Supporting Information

Tunable Optical Responses in a Cyanoester-Based Organic π-Conjugates for Selective Sensing of Aliphatic Diamine Vapors

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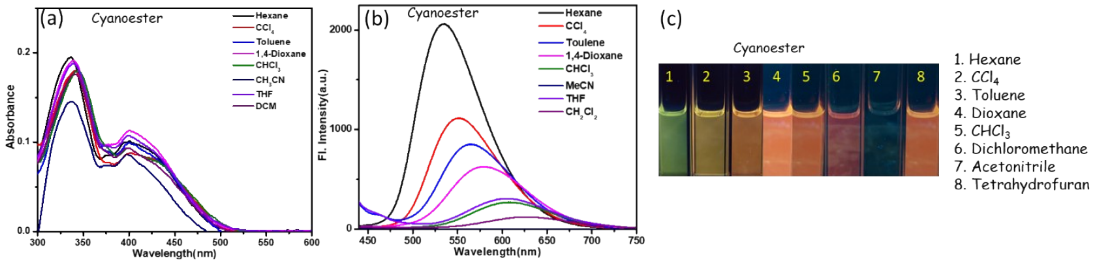

Figure S1: (a) absorption and (b) emission spectra of **CYE** (c)Photographs taken under 365 nm UV-vis lamp. λ_{ex}= 398 nm.

Table S1: Absorbance and Emission wavelength of Solvatochromic studies for **CYE**

Solvents	Cyanoester [$\lambda_{abs/em}$(nm)]	Φ_f(%)
Hexane	340, 399/535	12.4
CCl_4	340, 399/550	10.8
Toluene	340, 399/565	8.9
1,4-Dioxane	340, 399/579	7.5
THF	340, 399/606	3
$CHCl_3$	340, 399/607	5
CH_2Cl_2	340, 399/626	2
MeCN	340, 399/NE	NE

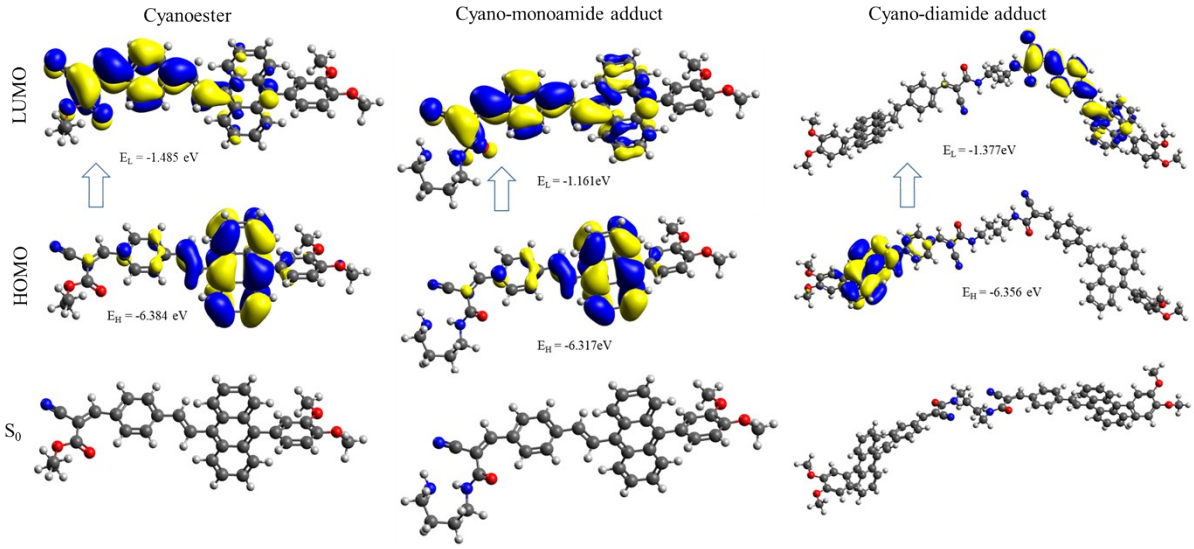

Figure S2: Frontier Molecular Orbital (FMO) contributions of **CYE** using CAM-B3LYP/6-31G(d) level of theory

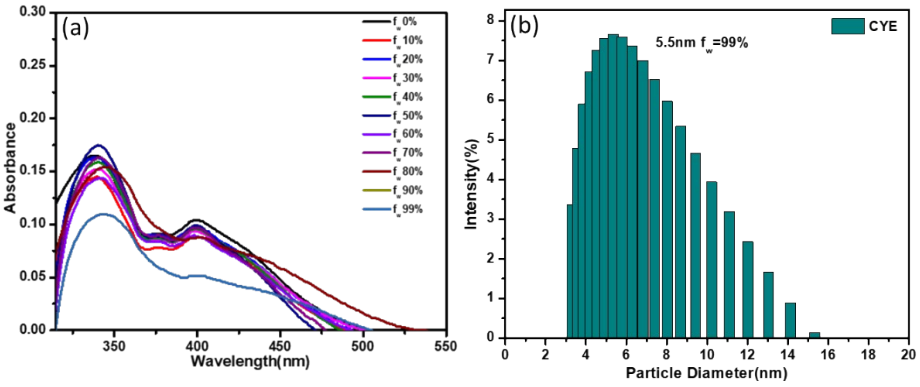

Figure S3: AIE study: (a) Absorption spectra of **CYE (**b) DLS study of **CYE**

Table S2: Absorbance and emission wavelength of AIE studies for **CYE**

f_w(v/v)(%)	Cyanoester [$\lambda_{abs/em}$(nm)]
0	340,399/NE
10	340,399/492
20	340,399/492
30	340,399/492
40	340,399/500
50	340,399/500
60	340,399/500
70	340,399/502
80	344,399/612
90	340,399/605
99	**343,399/597**

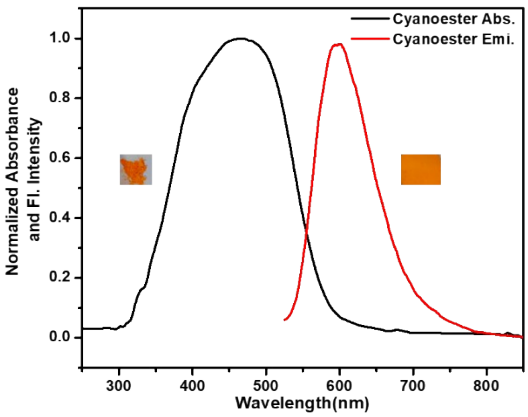

Figure S4: Solid-state UV-vis and Emission spectra of probes **CYE.** λ_{ex} = 398

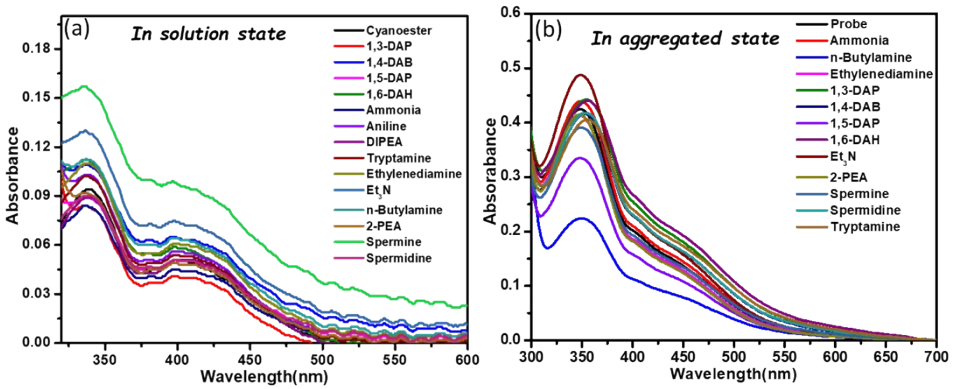

Figure S5: Absorption spectra of **CYE** in (a) solution state (10 μM in dioxane) (b) aggregated state after adding amines (100 μM in DMAc).

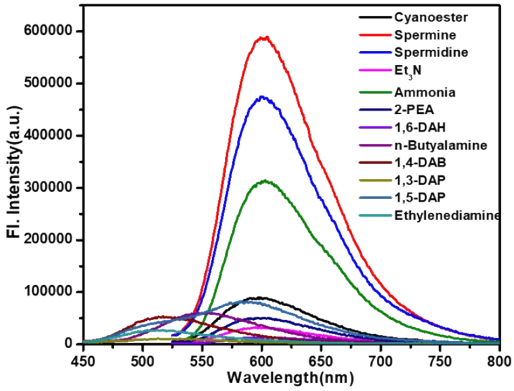

Figure S6: Solid-state emission profile of **CYE** before and after exposure to amine vapors. λ_{ex} = 450,525 nm.

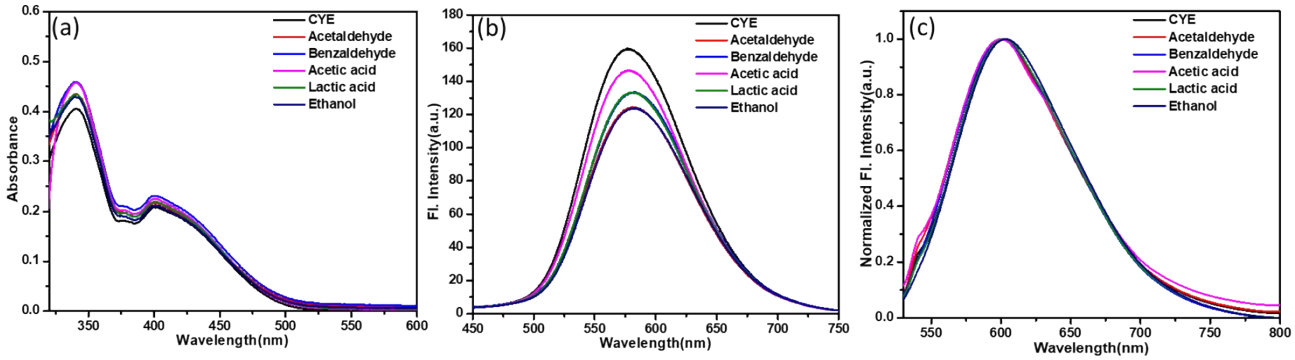

Figure S7: Solution state (10 μM in 1,4-dioxane) (a) Absorption spectra (b) Emission spectra (c) Solid-state emission spectra of **CYE** with interfering substances (exposed for 20 minutes,

the experiment was . λ_{ex} = 400 nm. The experiments were performed following the same procedure, used for other comparative studies.

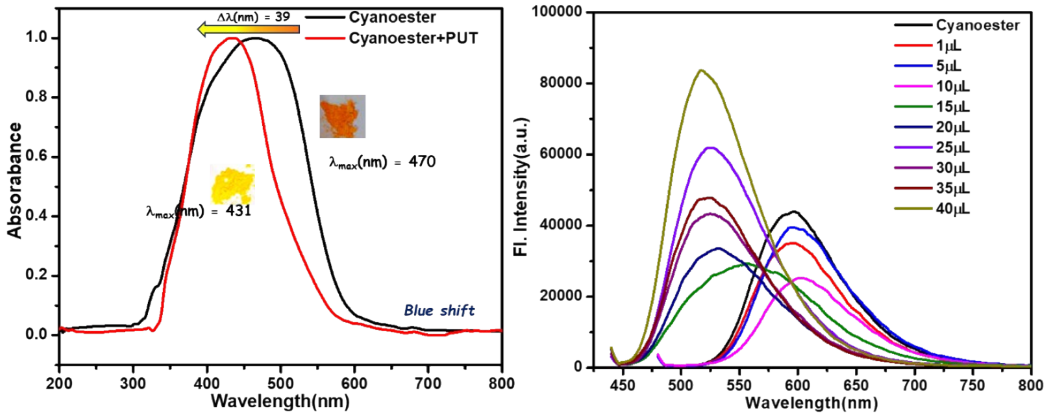

Figure S8: Solid-state (a) UV-Vis and (b) Emission spectra of **CYE** under different concentrations of PUT λ_{ex} = 440,480 nm

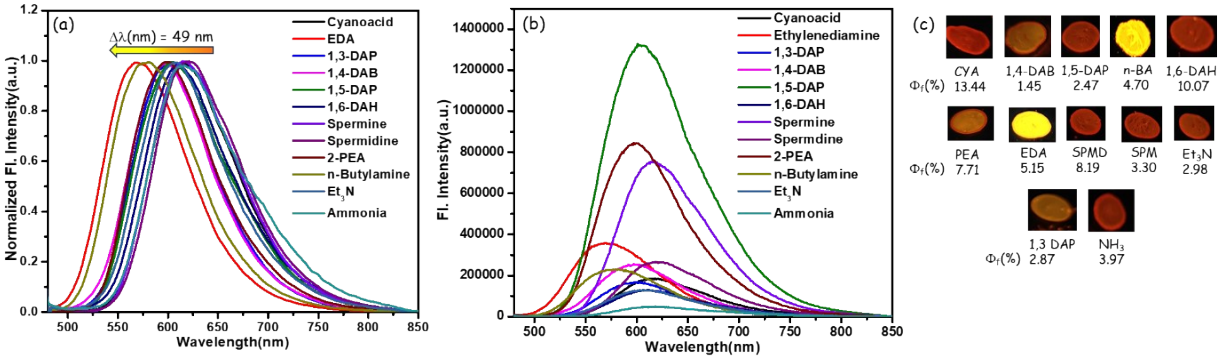

Figure S9: (a,b) Details of the solid-state emission profile of **CYA** with various amines. (c) Photographs of the coverslip are taken under a 365 nm UV lamp. λ_{ex} = 398 nm

Table S3: Details of solid-state emission profile of **CYA** with various amines. 30 μL of a 10 mM solution of **CYA** in 1,4-dioxane was drop-cast onto a glass coverslip and allowed to dry. The dried cover slips were exposed to 30 μL of amine vapors in a 200 mL air-tight bottle. λ_{ex}=400 nm

Amines	Cyanoacid			
Amines	λ_{em}(nm)	Δλ (nm)	Φ_f(%)	Concentration (mg/L)
Probe	618	-	13.44	-

1,3-DAP	600	18	2.87	133.2
1,4-DAB	596	22	1.45	131.55
1,5-DAP	604	14	2.47	130.5
1,6-DAH	612	6	10.07	126
Ethylenediamine	569	49	5.15	135
Spermidine	618	0	8.19	138.7
Spermine	618	0	3.30	140.5
N-Butylamine	580	38	4.70	111
Ammonia	618	0	3.97	109.5
Triethylamine	608	0	2.98	108.9
PEA	598	20	7.71	144.6

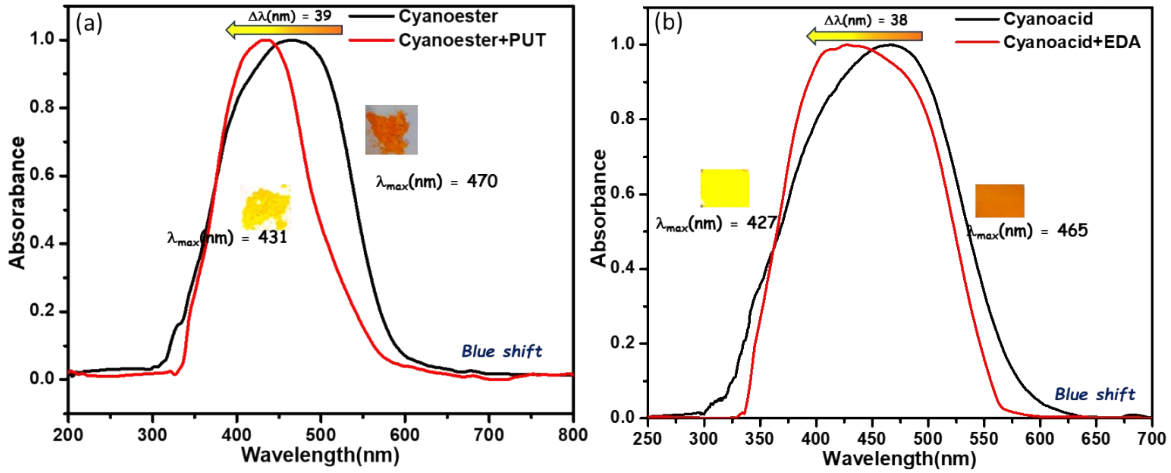

Figure S10: Solid state UV-Vis Spectra of (a) **CYE** and fumed **CYE** with 1,4-DAB (b) **CYA** and fumed **CYA** with EDA

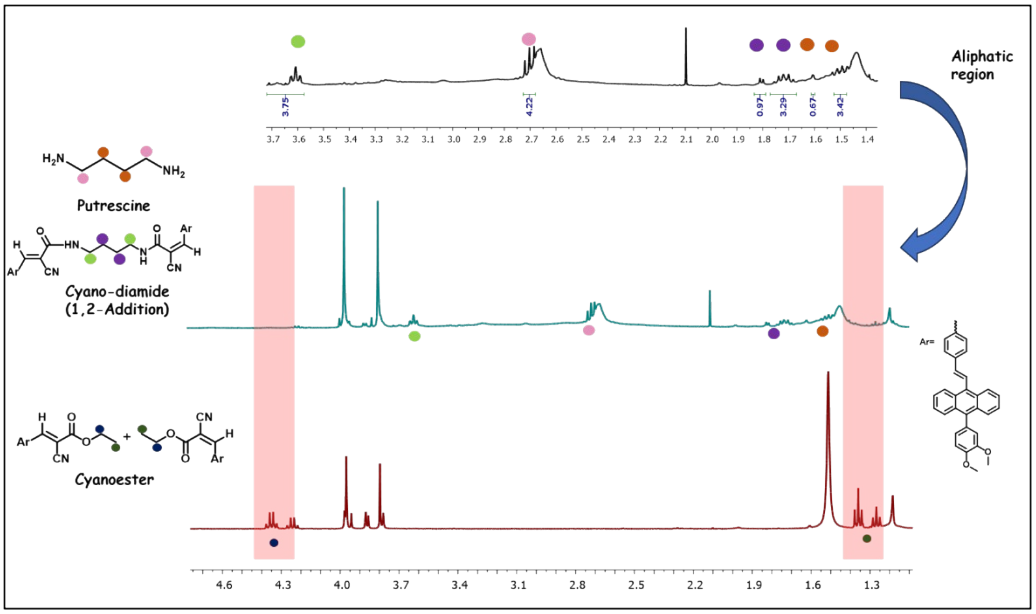

Figure S11: ^{1}H NMR Spectra(Aliphatic region) of **CYE** and fumed **CYE** with 1,4-DAB

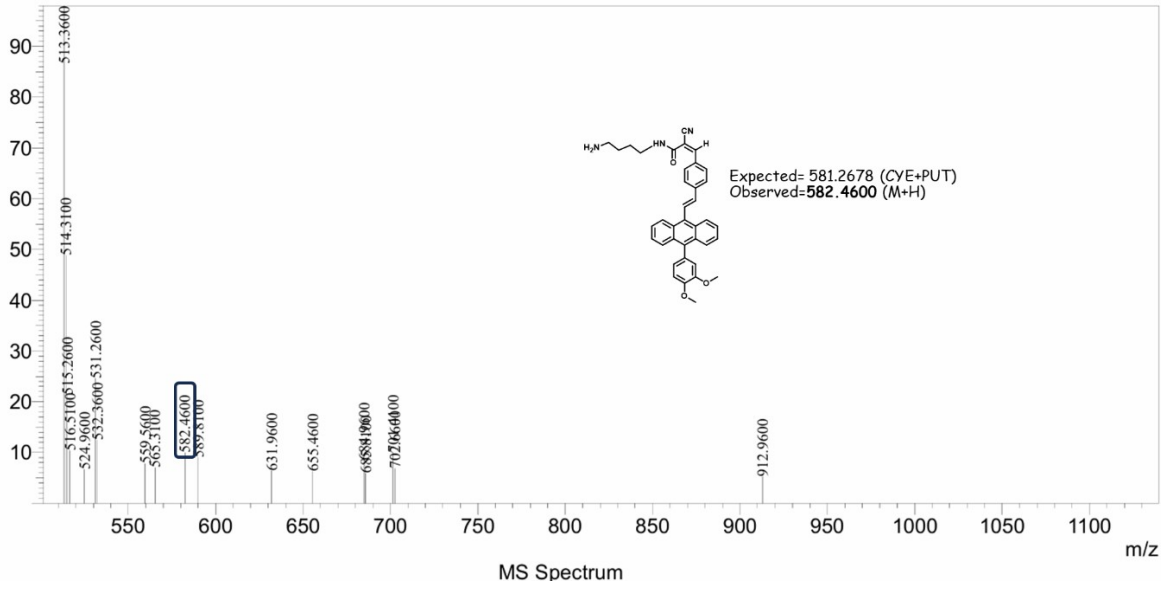

Figure S12: LC-MS spectra of fumed **CYE** with PUT/1,4-DAB(cyano-monoamide)

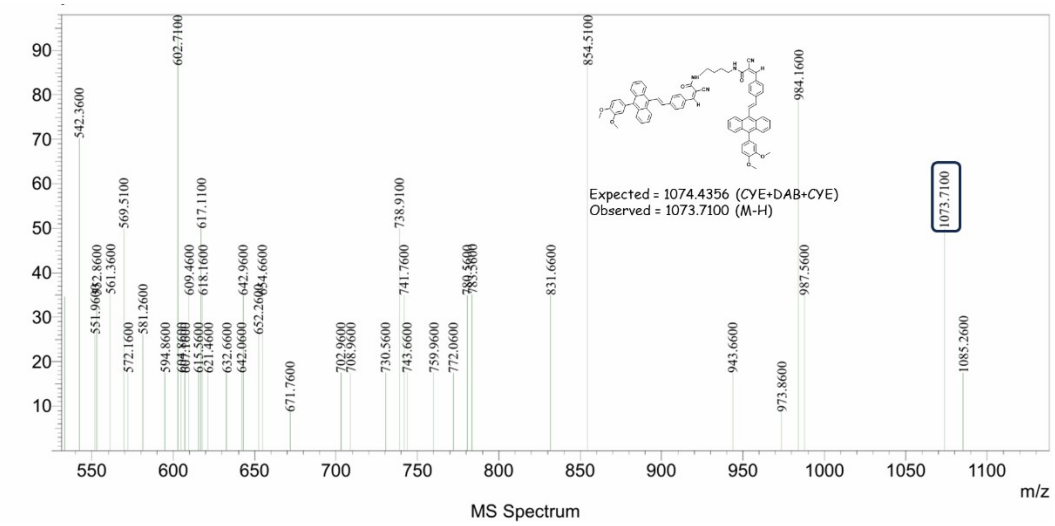

Figure S13: LC-MS spectra of fumed **CYE** with 1,4-DAB(cyano-diamide)

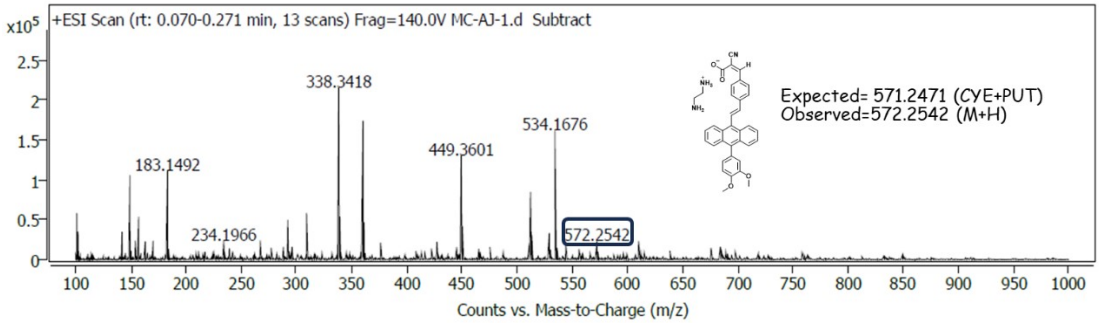

Figure S14: HR-MS spectra of fumed **CYA** with EDA (salt formation)

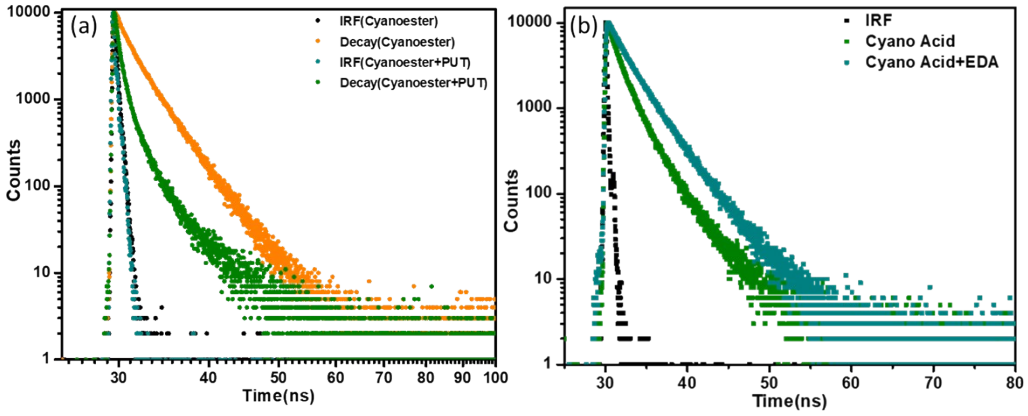

Figure S15: Lifetime decay plot of (a) fumed **CYE** with PUT (b) fumed **CYA** with EDA

Table S4: Lifetime components; All lifetimes (τ) are in ns, and λ_{ex} = 440, 510 nm

Sample	τ_1	τ_2	τ_3	α_1	α_2	α_3	$<\tau>$	χ^2	Φ_f%	K_r (x 10^6 s^{-1})	K_{nr} (x 10^6 s^{-1})
Cyanoester	1.74	0.2	4.04	0.29	0.63	0.08	0.96	1.01	8.09	83	957
Cyanoester + PUT	1.10	4.69	0.16	0.09	0.01	0.9	0.28	0.98	1.03	36	3534
Cyanoacid	0.49	1.55	3.31	0.35	0.53	0.11	1.37	1.04	13.44	98	631
Cyanoacid +EDA	0.91	2.54	4.18	0.22	0.64	0.13	2.40	1.01	5.15	21	395

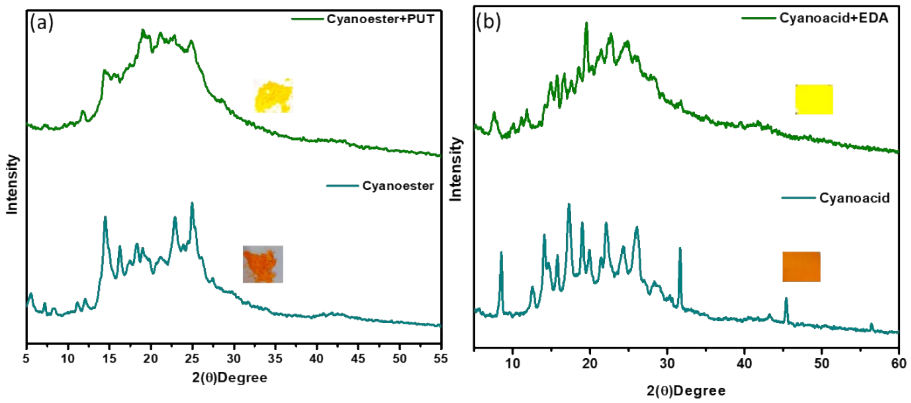

Figure S16: PXRD pattern of (a) **CYE** and fumed **CYE** with PUT (b) **CYA** and fumed **CYA** with EDA

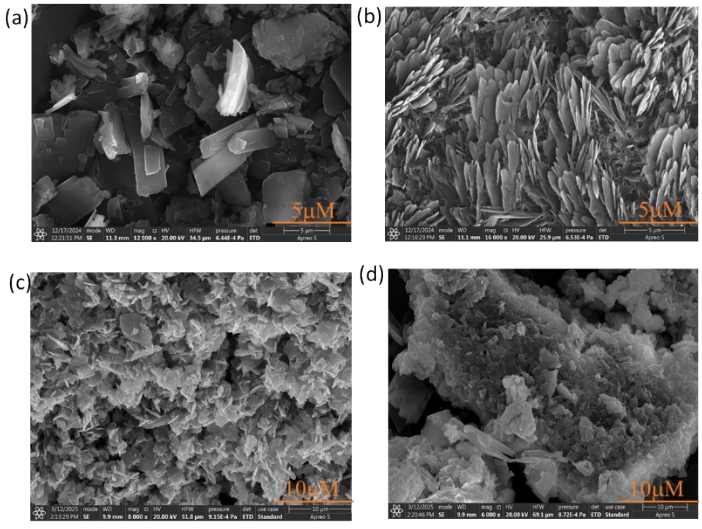

Figure S17: SEM images of (a) **CYE** (b) fumed **CYE** with PUT (c) **CYA** and (d) fumed **CYA** with EDA

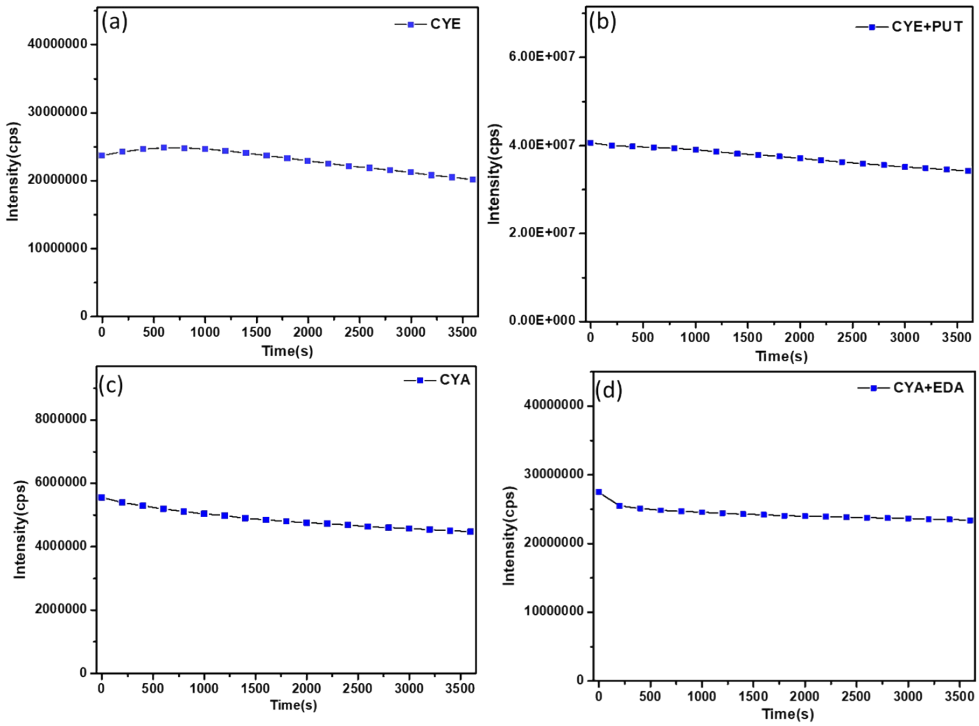

Figure S18: Photostability study of (a) **CYE** (b) **CYE** with PUT (c) **CYA** (d) **CYA** with EDA

Table S5 (a) Calculated lowest energy absorption (nm) and corresponding orbital contribution.

Molecules	Exp.	Calc.	*f*	Orbital contribution	%
Cyanoester	470	402.41	1.0985	H→L, H→L+1	65.3, 25
Cyano-monoamide adduct	431	391.13	1.0571	H→L, H→L+1	65, 27.2
Cyano-diamide adduct	431	398.84	1.6049	H→L+1, H-1→L, H→L+3	37, 26.4, 15.2

Table S5 (b) Calculated fluorescence emission (nm) and corresponding orbital contribution

Molecules	Exp.	Calc.	*f*	Orbital contribution	%
Cyanoester	596	615.85	1.4326	H→L	94.7
Cyano-monoamide adduct	557	604.65	1.3778	H→L	95.7
Cyano-	532-517	609.37	1.4122	H→L	95.2

diamide adduct					

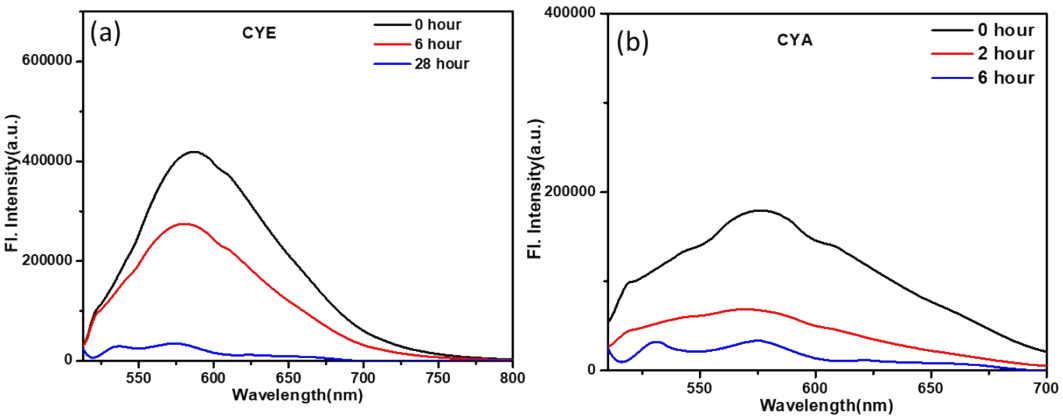

Figure S19: Emission spectra of (a) **CYE** (b) **CYA** after exposing to cottage-cheese at different time intervals.

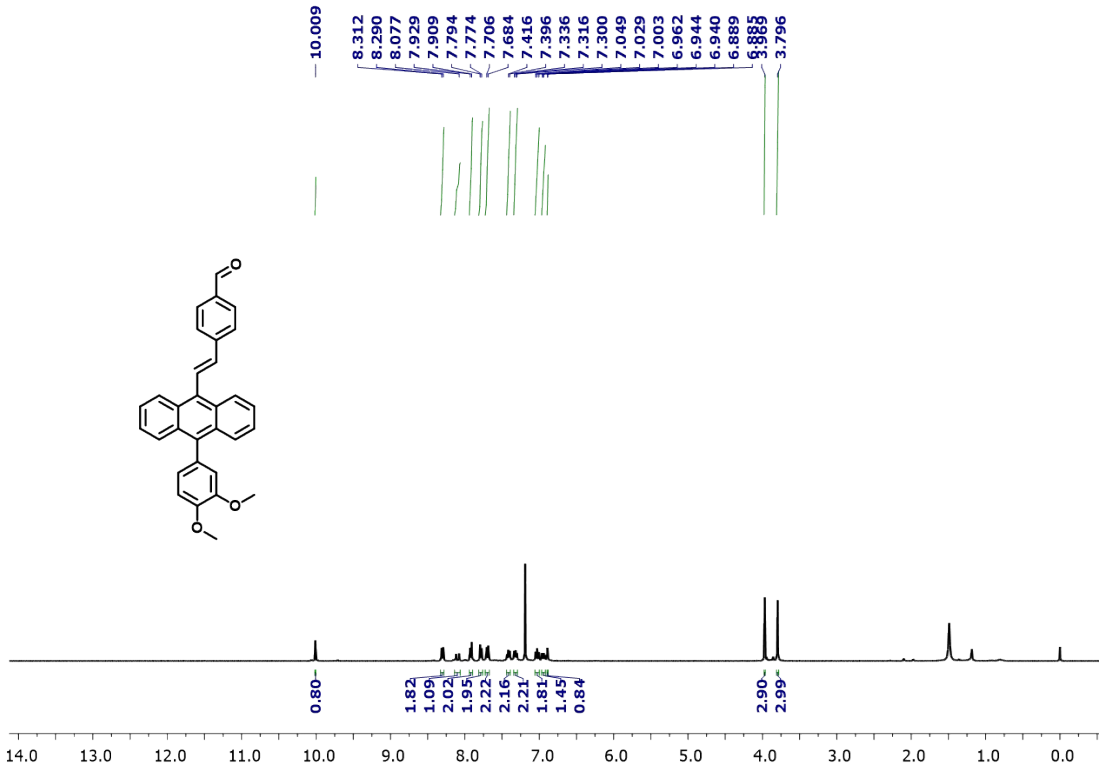

Figure S20: ^{1}H NMR (400 MHz) spectrum for **DAA** in $CDCl_3$

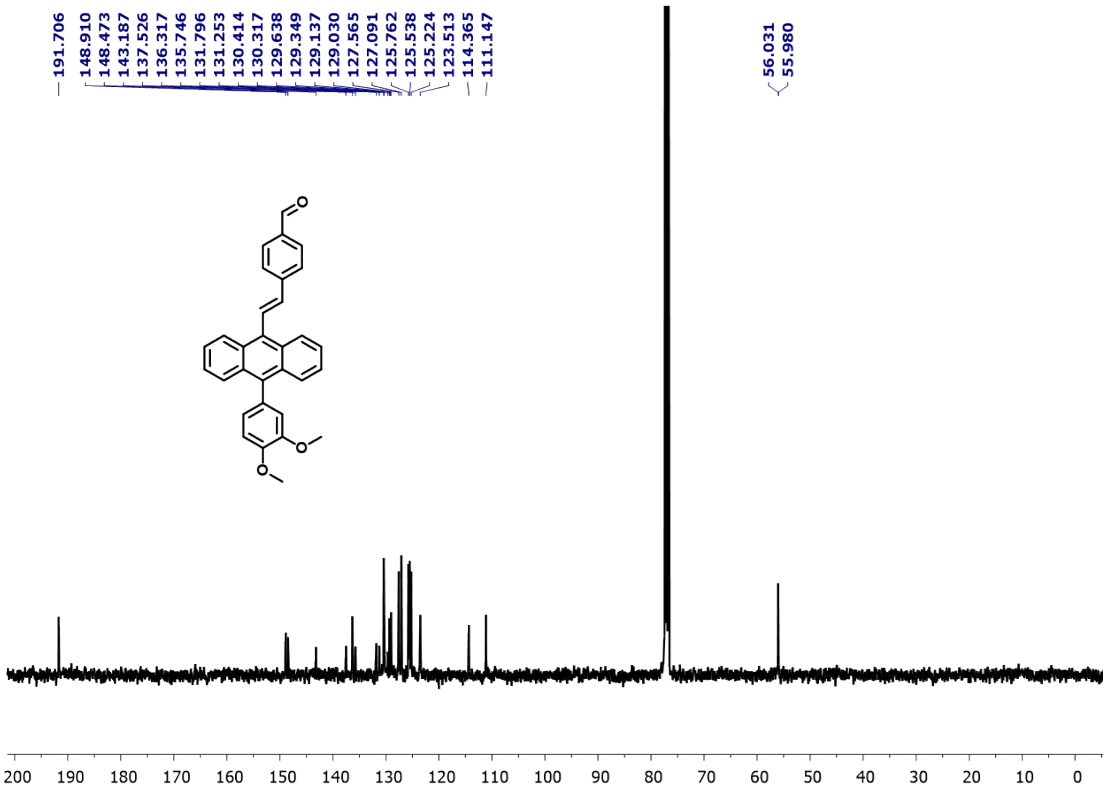

Figure S21: ^{13}C NMR (101 MHz) spectrum for **DAA** in $CDCl_3$

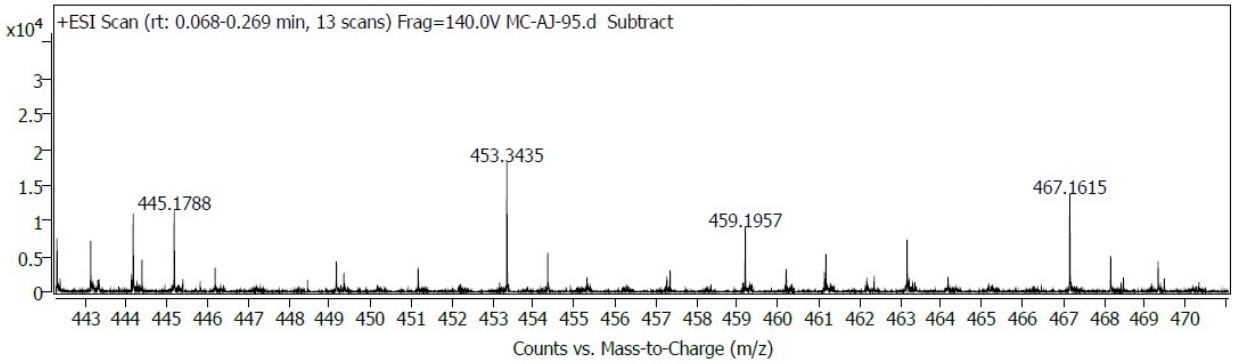

Figure S22: HRMS spectra for **DAA**

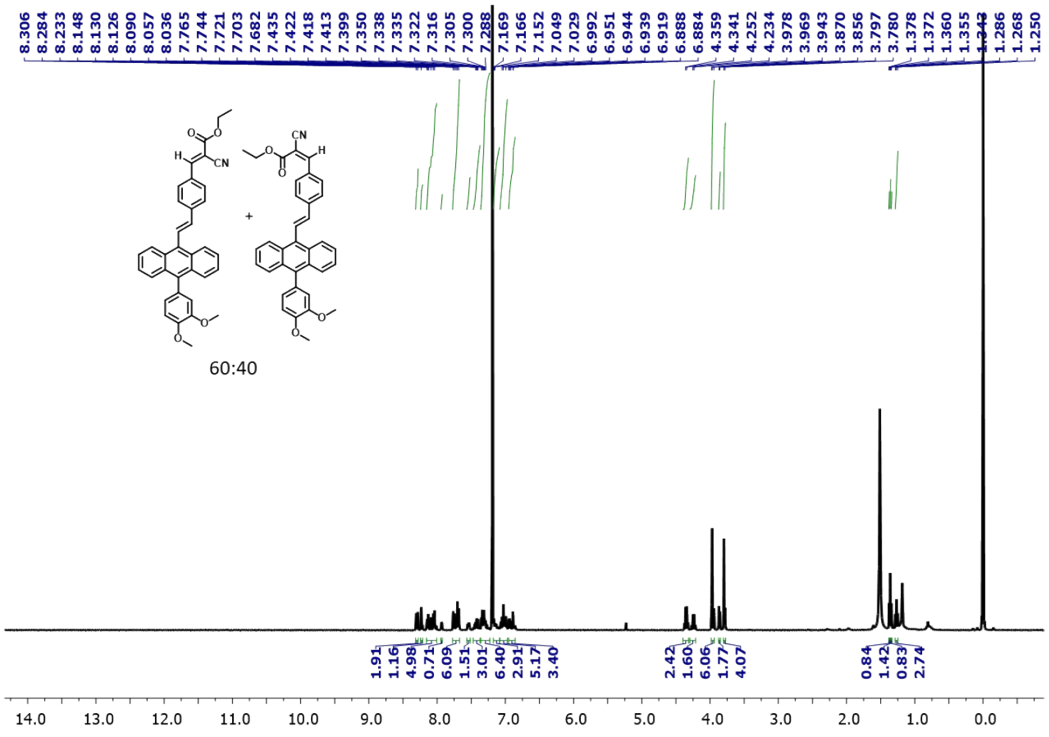

Figure S23: ^{1}H NMR (400 MHz) spectrum for **CYE** in $CDCl_3$

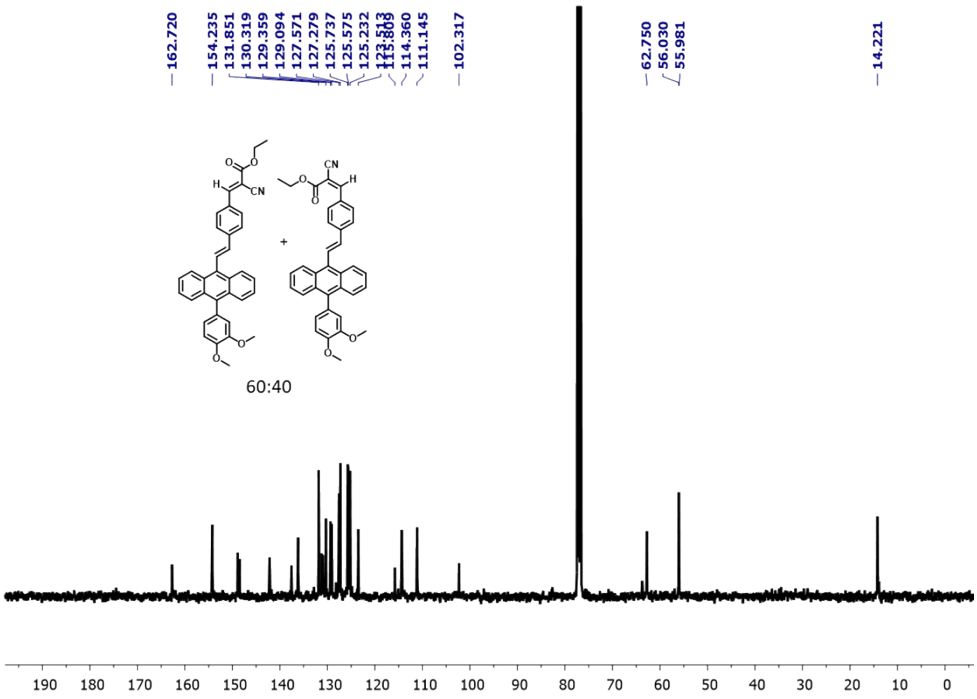

Figure S24: ^{13}C NMR (101 MHz) spectrum for **CYE** in $CDCl_3$

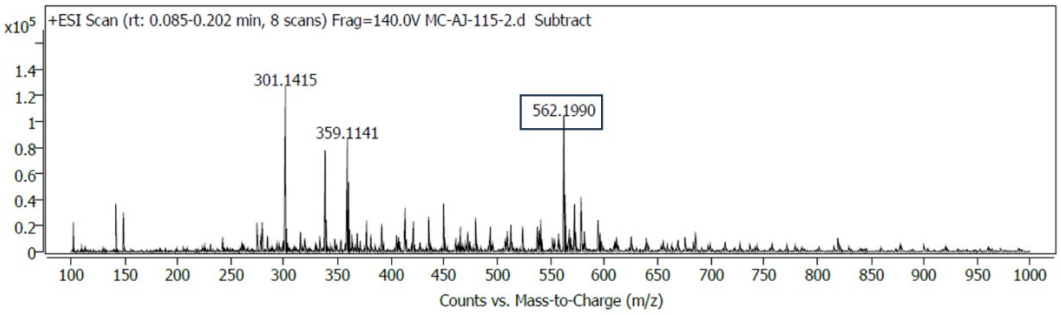

Figure S25: HRMS spectra of **CYE**

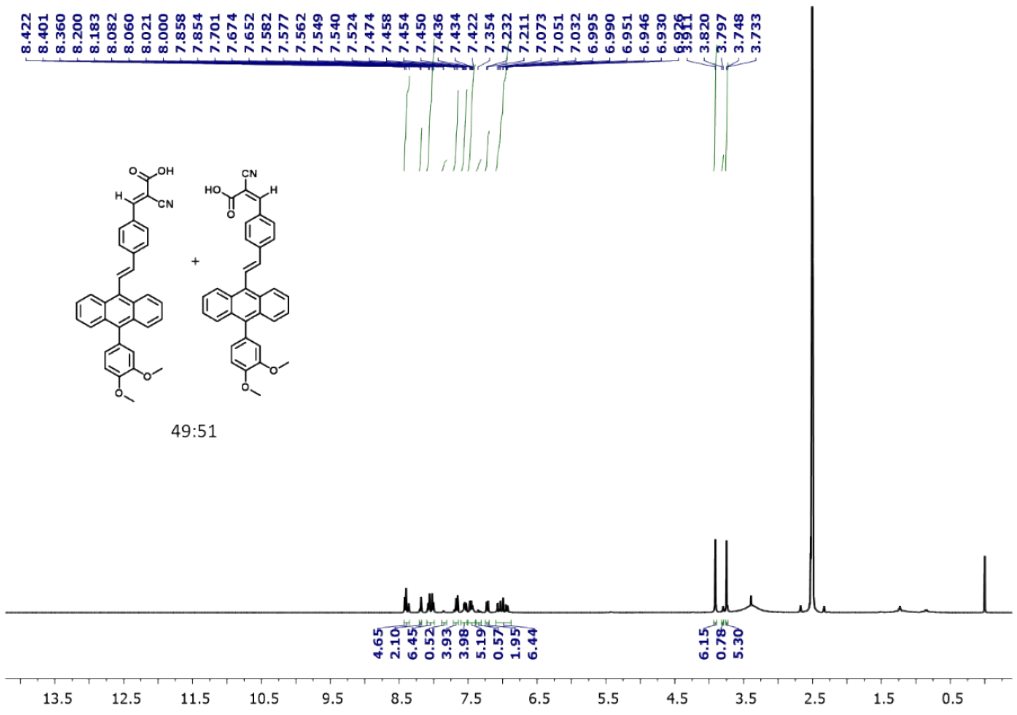

Figure S26: ^{1}H NMR (400 MHz) spectrum for **CYA** in DMSO-d_6

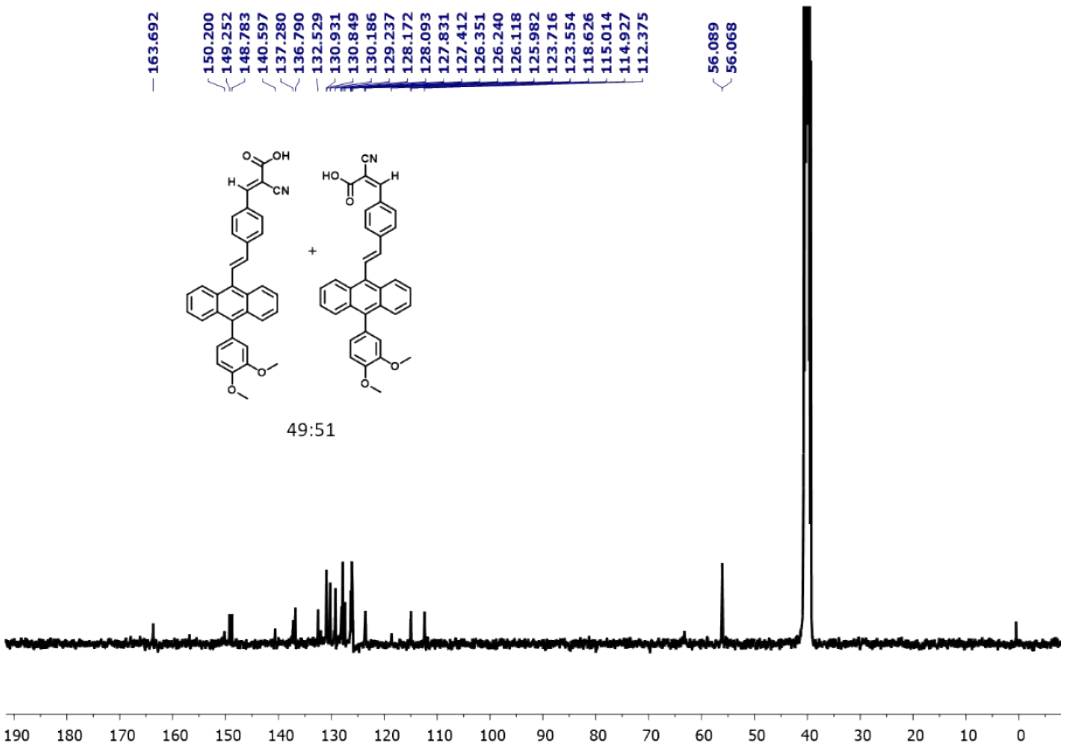

Figure S27: ^{13}C NMR (101 MHz) spectrum for **CYA** in DMSO-d_6

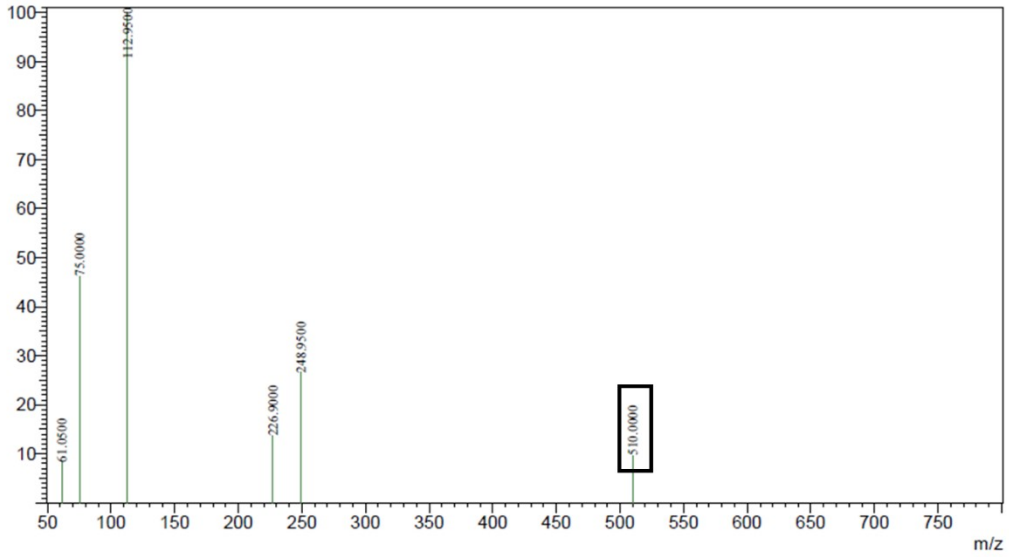

Figure S28: LCMS spectra of **CYA**

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