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Supporting Information

Photophysics and Peripheral Ring Size Dependent Aggregate Emission of Cross-Conjugated Enediynes: Applications to White Light Emission and Vapor Sensing

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General Experimental Procedure Section for Synthesis:

Melting points of the enediynyl dyes were recorded using Sigma melting point apparatus in capillary tubes. These values were uncorrected. IR spectra of the dyes were measured using JASCO FT-IR-4100 spectrometer. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectra of the derivatives were recorded on Bruker Avance 400 spectrometer and ^{1}H (500 MHz) on Bruker Avance 500 spectrometer for Variable Temperature NMR experiments. The chemical shifts (δppm) and coupling constants (Hz) from the NMR spectra were calculated with reference to chloroform. In the ^{13}C NMR spectra, the nature of the carbons (C, CH, CH_2 or CH_3) was confirmed through recording DEPT-135 experiment. High resolution mass measurements were carried out using Micromass Q-ToF ESI instrument with direct inlet mode. Analytical thin-layer chromatography (TLC) were done on glass plates (7.5 x 2.5 and 7.5 x 5.0 cm) coated with Acme's silica gel G containing 13% calcium sulfate as binder or on pre-coated 0.2 mm thick Merck 60 F_{245} silica plates. Various combinations of ethyl acetate and hexane were used as eluent. Visualization of the spots on the TLC plates was done by UV-chamber and then exposure to iodine vapor. All compounds were thoroughly purified using silica gel [Acme's silica gel (100–200 mesh)] column chromatography.

(2-(phenylethynyl)but-1-en-3-yne-1,4-diyl)dibenzene (Ph_3EDY):

Hexane was used as eluent to afford the enediyne as a yellow solid (55%).

Physical appearance: Brownish-white solid

R_f: 0.8

m.p.: 80–82 °C

IR (neat): 3057, 2360, 2334, 1488, 1441, 1375, 755, 689, 526 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, 2H), 7.55-7.54 (dd, 4H), 7.42-7.34 (m, 9H), 7.18 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, DEPT): δ 143.30 (1 x CH), 135.92 (2 x C), 131.87 (2 x CH), 131.83 (2 x CH), 129.32 (2 x CH), 129.24 (2 x CH), 128.90 (1 x C), 128.58 (2 x CH), 128.48 (2 x CH), 123.13 (2 x CH), 123.06 (1 x CH), 103.50 (1 x C), 94.74 (1 x C), 89.34 (1 x C), 88.45 (1 x C), 87.06 (1 x C).

HRMS (ESI, M+H$^+$): m/z calcd. for $C_{24}H_{16}$ 304.13, found 304.1325

1,1'-(3-(naphthalen-2-ylmethylene)penta-1,4-diyne-1,5-diyl)dinaphthalene (Nap_3EDY):

2% ethyl acetate in hexane was used as eluent to afford the enediyne as a yellow solid (51%).

Physical appearance: Yellow solid

R_f: 0.8

m.p.: 110–112 °C

IR (neat): 3051, 2368, 2341, 1488, 1461, 1332, 796, 734, 562, 446 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (d, 1H), 8.50 (d, 1H), 8.26-8.20 (dd, 2H), 8.06 (s, 1H), 7.94-7.83 (m, 7H), 7.71-7.44 (m, 9H), 7.42 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, DEPT): δ 140.37 (1 x CH), 133.81 (1 x C), 133.64 (2 x C), 133.47 (1 x C), 133.41 (1 x C), 133.28 (1 x C), 132.66 (1 x C), 131.64 (1 x CH), 130.98 (1 x

CH), 130.75 (1 x CH), 129.76 (1 x CH), 129.36 (1 x CH), 129.26 (1 x CH), 128.90 (1 x CH), 128.52 (1 x CH), 128.37 (1 x CH), 127.38 (1 x CH), 127.14 (1 x CH), 127.04 (1 x CH), 126.77 (1 x CH), 126.69 (1 x CH), 126.62 (1 x CH), 126.44 (1 x CH), 126.26 (1 x CH), 125.47 (1 x CH), 125.45 (1 x CH), 125.39 (1 x CH), 124.05 (1 x CH), 120.71 (1 x C), 120.65 (1 x C), 106.31 (1 x C), 94.22 (1 x C), 92.09 (1 x C), 91.89 (1 x C), 87.43 (1 x C).

HRMS (ESI, M+H$^+$): m/z calcd. for $C_{36}H_{22}$ 454.17, found 454.5788

9,9'-(3-(anthracen-9-ylmethylene)penta-1,4-diyne-1,5-diyl)dianthracene (An$_3$EDY):

2% ethyl acetate in hexane was used as eluent to afford the enediyne as a brownish yellow solid (58%).

Physical appearance: Orange-yellow solid

R_f: 0.8

m.p.: 166–168 ^{o}C

IR (neat): 3046, 2353, 2324, 1644, 1405, 730, 563 cm^{-1}.

^{1}H NMR (400 MHz, CDCl$_3$): δ 8.73-8.70 (dd, 4H), 8.48-8.45 (dd, 4H), 8.18 (s, 1H),8.14 (s, 1H), 8.05 (d, 4H), 7.69-7.63 (d, 4H), 7.58-7.50 (m, 8H), 6.67 (s, 1H), 6.63 (s, 1H).

^{13}C NMR (100 MHz, CDCl$_3$, DEPT): δ 138.12 (1 x CH), 134.19 (2 x C), 132.85 (2 x C), 131.60 (2 x C), 131.48 (2 x C), 131.40 (2 x C), 131.28 (2 x C), 129.67 (2 x CH), 129.05 (1 x CH), 128.93 (1 x CH), 128.07 (1 x CH), 127.54 (4 x CH), 127.42 (4 x CH), 126.97 (2 x CH), 126.87 (2 x CH), 126.83 (2 x CH), 126.12 (2 x CH), 126.08 (2 x CH), 125.91 (2 x CH), 125.87 (2 x CH), 125.48 (2 x C), 117.44 (1 x C), 117.44 (1 x C), 100.04 (1 x C), 88.99 (1 x C), 85.24 (1 x C), 81.84 (1 x C).

HRMS (ESI, M+H$^+$): m/z calcd. for $C_{48}H_{28}$ 604.22, found 604.2325

9-(4-(naphthalen-1-yl)-2-(naphthalen-1-ylethynyl)but-1-en-3-ynyl)anthracene (AnEDYNap):

2% ethyl acetate in hexane was used as eluent to afford the enediyne as a yellow solid (52%).

Physical appearance: Brownish-yellow solid

R_f: 0.7

m.p.: 154–156 ^oC

IR (neat): 3057, 2365, 2332, 1650, 1401, 1039, 779, 669, 566 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.65 (d, 1H),8.57 (s, 1H), 8.41 (d, 2H), 8.27 (s, 1H),8.11 (d, 2H),7.95-7.92 (dd, 2H), 7.72-7.50 (m, 10H), 7.32 (t, 1H),7.27-7.21 (m, 1H), 7.03 (t, 1H), 6.73 (d, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, DEPT): δ 141.69 (1 x CH), 133.64 (1 x C), 133.41 (2 x C), 133.07 (1 x C), 132.86 (1 x C), 131.61 (1 x C), 130.94 (1 x C), 130.68 (1 x C), 130.25 (1 x C), 129.72 (1 x CH), 129.41 (1 x CH), 129.12 (1 x CH), 128.86 (1 x CH), 128.55 (1 x CH), 127.99 (1 x CH), 127.94 (1 x CH), 127.19 (1 x CH), 126.73 (1 x CH), 126.61 (1 x CH), 126.45 (1 x CH), 126.26 (1 x CH), 126.23 (1 x CH), 125.91 (1 x CH), 125.61 (1 x CH), 125.49 (1 x CH), 125.03 (1 x CH), 120.55 (1 x C), 120.13 (1 x C), 111.54 (1 x C), 93.08 (1 x C), 92.49 (1 x C), 91.22 (1 x C), 87.34 (1 x C).

HRMS (ESI, $M+H^+$): m/z calcd. for $C_{40}H_{24}$ 504.19, found 504.1961

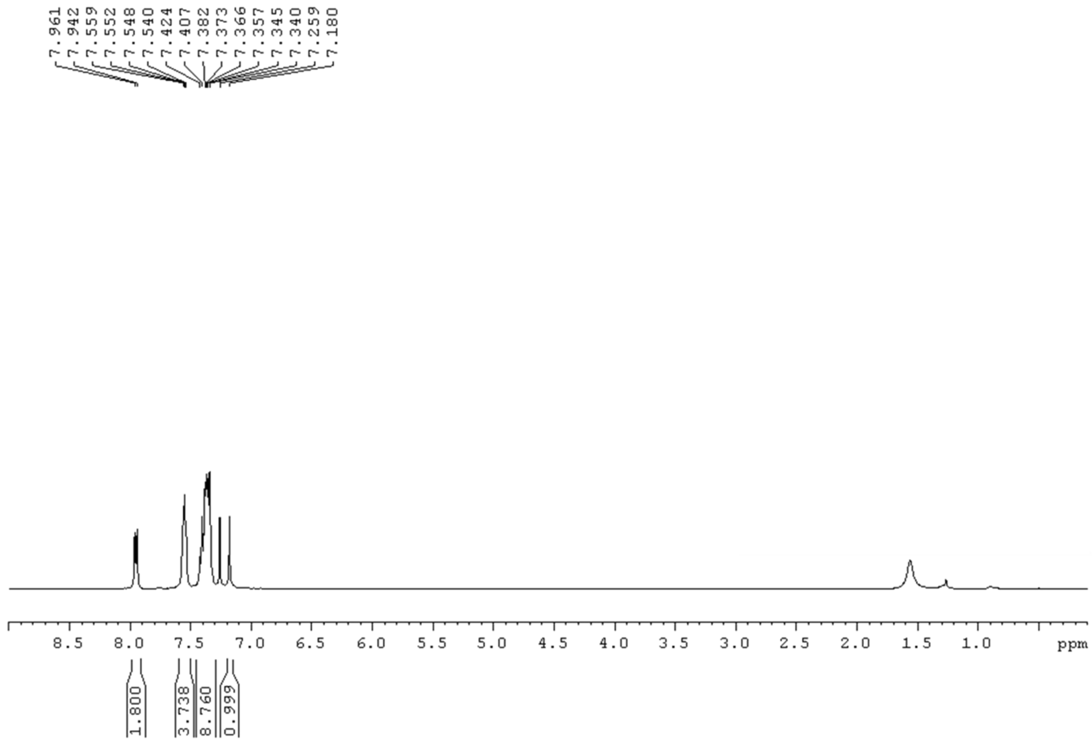

Figure S1. ^{1}H NMR spectrum of **Ph$_3$EDY** in $CDCl_3$ (400 MHz).

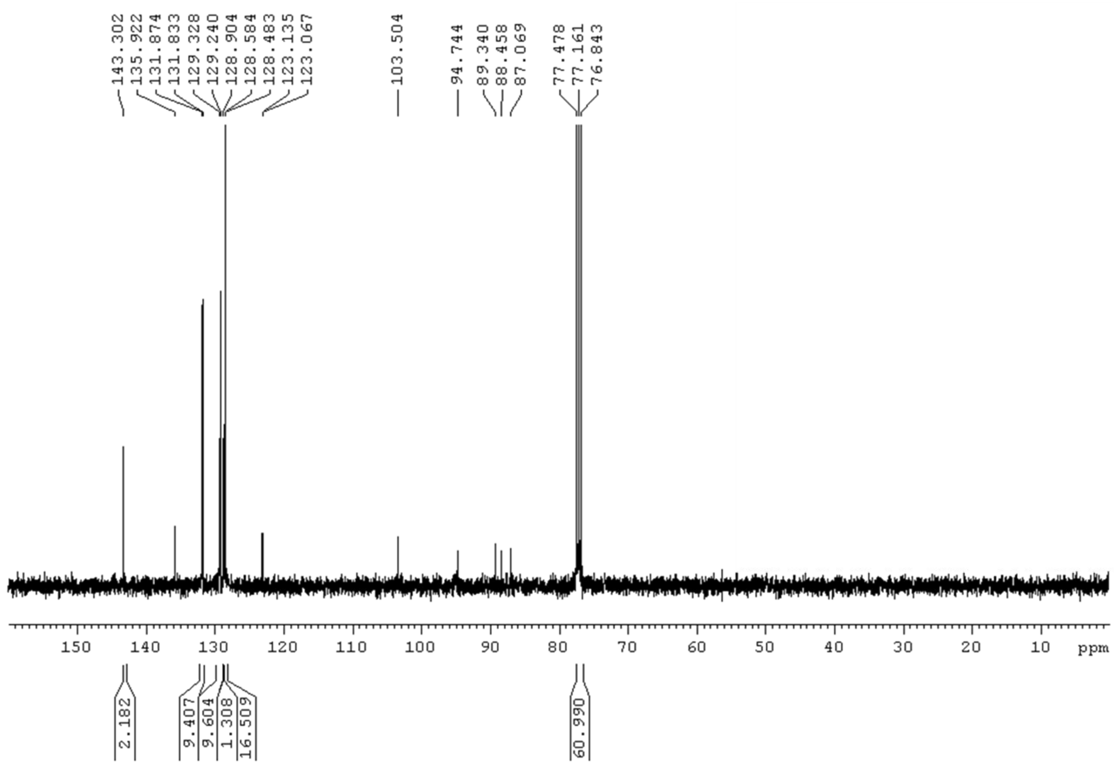

Figure S2. ^{13}C NMR spectrum of **Ph$_3$EDY** in $CDCl_3$ (100 MHz).

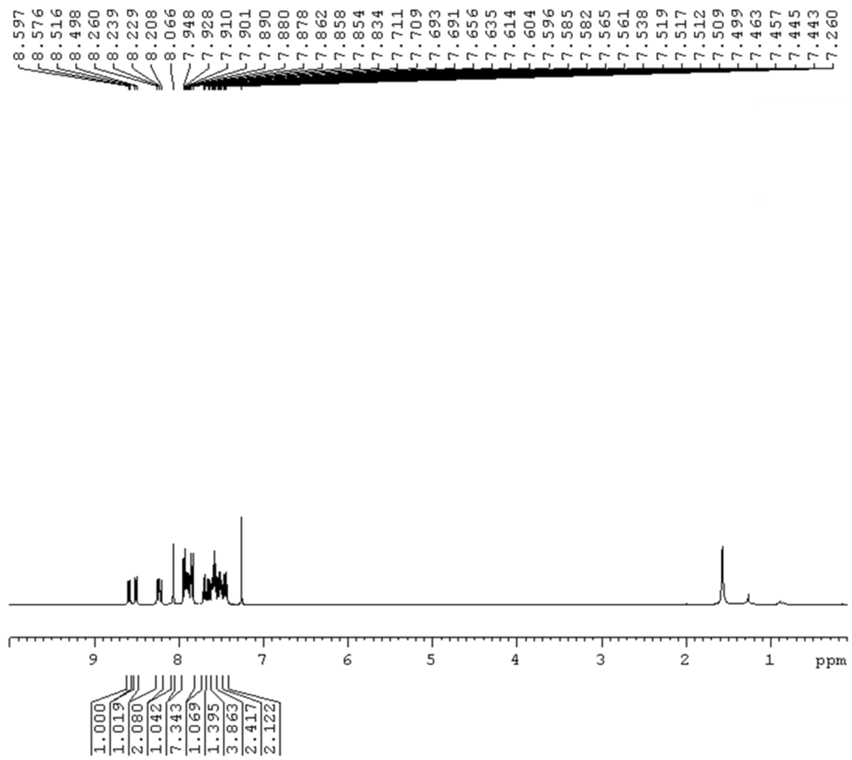

Figure S3. ^{1}H NMR spectrum of **Nap_3EDY** in $CDCl_3$ (400 MHz).

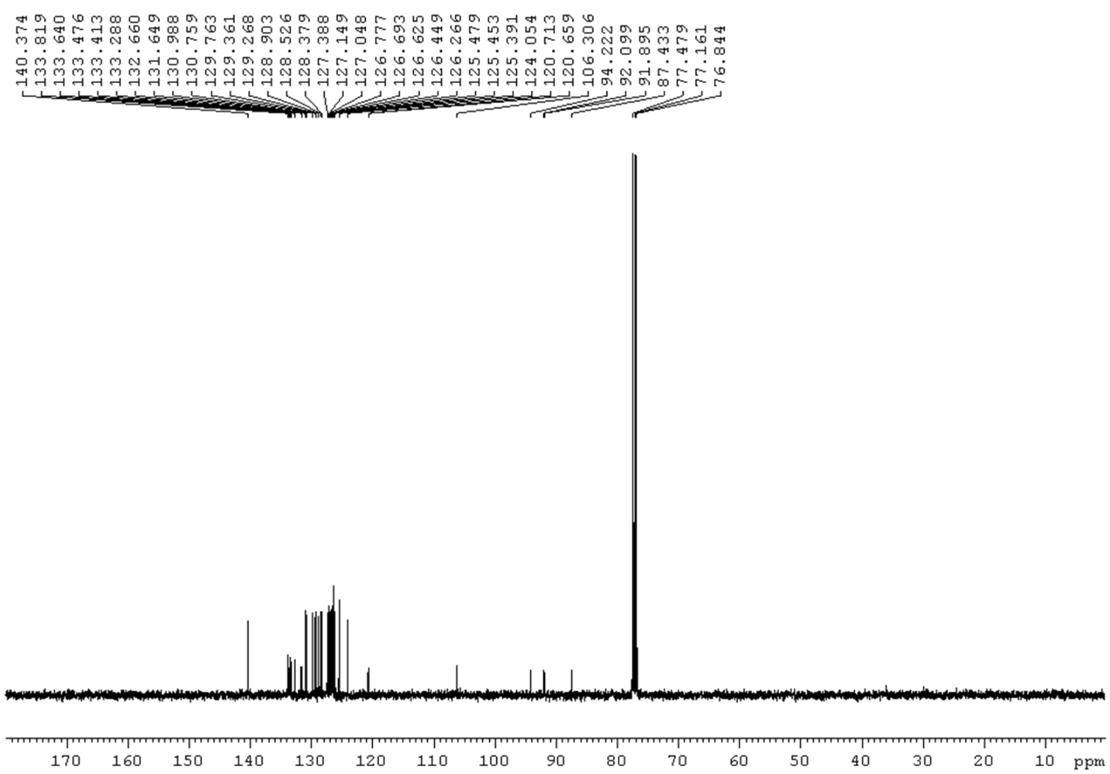

Figure S4. ^{13}C NMR spectrum of **Nap_3EDY** in $CDCl_3$ (100 MHz).

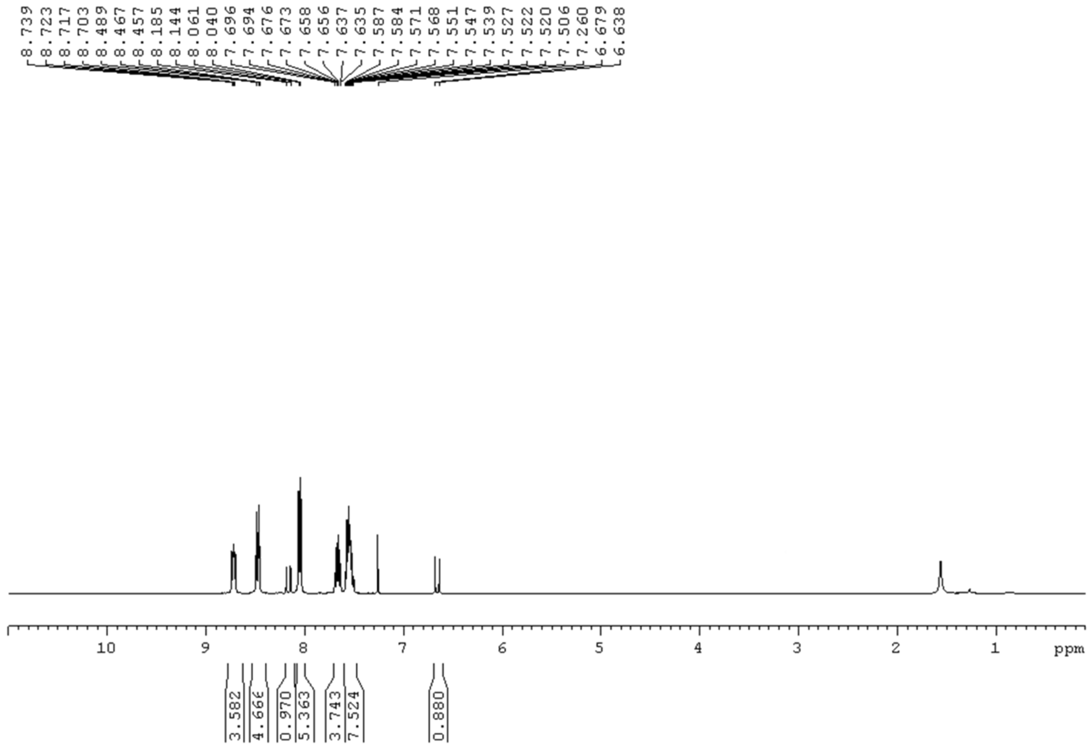

Figure S5. ^{1}H NMR spectrum of **An$_3$EDY** in $CDCl_3$ (400 MHz).

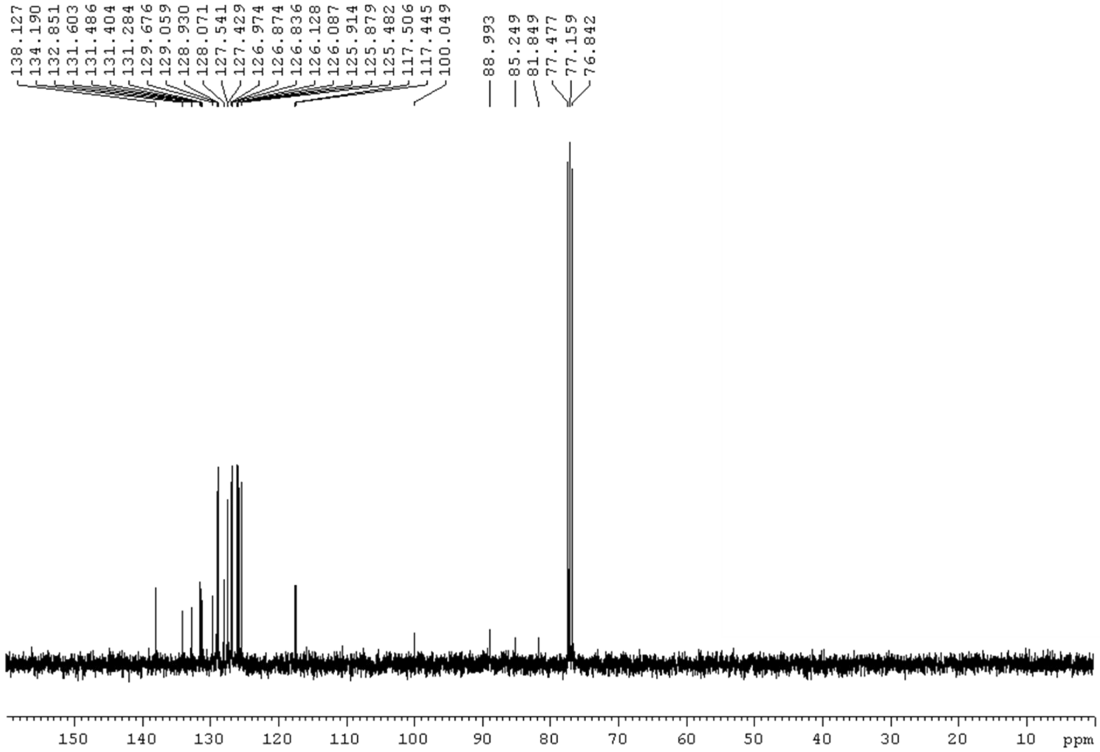

Figure S6. ^{13}C NMR spectrum of **An$_3$EDY** in $CDCl_3$ (100 MHz).

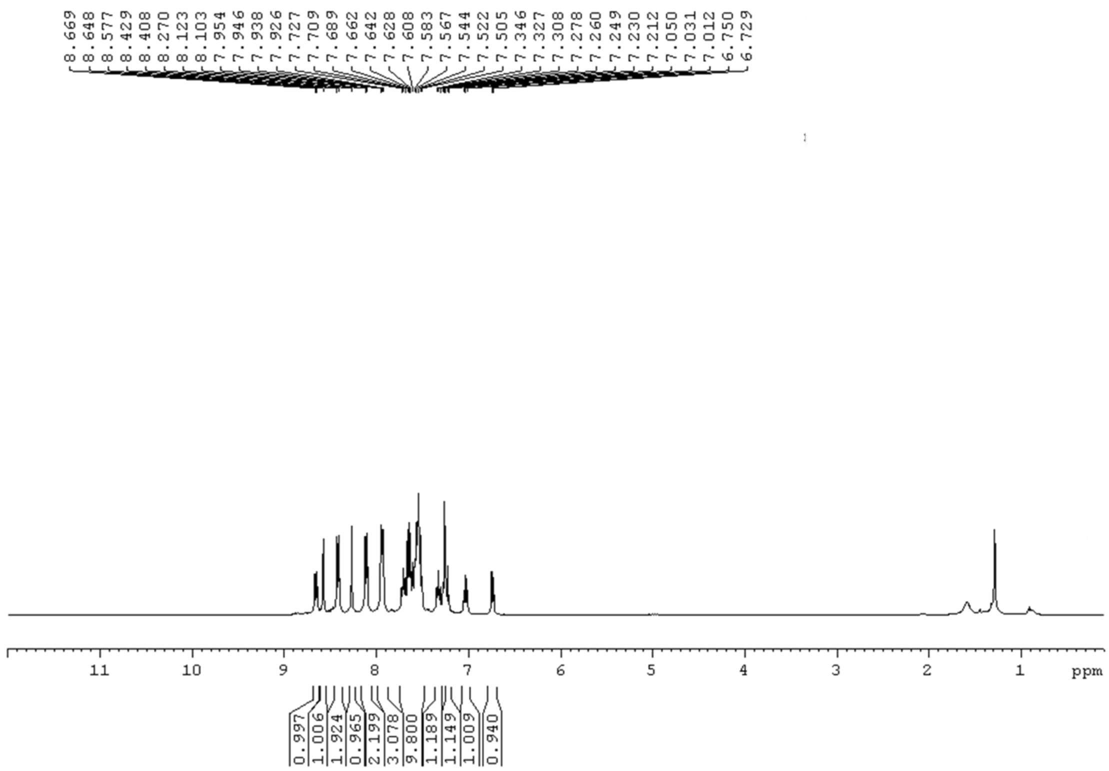

Figure S7. ^{1}H NMR spectrum of **AnEDYNap** in $CDCl_3$ (400 MHz).

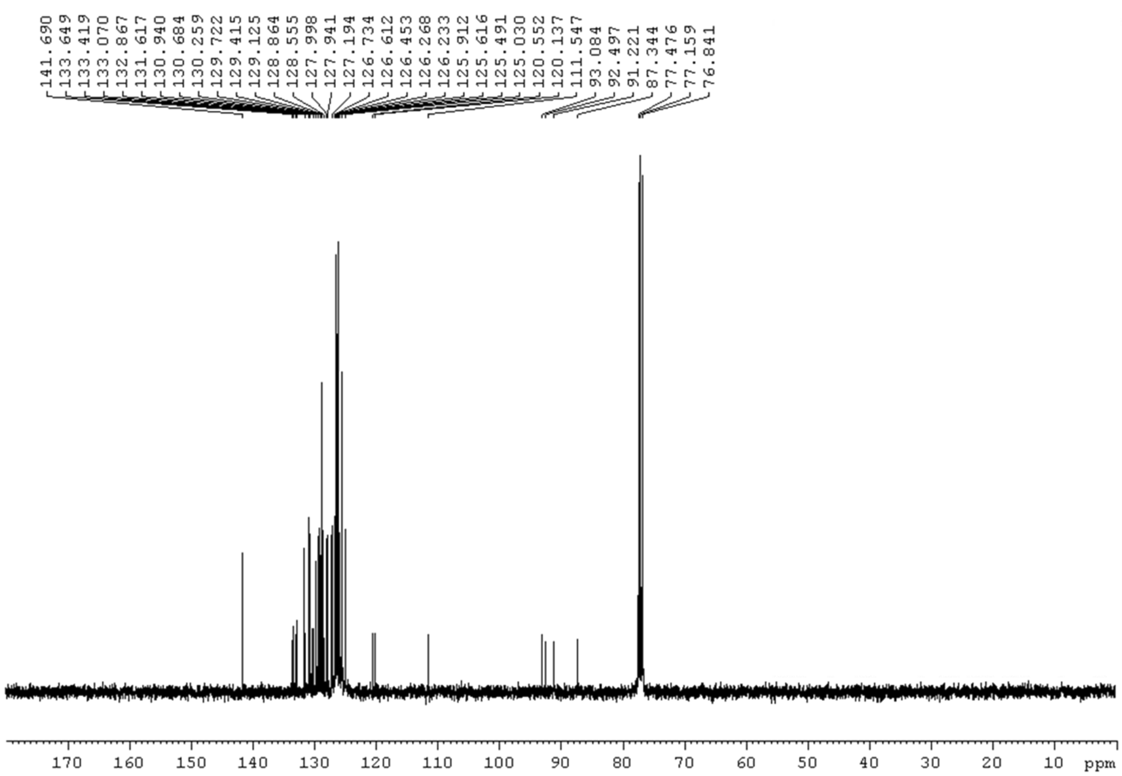

Figure S8. ^{13}C NMR spectrum of **AnEDYNap** in $CDCl_3$ (100 MHz).

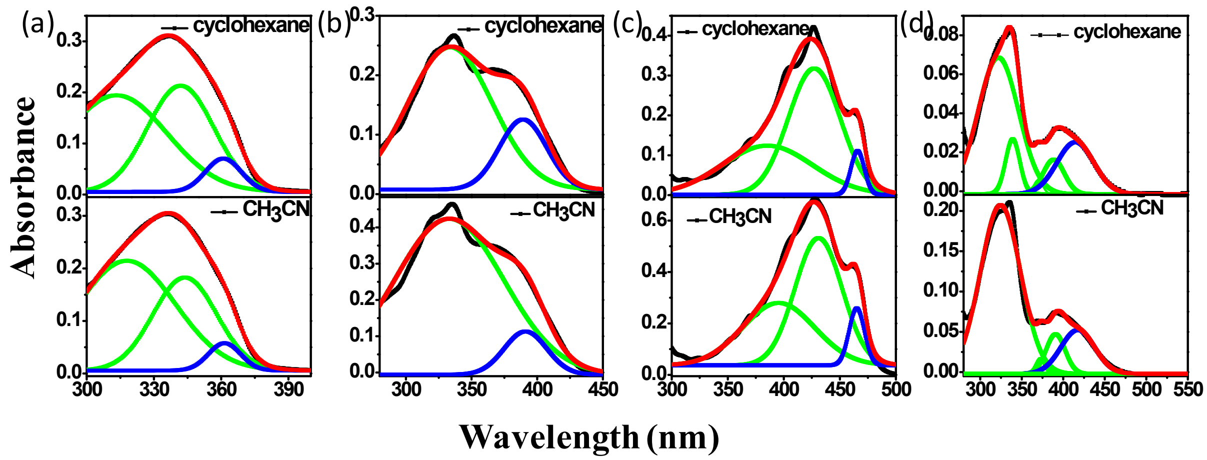

Figure S9. Gaussian fitting of absorption spectra of (a) **Ph_3EDY**, (b) **Nap_3EDY**, (c) **An_3EDY** (c = 1 x 10^{-5} M) and (d) **AnEDYNap** (c = 1 x 10^{-6} M) in cyclohexane and CH_3CN.

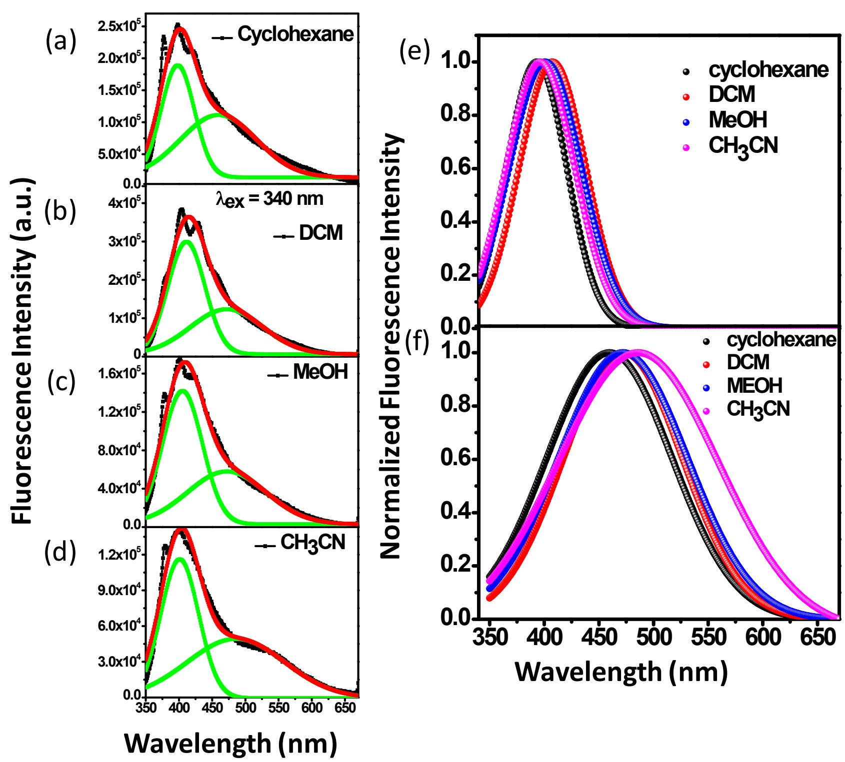

Figure S10. Gaussian fitting of emission spectra of **Ph_3EDY** in (a) cyclohexane, (b) DCM, (c) MeOH and (d) CH_3CN (c = 1 x 10^{-5} M, λ_{ex} = 340 nm) and resolved normalized emission spectra of **Ph_3EDY** (e) shorter wavelength and (f) longer wavelength band.

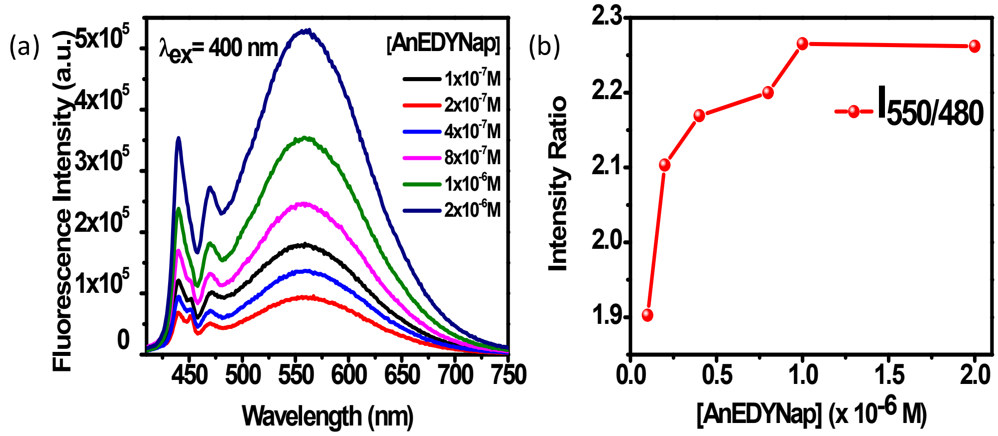

Figure S11. Steady-state (a) emission spectra in cyclohexane of **AnEDYNap** with varying concentration (λ_{ex} = 400 nm); (b) ratio of I_{550}/I_{480} vs. concentration of **AnEDYNap.**

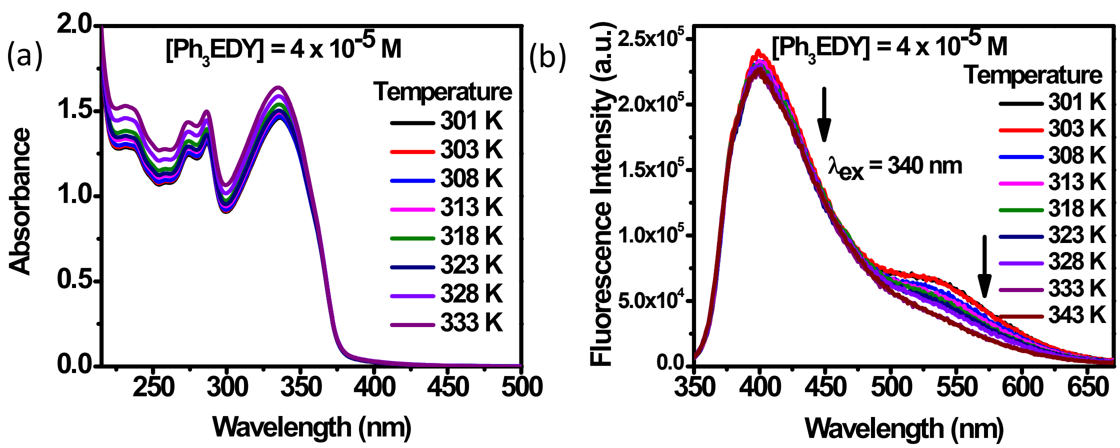

Figure S12. Steady-state (a) absorption and (b) emission spectra in CH_3CN of **Ph_3EDY** with varying temperature (λ_{ex} = 340 nm, c = 4 x10^{-5} M).

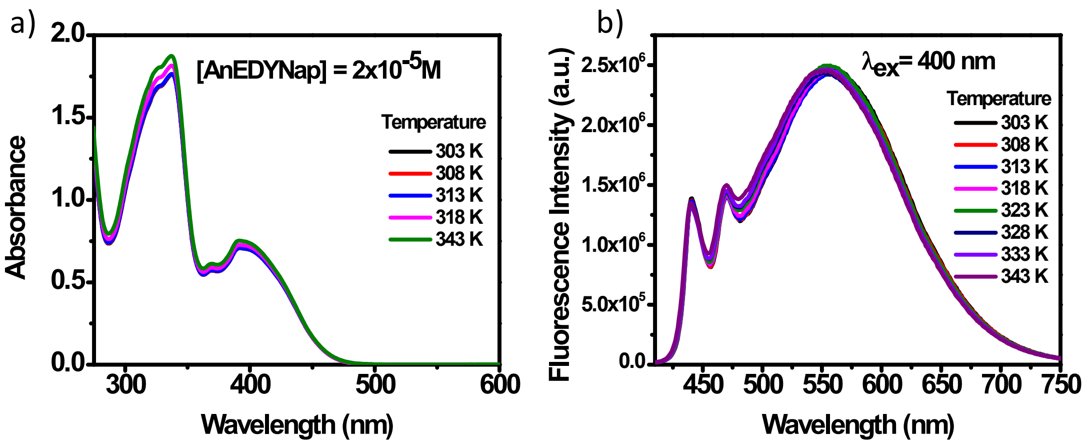

Figure S13. Steady-state (a) absorption and (b) emission spectra in cyclohexane of **AnEDYNap** with varying temperature (λ_{ex} = 400 nm, c = 2 x 10^{-5} M).

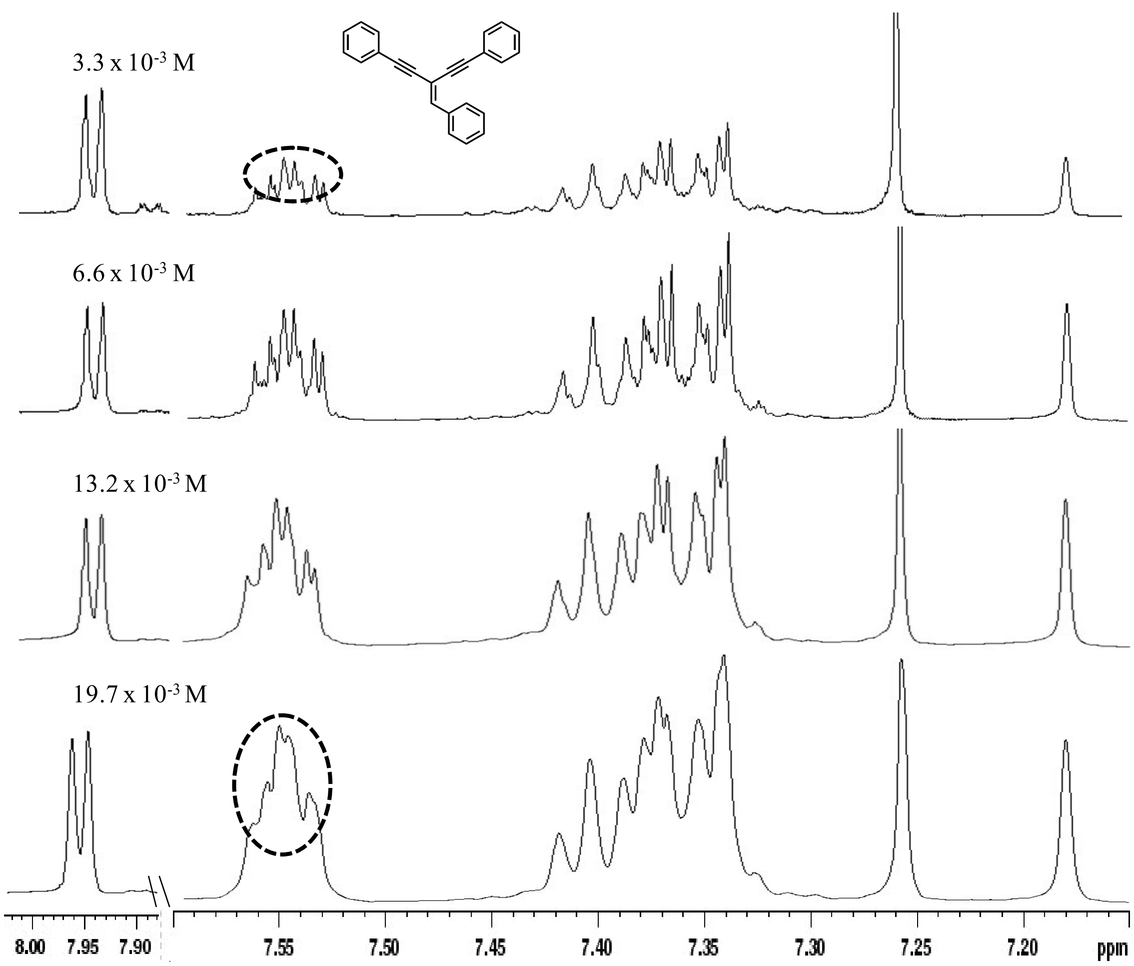

Figure S14. Concentration dependent ^{1}H NMR (500 MHz) of **Ph_3EDY** in $CDCl_3$.

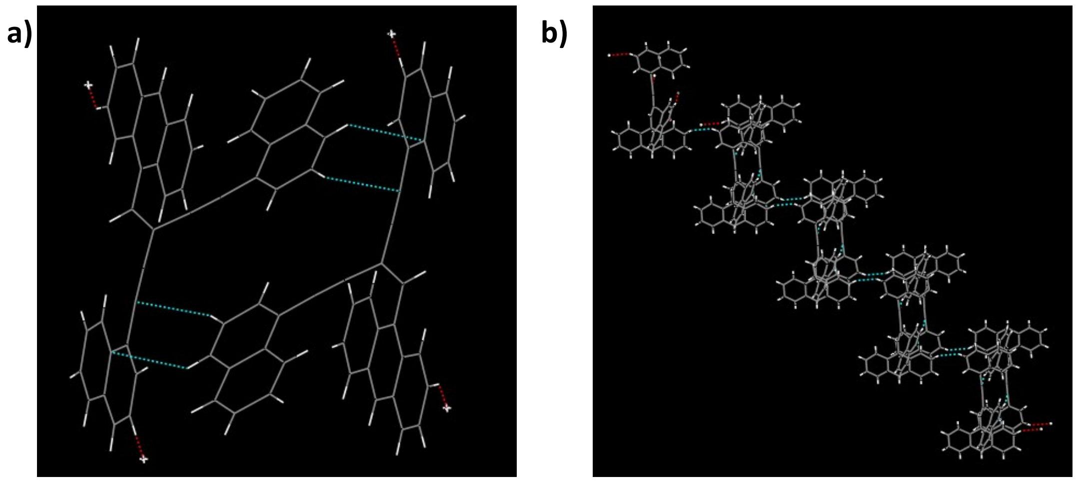

Figure S15. Crystal packing diagrams of **AnEDYNap** showing intermolecular interactions.

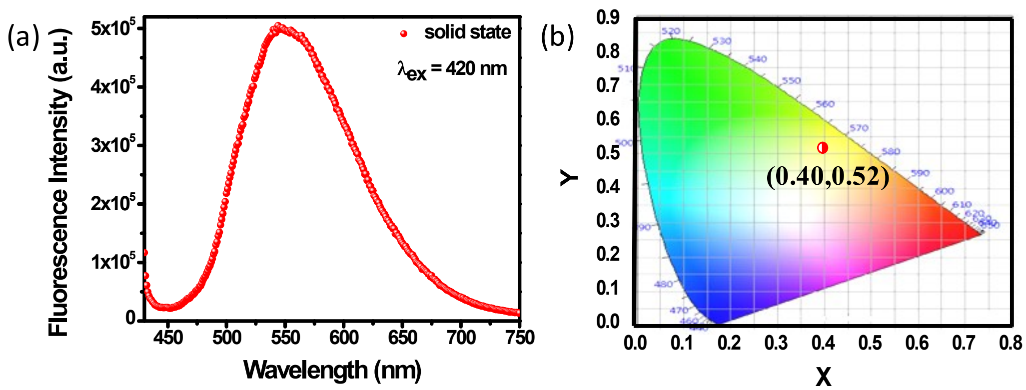

Figure S16. (a) Steady-state fluorescence spectrum of **AnEDYNap** in solid powder form (λ_{ex} = 420 nm), (b) CIE chromaticity diagram of **AnEDYNap** in solid powder form.

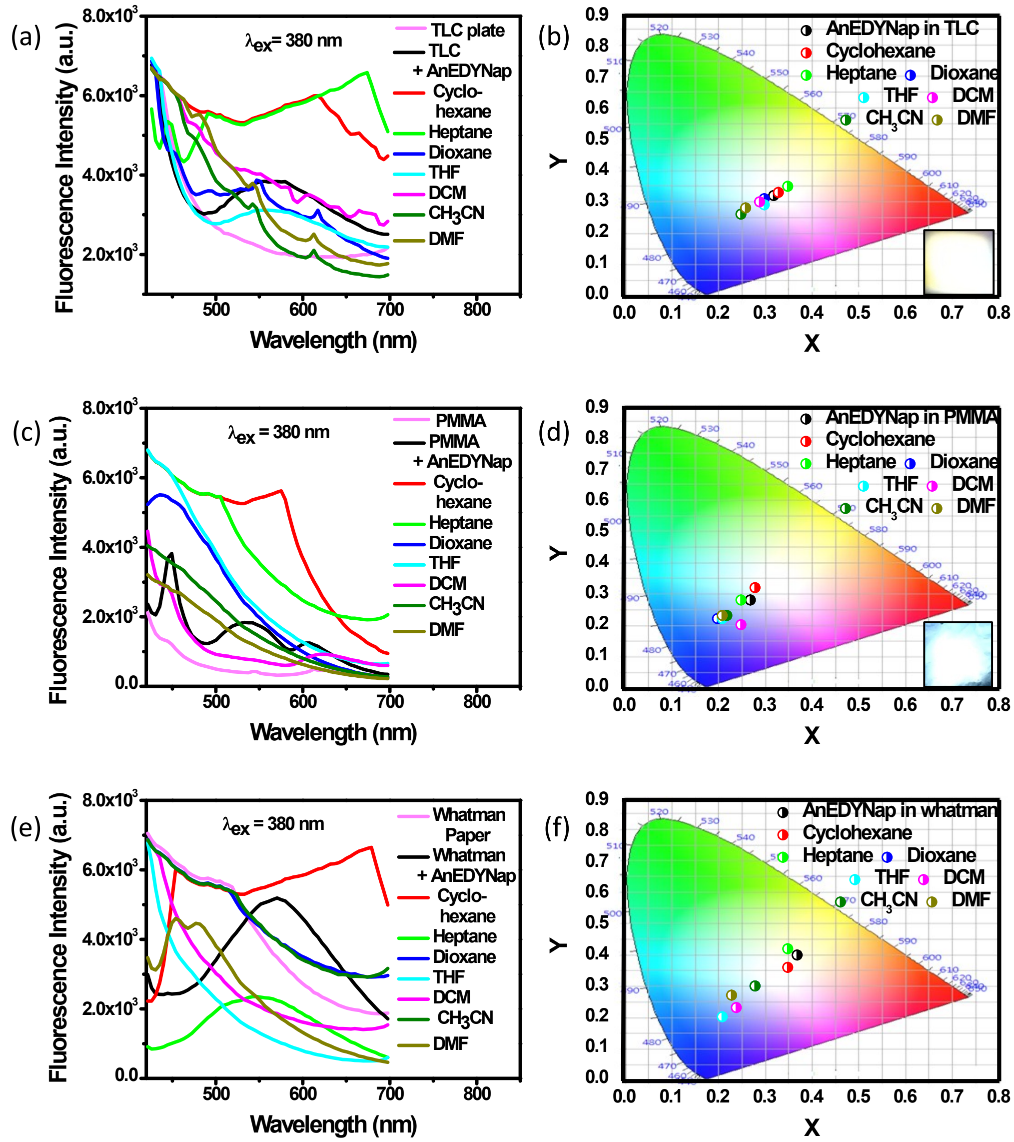

Figure S17. (a) Steady-state fluorescence spectrum of **AnEDYNap** in TLC plate and exposed to different solvent vapor (λ_{ex} = 380nm), (b) CIE chromaticity diagram of **AnEDYNap** in TLC plate, (c) steady-state fluorescence spectrum of **AnEDYNap** in PMMA film and exposed to different solvent vapor (λ_{ex} = 380 nm), (d) CIE chromaticity diagram of **AnEDYNap** in PMMA film (e) steady-state fluorescence spectrum of **AnEDYNap** in Whatman paper and exposed to different solvent vapor (λ_{ex} = 380 nm), (b) CIE chromaticity diagram of **AnEDYNap** in Whatman paper.

Table S1. Crystal data and structure refinement parameters for **AnEDYNap**.

Empirical Formula	C40 H24
Formula Weight	504.59
Crystal System	monoclinic
Space Group	P 21/n
a (Å)	12.6331(13)
b (Å)	15.3655(18)
c (Å)	14.1392(15)
α (°)	90
β (°)	95.557(3)
γ (°)	90
Volume (Å)	2731.7(5)
Z	4
Wavelength (Å)	0.71073
Temperature(K)	296(2)
Calculated density (g/cm^3)	1.227
Absorption coefficient (mm^{-1})	0.070
F(000)	1056
Crystal Dimensions (mm)	0.29 X 0.21 X 0.12
θ range for data collection (°)	2.27 to 17.56
Limiting indices	$-10 \leq h \leq 10$, $-12 \leq k \leq 13$, $-12 \leq l \leq 12$
Reflections collected	1770/1340
Data / restraints /Parameter	1340/ 0 / 362
GOF	1.025
Final [a]R indices [I>2\s (I)]	R1 = 0.0673, wR2 = 0.1111
R indices (all data)	R1 = 0.0478, wR2 = 0.0977
CCDC	1571708

Table S2. Screening of various functional and basis sets for the calculation of vertical absorption wavelength (λ_{abs}) of **Ph_3EDY** in cyclohexane. 'f' is oscillator strength.

Functional	Basis sets [λ_{abs} (nm) (f)]		
	6-311g(d,p)	6-311+g(d,p)	6-311++g(d,p)
B3LYP	395 (0.941)	399 (0.939)	399 (0.939)
CAM-B3LYP	385 (0.976)	389 (0.973)	389 (0.973)
LC-BLYP	327 (1.103)	330 (1.098)	330 (1.097)
LC-PBE	331 (1.098)	334 (1.096)	334 (1.096)
M05-2X	345 (1.069)	348 (1.065)	348 (1.065)
M06-2X	344 (1.056)	348 (1.050)	348 (1.049)
PBEO	377 (0.976)	379 (0.973)	379 (0.973)

Table S3. Quantum yield (ϕ), molar extinction coefficient (ε) and brightness (ϕ × ε) of **AnEDYNap** in various solvents using perylene (ϕ = 0.94 at 410 nm) as a reference standard.

Solvent	ϕ	$\varepsilon (x10^4)$	ε x ϕ $(x10^3)$
		$M^{-1}cm^{-1}$	$M^{-1}cm^{-1}$
Cyclohexane	0.08	3.2	2.5
DCM	0.02	4.8	0.9
MeOH	0.02	7.0	1.4
CH_3CN	0.02	6.2	1.2

Quantum Yield calculations. The fluorescence quantum yield (ϕ) of **AnEDYNap** in different solvents was measured using perylene[1] (ϕ = 0.94 at 410 nm) as a reference standard using the following relation:

$$\phi_u = \phi_r \frac{F_u A_r \eta_u^2 q_r}{F_r A_u \eta_r^2 q_u} \qquad (1)$$

where, *F* represents the corrected fluorescence peak area, *A* the absorbance at the excitation wavelength, *η* the refractive index of the solvent used, *q* the excitation light intensity, and the subscripts *r* and *u* refer to reference and unknown respectively.

Cartesian co-ordinates of the optimized ground state geometry of the fluorophores in cyclohexane (B3LYP/6-311G(d,p))

Optimized ground state geometry of Ph_3EDY

C	-2.10948	-2.45935	0.02163
C	-1.57635	-3.67261	-0.45078
C	-2.33822	-4.83398	-0.41886
C	-3.63903	-4.80940	0.08307
C	-4.17648	-3.61269	0.55560
C	-3.42248	-2.44599	0.52734
H	-0.56593	-3.68812	-0.84079
H	-1.91581	-5.76226	-0.78662
H	-4.22986	-5.71789	0.10706
H	-5.18627	-3.58900	0.94947
H	-3.83501	-1.51664	0.90117
C	-1.33393	-1.26692	-0.00980
C	-0.69250	-0.24002	-0.03726
C	0.14006	0.91546	-0.03737
C	1.54183	0.65024	-0.02073
C	2.72623	0.39935	-0.00400
C	-0.29507	2.21286	-0.02689
H	0.49727	2.95302	0.02510
C	4.11652	0.10061	0.01643
C	5.07481	1.13089	0.00460
C	4.55857	-1.23504	0.04952
C	6.43116	0.83028	0.02512
H	4.74129	2.16126	-0.02082
C	5.91687	-1.52588	0.06944
H	3.82543	-2.03240	0.06002
C	6.85794	-0.49682	0.05738
H	7.15845	1.63430	0.01584
H	6.24323	-2.55949	0.09508
H	7.91697	-0.72758	0.07336
C	-1.63697	2.77388	-0.05516
C	-1.76705	4.15443	0.20075
C	-2.81002	2.04699	-0.34058
C	-3.00769	4.77759	0.19599
H	-0.87552	4.73577	0.41148

C	-4.04868	2.67591	-0.35191
H	-2.74496	0.99318	-0.56899
C	-4.15766	4.03945	-0.07922
H	-3.07824	5.83960	0.40253
H	-4.93724	2.09819	-0.58146
H	-5.12807	4.52259	-0.08838

Optimized ground state geometry of Nap_3EDY

C	2.12153	-0.85245	-0.17275
C	1.09155	-0.20432	-0.06828
C	-0.22250	0.61416	0.05824
C	-1.60420	-0.06618	-0.13443
C	-2.67082	-0.60728	-0.28010
C	-0.16948	1.94692	0.28753
H	-1.07524	2.52212	0.33672
C	-4.03233	-1.29790	-0.46594
C	-5.20364	-0.66174	0.02199
C	-4.11914	-2.52234	-1.11074
C	-5.13059	0.59339	0.68180
C	-6.45751	-1.28859	-0.14723
C	-5.37201	-3.14869	-1.28041
H	-3.22014	-3.01286	-1.48977
C	-6.28822	1.19799	1.15569
H	-4.16167	1.07701	0.81244
C	-7.63089	-0.65691	0.34316
C	-6.52978	-2.54396	-0.80675
H	-5.42292	-4.11415	-1.78806
C	-7.54111	0.57167	0.98614
H	-6.23734	2.16336	1.66346
H	-8.59880	-1.14231	0.21138
H	-7.49849	-3.02779	-0.93770
H	-8.44002	1.06214	1.36536
C	3.41846	-1.67325	-0.30469
C	3.40165	-3.05174	0.03435
C	4.58983	-1.07614	-0.74433
C	2.21135	-3.67537	0.49283
C	4.58708	-3.81040	-0.07942
C	5.77310	-1.83535	-0.86360
H	4.60480	-0.01698	-1.00985
C	2.21602	-5.02528	0.82139
H	1.29643	-3.08828	0.58249
C	4.57446	-5.18902	0.26055
C	5.77775	-3.18543	-0.53534
H	6.68651	-1.35063	-1.21451

C	3.39997	-5.78388	0.70506
H	1.30269	-5.51000	1.17244
H	5.49053	-5.77423	0.17014
H	6.69279	-3.77219	-0.62519
H	3.38426	-6.84363	0.96793
C	1.19054	2.64055	0.46425
C	1.34989	3.97982	0.02501
C	2.25250	1.96513	1.04846
C	0.27413	4.68057	-0.58137
C	2.59807	4.62059	0.18386
C	3.49775	2.60760	1.21385
H	2.13148	0.93612	1.39343
C	0.45085	5.99080	-1.00833
H	-0.68908	4.18416	-0.70617
C	2.76165	5.96008	-0.25810
C	3.67443	3.91803	0.78718
H	4.32281	2.06351	1.67823
C	1.69716	6.63209	-0.84643
H	-0.37412	6.53486	-1.47284
H	3.72575	6.45456	-0.13230
H	4.63772	4.41412	0.91221
H	1.81708	7.66224	-1.18821

Optimized ground state geometry of An_3EDY

C	6.92199	-3.55511	1.11205
C	7.38970	-2.34469	0.68509
C	6.49219	-1.30505	0.29208
C	5.07481	-1.55054	0.34953
C	4.62994	-2.82631	0.80424
C	5.52228	-3.79626	1.17245
C	6.95968	-0.06139	-0.14049
C	4.17351	-0.52406	-0.04115
C	4.66654	0.73307	-0.48477
C	6.08743	0.95918	-0.52752
C	6.57155	2.22862	-0.96953
H	7.64408	2.38992	-0.99608
C	5.70951	3.21711	-1.35184
C	4.30629	2.99129	-1.31700
C	3.80273	1.78934	-0.89784
H	8.02996	0.11685	-0.17662
H	7.61361	-4.33577	1.40770
H	8.45587	-2.14974	0.63750
H	3.56495	-3.01490	0.85491
H	5.16185	-4.75950	1.51559

H	6.08995	4.17544	-1.68680
H	3.62934	3.77842	-1.62906
H	2.73330	1.62150	-0.88324
C	2.77411	-0.74788	0.01194
C	1.57603	-0.92785	0.05349
C	0.15853	-1.09091	0.09440
C	-0.39228	-2.33884	0.14069
H	0.30862	-3.16590	0.07583
C	-0.59781	0.11469	0.03996
C	-1.18169	1.17498	-0.02221
C	-4.00143	1.28223	-0.66966
C	-3.23925	2.46096	-0.42161
C	-5.33126	1.35654	-0.98402
C	-1.85662	2.41927	-0.09650
C	-3.90433	3.73483	-0.50887
C	-5.98836	2.61413	-1.07148
H	-5.89175	0.44707	-1.16767
C	-1.13929	3.62143	0.14956
C	-3.18276	4.90739	-0.27029
C	-5.29357	3.76730	-0.83979
H	-7.04233	2.65179	-1.32274
C	0.24444	3.62939	0.49282
C	-1.82441	4.88378	0.05617
H	-3.69211	5.86370	-0.33960
H	-5.78560	4.73209	-0.90403
C	0.90902	4.80376	0.72359
H	0.76419	2.68346	0.57741
C	-1.09362	6.08642	0.30262
C	0.23336	6.05082	0.62577
H	1.96058	4.78384	0.98652
H	-1.61922	7.03268	0.22868
H	0.77607	6.97064	0.81205
C	-2.19509	-1.46158	2.34534
C	-2.66148	-2.25553	1.25130
C	-3.03794	-1.05626	3.34255
C	-1.81755	-2.69704	0.19935
C	-4.04792	-2.65912	1.26660
C	-4.41307	-1.41711	3.32685
H	-2.65387	-0.45501	4.15875
C	-2.32828	-3.57140	-0.79615
C	-4.53261	-3.50529	0.26875
C	-4.89777	-2.20177	2.32117
H	-5.06683	-1.07757	4.12212
C	-1.52952	-4.04807	-1.88154
C	-3.70834	-3.98260	-0.75217
H	-5.57471	-3.80903	0.29345

H	-5.93988	-2.50341	2.30769
C	-2.04283	-4.89503	-2.82619
H	-0.50225	-3.71729	-1.96631
C	-4.20713	-4.86186	-1.76092
C	-3.39954	-5.31305	-2.76606
H	-1.41282	-5.24322	-3.63697
H	-5.24815	-5.16359	-1.71111
H	-3.78966	-5.98108	-3.52549
H	-3.50896	0.32065	-0.60133
H	-1.15157	-1.18374	2.38451

Optimized ground state geometry of AnEDYNap

C	-4.26266	-1.20818	3.24792
C	-4.66570	-2.08540	2.28282
C	-3.77426	-2.50303	1.24567
C	-2.43627	-1.96083	1.20356
C	-2.05332	-1.06942	2.25455
C	-2.93218	-0.70563	3.23696
C	-4.17122	-3.44025	0.29121
C	-1.55169	-2.36670	0.17148
C	-1.96998	-3.33514	-0.77819
C	-3.30236	-3.87952	-0.70987
C	-3.71019	-4.85048	-1.67499
H	-4.71633	-5.25086	-1.60825
C	-2.85988	-5.26594	-2.66053
C	-1.55039	-4.71946	-2.74367
C	-1.12486	-3.78221	-1.84132
H	-5.17785	-3.84445	0.33371
H	-4.94620	-0.90183	4.03157
H	-5.67114	-2.49304	2.29038
H	-1.04397	-0.68360	2.27342
H	-2.61140	-0.02937	4.02117
H	-3.18049	-6.00396	-3.38688
H	-0.88723	-5.04248	-3.53823
H	-0.13380	-3.35837	-1.94284
C	-0.16837	-1.87035	0.09156
H	0.61387	-2.62382	0.08371
C	0.24942	-0.57825	-0.03407
C	1.64380	-0.27215	-0.08458
C	-0.63521	0.53119	-0.16406
C	2.81848	0.01931	-0.13432
C	-1.35084	1.49927	-0.29301
C	-2.20796	2.62200	-0.44658

C	-1.68549	3.95946	-0.35837
C	-3.56200	2.42788	-0.68644
C	-0.31660	4.22755	-0.10700
C	-2.58275	5.06048	-0.52727
C	-4.43323	3.52107	-0.84988
H	-3.94475	1.41673	-0.74848
C	0.14517	5.52027	-0.02786
H	0.36279	3.39427	0.02579
C	-2.07153	6.38257	-0.44141
C	-3.95700	4.80840	-0.77398
H	-5.48485	3.33772	-1.03748
C	-0.73928	6.60959	-0.19758
H	1.19498	5.70786	0.16732
H	-2.75639	7.21391	-0.57139
H	-4.62793	5.65125	-0.90138
H	-0.36186	7.62386	-0.13348
C	4.19329	0.37558	-0.20165
C	5.21745	-0.55769	0.18511
C	4.55284	1.64088	-0.64764
C	4.92284	-1.86248	0.65338
C	6.58658	-0.15242	0.09610
C	5.90389	2.02633	-0.72912
H	3.77499	2.33583	-0.93943
C	5.92929	-2.72691	1.01417
H	3.88650	-2.16934	0.72490
C	7.60093	-1.07048	0.47657
C	6.90014	1.15147	-0.36657
H	6.15147	3.02068	-1.08231
C	7.28245	-2.32865	0.92512
H	5.68563	-3.72127	1.37079
H	8.63728	-0.75736	0.40666
H	7.94192	1.44711	-0.42926
H	8.06652	-3.01982	1.21270

Reference

1) A. M. Brouwer, *Pure Appl. Chem.*, 2011, **83**, 2213–2228.