

Supporting Information

Amplified spontaneous emission from oligo(*p*-phenylenevinylene) derivatives

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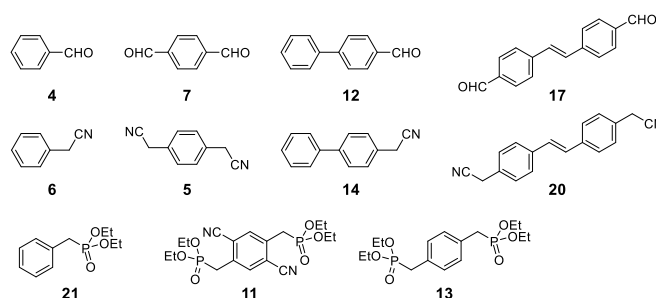
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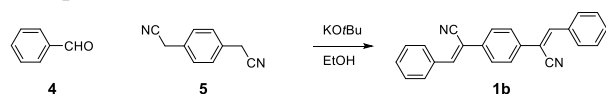
Methods S1. Synthesis

Benzaldehyde (**4**), *p*-xylylene dicyanide (**5**), phenylacetonitrile (**6**), terephthalaldehyde (**7**), *p*-phenylbenzaldehyde (**12**), tetraethyl *p*-xylylenediphosphonate (**13**), 4-biphenylacetonitrile (**14**), diethyl benzylphosphonate (**21**) were purchased. 1,4-Bis(diethylphosphorylmethyl)-2,5-dicyanobenze (**11**, CAS: 314270-67-2)^[S1,S2] and 4,4'-stilbenedicarboxaldehyde (**17**, CAS: 4720-99-4)^[S3] were synthesized according to the literature, and 4,4'-trans-stilbene-bis(acetonitrile) (**20**, CAS: 1000515-15-0) was prepared by modifying the literature.^[S4,S5]

Building blocks

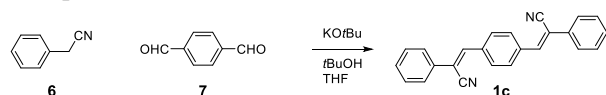


Compound **1b**^[S6,S7]



To a solution of benzaldehyde **4** (3.40 g, 32.0 mmol) and *p*-xylylene dicyanide **5** (2.35 g, 15.1 mmol) in ethanol (100 ml) under argon, a solution of potassium *tert*-butoxide (0.86 g, 7.67 mmol) in ethanol (20 ml) was added dropwise over a period of 10 min. The reaction mixture was refluxed for 2 h, and filtered at rt, washed with ethanol to give a colorless solid. The crude product was purified by vacuum sublimation at 250 °C. Pale yellow crystals. 3.87 g (77.2%). ¹H NMR (500 MHz, CDCl₃, 300 K, δ): 7.92 (d, *J* = 6.8 Hz, 4H), 7.770 (s, 4H), 7.62 (s, 2H), 7.51–7.46 (m, 6H); ¹³C NMR (125 MHz, CDCl₃, δ): 142.98, 135.39, 133.66, 131.06, 129.60, 129.21, 126.76, 117.80, 110.90. Anal. calcd for C₂₄H₁₆N₂: C 86.72, H 4.85, N 8.43; found: C 86.61, H 4.82, N 8.49.

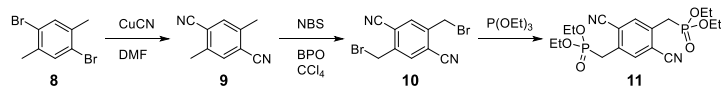
Compound **1c**^[S6,S8]



To a solution of phenylacetonitrile **6** (0.76 g, 6.49 mmol) and terephthalaldehyde **7** (0.40 g, 3.00 mmol) in ethanol (50 ml) under argon, a solution of potassium *tert*-butoxide (0.19 g, 1.68 mmol) in ethanol (20 ml) was added dropwise over a period of 10 min. The reaction mixture was refluxed for 2 h, and filtered at rt, washed with ethanol to give a colorless solid. The crude product was purified by vacuum sublimation at 240 °C. Pale yellow crystals. 0.62 g (62.5%). ¹H NMR (500 MHz, CDCl₃, 300 K, δ): 8.01 (s, 4H), 7.71 (d, *J* = 7.6 Hz, 4H), 7.56 (s, 2H), 7.48 (dd, *J* = 7.3 Hz, 4H),

7.71 (t, $J = 7.3$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3 , δ): 140.80, 135.65, 134.40, 129.92, 129.74, 129.32, 126.30, 117.89, 113.25. Anal. calcd for $\text{C}_{24}\text{H}_{16}\text{N}_2$: C 86.72, H 4.85, N 8.43; found: C 86.62, H 4.89, N 8.43.

Compound **11**^[S1,S2]

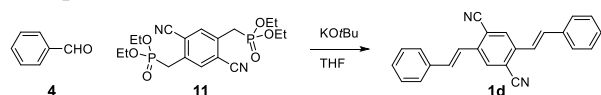


2,5-Dibromo-*p*-xylene **8** (5.34 g, 20.2 mmol) was dissolved in DMF (100 ml) under argon, followed by addition of copper cyanide (6.99 g, 78.0 mmol). The suspension solution was heated to 150 °C and stirred for 48 h. After cooling, the mixture was poured onto ice-cold NH_4OH aq. and filtered. The residue was extracted with DCM, dried over Na_2SO_4 and concentrated to dryness. The crude product was purified by column chromatography on a silica gel using DCM to give product **9** (1.57 g, 49.6%). ^1H NMR (500 MHz, CDCl_3 , 300 K, δ): 7.56 (s, 2H), 2.55 (s, 6H).

A solution of **9** (1.57 g, 10.0 mmol) and NBS (3.65 g, 20.5 mmol) in carbon tetrachloride (100 ml) was degassed and purged with argon. BPO (0.14 g, 0.58 mmol) was added and the mixture was refluxed for 72 h. The solution was evaporated, and the residue was purified by column chromatography on a silica gel using hexane/DCM (1:1) mixture ($R_f = 0.32$) to give a colorless crystal of **10** (1.26 g, 39.9%). ^1H NMR (500 MHz, CDCl_3 , 300 K, δ): 7.86 (s, 2H), 4.61 (s, 4H).

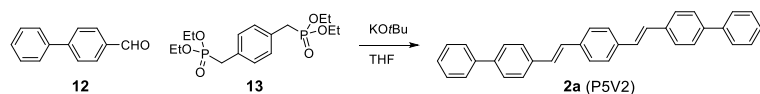
A mixture of **10** (1.26 g, 4.00 mmol) and triethyl phosphite (2.26 g, 13.6 mmol) was heated to 160 °C for 18 h. Then the excess of triethyl phosphite was removed using rotary evaporation and the residue was crystallized from hexane/EtOAc to give a colorless solid of **11** (1.11 g, 64.9%). ^1H NMR (500 MHz, CDCl_3 , 300 K, δ): 7.80 (s, 2H), 4.12 (m, 8H), 3.38 (d, $J = 21$ Hz, 4H), 1.29 (t, $J = 7.1$ Hz, 12H).

Compound **1d**



To a solution of benzaldehyde **4** (0.336 g, 3.17 mmol) and compound **11** (0.563 g, 1.32 mmol) in THF (30 ml) under argon at 0 °C, a solution of potassium *tert*-butoxide (0.316 g, 2.82 mmol) in THF (30 ml) was added dropwise over a period of 10 min. The reaction mixture was stirred at 0 °C for 1h and at rt for 18 h. The reaction was quenched with water and THF was evaporated. The crude solid was collected by filtration and washed with ethanol to give a yellow solid. The product was purified by vacuum sublimation at 240 °C. Yellow crystals. 0.37 g (83.6%). ^1H NMR (500 MHz, CDCl_3 , 300 K, δ): 8.06 (s, 2H), 7.60 (d, $J = 8.0$ Hz, 4H), 7.43–7.31 (m, 10H); ^{13}C NMR (125 MHz, CDCl_3 , δ): 139.1, 135.6, 135.4, 129.9, 129.7, 129.2, 127.5, 121.9, 116.7, 115.3. Anal. calcd for $\text{C}_{24}\text{H}_{16}\text{N}_2$: C 86.72, H 4.85, N 8.43; found: C 86.81, H 4.91, N 8.41.

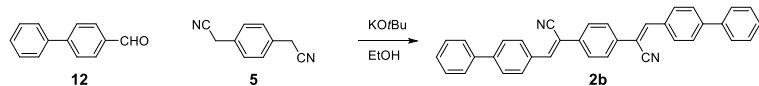
Compound **2a**



To a solution of *p*-phenylbenzaldehyde **12** (1.94 g, 10.7 mmol) and *p*-xylylenediphosphonate **13** (1.90 g, 5.01 mmol) in THF (80 ml) under argon at 0 °C, a solution of potassium *tert*-butoxide (1.22 g, 10.9 mmol) in THF (30 ml) was

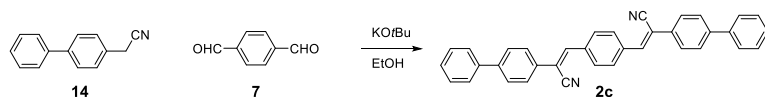
added dropwise over a period of 10 min. The reaction mixture was stirred at 0 °C for 1h and at rt for 18 h. The precipitate was filtered, washed with THF, water, methanol to give a pale yellow solid. The crude product was purified by vacuum sublimation at 300 °C. Pale yellow crystals. 1.89 g (78.0%). ¹H-NMR and ¹³C-NMR could not be recorded because of its poor solubility. Anal. calcd for C₃₄H₂₆: C 93.97, H 6.03; found: C 93.94, H 5.99.

Compound 2b



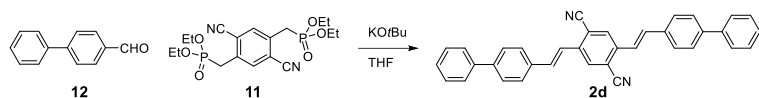
To a solution of *p*-phenylbenzaldehyde **12** (1.56 g, 8.56 mmol) and *p*-xylylene dicyanide **5** (0.640 g, 4.10 mmol) in ethanol (70 ml) under argon, a solution of potassium *tert*-butoxide (0.248 g, 2.21 mmol) in ethanol (30 ml) was added dropwise over a period of 10 min. The reaction mixture was refluxed for 6 h, and filtered at rt, washed with ethanol to give a colorless solid. The crude product was purified by vacuum sublimation at 330 °C. Pale yellow crystals. 1.60 g (80.8%). ¹H-NMR and ¹³C-NMR could not be recorded because of its poor solubility. Anal. calcd for C₃₆H₂₄N₂: C 89.23, H 4.99, N 5.78; found: C 89.24, H 5.02, N 5.73.

Compound 2c



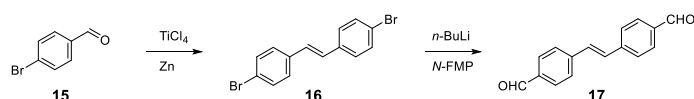
To a solution of 4-biphenylacetonitrile **14** (1.23 g, 6.39 mmol) and terephthalaldehyde **7** (0.373 g, 2.78 mmol) in ethanol (50 ml) under argon, a solution of potassium *tert*-butoxide (0.194 g, 1.73 mmol) in ethanol (20 ml) was added dropwise over a period of 10 min. The reaction mixture was refluxed for 3 h, and filtered at rt, washed with ethanol to give a colorless solid. The crude product was purified by vacuum sublimation at 320 °C. Pale yellow crystals. 1.19 g (88.6%). ¹H-NMR and ¹³C-NMR could not be recorded because of its poor solubility. Anal. calcd for C₃₆H₂₄N₂: C 89.23, H 4.99, N 5.78; found: C 89.26, H 5.02, N 5.73.

Compound 2d



To a solution of *p*-phenylbenzaldehyde **12** (0.410 g, 2.25 mmol) and compound **11** (0.444 g, 1.04 mmol) in THF (80 ml) under argon at 0 °C, a solution of potassium *tert*-butoxide (0.278 g, 2.48 mmol) in THF (30 ml) was added dropwise over a period of 10 min. The reaction mixture was stirred at 0 °C for 1h and at rt for 18 h. The reaction was quenched with water and THF was evaporated. The crude solid was collected by filtration and washed with ethanol to give a yellow solid. The product was purified by vacuum sublimation at 320 °C. Yellow crystals. 0.43 g (85.1%). ¹H-NMR and ¹³C-NMR could not be recorded because of its poor solubility. Anal. calcd for C₃₆H₂₄N₂: C 89.23, H 4.99, N 5.78; found: C 89.26, H 5.02, N 5.81.

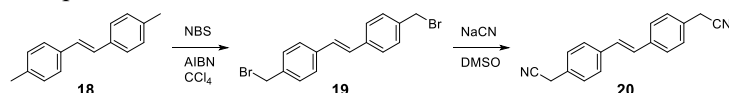
Compound 17^[S3]



To a three-neck flask equipped with dropping funnel, Zn powder (20.1 g, 307 mmol) and dry THF (250 ml) were added. The suspension was cooled to -10°C and titanium chloride (16.6 ml, 151 mmol) was added slowly within 1 h under vigorous stirring. Subsequently a solution of 4-bromobenzaldehyde **15** (10.1 g, 54.6 mmol) in dry THF (150 ml) was added dropwise. After complete addition, the reaction mixture was refluxed for 5 h. The flask was cooled to rt overnight. Saturated NaHCO_3 solution was added and THF was removed. The crude product was filtered and washed with EtOAc. The organic phase was collected, dried over Na_2SO_4 and concentrated to dryness. The residue was recrystallized by DCM/MeOH, then purified by vacuum sublimation at 190°C to give a colorless solid of **16** (7.27 g, 78.7%). $^1\text{H NMR}$ (500 MHz, CDCl_3 , 300 K, δ): 7.48 (d, $J = 8.5$ Hz, 4H), 7.36 (d, $J = 8.5$ Hz, 4H), 7.02 (s, 2H).

Compound **16** (0.667 g, 1.97 mmol) was dissolved in dry THF (50 ml). The solution was cooled to -78°C and n -butyllithium (1.6 M in hexane, 2.6 ml, 4.2 mmol) was added. The reaction mixture was stirred at -78°C for 30 min and then at rt for 30 min. The temperature was lowered again to -78°C and N -formylmorpholine (0.609 g, 5.29 mmol) was added slowly. The reaction mixture was stirred at -78°C for 1 h and rt overnight. The solvent was removed in vacuo and the residue was extracted with DCM with 5% HCl, dried over Na_2SO_4 and concentrated to dryness. The product was purified by column chromatography on a silica gel using DCM ($R_f = 0.46$) to give a colorless solid of **17** (0.38 g, 81.4%). $^1\text{H NMR}$ (500 MHz, CDCl_3 , 300 K, δ): 10.0 (s, 2H), 7.91 (d, $J = 8.3$ Hz, 4H), 7.70 (d, $J = 8.3$ Hz, 4H), 7.30 (s, 2H).

Compound 20^[S4,S5]

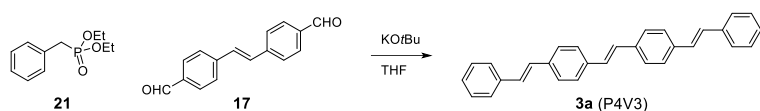


A solution of 4,4'-dimethyl-*trans*-stilbene **18** (2.50 g, 12.0 mmol) and NBS (4.28 g, 24.0 mmol) in carbon tetrachloride (100 ml) was degassed and purged with nitrogen. AIBN (0.083 g, 0.50 mmol) was added and the mixture was refluxed for 24 h. The solution was evaporated, and the residue was purified by column chromatography on a silica gel using hexane/DCM (1:1) mixture ($R_f = 0.61$) to give a colorless crystal of **19** (2.49 g, 56.8%). $^1\text{H NMR}$ (500 MHz, CDCl_3 , 300 K, δ): 7.49 (d, $J = 8.3$ Hz, 4H), 7.39 (d, $J = 8.3$ Hz, 4H), 7.10 (s, 2H), 4.52 (s, 4H).

Compound **19** (2.56 g, 7.00 mmol) was added in small portions to a suspension of sodium cyanide (0.72 g, 14.7 mmol) in DMSO, and the mixture was heated to 40°C . Water was added and the mixture was filtered. The residue was purified by column chromatography on a silica gel using DCM ($R_f = 0.48$) to give a colorless solid of **20** (0.33 g, 18.3%). $^1\text{H NMR}$ (500 MHz, CDCl_3 , 300 K, δ): 7.53 (d, $J = 8.3$ Hz, 4H), 7.33 (d, $J = 8.3$ Hz, 4H), 7.10 (s, 2H), 3.77 (s, 4H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3 , δ): 137.1, 129.4, 128.6, 128.5, 127.4, 117.8, 23.6.

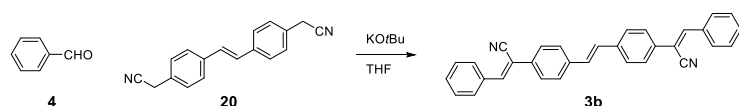
Anal. calcd for $\text{C}_{18}\text{H}_{14}\text{N}_2$: C 83.69, H 5.46, N 10.84; found: C 83.46, H 5.49, N 10.73.

Compound **3a**^[S9]



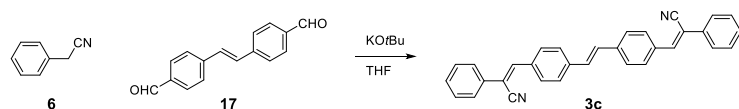
To a solution of diethyl benzylphosphonate **21** (1.49 g, 6.52 mmol) and compound **17** (0.536 g, 2.27 mmol) in THF (50 ml) under argon at 0 °C, a solution of potassium *tert*-butoxide (0.593 g, 5.29 mmol) in THF (30 ml) was added dropwise over a period of 10 min. The reaction mixture was stirred overnight. THF was reduced and the mixture was filtered, washed with methanol, water and ether to give a yellow solid. The crude product was purified by vacuum sublimation at 270 °C. Yellow crystals. 0.44 g (50.4%). ¹H-NMR and ¹³C-NMR could not be recorded because of its poor solubility. Anal. calcd for C₃₀H₂₄: C 93.71, H 6.29; found: C 93.70, H 6.30.

Compound **3b**



To a solution of benzaldehyde **4** (0.357 g, 3.36 mmol) and compound **20** (0.330 g, 1.27 mmol) in THF (80 ml) under argon, a solution of potassium *tert*-butoxide (0.081 g, 0.725 mmol) in THF (20 ml) was added dropwise over a period of 10 min. The reaction mixture was refluxed overnight. After cooling, THF was evaporated and ethanol was added to the solid. The mixture was filtered, washed with ethanol to give a yellow solid. The crude product was purified by vacuum sublimation at 290 °C. Yellow crystals. 0.19 g (34.2%). ¹H NMR (500 MHz, CDCl₃, 300 K, δ): 7.91 (d, J = 7.1 Hz, 4H), 7.71 (d, J = 8.5 Hz, 4H), 7.62 (d, J = 8.5 Hz, 4H), 7.59 (s, 2H), 7.51–7.44 (m, 6H), 7.20 (s, 2H); ¹³C NMR (125 MHz, CDCl₃, δ): 141.88, 138.11, 133.98, 133.89, 130.76, 129.48, 129.16, 128.96, 127.38, 126.50, 118.04, 111.45. Anal. calcd for C₃₂H₂₂N₂: C 88.45, H 5.10, N 6.45; found: C 88.38, H 5.08, N 6.50.

Compound **3c**



To a solution of phenylacetonitrile **6** (0.703 g, 6.00 mmol) and compound **17** (0.626 g, 2.65 mmol) in THF (100 ml) under argon, a solution of potassium *tert*-butoxide (0.151 g, 1.35 mmol) in THF (50 ml) was added dropwise over a period of 10 min. The reaction mixture was refluxed overnight. After cooling, THF was evaporated and ethanol was added to the solid. The mixture was filtered, washed with ethanol to give a yellow solid. The crude product was purified by vacuum sublimation at 290 °C. Orange crystals. 0.64 g (55.9%). ¹H NMR (500 MHz, CDCl₃, 300 K, δ): 7.94 (d, J = 8.3 Hz, 4H), 7.70 (d, J = 7.3 Hz, 4H), 7.64 (d, J = 8.3 Hz, 4H), 7.54 (s, 2H), 7.47 (dd, J = 7.3 Hz, 4H), 7.41 (t, J = 7.3 Hz, 2H), 7.24 (s, 2H); ¹³C NMR (125 MHz, CDCl₃, δ): 141.62, 139.27, 134.71, 133.48, 130.00, 129.66, 129.37, 129.25, 127.34, 126.15, 118.30, 111.38. Anal. calcd for C₃₂H₂₂N₂: C 88.45, H 5.10, N 6.45; found: C 88.50, H 5.15, N 6.40.

Methods S2. Theoretical calculations

The computations were performed using the computer facilities at the Research Institute for Information Technology, Kyushu University. Molecular orbital calculations were performed using the program Gaussian 16.^{S10} The geometries were optimized at the B3LYP/6-31G(d,p) level. The presence of energy minima was confirmed by the absence of imaginary modes (no imaginary frequencies). The time-dependent density functional theory (TD-DFT) calculations were conducted at the B3LYP/6-31G(d,p) level. To numerically achieve accurate values, we used a fine grid.

Table S1. Calculated energies. Ground state energies, HOMO-LUMO energies, vertical excitation energies (VEE) for singlet and triplet excited states, wavelength, and oscillator strength (f) at the B3LYP/6-31G(d,p)

	S₀ (hartrees)	HOMO (eV)	LUMO (eV)	States	VEE (eV)	Wavelength (nm)	f(-)
1a	-849.200748946	-5.179	-1.793	T ₁	1.8704	662.89	0
				S ₁	3.2074	386.55	1.8319
1b	-1033.67638569	-5.931	-2.473	T ₁	1.9765	627.29	0
				S ₁	3.1983	387.66	1.3509
1c	-1033.67676451	-5.946	-2.749	T ₁	1.7573	705.53	0
				S ₁	3.0076	412.24	1.5085
1d	-1033.68109303	-5.796	-2.602	T ₁	1.7788	696.99	0
				S ₁	3.0026	412.92	1.3172
2a	-1311.32939368	-5.093	-1.904	T ₁	1.7999	688.84	0
				S ₁	2.9372	422.12	2.6249
2b	-1495.80540090	-5.714	-2.506	T ₁	1.8768	660.63	0
				S ₁	2.9057	426.69	2.0602
2c	-1495.80517131	-5.750	-2.760	T ₁	1.6897	733.78	0
				S ₁	2.7334	453.60	1.9472
2d	-1495.80986380	-5.600	-2.616	T ₁	1.7069	726.35	0
				S ₁	2.7385	452.75	2.1391
3a	-1157.67267740	-5.027	-1.985	T ₁	1.6949	731.53	0
				S ₁	2.8169	440.14	2.5891
3b	-1342.14833965	-5.528	-2.446	T ₁	1.7791	696.88	0
				S ₁	2.8082	441.52	2.0265
3c	-1342.14952669	-5.585	-2.664	T ₁	1.6274	761.84	0
				S ₁	2.6933	460.35	2.3871

Table S2. Optimized geometries and molecular orbitals at the B3LYP/6-31G(d,p)

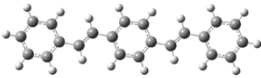
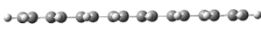

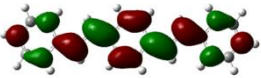
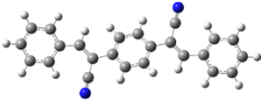
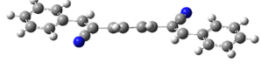
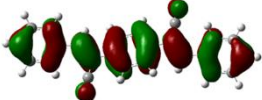
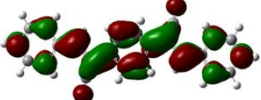
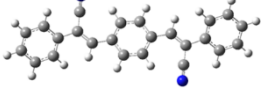
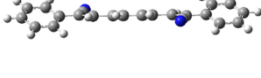


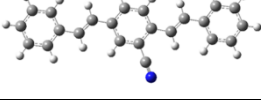
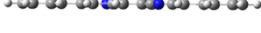
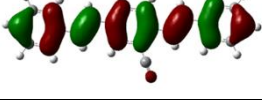

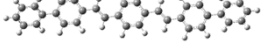
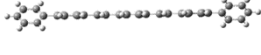


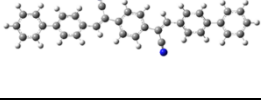
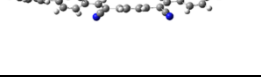


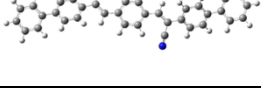


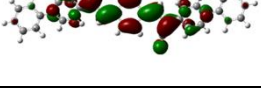
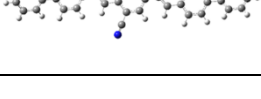







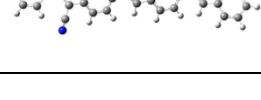
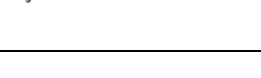

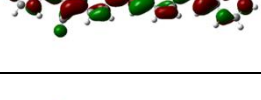
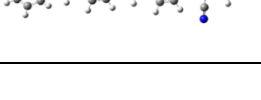



	Front view	Side view	HOMO	LUMO
1a				
1b				
1c				
1d				
2a				
2b				
2c				
2d				
3a				
3b				
3c				

Table S3. Calculated adiabatic excitation energies for S₁ state, the first vertical excitation energies (VEE), wavelength, and oscillator strength (*f*) at the B3LYP/6-31G(d,p)

	S₁-adiabatic (hartrees)	S₀@S₁ geometry (hartrees)	VEE (eV)	Wavelength (nm)	<i>f</i> (-)	Δ<i>E</i> (Stokes shift) (eV)^a
1a	-849.090240455	-849.194005448	2.8236	439.10	1.9493	0.3838
1b	-1033.56910605	-1033.66873379	2.7110	457.34	1.5560	0.4873
1c	-1033.57455550	-1033.66974947	2.5904	478.64	1.6538	0.4172
1d	-1033.57602194	-1033.67611390	2.7236	455.21	1.3535	0.2790
2a	-1311.22928661	-1311.32230473	2.5312	489.83	2.8611	0.4060
2b	-1495.70824067	-1495.79797200	2.4417	507.78	2.4194	0.4640
2c	-1495.71305557	-1495.79831272	2.3200	534.42	2.2643	0.4134
2d	-1495.71483265	-1495.80464722	2.4440	507.30	2.4587	0.2945
3a	-1157.57586925	-1157.66655972	2.4678	502.41	2.7968	0.3491
3b	-1342.05329878	-1342.14161820	2.4033	515.89	2.3409	0.4048
3c	-1342.05741400	-1342.14344218	2.3409	529.63	2.6245	0.3524

^aVEE at the ground state geometry minus VEE at the first singlet excited state geometry

Table S4. Crystal data and structure refinement for **1d**

CCDC number	2034947
Identification code	Compound_1d
Empirical formula	C ₂₄ H ₁₆ N ₂
Formula weight	332.39
Temperature	100 K
Wavelength	0.71075 Å
Crystal system	Triclinic
Space group	<i>P</i> -1
Unit cell dimensions	<i>a</i> = 3.8901 (6) <i>α</i> = 81.896 (14) <i>b</i> = 6.4671 (9) <i>β</i> = 85.023 (15) <i>c</i> = 17.778 (4) <i>γ</i> = 85.150 (12)
Volume	439.93 (13)
<i>Z</i>	1
Density (calculated)	1.255 g/cm ³
Absorption coefficient	0.074 mm ⁻¹
<i>F</i> (000)	174
Crystal size	0.3 × 0.02 × 0.01 mm ³
Theta range for data collection	2.321 to 27.559°.
Index ranges	-5 ≤ <i>h</i> ≤ 5, -8 ≤ <i>k</i> ≤ 8, -22 ≤ <i>l</i> ≤ 23
Reflections collected	2899
Independent reflections	2899 [R(int) = 0.050]
Completeness to theta = 27.559°	143.2
Absorption correction	multi-scan
Max. and min. transmission	1.00000 and 0.65654
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	2899 / 0 / 119
Goodness-of-fit on <i>F</i> ²	1.160
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0986, <i>wR</i> ₂ = 0.2696
R indices (all data)	<i>R</i> ₁ = 0.1139, <i>wR</i> ₂ = 0.2775
Largest diff. peak and hole	0.445 and -0.432 e.Å ⁻³

Table S5. Crystal data and structure refinement for **2b**

CCDC number	2034948	
Identification code	Compound_2b	
Empirical formula	C ₃₆ H ₂₄ N ₂	
Formula weight	484.60	
Temperature	123 K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	<i>a</i> = 26.029 (7)	<i>α</i> = 90
	<i>b</i> = 6.7825 (15)	<i>β</i> = 97.398 (7)
	<i>c</i> = 7.1139 (17)	<i>γ</i> = 90
Volume	1245.4 (5)	
<i>Z</i>	2	
Density (calculated)	1.292 g/cm ³	
Absorption coefficient	0.075 mm ⁻¹	
<i>F</i> (000)	508	
Crystal size	0.150 × 0.100 × 0.050 mm ³	
Theta range for data collection	3.105 to 27.494°.	
Index ranges	-33 ≤ <i>h</i> ≤ 33, -8 ≤ <i>k</i> ≤ 8, -9 ≤ <i>l</i> ≤ 9	
Reflections collected	10610	
Independent reflections	2835 [R(int) = 0.0618]	
Completeness to theta = 27.494°	99.3	
Absorption correction	multi-scan	
Max. and min. transmission	0.996 and 0.879	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	2835 / 0 / 172	
Goodness-of-fit on <i>F</i> ²	1.119	
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0662, <i>wR</i> ₂ = 0.1546	
R indices (all data)	<i>R</i> ₁ = 0.0749, <i>wR</i> ₂ = 0.1599	
Largest diff. peak and hole	0.42 and -0.38 e.Å ⁻³	

Table S6. Crystal data and structure refinement for **2c**

CCDC number	2034949
Identification code	Compound_2c
Empirical formula	C ₃₆ H ₂₄ N ₂
Formula weight	484.60
Temperature	183 K
Wavelength	1.54187 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 26.5004 (14) <i>α</i> = 90 <i>b</i> = 6.9730 (4) <i>β</i> = 90.180 (6) <i>c</i> = 6.8292 (4) <i>γ</i> = 90
Volume	1261.95 (11)
<i>Z</i>	2
Density (calculated)	1.275 g/cm ³
Absorption coefficient	0.571 mm ⁻¹
<i>F</i> (000)	508
Crystal size	0.200 × 0.100 × 0.050 mm ³
Theta range for data collection	3.336 to 68.235°
Index ranges	-31 ≤ <i>h</i> ≤ 31, -8 ≤ <i>k</i> ≤ 8, -8 ≤ <i>l</i> ≤ 8
Reflections collected	14004
Independent reflections	2309 [R(int) = 0.0528]
Completeness to theta = 68.235°	99.9
Absorption correction	multi-scan
Max. and min. transmission	0.972 and 0.713
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	2309 / 0 / 172
Goodness-of-fit on <i>F</i> ²	1.029
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0606, <i>wR</i> ₂ = 0.1286
R indices (all data)	<i>R</i> ₁ = 0.0910, <i>wR</i> ₂ = 0.1434
Largest diff. peak and hole	0.42 and -0.19 e.Å ⁻³

Table S7. Crystal data and structure refinement for **2d**

CCDC number	2034950	
Identification code	Compound_2d	
Empirical formula	C ₃₆ H ₂₄ N ₂	
Formula weight	484.57	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 6.6708 (4)	<i>α</i> = 93.342 (4)
	<i>b</i> = 7.2930 (3)	<i>β</i> = 91.641 (4)
	<i>c</i> = 26.0182 (11)	<i>γ</i> = 91.948 (4)
Volume	1262.31 (11)	
<i>Z</i>	2	
Density (calculated)	1.275 g/cm ³	
Absorption coefficient	0.074 mm ⁻¹	
<i>F</i> (000)	508	
Crystal size	0.3 × 0.2 × 0.03 mm ³	
Theta range for data collection	2.353 to 27.483°	
Index ranges	-8 ≤ <i>h</i> ≤ 7, -9 ≤ <i>k</i> ≤ 9, -33 ≤ <i>l</i> ≤ 33	
Reflections collected	20689	
Independent reflections	5798 [R(int) = 0.0319]	
Completeness to theta = 27.483°	99.91	
Absorption correction	multi-scan	
Max. and min. transmission	1.000 and 0.83192	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	5798 / 0 / 343	
Goodness-of-fit on <i>F</i> ²	1.024	
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0422, <i>wR</i> ₂ = 0.1011	
R indices (all data)	<i>R</i> ₁ = 0.0531, <i>wR</i> ₂ = 0.1062	
Largest diff. peak and hole	0.304 and -0.202 e.Å ⁻³	

Table S8. Crystal data and structure refinement for **3a**

CCDC number	2034951
Identification code	Compound_3a
Empirical formula	C ₃₀ H ₂₄
Formula weight	384.49
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 26.100 (3) <i>α</i> = 90 <i>b</i> = 7.4249 (8) <i>β</i> = 102.784 (10) <i>c</i> = 15.9316 (11) <i>γ</i> = 90
Volume	3010.8 (6)
<i>Z</i>	6
Density (calculated)	1.272 g/cm ³
Absorption coefficient	0.072 mm ⁻¹
<i>F</i> (000)	1224
Crystal size	0.108 × 0.039 × 0.012 mm ³
Theta range for data collection	2.401 to 27.482°
Index ranges	-32 ≤ <i>h</i> ≤ 33, -9 ≤ <i>k</i> ≤ 9, -20 ≤ <i>l</i> ≤ 20
Reflections collected	22613
Independent reflections	6907 [R(int) = 0.0700]
Completeness to theta = 27.482°	99.75
Absorption correction	gaussian
Max. and min. transmission	1.000 and 0.967
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	6907 / 0 / 406
Goodness-of-fit on <i>F</i> ²	0.980
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0655, <i>wR</i> ₂ = 0.1490
R indices (all data)	<i>R</i> ₁ = 0.1475, <i>wR</i> ₂ = 0.1870
Largest diff. peak and hole	0.571 and -0.269 e.Å ⁻³

Table S9. Crystal data and structure refinement for **3b**

CCDC number	2034952
Identification code	Compound_3b
Empirical formula	C ₃₂ H ₂₂ N ₂
Formula weight	434.54
Temperature	123 K
Wavelength	0.71075 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 24.094 (9) <i>α</i> = 90 <i>b</i> = 6.955 (2) <i>β</i> = 92.698 (8) <i>c</i> = 6.805 (2) <i>γ</i> = 90
Volume	1139.2 (7)
<i>Z</i>	2
Density (calculated)	1.267 g/cm ³
Absorption coefficient	0.074 mm ⁻¹
<i>F</i> (000)	456
Crystal size	0.200 × 0.200 × 0.180 mm ³
Theta range for data collection	3.049 to 27.484°.
Index ranges	-31 ≤ <i>h</i> ≤ 31, -9 ≤ <i>k</i> ≤ 9, -8 ≤ <i>l</i> ≤ 8
Reflections collected	10089
Independent reflections	2592 [R(int) = 0.0331]
Completeness to theta = 27.484°	99.5
Absorption correction	multi-scan
Max. and min. transmission	0.987 and 0.830
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	2592 / 0 / 154
Goodness-of-fit on <i>F</i> ²	1.176
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0655, <i>wR</i> ₂ = 0.1646
R indices (all data)	<i>R</i> ₁ = 0.0706, <i>wR</i> ₂ = 0.1680
Largest diff. peak and hole	0.34 and -0.38 e.Å ⁻³

Table S10. Crystal data and structure refinement for **3c**

CCDC number	2034953
Identification code	Compound_3c
Empirical formula	C ₃₂ H ₂₂ N ₂
Formula weight	434.51
Temperature	123 K
Wavelength	0.71075 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁
Unit cell dimensions	<i>a</i> = 14.024 (4) <i>α</i> = 90 <i>b</i> = 6.820 (2) <i>β</i> = 93.483 (10) <i>c</i> = 23.678 (7) <i>γ</i> = 90
Volume	2260.6 (12)
<i>Z</i>	4
Density (calculated)	1.277 g/cm ³
Absorption coefficient	0.074 mm ⁻¹
<i>F</i> (000)	912
Crystal size	0.120 × 0.060 × 0.030 mm ³
Theta range for data collection	3.043 to 24.998°.
Index ranges	-16 ≤ <i>h</i> ≤ 16, -7 ≤ <i>k</i> ≤ 8, -28 ≤ <i>l</i> ≤ 25
Reflections collected	17932
Independent reflections	7473 [R(int) = 0.0920]
Completeness to theta = 24.998°	1.72/0.94
Absorption correction	multi-scan
Max. and min. transmission	0.998 and 0.751
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	7473 / 2 / 613
Goodness-of-fit on <i>F</i> ²	1.106
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0998, <i>wR</i> ₂ = 0.1940
R indices (all data)	<i>R</i> ₁ = 0.1331, <i>wR</i> ₂ = 0.2182
Largest diff. peak and hole	0.552 and -0.317 e.Å ⁻³

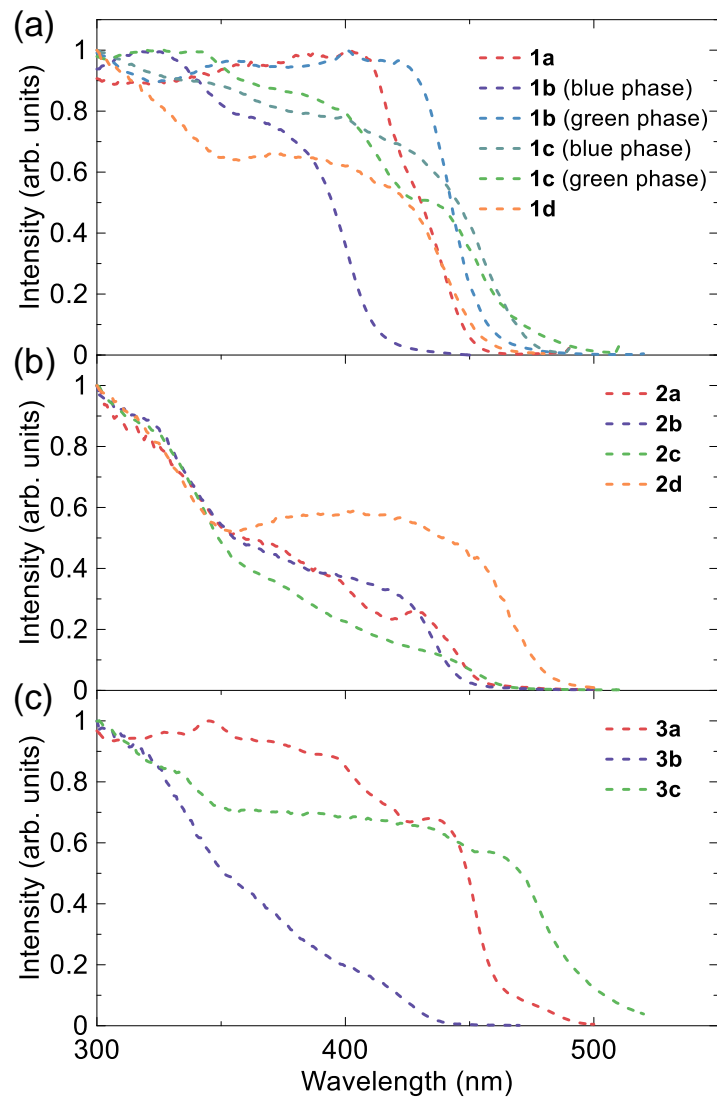


Fig. S1. Excitation spectra for crystals.

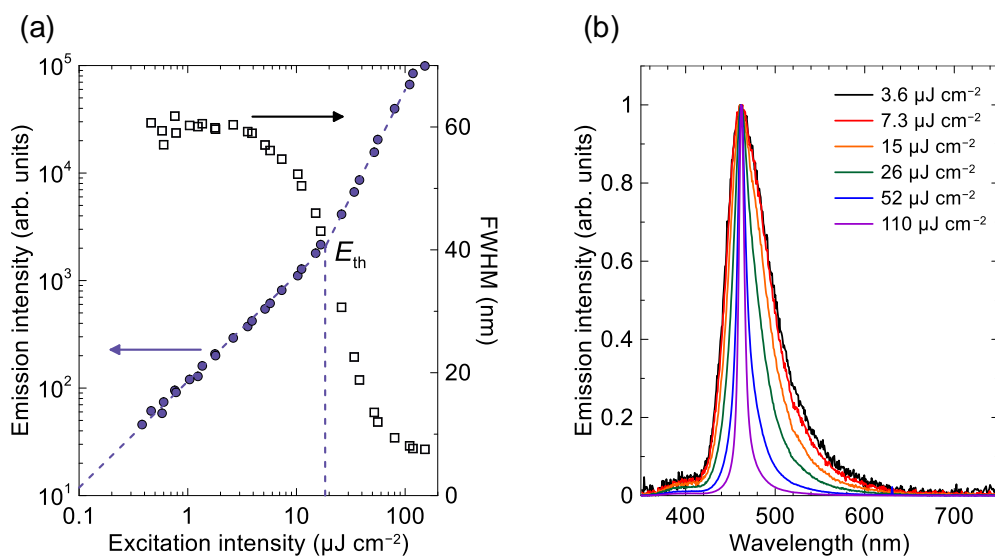


Fig. S2. ASE characteristics of the crystal of **1b** blue phase. (a) Output PL intensity and FWHM values as a function of the excitation energy and (b) PL spectra for different excitation powers below and above the ASE threshold.

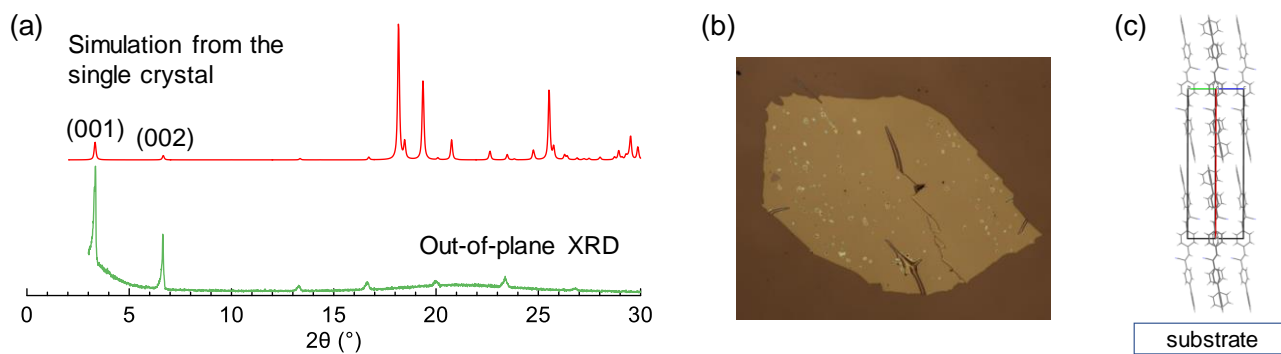


Fig. S3. Out-of-plane X-ray diffractogram of **2c**. (a) XRD and the simulated pattern from the single crystal analysis, (b) a photo of the crystal on the substrate, and (c) schematic image of the molecular orientation on the substrate.

Methods S3. FET fabrications

Bottom-gate/top-contact (BG/TC) FETs were constructed on heavily doped n-type silicon wafers covered with thermally grown silicon dioxide (300 nm) which was cleaned by piranha solution. The silicon dioxide acts as a gate dielectric layer and the silicon wafer serves as a gate electrode. A 20 nm-thick poly(methyl methacrylate) (PMMA) layer was dip-coated (0.5 mm s^{-1}) from a toluene solution (10 mg ml^{-1}) onto wafer. After the PMMA deposition, the substrates were baked at $80 \text{ }^\circ\text{C}$ for 8 h in a glove box ($<1 \text{ ppm O}_2$; $<1 \text{ ppm H}_2\text{O}$). A single crystal was carefully placed on the substrate. A source and drain electrodes were deposited with the deposition rate of 2 \AA s^{-1} using conventional thermal evaporation through a shadow mask under a vacuum of $<1 \times 10^{-4} \text{ Pa}$. The actual lengths of L/W were measured by the optical microscope.

The FET measurements were carried out at room temperature in a glovebox without exposure to air with a semiconductor parameter analyzer. Mobilities (μ) were calculated in the saturation regime by the relationship: $\mu_{\text{sat}} = (2I_{\text{D}}L)/[WC_i(V_{\text{G}} - V_{\text{th}})^2]$ where I_{D} is the source-drain saturation current; C_i is the capacitance of the insulating layer; V_{G} is the gate voltage and V_{th} is the threshold voltage. The latter can be estimated as the intercept of the linear section of the plot of $V_{\text{G}} (I_{\text{D}})^{1/2}$.

Table S11. Mobilities

Compound	Device configuration	μ_{h} [$\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$]	μ_{e} [$\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$]	Ref.
1a (crystal)	Ca-Au electrodes, PMMA-treated SiO_2	0.12	1.3×10^{-2}	S9
1c (green-emissive crystal)	Ca-Au electrodes, PMMA-treated SiO_2	2.1	2.5	S11
2a (thin-film)	Au electrodes	1.6×10^{-4}	-	S12
2a (crystal)	Ca-Au electrodes, PMMA-treated SiO_2	0.05	0.25	-
3a (crystal)	Ca-Au electrodes, PMMA-treated SiO_2	0.12	0.11	S9

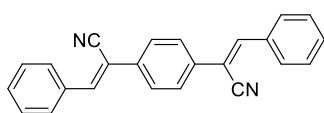
Table S12. Materials

Reagents	CAS No.	Supplier, code, and grade
Benzaldehyde	100-52-7	WAKO Chemical Industries, 025-12206
<i>p</i> -Xylylene dicyanide	622-75-3	Tokyo Kasei Co., Ltd., X0061
Phenylacetonitrile	140-29-4	WAKO Chemical Industries, 161-01243
Terephthalaldehyde	623-27-8	WAKO Chemical Industries, 203-03592
<i>p</i> -Phenylbenzaldehyde	3218-36-8	WAKO Chemical Industries, 165-17231
Tetraethyl <i>p</i> -xylylenediphosphonate	4546-04-7	Tokyo Kasei Co., Ltd., T1582
4-Biphenylacetonitrile	31603-77-7	Tokyo Kasei Co., Ltd., B1545
Diethyl benzylphosphonate	1080-32-7	WAKO Chemical Industries, 329-62002
2,5-Dibromo- <i>p</i> -xylene	1074-24-4	Tokyo Kasei Co., Ltd., D1841
4-Bromobenzaldehyde	1122-91-4	Tokyo Kasei Co., Ltd., B0549
4,4'-Dimethyl- <i>trans</i> -stilbene	18869-29-9	Tokyo Kasei Co., Ltd., D2708
Copper cyanide	544-92-3	WAKO Chemical Industries, 032-19152
<i>N</i> -Bromosuccinimide (NBS)	128-08-5	WAKO Chemical Industries, 025-07235
Triethyl phosphite	122-52-1	WAKO Chemical Industries, 200-02723
KOtBu	865-47-4	Tokyo Kasei Co., Ltd., P1008
Titanium chloride	7550-45-0	WAKO Chemical Industries, 202-12592
Zinc powder	7440-66-6	WAKO Chemical Industries, 263-00215
Sodium cyanide	143-33-9	WAKO Chemical Industries, 192-01852
Benzoyl peroxide (BPO)	94-36-0	Tokyo Kasei Co., Ltd., B3152
AIBN	78-67-1	WAKO Chemical Industries, 019-04932

Table S13. Instruments

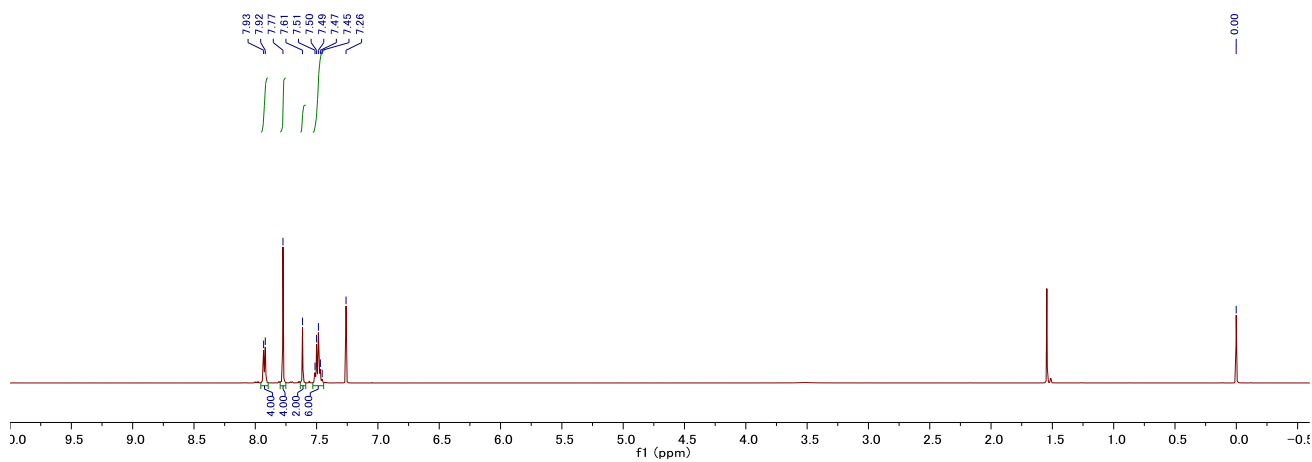
Instruments	Brands and Types	Conditions
Sublimation	ALS technology	Three-zone sublimation apparatus.
Elemental Analysis	Yanaco MT-5 CHN corder	
MS	Waters 3100 Mass Spectrometer	Direct probe ionization, ASAP-MS.
NMR	Bruker AVANCE III 500 MHz spectrometer	Chemical shifts were calibrated to the corresponding deuterated solvents. 7.26 ppm for CDCl ₃ and 5.32 ppm for CD ₂ Cl ₂ in ¹ H NMR, and 77.2 ppm for CDCl ₃ in ¹³ C NMR
UV-Vis	Perkin-Elmer Lambda 950-PKA UV-vis spectrophotometer	The light source consisted of Deuterium (D2) and Tungsten Iodide (50W) lamps for the ultraviolet and visible regions.
PL	Horiba Jobin-Yvon FluoroMax-4 JASCO FP-8600 fluorometer	the excitation wavelength was set to the absorption maximum
PL quantum Yield	Hamamatsu Photonics Quantaaurus-QY C11347-01	Absolute PL quantum yield. The measurement error for the obtained values on this instrument is ± 3%.
Transient photoluminescence decay	Hamamatsu Photonics Quantaaurus-Tau C11367-03	
UV/ozone	Nippon Laser & Electronics Lab. NL-UV253	15 min
XRD	Rigaku Ultima IV diffractometer	40 kV and 40 mA using CuK α radiation.
Laser scanning microscope	Olympus LEXT	
Surface profiler	Bruker Dektak XT	A tip radius of 12.5 μ m and a scan resolution of 0.168 μ m/point

Data S1. NMR spectra

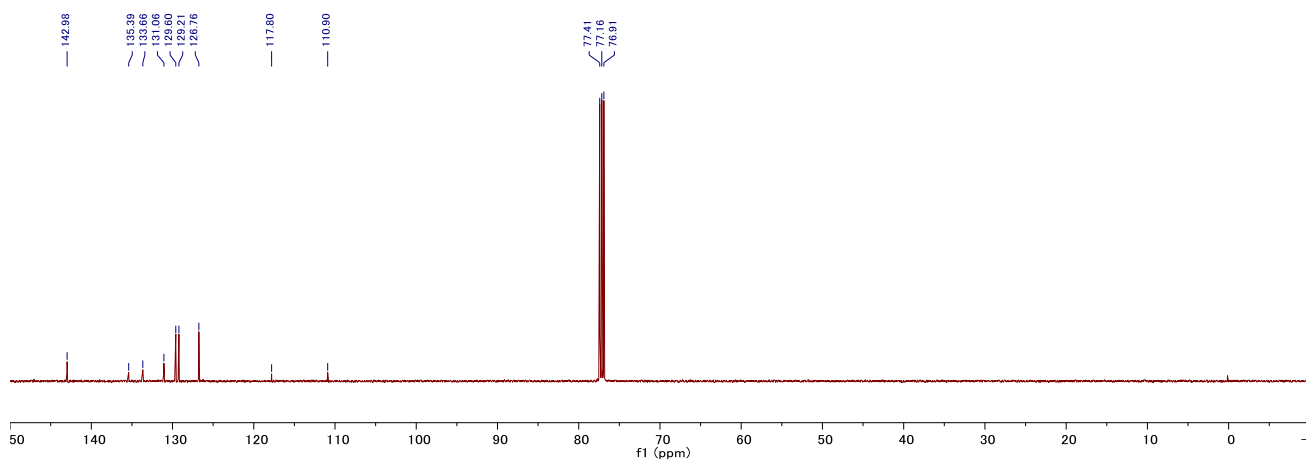


Compound 1b

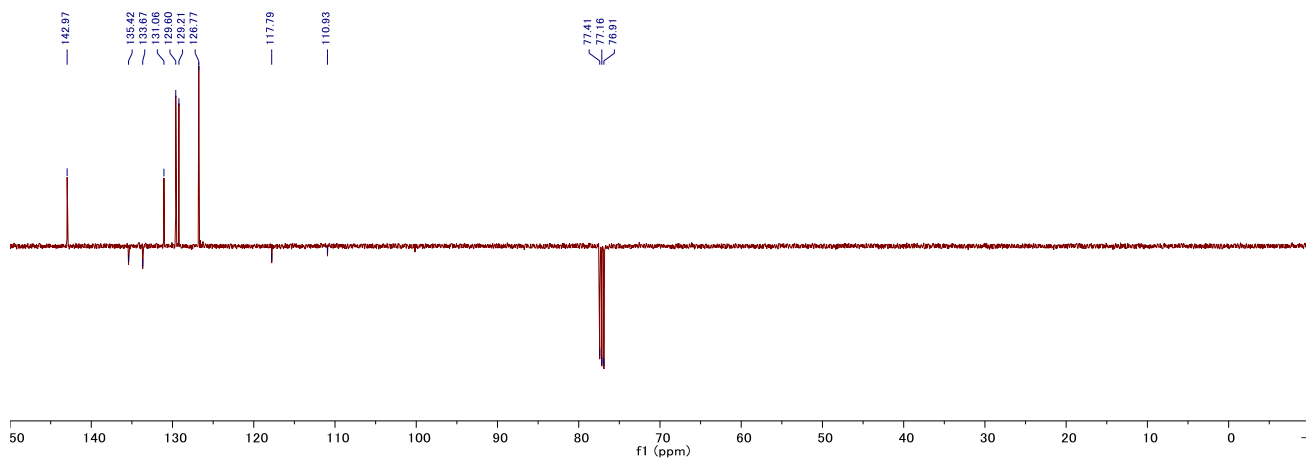
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)

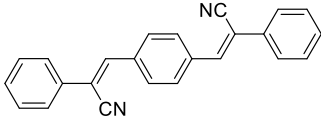


$^{13}\text{C-NMR}$ spectrum (125 MHz, CDCl_3 , 300 K)



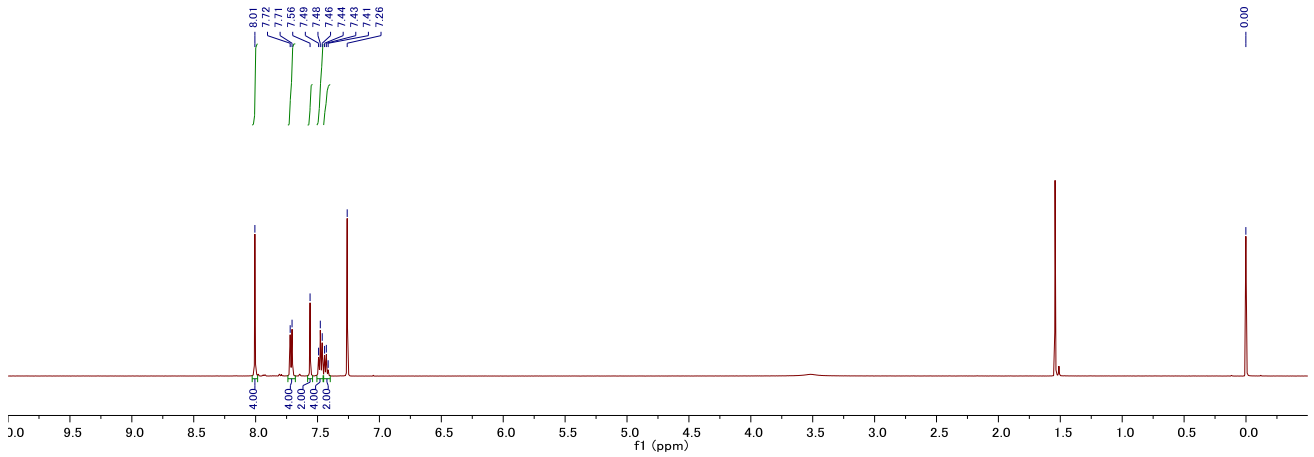
$^{13}\text{C-NMR}$ spectrum (APT) (125 MHz, CDCl_3 , 300 K)



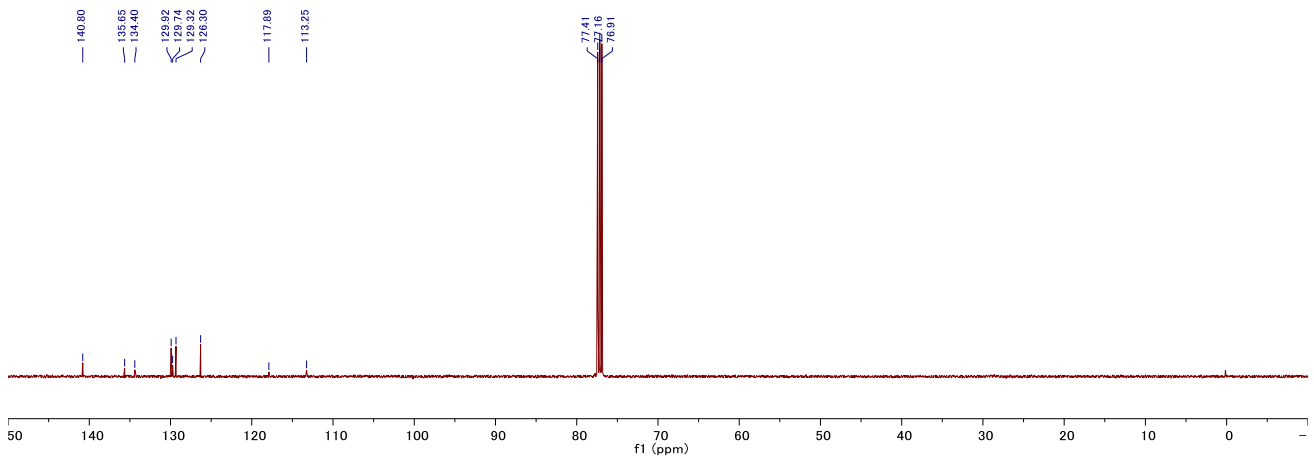


Compound **1c**

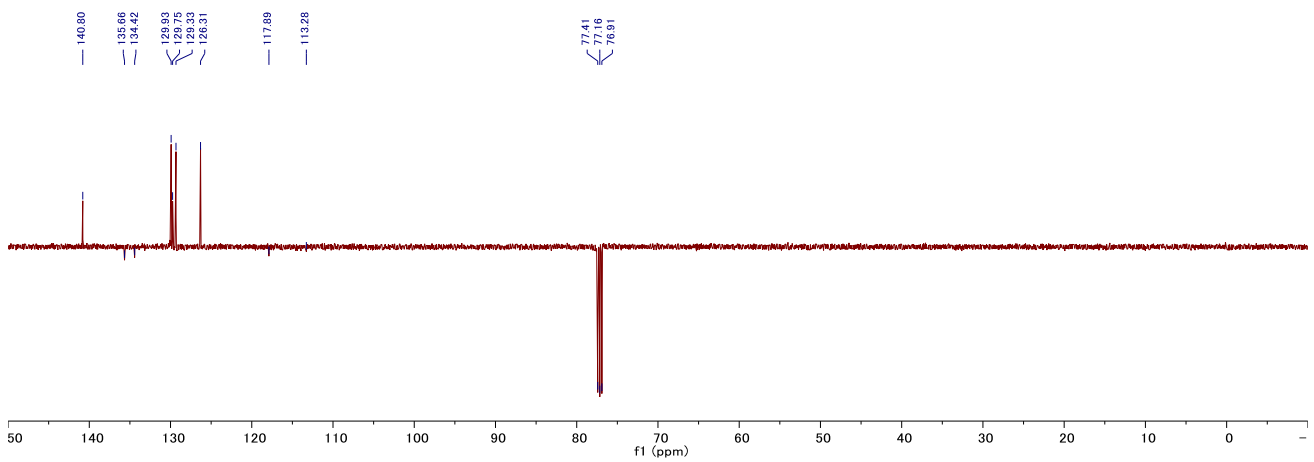
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)

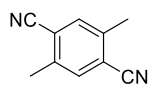


$^{13}\text{C-NMR}$ spectrum (125 MHz, CDCl_3 , 300 K)



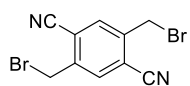
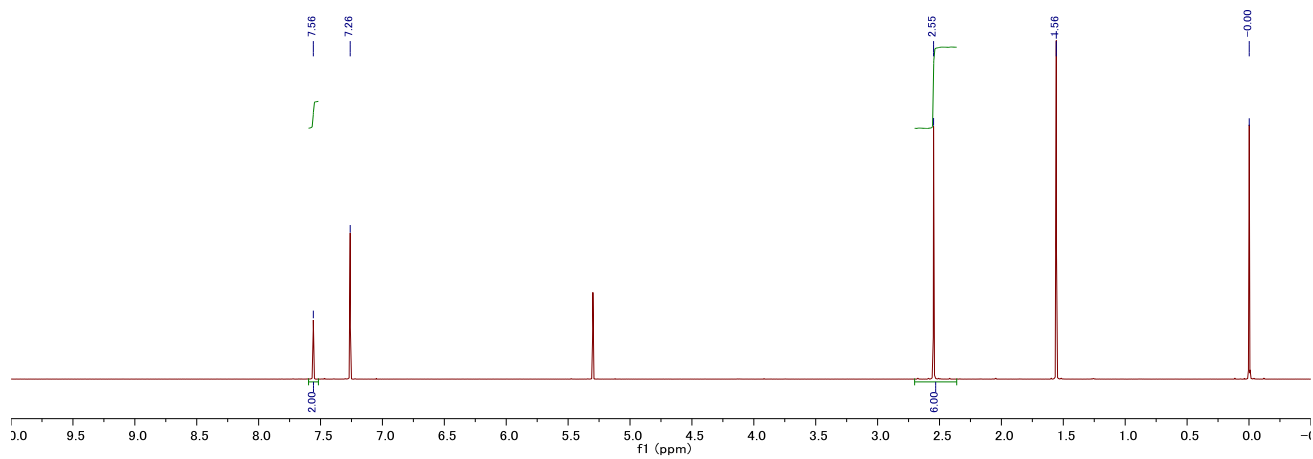
$^{13}\text{C-NMR}$ spectrum (APT) (125 MHz, CDCl_3 , 300 K)





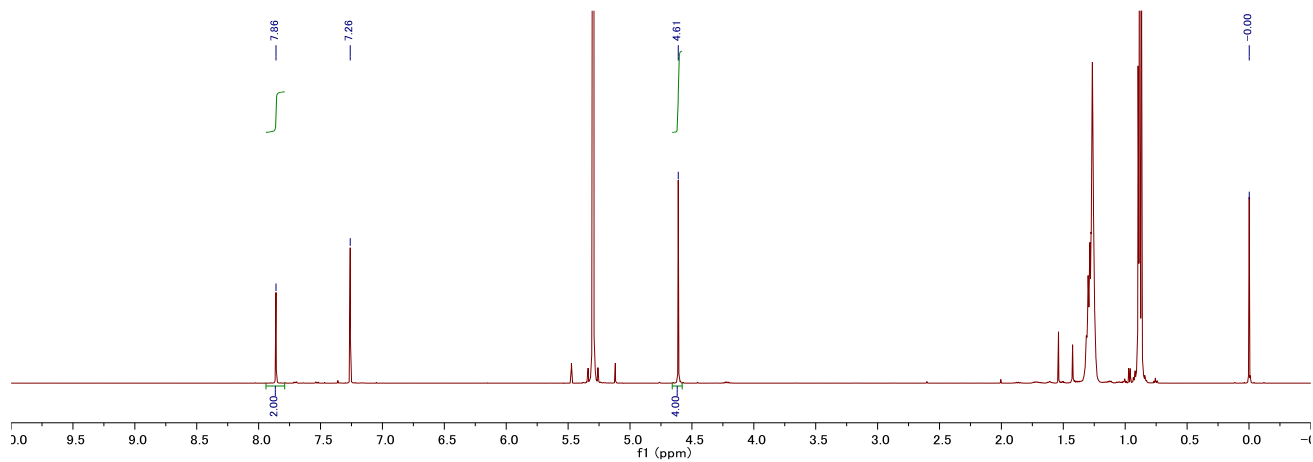
Compound **9**

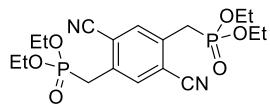
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)



Compound **10**

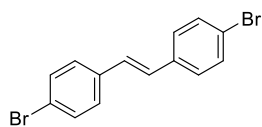
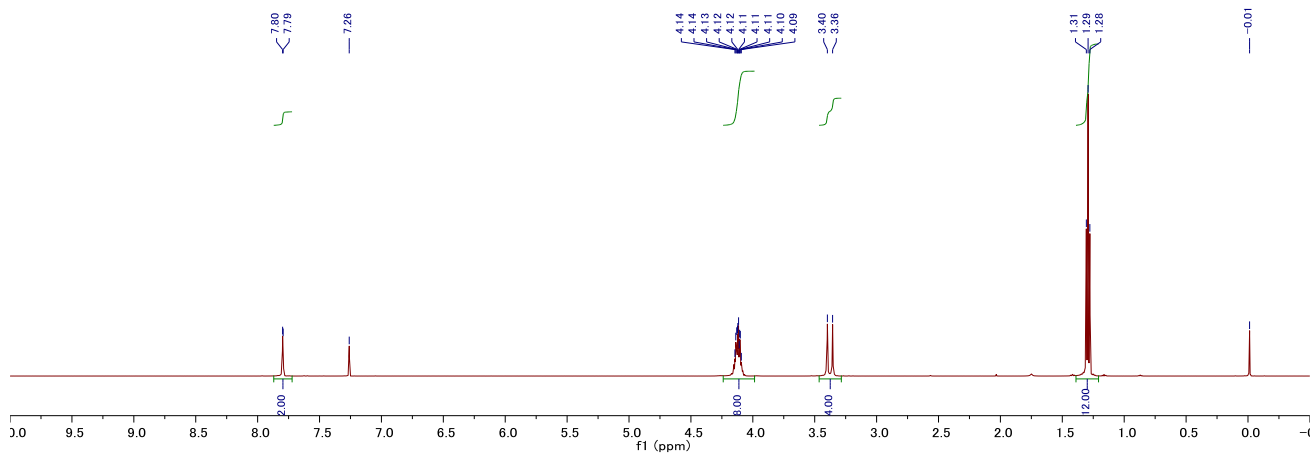
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)





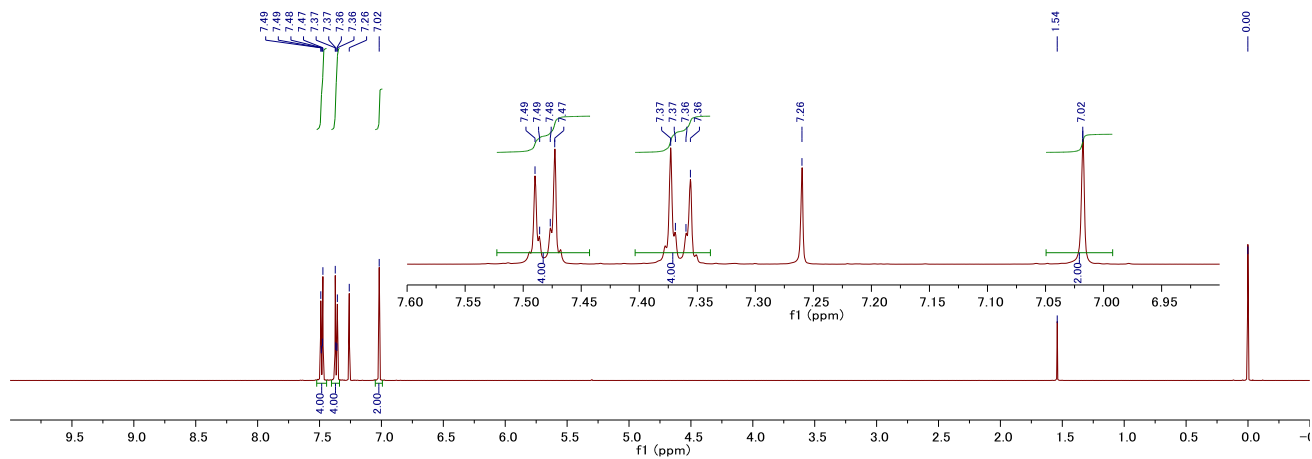
Compound 11

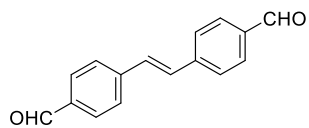
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)



Compound 16

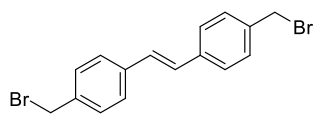
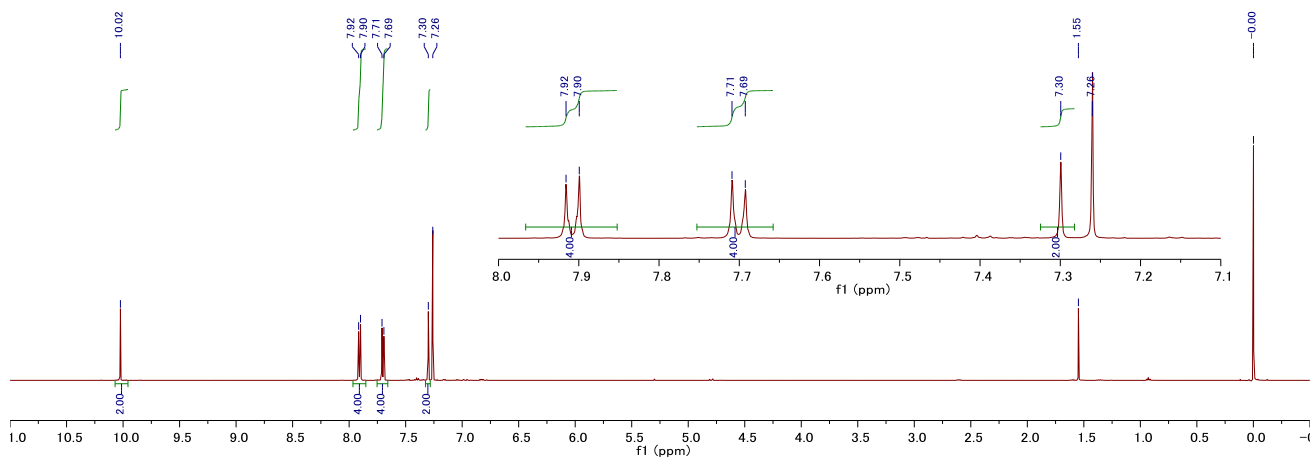
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)





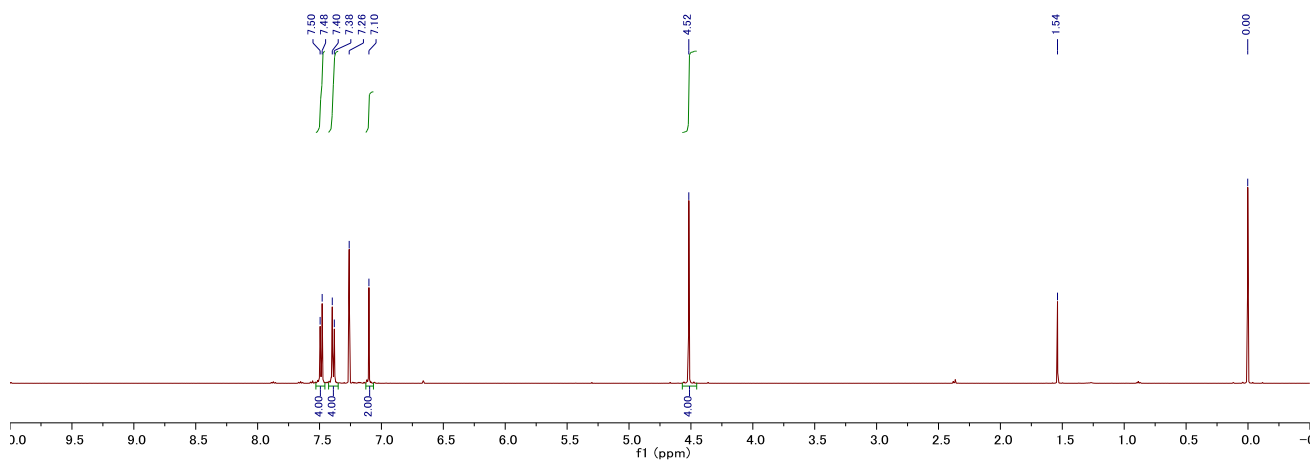
Compound 17

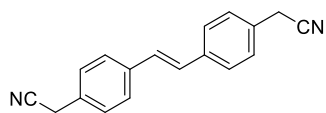
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)



Compound 19

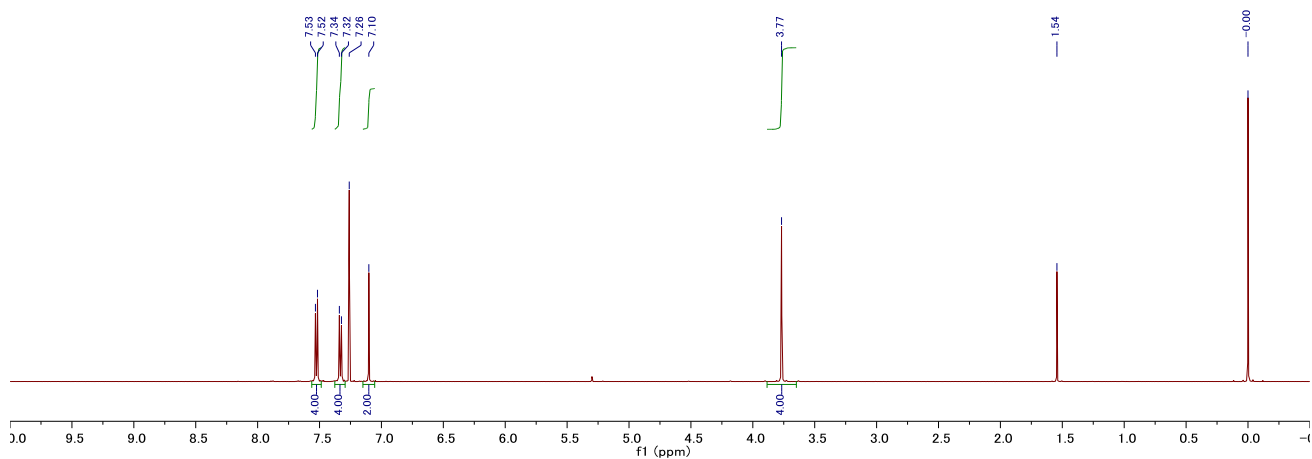
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)



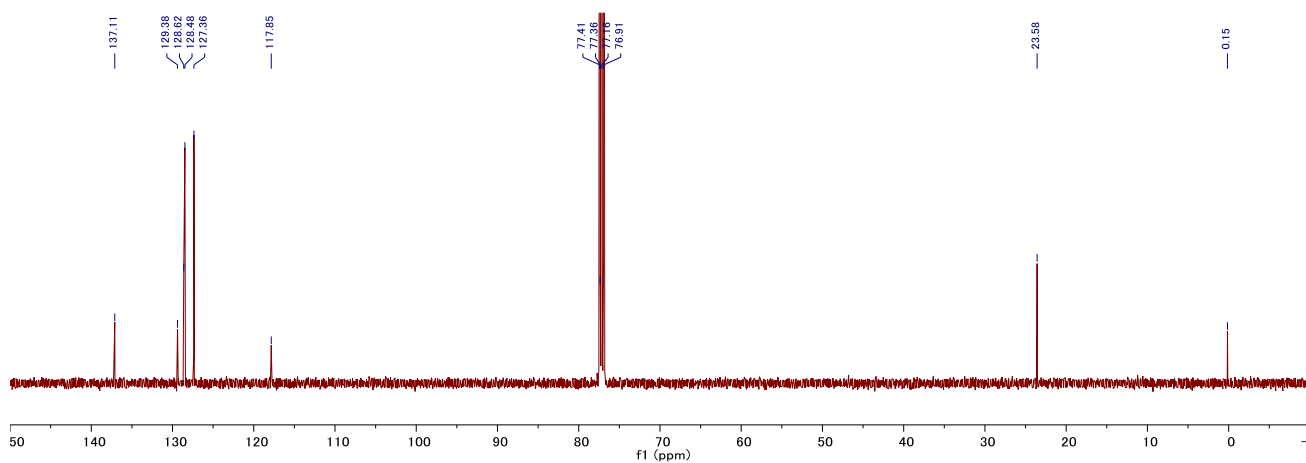


Compound **20**

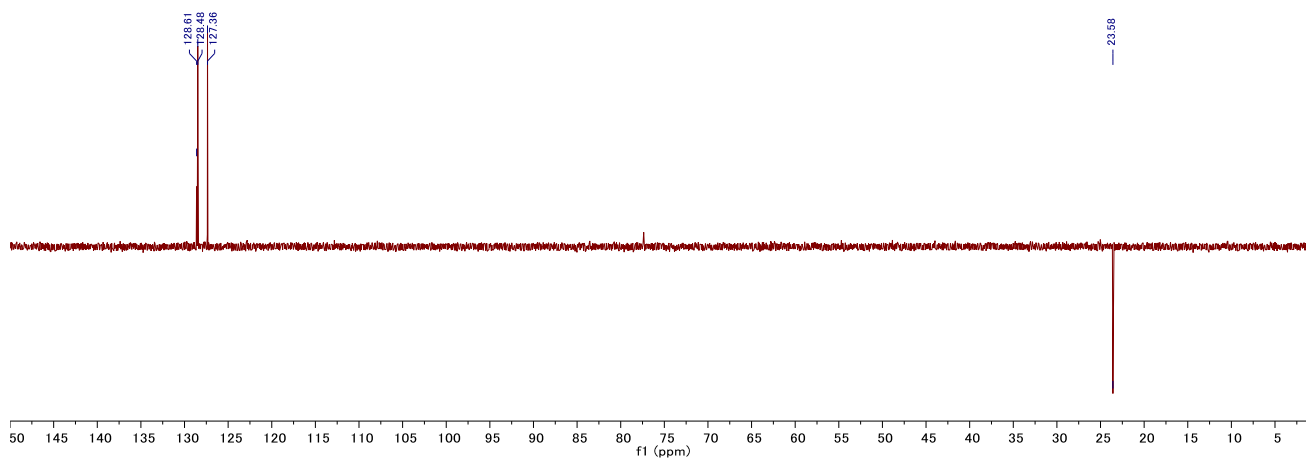
$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)

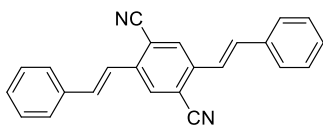


$^{13}\text{C-NMR}$ spectrum (125 MHz, CDCl_3 , 300 K)



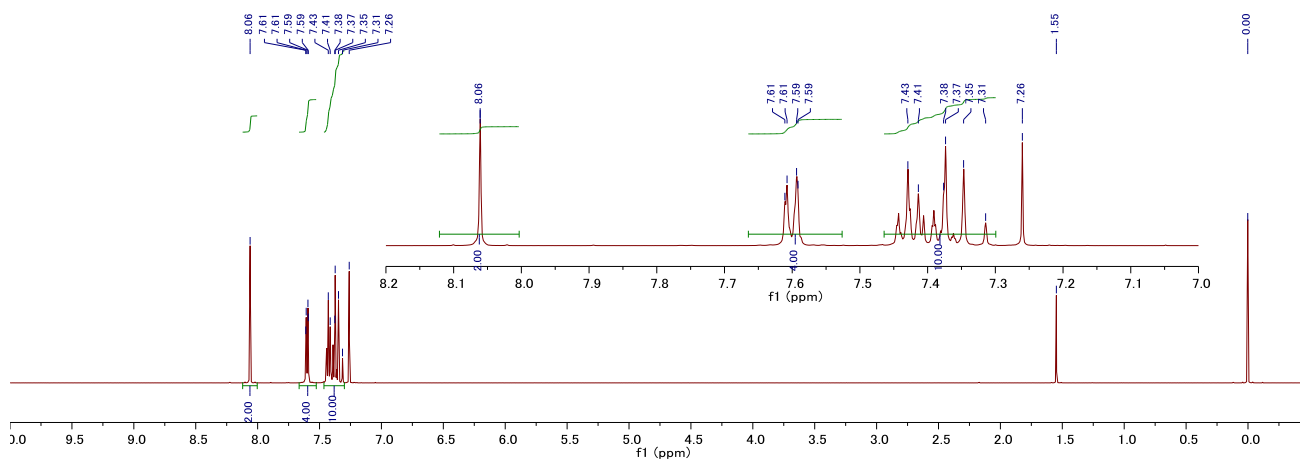
$^{13}\text{C-NMR}$ spectrum (DEPT135) (125 MHz, CDCl_3 , 300 K)



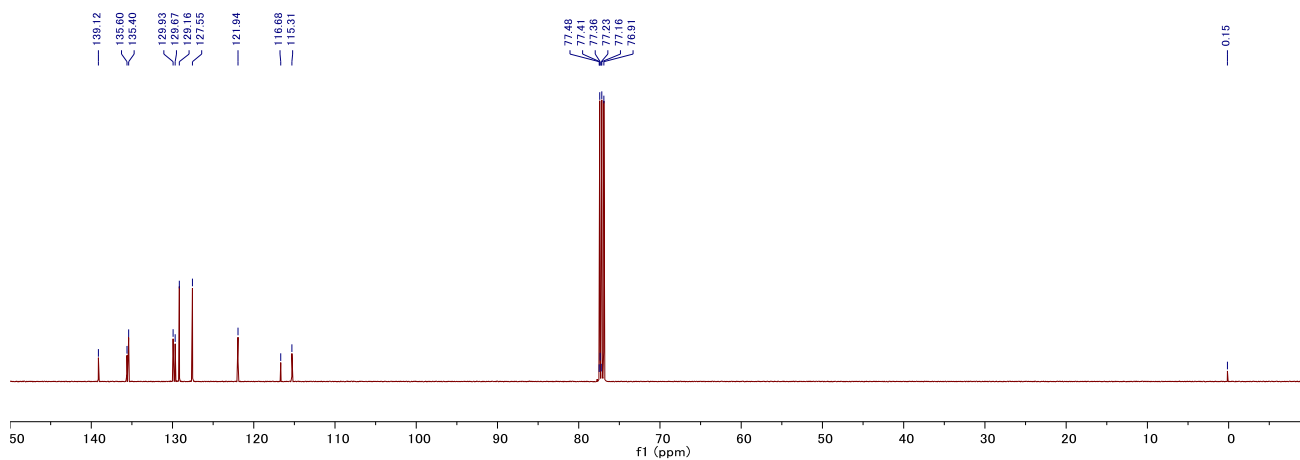


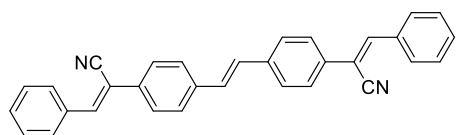
Compound **1d**

$^1\text{H-NMR}$ spectrum (500 MHz, CDCl_3 , 300 K)



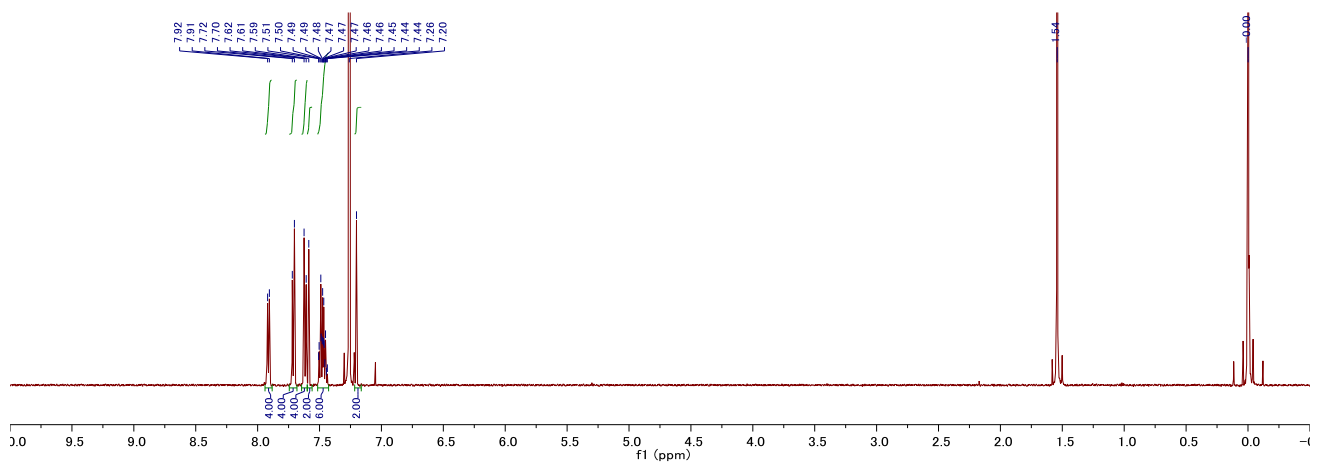
$^{13}\text{C-NMR}$ spectrum (125 MHz, CDCl_3 , 300 K)



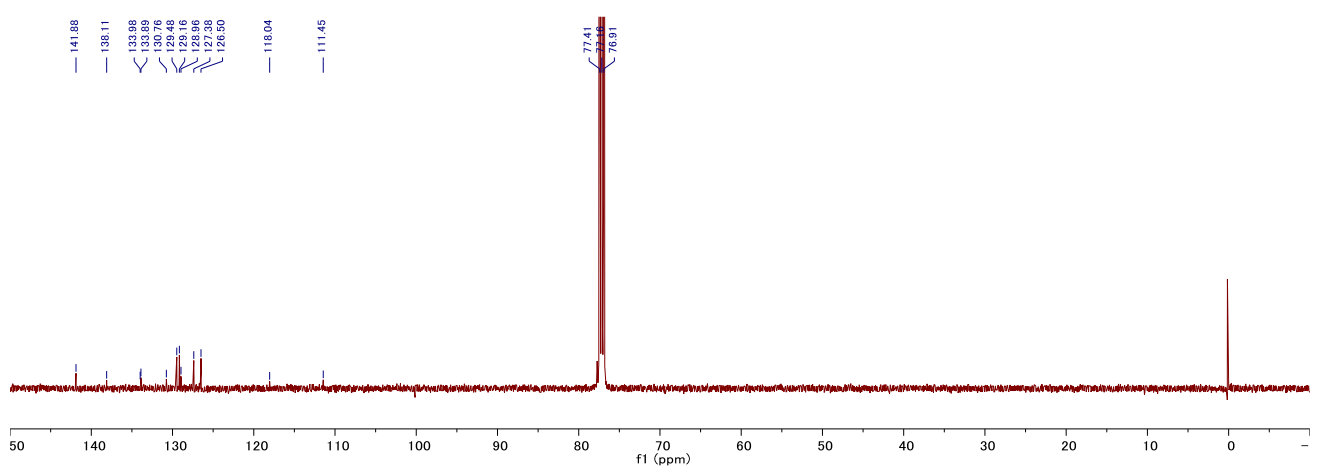


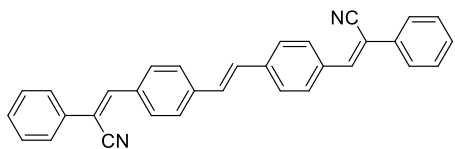
Compound **3b**

¹H-NMR spectrum (500 MHz, CDCl₃, 300 K)



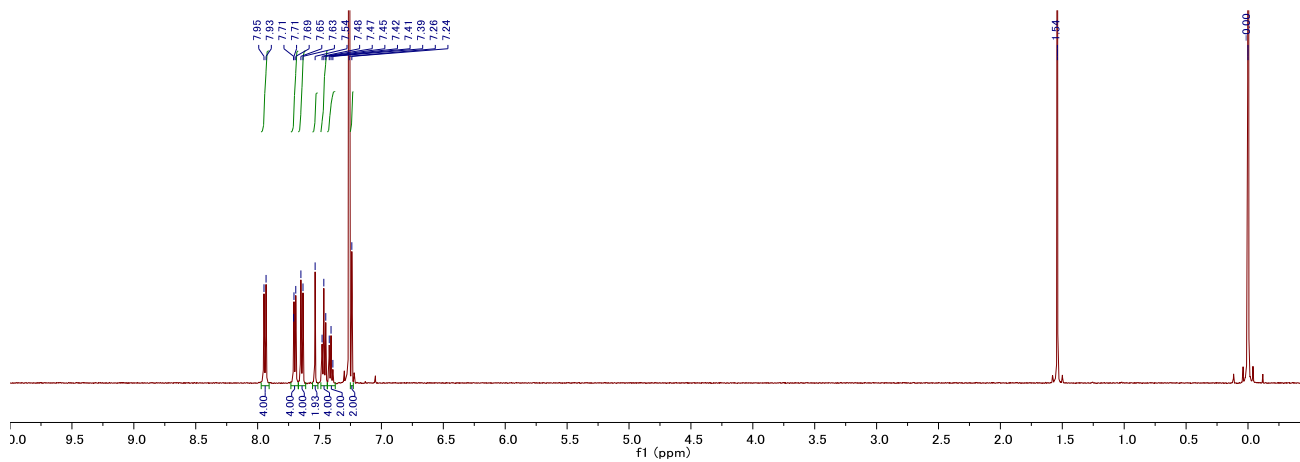
¹³C-NMR spectrum (125 MHz, CDCl₃, 300 K)



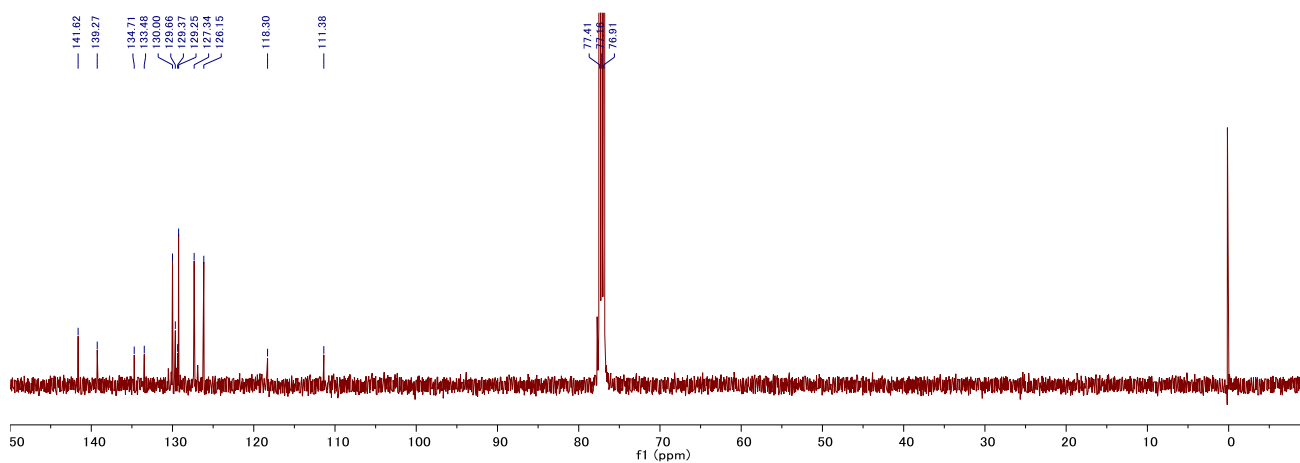


Compound 3c

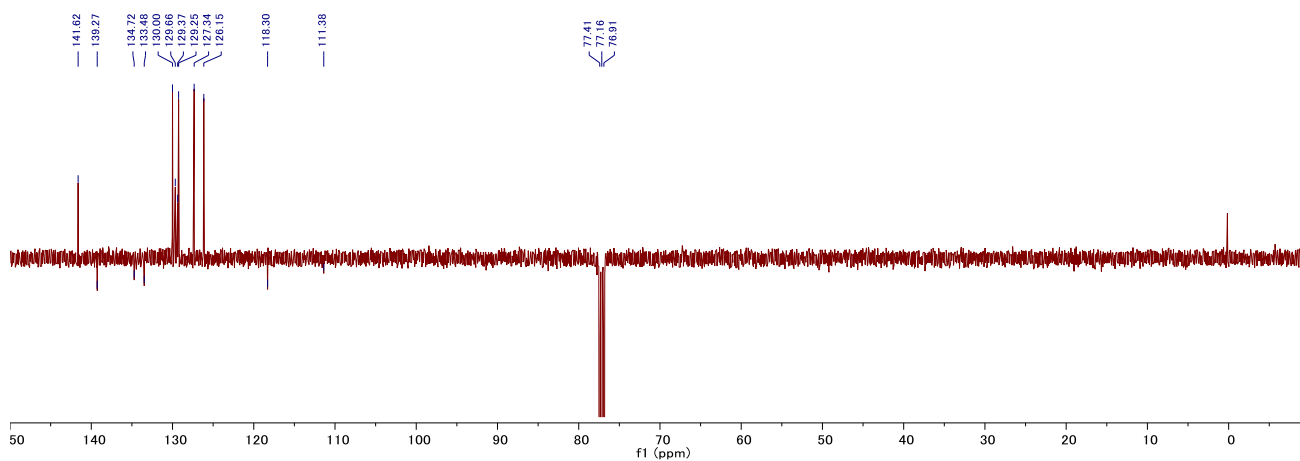
¹H-NMR spectrum (500 MHz, CDCl₃, 300 K)



¹³C-NMR spectrum (125 MHz, CDCl₃, 300 K)



¹³C-NMR spectrum (APT) (125 MHz, CDCl₃, 300 K)



Supplementary References

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