Electronic Supplementary Information

Experimental and theoretical investigation of fluorescence solvatochromism of dialkoxyphenyl-pyrene molecules

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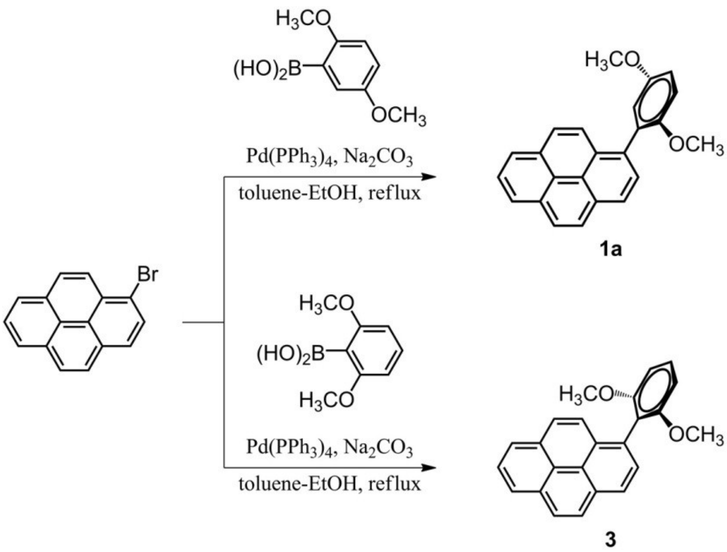
1. Methods

1.1 Materials

All starting materials and reagents, unless otherwise specified, were purchased from commercial suppliers (where noted) and used without further purification. 2,5-Dimethoxyphenylboronic acid,[1] and 2,6-dimethoxyphenylboronic acid[2] were synthesized and purified using reported methods. All reactions were performed under an argon atmosphere. Column chromatography was performed using Kanto Chemical silica gel 60 N (spherical, neutral). Spectroscopic grade solvents, dichloromethane (Wako Pure Chemical Industries, Ltd. (Wako)), toluene (Wako), chloroform (Wako), methanol (Wako), tetrahydrofuran (stabilizer free; Wako), *n*-hexane (Dojindo), acetonitrile (Dojindo) and dimethyl sulphoxide (Dojindo) were used for all spectroscopic studies without further purification.

1.2 Synthesis and characterization



General synthetic procedure for 1a and 3: A mixture of 1-bromopyrene (384 mg, 1.36 mmol, Wako), corresponding boronic acid (1.50 mmol), sodium carbonate (Na_2CO_3, 1.4 mL, 2 M a.q.), tetrakis(triphenylphosphine)palladium(0) ($Pd(PPh_3)_4$, 79 mg, 0.068 mmol, TCI) was refluxed in toluene-ethanol (54 mL-5.4 mL) under argon for 48–72 h until all starting material was consumed by TLC analysis. The reaction mixture was cooled, filtered and then evaporated to remove toluene. After evaporation, water (30 mL) was added and the aqueous layer was extracted with dichloromethane (3 × 30 mL). The combined organic layer was washed with brine (70 mL), dried over $MgSO_4$ and evaporated. The crude product was purified via column chromatography (SiO_2; dichloromethane/*n*-hexane, 1:5 v/v) and subsequent recycling HPLC with chloroform as the solvent to give the pure product.

1a: white powder (yield, 89%), T_m: 134.7-137.5 °C; TLC (SiO_2; dichloromethane/*n*-hexane, 1:1 v/v): R_f = 0.39; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.23-8.14 (m, 3H), 8.09 (d, J = 2.0 Hz, 2H), 8.01-7.95 (m, 3H), 7.89 (d, J = 9.2 Hz, 1H), 7.04-7.00 (m, 3H), 3.83 (s, 3H), 3.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 153.55, 151.63, 134.10, 131.38, 131.00, 130.90, 130.71, 129.14, 127.89, 127.44, 127.31, 127.13, 125.85, 124.98, 124.71, 124.47, 118.09, 113.72, 112.56, 56.37, 55.82; MALDI-TOF MS (matrix: dithranol) calculated for $C_{24}H_{18}O_2$: 338.1, found: 338.7 $[M]^+$.

3: white powder (yield, 87%), T_m: 232.6-235.3 °C; TLC (SiO_2; dichloromethane/*n*-hexane, 4:1 v/v): R_f = 0.19; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.23 (d, J = 8.0 Hz, 1H), 8.16-8.04 (m, 4H), 7.98-7.90 (m, 3H), 7.92 (d, J = 9.2 Hz, 1H), 7.44 (t, J = 8.0 Hz, 1H), 6.77 (d, J = 8.4 Hz, 2H), 3.64 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 158.55, 131.33, 131.12, 130.58, 130.32, 129.76, 129.32, 128.79, 127.60, 127.01, 126.85, 125.84, 125.63, 124.99, 124.87, 124.75, 124.66, 124.52, 118.06, 104.28, 55.94; MALDI-TOF MS (matrix: dithranol) calculated for $C_{24}H_{18}O_2$: 338.1, found: 338.5 $[M]^+$.

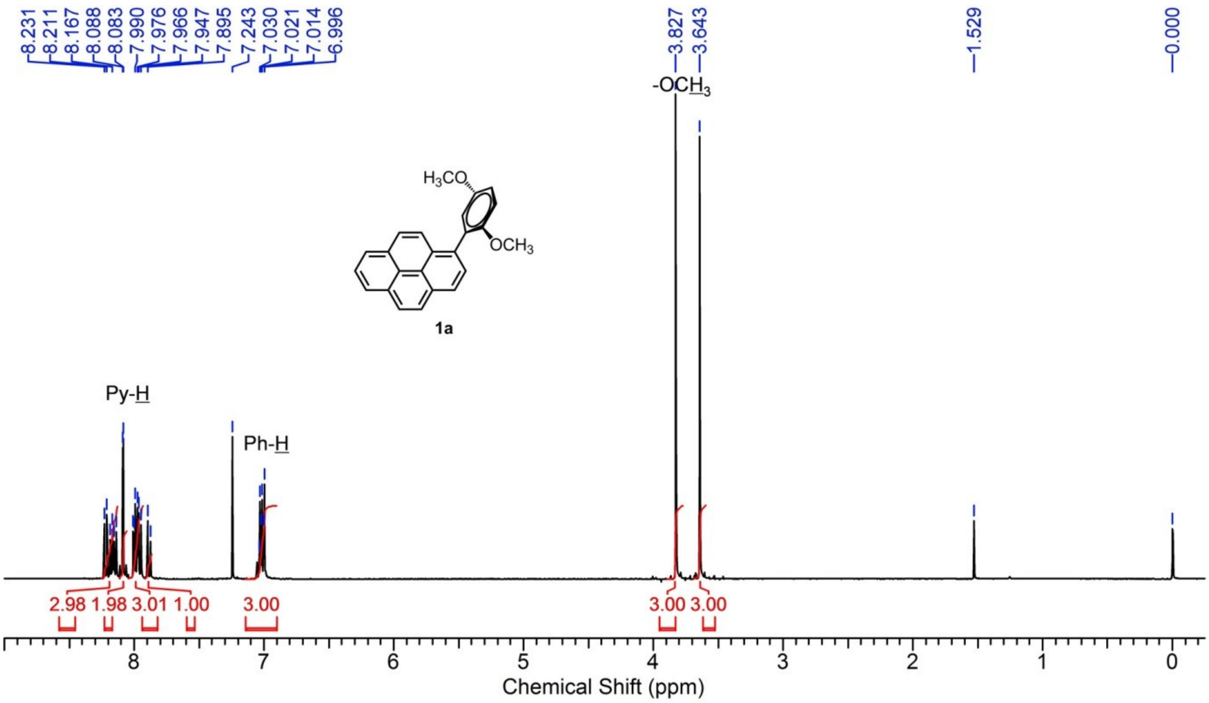


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1a**.

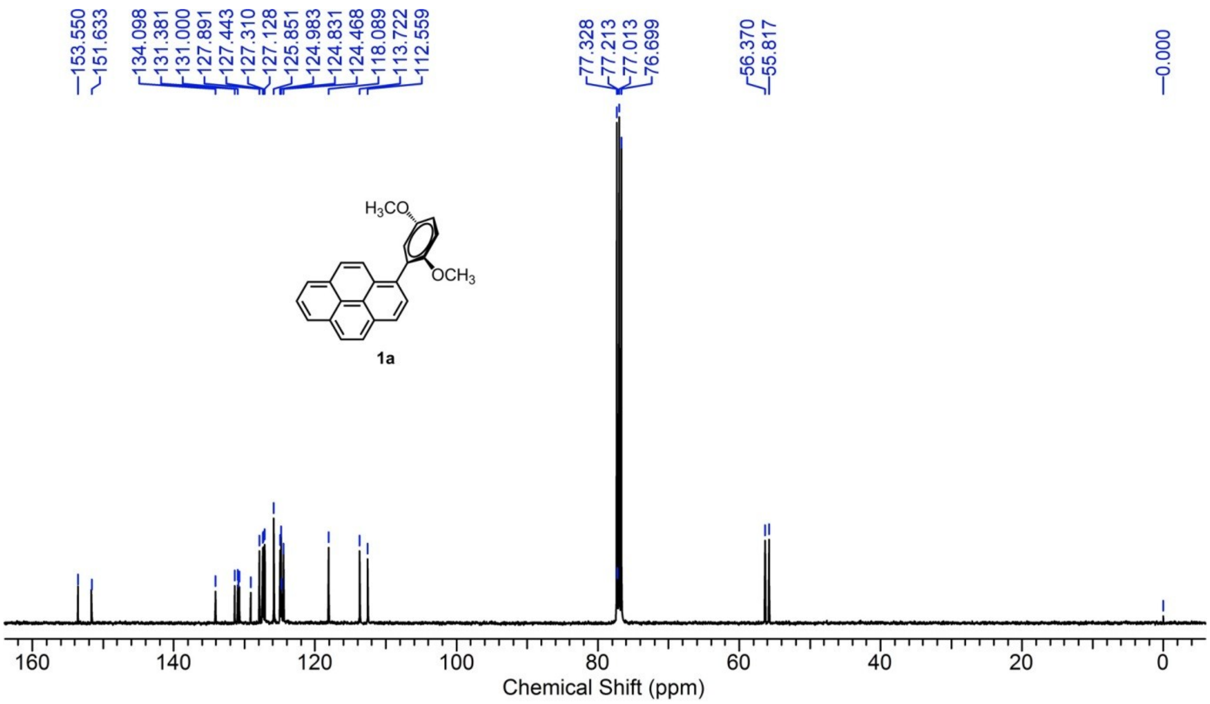


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **1a**.

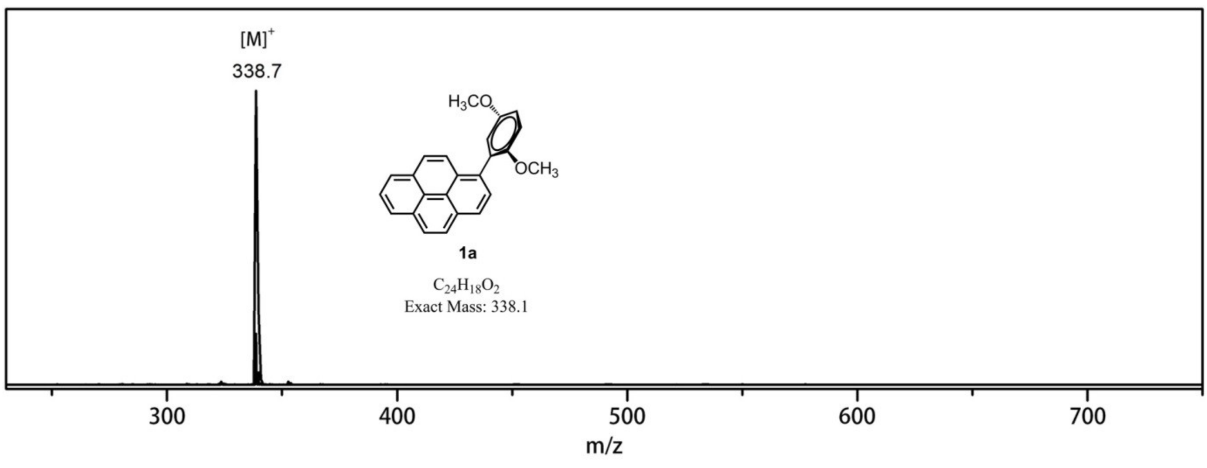


Figure S3. MALDI-TOF MS of **1a**. Matrix: dithranol.

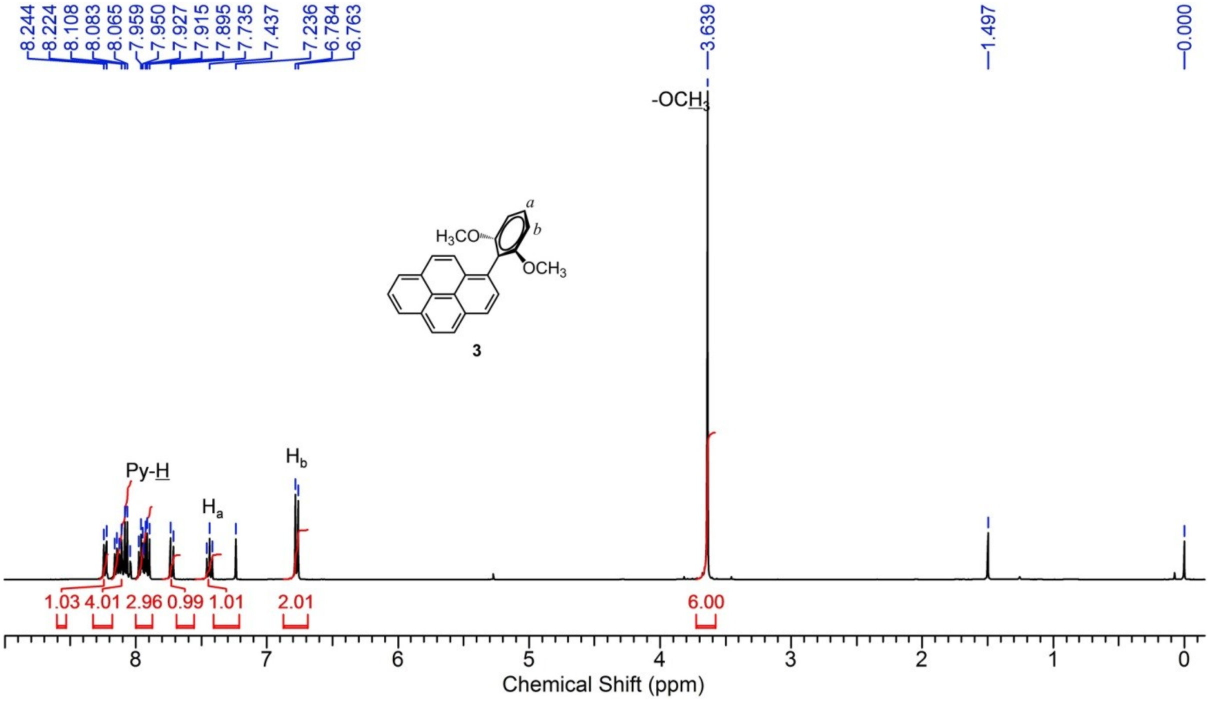


Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3**.

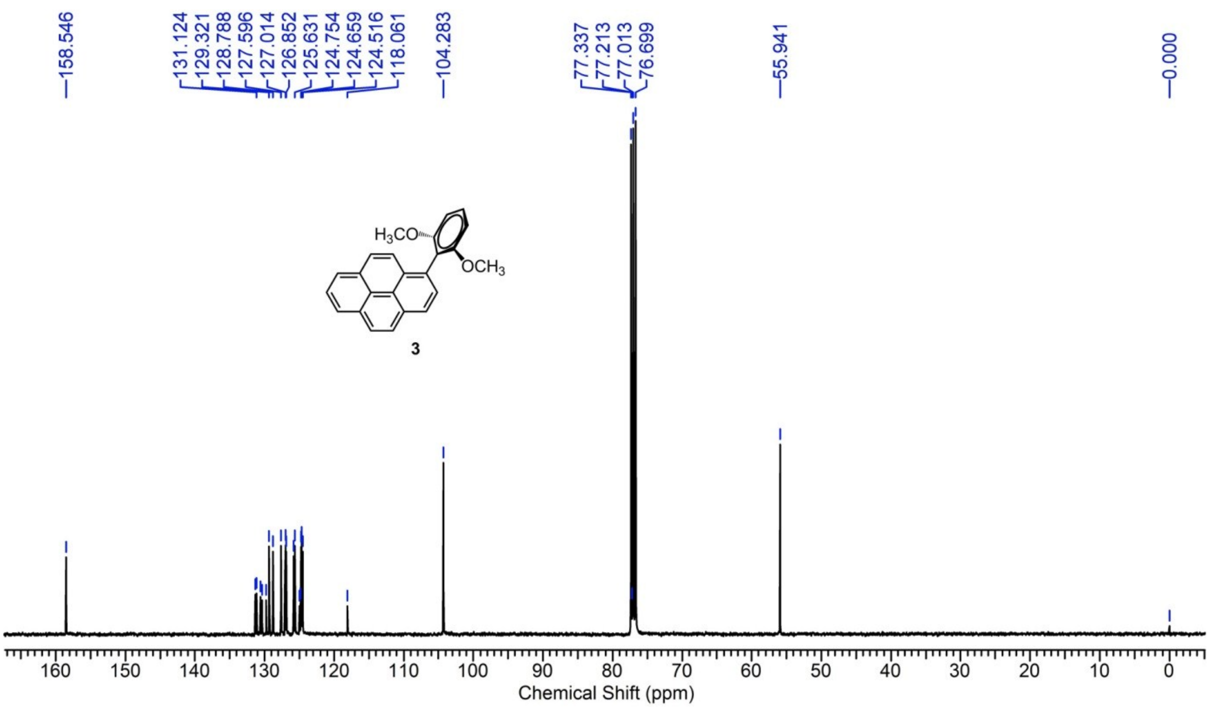


Figure S5. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3**.

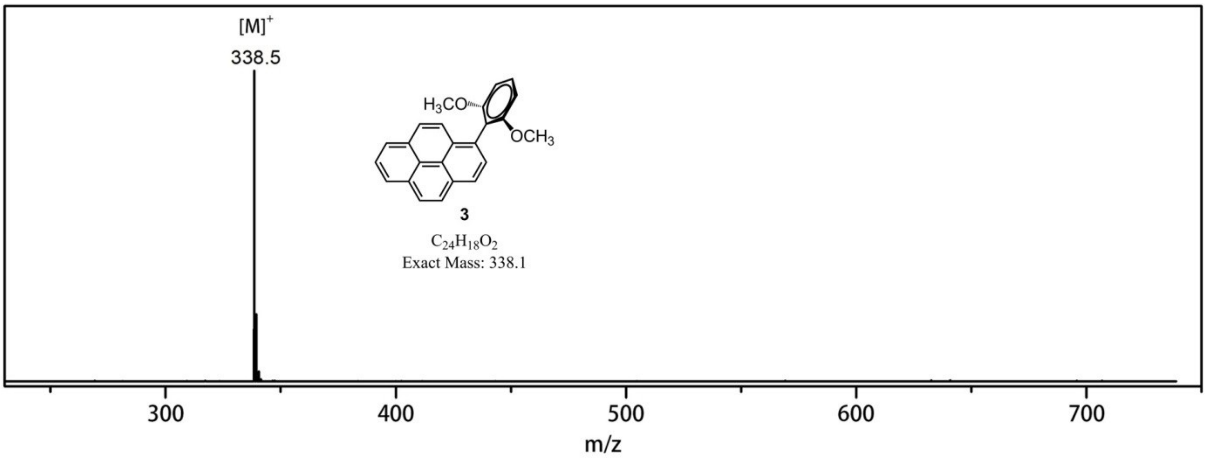


Figure S6. MALDI-TOF MS of **3**. Matrix: dithranol.

1.3 Techniques

Recycling high performance liquid chromatography (HPLC) was performed at room temperature using a GPC column (YMC-GPC T30000 ϕ 20 × 600 mm) on a LC-9225NEXT system, equipped with RI and UV-Vis detectors. Melting points were determined on a Yanaco melting point apparatus MP-500P. ^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer at 400 MHz and 100 MHz, respectively, with tetramethylsilane used as the internal standard. Matrix-assisted laser desorption ionization time-of-flight mass spectra (MALDI-TOF MS) were obtained by a Shimadzu AXIMA-CFR Plus station.

UV-Vis absorption and fluorescence spectra were recorded on a JASCO V-670 spectrophotometer and a JASCO FP-8300 spectrophotometer, respectively. Absolute quantum yields were determined on a Hamamatsu Photonics absolute PL quantum yield spectrometer C11347.

Nanosecond time-resolved fluorescence lifetime measurements were carried out by using time-correlated single photon counting (TCSPC) lifetime spectroscopy system HORIBA FluoroCube 3000U-UltraFast-SP spectrophotometer equipped with a nanosecond pulse LED (PB-280, 279 nm) and a nanosecond photon detection module (TBX). Decay analysis and the fitting routine to determine the lifetime(s) were performed using the DAS6 software provided by IBM. The quality of the fit has been judged by the fitting parameters such as chi-squared value χ^2 (< 1.20) as well as the visual inspection of the residuals.

A lab-built spectrometer equipped with a streak camera was used for recording picosecond time-resolved fluorescence spectra. Details of the spectrometer have been described elsewhere.[3,4] In short, pump pulses were prepared by using output of a femtosecond Ti:sapphire laser system (Coherent Micra-5/Legend-Elite USP/OPerA Solo). The pump wavelength was set at 345 nm. Fluorescence from samples was dispersed with a spectrograph (Acton SP-2358) and detected with a streak camera (Hamamatsu Photonics C10627). The polarization of the collected fluorescence was selected with an α-BBO Glan-Taylor prism analyzer set at 54.7^{o} with respect to the polarization of the pump pulse for avoiding effects of rotational relaxation on time-resolved spectra. The concentration of the sample solutions was 1 x 10^{-6} mol dm^{-3}. The sample solutions were held in a 1-cm cuvette and rapidly stirred for avoiding accumulation of photodamage. The measurements were performed at 25 ^{o}C.

2. Tables

Table S1. Photophysical parameters (λ: wavelength and Φ_{FL}: absolute fluorescence quantum yield) and fitting parameters (τ: decay time and χ^2: chi-squared value) of the fluorescence decays of **1b** in different solvents

Solvent	**Absorption Feature**[a]	**Fluorescence**[b]	**CIE**	**Fluorescence Decay**[b]	
	λ_{abs}, nm (ε, 10^4 dm^3 mol^{-1} cm^{-1})	λ_{max}, nm (Φ_{FL})	(x, y)	τ, ns[c]	χ^2
n-hexane	243 (4.38) 276 (3.08) 342 (2.50)	387 (0.09)	0.19, 0.11	7.7	1.05
Toluene	278 (0.31) 330 (1.85) 345 (2.53)	402 (0.43)	0.17, 0.06	8.5	1.13
$CHCl_3$	245 (4.01) 279 (3.02) 345 (2.55)	418 (0.50)	0.16, 0.07	5.0	1.19
THF	244 (4.81) 277 (3.31) 343 (2.59)	422 (0.48)	0.16, 0.08	5.3	1.07
CH_2Cl_2	244 (4.24) 278 (2.99) 344 (2.37)	432 (0.42)	0.16, 0.10	3.9	1.17
CH_3OH	243 (4.19) 276 (2.89) 341 (2.35)	443 (0.18)	0.17, 0.15	3.5	1.06
CH_3CN	243 (4.28) 276 (2.89) 342 (2.33)	462 (0.14)	0.18, 0.21	2.7	1.07
DMSO	279 (3.86) 346 (2.49)	471 (0.20)	0.19, 0.24	3.0	1.10

[a] Concentration: 10 μM;
[b] concentration: 1 μM. λ_{ex}: 342 nm for *n*-hexane and CH_3CN; 345 nm for toluene and $CHCl_3$; 343 nm for THF; 344 nm for CH_2Cl_2; 341 nm for CH_3OH and 346 nm for DMSO;
[c] monitored at their respective maximum emission wavelengths; λ_{ex}: 279 nm.

Table S2. Photophysical parameters (λ: wavelength and Φ_{FL}: absolute fluorescence quantum yield) and fitting parameters (τ: decay time and χ^2: chi-squared value) of the fluorescence decays of **2a** in different solvents

Solvent	Absorption Feature[a]	Fluorescence[b]	CIE	Fluorescence Decay[b]	
	λ_{abs}, nm (ε, 10^4 dm^3 mol^{-1} cm^{-1})	λ_{max}, nm (Φ_{FL})	(x, y)	τ, ns[c]	χ^2
n-hexane	238 (4.18) 277 (3.58) 341 (3.00)	379 (0.03)	0.21, 0.16	8.3	1.11
Toluene	282 (2.50) 345 (2.80)	381 (0.15)	0.19, 0.09	15.3	1.16
$CHCl_3$	245 (4.17) 280 (3.46) 345 (2.93)	381 (0.10)	0.19, 0.09	15.2	1.10
THF	243 (3.43) 279 (3.46) 343 (2.90)	380 (0.21)	0.18, 0.09	20.8	1.07
CH_2Cl_2	243 (4.19) 280 (3.51) 344 (2.88)	381 (0.27)	0.18, 0.08	22.8	1.05
CH_3OH	241 (4.39) 277 (3.62) 341 (2.95)	379 (0.06)	0.21, 0.14	15.6	1.18
CH_3CN	240 (4.26) 278 (3.43) 342 (2.80)	380 (0.10)	0.20, 0.13	14.2	1.10
DMSO	281 (3.17) 346 (2.62)	382 (0.41)	0.17, 0.05	39.4	1.10

[a] Concentration: 10 μM;
[b] concentration: 1 μM. λ_{ex}: 341 nm for *n*-hexane and CH_3OH; 345 nm for toluene and $CHCl_3$; 343 nm for THF; 344 nm for CH_2Cl_2; 342 nm for CH_3CN and 346 nm for DMSO;
[c] monitored at their respective maximum emission wavelengths; λ_{ex} = 279 nm.

Table S3. Photophysical parameters (λ: wavelength and Φ_{FL}: absolute fluorescence quantum yield) and fitting parameters (τ: decay time and χ^2: chi-squared value) of the fluorescence decays of **2b** in different solvents

Solvent	Absorption Feature[a]	Fluorescence[b]	CIE	Fluorescence Decay[b]	
	λ_{abs}, nm (ε, 10^4 dm^3 mol^{-1} cm^{-1})	λ_{max}, nm (Φ_{FL})	(x, y)	τ, ns[c]	χ^2
***n*-hexane**	240 (4.48) 279 (3.46) 341 (3.14)	379 (0.04)	0.21, 0.14	9.5	1.12
Toluene	282 (2.67) 345 (3.08)	381 (0.24)	0.18, 0.08	16.3	1.15
$CHCl_3$	244 (4.37) 281 (3.52) 345 (3.06)	381 (0.12)	0.19, 0.09	15.2	1.16
THF	241 (4.39) 279 (3.74) 343 (3.19)	380 (0.18)	0.18, 0.08	19.1	1.06
CH_2Cl_2	242 (4.68) 280 (3.72) 344 (3.11)	381 (0.21)	0.18, 0.07	22.4	1.13
CH_3OH	241 (4.64) 277 (3.71) 341 (3.10)	380 (0.07)	0.19, 0.11	16.3	1.13
CH_3CN	241 (4.67) 278 (3.64) 342 (3.01)	380 (0.17)	0.19, 0.11	14.8	1.18
DMSO	281 (3.56) 346 (2.98)	382 (0.44)	0.17, 0.04	37.0	1.09

[a]Concentration: 10 μM;
[b]concentration: 1 μM. λ_{ex}: 341 nm for *n*-hexane and CH_3OH; 345 nm for toluene and $CHCl_3$; 343 nm for THF; 344 nm for CH_2Cl_2; 342 nm for CH_3CN and 346 nm for DMSO;
[c]monitored at their respective maximum emission wavelengths; λ_{ex}: 279 nm.

Table S4. Photophysical parameters (λ: wavelength and Φ_{FL}: absolute fluorescence quantum yield) and fitting parameters (τ: decay time and χ^2: chi-squared value) of the fluorescence decays of **3** in different solvents

Solvent	**Absorption Feature**[a]	**Fluorescence**[b]	**CIE**	**Fluorescence Decay**[b]	
	λ_{abs}, nm (ε, 10^4 dm^3 mol^{-1} cm^{-1})	λ_{max}, nm (Φ_{FL})	(x, y)	τ, ns[c]	χ^2
***n*-hexane**	243 (5.15) 276 (3.72) 341 (3.49)	387 (0.02)	0.22, 0.17	7.6	1.07
Toluene	282 (1.71) 344 (3.24)	388 (0.07)	0.19, 0.13	14.3	1.03
$CHCl_3$	245 (4.57) 279 (3.36) 345 (3.13)	377 (0.07)	0.20, 0.13	14.2	1.10
THF	243 (4.98) 277 (3.69) 343 (3.37)	377 (0.11)	0.19, 0.11	35.6	1.18
CH_2Cl_2	244 (5.15) 278 (3.71) 344 (3.40)	377 (0.13)	0.19, 0.11	20.8	1.07
CH_3OH	242 (5.41) 275 (3.76) 341 (3.48)	395 (0.05)	0.20, 0.15	14.3	1.10
CH_3CN	242 (5.24) 276 (3.60) 341 (3.33)	376 (0.05)	0.20, 0.14	13.6	1.15
DMSO	278 (3.51) 345 (3.16)	378 (0.23)	0.18, 0.07	43.5	1.08

[a]Concentration: 10 μM.
[b]concentration: 1 μM. λ_{ex}: 341 nm for *n*-hexane, CH_3OH and CH_3CN; 344 nm for toluene and CH_2Cl_2; 345 nm for $CHCl_3$ and DMSO and 343 nm for THF;
[c]monitored at their respective maximum emission wavelengths; λ_{ex} = 279 nm.

Table S5. Cartesian coordinates (in Å) of the optimized geometries.

1a: min(GS) in CH_2Cl_2 solution

C	-0.407341	2.077521	0.877392
C	-0.585473	0.794762	0.356149
C	0.542159	0.055020	-0.052586
C	1.838887	0.622441	0.089793
C	1.994817	1.925283	0.634422
C	0.855622	2.636685	1.017698
C	0.435130	-1.259280	-0.633727
C	2.995474	-0.113885	-0.318321
C	2.854273	-1.412474	-0.874800
C	1.530067	-1.954613	-1.022163
C	3.997056	-2.118772	-1.266727
C	5.261506	-1.560535	-1.115992
C	5.408883	-0.287818	-0.574361
C	4.291481	0.451258	-0.170985
C	4.412667	1.772215	0.389694
C	3.319357	2.473173	0.771191
H	3.421690	3.470129	1.191300
H	5.406869	2.197079	0.498850
H	-0.551798	-1.690234	-0.760306
H	-1.281060	2.643083	1.187783
H	1.424210	-2.944108	-1.458913
H	6.139278	-2.120633	-1.424223
C	-1.973479	0.265847	0.220749
C	-2.433450	-0.810933	1.006060
C	-2.855757	0.871878	-0.663138
C	-3.743017	-1.252948	0.869928
C	-4.175678	0.430950	-0.799561
H	-2.519919	1.704471	-1.273897
C	-4.617938	-0.637725	-0.032151
H	-5.632359	-1.009420	-0.110493
H	3.886035	-3.112405	-1.692483
H	6.399308	0.144561	-0.460364
H	0.963948	3.635264	1.432309
O	-4.940658	1.108951	-1.706724
C	-6.289969	0.705987	-1.873002
H	-6.711514	1.370165	-2.627201
H	-6.353790	-0.330394	-2.223571
H	-6.852395	0.811968	-0.938367
H	-4.112973	-2.078528	1.465510
O	-1.533896	-1.347709	1.880987
C	-1.944666	-2.442078	2.682429
H	-2.237452	-3.298712	2.064585
H	-1.079216	-2.710961	3.287731
H	-2.776119	-2.163003	3.339698

1a: min(GS) in *n*-hexane solution

C	-0.411652	2.078194	0.868158
C	-0.587211	0.795039	0.348360
C	0.541357	0.056186	-0.057749
C	1.837001	0.624436	0.086762
C	1.990535	1.927587	0.630358
C	0.850224	2.638197	1.009953
C	0.436392	-1.257614	-0.638947
C	2.994758	-0.111178	-0.317753

C	2.855684	-1.409750	-0.873926
C	1.532408	-1.951864	-1.024537
C	3.999656	-2.114973	-1.262685
C	5.263187	-1.556689	-1.109114
C	5.408280	-0.284222	-0.567618
C	4.289924	0.454334	-0.167592
C	4.408485	1.775280	0.392247
C	3.314043	2.475767	0.769782
H	3.414885	3.473304	1.189219
H	5.402207	2.200934	0.503828
H	-0.550365	-1.687711	-0.768964
H	-1.287102	2.641524	1.177764
H	1.428083	-2.941162	-1.462442
H	6.142032	-2.116486	-1.415178
C	-1.974438	0.264285	0.215448
C	-2.427856	-0.816691	0.999561
C	-2.862736	0.871061	-0.660314
C	-3.736967	-1.260140	0.870850
C	-4.182933	0.428480	-0.789879
H	-2.533480	1.705149	-1.272236
C	-4.618814	-0.642727	-0.023569
H	-5.633438	-1.015204	-0.097049
H	3.889897	-3.108714	-1.688845
H	6.398217	0.148969	-0.451230
H	0.957232	3.637267	1.424108
O	-4.952948	1.108966	-1.690061
C	-6.298088	0.704890	-1.853356
H	-6.723949	1.371122	-2.603734
H	-6.362529	-0.330768	-2.208449
H	-6.859947	0.805429	-0.916840
H	-4.101320	-2.088199	1.466748
O	-1.519785	-1.354559	1.863725
C	-1.919377	-2.445448	2.668514
H	-2.218893	-3.304741	2.056109
H	-1.046685	-2.713134	3.264260
H	-2.744142	-2.167476	3.335906

1a: min(ICT) in CH_2Cl_2 solution

C	-0.484566	2.175949	0.627241
C	-0.632525	0.830439	0.225309
C	0.539446	0.090856	-0.140069
C	1.830277	0.689258	0.040659
C	1.942315	2.030109	0.514756
C	0.755515	2.761296	0.773148
C	0.490273	-1.207073	-0.716867
C	3.010173	-0.046768	-0.263283
C	2.919909	-1.377536	-0.789151
C	1.628019	-1.915660	-1.028715
C	4.104532	-2.091532	-1.073324
C	5.350701	-1.511284	-0.854296
C	5.453825	-0.215586	-0.357052
C	4.299574	0.539997	-0.056743
C	4.372269	1.872883	0.437757
C	3.234112	2.589117	0.703472
H	3.307380	3.610235	1.070247
H	5.350958	2.318869	0.594637
H	-0.473646	-1.651140	-0.937621

H	-1.375297	2.747693	0.873171
H	1.546865	-2.903106	-1.475239
H	6.253258	-2.073038	-1.078800
C	-1.982790	0.267361	0.148276
C	-2.330253	-0.985587	0.761177
C	-3.013566	0.950887	-0.483805
C	-3.632410	-1.509327	0.675370
C	-4.329431	0.436772	-0.541634
H	-2.821847	1.898706	-0.974500
C	-4.642331	-0.811177	0.027821
H	-5.642344	-1.221197	-0.012633
H	4.029553	-3.100225	-1.470359
H	6.431079	0.232870	-0.198649
H	0.834152	3.789359	1.117658
O	-5.214259	1.213661	-1.173742
C	-6.574014	0.791230	-1.294971
H	-7.077582	1.585151	-1.843023
H	-6.636098	-0.145109	-1.855557
H	-7.028006	0.674748	-0.307388
H	-3.869923	-2.450122	1.155859
O	-1.353150	-1.576144	1.449738
C	-1.561175	-2.845200	2.071608
H	-1.842173	-3.594714	1.327480
H	-0.605290	-3.106699	2.520759
H	-2.329044	-2.768947	2.845892

1a:min(ICT) in *n*-hexane solution

C	-0.485617	2.183771	0.606751
C	-0.633285	0.839183	0.205307
C	0.537540	0.096578	-0.155831
C	1.826412	0.693026	0.031500
C	1.939468	2.032262	0.504251
C	0.751562	2.767630	0.756397
C	0.489047	-1.200805	-0.730517
C	3.008293	-0.047472	-0.264533
C	2.917680	-1.377803	-0.787622
C	1.627712	-1.912996	-1.034210
C	4.102943	-2.094794	-1.064392
C	5.346293	-1.515908	-0.839808
C	5.449756	-0.220784	-0.343959
C	4.295068	0.537247	-0.051015
C	4.367487	1.870080	0.441929
C	3.229278	2.588512	0.699680
H	3.301704	3.610037	1.065615
H	5.346357	2.313837	0.603672
H	-0.474526	-1.640590	-0.963103
H	-1.376824	2.756285	0.851073
H	1.547936	-2.898999	-1.484580
H	6.249406	-2.079174	-1.059303
C	-1.982345	0.274417	0.138857
C	-2.323743	-0.975686	0.765033
C	-3.019806	0.940701	-0.495891
C	-3.624518	-1.507100	0.695266
C	-4.336826	0.421333	-0.534947
H	-2.836111	1.880688	-1.003943
C	-4.644064	-0.820402	0.049656
H	-5.643240	-1.233537	0.021710

H	4.028498	-3.103864	-1.460619
H	6.426776	0.226609	-0.181548
H	0.830830	3.796274	1.098492
O	-5.227379	1.190966	-1.167522
C	-6.584648	0.767946	-1.275316
H	-7.092897	1.556100	-1.827807
H	-6.651492	-0.174178	-1.826692
H	-7.033656	0.660482	-0.283756
H	-3.852474	-2.443543	1.189344
O	-1.337270	-1.557109	1.444075
C	-1.522234	-2.821631	2.073732
H	-1.806910	-3.579303	1.338359
H	-0.556230	-3.071258	2.507987
H	-2.278686	-2.750555	2.860757

1a: min(LE) in CH_2Cl_2 solution

C	-0.520186	2.164102	0.562053
C	-0.654434	0.802928	0.200294
C	0.554826	0.065627	-0.149566
C	1.829158	0.679240	0.051693
C	1.919938	2.021891	0.526137
C	0.701199	2.757538	0.740442
C	0.521136	-1.199077	-0.755008
C	3.022119	-0.032592	-0.250013
C	2.951968	-1.347062	-0.798744
C	1.685692	-1.894603	-1.062822
C	4.164369	-2.048972	-1.080512
C	5.394382	-1.460303	-0.833313
C	5.475965	-0.172097	-0.314066
C	4.297026	0.570107	-0.018129
C	4.346658	1.883317	0.487392
C	3.178390	2.595013	0.739215
H	3.237679	3.617266	1.102643
H	5.313078	2.345966	0.666684
H	-0.435161	-1.651971	-0.987940
H	-1.419232	2.731967	0.780962
H	1.618152	-2.881050	-1.513197
H	6.306377	-2.008275	-1.052526
C	-1.988644	0.226683	0.149754
C	-2.317998	-1.032988	0.734471
C	-3.037325	0.956503	-0.438700
C	-3.614387	-1.523988	0.650323
C	-4.335120	0.464903	-0.508045
H	-2.827678	1.914016	-0.903797
C	-4.626919	-0.790335	0.027020
H	-5.625424	-1.207281	-0.017263
H	4.105549	-3.051839	-1.494472
H	6.444082	0.286273	-0.132030
H	0.766281	3.787373	1.080144
O	-5.247996	1.266109	-1.132532
C	-6.582290	0.798759	-1.252030
H	-7.127239	1.580887	-1.780123
H	-6.626335	-0.130293	-1.831294
H	-7.036334	0.640455	-0.267488
H	-3.868393	-2.478843	1.093778
O	-1.330008	-1.652385	1.428302
C	-1.584452	-2.925956	1.998220

H	-1.870555	-3.652676	1.229806
H	-0.648636	-3.235670	2.462519
H	-2.368599	-2.867927	2.761042

1a: min(LE) *n*-hexane solution

C	-0.519904	2.171570	0.547152
C	-0.654552	0.809494	0.187753
C	0.551356	0.070951	-0.158608
C	1.826545	0.680435	0.045907
C	1.918056	2.023664	0.519825
C	0.702950	2.761213	0.728572
C	0.515263	-1.194350	-0.767000
C	3.017340	-0.034195	-0.251831
C	2.945620	-1.348509	-0.800902
C	1.676511	-1.892022	-1.070389
C	4.154416	-2.052177	-1.078419
C	5.385301	-1.467795	-0.827040
C	5.468257	-0.179857	-0.306896
C	4.293484	0.564195	-0.015912
C	4.344273	1.879685	0.490183
C	3.179765	2.593727	0.736663
H	3.239854	3.616158	1.100009
H	5.311996	2.338582	0.672686
H	-0.442951	-1.639924	-1.006895
H	-1.419032	2.739743	0.764402
H	1.608669	-2.877016	-1.524336
H	6.296487	-2.018134	-1.043568
C	-1.987890	0.232023	0.144285
C	-2.309881	-1.026176	0.737556
C	-3.041688	0.953874	-0.443005
C	-3.604131	-1.523285	0.663408
C	-4.337418	0.456226	-0.503169
H	-2.839388	1.908026	-0.917645
C	-4.622433	-0.796841	0.040842
H	-5.619907	-1.217122	0.003429
H	4.094261	-3.054299	-1.494135
H	6.437250	0.275545	-0.121979
H	0.769823	3.791236	1.067488
O	-5.255096	1.249582	-1.128957
C	-6.583561	0.776591	-1.246171
H	-7.132515	1.553726	-1.778046
H	-6.624820	-0.155745	-1.821740
H	-7.039031	0.620276	-0.261125
H	-3.851130	-2.476444	1.114693
O	-1.314186	-1.635834	1.427426
C	-1.557222	-2.898907	2.016325
H	-1.848188	-3.639579	1.261985
H	-0.615352	-3.198279	2.475672
H	-2.334510	-2.833942	2.786586

2a: min(GS) in CH_2Cl_2 solution

C	0.016213	-2.204368	0.740957
C	0.264202	-0.903851	0.293882
C	-0.825826	-0.064382	-0.019597
C	-2.153423	-0.550916	0.156032
C	-2.376536	-1.870959	0.630578
C	-1.274442	-2.682976	0.909595

C	-0.658868	1.268307	-0.546188
C	-3.274140	0.284733	-0.148481
C	-3.070703	1.600794	-0.640928
C	-1.721226	2.055658	-0.838218
C	-4.178391	2.405614	-0.929541
C	-5.470074	1.927842	-0.738959
C	-5.679500	0.638599	-0.261130
C	-4.598480	-0.197939	0.037954
C	-4.786088	-1.538321	0.528489
C	-3.727742	-2.334564	0.807695
H	-3.879440	-3.346107	1.174568
H	-5.801341	-1.899657	0.667916
H	0.345478	1.637709	-0.716609
H	0.859618	-2.845820	0.978475
H	-1.567077	3.054463	-1.237750
H	-6.320314	2.563800	-0.966523
C	1.681082	-0.458268	0.166629
C	2.152830	0.635993	0.892737
C	2.556047	-1.172568	-0.651759
C	3.491184	1.011475	0.793568
H	1.498169	1.196481	1.551345
C	3.892597	-0.786691	-0.746735
H	2.211868	-2.023542	-1.229861
C	4.376598	0.308286	-0.027479
H	5.412608	0.603974	-0.102939
H	-4.018345	3.411932	-1.307008
H	-6.690919	0.268570	-0.116351
H	-1.434931	-3.695294	1.270307
O	4.668024	-1.538475	-1.575237
O	3.860699	2.087066	1.541956
C	6.039885	-1.203388	-1.721557
H	6.450152	-1.928467	-2.423813
H	6.158810	-0.193731	-2.129333
H	6.569907	-1.281549	-0.766128
C	5.211487	2.521927	1.498319
H	5.496375	2.827356	0.485698
H	5.268965	3.381601	2.165335
H	5.890508	1.739343	1.853739

2a: min(GS) in *n*-hexane solution

C	0.017767	-2.201775	0.743741
C	0.264789	-0.902317	0.294319
C	-0.825434	-0.064148	-0.020128
C	-2.152491	-0.550594	0.156468
C	-2.374755	-1.869711	0.632786
C	-1.272418	-2.680269	0.912942
C	-0.658552	1.267477	-0.548322
C	-3.273226	0.284082	-0.148758
C	-3.070150	1.599311	-0.642526
C	-1.721104	2.053787	-0.840477
C	-4.177945	2.403065	-0.931515
C	-5.469168	1.925725	-0.740419
C	-5.677942	0.637432	-0.261252
C	-4.597123	-0.198383	0.038376
C	-4.783786	-1.537833	0.530362
C	-3.725441	-2.333076	0.810292
H	-3.876795	-3.344356	1.178409

H	-5.798999	-1.899426	0.670268
H	0.346123	1.635403	-0.719881
H	0.862455	-2.840817	0.983268
H	-1.567383	3.052224	-1.241390
H	-6.319603	2.561387	-0.968519
C	1.681245	-0.456558	0.166223
C	2.153256	0.637028	0.892877
C	2.555224	-1.170332	-0.653258
C	3.490829	1.011917	0.793508
H	1.500475	1.196504	1.553891
C	3.891078	-0.785511	-0.748306
H	2.211132	-2.018963	-1.234432
C	4.375653	0.308773	-0.028321
H	5.411846	0.604089	-0.103781
H	-4.017955	3.409117	-1.310038
H	-6.689293	0.267187	-0.115687
H	-1.432756	-3.692063	1.275653
O	4.665362	-1.537855	-1.578056
O	3.860460	2.087395	1.542829
C	6.032801	-1.204668	-1.726779
H	6.441996	-1.929803	-2.430140
H	6.153959	-0.194655	-2.135391
H	6.567347	-1.283012	-0.772877
C	5.208258	2.517557	1.505187
H	5.499767	2.826626	0.494565
H	5.266486	3.375336	2.175139
H	5.886442	1.733034	1.860638

2a: min(ICT) in CH_2Cl_2 solution

C	0.061875	-2.299574	0.333882
C	0.302773	-0.925305	0.055174
C	-0.842057	-0.069947	-0.146644
C	-2.155565	-0.598311	0.062878
C	-2.342592	-1.965394	0.412070
C	-1.199401	-2.800775	0.514575
C	-0.747700	1.268328	-0.622844
C	-3.306872	0.240459	-0.098491
C	-3.157592	1.597395	-0.513002
C	-1.843068	2.070840	-0.797076
C	-4.300141	2.407363	-0.652459
C	-5.565190	1.892829	-0.396785
C	-5.729130	0.568572	-0.006736
C	-4.616037	-0.278805	0.143702
C	-4.753106	-1.650288	0.523861
C	-3.655671	-2.455471	0.639197
H	-3.774386	-3.501322	0.914049
H	-5.749569	-2.042822	0.708404
H	0.223820	1.667800	-0.892428
H	0.908051	-2.964794	0.478542
H	-1.721745	3.084779	-1.169151
H	-6.437670	2.531437	-0.508555
C	1.667718	-0.457073	0.032855
C	2.067720	0.820668	0.486005
C	2.730886	-1.287528	-0.385612
C	3.430382	1.243336	0.475520
H	1.357502	1.510348	0.923058
C	4.091779	-0.854721	-0.380386

H	2.548909	-2.283354	-0.770920
C	4.475517	0.423335	0.033665
H	5.501120	0.754335	0.014892
H	-4.180168	3.440519	-0.967734
H	-6.723083	0.171621	0.182065
H	-1.335217	-3.848791	0.770112
O	4.940188	-1.774173	-0.829902
O	3.606708	2.472343	0.950007
C	6.336873	-1.476096	-0.919988
H	6.801120	-2.378738	-1.311152
H	6.502502	-0.641416	-1.605461
H	6.739446	-1.245758	0.069510
C	4.923985	3.024731	1.039542
H	5.368564	3.104016	0.044593
H	4.793893	4.015093	1.470223
H	5.549425	2.410276	1.691711

2a: min(ICT) in *n*-hexane solution

C	0.064470	-2.295697	0.335038
C	0.301377	-0.923284	0.050327
C	-0.842318	-0.067401	-0.150533
C	-2.154321	-0.597194	0.062163
C	-2.338468	-1.963806	0.414503
C	-1.195028	-2.798083	0.519040
C	-0.750742	1.269602	-0.628077
C	-3.306357	0.239130	-0.098680
C	-3.160285	1.595158	-0.514396
C	-1.848226	2.069550	-0.800866
C	-4.303941	2.403021	-0.653298
C	-5.567108	1.887174	-0.395682
C	-5.727774	0.563563	-0.004277
C	-4.613598	-0.281551	0.145635
C	-4.747710	-1.651532	0.527558
C	-3.649659	-2.455128	0.643540
H	-3.766439	-3.500582	0.920504
H	-5.743517	-2.045061	0.713479
H	0.218423	1.670344	-0.904243
H	0.911733	-2.959024	0.484157
H	-1.729739	3.082969	-1.175466
H	-6.440903	2.524065	-0.507054
C	1.666156	-0.454396	0.028779
C	2.067819	0.822721	0.481258
C	2.731115	-1.282183	-0.391798
C	3.429454	1.243663	0.474832
H	1.355040	1.514232	0.910804
C	4.091387	-0.853104	-0.381022
H	2.547411	-2.275689	-0.781863
C	4.477416	0.423328	0.037395
H	5.503409	0.753612	0.021231
H	-4.185710	3.435978	-0.969944
H	-6.720575	0.164747	0.186503
H	-1.329966	-3.845030	0.778840
O	4.941167	-1.775137	-0.831794
O	3.605712	2.475016	0.950253
C	6.334006	-1.479701	-0.918720
H	6.799317	-2.381587	-1.311464
H	6.504956	-0.643559	-1.602366

H	6.738592	-1.252321	0.071548
C	4.918945	3.024051	1.047409
H	5.373359	3.102145	0.055927
H	4.788705	4.016249	1.474745
H	5.541211	2.412064	1.706226

2a: min(LE) in CH_2Cl_2 solution

C	0.082861	-2.304161	0.345193
C	0.320171	-0.940857	0.045746
C	-0.838851	-0.080791	-0.182381
C	-2.150625	-0.594666	0.068888
C	-2.333444	-1.952863	0.464435
C	-1.173787	-2.800987	0.560512
C	-0.735350	1.215965	-0.708169
C	-3.291567	0.233925	-0.106425
C	-3.140860	1.573539	-0.573225
C	-1.852623	2.029036	-0.887460
C	-4.300942	2.395273	-0.725776
C	-5.559813	1.897758	-0.433609
C	-5.721677	0.586922	0.005280
C	-4.598369	-0.272297	0.172511
C	-4.735832	-1.608295	0.594732
C	-3.622293	-2.431476	0.722452
H	-3.749307	-3.467472	1.024267
H	-5.726845	-1.998201	0.808614
H	0.234203	1.599943	-0.999119
H	0.934924	-2.960410	0.487610
H	-1.724543	3.034206	-1.279155
H	-6.431771	2.534059	-0.553879
C	1.691584	-0.457444	0.024187
C	2.041406	0.813534	0.527125
C	2.726901	-1.288988	-0.454503
C	3.368055	1.224162	0.549636
H	1.296684	1.466628	0.965140
C	4.045289	-0.855856	-0.442054
H	2.510810	-2.259948	-0.884890
C	4.391245	0.405416	0.059167
H	5.419258	0.736020	0.067828
H	-4.177603	3.415530	-1.077941
H	-6.713781	0.200057	0.220994
H	-1.310939	-3.840739	0.843531
O	4.959168	-1.727416	-0.953055
O	3.593796	2.457458	1.083599
C	6.325757	-1.344952	-0.995159
H	6.855247	-2.183814	-1.446059
H	6.467591	-0.451155	-1.612264
H	6.718641	-1.166436	0.011569
C	4.927672	2.936142	1.166678
H	5.376489	3.033339	0.172279
H	4.862163	3.919694	1.631133
H	5.545610	2.280130	1.789301

2a: min(LE) in *n*-hexane solution

C	0.081977	-2.305376	0.350519
C	0.319004	-0.943453	0.045280
C	-0.836624	-0.085228	-0.184863
C	-2.149070	-0.595174	0.068672

C	-2.332447	-1.952302	0.470039
C	-1.175891	-2.799205	0.568913
C	-0.730327	1.211074	-0.716538
C	-3.287487	0.233923	-0.108820
C	-3.135224	1.572273	-0.579371
C	-1.844412	2.024502	-0.896083
C	-4.291742	2.394512	-0.732832
C	-5.551106	1.900547	-0.438636
C	-5.714343	0.590613	0.003701
C	-4.595499	-0.268592	0.172608
C	-4.734448	-1.605030	0.600154
C	-3.624248	-2.428015	0.730276
H	-3.751840	-3.462832	1.036454
H	-5.726514	-1.991453	0.815907
H	0.240670	1.588988	-1.011201
H	0.934868	-2.959779	0.495978
H	-1.715465	3.028222	-1.291591
H	-6.422125	2.537930	-0.559767
C	1.690632	-0.459129	0.022930
C	2.038036	0.809643	0.531938
C	2.725078	-1.286987	-0.461744
C	3.363432	1.221933	0.554744
H	1.293664	1.458294	0.977042
C	4.042144	-0.852964	-0.447900
H	2.510163	-2.255193	-0.898552
C	4.386832	0.406563	0.059411
H	5.414613	0.738094	0.069500
H	-4.166624	3.413722	-1.087540
H	-6.707256	0.206355	0.220615
H	-1.314062	-3.837760	0.856124
O	4.956632	-1.721973	-0.963226
O	3.587195	2.453740	1.094092
C	6.318779	-1.339913	-1.005216
H	6.849094	-2.176685	-1.459875
H	6.462045	-0.443307	-1.619425
H	6.714981	-1.164737	0.001784
C	4.916536	2.930455	1.184979
H	5.371100	3.035834	0.192985
H	4.850109	3.911133	1.656185
H	5.534498	2.271020	1.805484

3: min(GS) in CH_2Cl_2 solution

C	-0.722875	1.169482	1.804170
C	-0.873848	0.414177	0.641395
C	0.271135	-0.028037	-0.046281
C	1.560752	0.301834	0.455305
C	1.689874	1.071926	1.641249
C	0.532259	1.495482	2.299762
C	0.189294	-0.811324	-1.253158
C	2.734308	-0.140390	-0.231952
C	2.617642	-0.911226	-1.419044
C	1.300738	-1.229864	-1.903687
C	3.777369	-1.334930	-2.077521
C	5.034364	-1.008427	-1.580243
C	5.157589	-0.253964	-0.418267
C	4.022720	0.189336	0.269933
C	4.117533	0.971884	1.475130

C	3.007314	1.391212	2.126691
H	3.090867	1.981202	3.035486
H	5.105963	1.219912	1.852496
H	-0.793504	-1.063837	-1.637548
H	-1.611771	1.507227	2.329358
H	1.215144	-1.819796	-2.812377
H	5.925328	-1.344497	-2.102252
C	-2.246591	0.091591	0.153085
C	-2.892658	-1.084817	0.557452
C	-2.925855	0.967673	-0.704578
C	-4.186786	-1.383221	0.122266
C	-4.220352	0.683374	-1.148440
C	-4.831744	-0.491184	-0.726299
H	-5.837513	-0.717486	-1.067792
H	3.685973	-1.924615	-2.985767
H	6.142311	-0.001733	-0.034027
H	0.621126	2.085242	3.208268
H	-4.688320	-2.290409	0.433476
O	-2.175406	-1.892900	1.384165
C	-2.763296	-3.105406	1.831119
H	-2.997188	-3.765873	0.989310
H	-2.016853	-3.579517	2.467816
H	-3.670928	-2.913871	2.413460
H	-4.747475	1.357978	-1.810596
O	-2.239272	2.085746	-1.064328
C	-2.863901	3.020177	-1.931587
H	-3.102294	2.564676	-2.898671
H	-3.774600	3.429968	-1.481841
H	-2.138757	3.820516	-2.076487

3: min(GS) in *n*-hexane solution

C	-0.722392	0.299812	2.132016
C	-0.874079	0.107008	0.759632
C	0.269121	-0.006418	-0.051152
C	1.559024	0.077100	0.541371
C	1.689489	0.273445	1.941106
C	0.532973	0.382479	2.717285
C	0.185222	-0.205780	-1.475310
C	2.731267	-0.036355	-0.269106
C	2.612819	-0.232603	-1.670398
C	1.295359	-0.312865	-2.242478
C	3.771444	-0.341263	-2.446679
C	5.028984	-0.258836	-1.859743
C	5.153716	-0.066847	-0.488367
C	4.020244	0.046846	0.323569
C	4.116365	0.246167	1.746025
C	3.007271	0.353874	2.514284
H	3.092288	0.504297	3.587349
H	5.105409	0.308753	2.192182
H	-0.798502	-0.269301	-1.928651
H	-1.611290	0.386231	2.750250
H	1.208305	-0.462934	-3.315464
H	5.919183	-0.345073	-2.475865
C	-2.246669	0.024482	0.180975
C	-2.905962	-1.207187	0.074406
C	-2.911435	1.178687	-0.253574
C	-4.199303	-1.290640	-0.448970

C	-4.204978	1.111936	-0.778861
C	-4.830071	-0.125755	-0.868279
H	-5.835174	-0.184002	-1.275665
H	3.678549	-0.491439	-3.519096
H	6.139021	-0.003251	-0.034108
H	0.623341	0.533011	3.789935
H	-4.710371	-2.241210	-0.531751
O	-2.200629	-2.286217	0.506196
C	-2.794581	-3.568251	0.418220
H	-3.025415	-3.828948	-0.621039
H	-2.054363	-4.265498	0.810374
H	-3.706511	-3.626708	1.023495
H	-4.720582	2.002535	-1.114429
O	-2.211189	2.337334	-0.129641
C	-2.811634	3.546035	-0.557104
H	-3.043882	3.517751	-1.627854
H	-3.723737	3.760021	0.011767
H	-2.074901	4.326402	-0.367083

3: min(ICT) in CH_2Cl_2 solution

C	-0.842286	1.896272	0.915228
C	-0.931843	0.641797	0.282107
C	0.282598	-0.008246	-0.139594
C	1.541831	0.592338	0.173705
C	1.593534	1.843090	0.867454
C	0.383257	2.480990	1.205122
C	0.293328	-1.212160	-0.883373
C	2.760346	-0.046289	-0.212262
C	2.732491	-1.282262	-0.932922
C	1.467141	-1.828539	-1.270517
C	3.947070	-1.900035	-1.295654
C	5.172722	-1.313734	-0.960025
C	5.215158	-0.116451	-0.269209
C	4.017336	0.544122	0.117579
C	4.030925	1.784258	0.821047
C	2.865298	2.407984	1.175329
H	2.893967	3.357174	1.705241
H	4.989978	2.231788	1.069192
H	-0.648683	-1.662384	-1.178144
H	-1.754954	2.400331	1.214969
H	1.429372	-2.743654	-1.855385
H	6.098651	-1.803871	-1.248097
C	-2.243344	0.026949	0.116982
C	-2.524971	-1.289875	0.642216
C	-3.325191	0.697084	-0.523305
C	-3.773103	-1.905689	0.493844
C	-4.566453	0.093245	-0.646421
C	-4.780652	-1.206842	-0.143096
H	-5.760644	-1.658152	-0.255582
H	3.919359	-2.839413	-1.841206
H	6.168295	0.340238	-0.016199
H	0.413770	3.447377	1.702233
H	-3.960128	-2.891425	0.898504
O	-1.507545	-1.839186	1.298951
C	-1.631321	-3.147283	1.860524
H	-1.849736	-3.878187	1.077895
H	-0.665252	-3.359705	2.313272

H	-2.415217	-3.158649	2.622230
H	-5.382626	0.600708	-1.143868
O	-3.035272	1.924616	-1.014063
C	-4.055742	2.647977	-1.687670
H	-4.403701	2.104017	-2.572430
H	-4.900416	2.850288	-1.020587
H	-3.598269	3.587868	-1.993669

3: min(ICT) in *n*-hexane solution

C	-0.844915	1.961821	0.835480
C	-0.935182	0.678278	0.255739
C	0.274715	0.024146	-0.153455
C	1.531385	0.633898	0.139143
C	1.585996	1.902948	0.784771
C	0.368424	2.557159	1.096959
C	0.290315	-1.206349	-0.865786
C	2.754887	-0.027644	-0.215697
C	2.726326	-1.290446	-0.894305
C	1.463999	-1.838407	-1.226249
C	3.942900	-1.925963	-1.227312
C	5.157497	-1.332081	-0.903935
C	5.199963	-0.106647	-0.252407
C	4.008134	0.568941	0.102832
C	4.018714	1.833210	0.762573
C	2.852187	2.471772	1.081877
H	2.879372	3.439403	1.577595
H	4.977342	2.285549	1.003011
H	-0.649274	-1.652869	-1.173585
H	-1.759336	2.475766	1.112916
H	1.427059	-2.765903	-1.791682
H	6.086468	-1.830789	-1.167648
C	-2.240314	0.038973	0.130480
C	-2.464225	-1.292013	0.641413
C	-3.362545	0.659374	-0.463846
C	-3.692075	-1.976463	0.511239
C	-4.587412	-0.005847	-0.565325
C	-4.749547	-1.324608	-0.086129
H	-5.712626	-1.812510	-0.183115
H	3.915289	-2.882281	-1.742270
H	6.154525	0.353623	-0.011809
H	0.401712	3.540052	1.559944
H	-3.814488	-2.973029	0.915415
O	-1.416806	-1.807358	1.270550
C	-1.438702	-3.137156	1.789496
H	-1.642334	-3.854524	0.990819
H	-0.443527	-3.301507	2.196613
H	-2.189177	-3.218915	2.580350
H	-5.433464	0.481982	-1.032417
O	-3.162730	1.909171	-0.943781
C	-4.217460	2.570656	-1.620115
H	-4.538781	2.005785	-2.502794
H	-5.072599	2.740182	-0.955782
H	-3.808277	3.530172	-1.934364

3: min(LE) in CH_2Cl_2 solution

C	-0.852237	1.922109	0.852309
C	-0.939450	0.632421	0.279611

C	0.295902	-0.020220	-0.135778
C	1.549343	0.589310	0.177391
C	1.592713	1.849444	0.846120
C	0.348909	2.509275	1.149176
C	0.307348	-1.197285	-0.898439
C	2.766407	-0.042442	-0.197366
C	2.742029	-1.270776	-0.922660
C	1.496650	-1.813991	-1.275527
C	3.979786	-1.893970	-1.278179
C	5.187616	-1.311001	-0.931623
C	5.224653	-0.105378	-0.236706
C	4.019978	0.555362	0.140241
C	4.023047	1.782747	0.829439
C	2.830758	2.417954	1.163811
H	2.855808	3.376346	1.675258
H	4.972971	2.241357	1.089561
H	-0.633235	-1.641440	-1.203538
H	-1.771508	2.430727	1.120117
H	1.464105	-2.735257	-1.850793
H	6.118517	-1.797574	-1.209034
C	-2.244954	0.002939	0.125844
C	-2.513754	-1.300776	0.626180
C	-3.326710	0.689139	-0.492849
C	-3.763170	-1.897450	0.476364
C	-4.579651	0.097667	-0.633528
C	-4.783639	-1.192474	-0.153679
H	-5.759661	-1.654479	-0.266562
H	3.955939	-2.831219	-1.827368
H	6.176310	0.349146	0.024865
H	0.379454	3.475941	1.644220
H	-3.956640	-2.887785	0.867626
O	-1.498484	-1.882385	1.307851
C	-1.661919	-3.204856	1.797310
H	-1.872857	-3.904440	0.981491
H	-0.713208	-3.465522	2.265403
H	-2.462528	-3.253725	2.542939
H	-5.389382	0.620179	-1.125902
O	-3.038697	1.922354	-0.978158
C	-4.058831	2.661926	-1.633274
H	-4.413381	2.137696	-2.527016
H	-4.900184	2.856721	-0.960069
H	-3.598016	3.605519	-1.923857

3: min(LE) in *n*-hexane solution

C	-0.855393	1.937895	0.827649
C	-0.941307	0.642906	0.264762
C	0.291844	-0.009746	-0.148061
C	1.545214	0.597336	0.167237
C	1.587303	1.859978	0.832200
C	0.346169	2.523238	1.124682
C	0.303070	-1.187514	-0.913068
C	2.761148	-0.037222	-0.201059
C	2.737497	-1.266338	-0.925093
C	1.490145	-1.806108	-1.284323
C	3.972660	-1.891622	-1.273446
C	5.180314	-1.312184	-0.921750
C	5.216416	-0.105499	-0.228028

C	4.015006	0.557265	0.141257
C	4.017026	1.788355	0.828954
C	2.827473	2.426617	1.154565
H	2.851432	3.386554	1.663510
H	4.967517	2.243974	1.092671
H	-0.638595	-1.625168	-1.224719
H	-1.774812	2.448774	1.089274
H	1.458855	-2.726207	-1.861883
H	6.111333	-1.801180	-1.194306
C	-2.243299	0.004035	0.128067
C	-2.493189	-1.302112	0.632575
C	-3.340326	0.676125	-0.478432
C	-3.735771	-1.915258	0.493215
C	-4.585849	0.068139	-0.609595
C	-4.770352	-1.224848	-0.129028
H	-5.741291	-1.699301	-0.234363
H	3.949181	-2.829041	-1.822498
H	6.168270	0.346914	0.036585
H	0.377057	3.493234	1.613219
H	-3.912633	-2.907713	0.887425
O	-1.464081	-1.868446	1.304842
C	-1.601622	-3.187641	1.799968
H	-1.811303	-3.895628	0.990016
H	-0.643477	-3.432087	2.258055
H	-2.393280	-3.246491	2.555447
H	-5.406035	0.580930	-1.095020
O	-3.073522	1.915711	-0.960295
C	-4.096014	2.630066	-1.631303
H	-4.435128	2.090682	-2.522894
H	-4.948215	2.821015	-0.969415
H	-3.647030	3.577442	-1.929138

3. Figures

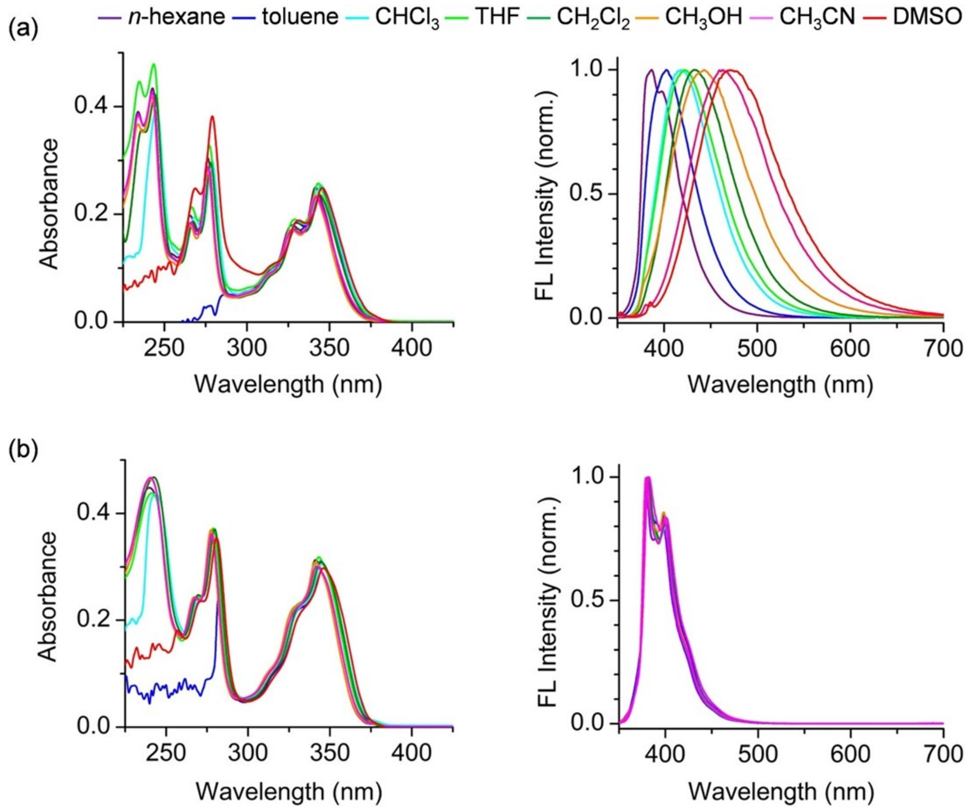


Fig. S7 UV-vis absorption (left) and normalized fluorescence emission (right) spectra of (a) **1b** and (b) **2b** in various solvents (UV-vis: 10 μM; FL: 1 μM) at 298 K. The solvents used were: *n*-hexane, toluene, chloroform ($CHCl_3$), tetrahydrofuran (THF), dichloromethane (CH_2Cl_2), methanol (CH_3OH), acetonitrile (CH_3CN) and dimethyl sulphoxide (DMSO).

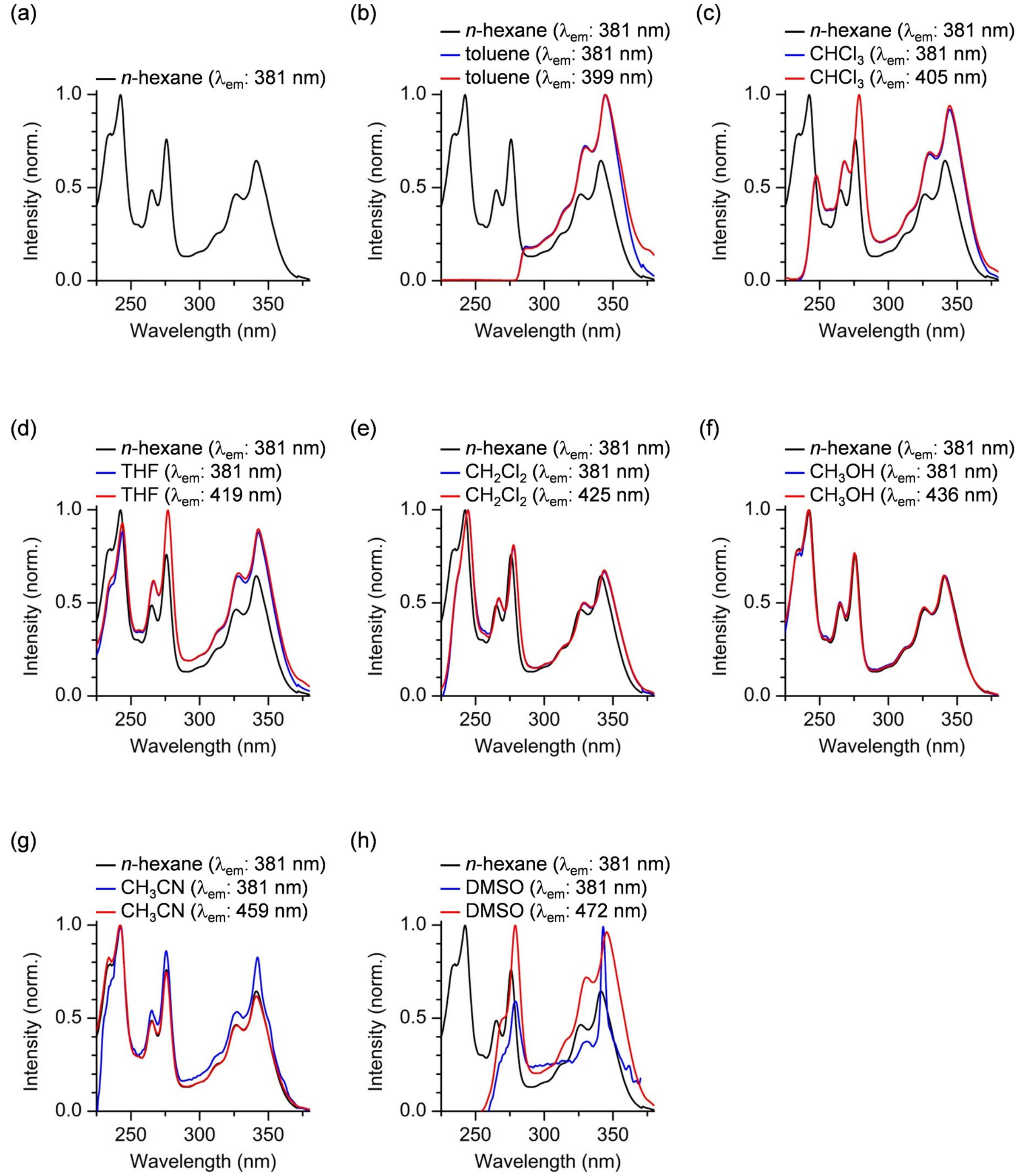


Fig. S8 Normalized excitation spectra of **1a** (1 μM) in (a) *n*-hexane, (b) toluene, (c) $CHCl_3$, (d) THF, (e) CH_2Cl_2, (f) CH_3OH, (g) CH_3CN and (h) DMSO monitored at the wavelength of monomer emission (381 nm) and the respective maximum emission wavelengths in each solvent.

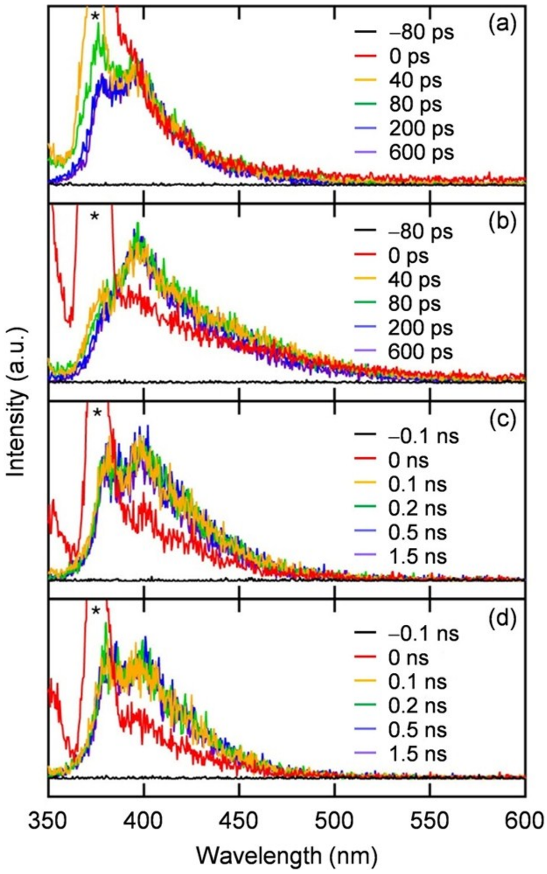


Fig. S9 Picosecond time-resolved fluorescence spectra of **2b** in (a) *n*-hexane, (b) CH_2Cl_2, (c) C_2H_5OH and (d) 1-C_4H_9OH with photoexcitation at 345 nm. * denotes Raman scattering signals from solvents, which are confirmed by the measurements of the blank solutions without the solute.

4. Supplementary References

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