Electronic Supplementary Material (ESI) for RSC Advances.

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1. General Remarks

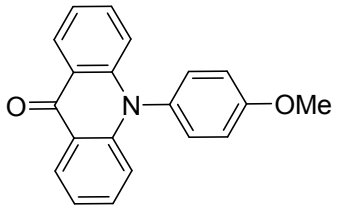
All reagents and solvents were commercially available and were used without further purification unless otherwise noted. For thin layer chromatography Silica gel 60 F254 plates from Merck were used and examined under UV-light irradiation (254 nm and 365 nm). Flash column chromatography was performed on silica gel (particle size: 200-300 mesh). IR-Spectra were recorded as KBr-pellets on a Bruker VERTEX 80V spectrometer. NMR spectra were taken on a Bruker AVANCE III HD (600MHz). Chemical shifts (δ) are reported in parts per million (ppm) relative to traces of $CHCl_3$ in the corresponding deuterated solvent. HRMS experiments were carried out on a Bruke Fourier Transform SolariX XR. Absorption spectra were recorded on a shimadzu UV2600. Emission spectra and absolute quantum yields were measured on FluoroMax-4 spectrometer equipped with an integral sphere. The particle distribution was measured on a Malvern Zetasizer Nano ZS. Electrochemical data were obtained in dichloromethane or tetrahydrofuran solution of tetrabutylammonium hexafluorophosphate (0.1 M) and ferrocene was used as an internal standard. Cyclic voltammagrams were obtained using a glassy carbon working electrode, a platinum counter electrode, and a Ag reference electrode tested on CHI660E station.

Acridone,[S1] 4-bromo-*N*,*N*-bis(4-methoxyphenyl)aniline[S2] and 4'-bromo-*N*,*N*-bis(4-methoxyphenyl)-[1,1'-biphenyl]-4-amine[S3] were prepared according to the reported methods.

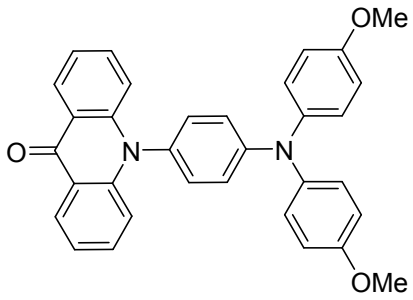
2. Experimental part

Genaral Procedure (GP) for the cross coupling reactions of acridone and bromide.

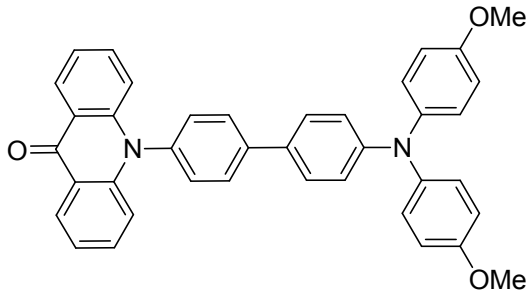
An 8 or 120 mL screw capped glass vial was charged with acridone **1**, bromide, CuI, 2,2,6,6-tetramethylheptane-3,5-dione, K_2CO_3 and dry DMF. The mixture was heated at 150 ^oC for 48 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (150 mL) and washed with water (6×200 mL) and dried over Na_2SO_4. The solvent was removed by a rotatory evaporation and the crude product was purified by silica gel column chromatography to give the product **2**.



According to **GP**, an 8 mL glass vial, acridone (390 mg, 2 mmol)), 4-bromoanisole (561 mg, 3 mmol), CuI (39 mg, 0.2 mmol), 2,2,6,6-tetramethylheptane-3,5-dione (73 mg, 0.4 mmol), K_2CO_3 (414 mg, 3 mmol) and dry DMF (3 mL), after workup, silica gel column (dichloromethane), the product **2a** was obtained as light yellow solid (463 g, 77 %). m.p. 232 ^oC. ^1H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 8.50 (d, J = 8.0 Hz, 2H), 7.52 (ddd, J = 8.5, 6.9, 1.6 Hz, 2H), 7.29-7.25 (m, 4H), 7.20 (d, J = 8.8 Hz, 2H), 6.85 (d, J = 8.6 Hz, 2H), 3.94 (s, 3H). ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 178.1, 160.7, 144.0, 133.5, 131.8, 131.4, 127.3, 122.3, 121.7, 117.5, 116.6, 56.1. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3104, 3064, 3050, 3037, 3002, 2960, 2937, 2836, 1631, 1596, 1512, 1490, 1457, 1361, 1348, 1294, 1270, 1249, 1182, 1162, 1106, 1029, 937, 839, 763, 756, 675, 621, 549, 530. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{20}H_{16}NO_2$, 302.11755; found, 302.11740.



According to **GP**, a 120 mL glass vial, acridone (976 mg, 5 mmol)), 4-bromo-*N*,*N*-bis(4-methoxyphenyl)aniline (2.11 g, 5.5 mmol), CuI (95 mg, 0.5 mmol), 2,2,6,6-tetramethylheptane-3,5-dione (184 mg, 1 mmol), K_2CO_3 (1.04 g, 7.5 mmol) and dry DMF (15 mL), after workup, silica gel column (dichloromethane), the product **2b** was obtained as light yellow solid (2.06 g, 83 %). m.p. 253 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 8.49 (dd, J = 8.0, 1.7 Hz, 2H), 7.56 (ddd, J = 8.6, 6.9, 1.7 Hz, 2H), 7.27 (ddd, J = 7.9, 6.9, 1.0 Hz, 2H), 7.25-7.21 (m, 4H), 7.12-7.08 (m, 4H), 6.99 (dd, J = 8.7, 0.9 Hz, 2H), 6.95-6.90 (m, 4H), 3.81 (s, 6H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 178.1, 157.2, 150.1, 144.1, 140.4, 133.5, 130.5, 130.1, 127.9, 127.2, 122.3, 121.7, 120.5, 117.6, 115.3, 55.9; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3060, 3043, 2995, 2952, 2933, 2906, 2831, 1631, 1598, 1504, 1483, 1457, 1359, 1303, 1290, 1268, 1241, 1176, 1159, 1103, 1031, 935, 825, 752, 675, 619, 603, 574, 559, 530; HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{33}H_{27}N_2O_3$, 499.20162; found, 499.20205.



According to **GP**, an 8 mL glass vial, acridone (390 mg, 2 mmol)), 4'-bromo-*N*,*N*-bis(4-methoxyphenyl)-[1,1'-biphenyl]-4-amine (1.01 g, 2.2 mmol), CuI (39 mg, 0.2 mmol), 2,2,6,6-tetramethylheptane-3,5-dione (73 mg, 0.4 mmol), K_2CO_3 (1.04 g, 7.5 mmol) and dry DMF (3 mL), after workup, silica gel column (dichloromethane), the product **2b** was obtained as light yellow solid (900 mg, 78 %). m.p. 251 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 8.51 (d, J = 8.0 Hz, 2H), 7.87 (d, J = 7.1 Hz, 2H), 7.56-7.51 (m, 4H), 7.39 (d, J = 7.6 Hz, 2H), 7.28 (t, J = 7.4 Hz, 2H), 7.12 (d, J = 7.9 Hz, 4H), 7.02 (d, J = 7.8 Hz, 2H), 6.91-6.88 (m, 6H), 3.81 (s, 6H). ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 178.1, 156.8, 149.4, 143.7, 142.5, 140.9, 137.5, 133.6, 131.3, 130.6, 129.1, 128.0, 127.4, 127.3, 122.3, 121.8, 120.4, 117.5, 115.1, 55.9. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3070, 3035, 3002, 2958, 2935, 2910, 2833, 1631, 1600, 1506, 1492, 1459, 1357, 1321, 1301, 1276, 1240, 1176, 1105, 1029, 935, 833, 821, 756, 719, 675, 576, 534. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{39}H_{31}N_2O_3$, 575.23292; found, 575.23388.

3. X-ray crystallographic structure determination

Table S1. Crystal data and structure refinement for 2a (CCDC 1972073)

Empirical formula	$C_{20}H_{15}NO_2$
Formula weight	301.33
Temperature/K	283.36
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.4255(10)
b/Å	12.9799(13)
c/Å	24.692(2)
α /°	90
β /°	92.779(3)
γ /°	90
Volume/Å^3	3017.3(5)
Z	8
ρcalc. g/cm^3	1.327
μ/mm^{-1}	0.086
F(000)	1264
Radiation	Mo K_α (λ = 0.71076)
2θ range for data collection/°	4.556 to 54
Index ranges	$-11 \le h \le 12$, $-16 \le k \le 16$, $-31 \le l \le 30$
Reflections collected	44195
Independent reflections	6580 [R_{int} = 0.1091, R_{sigma} = 0.1014]
Data/restraints/parameters	6580/0/417
Goodness-of-fit on F^2	1.203
Final R indexes [I>=2σ (I)]	R_1 = 0.1289, wR_2 = 0.1506
Final R indexes [all data]	R_1 = 0.2532, wR_2 = 0.1860
Largest diff. peak/hole / e Å^{-3}	0.19/-0.17

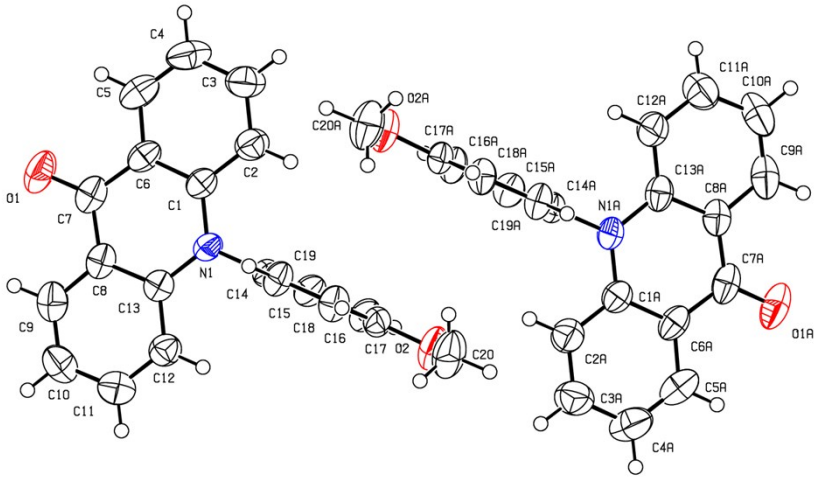


Table S2. Crystal data and structure refinement for 2b (CCDC 1972074)

Empirical formula	$C_{33}H_{26}N_2O_3$
Formula weight	498.56
Temperature/K	293.3
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.3406(5)
b/Å	9.8838(5)
c/Å	23.6490(12)
α/°	90
β/°	100.0920(10)
γ/°	90
Volume/Å^3	2609.8(2)
Z	4
ρcalc. g/cm^3	1.269
μ/mm^{-1}	0.082
F(000)	1048.0
Radiation	Mo K_α (λ = 0.71076)
2θ range for data collection/°	4.314 to 57.182
Index ranges	$-15 \le h \le 15$, $-13 \le k \le 13$, $-30 \le l \le 31$
Reflections collected	42064
Independent reflections	6642 [R_{int} = 0.0706, R_{sigma} = 0.0782]
Data/restraints/parameters	6642/0/345
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0748, wR_2 = 0.1239
Final R indexes [all data]	R_1 = 0.1695, wR_2 = 0.1516
Largest diff. peak/hole / e Å^{-3}	0.21/-0.20

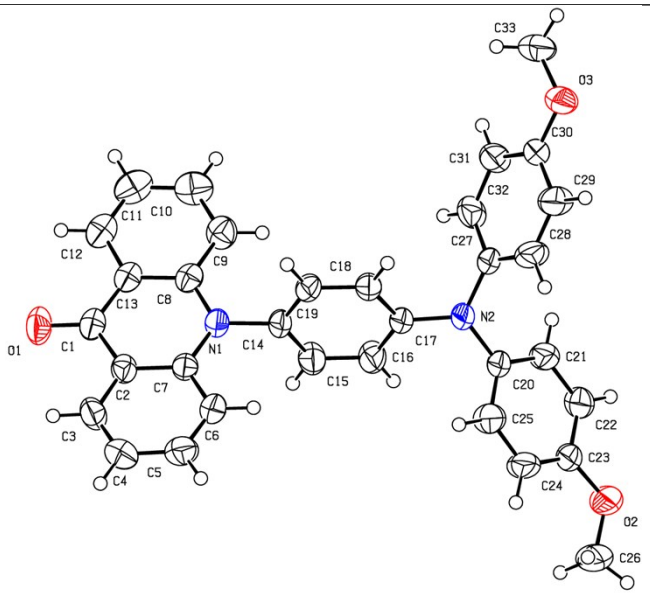
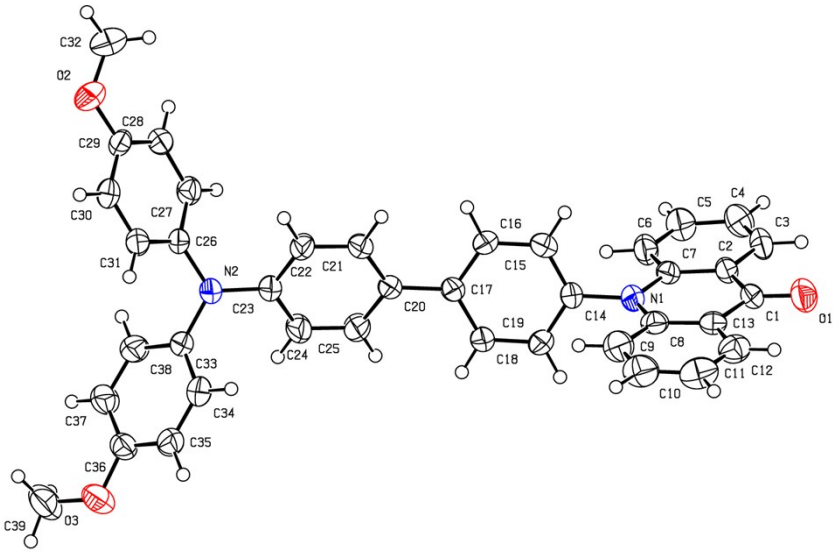


Table S3. Crystal data and structure refinement for 2c (CCDC 1972075)

Empirical formula	$C_{39}H_{30}N_2O_3$
Formula weight	574.68
Temperature/K	293.3
Crystal system	triclinic
Space group	Pī
a/Å	9.8465(8)
b/Å	12.7204(10)
c/Å	13.4275(10)
α /°	69.672(2)
β /°	71.642(2)
γ /°	77.107(2)
Volume/Å^3	1484.5(2)
Z	2
ρcalc. g/cm^3	1.281
μ/mm^{-1}	0.078
F(000)	604.0
Radiation	Mo K_α (λ = 0.71076)
2θ range for data collection/°	4.394 to 52.896
Index ranges	$-12 \le h \le 12$, $-15 \le k \le 15$, $-16 \le l \le 16$
Reflections collected	35328
Independent reflections	6114 [R_{int} = 0.0989, R_{sigma} = 0.1094]
Data/restraints/parameters	6114/0/399
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0852, wR_2 = 0.1120
Final R indexes [all data]	R_1 = 0.1916, wR_2 = 0.1365
Largest diff. peak/hole / e Å^{-3}	0.19/-0.18



4. NMR Spectra

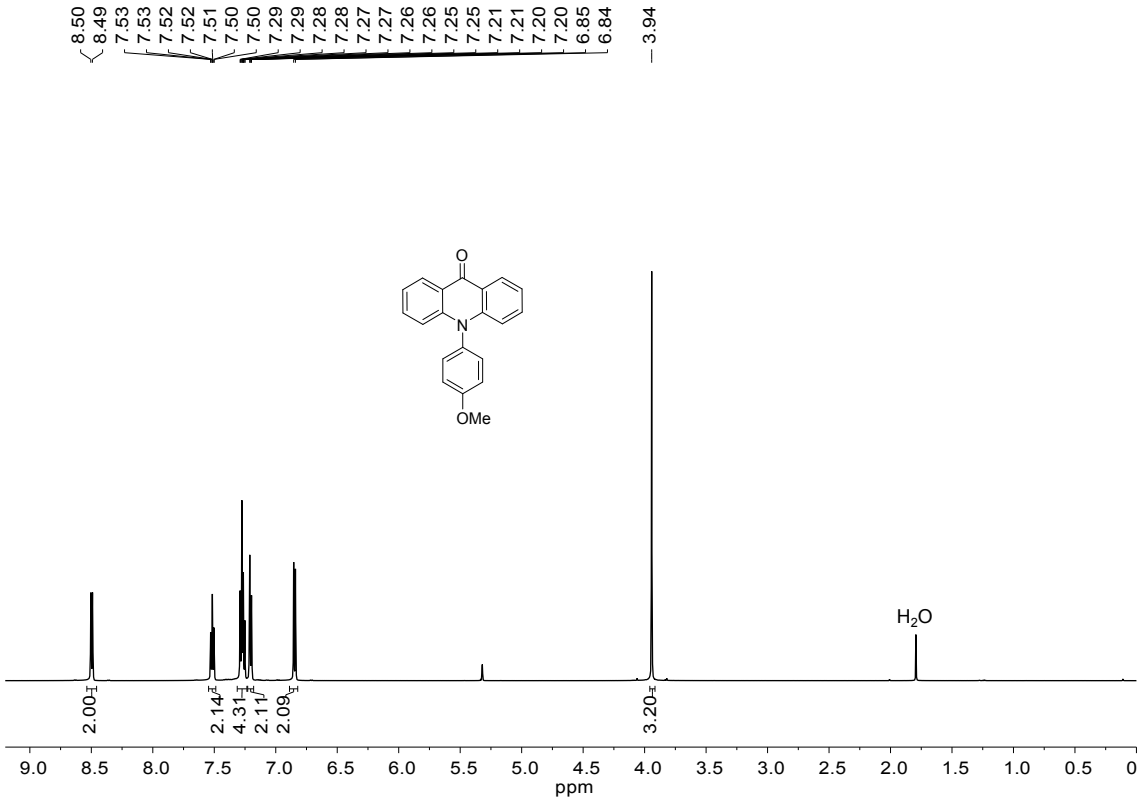


Figure S1. ^{1}H NMR spectrum (CD_2Cl_2, 600 MHz) of **2a**.

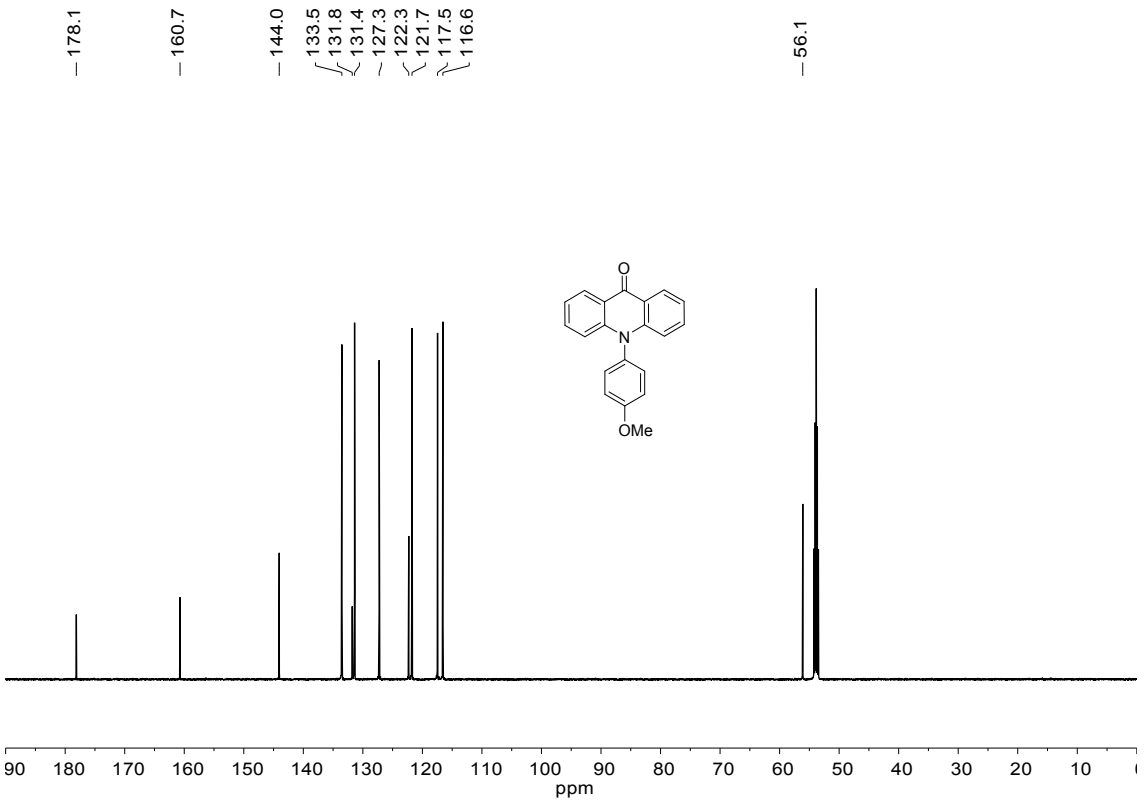


Figure S2. ^{13}C NMR spectrum (CD_2Cl_2, 150 MHz) of **2a**.

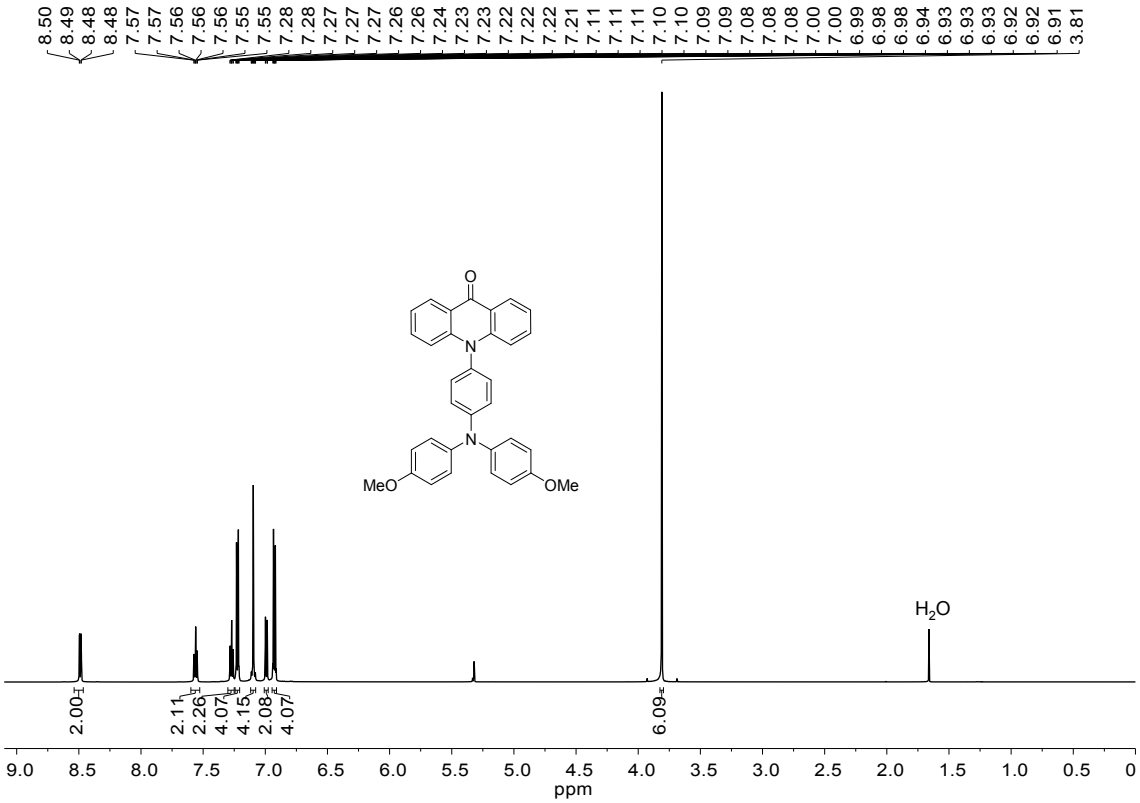


Figure S3. ^{1}H NMR spectrum (CD_2Cl_2, 600 MHz) of **2b**.

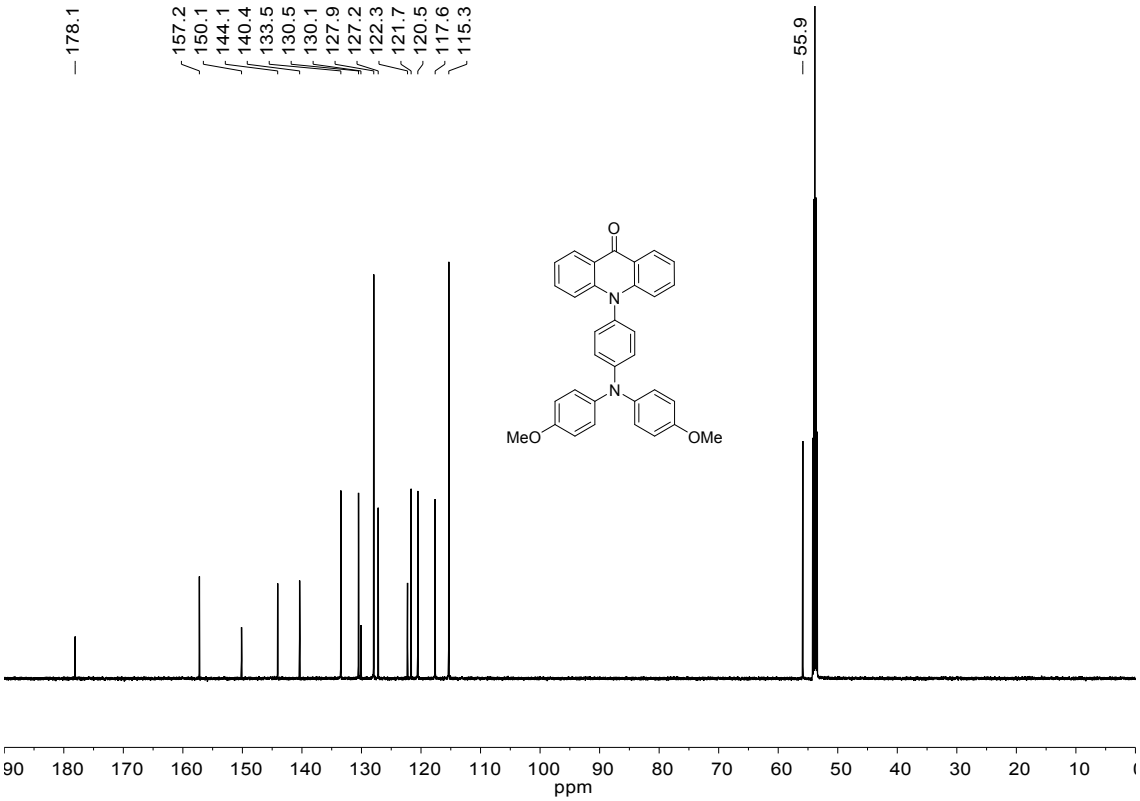


Figure S4. ^{13}C NMR spectrum (CD_2Cl_2, 150 MHz) of **2b**.

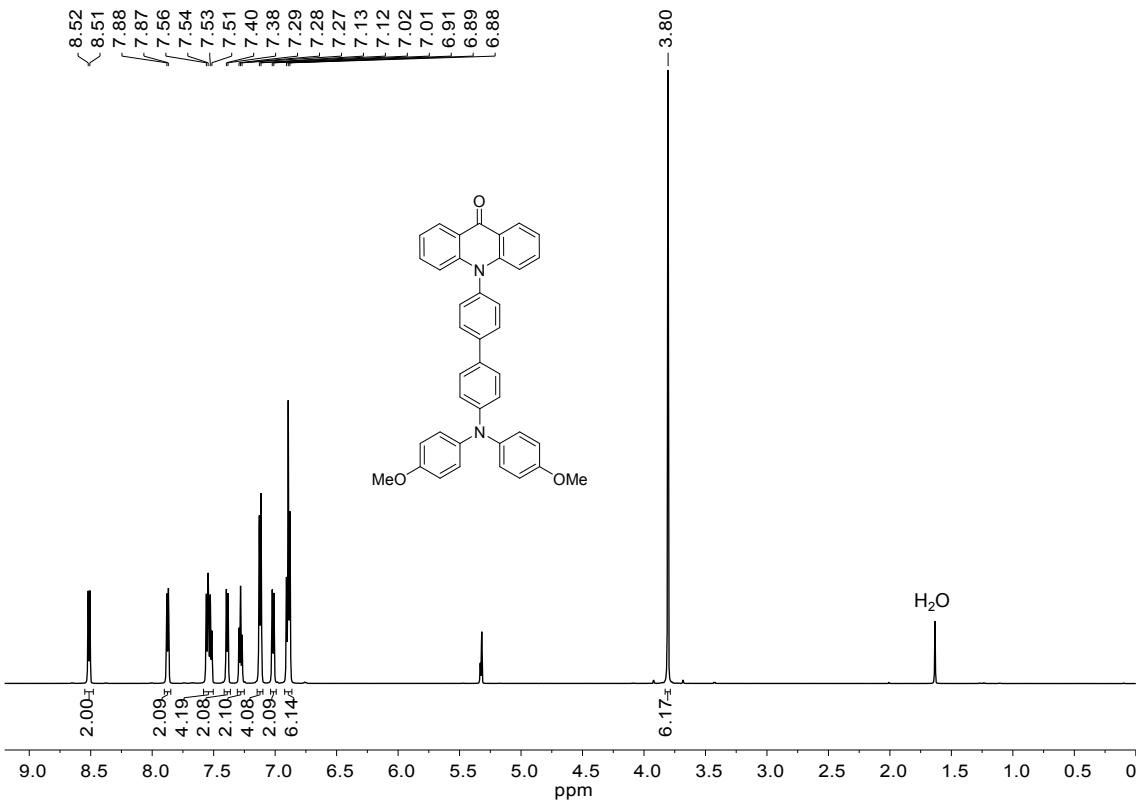


Figure S5. ^{1}H NMR spectrum (CD_2Cl_2, 600 MHz) of **2c**.

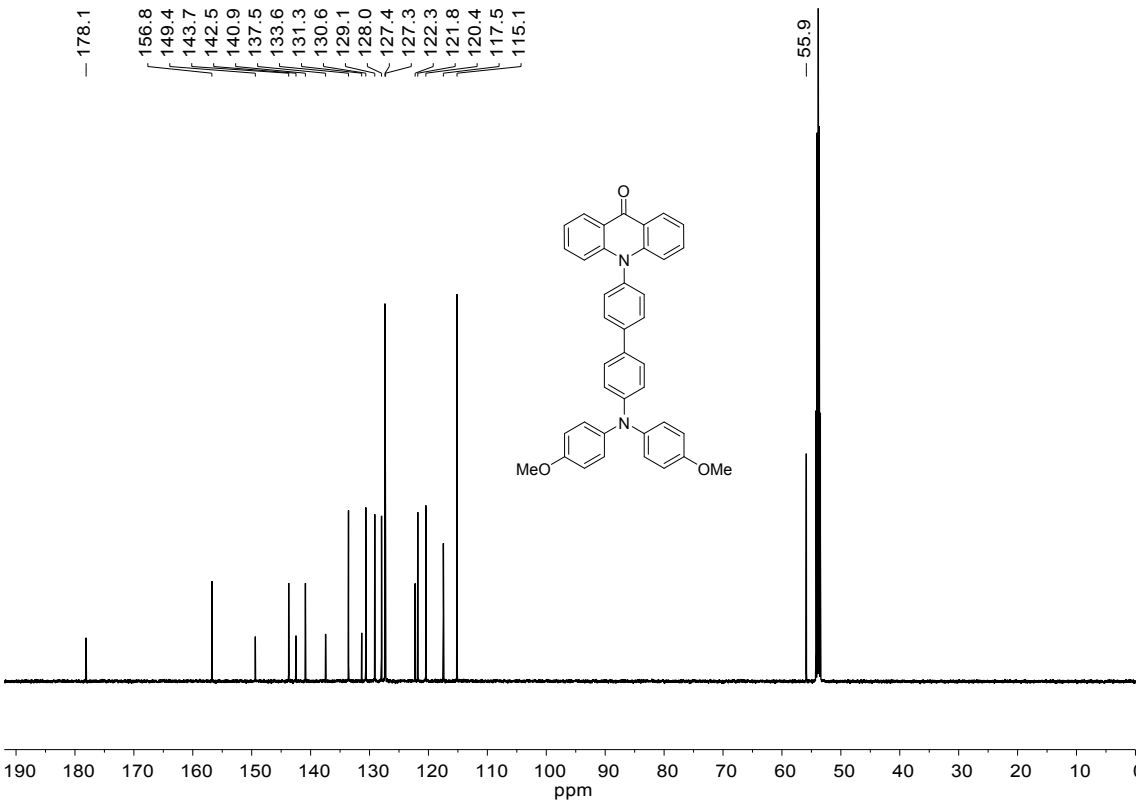


Figure S6. ^{13}C NMR spectrum (CD_2Cl_2, 150 MHz) of **2c**.

5. UV/vis and fluorescence spectra

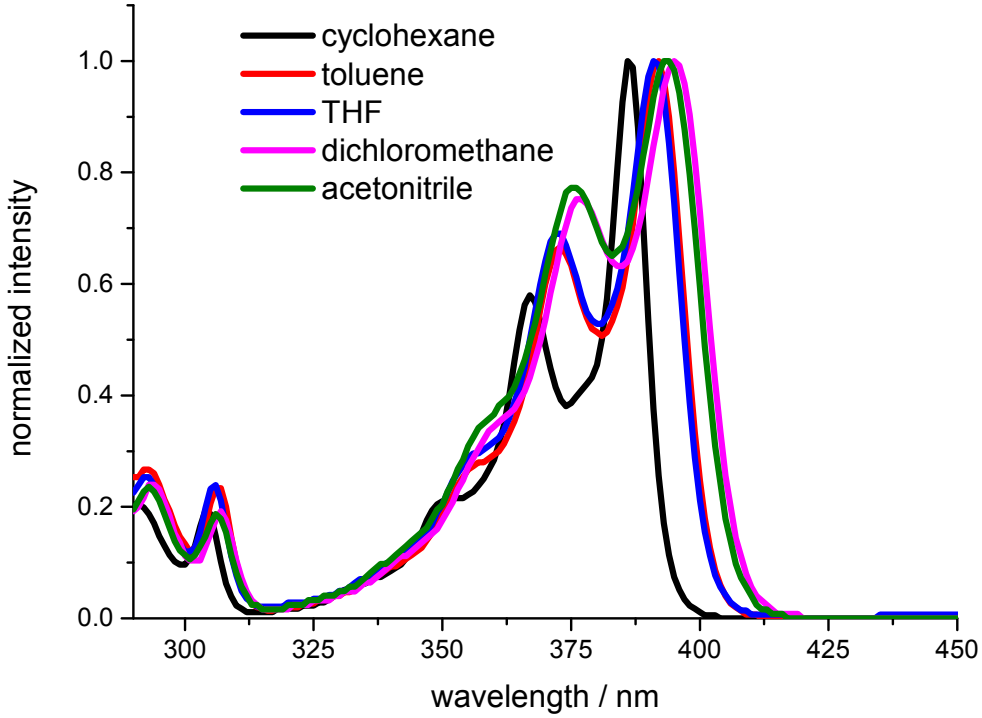


Figure S7. UV/vis absorption spectra of compound **2a** measured in different solvents at room temperature.

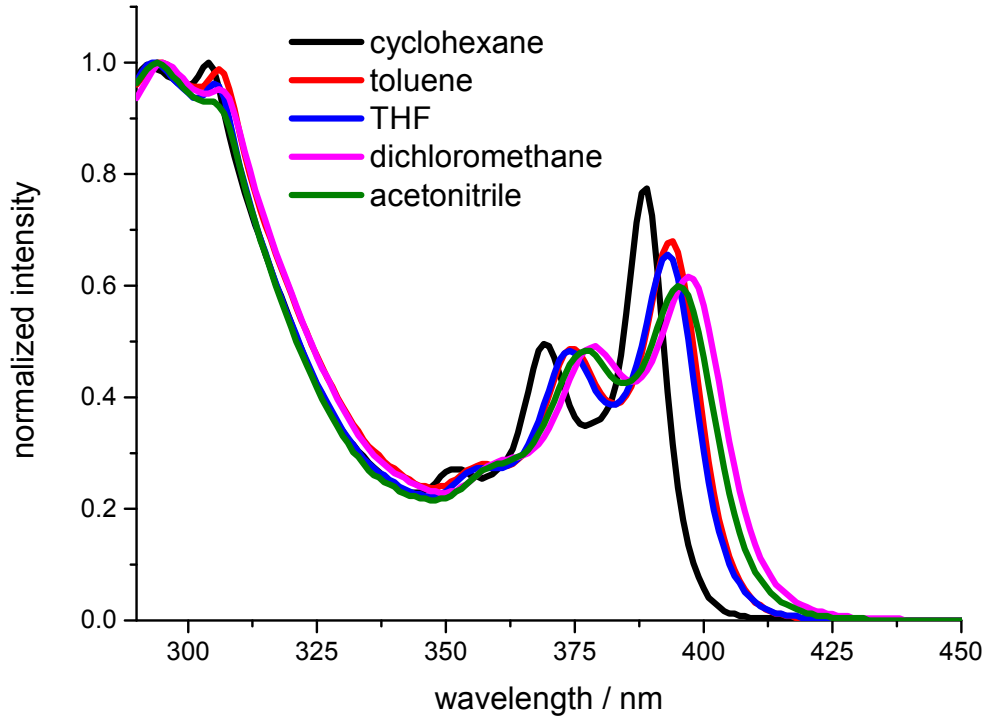


Figure S8. UV/vis absorption spectra of compound **2b** measured in different solvents at room temperature.

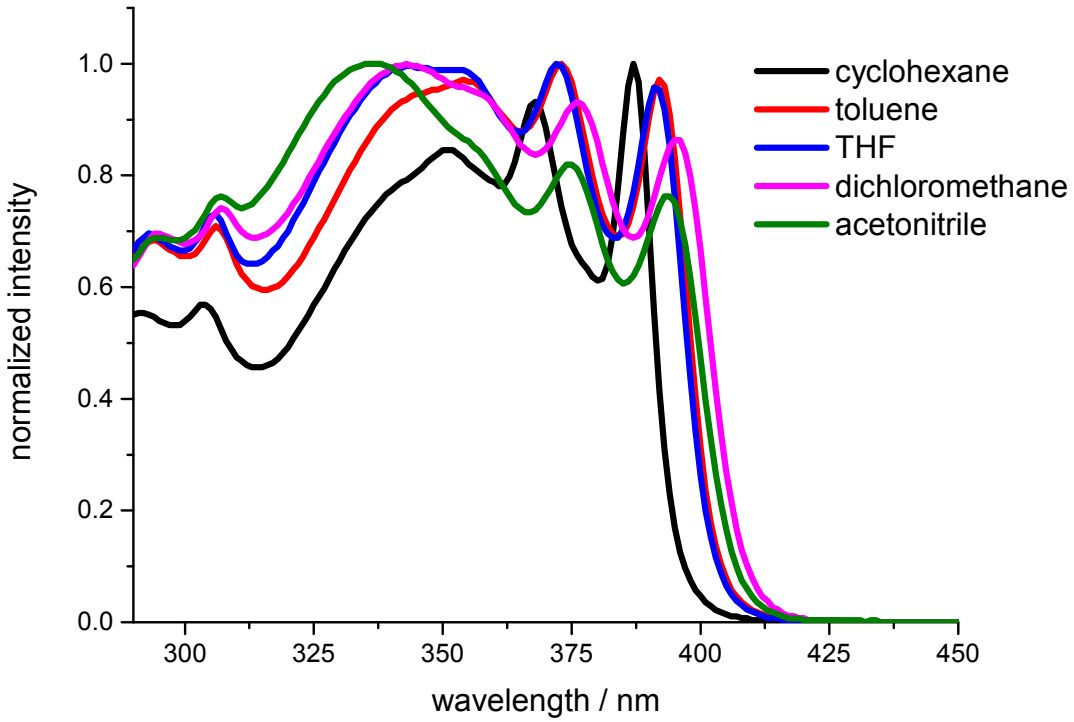


Figure S9. UV/vis absorption spectra of compound **2c** measured in different solvents at room temperature.

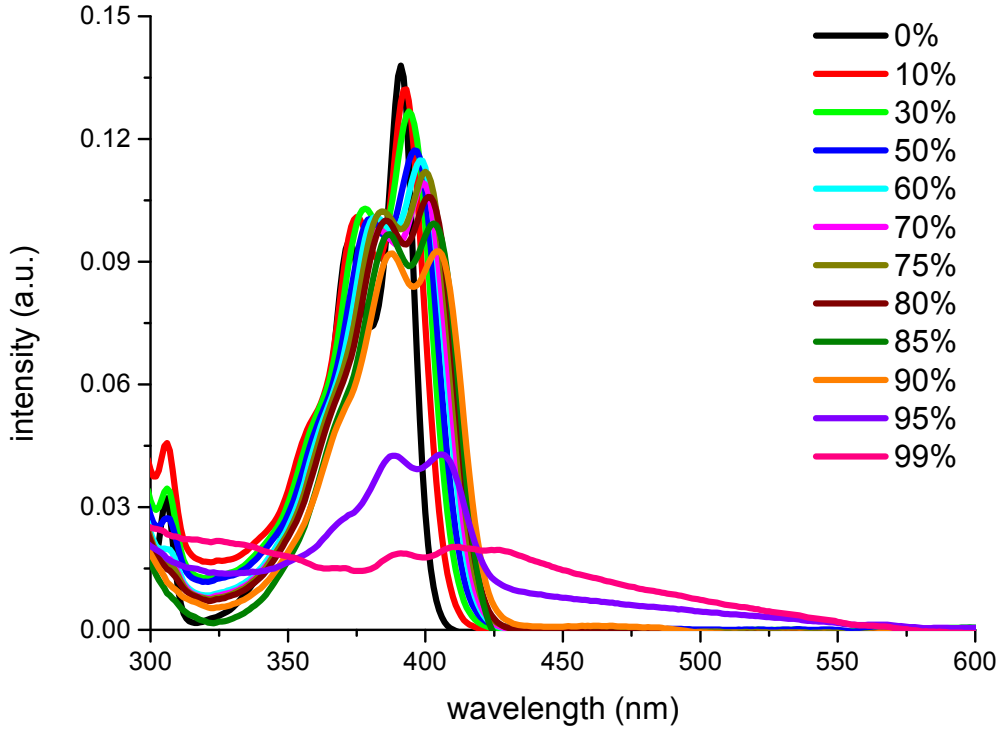


Figure S10. UV/vis absorption spectra of compound **2a** measured in THF/water with different water fractions at room temperature, concentration: 10 μM.

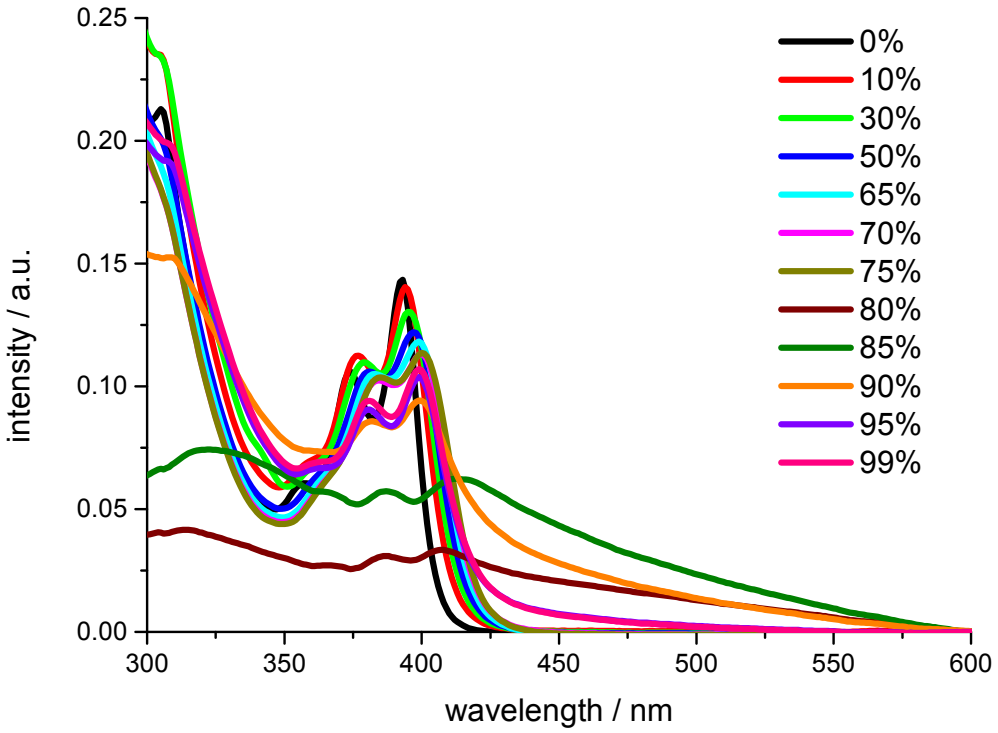


Figure S11. UV/vis absorption spectra of compound **2b** measured in THF/water with different water fractions at room temperature, concentration: 10 μM.

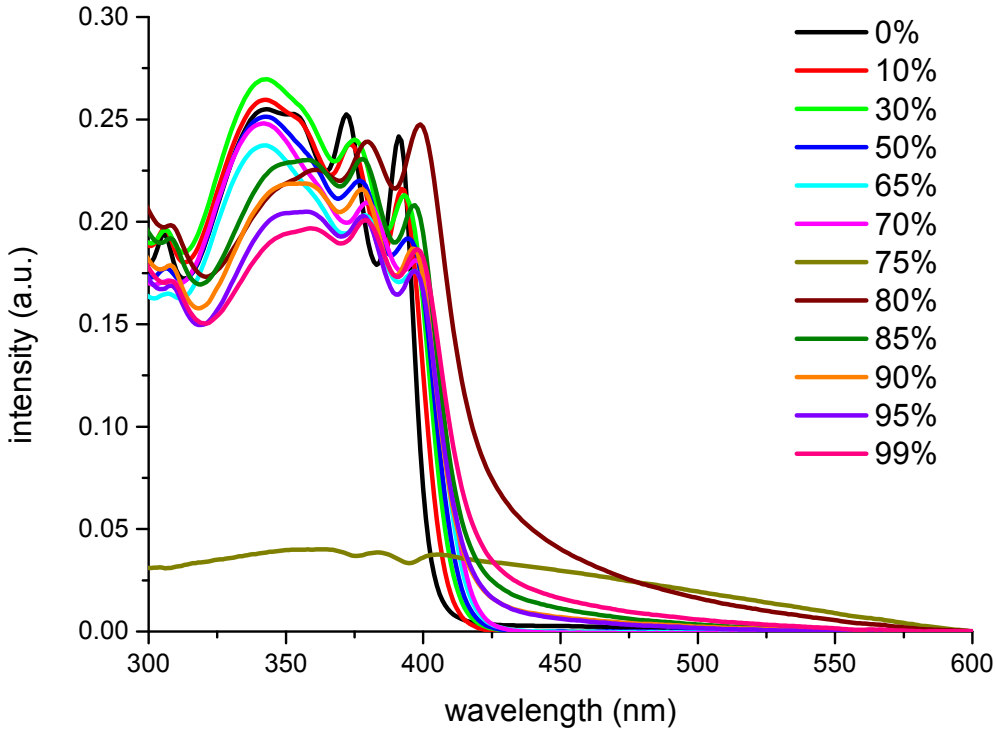


Figure S12. UV/vis absorption spectra of compound **2c** measured in THF/water with different water fractions at room temperature, concentration: 10 μM.

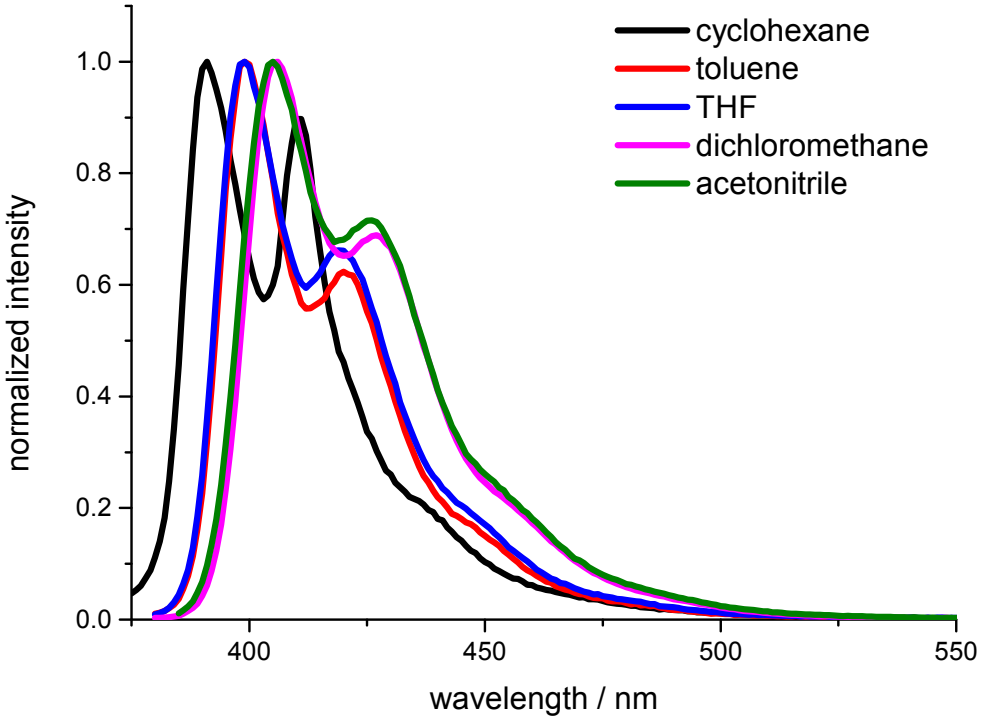


Figure S13. Fluorescence spectra of compound **2a** measured in different solvents at room temperature, concentration: 10 μM.

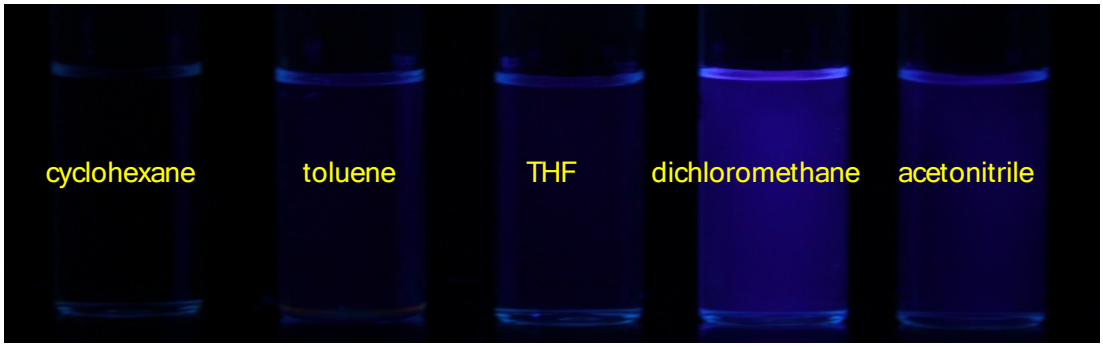


Figure S14. Photographs of compound **2a** in different solvents under 365 nm UV light, concentration: 10 μM.

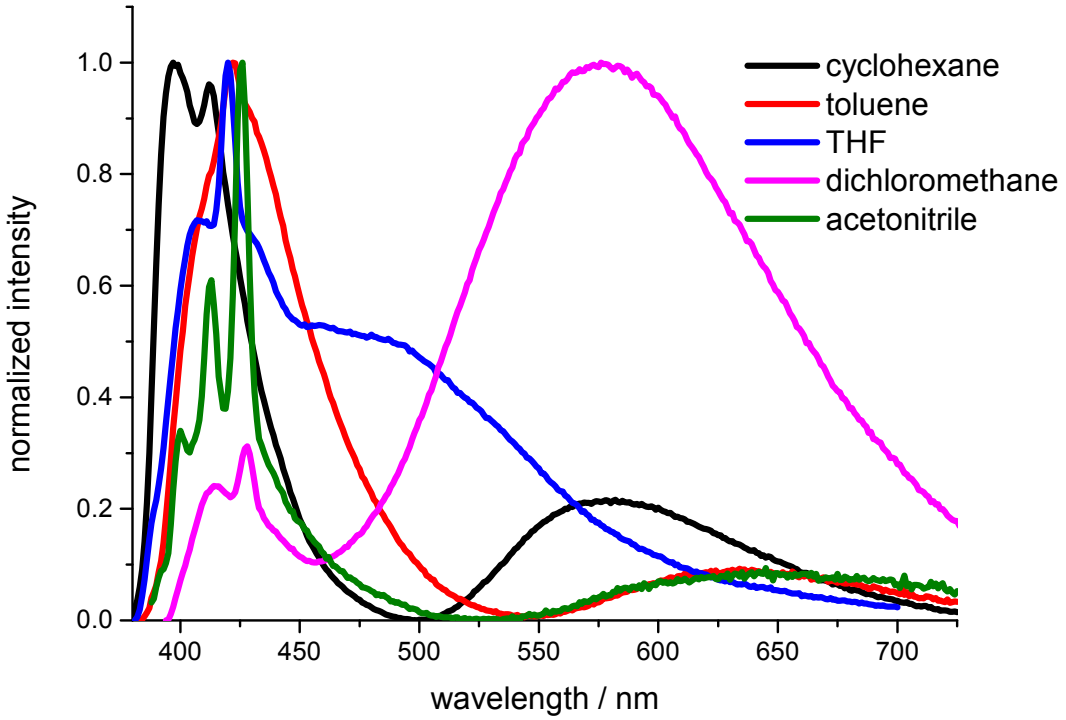


Figure S15. Fluorescence spectra of compound **2b** measured in different solvents at room temperature, concentration: 10 μM.

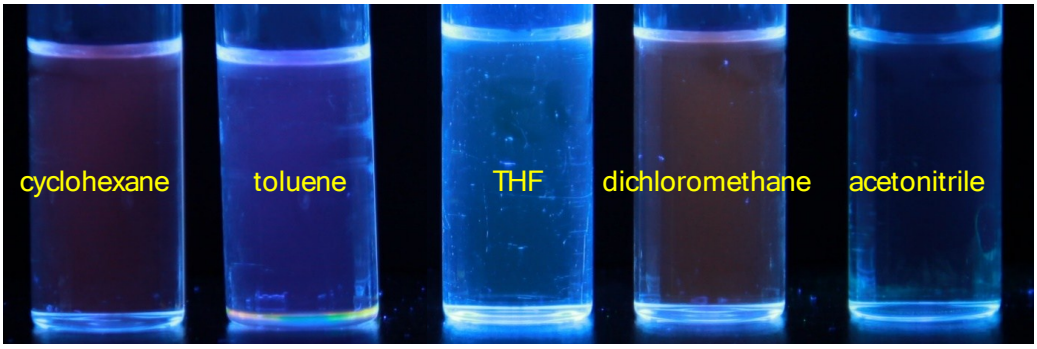


Figure S16. Photographs of compound **2b** in different solvents under 365 nm UV light, concentration: 10 μM.

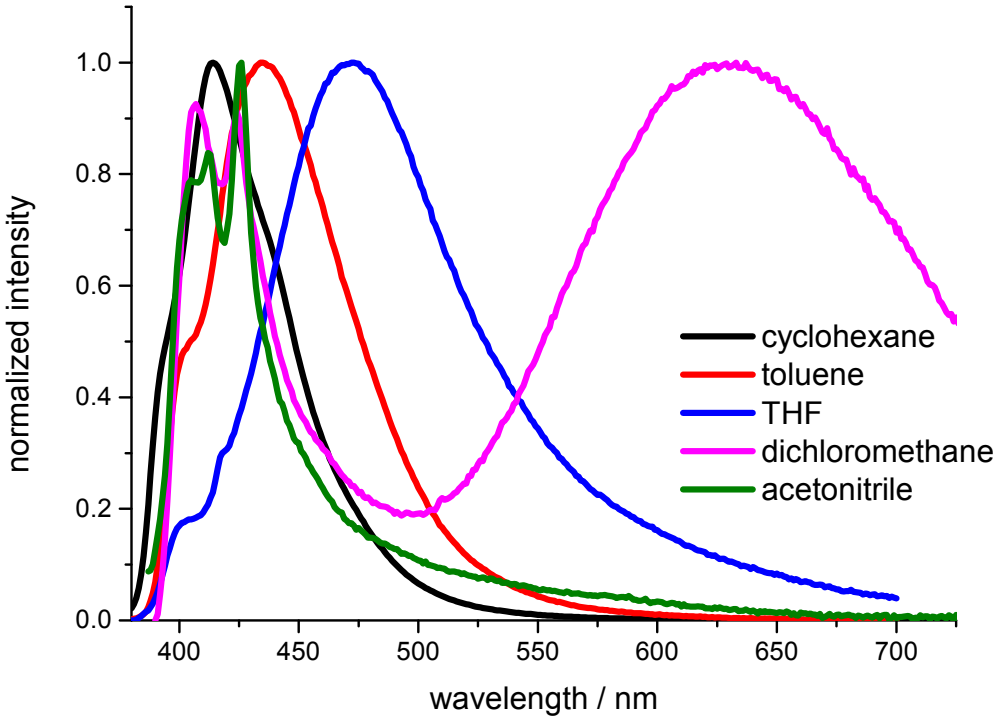


Figure S17. Fluorescence spectra of compound **2c** measured in different solvents at room temperature, concentration: 10 μM.

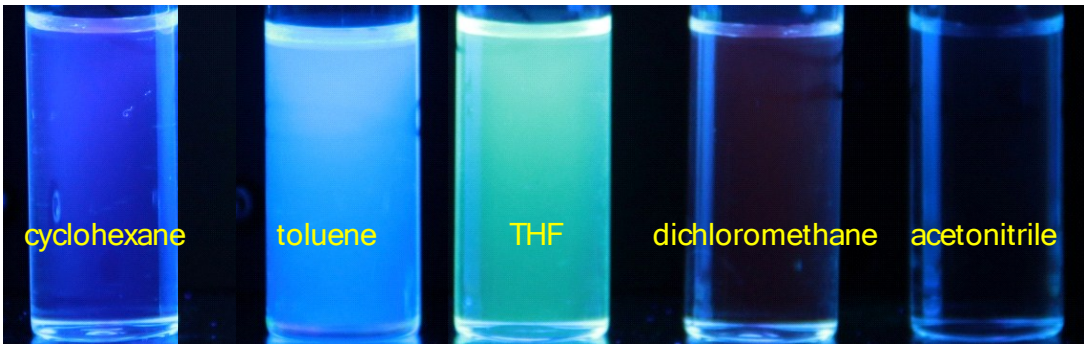


Figure S18. Photographs of compound **2c** in different solvents under 365 nm UV light, concentration: 10 μM.

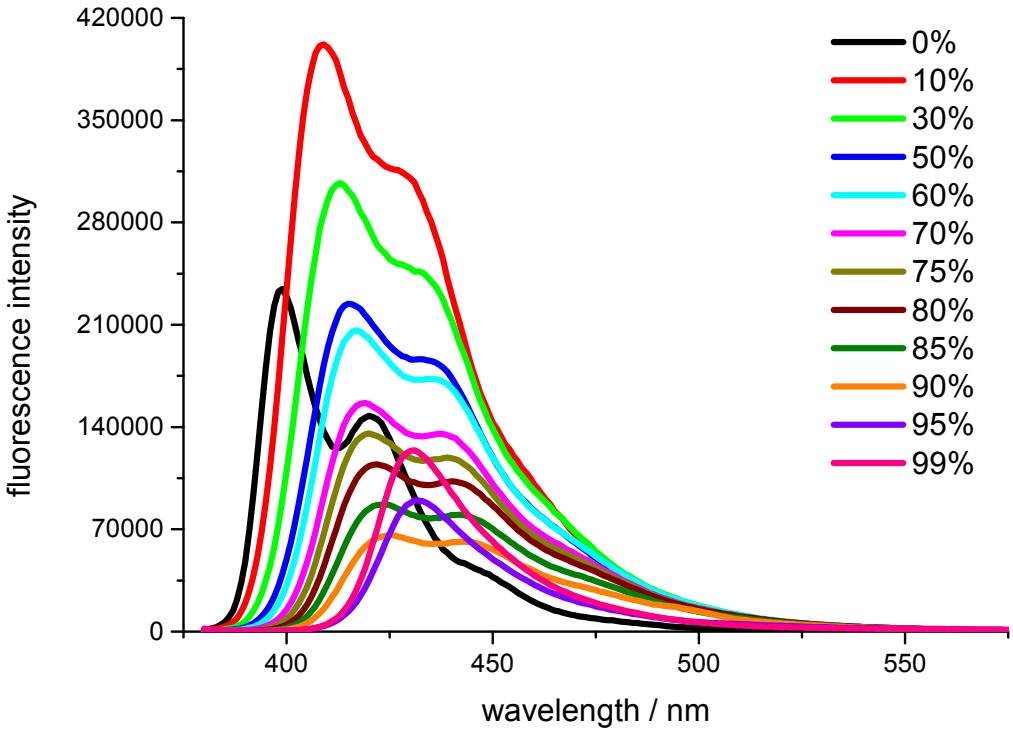


Figure S19. Fluorescence emission spectra of compound **2a** measured in THF/water with different water fractions at room temperature, concentration: 10 μM.

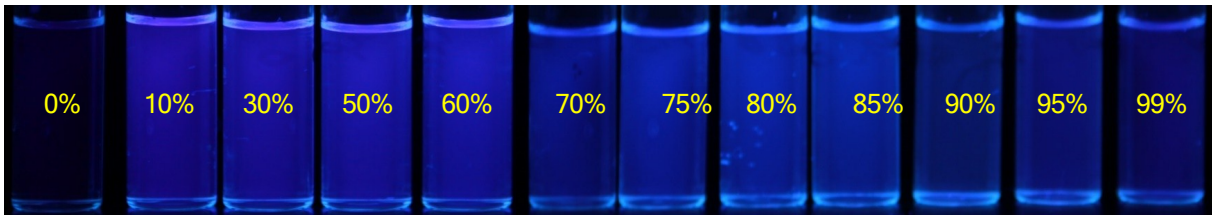


Figure S20. Photographs of compound **2a** in THF/water with different water fractions under 365 nm UV light, concentration: 10 μM.

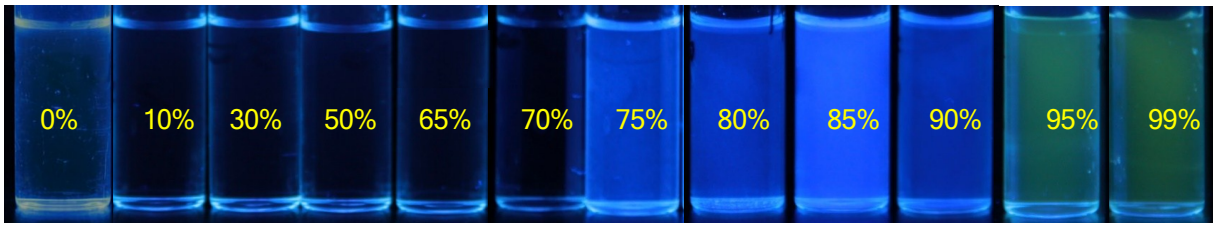


Figure S21. Photographs of compound **2b** in THF/water with different water fractions under 365 nm UV light, concentration: 10 μM.

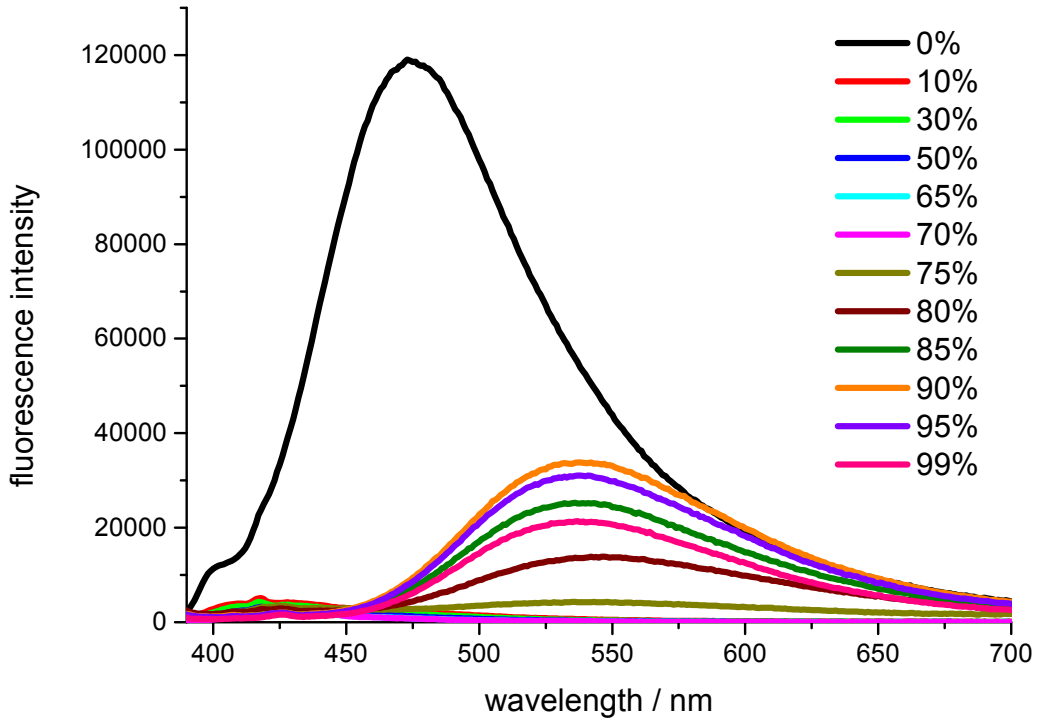


Figure S22. Fluorescence emission spectra of compound **2c** measured in THF/water with different water fractions at room temperature, concentration: 10 μM.

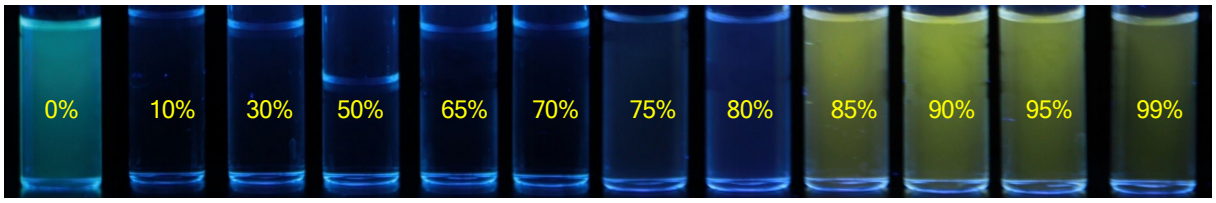


Figure S23. Photographs of compound **2c** in THF/water with different water fractions under 365 nm UV light, concentration: 10 μM.

Table S4 Summary of photoluminescence of **2a**-**2c** in different solvents at the concentration of 10 μM.

		LE					ICT				
compd.	sol.	$\lambda_{em}/\lambda_{ex}$ (nm)	Φ_F (%)	τ (ns)	k_r ($\times 10^7$ s^{-1})	k_{nr} ($\times 10^7$ s^{-1})	λ_{em} (nm)	Φ_F (%)	τ (ns)	k_r ($\times 10^7$ s^{-1})	k_{nr} ($\times 10^7$ s^{-1})
2a	CHX	391/367	4.4	0.014	326	7080	-	-	-	-	-
	TOL	399/373	8.2	0.013	656	7340	-	-	-	-	-
	THF	399/372	10	1.1	9.1	82	-	-	-	-	-
	DCM	406/377	35	1.8	19	36	-	-	-	-	-
	MeCN	405/375	23	2.0	11	38	-	-	-	-	-
2b	CHX	397/369	2.7	0.021	1270	45900	578	2.2	0.84	2.6	116
	TOL	422/374	3.6	4.6	0.8	21	636	1.3	0.021	61	4700
	THF	420/374	1.6	5.6	0.3	18	480	1.9	1.7	1.1	58
	DCM	426/379	1.7	3.9	0.4	25	571	3.3	0.69	4.8	140
	MeCN	426/378	3.8	3.7	1.0	26	652	1.4	1.5	0.9	66
2c	CHX[a]	414/368	3.5	0.011	320	8770	-	-	-	-	-
	TOL[a]	435/373	32	2.3	14	29	-	-	-	-	-
	THF[a]	473/372	10	2.9	3.4	31	-	-	-	-	-
	DCM	407/376	1.7	4.7	0.4	21	627	1.2	4.4	0.3	22
	MeCN[b]	426/378	3.8	4.3	0.9	22	-	-	-	-	-

[a] The fluorescence at the ICT and LE state are overlapped, thus only the peaks at the emission maxima are listed. [b]No fluorescence at the ICT state was observed. CHX: cyclohexane; TOL: toluene; THF: tetrahydrofuran; DCM: dichloromethane; MeCN: acetonitrile.

Table S5 Summary of photoluminescence of **2a-2c** in solid state

compd	$\lambda_{em}/\lambda_{ex}$ (nm)	Φ_F (%)	τ (ns)	k_r ($\times 10^7$ s^{-1})	k_{nr} ($\times 10^7$ s^{-1})
2a	464/365	13	3.9	3.3	22.3
2b	457/365	17	3.2	5.3	25.9
2c	496/365[a]	2.1	37.9	0.06	2.6

[a] The fluorescence of 2c has a broad emission in the range 458-504 nm, thus only the peak with the highest intensity is listed.

Table S6 Summary of photoluminescence of **2a-2c** in THF/water at the concentration of 10 μM in solution and aggregation states.

compd	water content	$\lambda_{em}/\lambda_{ex}$ (nm)	Φ_F (%)	τ (ns)	k_r ($\times 10^7$ s^{-1})	k_{nr} ($\times 10^7$ s^{-1})
2a	0	399/372	10	1.1	9.1	81.8
	0.99	431/372	7.3	1.3	5.7	72.4
2b	0[a]	420/374	1.6	5.6	0.3	17.6
	0.85	433/374	21	3.4	6.1	23.1
	0.95	525/374	1.9	89	0.02	1.1
2c	0[b]	473/372	10	2.9	3.4	31
	0.9	538/372	1.5	31.5	0.05	3.1

[a] Only the fluorescence of the LE state is listed. [b] The fluorescence at the ICT and LE state are overlapped, thus only the peaks at the emission maxima are listed.

6. CV spectra

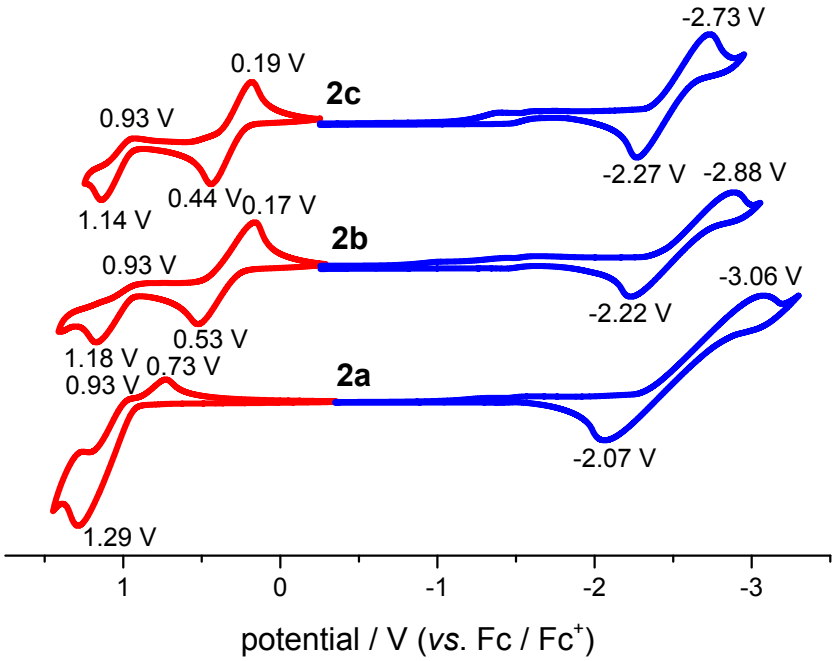


Figure S24. Cyclic voltammograms of compound **2a-2c** measured in 0.1 M Bu_4NClO_4 in dichloromethane for oxidation and in THF for reduction at room temperature. The scan speed was 100 mV/s, and ferrocene/ferrocenium (Fc/Fc^+) was used as internal reference.

7. Particle size distribution

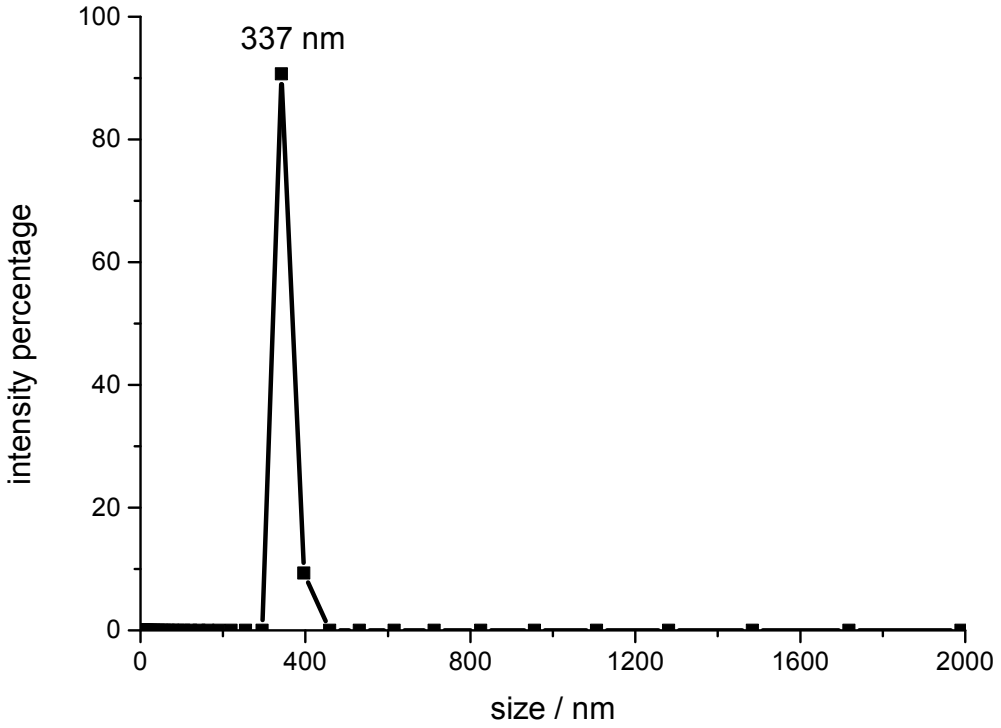


Figure S25. Particle size distribution of compound **2a** in 99% water in THF, concentration: 10 μM.

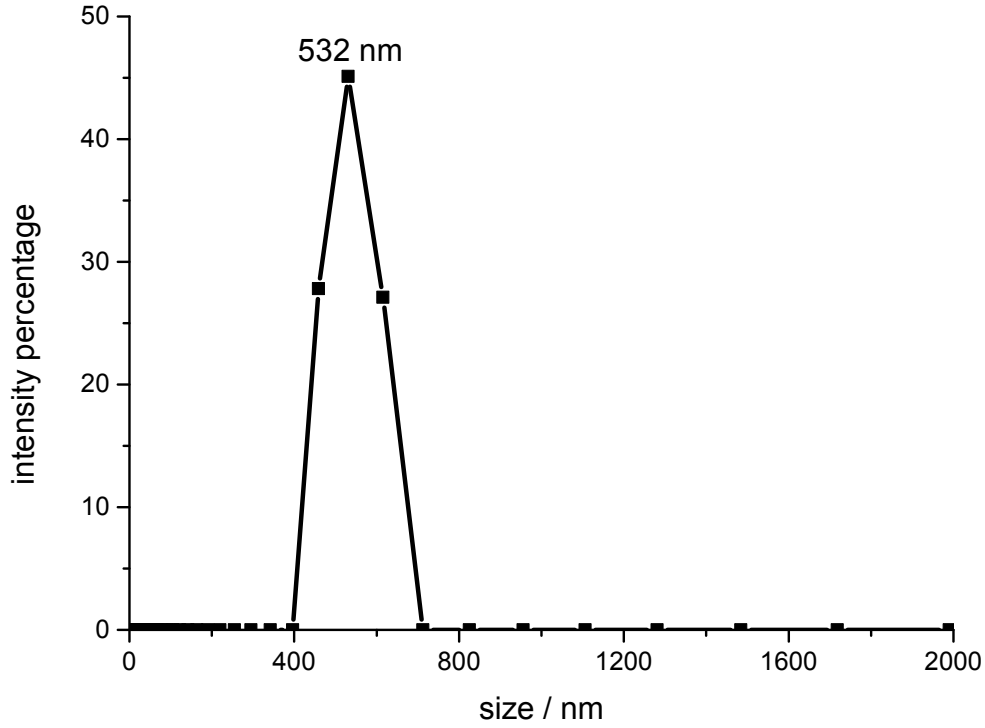


Figure S26. Particle size distribution of compound **2b** in 85% water in THF, concentration: 10 μM.

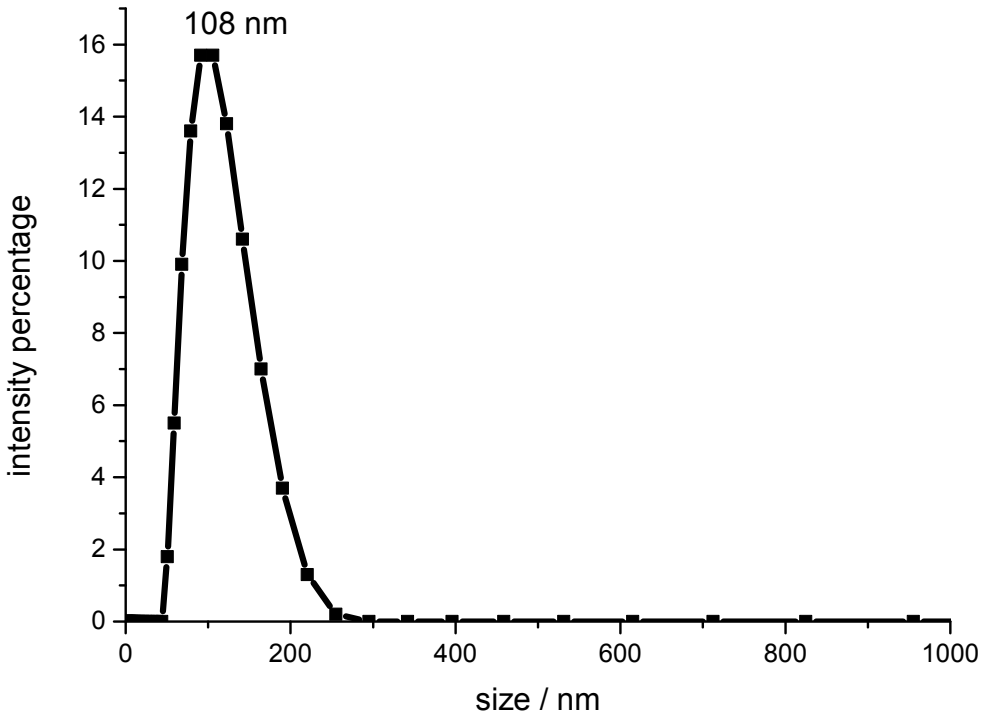


Figure S27. Particle size distribution of compound **2b** in 95% water in THF, concentration: 10 μM.

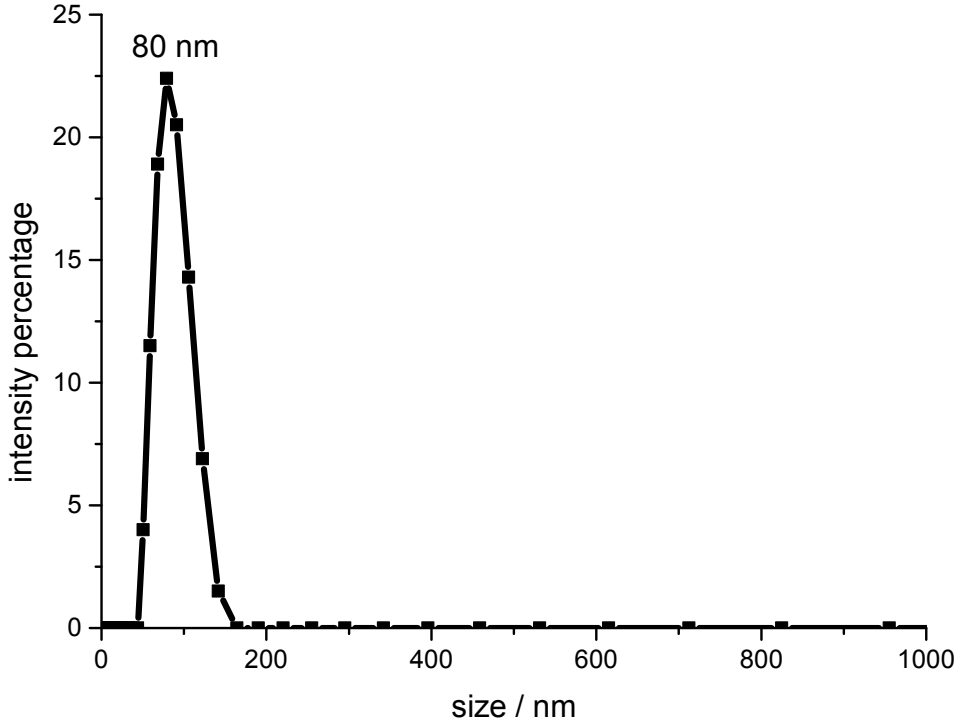


Figure S28. Particle size distribution of compound **2c** in 90% water in THF, concentration: 10 μM.

8. Calculations

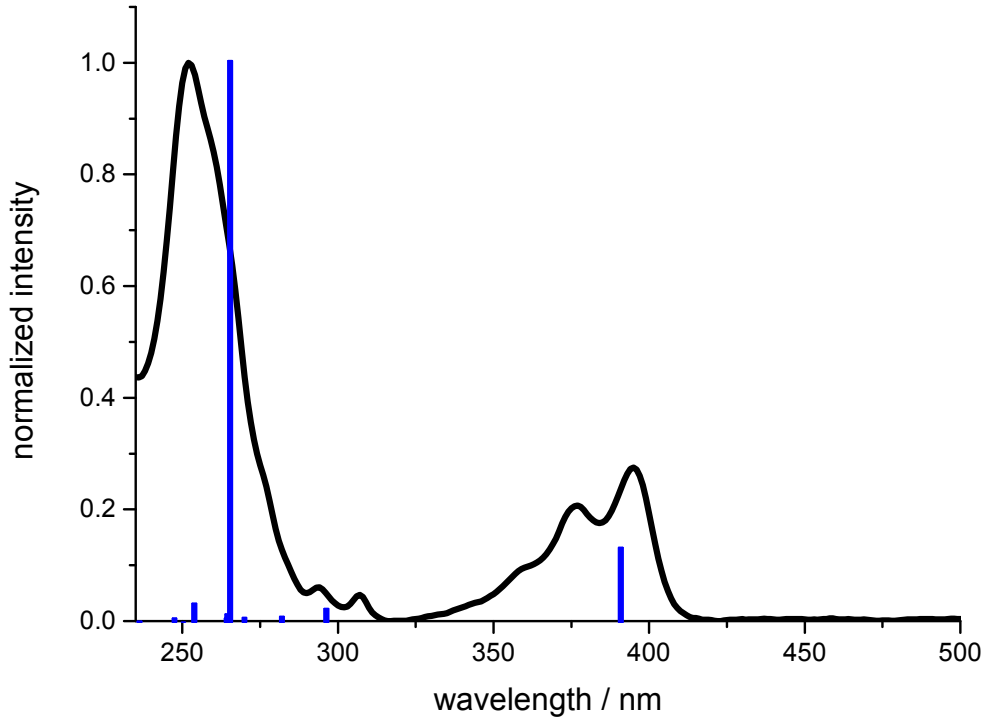


Figure S29. UV/Vis absorption spectrum of **2a** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at APFD/6-311G+(2d,p) level.

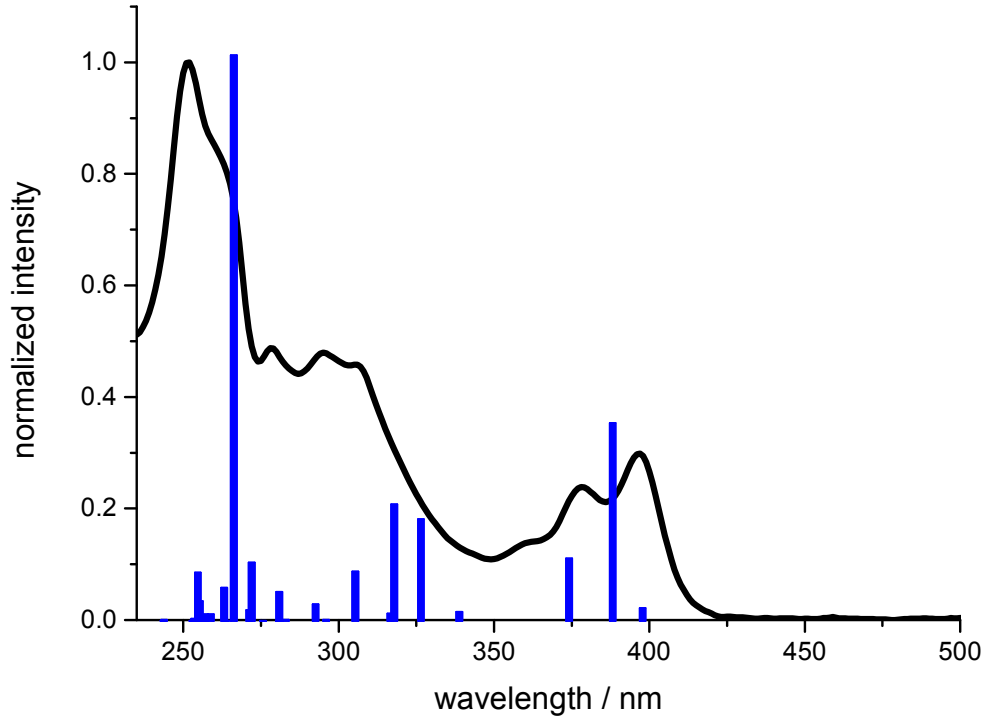


Figure S30. UV/Vis absorption spectrum of **2b** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at APFD/6-311G+(2d,p) level.

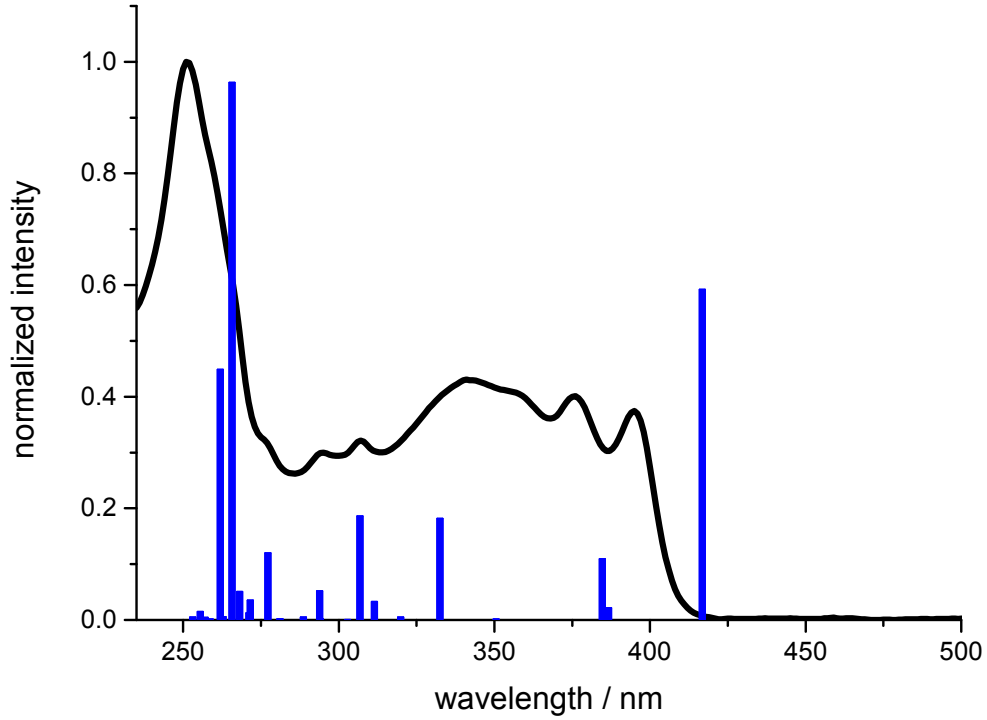


Figure S31. UV/Vis absorption spectrum of **2c** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at APFD/6-311G+(2d,p) level.

Table S7. TD-DFT calculated electron transitions of **2a** in dichloromethane at APFD /6-311G+(2d,p) level and the corresponding contributions.

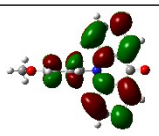
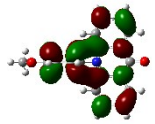
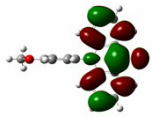
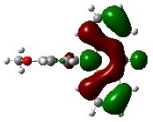
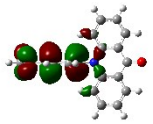
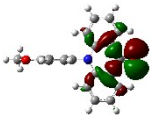
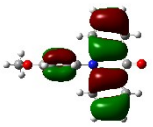
	transitions	contributions	Energy eV	Wavelength nm	Oscillator strength	
Excited 1	HOMO→LUMO	98.39%	3.1714	390.94	0.2066	 LUMO+2
Excited 2	HOMO-2→LUMO	96.54%	3.5927	345.10	0	 LUMO+1
Excited 3	HOMO-1→LUMO	98.59%	3.9362	314.99	0	 LUMO
Excited 4	HOMO-5→LUMO HOMO-3→LUMO HOMO→LUMO+1 HOMO→LUMO+2	12.72% 3.56% 79.25% 2.49%	4.1836	296.36	0.0368	 HOMO
Excited 5	HOMO-5→LUMO HOMO-3→LUMO HOMO→LUMO+1 HOMO→LUMO+2	10.00% 5.31% 10.85% 72.91%	4.3952	282.09	0.0155	 HOMO-1  HOMO-2  HOMO-5

Table S8. TD-DFT calculated electron transitions of **2b** in dichloromethane at APFD /6-311G+(2d,p) level and the corresponding contributions.

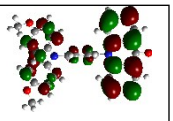
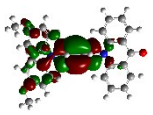
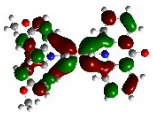
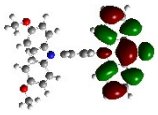
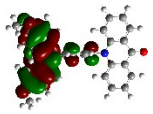
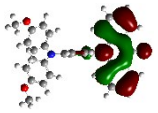
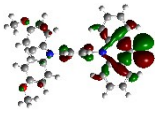
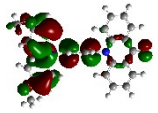
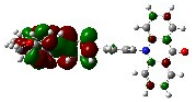
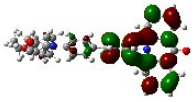
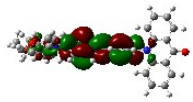
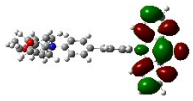
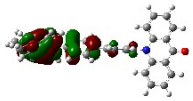
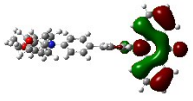
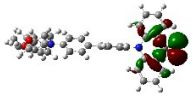
	transitions	contributions	Energy eV	Wavelength nm	Oscillator strength	 LUMO+3
Excited 1	HOMO→LUMO	99.75%	2.3690	523.37	0.0007	 LUMO+2
Excited 2	HOMO→LUMO+1 HOMO→LUMO+3	90.74% 6.32%	3.1183	397.61	0.0300	 LUMO+1
Excited 3	HOMO-1→LUMO HOMO→LUMO+2	82.39% 15.32%	3.1956	387.99	0.4523	 LUMO
Excited 4	HOMO-1→LUMO HOMO→LUMO+2	15.46% 82.19%	3.3150	374.01	0.1431	 HOMO
Excited 5	HOMO-4→LUMO HOMO-3→LUMO	6.05% 91.44%	3.5032	353.92	0	 HOMO-1  HOMO-3  HOMO-4

Table S9. TD-DFT calculated electron transitions of **2c** in dichloromethane at APFD /6-311G+(2d,p) level and the corresponding contributions.

	transitions	contributions	Energy eV	Wavelength nm	Oscillator strength	
Excited 1	HOMO→LUMO	99.79%	2.4349	509.19	0.0001	 LUMO+3
Excited 2	HOMO→LUMO+1	96.44%	2.9743	416.85	0.8064	 LUMO+2
Excited 3	HOMO→LUMO+2 HOMO→LUMO+3	10.63% 87.75%	3.2059	386.74	0.0290	 LUMO+1
Excited 4	HOMO-1→LUMO	96.89%	3.2226	384.73	0.1483	 LUMO  HOMO
Excited 5	HOMO-4→LUMO	97.19%	3.5001	354.23	0	 HOMO-1  HOMO-4

Cartesian coordinates for theoretically optimized structures of 2a-2c

2a opt B3LYP/6-31G(d)

HF = -976.4006948 hartree

C	1.03117322	-3.64598290	0.01987237
C	0.33858264	-2.44542508	0.04866693
C	1.03861455	-1.21955241	0.01533471
C	2.45175185	-1.24483194	-0.04770624
C	3.12575666	-2.47781091	-0.07612261
C	2.43292936	-3.67478426	-0.04310324
C	2.45162277	1.24497350	-0.04782586
C	1.03849414	1.21954993	0.01536916
C	0.33835358	2.44536159	0.04893149
H	-0.74289174	2.44843152	0.09810538
C	1.03082223	3.64598321	0.02007496
C	2.43256637	3.67492525	-0.04317909
C	3.12550298	2.47802261	-0.07632288
H	0.47041689	-4.57606851	0.04712089
H	-0.74267237	-2.44860165	0.09762841
H	4.20895428	-2.44074319	-0.12465690
H	2.96220404	-4.62198801	-0.06508103
H	0.46998691	4.57601546	0.04752610
H	2.96173776	4.62218401	-0.06526661
H	4.20869956	2.44105602	-0.12496081
C	-1.08593471	-0.00009248	0.10806462
C	-1.73622820	-0.00017420	1.34883708
C	-1.84146818	-0.00004932	-1.06301382
C	-3.12272668	-0.00020335	1.41229789
H	-1.14588170	-0.00023626	2.25961842
C	-3.23726738	-0.00005654	-1.01124520
H	-1.33465550	-0.00000560	-2.02289937
C	-3.88344580	-0.00011928	0.23176827
H	-3.64315599	-0.00027746	2.36390287
H	-3.80221557	-0.00007500	-1.93522462
C	-6.06185572	0.00001420	-0.75247836

H	-5.89817109	-0.89427998	-1.36652166
H	-7.08840513	0.00017255	-0.38459636
H	-5.89800266	0.89421773	-1.36661934
O	-5.23368710	-0.00001663	0.40237776
C	3.23956458	0.00011384	-0.08430074
O	4.47170940	0.00017156	-0.14086147
N	0.35271775	-0.00002997	0.04375395

2b opt B3LYP/6-31G(d)

HF = -1608.3871845 hartree

C	-3.91872108	2.39479425	2.74170961
C	-3.24481528	1.59246638	1.83430675
C	-3.96471696	0.77438843	0.93588489
C	-5.37878198	0.79298419	0.98382447
C	-6.03367688	1.61728145	1.91506378
C	-5.32133630	2.41589203	2.79165263
C	-6.18700837	-0.03794263	0.07406117
C	-5.41776975	-0.87045567	-0.86729886
C	-4.00290593	-0.85400692	-0.87695786
C	-3.32121172	-1.67366119	-1.80317023
H	-2.23913564	-1.67495302	-1.82660698
C	-4.03257875	-2.47568911	-2.68180353
C	-5.43610527	-2.49462582	-2.67474757
C	-6.11117975	-1.69439446	-1.77062449
H	-3.34280058	3.01492747	3.42300987
H	-2.16266846	1.59164742	1.81394910
H	-7.11834212	1.59346982	1.90944156
H	-5.83592154	3.04893945	3.50744378
H	-3.48566098	-3.09741695	-3.38513193
H	-5.98018457	-3.12754525	-3.36848630
H	-7.19468255	-1.66907202	-1.72101778
C	-1.85673311	-0.03982717	-0.01495710
C	-1.13196640	-0.93361776	0.77763142

C	-1.16644145	0.85471360	-0.83759756
C	0.25873528	-0.93187082	0.75635100
H	-1.66413920	-1.62415147	1.42466994
C	0.22355947	0.85464681	-0.87428045
H	-1.72608843	1.54414738	-1.46225362
C	0.96473013	-0.03828537	-0.07400830
H	0.80635838	-1.62198819	1.38740868
H	0.74389859	1.54499611	-1.52780717
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O	5.25201977	-4.74576903	0.87242125

2c opt B3LYP/6-31G(d)

HF = -1839.4509874 hartree

C	-6.25461854	0.79767828	-3.55739511
C	-5.56167442	0.53477352	-2.38591535
C	-6.26315380	0.26716023	-1.18994700
C	-7.67771507	0.27292616	-1.21461854
C	-8.35189413	0.54302948	-2.41790623
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H	0.37429441	-1.97814449	0.83976042
C	3.01494639	-0.00003882	0.00010899
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C	4.84242095	-2.10425269	-1.21001673
C	6.94304671	-2.71085600	0.52562353
H	6.45483259	-0.86067912	1.50583804
C	5.55698882	-3.28222169	-1.37269944
H	4.03338854	-1.86424683	-1.89215750
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C	8.33963109	5.14048641	-0.08439871
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H	8.70445954	-6.09767314	-0.29115028
H	9.15433851	-4.40545707	0.04791654
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O	7.26272464	4.77194433	0.76221932
C	-8.46641656	-0.00001880	-0.00005701
O	-9.69997429	-0.00002905	-0.00007796

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