

Donor- π -Acceptor-Type Fluorinated Tolane Containing a Semifluoroalkoxy Chain as a Condensed-Phase Luminophore

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NMR spectrum

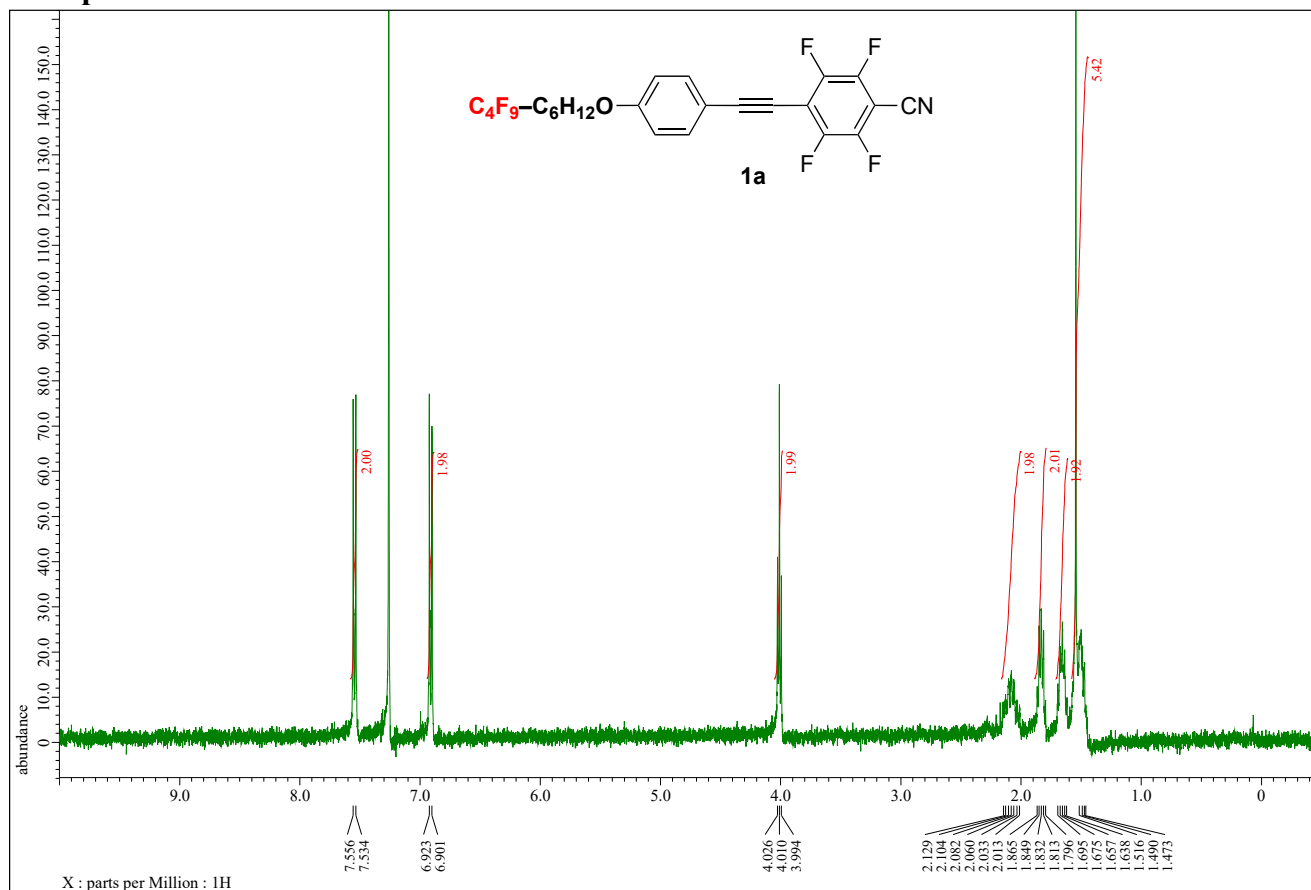


Figure S1. ¹H NMR spectrum of **1a** (CDCl₃, 400 MHz).

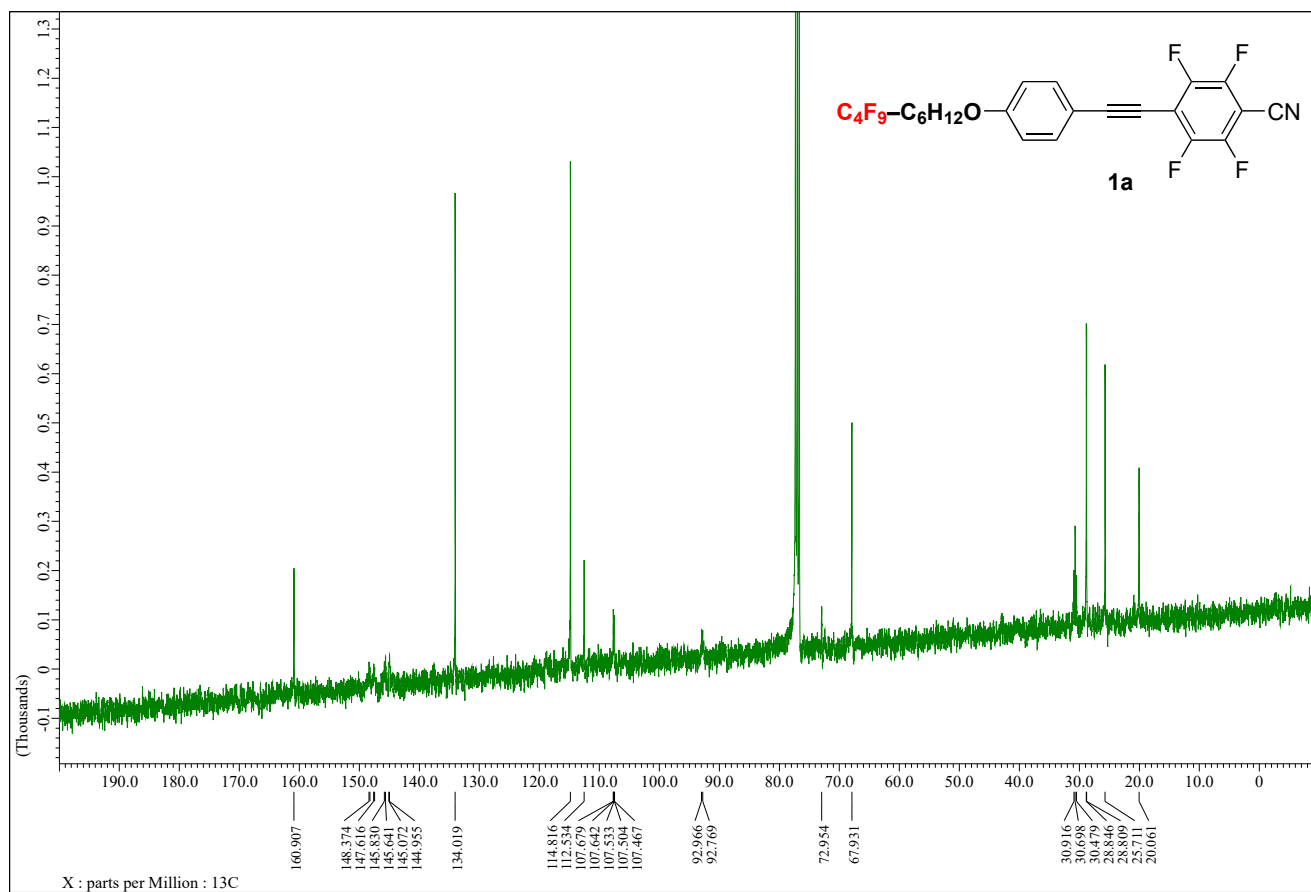


Figure S2. ¹³C NMR spectrum of **1a** (CDCl₃, 100 MHz).

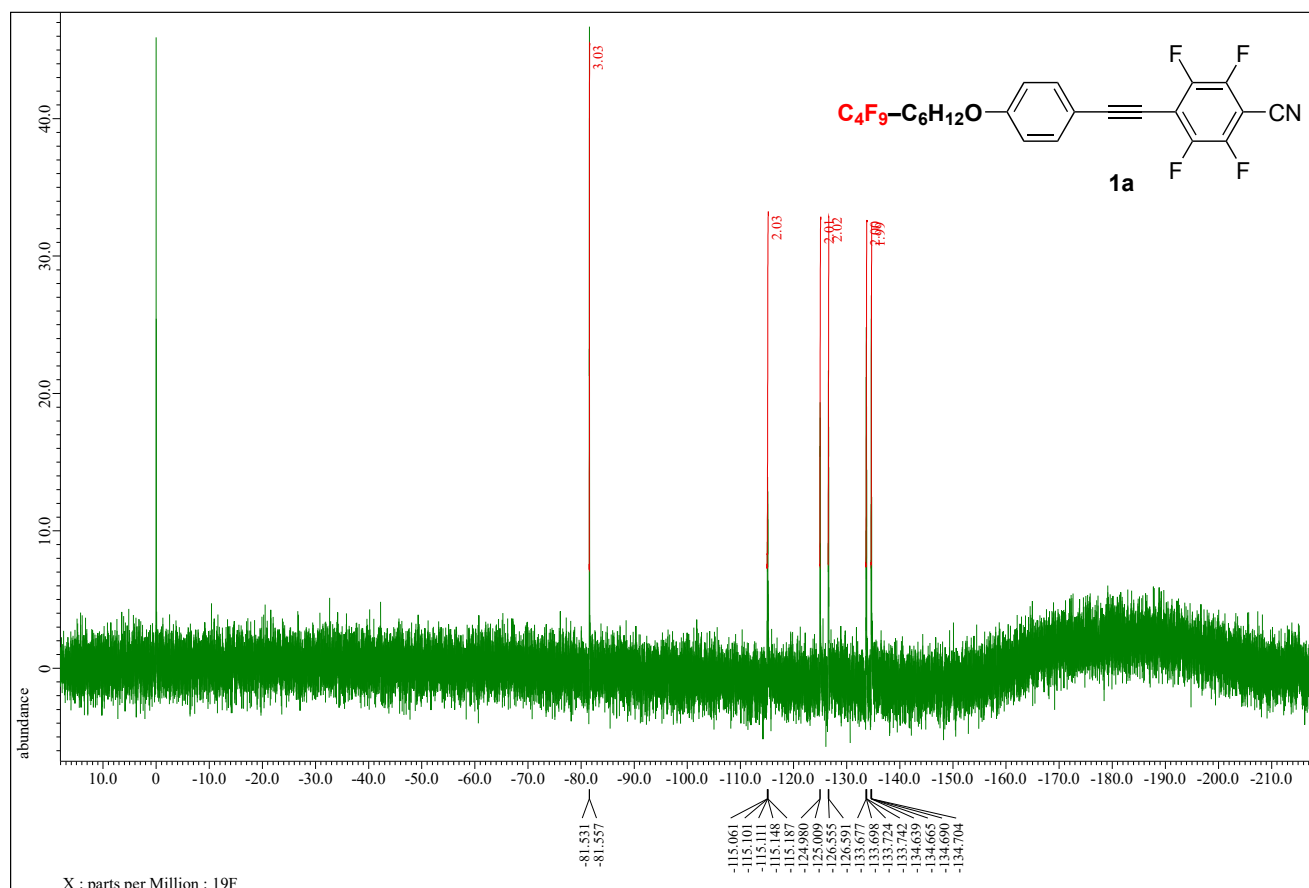


Figure S3. ^{19}F NMR spectrum of **1a** (CDCl_3 , CFCl_3 , 376 MHz).

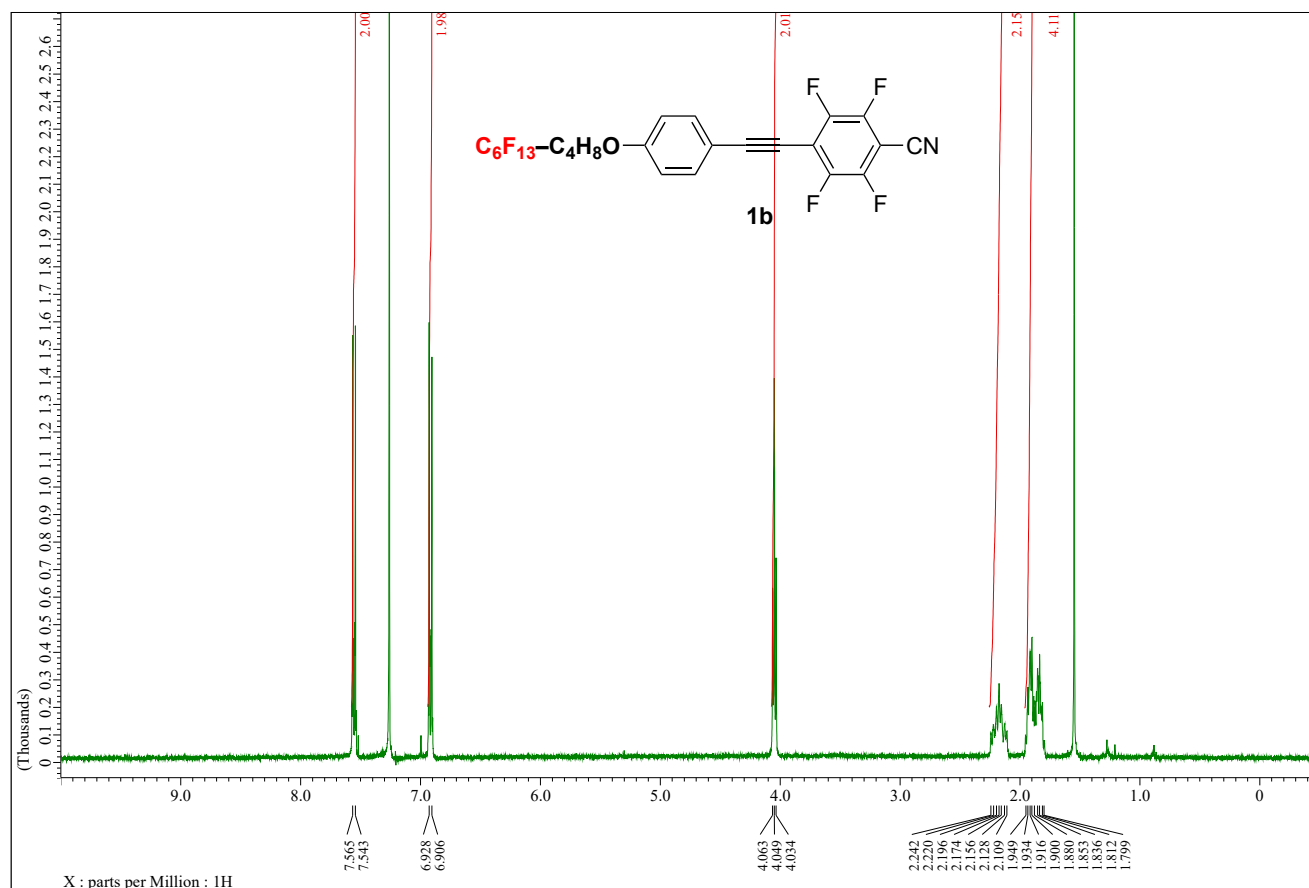


Figure S4. ¹H NMR spectrum of **1b** (CDCl₃, 400 MHz).

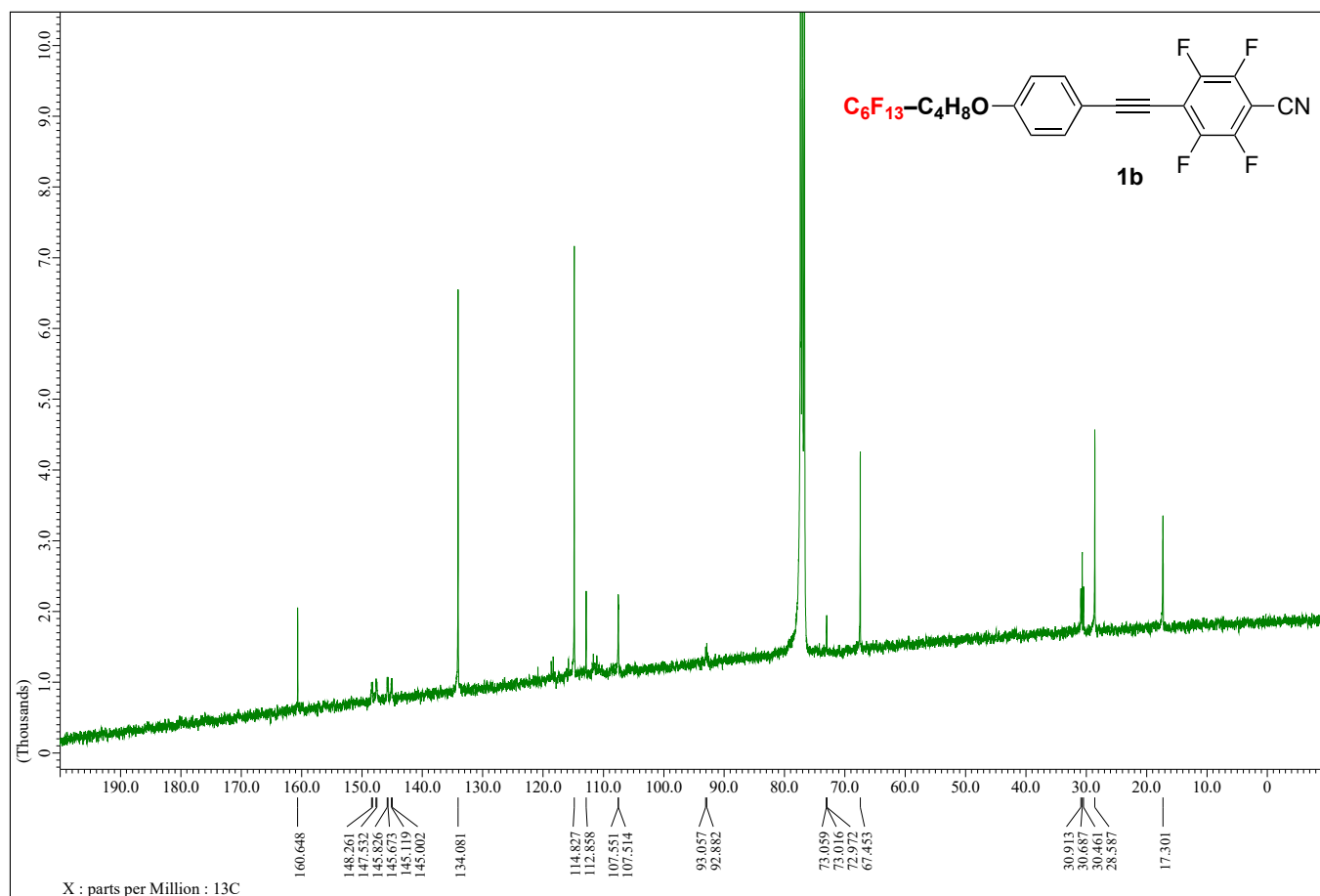


Figure S5. ¹³C NMR spectrum of **1b** (CDCl₃, 100 MHz).

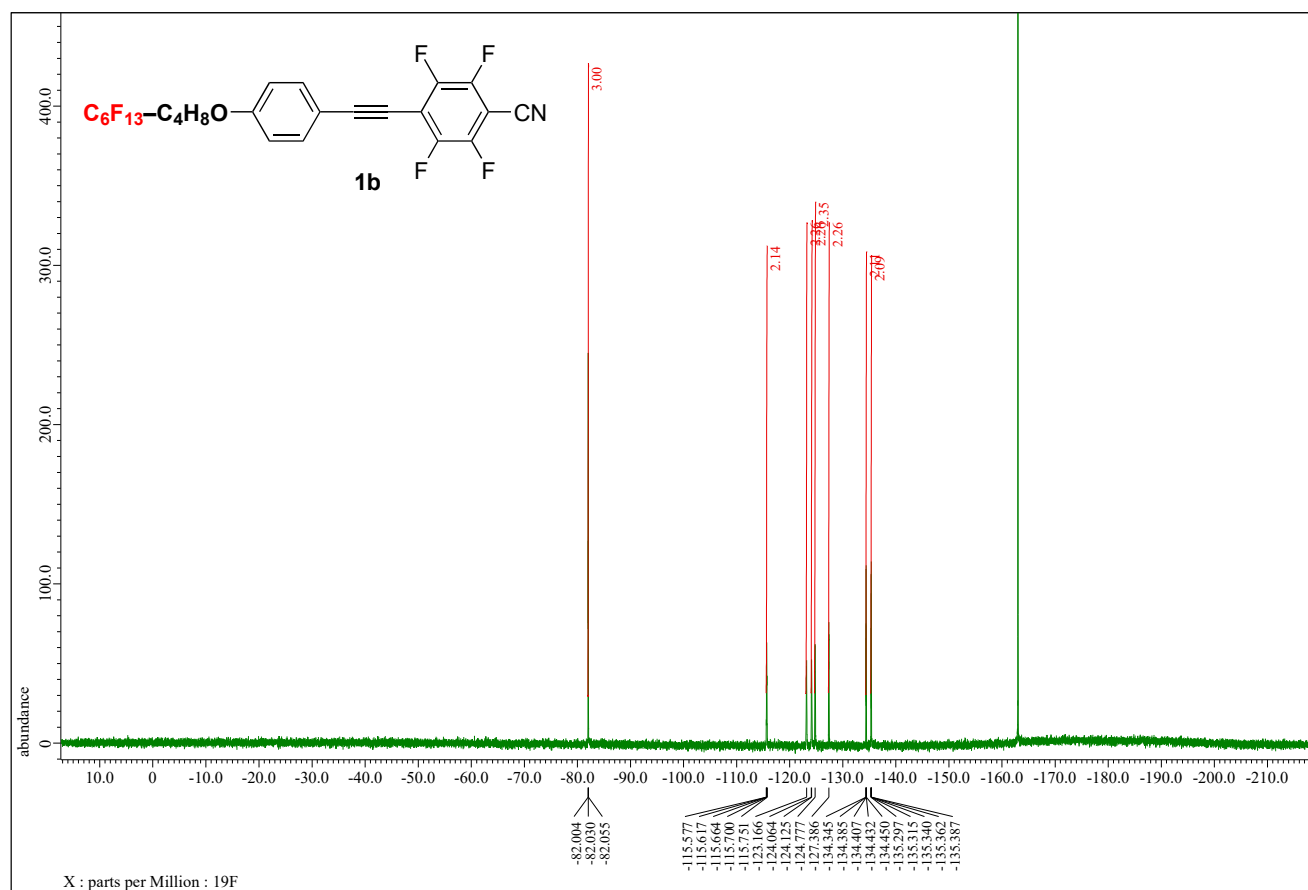


Figure S6. ^{19}F NMR spectrum of **1b** (CDCl_3 , C_6F_6 , 376 MHz).

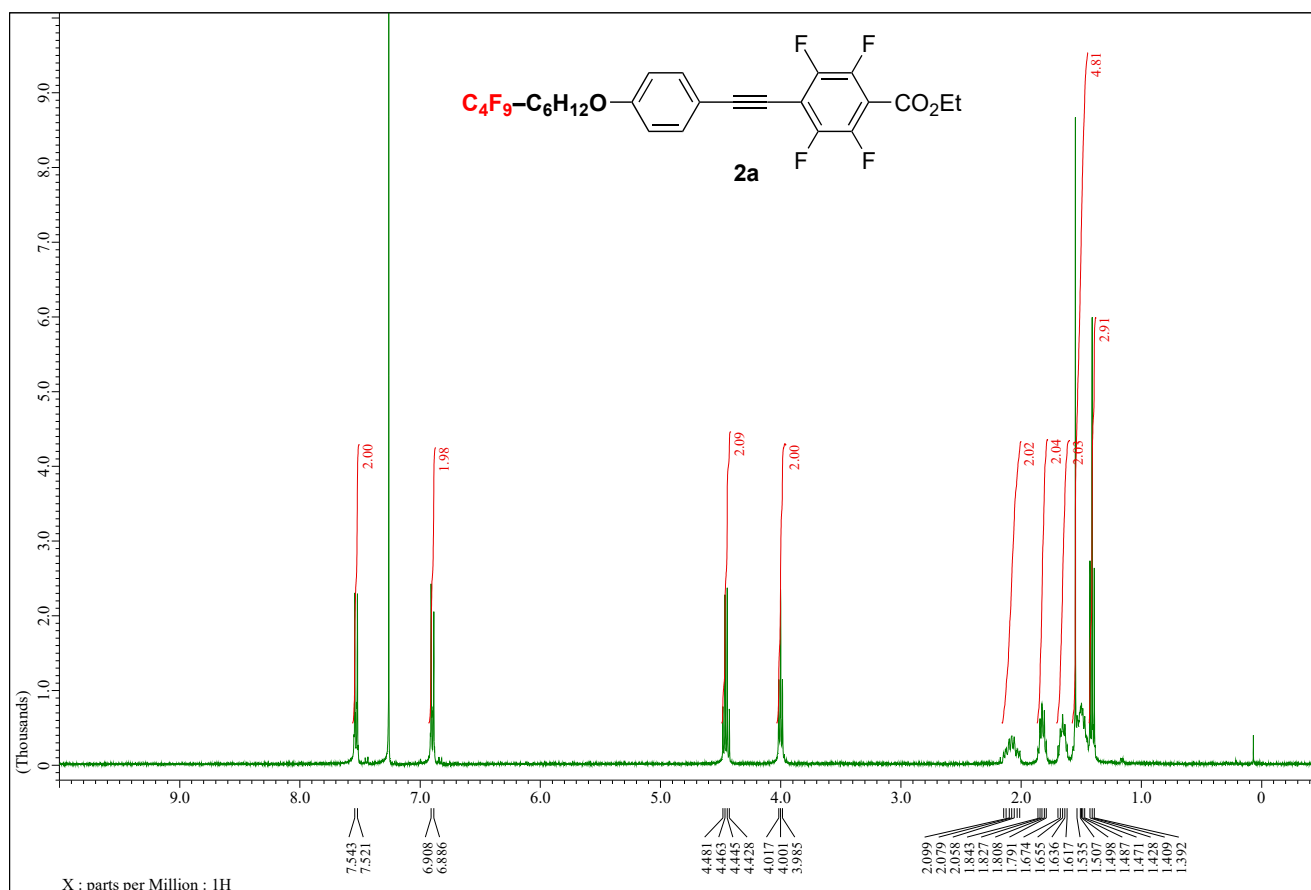


Figure S7. ¹H NMR spectrum of **2a** (CDCl₃, 400 MHz).

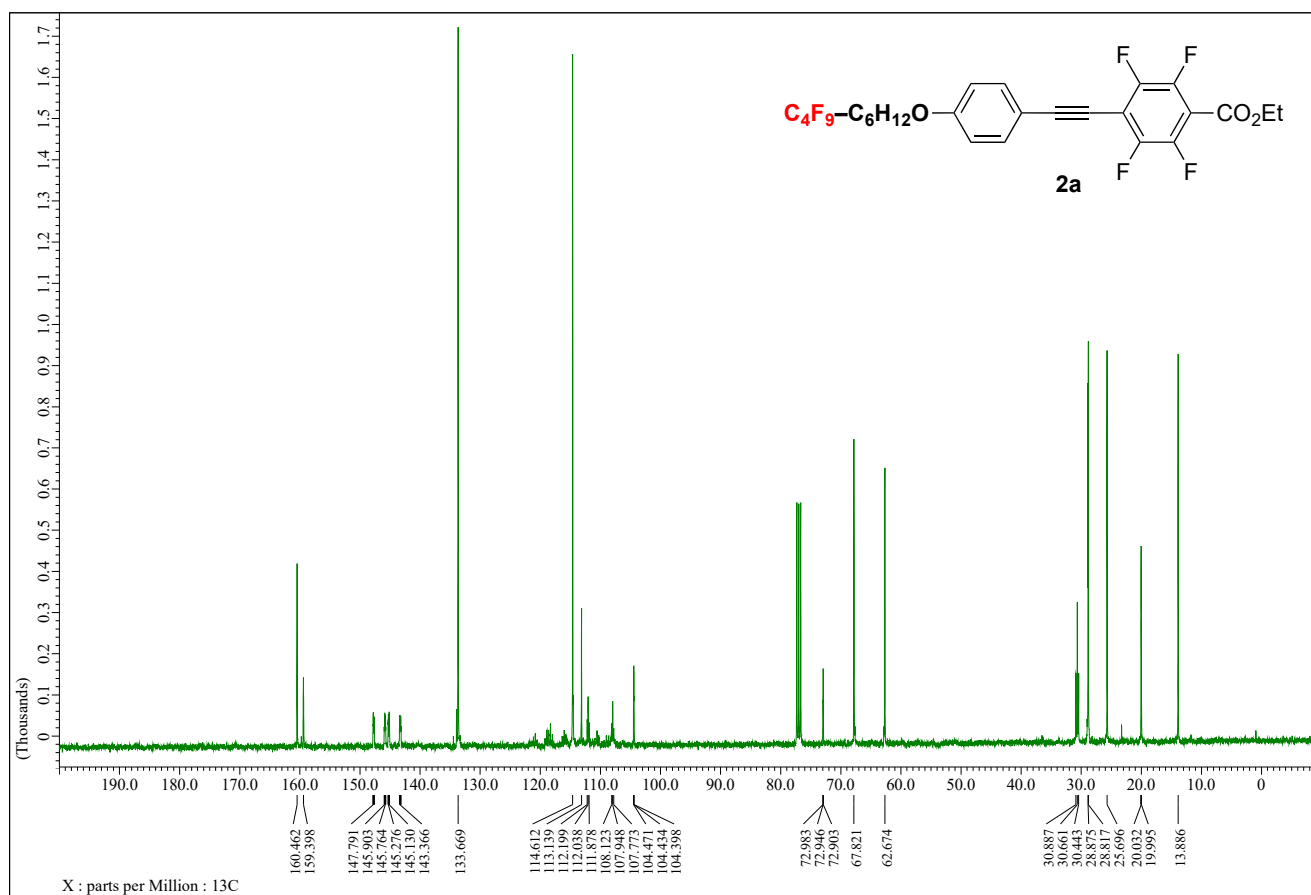


Figure S8. ¹³C NMR spectrum of **2a** (CDCl₃, 100 MHz).

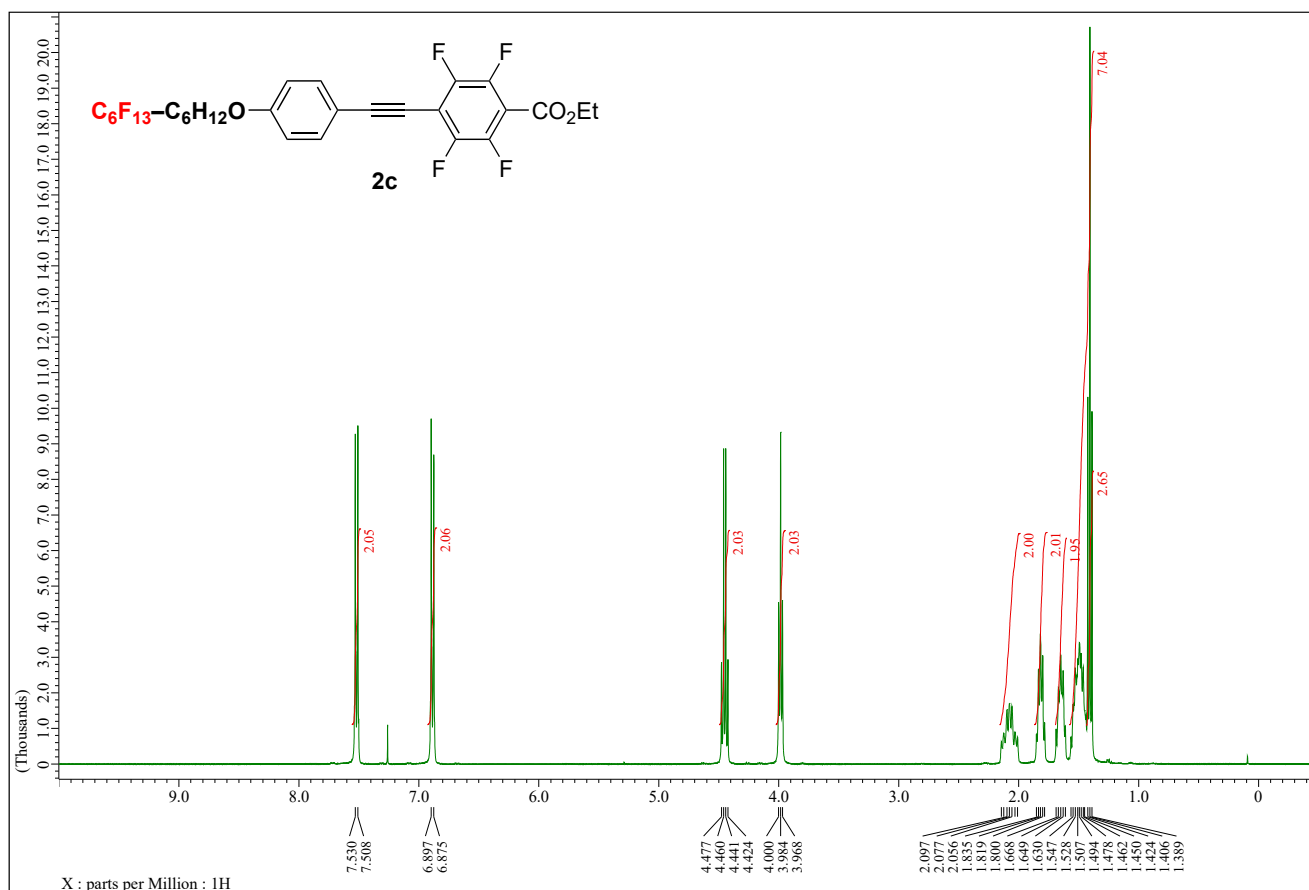


Figure S10. ¹H NMR spectrum of **2c** (CDCl₃, 400 MHz).

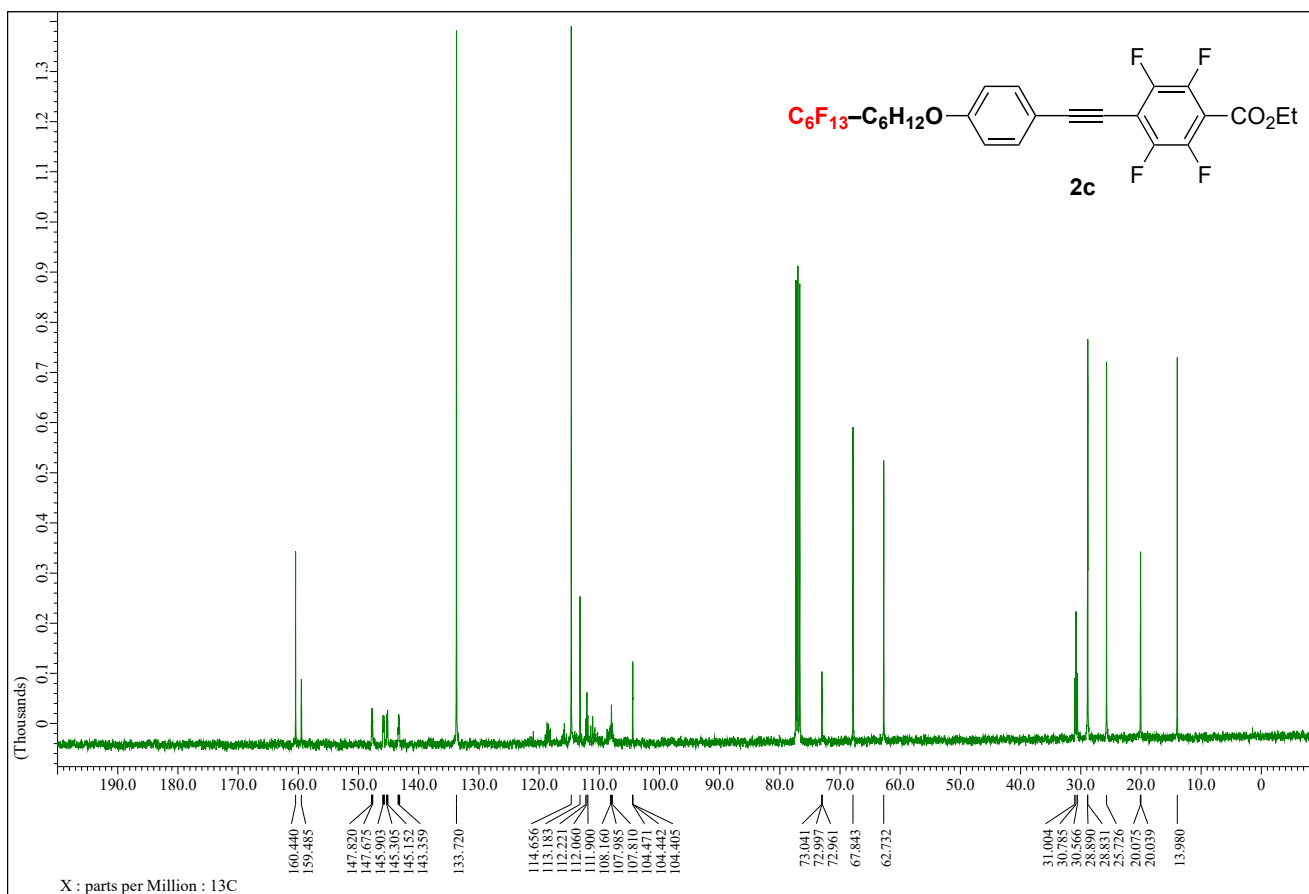


Figure S11. ¹³C NMR spectrum of **2c** (CDCl₃, 100 MHz).

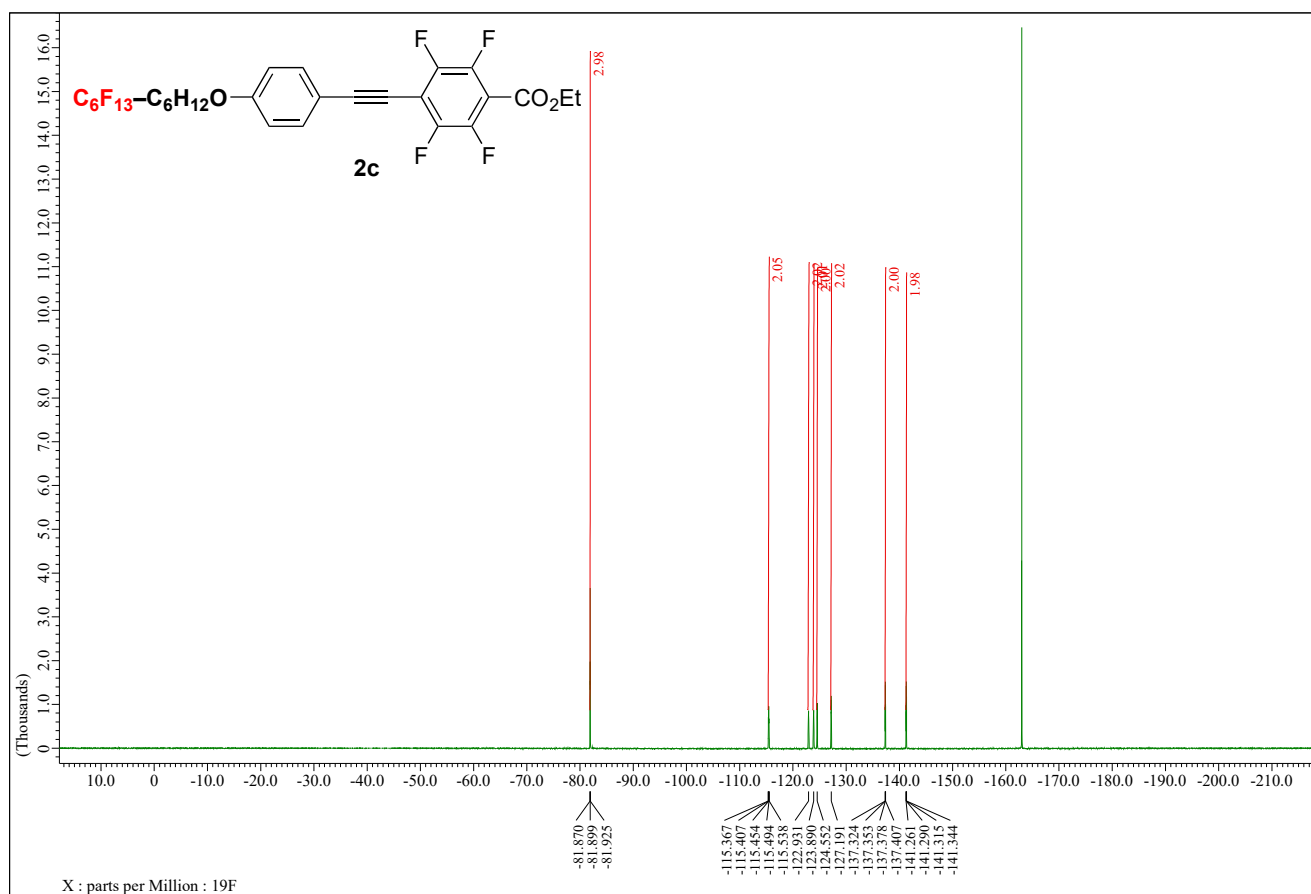


Figure S12. ^{19}F NMR spectrum of **2c** (CDCl_3 , C_6F_6 , 376 MHz).

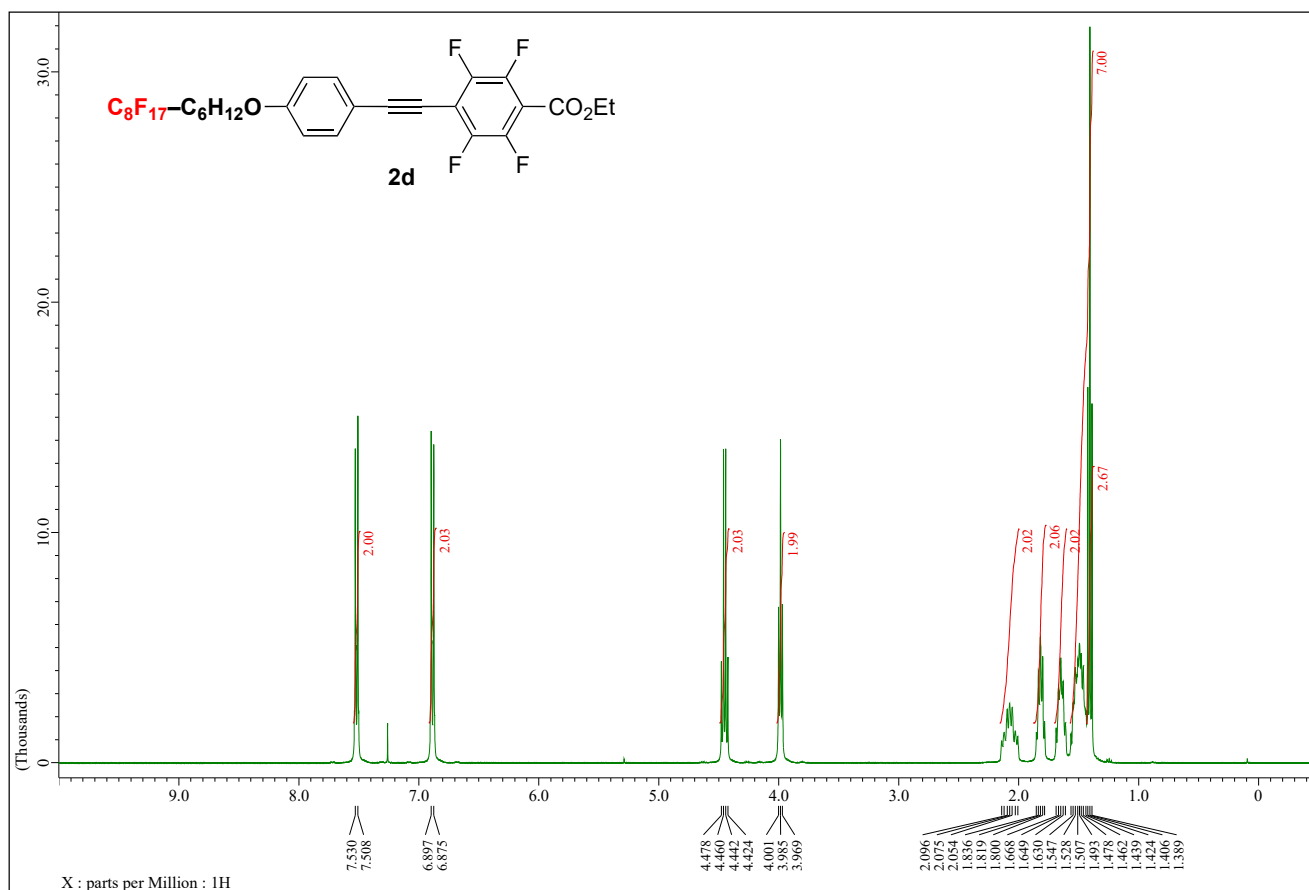


Figure S13. ¹H NMR spectrum of **2d** (CDCl₃, 400 MHz).

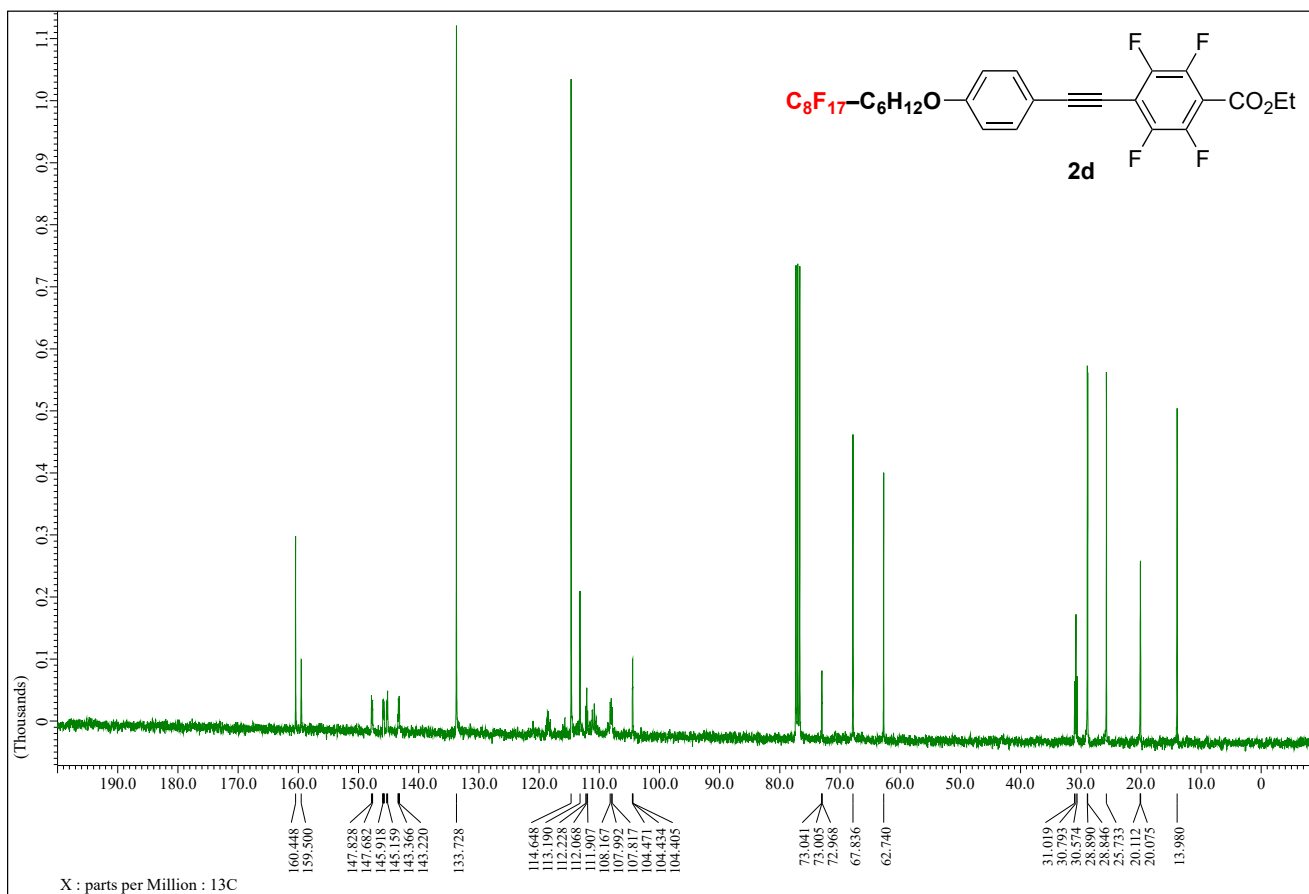


Figure S14. ¹³C NMR spectrum of **2d** (CDCl₃, 100 MHz).

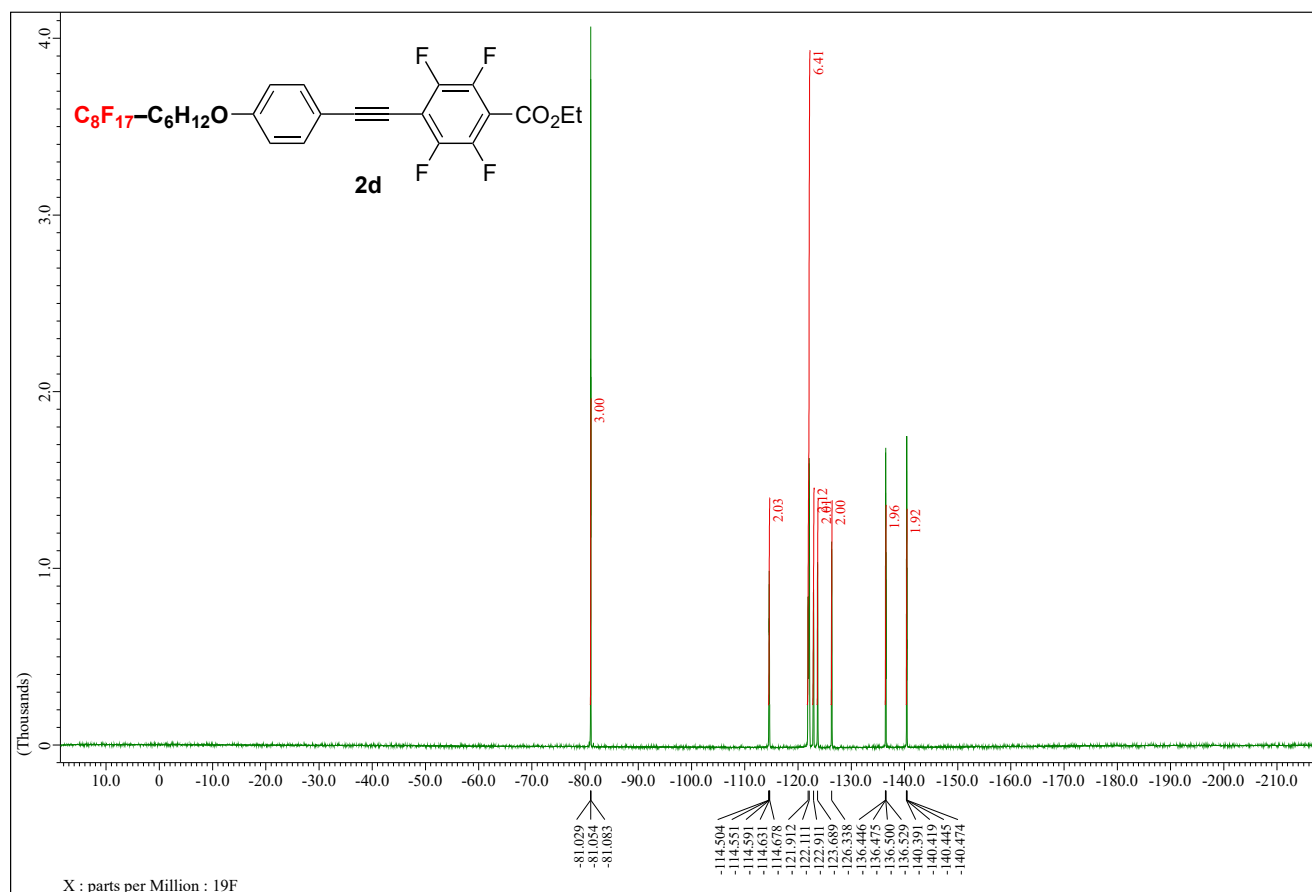
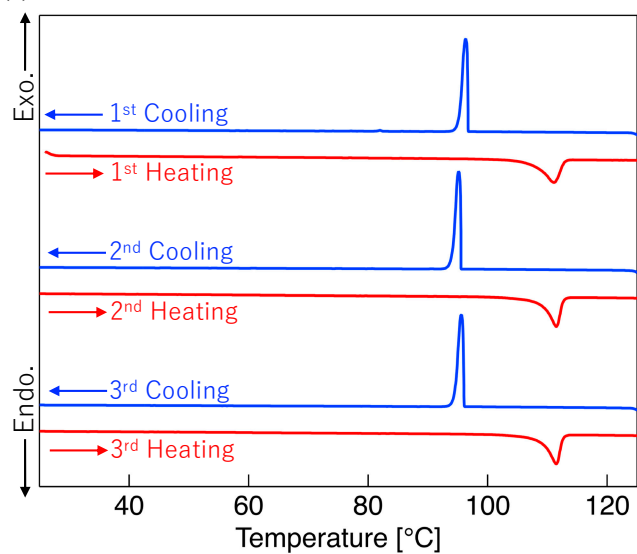


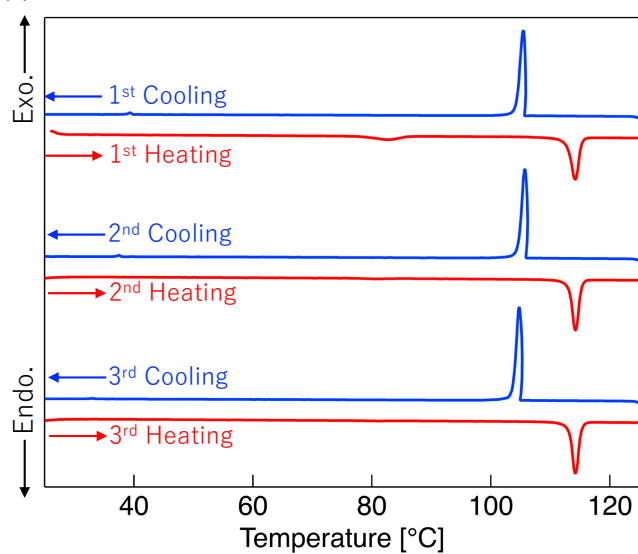
Figure S15. ¹⁹F NMR spectrum of **2d** (CDCl₃, CFCl₃, 376 MHz).

Phase transition behavior

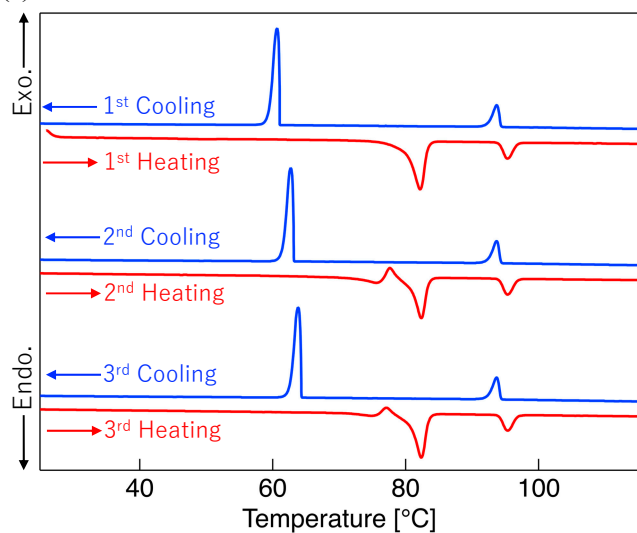
(a) **1a**



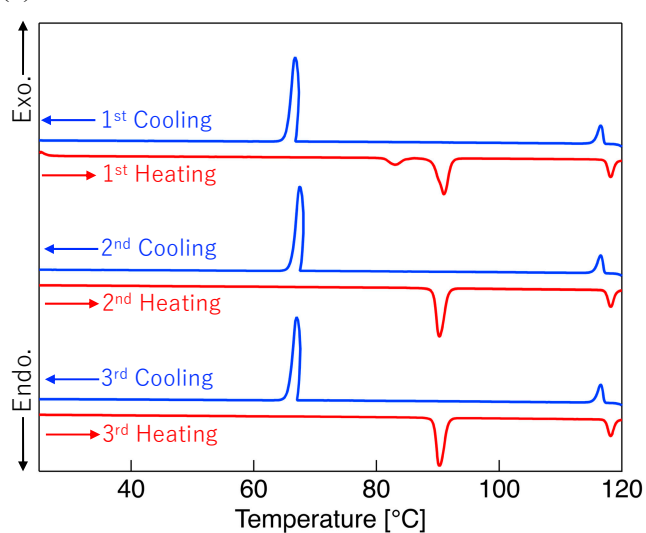
(b) **1b**



(c) **2a**



(d) **2c**



(e) **2d**

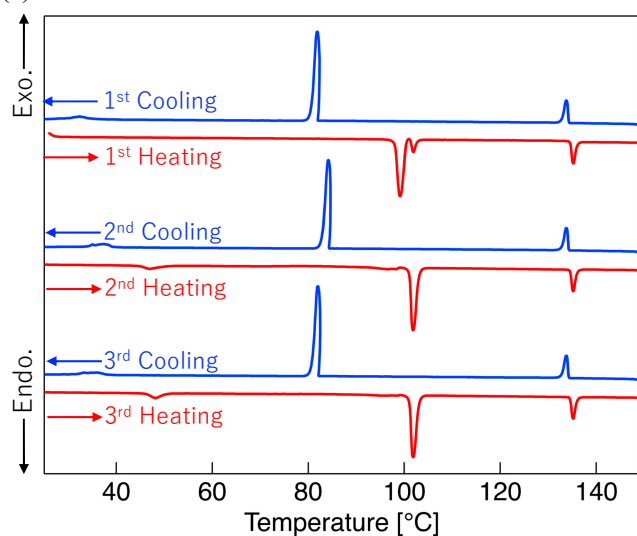
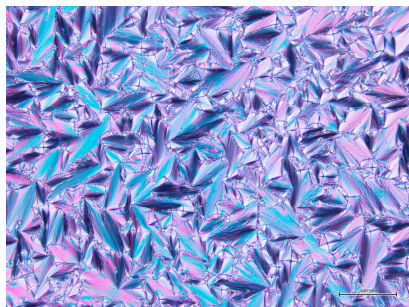
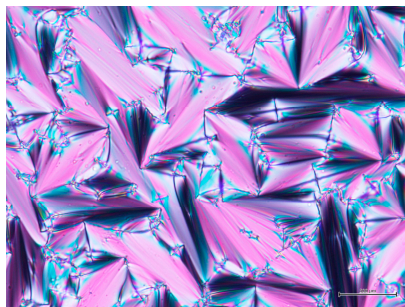
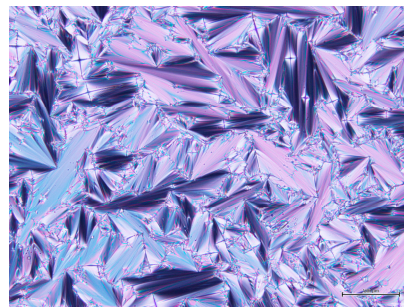


Figure S16. DSC Thermograms of **1a**, **1b**, **2a**, **2c**, and **2d** under N₂ atmosphere. Scan rate: 5.0 °C min⁻¹.

(a) **2a** at 84 °C(b) **2c** at 110 °C(c) **2d** at 130 °C**Figure S17.** Optical texture of (a) **2a**, (b) **2c**, and **2d** observed by POM.**Table S1.** Phase transition behavior of **1a**, **1b**, **2a**, **2c**, and **2d** observed by DSC measurement.

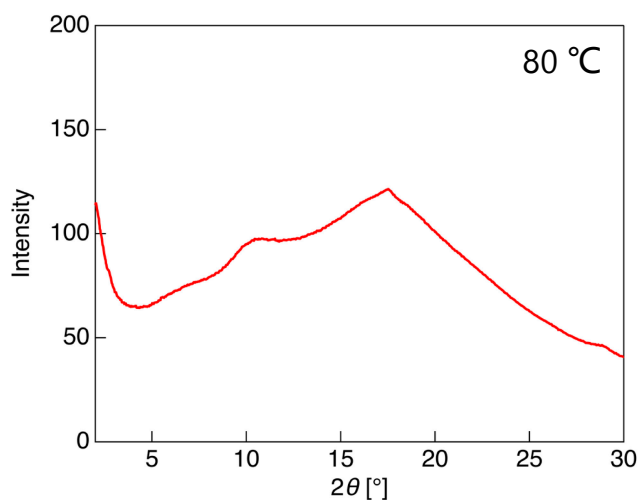
Molecule	Phase sequence		Temperature	Enthalpy (ΔH)	Entropy (ΔS)
			[°C]	[kJ mol ⁻¹]	[J mol ⁻¹ K ⁻¹]
1a	1 st Heating	Cry-Iso	108	29.6	77.6
	1 st Cooling	Iso-Cry	97	-27.7	-75.1
	2 nd Heating	Cry-Iso	109	28.6	75.0
	2 nd Cooling	Iso-Cry	96	-28.1	-76.2
	3 rd Heating	Cry-Iso	109	28.8	75.5
	3 rd Cooling	Iso-Cry	96	-28.2	-76.4
1b	1 st Heating	Cry ¹ -Cry ²	79	5.02	14.3
		Cry ² -Iso	113	22.1	57.2
	1 st Cooling	Iso-Cry	106	-20.7	-54.7
	2 nd Heating	Cry-Iso	113	21.6	55.9
	2 nd Cooling	Iso-Cry	106	-20.7	-54.6
	3 rd Heating	Cry-Iso	113	23.7	61.3
2a	3 rd Cooling	Iso-Cry	105	-20.8	-55.1
	1 st Heating	Cry-SmA	80	29.7	84.1
		SmA-Iso	94	6.74	18.4
	1 st Cooling	Iso-SmA	95	-6.69	-18.2
		SmA-Cry	61	-21.9	-65.5
	2 nd Heating	Cry ¹ -Cry ²	77	19.3	55.2
		Cry ² -SmA	80	22.4	63.3
		SmA-Iso	94	6.72	18.3
	2 nd Cooling	Iso-SmA	94	-6.71	-18.3
		SmA-Cry ¹	63	-21.4	-63.7
	3 rd Heating	Cry ¹ -Cry ²	76	6.61	19.0
		Cry ² -SmA	80	22.5	63.6
		SmA-Iso	94	6.76	18.4
	3 rd Cooling	Iso-SmA	94	-6.64	-18.1
		SmA-Cry ¹	64	-21.8	-64.6

Table S1 (continue). Phase transition behavior of **1a**, **1b**, **2a**, **2c**, and **2d** observed by DSC measurement.

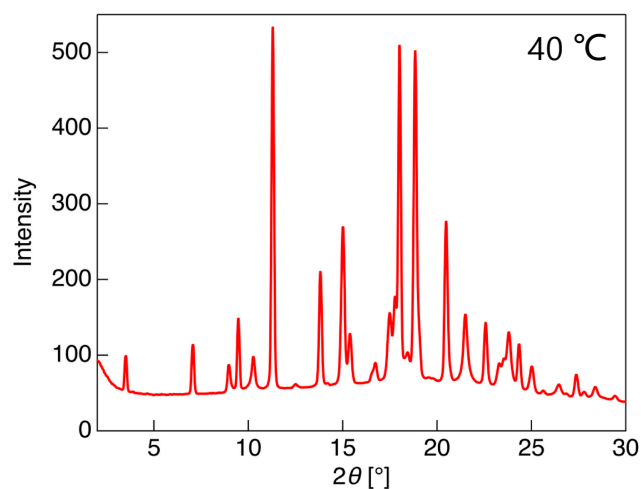
Molecule	Phase sequence		Temperature [°C]	Enthalpy (ΔH) [kJ mol ⁻¹]	Entropy (ΔS) [J mol ⁻¹ K ⁻¹]
2c	1 st Heating	Cry ¹ -Cry ²	81	6.43	18.2
		Cry ² -SmA	89	29.3	80.9
		SmA-Iso	117	8.31	21.3
	1 st Cooling	Iso-SmA	117	-8.29	-21.2
		SmA-Cry ¹	67	-27.6	-81.1
	2 nd Heating	Cry-SmA	89	29.8	82.3
		SmA-Iso	117	8.22	21.1
	2 nd Cooling	Iso-SmA	117	-8.3	-21.3
		SmA-Cry	67	-27.7	-81.3
	3 rd Heating	Cry-SmA	89	29.7	81.8
		SmA-Iso	117	8.57	21.9
	3 rd Cooling	Iso-SmA	117	-8.40	-21.5
		SmA-Cry	67	-27.5	-81.0
2d	1 st Heating	Cry-SmA	98	39.2	105.6
		SmA-Iso	135	10.6	26.0
	1 st Cooling	Iso-SmA	134	-10.2	-25.0
		SmA-Cry ²	82	-34.6	-97.7
		Cry ² -Cry ¹	35	-5.64	-18.3
	2 nd Heating	Cry ¹ -Cry ²	45	5.29	16.6
		Cry ² -SmA	101	38.0	101.6
		SmA-Iso	135	10.1	24.8
	2 nd Cooling	Iso-SmA	134	-10.1	-24.9
		SmA-Cry ²	84	-35.1	-98.1
		Cry ² -Cry ¹	39	-5.39	-17.3
	3 rd Heating	Cry ¹ -Cry ²	46	6.05	18.9
		Cry ² -SmA	101	38.1	101.7
		SmA-Iso	135	9.82	24.1
	3 rd Cooling	Iso-SmA	134	-10.2	-25.1
		SmA-Cry ²	82	-34.7	-97.6
		Cry ² -Cry ¹	38	-5.13	-16.5

Varied Temperature Powder X-ray Diffraction (VT-PXRD)

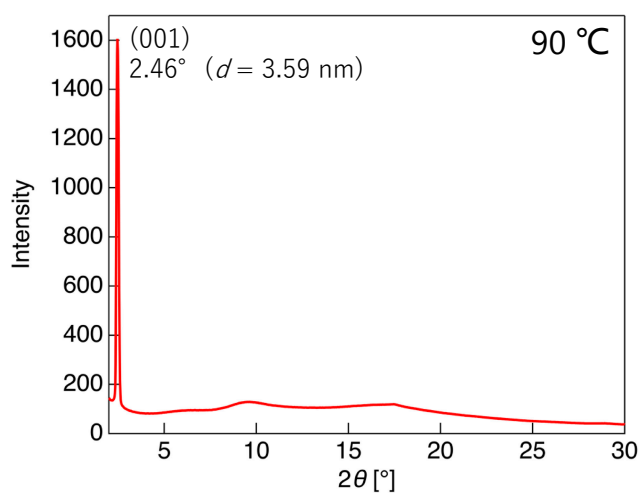
(a) **2a** in SmA phase at 80 °C



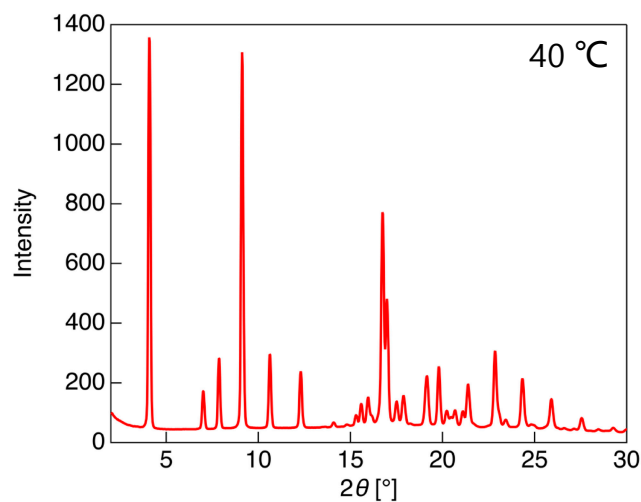
(b) **2a** in Cry phase at 40 °C



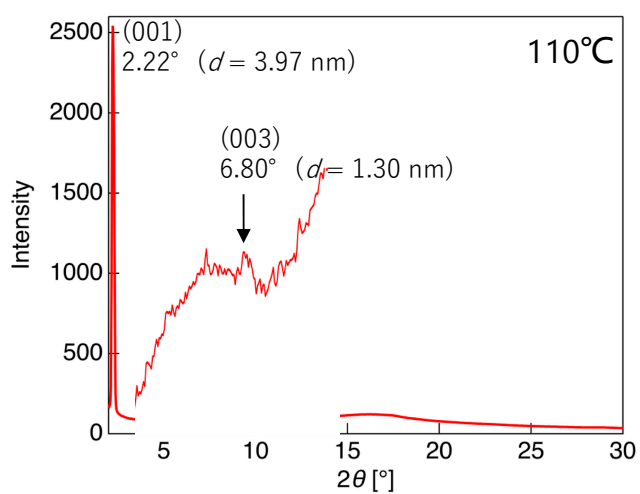
(c) **2c** in SmA phase at 90 °C



(d) **2c** in Cry phase at 40 °C



(e) **2d** in SmA phase at 110 °C



(f) **2d** in Cry phase at 40 °C

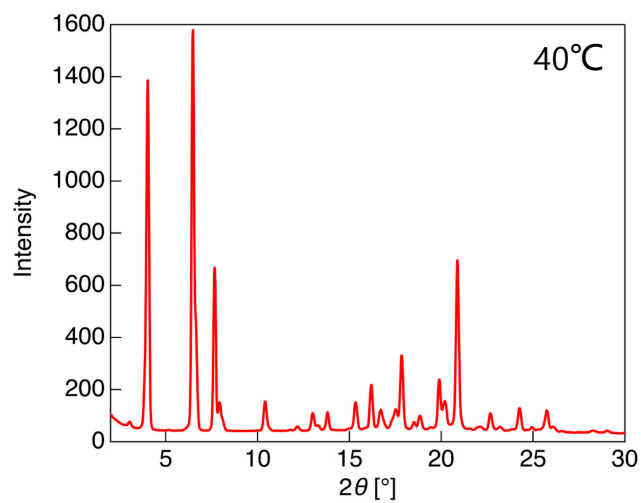
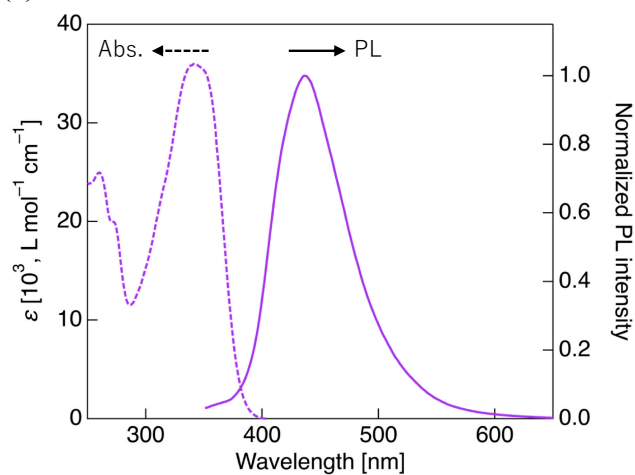


Figure S18. VT-PXRD patterns of (a) **2a** in SmA phase at 80 °C, (b) **2a** in Cry phase at 40 °C, (c) **2c** in SmA phase at 90 °C, (d) **2c** in Cry phase at 40 °C, (e) **2d** in SmA phase at 110 °C, and (f) **2d** in Cry phase at 40 °C.

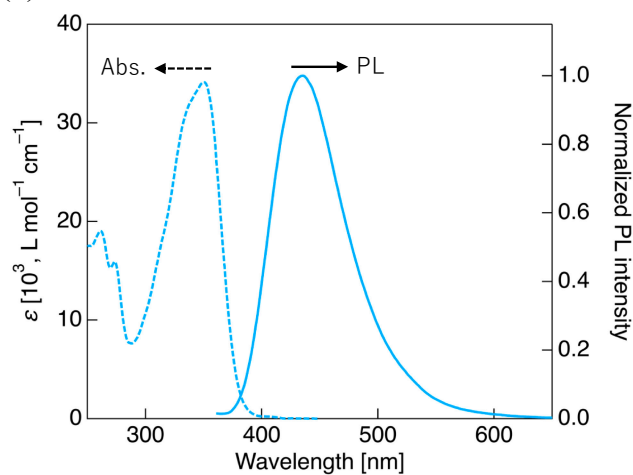
Photophysical behavior

CH₂Cl₂ solution phase

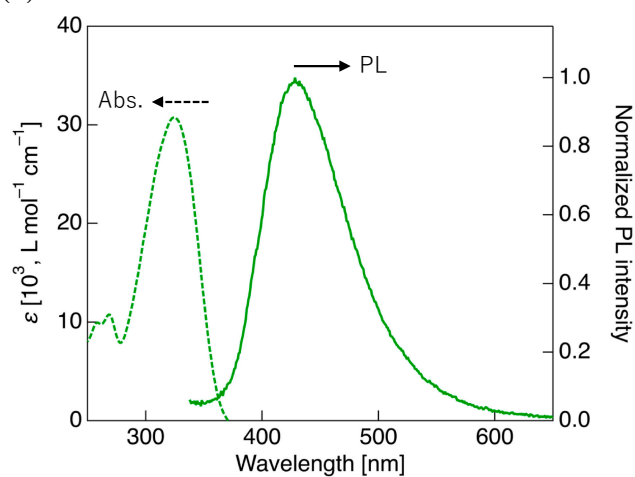
(a) **1a**



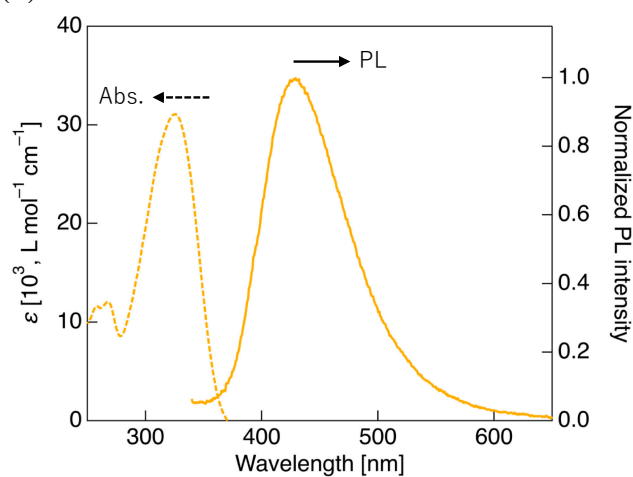
(b) **1b**



(c) **2a**



(d) **2c**



(e) **2d**

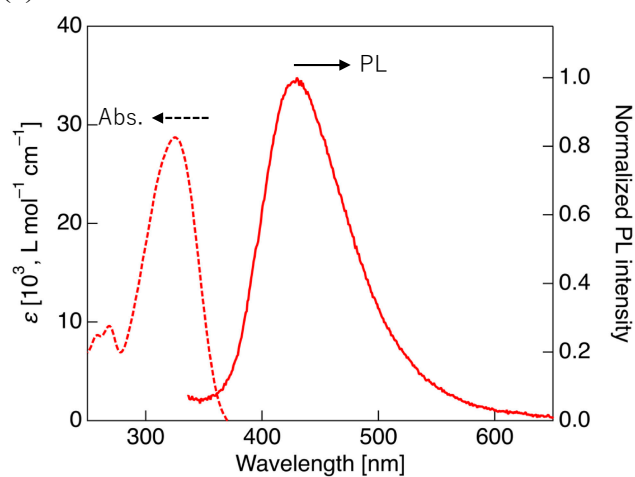
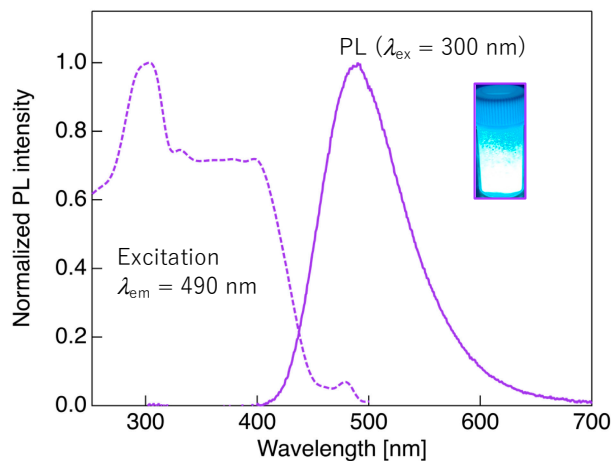


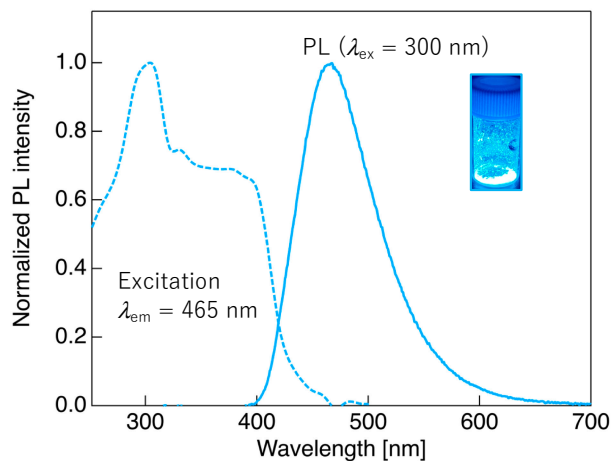
Figure S19. UV-vis absorption (1.0×10^{-5} mol L⁻¹) and PL spectrum (1.0×10^{-6} mol L⁻¹) of (a) **1a**, (b) **1b**, (c) **2a**, (d) **2c**, and (e) **2d** in CH₂Cl₂ solution. Excitation wavelength: λ_{abs} at the long-wavelength side.

Cry phase

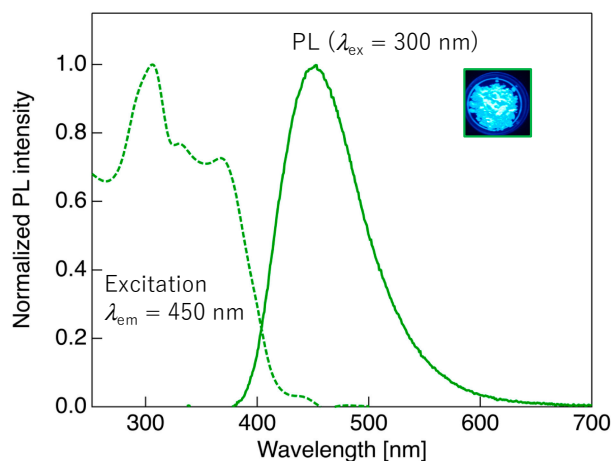
(a) **1a**



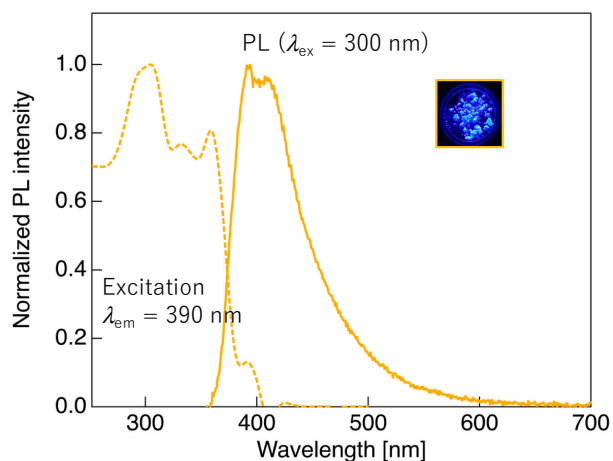
(b) **1b**



(c) **1c**



(d) **1d**



(e) **1e**

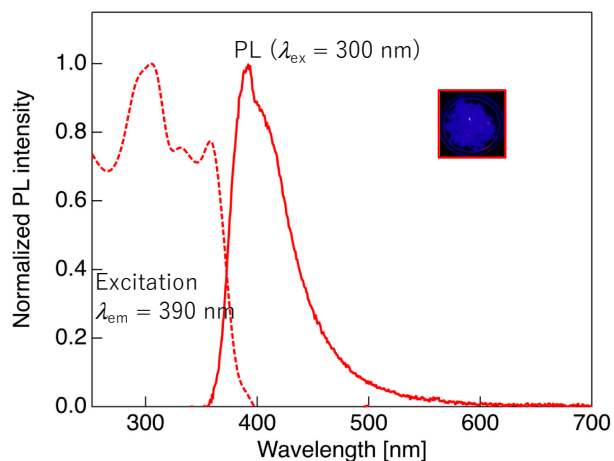
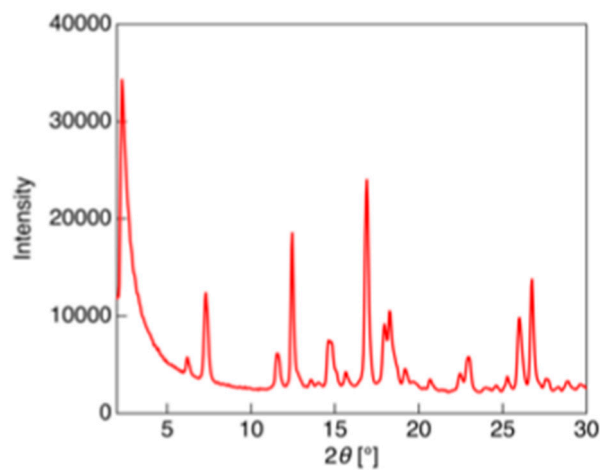


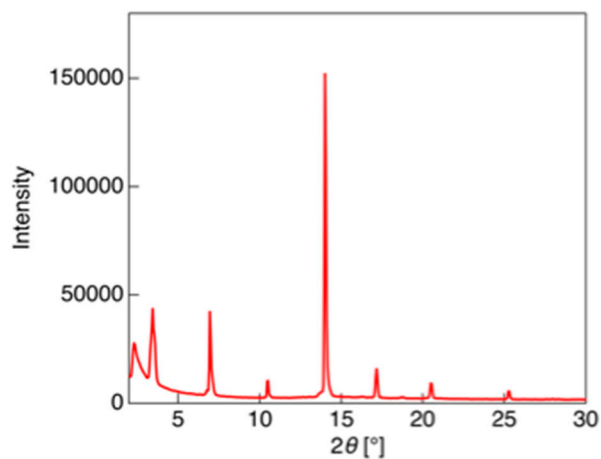
Figure S20. Excitation and PL spectra of (a) **1a**, (b) **1b**, (c) **2a**, (d) **2c**, and (e) **2d** in Cry phase. Measured using a PL quantum yield measurement system.

PXRD Measurement at 25 °C

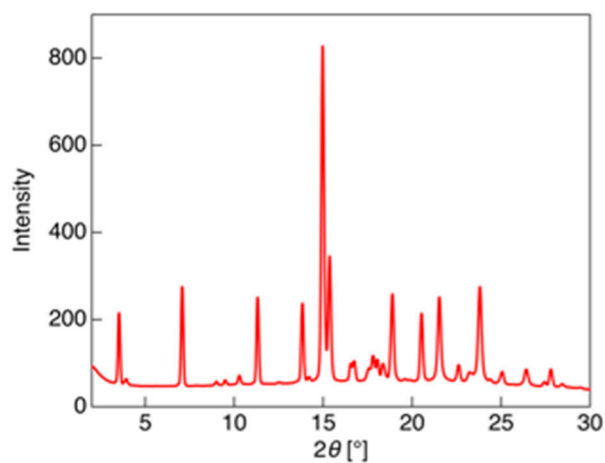
(a) 1a



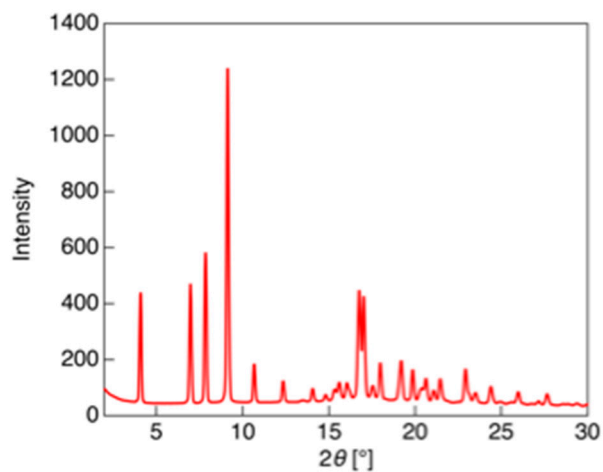
(b) 1b



(c) 2a



(d) 2c



(e) 2d

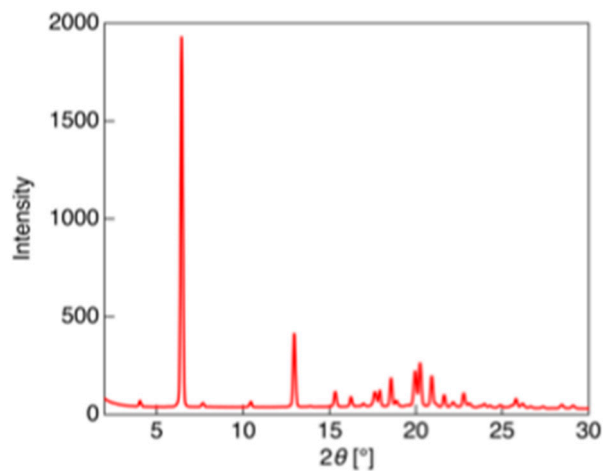


Figure S21. PXRD patterns of (a) **1a**, (b) **1b**, (c) **2a**, (d) **2c**, and (e) **2d** measured at 25 °C.

Varied-temperature PL behavior

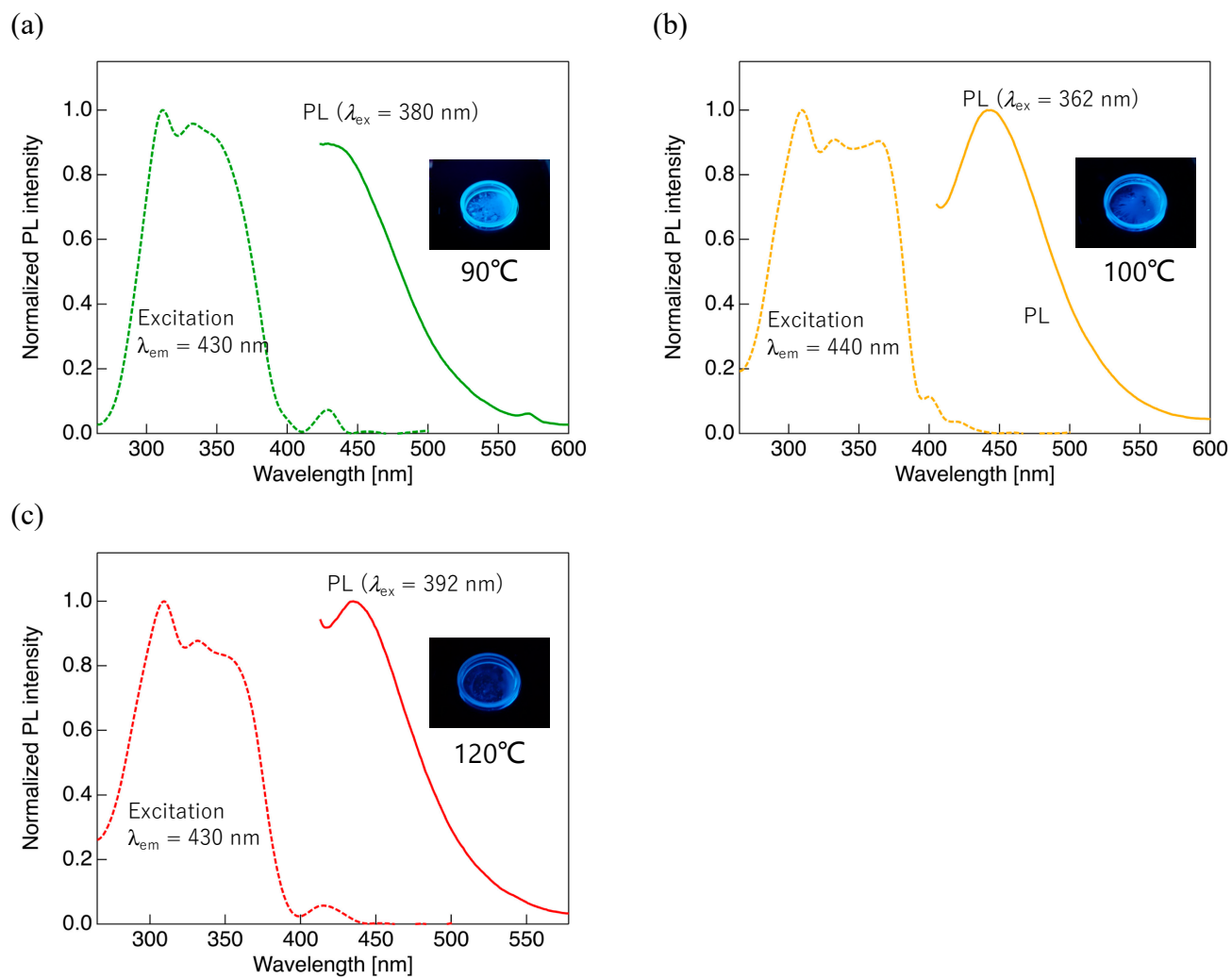
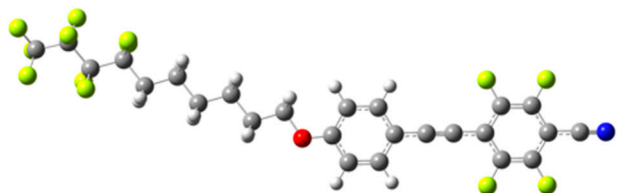


Figure S22. (a) Excitation and PL spectrum of (a) **2a** (90 °C), (b) **2c** (100 °C), and (c) **2d** (120 °C).

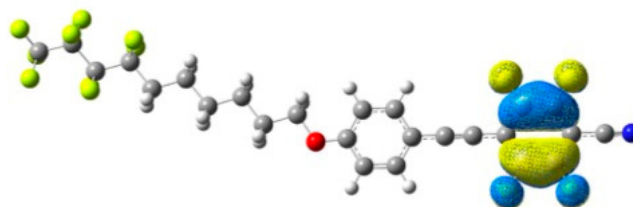
Quantum chemical calculation

Quantum chemical calculation was performed using the Gaussian 16 program set. The initial structure for quantum chemical calculations was optimized by the structural optimization calculation with the M06-2X functional and the 6-31+G(d,p) basis set. Theoretical vertical electronic transitions were determined by time-dependent self-consistent field (TD-SCF) approximation.

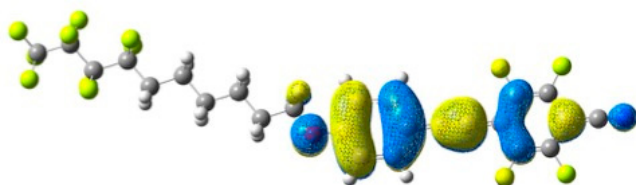
(a) Optimized structure



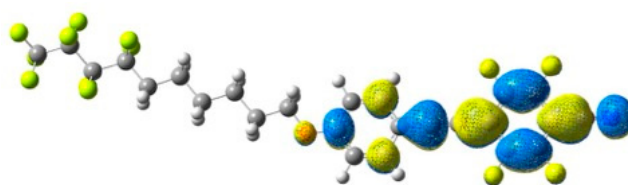
(b) HOMO-2 (-9.07 eV)



(c) HOMO (-7.50 eV)



(d) LUMO (-1.96 eV)



(e) Theoretical data

<Optimization>

SCF Done: E(RM062X) = -2389.37511332 Hartree A.U. after 15 cycles

Dipole moment (field-independent basis, Debye):

X= 6.6457 Y= -1.8662 Z= -0.0796 Tot= 6.9032

<TD-SCF>

Excited State 1: Singlet-A 3.6540 eV 339.31 nm f=1.6440 <S**2>=0.000

146 → 150 -0.11526

149(H) → 150(L) 0.68057

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -2389.24083271

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.6453 eV 266.91 nm f=0.0943 <S**2>=0.000

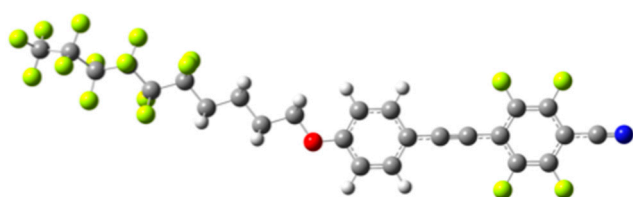
146 → 153 -0.14106

147(H-2) → 150(L) 0.65614

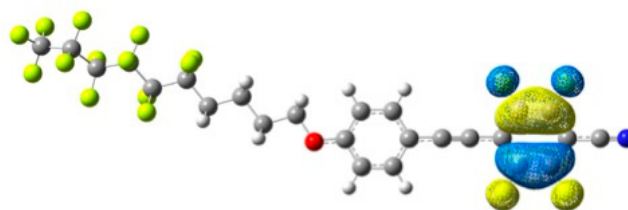
149 → 153 0.16648

Figure S23. (a) Optimized structure of **1a** and its orbital distributions for (b) HOMO-1, (c) HOMO, and (d) LUMO. (e) Theoretical data calculated by optimization and TD-SCF calculation.

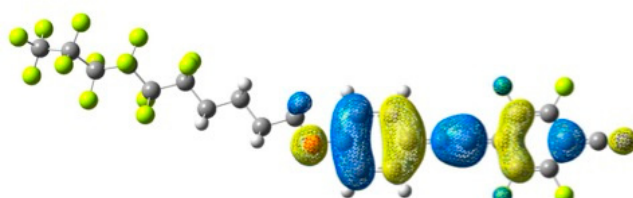
(a) Optimized structure



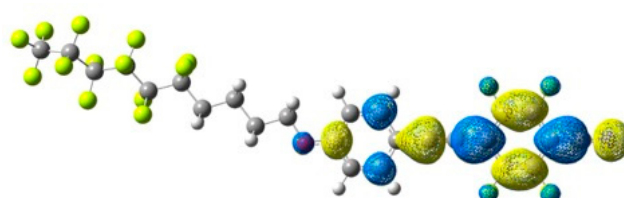
(b) HOMO-2 (-9.08 eV)



(c) HOMO (-7.52 eV)



(d) LUMO (-1.97 eV)



(e) Theoretical data

<Optimization>

SCF Done: E(RM062X) = -2786.21904838 Hartree A.U. after 15 cycles

Dipole moment (field-independent basis, Debye):

X= -6.5295 Y= -1.7437 Z= -0.1083 Tot= 6.7592

<TD-SCF>

Excited State	1:	Singlet-A	3.6639 eV	338.40 nm	f=1.6457	<S**2>=0.000
	162 → 166	-0.11461				
	165(H) → 166(L)	0.68073				

This state for optimization and/or second-order correction.

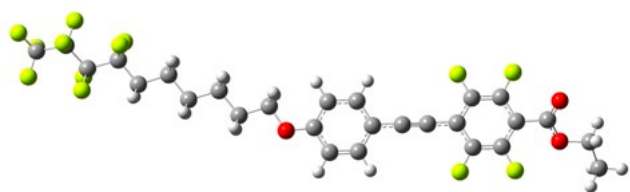
Total Energy, E(TD-HF/TD-DFT) = -2786.08440435

Copying the excited state density for this state as the 1-particle RhoCI density.

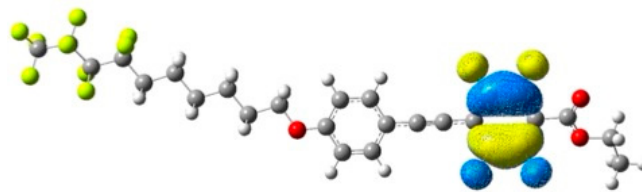
Excited State	2:	Singlet-A	4.6443 eV	266.96 nm	f=0.0948	<S**2>=0.000
	162 → 169	-0.14122				
	163(H-2) → 166(L)	0.65640				
	165 → 169	0.16723				

Figure S24. (a) Optimized structure of **1b** and its orbital distributions for (b) HOMO-1, (c) HOMO, and (d) LUMO. (e) Theoretical data calculated by optimization and TD-SCF calculation.

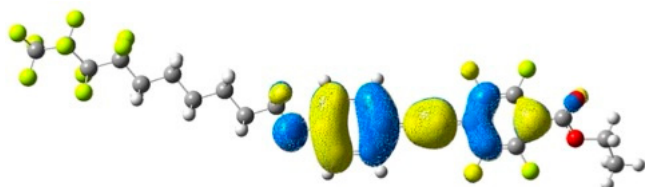
(a) Optimized structure



(b) HOMO-1 (-8.81 eV)



(c) HOMO (-7.43 eV)



(d) LUMO (-1.65 eV)



(e) Theoretical data

<Optimization>

SCF Done: E(RM062X) = -2564.26027788 Hartree A.U. after 15 cycles

Dipole moment (field-independent basis, Debye):

X= 0.7107 Y= -2.9916 Z= 1.5545 Tot= 3.4454

<TD-SCF>

Excited State	1:	Singlet-A	3.8346 eV	323.33 nm	f=1.6274	<S**2>=0.000
	159 → 163		0.11378			
	162(H) → 163(L)		0.67822			

This state for optimization and/or second-order correction.

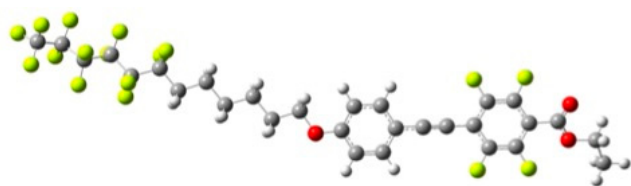
Total Energy, E(TD-HF/TD-DFT) = -2564.11935728

Copying the excited state density for this state as the 1-particle RhoCI density.

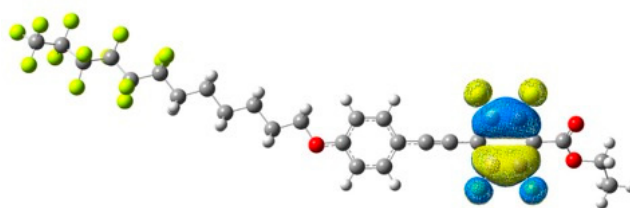
Excited State	2:	Singlet-A	4.6777 eV	265.05 nm	f=0.0842	<S**2>=0.000
	159 → 167		0.14092			
	161(H-1) → 163(L)		0.65489			
	162 → 167		0.16542			

Figure S25. (a) Optimized structure of **2a** and its orbital distributions for (b) HOMO-1, (c) HOMO, and (d) LUMO. (e) Theoretical data calculated by optimization and TD-SCF calculation.

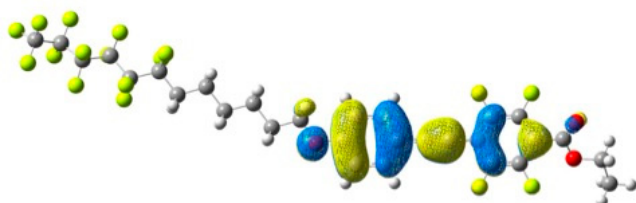
(a) Optimized structure



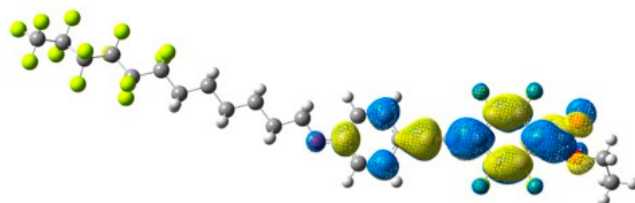
(b) HOMO-1 (-8.81 eV)



(c) HOMO (-7.43 eV)



(d) LUMO (-1.65 eV)



(e) Theoretical data

<Optimization>

SCF Done: E(RM062X) = -3039.69615877 Hartree A.U. after 15 cycles

Dipole moment (field-independent basis, Debye):

X= 0.6070 Y= -2.9027 Z= 1.3423 Tot= 3.2551

<TD-SCF>

Excited State	1:	Singlet-A	3.8349 eV	323.30 nm	f=1.6297	<S**2>=0.000
	183 → 187	0.11418				
	186(H) → 187(L)	0.67828				

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -3039.55522848

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State	2:	Singlet-A	4.6784 eV	265.02 nm	f=0.0842	<S**2>=0.000
	183 → 191	0.14100				
	185(H-1) → 187(L)	0.65477				
	186 → 191	0.16579				

Figure S26. (a) Optimized structure of **2c** and its orbital distributions for (b) HOMO-1, (c) HOMO, and (d) LUMO. (e) Theoretical data calculated by optimization and TD-SCF calculation.

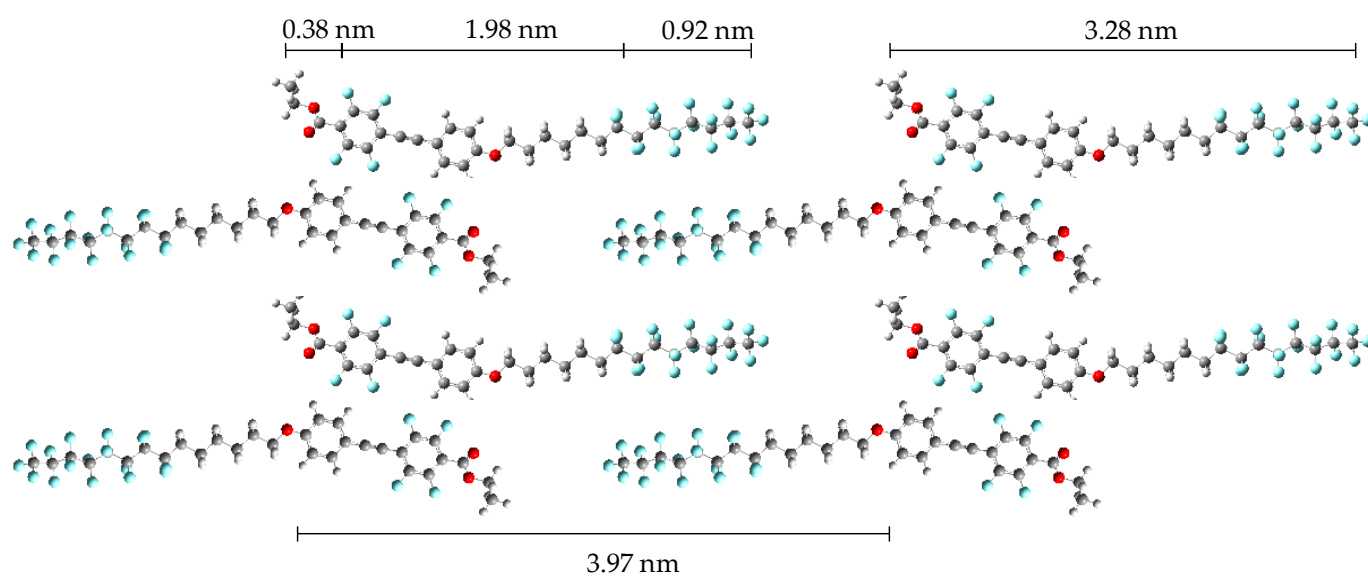


Figure S27. Possible aggregated structures of **2d** in the mesophase.

Table S2. Cartesian coordinate for **1a**.

No.	Atom Type		Coordinates (Angstroms)								
	No.		x	y	z						
1	6	0	-3.260098	-2.264895	-0.06752	28	1	0	2.368589	0.48243	-0.850616
2	6	0	-4.615129	-1.99364	-0.055201	29	6	0	3.837656	-0.882727	-0.062504
3	6	0	-5.073541	-0.662135	-0.023511	30	1	0	3.925744	-1.465041	-0.989154
4	6	0	-4.137842	0.380299	-0.003811	31	1	0	3.929588	-1.595718	0.767492
5	6	0	-2.77223	0.114458	-0.015274	32	6	0	4.977014	0.132327	0.011956
6	6	0	-2.329259	-1.213593	-0.04789	33	1	0	4.900445	0.701276	0.944993
7	1	0	-2.892411	-3.285081	-0.092173	34	1	0	4.885536	0.848082	-0.813011
8	1	0	-5.333005	-2.807056	-0.070208	35	6	0	6.34125	-0.556333	-0.059531
9	1	0	-4.483445	1.408574	0.020851	36	1	0	6.443052	-1.116508	-0.993521
10	1	0	-2.071649	0.939723	0.000775	37	1	0	6.463394	-1.261927	0.769475
11	6	0	-6.472447	-0.380959	-0.011893	38	6	0	7.475878	0.43591	0.01077
12	6	0	-7.662914	-0.147164	-0.00253	39	6	0	8.87659	-0.218512	0.013877
13	6	0	-9.055666	0.120643	0.008495	40	6	0	10.057678	0.756608	-0.226239
14	6	0	-9.546467	1.432534	0.003399	41	6	0	11.435136	0.187767	0.195548
15	6	0	-9.995001	-0.918388	0.02522	42	6	0	-13.237066	0.91798	0.041534
16	6	0	-10.90398	1.693819	0.014279	43	7	0	-14.373251	1.134654	0.049999
17	6	0	-11.353269	-0.661669	0.036305	44	9	0	12.395406	0.976218	-0.282222
18	6	0	-11.832449	0.650377	0.030934	45	9	0	11.542589	0.142337	1.520192
19	8	0	-1.028725	-1.579961	-0.063026	46	9	0	11.599275	-1.039259	-0.298124
20	6	0	-0.031596	-0.558939	-0.036581	47	9	0	9.864751	1.896868	0.460119
21	1	0	-0.156046	0.096673	-0.908382	48	9	0	10.123214	1.042853	-1.537725
22	1	0	-0.150037	0.043337	0.873845	49	9	0	9.05821	-0.831995	1.203755
23	6	0	1.324135	-1.236199	-0.061753	50	9	0	8.925255	-1.156077	-0.955348
24	1	0	1.401963	-1.841653	-0.972545	51	9	0	7.388718	1.194257	1.137345
25	1	0	1.394963	-1.92029	0.792101	52	9	0	7.445072	1.297155	-1.046964
26	6	0	2.462935	-0.219014	-0.01097	53	9	0	-12.211273	-1.677425	0.052264
27	1	0	2.382092	0.377071	0.907694	54	9	0	-9.578986	-2.183529	0.030744
						55	9	0	-8.69387	2.455627	-0.012369
						56	9	0	-11.327487	2.954292	0.008771

Table S3. Cartesian coordinate for **1b**.

No.	Atom	Type	Coordinates (Angstroms)								
	No.		x	y	z						
1	6	0	3.807288	-2.231143	0.057314	28	1	0	-1.829082	0.478661	0.914966
2	6	0	5.163832	-1.967287	0.04684	29	6	0	-3.261384	-0.859064	0.010688
3	6	0	5.629431	-0.63821	0.021122	30	1	0	-3.366948	-1.526446	0.870639
4	6	0	4.699723	0.409572	0.007346	31	1	0	-3.376109	-1.460664	-0.897428
5	6	0	3.332571	0.151216	0.017962	32	6	0	-4.397423	0.133776	0.056522
6	6	0	2.882992	-1.174431	0.042244	33	6	0	-5.794125	-0.517215	-0.074897
7	1	0	3.433802	-3.249315	0.076718	34	6	0	-6.982563	0.409486	0.297934
8	1	0	5.87721	-2.784685	0.058133	35	6	0	-8.337416	-0.084774	-0.279267
9	1	0	5.051028	1.435996	-0.012055	36	6	0	-9.563283	0.524373	0.4508
10	1	0	2.636577	0.980507	0.007127	37	6	0	-10.882438	0.412896	-0.35395
11	6	0	7.030045	-0.365103	0.008631	38	6	0	13.803814	0.884361	-0.052128
12	6	0	8.22192	-0.139006	-0.002504	39	7	0	14.94158	1.092478	-0.061921
13	6	0	9.616647	0.118655	-0.015366	40	9	0	-11.903326	0.707624	0.445587
14	6	0	10.117016	1.426665	-0.040744	41	9	0	-10.882733	1.259327	-1.378372
15	6	0	10.548236	-0.927352	-0.002892	42	9	0	-11.033434	-0.829567	-0.811127
16	6	0	11.476479	1.677666	-0.052887	43	9	0	-9.335418	1.827224	0.693744
17	6	0	11.90841	-0.680928	-0.015039	44	9	0	-9.738479	-0.118046	1.61549
18	6	0	12.397207	0.627339	-0.04009	45	9	0	-8.400799	0.248138	-1.580891
19	8	0	1.579743	-1.534388	0.052499	46	9	0	-8.40351	-1.423222	-0.16723
20	6	0	0.589311	-0.50885	0.035041	47	9	0	-6.754156	1.64847	-0.169467
21	1	0	0.708855	0.132738	0.917848	48	9	0	-7.086186	0.461474	1.639221
22	1	0	0.713422	0.106718	-0.865402	49	9	0	-5.955007	-0.928046	-1.351408
23	6	0	-0.766713	-1.187331	0.04047	50	9	0	-5.848866	-1.597563	0.730259
24	1	0	-0.842718	-1.822965	0.929939	51	9	0	-4.284956	1.04737	-0.9448
25	1	0	-0.840376	-1.839836	-0.837057	52	9	0	-4.394508	0.831004	1.22904
26	6	0	-1.899807	-0.162371	0.029092	53	9	0	12.758935	-1.702977	-0.00246
27	1	0	-1.807933	0.484338	-0.849884	54	9	0	10.122904	-2.189151	0.020904
						55	9	0	9.271919	2.45597	-0.053458
						56	9	0	11.909249	2.934756	-0.076536

Table S4. Cartesian coordinate for **2a**.

No.	Atom	Type	Coordinates (Angstroms)								
	No.		x	y	z						
1	6	0	-2.046539	-2.283436	-0.135594	32	6	0	6.186442	0.129566	-0.004332
2	6	0	-3.402365	-2.013825	-0.143562	33	1	0	6.085074	0.78798	0.865287
3	6	0	-3.863795	-0.683748	-0.110269	34	1	0	6.118681	0.760084	-0.898344
4	6	0	-2.929648	0.359038	-0.069871	35	6	0	7.550922	-0.56127	0.032144
5	6	0	-1.563158	0.095217	-0.062501	36	1	0	7.66306	-1.241861	-0.816894
6	6	0	-1.117579	-1.231562	-0.094923	37	1	0	7.662759	-1.149352	0.949636
7	1	0	-1.677443	-3.303164	-0.16041	38	6	0	8.68604	0.431341	-0.023
8	1	0	-4.11848	-2.828356	-0.175189	39	6	0	10.083823	-0.213397	0.12068
9	1	0	-3.27676	1.386816	-0.044373	40	6	0	11.272437	0.708177	-0.255394
10	1	0	-0.864354	0.921622	-0.03165	41	6	0	12.636352	0.226101	0.297596
11	6	0	-5.26437	-0.403836	-0.117553	42	9	0	-10.982291	-1.698353	-0.379732
12	6	0	-6.454478	-0.170004	-0.12325	43	9	0	-8.381774	-2.188138	-0.359864
13	6	0	-7.848841	0.101174	-0.130414	44	9	0	-7.491323	2.42505	0.094935
14	6	0	-8.342959	1.405051	-0.025687	45	9	0	-10.092396	2.936759	0.084159
15	6	0	-8.792903	-0.923968	-0.24327	46	6	0	-12.103906	0.964919	-0.172013
16	6	0	-9.70214	1.667882	-0.039584	47	8	0	-12.554744	1.944939	-0.718971
17	6	0	-10.152862	-0.662471	-0.243437	48	8	0	-12.824395	0.05991	0.477507
18	6	0	-10.641537	0.640821	-0.142978	49	6	0	-14.256089	0.270404	0.482924
19	8	0	0.184523	-1.596331	-0.089691	50	1	0	-14.457039	1.233978	0.957868
20	6	0	1.178547	-0.573146	-0.053946	51	1	0	-14.59765	0.31556	-0.554244
21	1	0	1.066357	0.076439	-0.932111	52	6	0	-14.873223	-0.882199	1.240704
22	1	0	1.045103	0.035421	0.850161	53	1	0	-14.502917	-0.912801	2.26803
23	6	0	2.536103	-1.247276	-0.052609	54	1	0	-15.958313	-0.757887	1.266898
24	1	0	2.620437	-1.877418	-0.945865	55	1	0	-14.644388	-1.832684	0.753203
25	1	0	2.603734	-1.907482	0.820185	56	9	0	12.80854	-1.069346	0.035694
26	6	0	3.672559	-0.226587	-0.02511	57	9	0	12.708342	0.418549	1.611487
27	1	0	3.570782	0.414549	0.860564	58	9	0	11.373816	0.759289	-1.594503
28	1	0	3.596515	0.431741	-0.900746	59	9	0	11.062489	1.950976	0.213829
29	6	0	5.048432	-0.889706	-0.011226	60	9	0	10.149824	-1.301564	-0.674449
30	1	0	5.147546	-1.541454	-0.889258	61	9	0	10.238225	-0.617096	1.400673
31	1	0	5.131505	-1.536567	0.872171	62	9	0	8.685657	1.11519	-1.203689
						63	9	0	8.572202	1.357962	0.96702
						64	9	0	13.612148	0.917069	-0.28743

Table S5. Cartesian coordinate for **2c**.

No.	Atom	Type	Coordinates (Angstroms)			No.	Atom	Type			
	No.		x	y	z						
1	6	0	-4.01683	-2.371867	-0.099891	35	6	0	5.607544	-0.774946	0.001415
2	6	0	-5.367898	-2.079217	-0.115029	36	1	0	5.721912	-1.355805	-0.920407
3	6	0	-5.806733	-0.741296	-0.09472	37	1	0	5.706022	-1.463847	0.845336
4	6	0	-4.855143	0.28574	-0.058214	38	6	0	6.750739	0.207541	0.073078
5	6	0	-3.493467	-0.00131	-0.042721	39	6	0	8.144693	-0.449128	-0.059421
6	6	0	-3.070276	-1.335631	-0.064219	40	6	0	9.336198	0.465255	0.334114
7	1	0	-3.665183	-3.39792	-0.115587	41	6	0	10.691651	-0.026663	-0.243367
8	1	0	-6.097637	-2.881694	-0.143099	42	9	0	-12.948074	-1.625373	-0.286722
9	1	0	-5.184649	1.319484	-0.042101	43	9	0	-10.358521	-2.168841	-0.243228
10	1	0	-2.781078	0.813465	-0.014395	44	9	0	-9.3685	2.442626	-0.055587
11	6	0	-7.202146	-0.437188	-0.112056	45	9	0	-11.957895	3.008549	-0.09233
12	6	0	-8.38769	-0.181596	-0.127515	46	6	0	-14.012115	1.069224	-0.227183
13	6	0	-9.776134	0.117775	-0.146626	47	8	0	-14.444965	2.024593	-0.829478
14	6	0	-10.241979	1.435796	-0.11582	48	8	0	-14.747942	0.220309	0.478434
15	6	0	-10.742265	-0.891524	-0.199209	49	6	0	-16.174813	0.461364	0.478164
16	6	0	-11.595281	1.726508	-0.142695	50	1	0	-16.35261	1.454909	0.897409
17	6	0	-12.09637	-0.601317	-0.211945	51	1	0	-16.521513	0.453543	-0.558253
18	6	0	-12.556774	0.715757	-0.185107	52	6	0	-16.811411	-0.631969	1.304565
19	8	0	-1.774254	-1.721601	-0.053164	53	1	0	-16.435221	-0.611121	2.329999
20	6	0	-0.764697	-0.713591	-0.021836	54	1	0	-17.893437	-0.48307	1.329174
21	1	0	-0.869895	-0.063295	-0.900287	55	1	0	-16.605896	-1.613754	0.871747
22	1	0	-0.886331	-0.102135	0.882046	56	6	0	11.916731	0.566583	0.501212
23	6	0	0.583314	-1.406581	-0.025229	57	6	0	13.238548	0.462414	-0.30018
24	1	0	0.659035	-2.031573	-0.922897	58	9	0	13.24708	1.326456	-1.309736
25	1	0	0.642623	-2.073469	0.843025	59	9	0	13.385156	-0.772656	-0.778395
26	6	0	1.732467	-0.400346	0.009033	60	9	0	14.257912	0.737957	0.508199
27	1	0	1.647002	0.22515	0.907544	61	9	0	11.693206	1.866408	0.763668
28	1	0	1.655472	0.275279	-0.853232	62	9	0	10.763262	0.324365	-1.539871
29	6	0	3.100937	-1.078631	-0.004365	63	9	0	10.751534	-1.366853	-0.150032
30	1	0	3.189483	-1.701234	-0.904498	64	9	0	9.11756	1.712968	-0.11446
31	1	0	3.180671	-1.755801	0.856217	65	9	0	9.433434	0.495363	1.676675
32	6	0	4.249278	-0.071604	0.031728	66	9	0	8.311664	-0.842415	-1.340834
33	1	0	4.173198	0.53907	0.938735	67	9	0	8.189605	-1.541613	0.730043
34	1	0	4.168622	0.607426	-0.824082	68	9	0	6.652941	1.139603	-0.913176
						69	9	0	6.745498	0.884889	1.257657
						70	9	0	12.08483	-0.09447	1.656519