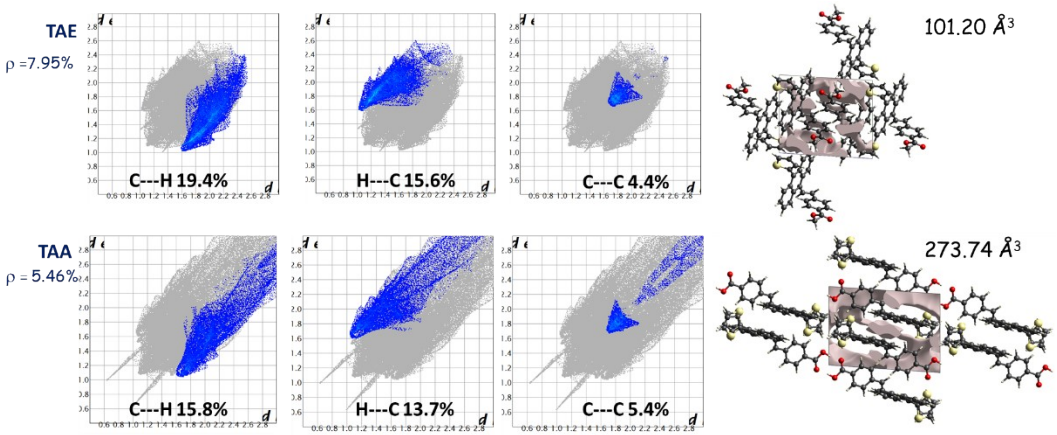
Table S5: Solid state photophysical parameters for all the compounds with absorption and emission wavelength

Samples	**States**	**λ^{max}_{abs}(nm)**	**λ^{max}_{em} (nm)**	**Φ_f (%)**	**<τ>**	**k_r/k_{nr} (in s^{-1})**
TAA	Pristine	415	512	3.7	0.62	0.06/1.55
	Ground	442	535	5	0.64	0.08/1.48
TAE	Pristine	419	491	2.7	0.73	0.04/1.33
	Ground	420	492	10	0.77	0.13/1.17
DMAA	Pristine	429	494	10.33	1.07	0.096/0.838
	Ground	437	520	31.33	0.75	0.418/0.916
DMAE	Pristine	434	483	24.91	1.52	0.164/0.494
	Ground	440	512	42.64	1.43	0.298/0.401

Table S6: Quantitative interactions (%) of all the compounds

Type of Interactions	**TAE**	**TAA**	**DMAE**	**DMAA**
C···H	19.4	15.8	16.6	15.7
H···C	15.6	13.7	13.4	12.9

H···H	43.6	50.7	52.4	49.5
C···C	4.4	5.4	1.1	4.7
C···O	0.4	1	0.8	0.5
C···S	0.2	0	-	-
O···H	5	6.5	7.9	8.1
O···C	0.3	0.5	3.9	0.7
O···O	-	-	0.2	1
S···S	0.6	0	-	-
S···H	3.9	0.7	-	-
S···C	0.2	0	-	-
H···S	2.5	0.7	-	-
H···O	4	4.9	6.9	7.2



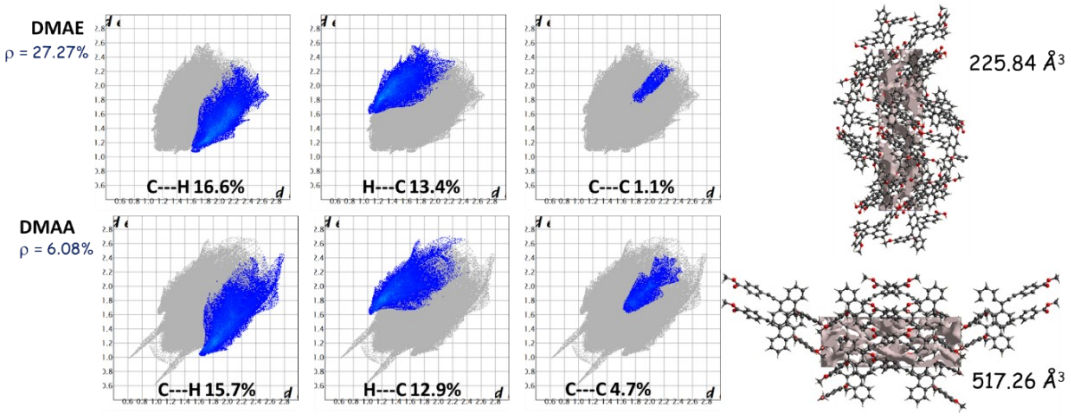


Figure S13: d_{norm} Hirshfeld surfaces for **TAA**, **TAE**, **DMAE** and **DMAA** and their 2D finger plots of C…H, H…C and C…C interactions

Table S7: Crystallographic parameters of all the compounds

Compounds	TAE	TAA	DMAE	DMAA
Emp. Formula	$C_{28}H_{20}O_2S$	$C_{27}H_{18}O_2S$	$C_{32}H_{26}O_4$	$C_{31}H_{24}O_4$
Formula Weight	420.50	406.47	474.525	459.49
Crystal System	Triclinic	Triclinic	Monoclinic	Monoclinic
Space Group	P-1	P-1	P-2_1	P-2_1/c
a /Å	8.9516	9.2745	12.0602	15.2306
b /Å	10.6649	9.8947	8.4487	33.5647
c /Å	12.0474	13.5650	23.7592	9.16660
α/degree	81.820	86.663	90	90
β/degree	77.034	81.113	92.455	93.3160
γ/degree	67.133	72.576	90	90
V /Å^3	1030.78(8)	1170.74 (4)	2418.67(14)	4678.22(11)
Z	4	2	2	8
$\rho_{calc.}$ /g cm-3	2.710	1.153	1.303	1.305
μ /mm^{-1}	3.146	1.370	0.680	0.687
F (000)	880.0	424	1000	1928
Data/ restraints/ parameters	4331/0/281	4914/1/282	6832/1/655	9936/0/636
S	1.080	1.093	1.069	1.036
R1 [I>2σ(I)]	0.0543	0.0402	0.1054	0.059
wR2 [all data]	0.1648	0.1249	0.2986	0.1646
Max/min. residual electron dens. [eÅ^{-3}]	0.34/-0.64	0.25/-0.30	1.16/-0.46	0.68/-0.39

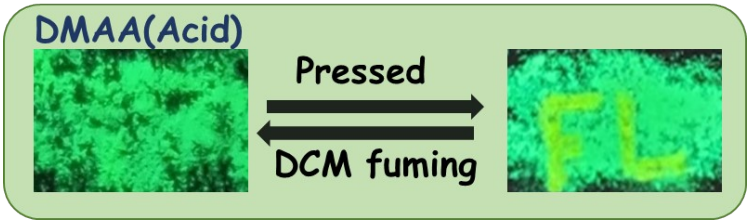


Figure S14: Application of DMAA as a rewritable optical recorder

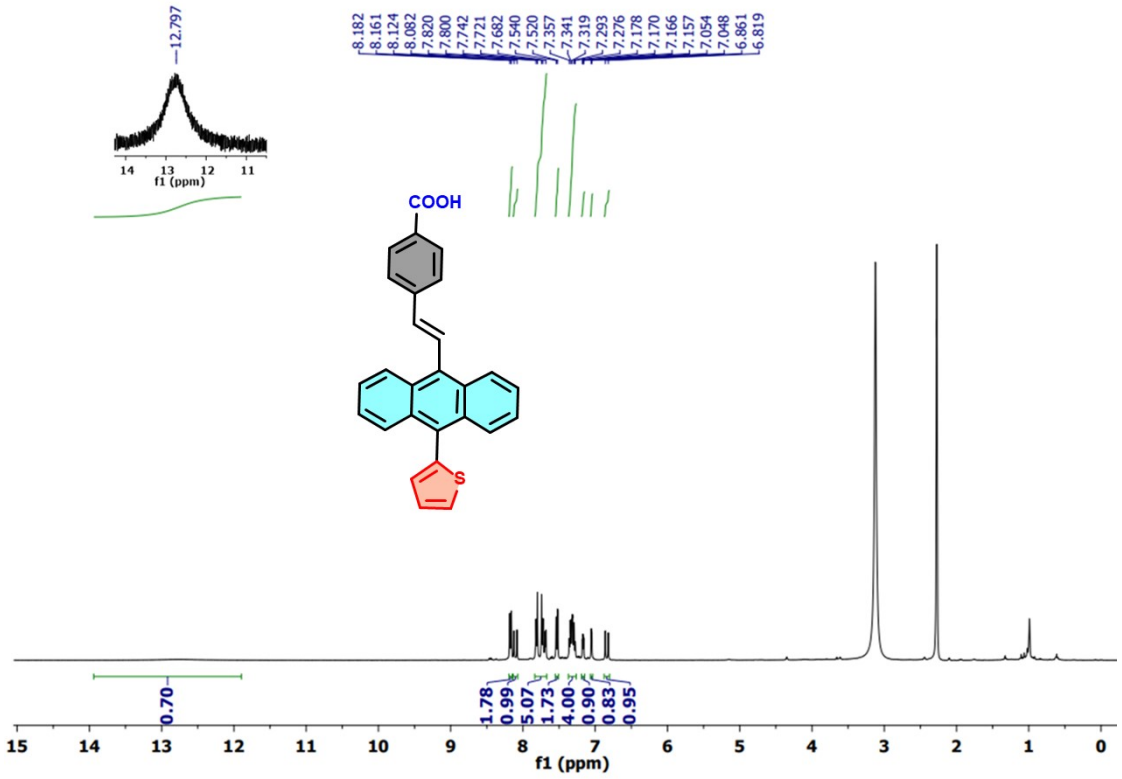


Figure S15: ^{1}H-NMR spectrum of **TAA** in DMSO-d_6

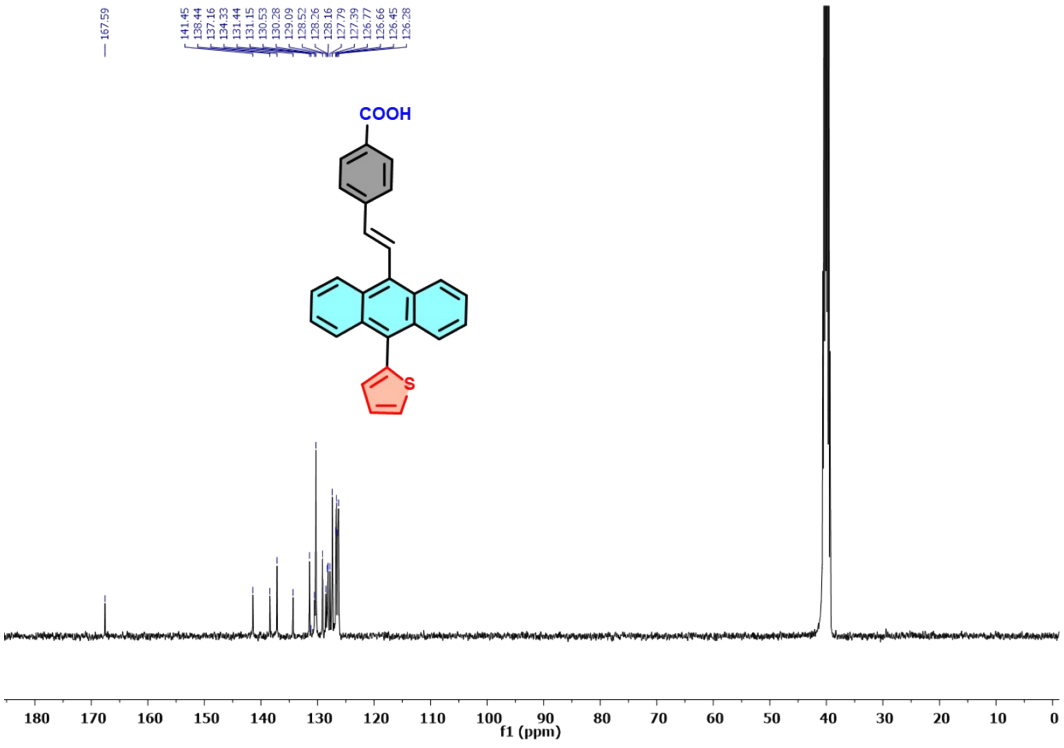


Figure S16: ^{13}C-NMR spectrum of **TAA** in DMSO-d_6

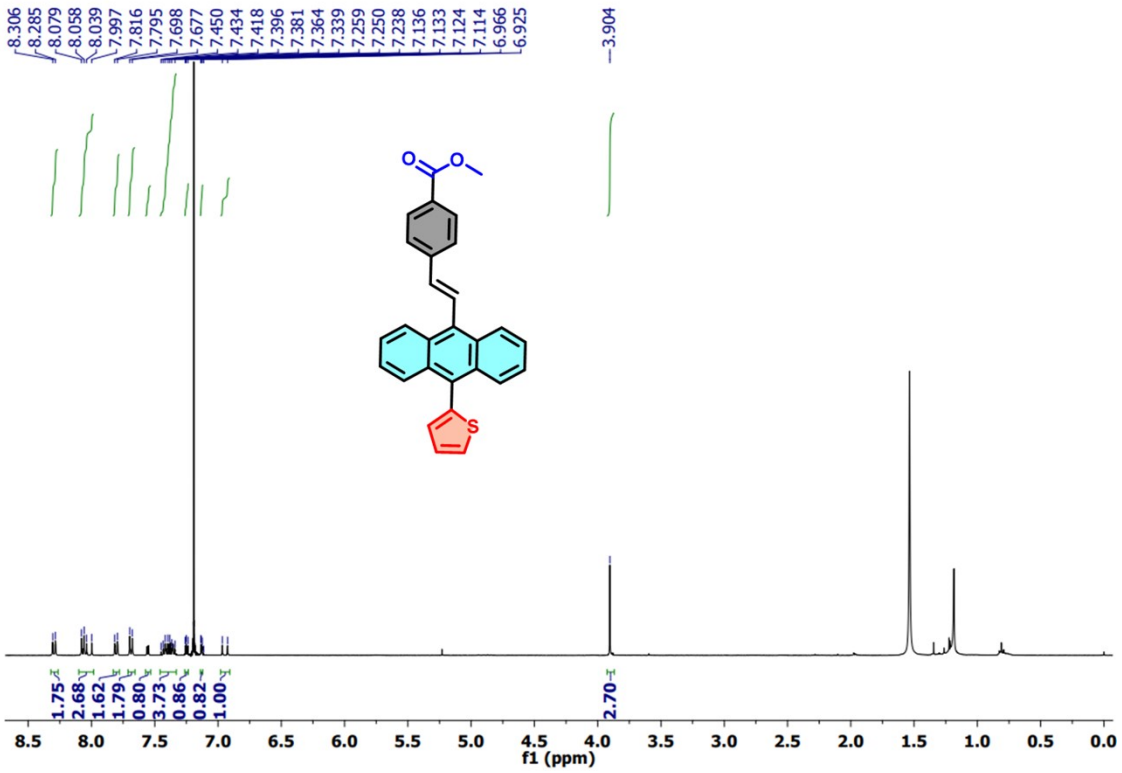


Figure S17: ^{1}H-NMR spectrum of **TAE** in $CDCl_3$

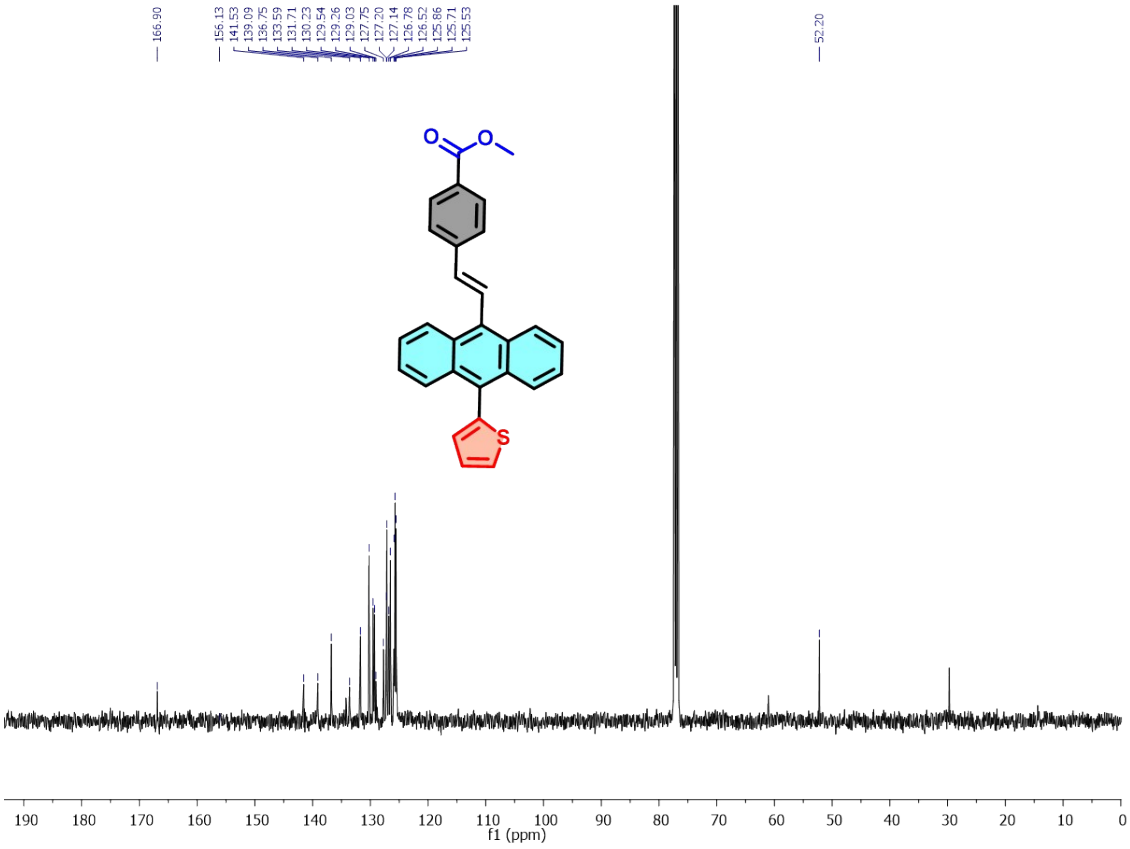


Figure S18: ^{13}C-NMR spectrum of **TAE** in $CDCl_3$

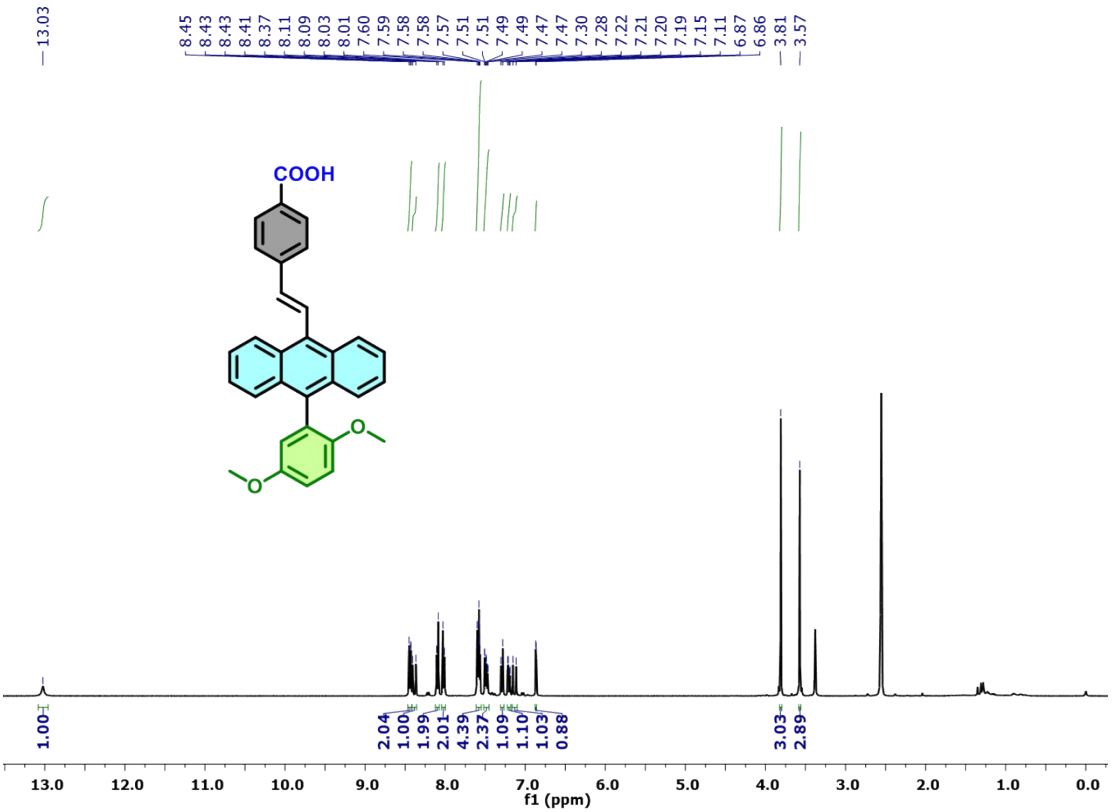


Figure S19: ^{1}H-NMR spectrum of **DMAA** in DMSO-d_6

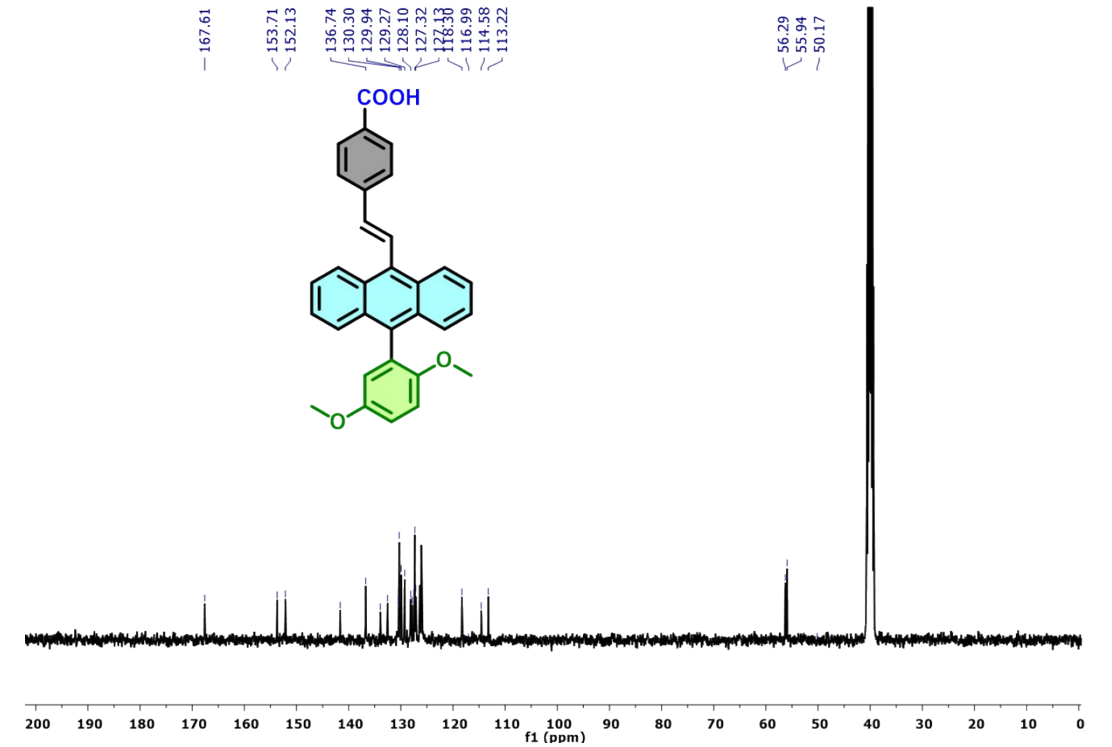


Figure S20: ^{13}C-NMR spectrum of **DMAA** in DMSO-d_6

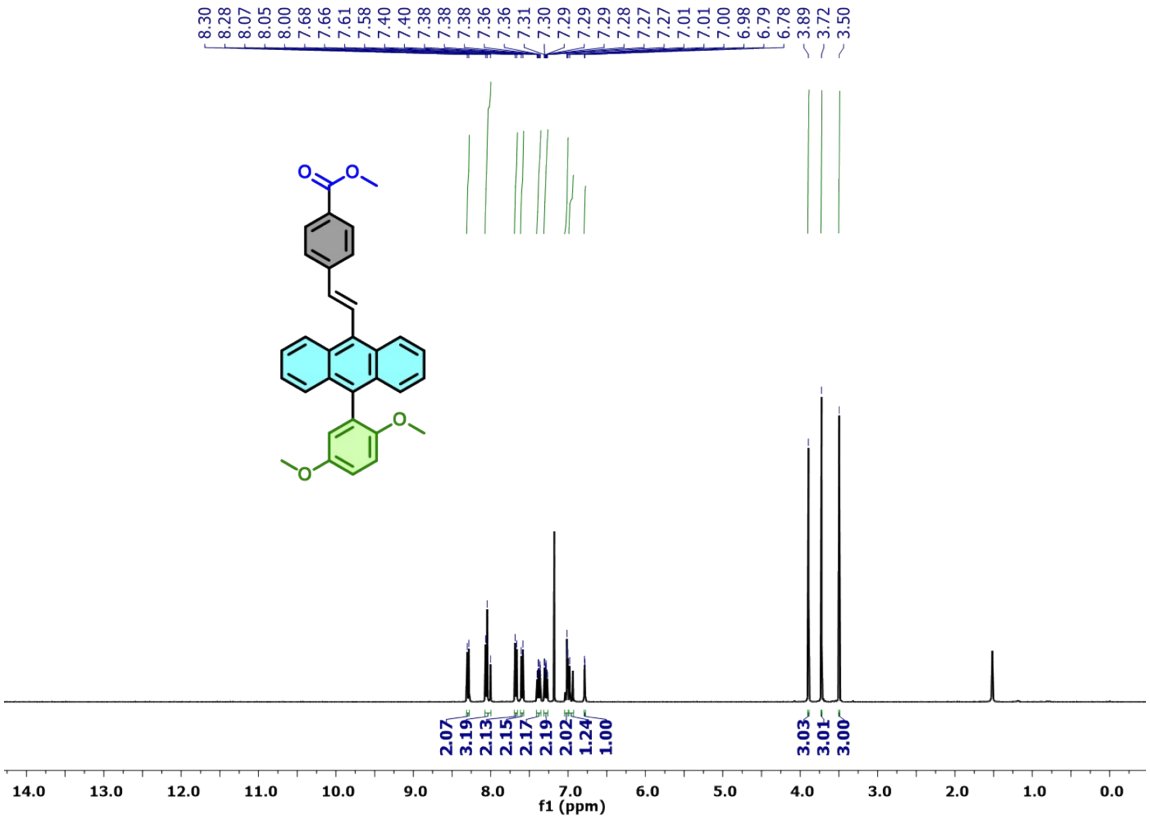


Figure S21: ^{1}H NMR spectrum for **DMAE** in $CDCl_3$

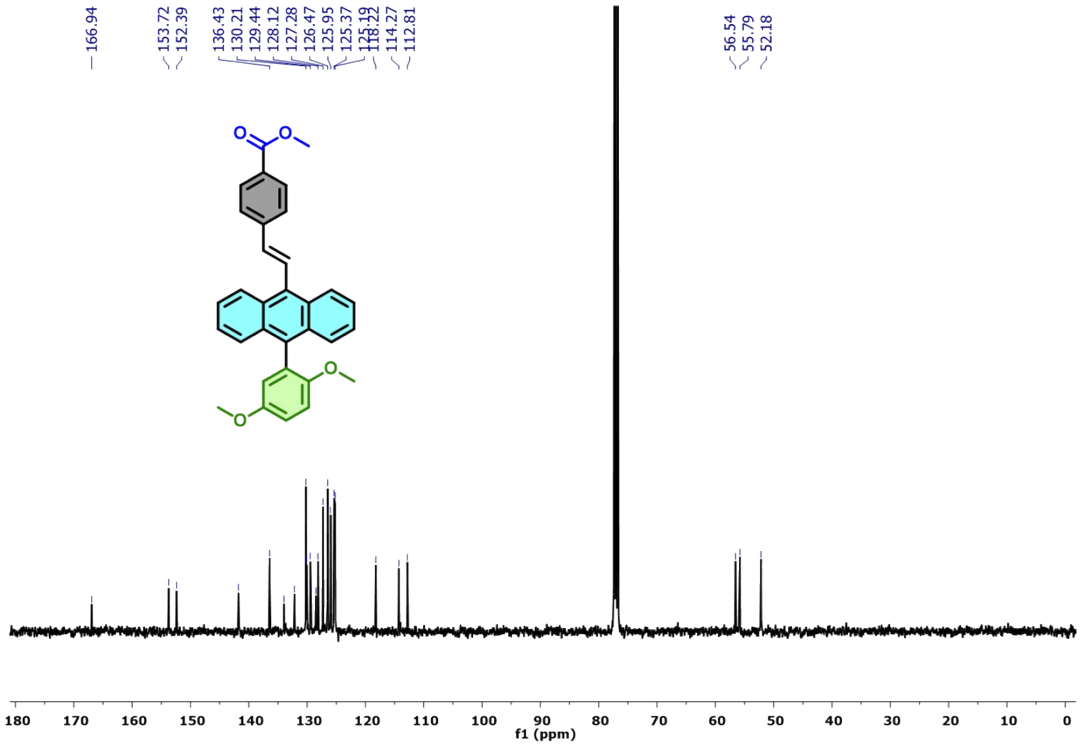


Figure S22: ^{13}C NMR spectrum for **DMAE** in $CDCl_3$

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