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Access to Indenofluorene Skeletons via Pd-Catalyzed Sequential Reaction Involving Cyclization of Indenone-Allenyne intermediates

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I. General information

Where possible, reagents were purchased form commercial sources (Adamas, Aladdin, Innochem, Bidepharm and Leyan) Solvents were purified and dried by distillation: tetrahydrofuran and toluene from sodium/benzophenone, acetonitrile, triethylamine and diisopropylamine from calcium hydride. Other solvents and all reagents were used without further purification unless otherwise noted. All reactions were performed under nitrogen atmosphere unless otherwise noted. All reactions were isolated from moisture and oxygen by a nitrogen atmosphere with a sealed 25.0 mL schlenk tube and heated in a heating module (heater + magnetic stirrer). All work-up and purification procedures were carried out with reagent-grade solvents in air.

Analytical thin-layer chromatography (TLC) was performed using Huang Hai HSGF254 (0.25 mm) precoated plates. The developed chromatogram was analyzed by UV lamp (254 nm). Flash column chromatography was performed with silica gel (200–300 mesh) or Neutral alumina (200–300 mesh). The ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE III 400 MHz Spectrometer as solutions in $CDCl_3$. Chemical shifts are given in δ-scale. ^{1}H NMR and ^{13}C NMR spectra were referenced to residual peak of $CDCl_3$ (^{1}H, δ = 7.26; ^{13}C, δ = 77.16), coupling constants *J* are given in Hz. High resolution mass spectra (HRMS) were obtained from Agilent 6545 Q-TOF LCMS with electrospray ionization (ESI). Single-crystal diffraction data were collected on a Rigaku synergy diffractometer using Mo-Kα （λ= 0.71073 Å) radiation from a graphite monochromator.

II. General Procedure for the Synthesis of 1-(2-iodoaryl)ynones 1:

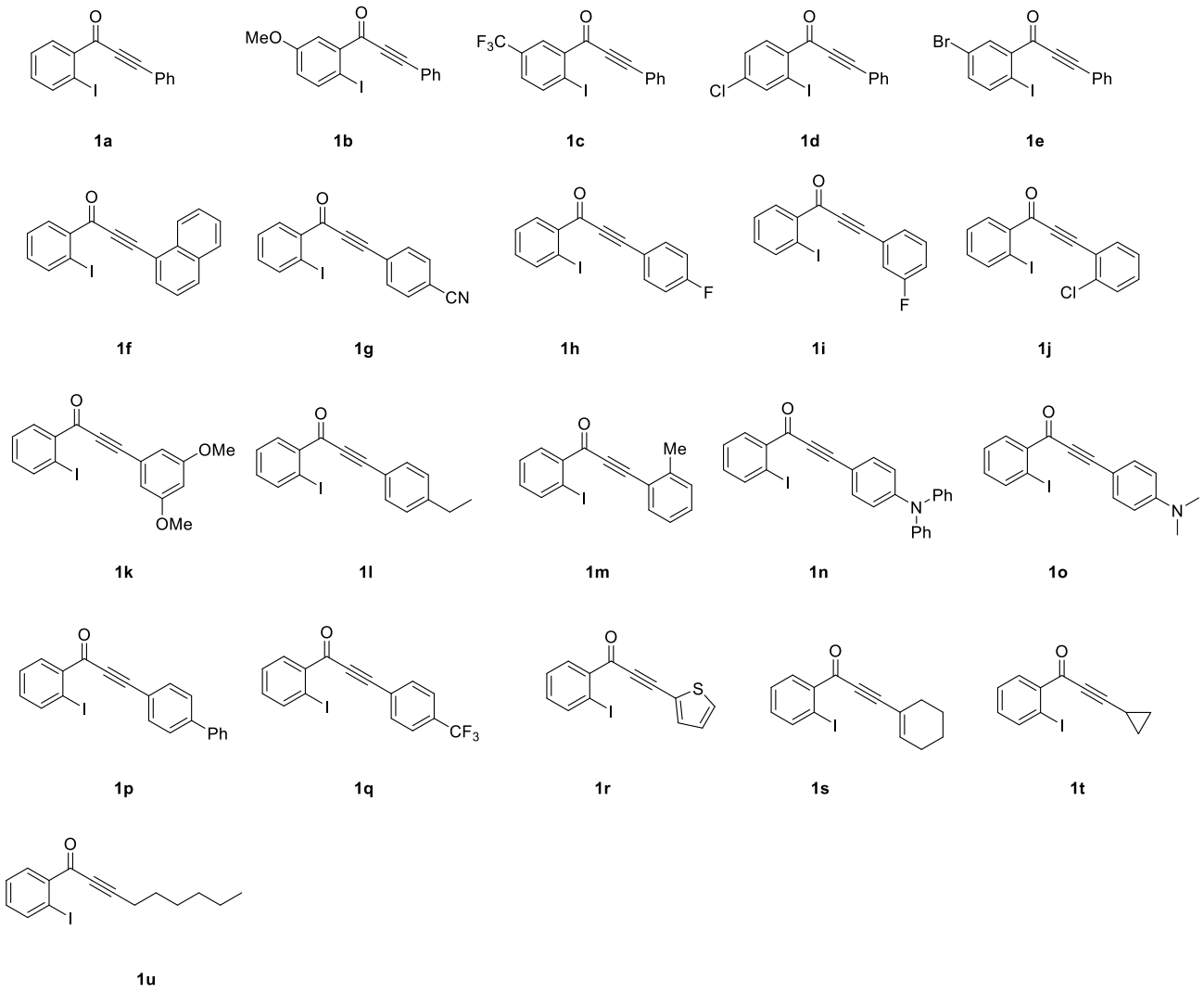
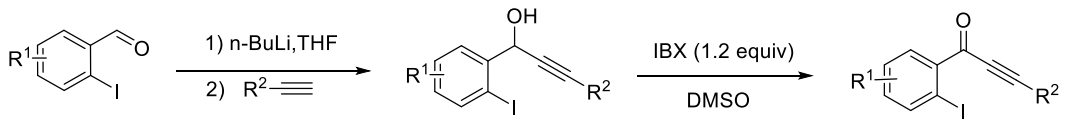


Figure S1. Structures of Substrates 1

Procedure A: General Procedure for the preparation of 1a-1e an1g-1y[1, 2]

1a-1e, 1g, 1l, 1q, 1s, 1u were known compounds. Other 1-(2-iodophenyl)-3-arylprop-2-yn-1-ones were synthesized as follows:

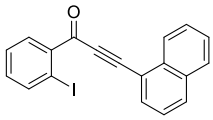


Step 1: n-BuLi (2.4 mL, 6.0 mmol, 2.5 M solution in hexanes, 1.2 equiv) was added dropwise to a solution of alkyne (6.0 mmol, 1.2 equiv) in anhydrous THF (10 mL) under nitrogen at -78 °C. After 30 min of stirring, 2-iodoaryl aldehyde (5.0 mmol) in THF (5.0 mL) was added and the reaction

mixture was stirred for 4 h at ambient temperature. Then NH_4Cl_{aq} was used to quench the reaction mixture, it was extracted with ethyl acetate for three times, the combined organic fractions were washed with the saturated aqueous solution of NaCl, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. the residue was purified by column chromatography on silica gel (petroleum ether / ethyl acetate) to afford propargyl alcohol.

Step 2: To a solution of substituted alkynol (4.0 mmol) in DMSO (8.0 mL) in round-bottom flask, IBX (1.34 g, 4.8 mmol) was added at room temperature. The reaction was stirred in air until the full conversion of substituted alkynol monitored by TLC. The resulting mixture was quenched with water and filtered. Then the filtrate was extracted with ethyl acetate (3× 15.0 mL). The organic layers was combined, washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. Purification by column chromatography with petroleum ether/ethyl acetate.

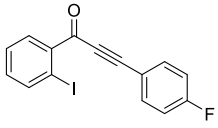
1-(2-iodophenyl)-3-(naphthalen-1-yl)prop-2-yn-1-one (1f)



Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a yellow foam after column chromatography (1.45 g, total yield: 76%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.38 (d, *J* = 8.3 Hz, 1 H), 8.23 (d, *J* = 7.7 Hz, 1 H), 8.09 (d, *J* = 7.9 Hz, 1 H), 7.99 (d, *J* = 8.3 Hz, 1 H), 7.95–7.88 (m, 2 H), 7.64 (t, *J* = 7.5 Hz, 1 H), 7.60–7.48 (m, 3 H), 7.26–7.21 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.22, 142.32, 133.90, 133.55, 133.54, 133.49, 133.24, 133.10, 133.08, 131.89, 128.73, 128.27, 127.95, 127.14, 125.97, 125.33, 117.67, 93.01, 92.06 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{19}H_{12}IO^+$ 382.9927; found 382.9926.

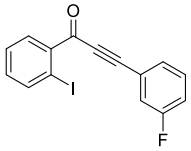
3-(4-fluorophenyl)-1-(2-iodophenyl)prop-2-yn-1-one (1h)

Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was



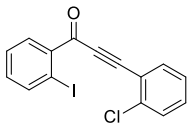
obtained as a yellow foam after column chromatography (1.28 g, total yield: 73%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.12–8.01 (m, 2 H), 7.68–7.61 (m, 2 H), 7.50 (t, *J* = 7.6 Hz, 1 H), 7.24–7.18 (m, 1 H), 7.14–7.08 (m, 2 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.06, 164.23 (d, *J* = 254.1 Hz), 142.24, 139.49, 135.52 (d, *J* = 8.9 Hz), 133.57, 133.02, 128.20, 116.38 (d, *J* = 22.3 Hz), 116.18 (d, *J* = 3.4 Hz), 93.42, 92.94, 87.23 (d, *J* = 1.5 Hz) ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{15}H_9FIO^+$ 350.9677; found 350.9673.

3-(3-fluorophenyl)-1-(2-iodophenyl)prop-2-yn-1-one (1i)



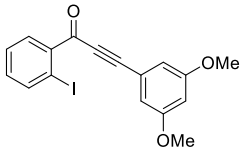
Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a yellow foam after column chromatography (1.37 g, total yield: 78%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.09 (ddd, *J* = 16.4, 7.8, 1.4 Hz, 2 H), 7.51 (td, *J* = 7.7, 1.2 Hz, 1 H), 7.46–7.42 (m, 1 H), 7.42–7.37 (m, 1 H), 7.37–7.32 (m, 1 H), 7.25–7.16 (m, 2 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 177.77, 162.31 (d, *J* = 248.6 Hz), 142.29, 139.12, 133.71, 133.19, 130.54 (d, *J* = 8.5 Hz), 129.02 (d, *J* = 3.2 Hz), 128.22, 121.78 (d, *J* = 9.4 Hz), 119.69 (d, *J* = 23.1 Hz), 118.48 (d, *J* = 21.2 Hz), 92.96, 92.35 (d, *J* = 3.4 Hz), 87.38 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{15}H_9FIO^+$ 350.9677; found 350.9673.

3-(2-chlorophenyl)-1-(2-iodophenyl)prop-2-yn-1-one (1j)



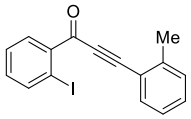
Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a yellow foam after column chromatography (1.32 g, total yield: 72%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.34 (d, *J* = 7.8 Hz, 1 H), 8.08 (d, *J* = 7.8 Hz, 1 H), 7.69 (d, *J* = 7.7 Hz, 1 H), 7.56–7.44 (m, 2 H), 7.44–7.38 (m, 1 H), 7.32 (t, *J* = 7.0 Hz, 1 H), 7.25–7.19 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 177.32, 142.43, 138.48, 137.66, 135.05, 134.09, 133.78, 132.02, 129.75, 128.20, 126.94, 120.28, 92.95, 91.05, 90.03 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{15}H_9ClIO^+$ 366.9381; found 366.9376.

3-(3,5-dimethoxyphenyl)-1-(2-iodophenyl)prop-2-yn-1-one (1k)



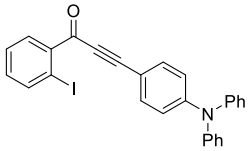
Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a yellow foam after column chromatography (1.49 g, total yield: 76%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.11 (d, *J* = 7.7 Hz, 1 H), 8.04 (d, *J* = 7.9 Hz, 1 H), 7.49 (t, *J* = 7.5 Hz, 1 H), 7.20 (t, *J* = 8.3 Hz, 1 H), 6.80–6.74 (m, 2 H), 6.57 (s, 1 H), 3.79 (s, 6 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.13, 160.81, 142.27, 139.51, 133.57, 133.17, 128.21, 121.25, 110.81, 104.51, 94.44, 92.96, 86.59, 55.71 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{14}IO_3^+$ 392.9982; found 392.9987.

1-(2-iodophenyl)-3-(o-tolyl)prop-2-yn-1-one (1m)



Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a yellow foam after column chromatography (1.25 g, total yield: 72%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.16 (d, *J* = 7.8 Hz, 1 H), 8.06 (d, *J* = 7.9 Hz, 1 H), 7.61 (d, *J* = 7.7 Hz, 1 H), 7.50 (t, *J* = 7.6 Hz, 1 H), 7.37 (t, *J* = 7.5 Hz, 1 H), 7.27 (d, *J* = 7.8 Hz, 1 H), 7.25–7.18 (m, 2 H), 2.54 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.11, 142.58, 142.25, 139.59, 133.75, 133.46, 133.07, 131.13, 130.01, 128.15, 126.04, 119.86, 93.62, 92.88, 91.09, 20.91 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{16}H_{12}IO^+$ 346.9927; found 346.9929.

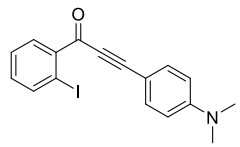
3-(4-(diphenylamino)phenyl)-1-(2-iodophenyl)prop-2-yn-1-one (1n)



Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a black foam after column chromatography (1.71 g, total yield: 68%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.06 (dd, *J* = 16.6, 7.4 Hz, 2 H), 7.51–7.28 (m, 7 H), 7.06 (dd, *J* = 70.4, 6.4 Hz, 9 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.35, 150.64, 146.46, 142.05, 140.25, 134.77, 133.89, 133.18, 132.73, 130.33, 129.78, 128.62,

128.12, 126.04, 124.84, 120.48, 111.06, 96.97, 92.89, 88.11 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{27}H_{19}INO^+$ 500.0506; found 500.0497.

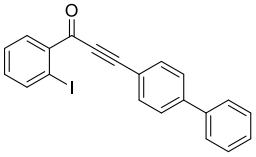
3-(4-(dimethylamino)phenyl)-1-(2-iodophenyl)prop-2-yn-1-one (1o)



Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a black foam after column chromatography (1.52 g, total yield: 81%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.24–7.99 (m, 2 H), 7.58 (q, *J* = 9.0, 8.2 Hz, 1 H), 7.53–7.43 (m, 3 H), 7.15 (t, *J* = 7.6 Hz, 1 H), 6.62 (d, *J* = 8.6 Hz, 1 H), 3.01 (s, 6 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.27, 151.93, 141.80, 135.30, 135.20, 133.64, 133.57, 132.88, 132.45, 130.18, 129.38, 128.50, 128.47, 128.02, 111.59, 105.25, 99.59, 92.69, 88.74, 40.01 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{15}INO^+$ 376.0193; found 376.0203.

3-([1,1'-biphenyl]-4-yl)-1-(2-iodophenyl)prop-2-yn-1-one (1p)

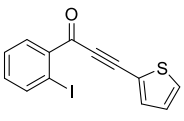
Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was



obtained as a yellow foam after column chromatography (1.47 g, total yield: 72%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.15 (dd, *J* = 7.8, 1.6 Hz, 1 H), 8.07 (d, *J* = 7.6 Hz, 1 H), 7.73 (d, *J* = 8.3 Hz, 2 H), 7.66–7.60 (m, 4 H), 7.54–7.45 (m, 3 H), 7.43–7.37 (m, 1 H), 7.22 (td, *J* = 7.7, 1.6 Hz, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.17, 143.90, 142.24, 139.83, 139.64, 133.75, 133.52, 133.10, 129.11, 128.36, 128.21, 127.45, 127.26, 118.76, 94.64, 92.98, 88.04 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{21}H_{14}IO^+$ 409.0084; found 409.0080.

1-(2-iodophenyl)-3-(thiophen-2-yl)prop-2-yn-1-one (1r)

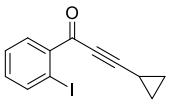
Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was



obtained as a yellow oil after column chromatography (1.34 g, total yield: 79%). **^{1}H**

NMR (400 MHz, $CDCl_3$): δ = 8.08–7.99 (m, 2 H), 7.58–7.51 (m, 2 H), 7.49 (t, *J* = 7.6 Hz, 1 H), 7.19 (td, *J* = 7.5, 1.2 Hz, 1 H), 7.10–7.05 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 177.69, 142.12, 139.35, 137.08, 133.50, 132.86, 132.24, 128.18, 127.93, 119.72, 92.90, 92.05, 88.71 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{13}H_8ISO^+$ 338.9335; found 338.9335.

3-cyclopropyl-1-(2-iodophenyl)prop-2-yn-1-one (1t)



Following the general procedure A starting with 5.0 mmol of 2-iodobenzaldehyde. The product was obtained as a yellow oil after column chromatography (1.29 g, total yield: 87%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.97 (t, *J* = 7.4 Hz, 2 H), 7.43 (t, *J* = 7.6 Hz, 1 H), 7.14 (t, *J* = 7.6 Hz, 1 H), 1.55–1.44 (m, 1 H), 1.05–0.97 (m, 4 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 178.02, 141.99, 139.70, 133.18, 132.87, 128.01, 102.69, 92.61, 76.04, 10.01 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{12}H_{10}IO^+$ 296.9771; found 296.9774.

III. General procedure for the synthesis of 1-(2-alkynylphenyl)propargyl ethers 2 and 8:

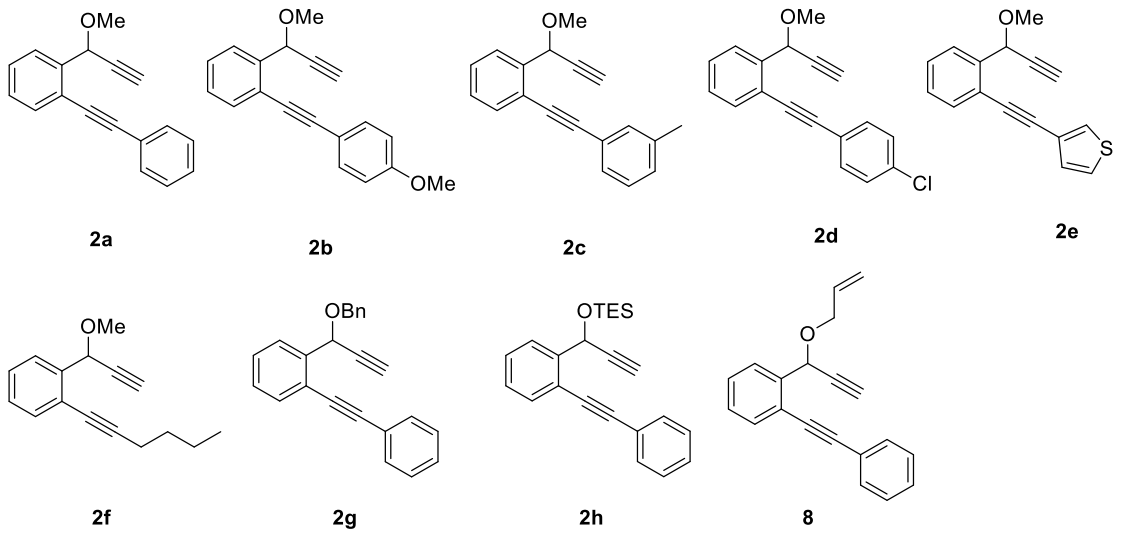
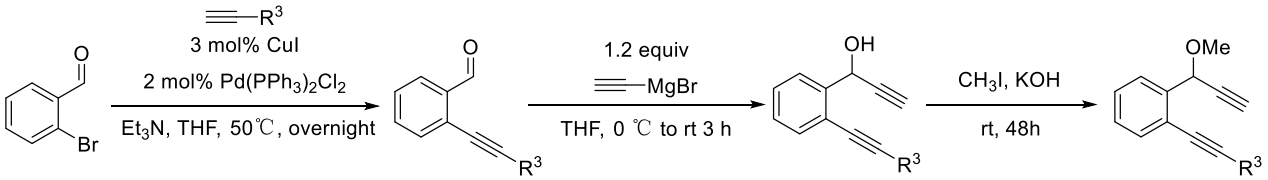


Figure S2. Structures of Substrates 2 and 8

Procedure B: General procedure for the synthesis of 2a–2f [3]



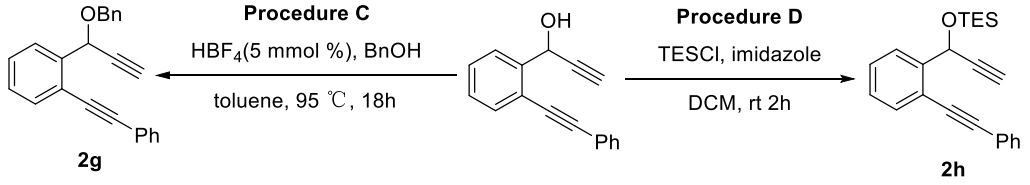
Step 1: To a stirred mixture of of 2-bromobenzaldehyde (1.850 g, 10.0 mmol, 1.0 equiv), 57 mg (3.0 mol %) of CuI, and 141 mg (2.0 mol %) of $Pd(PPh_3)_2Cl_2$ in 10 mL of THF was added of triethylamine (2.1 ml, 15.0 mmol, 1.5 equiv) under an atmosphere of N_2. A solution of terminal alkyne (12.0 mmol, 1.2 euqiv) in 10 mL of THF was then added. The reaction mixture was stirred at 50 ℃ overnight. After the reaction was complete (monitored by TLC), the reaction mixture was filtered and the solvent of the filtrate was reduced under the reduced pressure. After filtration and removal of the solvent in vacuo, the residue was purified by column chromatography on silica gel (eluent: petroleum ether/ ethyl acetate = 20/1) to afford aldehyde.

Step 2: To a solution of benzaldehyde (8.0 mmol) in THF (20.0 mL) was added ethynylmagnesium bromide (19.2 mL, 9.6 mmol, 0.5 M solution in THF, 1.2 euqiv) dropwise at 0 ℃. The resulting solution was warmed up to room temperature and stirred for 3 h. Then the mixture was quenched with

saturated ammonium chloride solution, extracted with ethyl acetate, washed with brine, and dried over anhydrous Na_2SO_4. The solvent was evaporated under the reduced pressure and the residue was purified by column chromatography on silica gel (eluent: petroleum ether / ethyl acetate = 8/1) to afford propargyl alcohol.

Step 3: To a solution of propargyl alcohol (6.0 mmol) and water (2.0 mL) was added potassium hydroxide (672 mg, 12.0 mmol, 2.0 equiv) and MeI (1.703 g, 12.0 mmol, 2.0 equiv). The mixture was stirred rapidly for 48 h. The crude mixture was then extracted with Et_2O. The organic layer was dried over anhydrous Na_2SO_4, filtered, and the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether / ethyl acetate = 60/1) to afford **2**.

Procedure C and Procedure D: General procedure for the synthesis of 2g and 2h [4, 5]

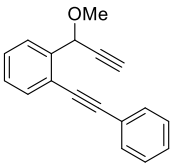


Procedure C: In a vial fitted with a screw cap and a stirring bar, the propargylic alcohol (10.0 mmol, 1.0 equiv), benzylalcohol (5.0 ml, 5.0 equiv) and toluene (20.0 mL) were introduced. An aqueous solution of HBF_4 (40 wt.%, 80 μL, 5.0 mol%) was then added, and the reaction mixture was stirred at 95 °C for 18 h. The reaction was quenched with a saturated aqueous solution of $NaHCO_3$ and the mixture extracted with EtOAc. The combined organic extracts were washed with brine, dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification of the crude product with silica gel flash column chromatography.

Procedure D: To a solution of the propargylic alcohol (0.75 mL, 6.0 mmol) in 30 mL of DCM was added imidazole (1.086 g, 8.4 mmol, 1.4 equiv). Then chlorotriethylsilane (0.9 g, 7.2 mmol, 1.2 equiv) was added dropwise to the solution at 0 °C. The reaction was quenched with water (15.0 mL) at room

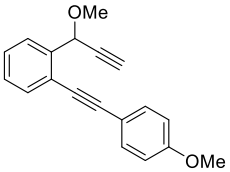
temperature and the resulting mixture was extracted with DCM (3 × 15.0 mL). The organic layer was dried (Na_2SO_4) and concentrated to leave a residue, which was chromatographed on silica gel with petroleum ether–ethyl acetate (100:1) to give the **2i** (1.517 g, 73%) as a colorless oil.

1-(1-methoxyprop-2-yn-1-yl)-2-(phenylethynyl)benzene (2a)



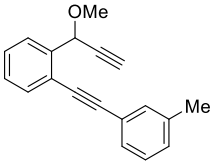
Following the general procedure B starting with 15.0 mmol of 2-bromobenzaldehyde. The product was obtained as a pale yellow oil after column chromatography (2.59 g, total yield: 70%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.75 (d, *J* = 7.7 Hz, 1 H), 7.58–7.53 (m, 3 H), 7.42–7.31 (m, 5 H), 5.58 (d, *J* = 2.0 Hz, 1 H), 3.54 (d, *J* = 0.8 Hz, 3 H), 2.64 (d, *J* = 2.2 Hz, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.73, 132.30, 131.66, 128.89, 128.64, 128.54, 128.52, 127.26,123.34, 123.14, 122.52, 94.41, 86.77, 81.40, 75.46, 71.04, 57.04 ppm. **HRMS** (ESI) m/z: [M + H]$^+$ calcd for $C_{18}H_{15}O^+$ 247.1117; found 247.1109.

1-((4-methoxyphenyl)ethynyl)-2-(1-methoxyprop-2-yn-1-yl)benzene (2b)



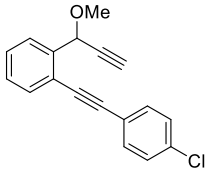
Following the general procedure B starting with 5.0 mmol of 2-bromobenzaldehyde. The product was obtained as a pale yellow oil after column chromatography (0.82 g, total yield: 60%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.82–7.75 (m, 1 H), 7.60–7.52 (m, 3 H), 7.40 (td, *J* = 7.6, 1.6 Hz, 1 H), 7.34 (td, *J* = 7.5, 1.5 Hz, 1 H), 6.94 –6.89 (m, 2 H), 5.66–5.61 (m, 1 H), 3.81 (s, 3 H), 3.57 (s, 3 H), 2.73–2.66 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 159.90, 139.46, 133.07, 132.06, 128.49, 128.46, 127.16, 122.83, 115.17, 114.14, 94.48, 85.45, 81.44, 75.36, 71.00, 56.94, 55.33 ppm. **HRMS** (ESI) m/z: [M + Na]$^+$ calcd for $C_{19}H_{16}NaO_2^+$ 299.1043; found 299.1043.

1-(1-methoxyprop-2-yn-1-yl)-2-(m-tolylethynyl)benzene (2c)



Following the general procedure B starting with 5.0 mmol of 2-bromobenzaldehyde. The product was obtained as a pale yellow oil after column chromatography (0.74 g, total yield: 57%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.75 (d, *J* = 7.7 Hz, 1 H), 7.55 (d, *J* = 7.5 Hz, 1 H), 7.42–7.30 (m, 4 H), 7.26 (t, *J* = 7.6 Hz, 1 H), 7.18 (d, *J* = 7.6 Hz, 1 H), 5.65–5.51 (m, 1 H), 3.54 (d, *J* = 1.6 Hz, 3 H), 2.68–2.59 (m, 1 H), 2.38 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.73, 138.26, 132.33, 132.22, 129.59, 128.86, 128.82, 128.57, 128.46, 127.28, 122.99, 122.68, 94.64, 86.43, 81.50, 75.42, 71.06, 57.07, 21.40 ppm. **HRMS** (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{16}NaO^+$ 283.1093; found 283.1095.

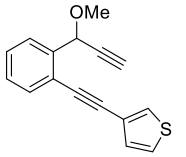
1-((4-chlorophenyl)ethynyl)-2-(1-methoxyprop-2-yn-1-yl)benzene (2d)



Following the general procedure B starting with 5.0 mmol of 2-bromobenzaldehyde. The product was obtained as a pale yellow oil after column chromatography (0.77 g, total yield: 55%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 7.8 Hz, 1 H), 7.56 (d, *J* = 7.6 Hz, 1 H), 7.52–7.46 (m, 2 H), 7.42 (td, *J* = 7.7, 1.3 Hz, 1 H), 7.38–7.32 (m, 3 H), 5.59–5.53 (m, 1 H), 3.56–3.53 (m, 3 H), 2.69–2.66 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.64, 134.62, 132.83, 132.31, 129.10, 128.85, 128.59, 127.27, 122.10, 121.55, 93.23, 87.67, 81.19, 75.62, 70.96, 56.99 ppm. **HRMS** (ESI) m/z: $[M + Na]^+$ calcd for $C_{18}H_{13}ClNaO^+$ 303.0547; found 303.0547.

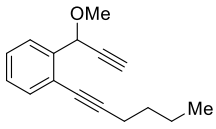
3-((2-(1-methoxyprop-2-yn-1-yl)phenyl)ethynyl)thiophene (2e)

Following the general procedure B starting with 5.0 mmol of 2-bromobenzaldehyde. The product was



obtained as a colorless oil after column chromatography (0.91 g, total yield: 72%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.76 (d, *J* = 7.7 Hz, 1 H), 7.61–7.46 (m, 2 H), 7.40 (t, *J* = 7.6 Hz, 1 H), 7.36–7.30 (m, 2 H), 7.25–7.19 (m, 1 H), 5.57 (s, 1 H), 3.54 (s, 3 H), 2.69–2.59 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.65, 132.23, 129.87, 128.95, 128.83, 128.55, 127.27, 125.64, 122.50, 122.16, 89.54, 86.28, 81.38, 75.46, 71.01, 57.01 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{16}H_{13}OS^+$ 253.0682; found 253. 0683.

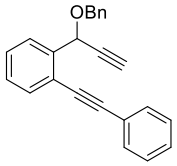
1-(hex-1-yn-1-yl)-2-(1-methoxyprop-2-yn-1-yl)benzene (2f)



Following the general procedure B starting with 5.0 mmol of 2-bromobenzaldehyde. The product was obtained as a colorless oil after column chromatography (0.75 g, total yield: 66%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.69 (dd, *J* = 7.8, 1.4 Hz, 1 H), 7.42 (dd, *J* = 7.6, 1.3 Hz, 1 H), 7.33 (td, *J* = 7.6, 1.5 Hz, 1 H), 7.26 (td, *J* = 7.5, 1.5 Hz, 1 H), 5.51 (d, *J* = 2.2 Hz, 1 H), 3.49 (s, 3 H), 2.61 (d, *J* = 2.2 Hz, 1 H), 2.48 (t, *J* = 7.0 Hz, 2 H), 1.67–1.59 (m, 2 H), 1.57–1.47 (m, 2 H), 0.97 (t, *J* = 7.3 Hz, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.53, 132.27, 128.37, 128.07, 127.08, 123.35, 95.68, 81.62, 77.98, 75.10, 70.90, 56.80, 30.90, 22.12, 19.35, 13.71 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{16}H_{19}O^+$ 227.1430; found 227.1429.

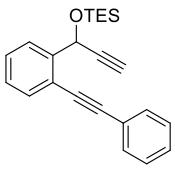
1-(1-(benzyloxy)prop-2-yn-1-yl)-2-(phenylethynyl)benzene (2g)

Following the general procedure B Step 1, 2 and procedure C starting with 5.0 mmol of 2-



bromobenzaldehyde. The product was obtained as a colorless oil after column chromatography (0.77 g, total yield: 48%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.89 (dd, *J* = 7.8, 1.4 Hz, 1 H), 7.61 (dd, *J* = 7.6, 1.1 Hz, 1 H), 7.50–7.42 (m, 5 H), 7.42–7.26 (m, 7 H), 5.82 (d, *J* = 2.2 Hz, 1 H), 4.91–4.74 (m, 2 H), 2.72 (d, *J* = 2.2 Hz, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.87, 137.49, 132.27, 131.66, 128.95, 128.56, 128.54, 128.45, 128.41, 128.28, 127.86, 127.60, 122.99, 122.41, 94.34, 86.75, 81.62, 75.63, 71.06, 68.61 ppm. **HRMS** (ESI) m/z: $[M + Na]^+$ calcd for $C_{24}H_{18}NaO^+$ 345.1250; found 345.1255.

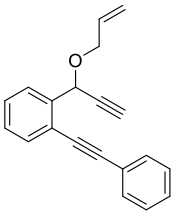
triethyl((1-(2-(phenylethynyl)phenyl)prop-2-yn-1-yl)oxy)silane (2h)



Following the general procedure B Step 1, 2 and procedure D starting with 10.0 mmol of 2-bromobenzaldehyde. The product was obtained as a colorless oil after column chromatography (1.42 g, total yield: 82%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.80 (d, *J* = 7.9 Hz, 1 H), 7.61–7.51 (m, 3 H), 7.45–7.36 (m, 4 H), 7.30 (t, *J* = 7.5 Hz, 1 H), 6.03 (s, 1H), 2.54

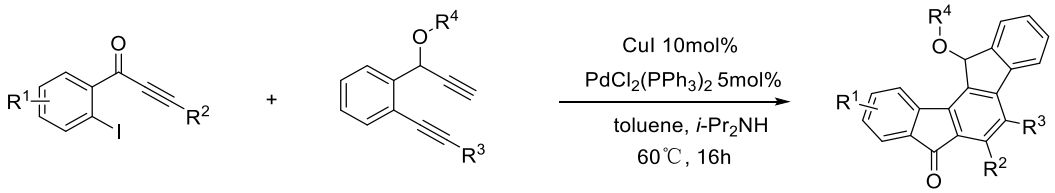
(s, 1 H), 0.99 (t, J = 7.9 Hz, 9 H), 0.76–0.66 (m, 6 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 143.40, 132.04, 131.63, 129.06, 128.57, 128.54, 127.88, 126.50, 123.33, 120.70, 94.70, 86.86, 84.66, 73.03, 62.59, 6.86, 4.92 ppm. **HRMS** (ESI) m/z: $[M + Na]^+$ calcd for $C_{23}H_{26}NaOSi^+$ 369.1645; found 369.1660.

triethyl((1-(2-(phenylethynyl)phenyl)prop-2-yn-1-yl)oxy)silane (8)



8 were prepared according to the known methods.[3] **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.79 (d, J = 7.7 Hz, 1 H), 7.58–7.53 (m, 3 H), 7.43–7.31 (m, 5 H), 6.04–5.93 (m, 1 H), 5.73 (s, 1 H), 5.35 (d, J = 17.2 Hz, 1 H), 5.20 (d, J = 10.4 Hz, 1 H), 4.34–4.28 (m, 1 H), 4.20–4.14 (m, 1 H), 2.63 (s, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 139.97, 134.23, 132.33, 131.68, 129.00, 128.65, 128.54, 127.54, 123.22, 122.46, 118.15, 94.39, 86.85, 81.73, 75.31, 70.22, 68.53 ppm.

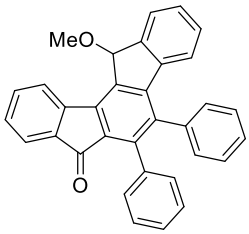
IV. General procedure for the synthesis of 3:



1 2 3

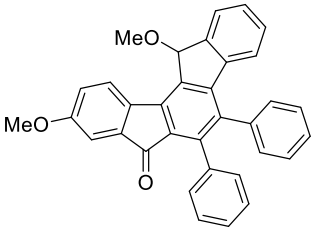
Procedure E: An oven-dried 25 mL Schlenk tube was charged with the substrates **1** (0.25 mmol, 1.0 equiv), **2** (0.3 mmol, 1.2 equiv), $Pd(PPh_3)_2Cl_2$ (8.8 mg, 5 mol%), CuI (4.8 mg, 10 mol%), DIPA (0.1 mL) and toluene (2.0 mL) under nitrogen atmosphere. Then the reaction mixture was stirred at 60 °C for 16 h. After cooling the reaction mixture to room temperature, the reaction mixture was purified by flash column chromatography on silica gel (PE/EA = 10/1) to afford the desired products **3**.

12–methoxy–5,6–diphenylindeno[1,2–a]fluoren–7(12H)–one (3aa)



Yellow foam (103.6 mg, 92% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.24 (d, *J* = 7.4 Hz, 1 H), 7.69 (d, *J* = 7.4 Hz, 1 H), 7.63–7.58 (m, 2 H), 7.38–7.32 (m, 2 H), 7.31–7.28 (m, 3 H), 7.25–7.11 (m, 6 H), 7.09–7.01 (m, 2 H), 6.30 (d, *J* = 7.9 Hz, 1 H), 6.05 (s, 1 H), 3.07 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.76, 144.94, 143.98, 142.84, 142.31, 141.42, 140.46, 137.96, 137.81, 136.21, 135.39, 135.26, 134.89, 134.66, 130.18, 130.06, 129.88, 129.66, 129.51, 129.32, 129.09, 128.67, 128.49, 128.45, 127.53, 127.39, 127.33, 127.07, 125.37, 124.66, 124.17, 123.85, 79.46, 51.12 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{23}O_2^+$ 451.1693; found 451.1695.

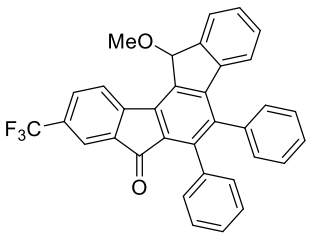
9,12-dimethoxy-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (3ba)



Yellow foam (85.3 mg, 71% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.11 (d, *J* = 8.3 Hz, 1 H), 7.67 (d, *J* = 7.5 Hz, 1 H), 7.35–7.26 (m, 4 H), 7.25–7.17 (m, 3 H), 7.17–6.98 (m, 7 H), 6.29 (d, *J* = 7.9 Hz, 1 H), 5.98 (s, 1 H), 3.85 (s, 3 H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.58, 161.05, 144.94, 144.03, 142.81,

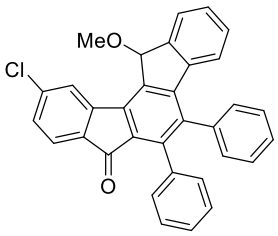
141.72, 140.51, 137.86, 137.28, 136.85, 136.26, 134.85, 134.66, 134.15, 130.28, 130.13, 130.10, 129.66, 129.52, 129.01, 128.59, 128.45, 128.40, 127.44, 127.36, 127.29, 127.01, 125.73, 125.32, 124.15, 120.17, 109.05, 79.47, 55.76, 51.03 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{25}O_3^+$ 481.1798; found 481.1800.

12-methoxy-5,6-diphenyl-10-(trifluoromethyl)indeno[1,2-a]fluoren-7(12H)-one (3ca)



Yellow foam (95.9 mg, 74% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.37 (d, *J* = 7.9 Hz, 1 H), 7.90–7.78 (m, 2 H), 7.68 (d, *J* = 7.4 Hz, 1 H), 7.36–7.32 (m, 1 H), 7.31–7.26 (m, 3 H), 7.25–7.16 (m, 3 H), 7.15–7.04 (m, 4 H), 7.02–6.97 (m, 1 H), 6.29 (d, *J* = 7.9 Hz, 1 H), 6.05 (s, 1 H), 3.05 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 191.07, 145.47, 145.30 (q, J_{C-F} = 1.0 Hz), 143.80, 143.39, 140.23, 140.07, 139.02, 137.47, 136.30, 135.79, 135.77, 131.74 (q, J_{C-F} = 3.7 Hz), 131.43 (q, J_{C-F} = 32.8 Hz), 130.05, 130.02, 129.93, 129.60, 129.44, 129.29, 129.02, 128.60, 128.56, 127.75, 127.53, 127.47, 127.34, 125.44, 124.92, 124.37, 123.92 (q, J_{C-F} = 272.4 Hz), 120.67 (q, J_{C-F} = 3.8 Hz) 79.45, 51.17 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -62.79 (s, 3 F) ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{22}F_3O_2^+$ 519.1566; found 519.1566.

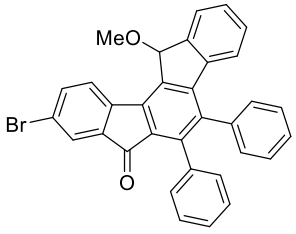
10-chloro-12-methoxy-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (3da)



Yellow foam (100.6 mg, 83% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.24 (d, *J* = 1.7 Hz, 1 H), 7.69 (d, *J* = 7.5 Hz, 1 H), 7.52 (d, *J* = 7.8 Hz, 1 H), 7.36–7.27 (m, 5 H), 7.16–7.25 (m, 3 H), 7.16–7.05 (m, 4 H), 7.04–6.96 (m, 1 H), 6.30 (d, *J* = 7.9 Hz, 1 H), 6.03 (s, 1 H), 3.08 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 191.32, 145.07, 143.90, 143.85, 143.07, 141.09, 140.31, 140.10, 138.59, 137.59, 135.93, 135.78, 133.64, 130.10, 129.95, 129.62, 129.46, 129.30, 129.18, 128.88, 128.55, 128.50, 127.64, 127.45, 127.38, 127.20, 125.42, 125.08, 124.84, 124.27, 79.38, 51.21 ppm. **HRMS** (ESI) m/z:

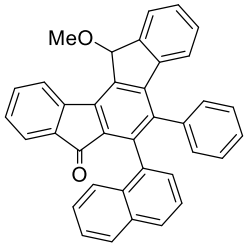
[M + H]$^+$ calcd for $C_{33}H_{22}ClO_2^+$ 485.1303; found 485.1303.

9–bromo–12–methoxy–5,6–diphenylindeno[1,2–a]fluoren–7(12H)–one (3ea)



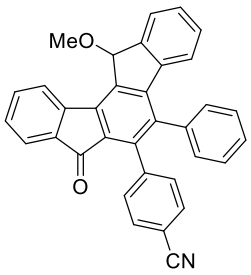
Yellow foam (113.8 mg, 86% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.09 (d, *J* = 7.8 Hz, 1 H), 7.73–7.59 (m, 3 H), 7.34–7.24 (m, 4 H), 7.23–7.14 (m, 3 H), 7.14–7.02 (m, 4 H), 7.02–6.94 (m, 1 H), 6.27 (d, *J* = 7.9 Hz, 1 H), 5.97 (s, 1 H), 3.02 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 191.18, 145.27, 143.84, 143.15, 140.87, 140.59, 140.27, 138.29, 137.58, 137.34, 137.02, 135.89, 135.43, 134.66, 130.08, 129.95, 129.58, 129.44, 129.17, 128.86, 128.53, 128.49, 127.63, 127.45, 127.39, 127.22, 126.99, 126.11, 125.36, 124.28, 123.48, 79.41, 51.08 ppm. **HRMS** (ESI) m/z: [M + H]$^+$ calcd for $C_{33}H_{22}BrO_2^+$ 529.0798; found 529.0801.

12-methoxy-6-(naphthalen-1-yl)-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3fa)



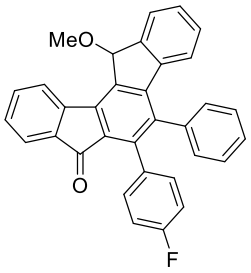
Yellow foam (101.4 mg, 81% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.77 (d, *J* = 8.2 Hz, 1 H), 7.69 (d, *J* = 7.9 Hz, 2 H), 7.61–7.53 (m, 2 H), 7.48 (d, *J* = 7.2 Hz, 1 H), 7.37 (t, *J* = 7.5 Hz, 1 H), 7.35–7.25 (m, 4 H), 7.24–7.18 (m, 2 H), 7.14–6.99 (m, 3 H), 6.92 (t, *J* = 7.5 Hz, 1 H), 6.89–6.83 (m, 1 H), 6.26 (d, *J* = 7.9 Hz, 1 H), 6.07 (s, 1 H), 3.13 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.17, 145.20, 144.00, 142.47, 141.25, 140.79, 140.47, 138.74, 137.64, 135.77, 135.33, 134.83, 134.63, 133.07, 132.81, 131.12, 130.05, 129.31, 129.11, 128.69, 128.50, 128.37, 128.30, 128.25, 128.13, 127.65, 127.51, 126.84, 125.77, 125.47, 125.38, 124.90, 124.72, 124.27, 123.88, 79.64, 51.33 ppm. **HRMS** (ESI) m/z: [M + H]$^+$ calcd for $C_{37}H_{25}O_2^+$ 501.1849; found 501.1849.

4-(12-methoxy-7-oxo-5-phenyl-7,12-dihydroindeno[1,2-a]fluoren-6-yl)benzonitrile (3ga)



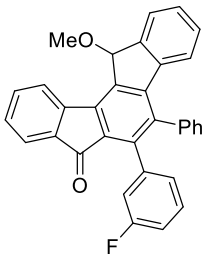
Yellow foam (80.8 mg, 68% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.69 (d, *J* = 7.5 Hz, 1 H), 7.58–7.64 (m, 2 H), 7.52 (d, *J* = 8.0 Hz, 1 H), 7.46 (d, *J* = 8.0 Hz, 1 H), 7.38–7.25 (m, 6 H), 7.14–7.06(m, 4 H), 6.31 (d, *J* = 7.9 Hz, 1 H), 6.03 (s, 1 H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.59, 145.31, 143.94, 142.22, 141.59, 141.53, 140.46, 140.05, 137.20, 137.00, 136.19, 135.24, 135.06, 131.22, 131.17, 130.65, 130.48, 130.01, 129.86, 129.60, 129.54, 129.23, 129.00, 128.81, 128.79, 128.04, 125.47, 124.88, 124.21, 123.99, 119.11, 110.95, 79.43, 51.23 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{22}NO_2^+$ 476.1645; found 476.1652.

6-(4-fluorophenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3ha)



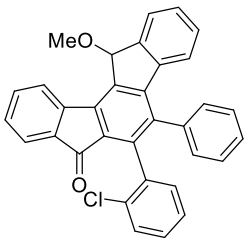
Yellow foam (90.2 mg, 77% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.4 Hz, 1 H), 7.69 (d, *J* = 7.5 Hz, 1 H), 7.64–7.56 (m, 2 H), 7.36–7.29 (m, 5 H), 7.14–7.05 (m, 4 H), 7.01–6.85 (m, 3 H), 6.30 (d, *J* = 7.9 Hz, 1 H), 6.02 (s, 1H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.77, 161.95 (d, $J_{C\text{-}F}$ = 245.7 Hz), 145.04, 143.96, 142.22, 141.70, 141.45, 140.32, 138.00, 137.64, 135.46, 135.28, 134.98, 134.67, 131.99 (d, $J_{C\text{-}F}$ = 3.5 Hz), 131.41 (d, $J_{C\text{-}F}$ = 8.1 Hz), 131.26 (d, $J_{C\text{-}F}$ = 8.1 Hz), 130.14, 129.98, 129.89, 129.37, 129.11, 128.75, 128.62, 128.60, 127.66, 125.38, 124.70, 124.16, 123.85, 114.54 (d, $J_{C\text{-}F}$ = 4.6 Hz), 114.32 (d, $J_{C\text{-}F}$ = 4.7 Hz), 79.41, 51.12 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -115.18–-115.29 (m, 1 F) ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{22}FO_2^+$ 469.1598; found 469.1598.

6-(3-fluorophenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3ia)



Yellow foam (83.2 mg, 71% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.4 Hz, 1 H), 7.69 (d, *J* = 7.5 Hz, 1 H), 7.64–7.57 (m, 2 H), 7.38–7.28 (m, 5 H), 7.23–7.04 (m, 4 H), 6.97–6.85 (m, 2 H), 6.83–6.71 (m, 1 H), 6.30 (d, *J* = 7.9 Hz, 1 H), 6.03 (s, 1 H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.56, 162.14 (d, *J* = 245.0 Hz), 145.07, 143.95, 142.25, 141.42, 141.20 (d, J_{C-F} = 1.9 Hz), 140.28, 138.51, 138.43, 137.67, 137.42 (d, J_{C-F} = 1.6 Hz), 135.65, 135.25, 135.01, 130.08, 130.01, 129.95, 129.86, 129.78, 129.42, 129.14, 128.92, 128.85 (d, J_{C-F} = 2.3 Hz), 128.79, 128.65 (d, J_{C-F} = 4.5 Hz), 128.57 (d, J_{C-F} = 2.6 Hz), 127.74 (d, J_{C-F} = 1.6 Hz), 125.54 (d, J_{C-F} = 2.9 Hz), 125.39, 125.37, 124.74, 124.19, 123.90, 116.88 (d, J_{C-F} = 14.5 Hz), 116.66 (d, J_{C-F} = 14.5 Hz), 114.02 (d, J_{C-F} = 21.0 Hz) 79.44, 51.16, 51.14 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -114.39–-114.63 (m, 1 F) ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{22}FO_2^+$ 469.1598; found 469.1597.

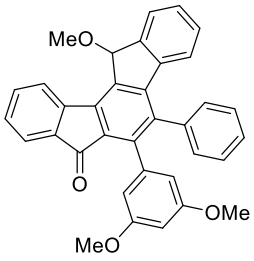
6-(2-chlorophenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3ja)



Yellow foam (116.4 mg, 96% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.24 (d, *J* = 7.4 Hz, 1 H), 7.69 (d, *J* = 7.5 Hz, 1 H), 7.64–7.57 (m, 2 H), 7.37–7.27 (m, 7 H), 7.21–7.14 (m, 2 H), 7.08 (t, *J* = 7.5 Hz, 2 H), 7.00–6.92 (m, 1 H), 6.33 (d, *J* = 7.8 Hz, 1 H), 6.06 (s, 1 H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.35, 145.12, 143.80, 142.47, 141.04, 140.28, 139.17, 137.54, 137.33, 135.87, 135.71, 135.16, 134.83, 134.67, 133.38, 130.60, 130.16, 129.79, 129.23, 128.98, 128.68, 128.65, 128.60, 128.14, 127.69, 125.97, 125.23, 124.65, 124.05, 123.83, 79.44, 51.01 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{22}ClO_2^+$ 485.1303; found 485.1300.

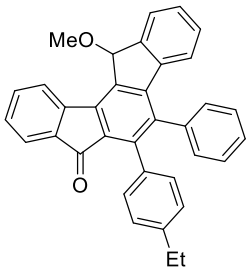
6-(3,5-dimethoxyphenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3ka)

Yellow foam (79.1 mg, 62% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.68 (d, *J* = 7.5 Hz, 1 H), 7.64–7.57 (m, 2 H), 7.36–7.29 (m, 5 H), 7.18–7.13 (m, 2 H), 7.06 (t, *J* = 7.6 Hz,



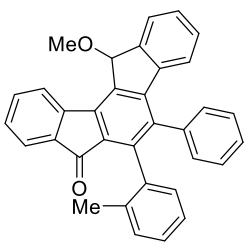
1 H), 6.37–6.24 (m, 3 H), 6.19 (s, 1 H), 6.03 (s, 1 H), 3.69 (s, 3 H), 3.63 (s, 3 H), 3.05 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.38, 159.84, 159.83, 144.89, 143.95, 142.52, 142.23, 141.41, 140.43, 137.94, 137.80, 137.73, 135.37, 135.27, 134.84, 134.65, 130.06, 129.92, 129.77, 129.30, 129.06, 128.65, 128.49, 128.48, 127.60, 125.34, 124.63, 124.19, 123.85, 108.24, 108.00, 99.52, 79.43, 55.32, 55.29, 51.08 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{35}H_{27}O_4^+$ 511.1904; found 511.1900.

6-(4-ethylphenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3la)



Yellow foam (92.1 mg, 77% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.68 (d, *J* = 7.5 Hz, 1 H), 7.64–7.56 (m, 2 H), 7.37–7.28 (m, 5 H), 7.16–7.10 (m, 2 H), 7.09–7.00 (m, 4 H), 6.93 (d, *J* = 7.8 Hz, 1 H), 6.28 (d, *J* = 7.9 Hz, 1 H), 6.04 (s, 1 H), 3.06 (s, 3 H), 2.62 (q, *J* = 7.6 Hz, 2 H), 1.22 (t, *J* = 7.6 Hz, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.83, 144.91, 143.98, 143.08, 142.76, 142.31, 141.44, 140.53, 138.14, 137.95, 135.44, 135.08, 134.84, 133.25, 130.21, 130.08, 129.95, 129.62, 129.44, 129.27, 129.05, 128.60, 128.45, 128.43, 127.43, 126.83, 126.77, 125.34, 124.62, 124.17, 123.81, 79.44, 51.08, 28.63, 15.26 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{35}H_{27}O_2^+$ 479.2006; found 455.1999.

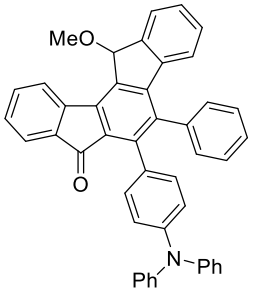
12-methoxy-5-phenyl-6-(o-tolyl)indeno[1,2-a]fluoren-7(12H)-one (3ma)



Yellow foam (90.6 mg, 78% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.70 (d, *J* = 7.5 Hz, 1 H), 7.63–7.58 (m, 2 H), 7.37–7.32 (m, 2 H), 7.32–7.24 (m, 3 H), 7.21–7.17 (m, 1 H), 7.14–7.09 (m, 3 H), 7.09–6.99 (m, 2 H), 6.88 (d, *J* = 7.5 Hz, 1 H), 6.31 (d, *J* = 7.9 Hz, 1 H), 6.05 (s, 1 H), 3.11 (s, 3 H), 2.13 (s, 3 H).ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.70, 145.23, 143.92, 142.51, 142.18, 141.22, 140.50, 137.83, 137.78, 136.14, 135.73, 135.36, 134.85, 130.33, 130.10, 129.29, 129.24,

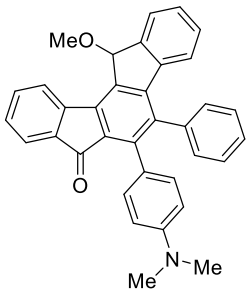
129.21, 129.08, 128.65, 128.52, 128.33, 127.64, 127.37, 125.38, 125.01, 124.67, 124.19, 123.83, 79.54, 51.25, 20.24 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{25}O_2^+$ 465.1849; found 465.1844

6-(4-(diphenylamino)phenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3na)



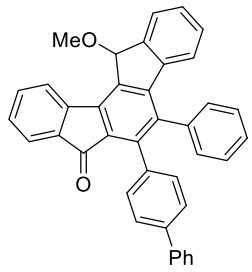
Yellow foam (137.4 mg, 89% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.25 (d, *J* = 7.5 Hz, 1 H), 7.71–7.65 (m, 2 H), 7.61 (t, *J* = 7.5 Hz, 1 H), 7.40–7.31 (m, 5 H), 7.25–7.21 (m, 3 H), 7.20–6.80 (m, 14 H), 6.43 (d, *J* = 7.9 Hz, 1 H), 6.05 (s, 1 H), 3.07 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 193.00, 147.86, 146.43, 144.80, 143.99, 142.82, 142.38, 141.44, 140.47, 138.35, 138.01, 135.43, 135.17, 134.93, 134.66, 130.88, 130.79, 130.63, 130.40, 130.28, 129.79, 129.34, 129.18, 129.08, 128.68, 128.42, 128.36, 127.37, 125.39, 124.70, 124.20, 124.08, 123.83, 123.31, 123.24, 122.53, 79.45, 51.11 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{45}H_{32}NO_2^+$ 618.2428; found 618.2418.

6-(4-(diphenylamino)phenyl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3oa)



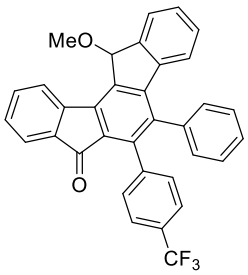
Yellow foam (49.4 mg, 40% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.22 (d, *J* = 7.5 Hz, 1 H), 7.67 (d, *J* = 7.5 Hz, 1 H), 7.63–7.56 (m, 2 H), 7.36–7.29 (m, 5 H), 7.16–7.11 (m, 2 H), 7.09–6.97 (m, 2 H), 6.93–6.81 (m, 1 H), 6.64 –6.51 (m, 2H), 6.25 (d, *J* = 7.9 Hz, 1 H), 6.04 (s, 1 H), 3.05 (s, 3 H), 2.92 (s, 6 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.92, 149.47, 144.89, 144.03, 143.58, 142.31, 141.60, 140.72, 138.52, 138.39, 135.64, 134.72, 134.57, 130.87, 130.68, 130.36, 130.22, 130.00, 129.17, 129.02, 128.52, 127.38, 125.33, 124.55, 124.19, 123.78, 111.35, 79.46, 51.03, 40.55 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{35}H_{28}NO_2^+$ 494.2115; found 494.2120.

6-([1,1'-biphenyl]-4-yl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3pa)



Yellow foam (105.3 mg, 80% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.24 (d, *J* = 7.5 Hz, 1 H), 7.69 (d, *J* = 7.6 Hz, 1 H), 7.64–7.57 (m, 4 H), 7.48 (d, *J* = 8.0 Hz, 1 H), 7.41 (q, *J* = 7.4 Hz, 3 H), 7.38–7.27 (m, 6 H), 7.22 (d, *J* = 8.0 Hz, 1 H), 7.16–7.11 (m, 2 H), 7.10–7.04 (m, 2 H), 6.29 (d, *J* = 7.9 Hz, 1 H), 6.06 (s, 1 H), 3.07 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.94, 145.08, 144.02, 142.59, 142.38, 141.55, 141.04, 140.51, 139.56, 138.11, 137.81, 135.43, 135.36, 135.27, 134.98, 130.26, 130.23, 130.10, 130.07, 129.94, 129.39, 129.14, 128.74, 128.59, 128.57, 127.62, 127.21, 127.16, 126.04, 125.98, 125.41, 124.73, 124.25, 123.93, 79.52, 51.16 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{39}H_{27}O_2^+$ 527.2006; found 527.2003.

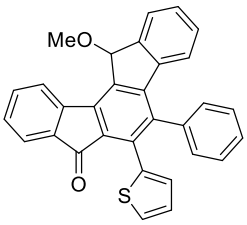
12-methoxy-5-phenyl-6-(4-(trifluoromethyl)phenyl)indeno[1,2-a]fluoren-7(12H)-one (3qa)



Yellow foam (95.9 mg, 74% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ =8.22 (d, *J* = 7.4 Hz, 1 H), 7.68 (d, *J* = 7.5 Hz, 1 H), 7.62–7.57 (m, 2 H), 7.47 (d, *J* = 8.0 Hz, 1 H), 7.42 (d, *J* = 8.1 Hz, 1 H), 7.37–7.24 (m, 6 H), 7.14–7.04 (m, 4 H), 6.28 (d, *J* = 7.9 Hz, 1 H), 6.02 (s, 1 H), 3.05 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.69, 145.26, 143.98, 142.27, 141.53, 141.13, 140.24, 140.16 (q, $J_{C\text{-}F}$ = 1.6 Hz), 137.58, 137.24, 135.92, 135.20, 135.15, 134.66, 130.19, 130.08, 130.02, 129.92, 129.75, 129.53, 129.20, 129.15 (q, $J_{C\text{-}F}$ = 32.4 Hz), 128.90, 128.73, 128.72, 127.90, 125.45, 124.83, 124.4 (q, $J_{C\text{-}F}$ = 272.7 Hz), 124.35 (q, $J_{C\text{-}F}$ = 3.6 Hz), 124.24, 123.96, 79.47, 51.20 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -62.41 (s, 3 F) ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{22}F_3O_2^+$ 519.1566; found 519.1570.

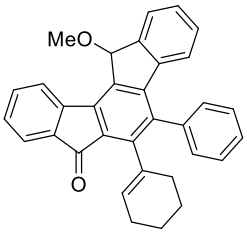
12-methoxy-5-phenyl-6-(thiophen-2-yl)indeno[1,2-a]fluoren-7(12H)-one (3ra)

Yellow foam (85.6 mg, 75% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.68 (d, *J* = 7.5 Hz, 1 H), 7.66–7.57 (m, 2 H), 7.38–7.30 (m, 5 H), 7.29–7.25 (m, 1 H), 7.23 –7.15 (m, 2 H),



7.07 (t, *J* = 7.7 Hz, 1 H), 6.91 (t, *J* = 4.3 Hz, 1 H), 6.80–6.75 (m, 1 H), 6.27 (d, *J* = 7.9 Hz, 1 H), 6.03 (s, 1 H), 3.04 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.26, 144.96, 143.91, 142.05, 141.52, 140.26, 139.03, 137.70, 136.18, 135.99, 135.34, 134.99, 131.12, 129.97, 129.78, 129.44, 129.16, 128.80, 128.57, 128.54, 128.38, 127.84, 126.40, 126.33, 125.40, 124.72, 124.21, 123.98, 79.43, 51.10 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{31}H_{21}O_2S^+$ 457.1257; found 457.1259.

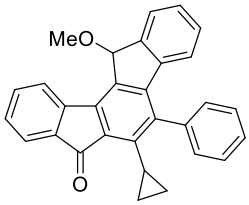
6-(cyclohex-1-en-1-yl)-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3sa)



Yellow foam (106.8 mg, 94% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.17 (d, *J* = 7.5 Hz, 1 H), 7.73–7.61 (m, 2 H), 7.60–7.55 (m, 1H), 7.49–7.41 (m, 3 H), 7.35 (t, *J* = 7.4 Hz, 1 H), 7.32–7.23 (m, 2 H), 7.23–7.14 (m, 1 H), 7.08–7.02 (m, 1 H), 6.29 (d, *J* = 7.9 Hz, 1 H), 5.97 (s, 1 H), 5.35 (d, *J* = 48.5 Hz, 1 H), 3.01 (d, *J* = 3.9 Hz, 3 H), 2.43–2.22 (m, 1 H), 2.16–2.01 (m, 1 H), 1.86–1.62 (m, 4 H), 1.47–1.34 (m, 1 H), 1.31–1.22 (m, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 193.43, 145.69, 145.65, 144.92, 144.89, 143.96, 143.92, 142.69, 142.67, 141.30, 140.66, 140.64, 138.53, 138.40, 137.59, 137.55, 135.51, 134.78, 134.67, 134.39, 134.36, 134.11, 133.95, 130.91, 130.89, 129.71, 129.66, 129.19, 129.04, 128.90, 128.66, 128.49, 128.29, 128.18, 127.59, 127.57, 127.26, 127.20, 125.32, 124.60, 124.17, 124.14, 123.68, 79.47, 79.43, 77.68, 77.16, 76.84, 51.08, 51.04, 30.28, 29.97, 25.28, 22.85, 21.88 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{27}O_2^+$ 455.2006; found 455.2009.

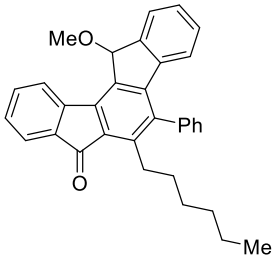
6-cyclopropyl-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3ta)

Yellow foam (59.1 mg, 57% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.14 (d, *J* = 7.5 Hz, 1 H), 7.69 (d, *J* = 7.3 Hz, 1 H), 7.62 (d, *J* = 7.4 Hz, 1 H), 7.58–7.48 (m, 4 H), 7.39–7.25 (m, 4 H), 7.03 (t, *J* = 7.6 Hz, 1 H), 6.23 (d, *J* = 7.9 Hz, 1 H), 5.91 (s, 1 H), 2.95 (s, 3 H), 2.01–1.93 (m, 1 H), 0.81–0.72 (m, 2



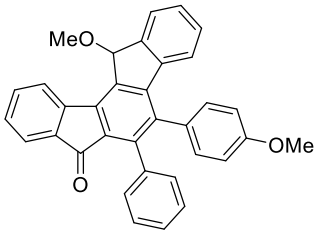
H), 0.38 (t, *J* = 5.2 Hz, 2 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 144.81, 144.49, 143.99, 142.14, 141.71, 140.57, 140.07, 139.34, 135.56, 134.66, 134.66, 134.08, 132.08, 129.88, 129.87, 129.11, 128.96, 128.91, 128.81, 128.45, 127.80, 125.32, 124.46, 124.31, 123.65, 79.21, 50.88, 12.31, 9.67, 9.66 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{30}H_{23}O_2^+$ 415.1693; found 415.1692.

6-hexyl-12-methoxy-5-phenylindeno[1,2-a]fluoren-7(12H)-one (3ua)



Yellow oil (37.8 mg, 33% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.16 (d, *J* = 7.5 Hz, 1 H), 7.70 (d, *J* = 7.4 Hz, 1 H), 7.63 (d, *J* = 7.5 Hz, 1 H), 7.60–7.50 (m, 4 H), 7.35 (t, *J* = 7.4 Hz, 2 H), 7.31–7.23 (m, 2 H), 7.04 (t, *J* = 7.6 Hz, 1 H), 6.11 (d, *J* = 7.9 Hz, 1 H), 5.95 (s, 1 H), 2.98 (s, 3 H), 2.91–2.82 (m, 2 H), 1.47–1.39 (m, 2 H), 1.28–1.11 (m, 6 H), 0.82 (t, *J* = 7.0 Hz, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 194.64, 145.50, 144.96, 144.01, 142.51, 141.82, 140.68, 138.42, 138.37, 135.58, 134.79, 133.56, 129.71, 129.64, 129.51, 129.20, 129.11, 129.04, 128.45, 128.08, 125.34, 124.54, 124.06, 123.69, 79.37, 50.93, 31.40, 30.96, 29.80, 28.33, 22.63, 14.19 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{31}O_2^+$ 459.2319; found 459.2324 ppm.

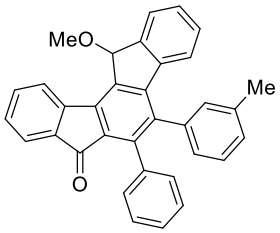
12-methoxy-5-(4-methoxyphenyl)-6-phenylindeno[1,2-a]fluoren-7(12H)-one (3ab)



Yellow foam (104.5 mg, 87% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.22 (d, *J* = 7.5 Hz, 1 H), 7.68 (d, *J* = 7.5 Hz, 1 H), 7.62–7.56 (m, 2 H), 7.36–7.31 (m, 2 H), 7.28–7.18 (m, 3 H), 7.16–7.07 (m, 2 H), 7.07–6.96 (m, 3 H), 6.86–6.78 (m, 2 H), 6.40 (d, *J* = 7.9 Hz, 1 H), 6.03 (s, 1 H), 3.81 (s, 3 H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.82, 158.85, 145.34, 143.97, 143.24, 142.35, 141.30, 140.64, 137.72, 136.38, 135.41, 135.25, 134.88, 134.68, 131.27, 131.14, 129.97, 129.90, 129.68, 129.51, 129.28, 129.12, 128.63, 127.45, 127.38, 127.03, 125.36, 124.64, 124.24, 123.84, 113.91, 113.90, 79.50, 55.27,

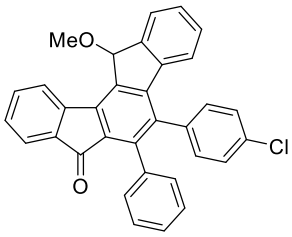
51.11 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{25}O_3^+$ 481.1798; found 481.1793.

12-methoxy-6-phenyl-5-(m-tolyl)indeno[1,2-a]fluoren-7(12H)-one (3ac)



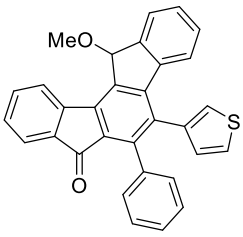
Yellow foam (101.0 mg, 87% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.24 (d, *J* = 7.6 Hz, 1 H), 7.70 (d, *J* = 7.6 Hz, 1 H), 7.65–7.56 (m, 2 H), 7.34 (t, *J* = 7.5 Hz, 2 H), 7.30–7.15 (m, 5 H), 7.13–7.02 (m, 3 H), 7.02–6.89 (m, 2 H), 6.37 (d, *J* = 7.8 Hz, 1H), 6.05 (d, *J* = 5.0 Hz, 1 H), 3.08 (dd, *J* = 3.0, 1.1 Hz, 3 H), 2.29 (d, *J* = 3.7 Hz, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.74, 144.87, 143.95, 143.92, 142.81, 142.80, 142.30, 141.25, 140.51, 138.14, 138.12, 137.97, 137.94, 137.59, 137.58, 136.25, 135.36, 135.20, 135.17, 134.83, 134.67, 130.75, 130.65, 129.82, 129.63, 129.60, 129.48, 129.43, 129.24, 129.06, 128.58, 128.29, 128.27, 128.17, 128.16, 127.33, 127.27, 127.20, 127.15, 127.01, 125.30, 125.29, 124.60, 124.23, 123.78, 79.42, 79.41, 51.06, 21.47, 21.45 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{34}H_{25}O_2^+$ 465.1849; found 465.1845.

5-(4-chlorophenyl)-12-methoxy-6-phenylindeno[1,2-a]fluoren-7(12H)-one (3ad)



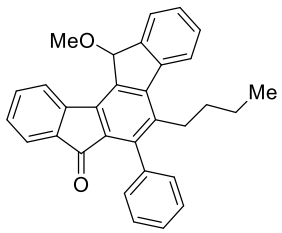
Yellow foam (111.5 mg, 92% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.21 (d, *J* = 7.6 Hz, 1 H), 7.68 (d, *J* = 7.5 Hz, 1 H), 7.61–7.54 (m, 2 H), 7.36–7.29 (m, 2 H), 7.29–7.17 (m, 5 H), 7.14–7.08 (m, 2 H), 7.05 (d, *J* = 8.6 Hz, 2 H), 6.96 (d, *J* = 6.7 Hz, 1 H), 6.36 (d, *J* = 7.9 Hz, 1 H), 6.01 (s, 1 H), 3.04 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.55, 144.84, 144.03, 142.79, 142.15, 141.67, 140.16, 136.47, 136.33, 135.92, 135.39, 135.31, 134.94, 134.67, 133.54, 131.66, 131.52, 129.93, 129.56, 129.45, 129.40, 129.19, 128.86, 128.79, 128.74, 127.60, 127.52, 127.27, 125.51, 124.73, 123.99, 123.89, 79.40, 51.14 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{22}ClO_2^+$ 485.1303; found 485.1305.

12-methoxy-6-phenyl-5-(thiophen-3-yl)indeno[1,2-a]fluoren-7(12H)-one (3ae)



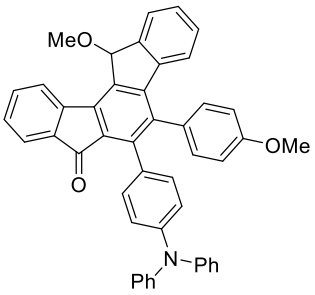
Yellow foam (95.9 mg, 84% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.69 (d, *J* = 7.5 Hz, 1 H), 7.64–7.55 (m, 2 H), 7.35 (q, *J* = 7.0 Hz, 2H), 7.32–7.05 (m, 7 H), 7.01–6.93 (m, 1 H), 6.89–6.81 (m, 1 H), 6.50 (d, *J* = 7.9 Hz, 1 H), 6.03 (s, 1 H), 3.06 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.61, 145.63, 145.58, 143.95, 143.57, 143.52, 142.25, 141.60, 140.37, 137.55, 137.46, 136.32, 136.30, 135.33, 135.24, 135.22, 134.89, 132.79, 129.85, 129.71, 129.52, 129.46, 129.38, 129.28, 129.25, 129.10, 128.89, 128.82, 127.46, 127.43, 127.39, 127.36, 127.19, 125.75, 125.37, 124.69, 124.40, 124.26, 123.91, 123.88, 123.86, 79.47, 51.13 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{31}H_{21}SO_2^+$ 457.1257; found 457.1256.

5-butyl-12-methoxy-6-phenylindeno[1,2-a]fluoren-7(12H)-one (3af)



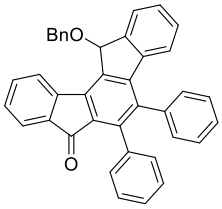
Yellow foam (56.0 mg, 52% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.15 (d, *J* = 7.4 Hz, 1 H), 7.85 (d, *J* = 7.2 Hz, 1 H), 7.76 (d, *J* = 6.9 Hz, 1 H), 7.57–7.44 (m, 7 H), 7.32–7.21 (m, 3 H), 5.98 (s, 1 H), 2.99 (s, 3 H), 2.84–2.73 (m, 2 H), 1.57–1.48 (m, 2 H), 1.31 (q, *J* = 7.3 Hz, 2 H), 0.80 (t, *J* = 7.3 Hz, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 193.05, 144.97, 144.21, 143.33, 142.62, 140.86, 139.77, 138.36, 137.27, 135.82, 135.23, 134.81, 134.66, 130.38, 129.64, 128.99, 128.79, 128.77, 128.47, 128.17, 127.58, 125.73, 124.45, 124.24, 123.76, 79.33, 50.90, 31.81, 29.19, 23.01, 13.77 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{31}H_{27}O_2^+$ 431.2006; found 431.2006.

6-(4-(diphenylamino)phenyl)-12-methoxy-5-(4-methoxyphenyl)indeno[1,2-a]fluoren-7(12H)-one (3nb)



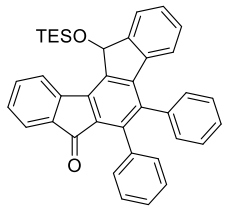
Yellow foam (124.7 mg, 77% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 7.5 Hz, 1 H), 7.66 (dd, *J* = 11.9, 7.4 Hz, 2 H), 7.60 (t, *J* = 7.1 Hz, 1 H), 7.38–7.30 (m, 2 H), 7.26–7.20 (m, 4 H), 7.11 (t, *J* = 7.6 Hz, 1 H), 7.07–6.82 (m, 14 H), 6.54 (d, *J* = 7.8 Hz, 1 H), 6.03 (s, 1 H), 3.88 (s, 3 H), 3.05 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.91, 158.84, 147.77, 146.24, 144.99, 143.85, 143.09, 142.30, 141.17, 140.51, 137.99, 135.33, 135.04, 134.77, 131.38, 131.27, 130.99, 130.70, 130.53, 130.03, 129.66, 129.16, 129.06, 128.97, 128.96, 128.52, 125.25, 124.55, 124.13, 123.94, 123.68, 123.27, 123.19, 122.40, 113.67, 113.65, 79.37, 55.24, 50.97 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{46}H_{34}NO_3^+$ 648.2533; found 648.2526.

12-(benzyloxy)-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (3ag)



Yellow foam (113.2 mg, 86% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.30 (d, *J* = 7.5 Hz, 1 H), 7.78 (d, *J* = 7.5 Hz, 1 H), 7.62 (d, *J* = 7.3 Hz, 1 H), 7.56 (t, *J* = 7.5 Hz, 1 H), 7.38–7.28 (m, 5 H), 7.26–7.07 (m, 12 H), 7.05–7.00 (m, 1 H), 6.33 (d, *J* = 7.9 Hz, 1 H), 6.21 (s, 1 H), 4.25 (d, *J* = 10.5 Hz, 1 H), 4.10 (d, *J* = 10.5 Hz, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.65, 144.71, 144.11, 142.82, 142.20, 141.40, 140.44, 138.05, 138.00, 137.78, 136.16, 135.35, 135.28, 134.72, 130.18, 130.01, 129.89, 129.60, 129.51, 129.36, 129.19, 128.80, 128.48, 128.46, 128.40, 128.32, 127.77, 127.53, 127.38, 127.32, 127.07, 125.47, 124.85, 124.19, 123.81, 79.06, 65.71 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{39}H_{27}O_2^+$ 527.2006; found 527.2003.

5,6-diphenyl-12-((triethylsilyl)oxy)indeno[1,2-a]fluoren-7(12H)-one (3ah)

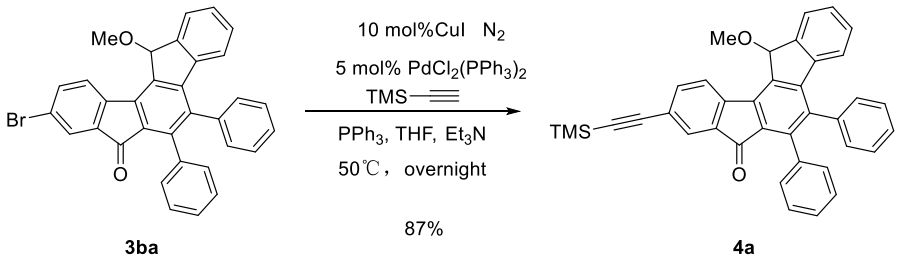


Yellow foam (101.9 mg, 74% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.18 (d, *J* = 7.5 Hz, 1 H), 7.70 (d, *J* = 7.5 Hz, 1 H), 7.62–7.56 (m, 2 H), 7.37–7.26 (m, 5 H), 7.24–7.17 (m, 3 H), 7.12–7.02 (m, 5 H), 6.25 (d, *J* = 7.8 Hz, 1 H), 6.16 (s, 1 H),

0.71 (t, J = 7.9 Hz, 9 H), 0.26 (q, J = 7.9 Hz, 6 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.92, 146.96, 144.17, 142.72, 142.30, 141.06, 139.46, 138.79, 137.93, 137.86, 136.32, 135.41, 134.41, 130.11, 130.06, 129.65, 129.61, 129.29, 129.07, 128.53, 128.51, 128.49, 127.51, 127.38, 127.37, 127.08, 126.00, 125.18, 124.12, 123.83, 74.60, 6.79, 5.99 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{38}H_{35}O_2Si^+$ 551.2401; found 551.2403.

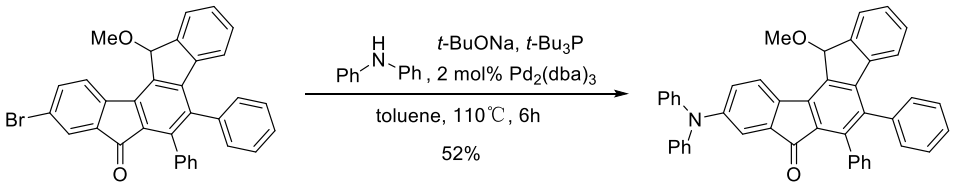
V. Application

(1) Synthesis of 4a, 4b:



3ba 4a

Procedure F: 9-bromo-12-methoxy-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (0.1 mmol, 1.0 equiv) was added to a 25 mL Schlenk flask with PPh_3 (2.6 mg, 0.01 mmol, 0.1 equiv) CuI (1.9 mg, 0.01 mmol, 0.1 equiv) and $Pd(PPh_3)_2Cl_2$ (3.5 mg, 0.005 mmol, 0.05 equiv), followed by the addition of triethylamine (1 mL) and ethynyltrimethylsilane (0.12 mmol, 1.2 equiv) under nitrogen. After the reaction mixture was stirred at 50 °C overnight. The mixture was concentrated under reduced pressure and purified by silica gel column chromatography to afford **4a** as a yellow foam.[6]

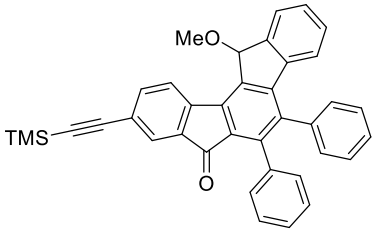


3ba 4b

Procedure G: To a mixture of 9-bromo-12-methoxy-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (0.1 mmol, 1.0 equiv, diphenylamine(25.4 mg, 0.15 mmol, 1.5 equiv), and sodium tert-butoxide (10.2 mg, 0.106 mmol, 1.06 equiv), tris(dibenzylideneacetone)dipalladium (1.9 mg, 0.002 mmol, 0.02 equiv) and toluene (2 mL) was added tri-tert-butylphosphine(0.3 μL, 0.002 mmol, 0.02 equiv) under nitrogen, and the mixture was stirred for 6 hours at 110 ℃。The mixture was concentrated under reduced pressure and purified by silica gel column chromatography to afford **4b** as a orangered foam.[7]

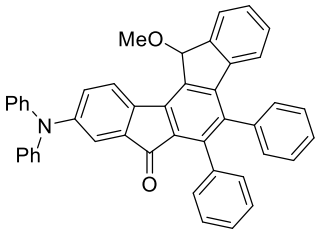
12-methoxy-5,6-diphenyl-9-((trimethylsilyl)ethynyl)indeno[1,2-a]fluoren-7(12H)-one (4a)

Yellow foam (47.6 mg, 87% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.18 (d, *J* = 7.8 Hz, 1 H), 7.72–



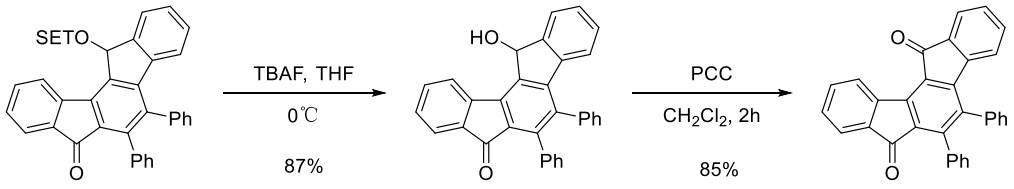
7.64 (m, 3 H), 7.33 (t, *J* = 7.4 Hz, 1 H), 7.31–7.27 (m, 3 H), 7.25–7.17 (m, 3 H), 7.16–7.04 (m, 4 H), 7.03–6.98 (dd, 1 H), 6.28 (d, *J* = 7.9 Hz, 1 H), 6.04 (s, 1 H), 3.05 (s, 3 H), 0.28 (s, 9 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 191.79, 145.14, 143.92, 142.99, 141.88, 140.88, 140.37, 138.40, 138.32, 137.70, 136.04, 135.57, 135.33, 130.14, 130.07, 130.02, 129.64, 129.50, 129.16, 128.80, 128.54, 128.49, 127.61, 127.46, 127.40, 127.19, 127.07, 125.38, 124.47, 124.25, 124.22, 104.46, 96.47, 79.47, 51.13, 0.06 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{23}O_2^+$ 451.1693; found 451.1695.

9-(diphenylamino)-12-methoxy-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (4b)



Red foam (32.1mg, 52% yield), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.03 (d, *J* = 8.1 Hz, 1 H), 7.67 (d, *J* = 7.5 Hz, 1 H), 7.34–7.26 (m, 9 H), 7.24–7.11 (m, 11 H), 7.10–7.04 (m, 3 H), 7.02–6.97 (m, 1 H), 6.30 (d, *J* = 7.9 Hz, 1 H), 5.98 (s, 1 H), 3.08 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.65, 149.38, 147.10, 144.92, 144.09, 142.83, 141.68, 140.58, 137.92, 136.86, 136.84, 136.31, 135.21, 134.29, 130.30, 130.20, 130.17, 129.66, 129.61, 129.47, 129.02, 128.57, 128.45, 128.42, 127.63, 127.46, 127.33, 127.27, 126.97, 125.40, 125.37, 125.12, 124.17, 123.88, 118.01, 79.54, 51.21 ppm. **HRMS** (ESI) m/z: $[M + Na]^+$ calcd for $C_{45}H_{31}NNaO_2^+$ 640.2247; found 640.2250.

(2) Synthesis of 5, 6:

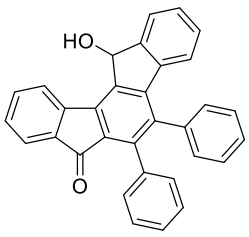


Procedure H: In nitrogen atmosphere，5,6-diphenyl-12-((triethylsilyl)oxy)indeno[1,2-a]fluoren-7(12H)-one (0.275 g, 0.5 mmol) and ultra-dry tetrahydrofuran (0.5 M, 1 mL) were added into a 25 mL round-bottomed flask equipped with a magnetic stirrer. After the mixture was cooled to 0 ℃,

tetrabutylammonium fluoride (0.6 mL, 0.6 mmol, 1.2 equiv, 1M in THF) was slowly added dropwise, then the mixture was heated to room temperature and stirred for 30 min. After the reaction was monitored by TCL plate is completed, it was quenched with water (5 ml), extracted with ethyl acetate for three times, and the organic layers were combined, dried with anhydrous sodium sulfate, and further purified by chromatography column (PE:EA = 3:1) to obtain **5** as a yellow foam (0.189 g) in 87% yield.[8, 9]

Procedure I: Pyridinium chlorochromate (0.185 g, 0.86 mmol, 2.0 equiv) and molecular sieve (0.6 g) were added to a solution of diols(0.189 g, 0.43 mmol, 1.0 equiv) in dry CH_2Cl_2 (15 mL) and the resulting mixture was stirred at 25 °C for 2 h. Afterwards, the reaction mixture was filtered through Celite®, washed by CH_2Cl_2 and concentrated under reduced pressure. Column chromatography of the residue on silica gel yielded the desired diketones **6**.[10]

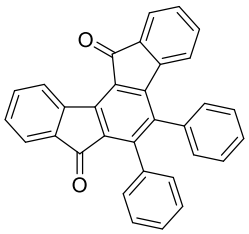
12-hydroxy-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one (5)



Following the general procedure H starting with 0.5 mmol of 5,6-diphenyl-12-((triethylsilyl)oxy)indeno[1,2-a]fluoren-7(12H)-one. The product was obtained as a yellow foam after column chromatography (189.1 mg, 87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.21 (d, *J* = 7.7 Hz, 1 H), 7.72 (d, *J* = 7.5 Hz, 1 H), 7.60–7.55 (m, 2 H), 7.34–7.24 (m, 5 H), 7.21–7.16 (m, 3 H), 7.14–7.10 (m, 1 H), 7.09–7.03 (m, 3 H), 7.02–6.97 (m, 1 H), 6.26 (d, *J* = 7.9 Hz, 1 H), 5.95 (s, 1 H), 2.13 (s, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.68, 147.15, 144.10, 142.98, 142.17, 141.05, 139.26, 138.14, 138.05, 137.75, 136.15, 135.43, 134.75, 130.28, 130.18, 129.93, 129.66, 129.46, 129.39, 129.29, 129.05, 128.53, 128.52, 127.58, 127.42, 127.38, 127.13, 125.23, 124.80, 124.25, 124.00, 73.56 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{23}O_2^+$ 451.1693; found 451.1695.

5,6-diphenylindeno[1,2-a]fluorene-7,12-dione (6)

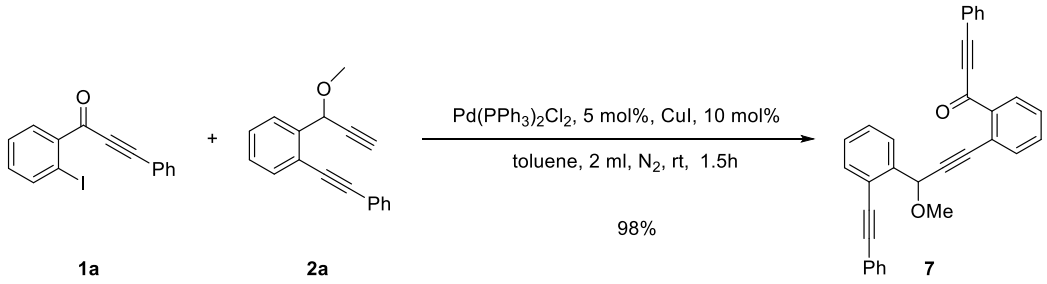
Following the general procedure **I** starting with 0.43 mmol of 12-hydroxy-5,6-diphenylindeno[1,2-



a]fluoren-7(12H)-one. The product was obtained as a yellow foam after column chromatography (159.0 mg, 85% yield).**^{1}H NMR** (400 MHz, $CDCl_3$): δ = 9.12 (d, *J* = 7.7 Hz, 1 H), 7.76 (d, *J* = 7.4 Hz, 1 H), 7.67–7.57 (m, 2 H), 7.41 (t, *J* = 6.7 Hz, 1 H), 7.35–7.27 (m, 4 H), 7.24–7.03 (m, 8 H), 6.13 (d, *J* = 7.7 Hz, 1 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.95, 191.92, 147.51, 146.43, 143.69, 141.65, 138.50, 136.92, 135.61, 135.57, 135.54, 135.13, 134.66, 132.21, 130.78, 129.94, 129.73, 129.14, 128.71, 127.98, 127.64, 127.57, 127.51, 124.30, 124.19, 123.72 ppm. **HRMS** (ESI) m/z: $[M + H]^+$ calcd for $C_{33}H_{23}O_2^+$ 451.1693; found 451.1695.

VI. Sonogashira coupling reaction:

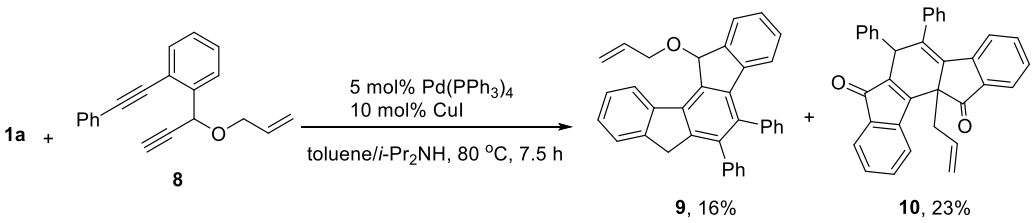
(1) Synthesis of 7:



1a 2a 7

Procedure J: An oven-dried 25 mL Schlenk tube equipped with a magnetic stirring bar and flushed with nitrogen gas. **1a** (0.5 mmol), **2a** (0.6 mmol), $Pd(PPh_3)_2Cl_2$ (5 mol%), CuI (10 mol%), *i*-Pr_2NH(0.2 mL) and toluene (4.0 mL) were added to the tube under nitrogen atmosphere. The reaction was stirred for 1.5 h at room temperature. The reaction mixture was evaporated under reduced pressure. The yield of the coupling products is obtained by column chromatography.

(2) Synthesis of 9, 10 via diverse reaction of 1a with an allylic diynylic ether 8:

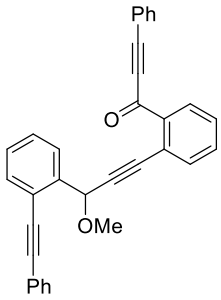


9, 16% **10**, 23%

Procedure k: An oven-dried 25 mL Schlenk tube equipped with a magnetic stirring bar and flushed with nitrogen gas. **1a** (0.25 mmol), **8** (0.3 mmol), $Pd(PPh_3)_2Cl_2$ (5 mol%, 8.8 mg), CuI (10 mol%, 4.8 mg), *i*-Pr_2NH(0.1 mL) and toluene (2.0 mL) were added to the tube under nitrogen atmosphere. The reaction was stirred at 25 °C for 7.5 h. The reaction mixture was evaporated under reduced pressure. The yield of the coupling products is obtained by column chromatography.

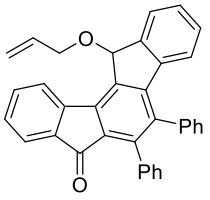
1-(2-(3-methoxy-3-(2-(phenylethynyl)phenyl)prop-1-yn-1-yl)phenyl)-3-phenylprop-2-yn-1-one (7)

Following the general procedure J starting with 0.5 mmol of **1a**. The product was obtained as a



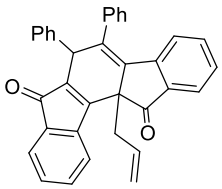
colorless oil after column chromatography (0.22 g, total yield: 98%). Brown oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.21 (d, *J* = 7.5 Hz, 1 H), 7.96 (d, *J* = 7.7 Hz, 1 H), 7.64 (t, *J* = 6.7 Hz, 3 H), 7.57 (d, *J* = 6.8 Hz, 3 H), 7.54–7.47 (m, 2 H), 7.44 (dd, *J* = 12.1, 5.4 Hz, 2 H), 7.40–7.31 (m, 6 H), 5.89 (s, 1 H), 3.66 (s, 3 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 177.36, 139.90, 138.53, 135.07, 133.13, 132.54, 132.27, 131.74, 131.69, 130.83, 128.86, 128.71, 128.53, 128.49, 128.48, 128.38, 128.10, 123.24, 122.73, 122.34, 120.21, 94.23, 93.44, 92.92, 87.96, 87.07, 85.99, 71.92, 57.07 ppm. **HRMS** (ESI) m/z: $[M+Na]^+$ calcd for $C_{33}H_{22}NaO_2^+$ 473.1512; found 473.1525.

12-(allyloxy)-5,6-diphenylindeno[1,2-a]fluoren-7(12H)-one and 11c-allyl-5,6-diphenyl-6,11c-dihydroindeno[1,2-a]fluorene-7,12-dione (9 and 10 as mixtures)



9

+



10

Yellow foam (47.6 mg, **9**, 16%, **10**, 23%), **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 9.50 (d, *J* = 8.0 Hz, 1 H), 8.27 (d, *J* = 7.5 Hz, ~ 0.7 H), 7.94 (d, *J* = 7.4 Hz, 1 H), 7.78 (t, *J* = 7.6 Hz, 1 H), 7.69 (t, *J* = 6.9 Hz, ~ 1.7 H), 7.61–7.50 (m, 3 H), 7.36 (q, *J* = 6.6, 5.6 Hz, 3 H), 7.31 (d, *J* = 7.8 Hz, ~ 2.3 H), 7.27 (s, ~ 1.3 H), 7.24 (s, 1 H), 7.23–7.16 (m, ~ 2.8 H), 7.16 – 7.08 (m, ~ 2.9 H), 7.02 (s, ~ 6.9 H), 6.75 (d, *J* = 7.8 Hz, 1 H), 6.27 (d, *J* = 7.9 Hz, ~ 0.7 H), 6.10 (s, ~ 0.7 H), 5.81 (ddt, *J* = 16.6, 11.3, 5.7 Hz, ~ 0.7 H), 5.69 (dq, *J* = 16.0, 8.6 Hz, 1 H), 5.18 (d, *J* = 17.2 Hz, ~ 0.7 H), 5.12–5.04 (m, ~ 1.7 H), 5.00 (d, *J* = 10.1 Hz, 1 H), 4.20 (s, 1 H), 3.75 (dd, *J* = 12.1, 5.5 Hz, ~ 0.8 H), 3.61 (dd, *J* = 12.0, 5.8 Hz, ~ 0.8 H), 2.80 (qd, *J* = 13.7, 7.3 Hz, 2 H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 145.10, 144.77, 144.59, 144.21, 143.32, 142.87, 142.26, 141.42, 140.32, 140.08, 138.90, 138.60, 138.16, 137.98, 137.79, 136.84, 136.20, 135.55, 135.44, 135.39, 134.81, 134.37, 132.25, 132.17, 130.17, 130.04, 129.95, 129.90, 129.65, 129.51, 129.46, 129.42, 129.35, 129.13, 128.71, 128.56, 128.50, 128.47, 128.43, 128.27, 128.22, 127.99, 127.54, 127.44, 127.40, 127.35, 127.09, 125.43, 124.82, 124.39, 124.18, 124.06, 123.85,

123.81, 119.59, 117.05, 78.99, 64.71, 58.65, 53.88, 43.77 ppm. **HRMS** (ESI) m/z: $[M + Na]^+$ calcd for $C_{35}H_{24}NaO_2^+$ 499.1669; found 499.1661.

VII. Computational Methods.

All DFT calculations were carried out using Gaussian 16 program. All the geometry optimizations and frequency calculations in this paper were performed with M06[11] functional in implicit toluene, at 6-31G(d) basis set by using the Solvation Model based on Density[12] (SMD) with keyword in the Gaussian code route section "SCRF = (SMD, Solvent = toluene)". The vibrational frequencies were computed at the same level of theory as for the geometry optimizations to confirm whether each optimized structure is an energy minimum or a transition state, and to evaluate the zero-point vibrational energy (ZPVE) and thermal corrections. Single-point energy calculations were performed on an optimized geometry using M06-L[13] functional with a higher level basis set 6-311+G(d,p). The Gibbs free energies presented in this paper are the M06-L calculated single-point energy in toluene solvent with M06 calculated thermodynamic corrections in toluene solvent.

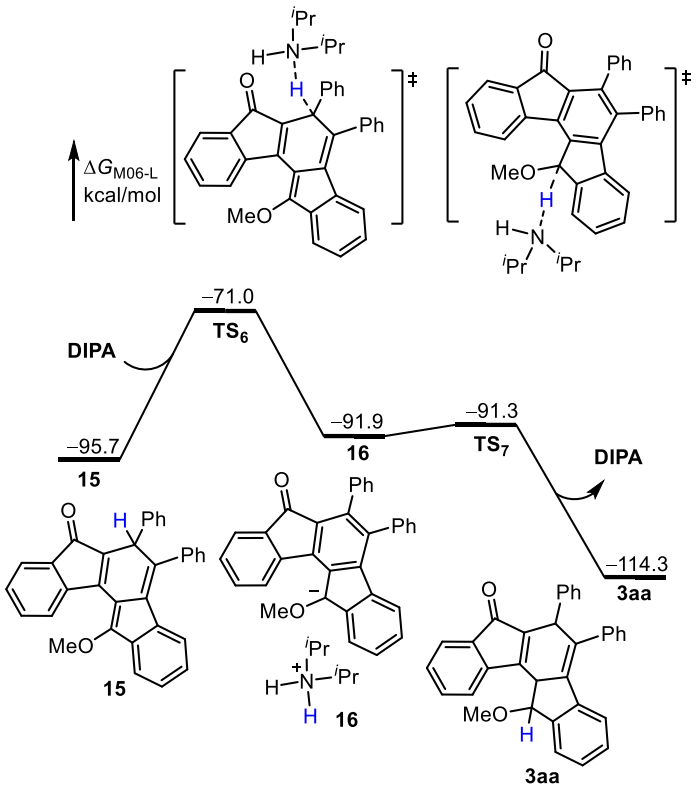


Figure S3. Free energy profile for the DIPA promoted isomerization of intermediate **15**. The energy values are in kcal/mol and represent the relative free energies calculated at M06-L/6-311+G(d,p)/SMD(toluene)//M06/6-31G(d)/SMD(toluene) level of theory in toluene solvent.

VIII. M06 and M06-L calculated absolute energies, enthalpies, and free energies of all structures.

Geometry	$E_{(elec\text{-}M06\text{-}L)}$[1]	$H_{(corr\text{-}M06)}$[2]	$G_{(corr\text{-}M06)}$[3]	$G_{(solv\text{-}M06\text{-}L)}$[4]	IF[5]
7	-1421.226093	0.475162	0.379635	-1419.967603	
DIPA	-292.461134	0.215500	0.172176	-292.101187	
TS_1	-1713.669924	0.687704	0.571767	-1712.029511	973.79*i*
11	-1713.682861	0.693221	0.574836	-1712.037522	
TS_2	-1713.668357	0.687585	0.568939	-1712.031283	1031.63*i*
12	-1421.228203	0.474725	0.378490	-1419.967004	
TS_3	-1421.194589	0.471288	0.381719	-1420.81287	474.31*i*
13	-1421.288938	0.476115	0.381563	-1420.907375	
TS_4	-1421.281162	0.473895	0.385403	-1420.895759	375.91*i*
14	-1421.295031	0.473986	0.383311	-1420.91172	
TS_5	-1421.295926	0.473104	0.387062	-1420.911065	70.46*i*
15	-1421.389224	0.478526	0.390175	-1420.999049	
TS_6	-1713.837696	0.690916	0.589098	-1713.248598	1156.26*i*
16	-1713.870204	0.696540	0.588306	-1713.281898	
TS_7	-1713.86391	0.691273	0.582850	-1713.28106	1067.02*i*
3aa	-1421.421217	0.478412	0.392537	-1421.02868	

[1]The electronic energy calculated by M06-L in toluene solvent. [2]The thermal correction to enthalpy calculated by M06 in toluene solvent. [3]The thermal correction to Gibbs free energy calculated by M06 in toluene solvent. [4]The Gibbs free energy calculated by M06-L in toluene solvent. [5]The M06 calculated imaginary frequencies for the transition states.

IX. M06 geometries for all the optimized compounds and transition states.

7

C	-0.53506200	2.12966400	1.11240900
C	0.25602100	3.26709000	1.38574000
C	-1.93388200	2.25011600	1.14907800
C	-0.37613300	4.47448000	1.69824500
C	-2.53945600	3.46270900	1.43893100
H	-2.53219800	1.36223400	0.94758600
C	-1.75769000	4.58174500	1.71840300
H	0.25382900	5.33346600	1.91896600
H	-3.62562200	3.53280300	1.45137800
H	-2.22672900	5.53581000	1.95143300
C	1.74684400	3.30019200	1.37625900
O	2.35954000	4.19627400	1.94274900
C	2.47677800	2.30508600	0.62991600
C	3.19226500	1.57146700	-0.02373400
C	3.98682900	0.68511000	-0.80079100
C	5.38592400	0.79820600	-0.78846200
C	3.37612000	-0.30239600	-1.59150200
C	6.15954600	-0.06272200	-1.55344300
H	5.84963600	1.56779200	-0.17388600
C	4.16082800	-1.15667600	-2.35475900
H	2.28894700	-0.39565100	-1.59401800
C	5.54904000	-1.03882300	-2.33800900
H	7.24406400	0.02891000	-1.54084300
H	3.68567600	-1.91716900	-2.97281400
H	6.15860800	-1.71017000	-2.94075000
C	-0.01558500	0.82888000	0.84151400
C	0.26900000	-0.32737900	0.61901100
C	0.69900200	-1.70147800	0.37548500
O	0.56802900	-1.95576200	-1.01356600
C	1.14648300	-3.17858000	-1.39559200
H	2.19881400	-3.25057200	-1.06499100
H	0.59738100	-4.04458100	-0.99281700
C	-0.05114700	-2.70468900	1.23227800
C	-1.45454300	-2.84016600	1.15321600
C	0.66306000	-3.53712600	2.08688500
C	-2.09297700	-3.80068500	1.95123400
C	0.01976200	-4.48566700	2.87683400
H	1.74830700	-3.43694200	2.13358300
C	-1.36331400	-4.61439700	2.80725800
H	-3.17569400	-3.89570200	1.88699100
H	0.59931600	-5.12368500	3.54150100
H	-1.87752000	-5.35288700	3.41978900
H	1.77307400	-1.77517500	0.64852500
H	1.11024200	-3.22100600	-2.48945800
C	-2.22925300	-2.01999200	0.28708000
C	-2.89363700	-1.32020800	-0.45104300
C	-3.57916900	-0.44464100	-1.33858400
C	-4.97574700	-0.47746700	-1.46680100
C	-2.83994500	0.48041900	-2.09453500
C	-5.61611800	0.39725500	-2.33422400
H	-5.54668100	-1.19515200	-0.87975300
C	-3.48945900	1.35214400	-2.95699200
H	-1.75546200	0.49678000	-1.98966800
C	-4.87693000	1.31302300	-3.07940500
H	-6.70029300	0.36496000	-2.42950800
H	-2.90961700	2.06703400	-3.53838100
H	-5.38334200	1.99783900	-3.75773500

DIPA

N	-0.02961900	-0.06933000	-0.85406800
H	-0.17754400	-0.91431300	-1.40237100
C	1.37801600	-0.03374500	-0.44925900
C	1.80766200	-1.22065700	0.41105200
C	1.71888000	1.28648600	0.22188900
H	1.95145300	-0.08185400	-1.39001600
H	1.59151300	-2.17240500	-0.09571900
H	2.88645200	-1.19163600	0.62054300
H	1.28742500	-1.23042800	1.38009300
H	1.43491100	2.13311800	-0.41630500
H	1.20245400	1.39759100	1.18655600
H	2.79682600	1.35062600	0.42225800
C	-1.03701200	-0.00681100	0.21555400
C	-1.98213800	-1.19299100	0.11629700
C	-1.80611700	1.30447200	0.13530300
H	-0.54093800	-0.05537600	1.20153900
H	-1.44535100	-2.14352400	0.24941900
H	-2.77642400	-1.14207100	0.87278400
H	-2.46734600	-1.21108300	-0.87205800
H	-1.12925400	2.16647400	0.19613800
H	-2.33784000	1.36960400	-0.82505400
H	-2.54474400	1.39005600	0.94566000

TS_1

C	1.43600700	-1.65883200	0.73350600
C	1.45153100	-3.07315900	0.63014100
C	2.46349400	-1.04706100	1.49034300
C	2.48669100	-3.79833600	1.24069800
C	3.46052100	-1.78597800	2.09569300
H	2.46454400	0.04007800	1.56196100
C	3.48255500	-3.17803400	1.97014000
H	2.46958800	-4.88035900	1.12633200
H	4.23788800	-1.27211000	2.66017500
H	4.26822100	-3.76518700	2.44165600
C	0.44014900	-3.88802200	-0.07541800
O	0.65426900	-5.05449600	-0.39068900
C	-0.87989200	-3.34655800	-0.32162800
C	-2.06141200	-3.11936700	-0.49715100
C	-3.44063200	-2.82865100	-0.68815500
C	-3.86805300	-1.49651000	-0.78569200
C	-4.38065200	-3.86659900	-0.77379500
C	-5.21538500	-1.21171500	-0.96435600
H	-3.12530500	-0.69823100	-0.73824600
C	-5.72621400	-3.57107800	-0.94460300
H	-4.04108400	-4.89841800	-0.70220400
C	-6.14629600	-2.24586600	-1.04009000
H	-5.54042900	-0.17474200	-1.05013900
H	-6.45256600	-4.37951700	-1.00768300
H	-7.20251400	-2.01979200	-1.17838000
C	0.54736400	-0.76638800	0.08716400
C	-0.00939600	0.20877900	-0.41341100
C	-0.74857000	1.32993300	-0.82960200
O	-2.00040800	1.04646200	-1.43835100
C	-1.87920900	0.55695500	-2.75860600
H	-1.35198800	1.27660800	-3.40540100

H	-1.33526000	-0.40176900	-2.77875800
C	-0.18812900	2.63358700	-1.18806400
C	1.18390100	3.00284500	-1.09418200
C	-1.09872800	3.65759600	-1.53531100
C	1.55688300	4.35123600	-1.25465000
C	-0.70395200	4.97207900	-1.72061000
H	-2.14557500	3.38377200	-1.66262100
C	0.63368900	5.33699400	-1.55698900
H	2.61492400	4.59704300	-1.16811800
H	-1.44694400	5.72185100	-1.99173500
H	0.95276800	6.36893800	-1.68965800
H	-1.37203500	1.79718100	0.50256400
H	-2.89248800	0.39972700	-3.14937600
C	2.24331800	2.06485300	-0.93085000
C	3.23323300	1.35913100	-0.86831300
C	4.32470400	0.44813500	-0.79810100
C	4.18436600	-0.85352800	-1.30784700
C	5.53459200	0.81399000	-0.18905400
C	5.22622800	-1.76348200	-1.20236400
H	3.24196100	-1.13784400	-1.77385100
C	6.57315100	-0.10303500	-0.08779700
H	5.64530300	1.82250400	0.20716100
C	6.42229500	-1.39328200	-0.59043400
H	5.09962100	-2.77255900	-1.59173700
H	7.50729300	0.19128500	0.38872600
H	7.23709900	-2.11071800	-0.50556800
N	-2.08225400	2.25432200	1.35587500
H	-2.49179800	3.07077900	0.89240800
C	-3.18966000	1.27540500	1.59917800
C	-4.30043500	1.89764100	2.42287400
C	-2.65557700	-0.00926600	2.19734300
H	-3.56464500	1.06217400	0.58735500
H	-4.66165000	2.83457500	1.97591900
H	-5.15019300	1.20506600	2.47665800
H	-3.98439800	2.10719300	3.45409200
H	-1.84655400	-0.43661200	1.58833900
H	-2.28296100	0.13892700	3.22064000
H	-3.46531200	-0.74831400	2.24775200
C	-1.28032700	2.72330800	2.53681800
C	-1.22211800	4.23817300	2.51449100
C	0.10535300	2.10410900	2.51431900
H	-1.81259200	2.39334700	3.44015100
H	-2.22576400	4.68143500	2.58629600
H	-0.62762200	4.61161500	3.35688400
H	-0.74764000	4.59319800	1.58688200
H	0.07039100	1.00833100	2.46474400
H	0.68085400	2.46673300	1.64999300
H	0.64941500	2.38781000	3.42415800

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C	3.58312600	-1.61436000	0.84727400
C	4.75167300	-0.82526600	0.65239800
C	3.74152300	-3.02355500	0.90171100
C	6.00756900	-1.45206900	0.61281400
C	4.98602600	-3.61174400	0.81489300
H	2.85262400	-3.63467200	1.05929100
C	6.13916000	-2.82489300	0.68469200
H	6.88030400	-0.81255500	0.49364600
H	5.07034100	-4.69657900	0.87210700
H	7.12188900	-3.28917400	0.63305400
C	4.74979600	0.62954600	0.41905500
O	5.76581200	1.31053700	0.52698400
C	3.55146100	1.29364600	-0.08184800
C	2.72958200	2.02891700	-0.59752700
C	1.75500400	2.86025100	-1.22494300
C	2.03481700	3.46028300	-2.46263800
C	0.50187700	3.06770400	-0.62854600
C	1.07146100	4.23608400	-3.09434100
H	3.01149100	3.30628000	-2.91898300
C	-0.45551800	3.84537200	-1.26729200
H	0.29480700	2.61373500	0.34001300
C	-0.17580700	4.42715000	-2.50199400
H	1.29641200	4.69790200	-4.05438200
H	-1.42396200	3.99754300	-0.79308800
H	-0.92764400	5.03717600	-3.00023800
C	2.29735900	-1.07256700	0.99573700
C	1.16379400	-0.74265900	1.38965900
C	-0.14260700	-0.39000600	1.60616000
O	-1.09948300	-1.34057100	1.19302200
C	-1.47485600	-2.25152000	2.20761200
H	-0.61681000	-2.86963600	2.51756500
H	-1.86664500	-1.71777000	3.08544400
C	-0.58994800	0.86835900	2.12491100
C	-1.93721400	1.33969900	2.05513500
C	0.36037600	1.73395100	2.72325900
C	-2.25278400	2.61786900	2.56266100
C	0.02423200	2.98363900	3.19919300
H	1.39046400	1.38566100	2.80005300
C	-1.29744600	3.44341400	3.12268400
H	-3.28996200	2.94584800	2.49265300
H	0.79617900	3.60924900	3.64595500
H	-1.57052200	4.42491300	3.50494700
H	1.06655100	-1.18516200	-0.89425600
H	-2.26409900	-2.89867700	1.80457500
C	-3.00879800	0.61378900	1.46743800
C	-3.99633900	0.08489900	0.98741500
C	-5.10156700	-0.58284800	0.39342100
C	-4.93884000	-1.86025300	-0.17079300
C	-6.37246200	0.01435500	0.34992200
C	-6.01166800	-2.51516000	-0.75888500
H	-3.95399900	-2.32678900	-0.13467800
C	-7.44119000	-0.64720000	-0.23916600
H	-6.50563800	1.00329100	0.78585800
C	-7.26722100	-1.91233400	-0.79590400
H	-5.86963800	-3.50532400	-1.18997300
H	-8.42033200	-0.17109600	-0.26395400
H	-8.10829600	-2.42811800	-1.25623000
N	0.12613200	-1.35771600	-1.29974700
H	-0.46492700	-1.52205700	-0.45557100
C	-0.36886800	-0.07413500	-1.92074400
C	-1.86388600	-0.15635800	-2.13462100
C	0.41844200	0.27288400	-3.16291300
H	-0.16334700	0.67084100	-1.13727200
H	-2.38577000	-0.37769100	-1.19268800
H	-2.22835400	0.81616300	-2.48873400
H	-2.14143200	-0.90778000	-2.88754300
H	1.49835200	0.30761700	-2.96350900
H	0.22972600	-0.43559200	-3.98197900
H	0.11429300	1.26823400	-3.51073000
C	0.15665000	-2.61988100	-2.12865900
C	-0.44422700	-3.73095200	-1.29098800
C	1.58000300	-2.92085300	-2.55068100

H	-0.47045600	-2.43359700	-3.01027400
H	-1.49109300	-3.51721400	-1.03332100
H	-0.41437700	-4.68169000	-1.83601100
H	0.12173500	-3.85623200	-0.35493900
H	2.02522800	-2.10423800	-3.13195000
H	2.21583300	-3.10174700	-1.67062300
H	1.60140600	-3.82595200	-3.16942800

TS_2

C	-3.06802600	-1.90255800	-0.58088100
C	-4.34121100	-1.31514100	-0.38676600
C	-3.02192900	-3.28769800	-0.84604500
C	-5.49448300	-2.11168400	-0.48281100
C	-4.17022800	-4.05473600	-0.92372900
H	-2.04454400	-3.74354400	-1.00820800
C	-5.42502000	-3.46637500	-0.74180300
H	-6.45374600	-1.61799500	-0.34102700
H	-4.09102900	-5.11990500	-1.13924900
H	-6.33230000	-4.06402500	-0.80527700
C	-4.58164800	0.11198900	-0.07980500
O	-5.71558000	0.57975900	-0.03488200
C	-3.48587400	1.00962000	0.24320700
C	-2.76538600	1.91970500	0.60841400
C	-1.89117900	2.93695800	1.08678800
C	-2.27961000	3.73492000	2.17451000
C	-0.62192600	3.11875900	0.51732800
C	-1.40294400	4.67799400	2.69366300
H	-3.26847600	3.59508600	2.60811600
C	0.24767100	4.06584200	1.04196900
H	-0.33161400	2.50545200	-0.33550100
C	-0.13754200	4.84187400	2.13302500
H	-1.70808500	5.28944300	3.54117300
H	1.23223600	4.19608100	0.59522100
H	0.54803000	5.58107600	2.54438800
C	-1.80389700	-1.21047900	-0.46634800
C	-0.90968900	-0.84607700	-1.31613700
C	0.25018100	-0.44987800	-1.85352500
O	1.27998500	-1.38605800	-1.91059100
C	1.74611700	-1.66506100	-3.21229300
H	0.95235700	-2.11911500	-3.82704600
H	2.11456200	-0.76258000	-3.72391900
C	0.49071700	0.92940200	-2.28718600
C	1.73748300	1.58825900	-2.11050400
C	-0.56445900	1.66712200	-2.84663300
C	1.88405600	2.92496300	-2.51883900
C	-0.41043800	2.99330000	-3.22138700
H	-1.52382600	1.16803200	-2.98188600
C	0.82378700	3.62682600	-3.06994100
H	2.85141100	3.40571100	-2.37624100
H	-1.25401300	3.53283400	-3.64900600
H	0.95567700	4.66208500	-3.37884600
H	-0.86269400	-1.19735500	0.73383400
H	2.57773900	-2.37310600	-3.11549300
C	2.82219400	0.93606500	-1.46362900
C	3.73204000	0.36005900	-0.89909500
C	4.68596900	-0.46859500	-0.24592300
C	4.36344800	-1.82109400	-0.03541100
C	5.92184300	0.01743000	0.20341100
C	5.25849300	-2.66172500	0.61120200
H	3.40063800	-2.18659100	-0.39793700
C	6.81237100	-0.83209800	0.84739700
H	6.17216500	1.06455700	0.04110500
C	6.48537400	-2.17001700	1.05437200
H	5.00069100	-3.70876300	0.76693300
H	7.77066500	-0.44647800	1.19182800
H	7.18764600	-2.83097900	1.55964100
N	0.17173000	-1.22031300	1.37308800
H	0.86085000	-1.31533100	0.61672300
C	0.39584600	0.12061400	1.98634500
C	1.82717800	0.27711900	2.45935900
C	-0.62459300	0.40865900	3.06618100
H	0.22359800	0.81457100	1.14925700
H	2.54095900	0.05816600	1.65168200
H	1.99780500	1.31302700	2.78106600
H	2.05631500	-0.37622900	3.31323300
H	-1.65030300	0.30053100	2.68775600
H	-0.49620400	-0.24748700	3.93892000
H	-0.50058600	1.44347800	3.41207600
C	0.23879100	-2.43118700	2.24925200
C	1.12439200	-3.45770700	1.56875600
C	-1.15511000	-2.97526300	2.50938700
H	0.69662400	-2.12873600	3.20229700
H	2.16071800	-3.09763900	1.48932000
H	1.13218500	-4.40149800	2.12759900
H	0.75070800	-3.66508300	0.55307100
H	-1.83554200	-2.20745100	2.89907800
H	-1.59900200	-3.37927800	1.58834600
H	-1.10554000	-3.78900800	3.24389400

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C	2.35073200	-2.00924500	0.78211300
C	3.58286700	-1.85613400	1.45146700
C	1.42929100	-2.93333500	1.28668800
C	3.86652800	-2.64809300	2.56944800
C	1.70954000	-3.68768100	2.41713400
H	0.48711600	-3.06968200	0.75577900
C	2.93907600	-3.55439000	3.05846700
H	4.82970800	-2.51478800	3.05815600
H	0.97072900	-4.39545100	2.78948800
H	3.17027100	-4.15287900	3.93759700
C	4.62316300	-0.84768500	1.09741600
O	5.80169000	-1.01116500	1.38171800
C	4.17407100	0.38427300	0.49453700
C	3.79017400	1.44481700	0.04119500
C	3.28098100	2.65482500	-0.50178300
C	4.15090600	3.69683800	-0.85812400
C	1.89624000	2.80896400	-0.68305500
C	3.64294900	4.87431100	-1.38711400
H	5.22177100	3.56627900	-0.71262400
C	1.40018300	3.99315800	-1.21063200
H	1.22392500	1.99559100	-0.40329800
C	2.26908100	5.02400300	-1.56264800
H	4.32017600	5.68073100	-1.66220100
H	0.32689300	4.11770800	-1.34607500
H	1.87262400	5.95040400	-1.97503700
C	2.03233100	-1.30616500	-0.47678600
C	0.82387200	-0.95456500	-0.84344000
C	-0.41634100	-0.62743600	-1.14681000
O	-0.89918500	0.59168300	-0.73627400
C	-1.34362800	1.42802800	-1.78924500
H	-0.49859600	1.73848900	-2.42459200
H	-2.09863500	0.93725500	-2.41966500

C	-1.31354700	-1.56158400	-1.86731100
C	-2.69867900	-1.65373900	-1.58709400
C	-0.76624200	-2.41698200	-2.82769600
C	-3.47421500	-2.59736300	-2.28125500
C	-1.54430400	-3.35143600	-3.49673300
H	0.29709600	-2.33375800	-3.04959600
C	-2.90732800	-3.43957100	-3.22442100
H	-4.53741600	-2.65798200	-2.05420000
H	-1.08806700	-4.00298400	-4.23976900
H	-3.52892100	-4.16280900	-3.74906300
H	2.86350300	-1.09921000	-1.15639500
H	-1.79876900	2.30720900	-1.32071800
C	-3.34033300	-0.83753800	-0.61462600
C	-3.92073800	-0.14679000	0.19875300
C	-4.50790300	0.71454100	1.16642800
C	-3.69497800	1.62231500	1.86487800
C	-5.88467800	0.68031300	1.43321300
C	-4.25213100	2.47450200	2.80765500
H	-2.62616700	1.63790500	1.65479700
C	-6.43322500	1.53678100	2.37795400
H	-6.51322200	-0.02436200	0.89103200
C	-5.62069900	2.43472500	3.06640100
H	-3.61479900	3.17397200	3.34625400
H	-7.50271000	1.50387500	2.57955500
H	-6.05465400	3.10436900	3.80717800

TS_3

C	-2.09958100	-2.05135000	-0.79913600
C	-2.94608900	-0.95667400	-1.00528400
C	-2.64740900	-3.31733600	-0.57412100
C	-4.32940400	-1.10346900	-0.98570200
C	-4.02898200	-3.46030000	-0.55896500
H	-1.98978100	-4.16909600	-0.41092200
C	-4.87074800	-2.36158000	-0.76154900
H	-4.95610300	-0.22641500	-1.14071800
H	-4.46190300	-4.44380300	-0.38328700
H	-5.95044500	-2.49732700	-0.74130900
C	-2.26065400	0.32780400	-1.21591600
O	-2.82384800	1.38887000	-1.42633800
C	-0.79231900	0.22611000	-1.15122000
C	0.27006200	0.88771100	-1.18130600
C	1.10179600	2.05005500	-1.25446400
C	0.47053100	3.30717100	-1.27922700
C	2.50202600	1.98329300	-1.28907300
C	1.23039100	4.46655800	-1.33270400
H	-0.61842800	3.34339400	-1.25338200
C	3.25423500	3.14849400	-1.35066000
H	2.99568400	1.01096900	-1.27260500
C	2.62171100	4.38906300	-1.36976900
H	0.73609800	5.43645400	-1.34912300
H	4.34066400	3.08847000	-1.37928200
H	3.21554300	5.30069100	-1.41333900
C	-0.69063300	-1.76730800	-0.81763900
C	0.50530100	-2.13008700	-0.71419900
C	1.81311500	-1.51672100	-0.75900700
O	2.58491800	-1.77237800	-1.89431500
C	1.90618300	-1.60759100	-3.11674600
H	1.10049300	-2.34677700	-3.24177500
H	1.47181500	-0.59824800	-3.20507500
C	2.69177700	-1.66766900	0.46174700
C	2.35974200	-1.05989200	1.69033000
C	3.86550100	-2.41311500	0.37230900
C	3.21674800	-1.21955200	2.78989100
C	4.70423500	-2.56534700	1.47051600
H	4.12124500	-2.87274300	-0.57863000
C	4.38071000	-1.96534600	2.68334900
H	2.94757700	-0.74153800	3.73030600
H	5.61512200	-3.15409900	1.37527600
H	5.03481300	-2.07713700	3.54626400
H	1.42653100	-0.40747600	-0.82488900
H	2.64931500	-1.74744200	-3.90794900
C	1.16944300	-0.29215800	1.85078300
C	0.14931800	0.35059700	1.99725200
C	-1.08770900	1.05319500	2.09421700
C	-1.12977700	2.45264900	2.01013000
C	-2.28700000	0.33800600	2.23512400
C	-2.34765500	3.11775900	2.06376200
H	-0.19831600	3.00596200	1.89827900
C	-3.50008300	1.01173600	2.29017300
H	-2.25125000	-0.74896500	2.29966000
C	-3.53376900	2.40108400	2.20434100
H	-2.37183800	4.20404800	1.99347200
H	-4.42525400	0.44730700	2.39751300
H	-4.48620300	2.92707700	2.24330500

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C	1.40147400	2.46140300	0.42542900
C	2.70739800	2.95365000	0.38407000
C	0.34131400	3.30279100	0.74524600
C	2.99308000	4.28666300	0.65762800
C	0.62441000	4.63689200	1.01842400
H	-0.67978100	2.92457900	0.77828900
C	1.93596000	5.12885600	0.97649400
H	4.02164900	4.64245900	0.61770600
H	-0.18993100	5.31468700	1.27022100
H	2.12153100	6.17883300	1.19590700
C	3.65151900	1.87772200	0.02404300
O	4.86143500	2.02325200	-0.07702000
C	2.83108800	0.64737400	-0.17601700
C	3.15806100	-0.61416200	-0.55209500
C	4.38869600	-1.30674000	-0.88870400
C	5.67703400	-0.74411200	-0.86287300
C	4.25952100	-2.65652200	-1.26858200
C	6.78159400	-1.51039400	-1.20719800
H	5.79247400	0.29658800	-0.57241800
C	5.36591100	-3.41740900	-1.61259100
H	3.26596700	-3.10566100	-1.29193600
C	6.63455600	-2.84382300	-1.58267400
H	7.77247600	-1.05950900	-1.18215500
H	5.24007900	-4.45876200	-1.90412400
H	7.50814800	-3.43591000	-1.85137400
C	1.41412000	1.02639600	0.09807400
C	0.36590900	0.23286800	0.07106800
C	-0.69836600	-0.54422500	0.08584800
O	-1.48681200	-0.61883900	-1.03215200
C	-1.60856100	-1.91768600	-1.58073000
H	-0.64221300	-2.26056100	-1.98341900
H	-1.96853900	-2.65089400	-0.84500900
C	-1.09029900	-1.29869800	1.30106500
C	-2.44280900	-1.50071800	1.66741900
C	-0.08679200	-1.79572900	2.13750800
C	-2.73152700	-2.19170200	2.85593900

C	-0.38866300	-2.46823000	3.31324700
H	0.95315700	-1.64583300	1.84691000
C	-1.71920000	-2.67016100	3.67246300
H	-3.77589300	-2.33764700	3.12714900
H	0.41513600	-2.84362200	3.94386300
H	-1.96774800	-3.20327400	4.58831400
H	2.28337500	-1.27232400	-0.62780300
H	-2.33655500	-1.84876300	-2.39526300
C	-3.52915800	-1.01643300	0.88710200
C	-4.47961300	-0.62845400	0.23768500
C	-5.51951100	-0.14025000	-0.60102600
C	-5.18729100	0.55640500	-1.77444700
C	-6.87046000	-0.34603800	-0.28419500
C	-6.18795600	1.03374400	-2.60894300
H	-4.13557100	0.71472400	-2.01022000
C	-7.86474800	0.13500300	-1.12517000
H	-7.12607000	-0.88635100	0.62594500
C	-7.52753300	0.82449800	-2.28755100
H	-5.92216100	1.57376500	-3.51630500
H	-8.91105000	-0.02891600	-0.87233000
H	-8.31041200	1.20042400	-2.94429600

TS_4

C	1.53293300	-2.35033300	0.25004200
C	0.47714600	-3.24086700	0.48270500
C	2.82001600	-2.67686700	0.66817500
C	0.67165000	-4.46181800	1.11054300
C	3.01888300	-3.90385300	1.29796400
H	3.65055400	-1.98695300	0.51623300
C	1.96144200	-4.79335300	1.51689100
H	-0.17248800	-5.12966700	1.27854200
H	4.01997600	-4.17563600	1.63026800
H	2.15175000	-5.74399100	2.01179000
C	-0.78749500	-2.64794600	-0.00358600
O	-1.88363200	-3.17937800	0.08296100
C	-0.41651300	-1.32869200	-0.60769100
C	-1.16272300	-0.36451000	-1.22687800
C	-2.57864800	-0.15275100	-1.43113700
C	-3.60702200	-0.91134800	-0.84410300
C	-2.93843100	0.94552500	-2.23692600
C	-4.93544200	-0.58243300	-1.07179500
H	-3.34711100	-1.76160300	-0.21984000
C	-4.26730800	1.26244700	-2.47270200
H	-2.14761700	1.55175400	-2.68113000
C	-5.27256100	0.49636300	-1.88745100
H	-5.72033700	-1.17835500	-0.60842800
H	-4.52068500	2.10989900	-3.10766800
H	-6.31896400	0.74092300	-2.06493900
C	1.01596100	-1.16273500	-0.43943500
C	1.69550900	-0.00159600	-0.63527200
C	2.89112800	0.50882500	-0.98923400
O	3.73113600	0.06355400	-1.94500500
C	3.35330700	-1.10025600	-2.65585200
H	3.31083600	-1.98105200	-2.00113300
H	2.37531700	-0.96296700	-3.13833400
C	3.27103100	1.76449800	-0.36125800
C	2.23314700	2.31453700	0.40356000
C	4.50006600	2.40851000	-0.46575800
C	2.43185900	3.51965300	1.07532200
C	4.69051400	3.61002400	0.20861200
H	5.29609700	1.96653700	-1.06198400
C	3.66159700	4.16236800	0.97318100
H	1.62070800	3.94893400	1.66137300
H	5.64749600	4.12431000	0.13710700
H	3.81821400	5.10813900	1.48938300
H	-0.55182500	0.42598700	-1.67305800
H	4.12070200	-1.25249800	-3.41978300
C	0.98614000	1.57222300	0.40135300
C	-0.19531000	1.60748200	0.80961000
C	-1.51569400	1.55949000	1.30056200
C	-2.51873600	2.38936300	0.76126200
C	-1.85397400	0.68173800	2.35153400
C	-3.81048100	2.34559500	1.26514600
H	-2.26219500	3.06873500	-0.05051600
C	-3.14689200	0.65196400	2.84947500
H	-1.08415600	0.02662500	2.75822500
C	-4.13021300	1.48150900	2.31002500
H	-4.57605300	2.98986600	0.83501600
H	-3.39427000	-0.02998200	3.66156900
H	-5.14528600	1.45105200	2.70234100

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C	-0.32857500	-1.69192500	0.80377400
C	-0.10257600	-3.02063000	0.39890500
C	-0.19757200	-1.36676400	2.15727700
C	0.28534000	-4.01103300	1.28286900
C	0.20992600	-2.35732000	3.04669600
H	-0.41959300	-0.36387000	2.51544400
C	0.45948100	-3.66717900	2.62326700
H	0.44221600	-5.02832500	0.92601000
H	0.32914500	-2.10589400	4.10014100
H	0.77470500	-4.41802800	3.34545400
C	-0.40037200	-3.14370600	-1.04072900
O	-0.32781900	-4.17958000	-1.68201600
C	-0.77177600	-1.76307500	-1.50522500
C	-0.93024700	-1.28505700	-2.78469800
C	-1.02261900	-1.88439400	-4.09774100
C	-1.17467200	-3.25762400	-4.37127200
C	-0.99875800	-0.99556300	-5.19421800
C	-1.28397400	-3.70692800	-5.67944000
H	-1.19312600	-3.96122600	-3.54517200
C	-1.10140000	-1.45024700	-6.49881200
H	-0.88933000	0.07284700	-5.00209400
C	-1.24541900	-2.81360900	-6.74819500
H	-1.40191000	-4.77318400	-5.86769600
H	-1.07255900	-0.74095700	-7.32462800
H	-1.33033400	-3.17789600	-7.77089800
C	-0.74404100	-0.90637300	-0.34230700
C	-1.05212300	0.49363400	-0.30970600
C	-2.08276000	1.13780400	-0.97013300
O	-3.02848900	0.46266500	-1.63972300
C	-3.57617800	1.02905700	-2.81857000
H	-3.82797500	0.19385700	-3.48136200
H	-4.49488000	1.58948100	-2.59919300
C	-2.04736900	2.57497200	-0.72190700
C	-0.94510900	2.82215100	0.12004200
C	-2.86948100	3.63220400	-1.11328900
C	-0.64114300	4.10049800	0.55372600
C	-2.55943000	4.91849200	-0.67671200
H	-3.74009500	3.47482700	-1.74579400
C	-1.45593500	5.15545600	0.14316400
H	0.21372800	4.27176600	1.20824600

H	-3.19232300	5.75102900	-0.97988800
H	-1.23468100	6.16947300	0.47178000
H	-0.97985000	-0.19342900	-2.82961200
H	-2.85634100	1.68509400	-3.32734800
C	-0.28411700	1.53368900	0.42100700
C	0.81659600	1.40372300	1.13097300
C	1.95492100	1.52252900	1.89683400
C	3.23441800	1.66505400	1.28451500
C	1.89348900	1.47833000	3.32088600
C	4.37335300	1.76347300	2.05987900
H	3.29380300	1.69324900	0.19793900
C	3.04728800	1.57783800	4.07378200
H	0.92233000	1.37419400	3.80296000
C	4.29340300	1.72038200	3.45525700
H	5.34229500	1.87413300	1.57528700
H	2.98172300	1.54666800	5.16041700
H	5.19697200	1.79635900	4.05722600

TS_5

C	-2.38773400	-1.70138400	0.26405100
C	-1.79130400	-2.96482500	0.40332500
C	-3.69227400	-1.52267800	0.71039600
C	-2.45586900	-4.04967500	0.93757300
C	-4.37434900	-2.61931700	1.24788300
H	-4.18373300	-0.55526900	0.65161900
C	-3.77734300	-3.87266500	1.35641000
H	-1.94521800	-5.00725600	1.03467400
H	-5.39909800	-2.48516900	1.59261400
H	-4.33606900	-4.70627100	1.77798800
C	-0.37470200	-2.88200800	-0.03279700
O	0.41725600	-3.80596200	-0.04667200
C	-0.17520800	-1.46336500	-0.47358800
C	0.94367000	-0.88907000	-1.08640600
C	2.29694800	-1.36584100	-1.11330800
C	2.86201000	-2.14000600	-0.08081800
C	3.13344900	-0.96266700	-2.17331700
C	4.19058100	-2.52678800	-0.13701600
H	2.24559800	-2.43009000	0.76535900
C	4.45818900	-1.36783600	-2.23703200
H	2.71184100	-0.34258100	-2.96584700
C	4.99222100	-2.14879800	-1.21484300
H	4.61243700	-3.12198500	0.67134300
H	5.08053100	-1.06336300	-3.07716600
H	6.03453700	-2.46187800	-1.25446600
C	-1.38589900	-0.78034600	-0.30773200
C	-1.47908900	0.62622500	-0.42857200
C	-2.60292300	1.39066600	-0.67083800
O	-3.68815500	0.82315800	-1.21092000
C	-4.92500800	1.50837100	-1.23794600
H	-5.67042000	0.76830700	-1.54400900
H	-5.19478400	1.89546700	-0.24563300
C	-2.37375200	2.79410200	-0.35065600
C	-1.02937600	2.89471300	0.06523100
C	-3.16851100	3.94492200	-0.38218200
C	-0.47615500	4.11129300	0.42963400
C	-2.60981200	5.16213300	-0.00450500
H	-4.21316500	3.91492200	-0.67801400
C	-1.27592000	5.25056500	0.39482000
H	0.56976700	4.16629700	0.73075600
H	-3.22688500	6.05889400	-0.02581400
H	-0.85628400	6.21599500	0.67222100
H	0.73254800	-0.08018600	-1.78892700
H	-4.91699800	2.32320800	-1.97397700
C	-0.36993300	1.56982900	-0.02092400
C	0.88614600	1.38110400	0.29254800
C	2.21431000	1.18234200	0.62229900
C	3.26674600	1.53992400	-0.26426200
C	2.56877000	0.66826500	1.90140700
C	4.58801200	1.39628600	0.12057400
H	3.01315600	1.94452600	-1.24346400
C	3.89636400	0.54489100	2.26646600
H	1.77281300	0.38382200	2.58833700
C	4.91773500	0.90680600	1.38439700
H	5.37734000	1.67089700	-0.57850900
H	4.14318300	0.15427500	3.25300000
H	5.96032800	0.80514400	1.67931100

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C	-2.46666500	-2.04305000	-0.58309100
C	-1.86267000	-3.19590900	-1.11435900
C	-3.82112700	-2.06629200	-0.30011000
C	-2.56320100	-4.35344200	-1.36682500
C	-4.54327400	-3.24424200	-0.55143800
H	-4.32516500	-1.19698800	0.10848100
C	-3.93327600	-4.37466300	-1.07548900
H	-2.05162200	-5.22083500	-1.78295200
H	-5.60932300	-3.26454700	-0.32832900
H	-4.51839700	-5.27390300	-1.26062600
C	-0.41640500	-2.91240900	-1.34257900
O	0.41319200	-3.66719600	-1.82383200
C	-0.21725700	-1.52966200	-0.89514600
C	1.10059900	-0.84103100	-0.92274600
C	2.10687400	-1.50113100	0.01615200
C	1.80061100	-1.66354000	1.36823700
C	3.35671300	-1.90312100	-0.44888400
C	2.73113600	-2.21829500	2.23980000
H	0.82349000	-1.34889100	1.73870100
C	4.28962600	-2.45907700	0.42116900
H	3.59952800	-1.77558800	-1.50471900
C	3.97957700	-2.61692900	1.76805800
H	2.48029800	-2.34112200	3.29268900
H	5.26229400	-2.77120600	0.04340500
H	4.70833700	-3.05243800	2.45018100
C	-1.40029500	-0.99752300	-0.46054100
C	-1.42572100	0.37466900	-0.04955200
C	-2.40910600	1.20763700	0.43529000
O	-3.64488700	0.76203200	0.68830400
C	-4.65605200	1.60919200	1.19563100
H	-5.54110600	0.97720800	1.31597700
H	-4.38214700	2.02046600	2.17583700
C	-1.88000600	2.56279500	0.60213100
C	-0.51734700	2.53309400	0.20609600
C	-2.45244000	3.76778300	1.02078900
C	0.24161200	3.69870100	0.20794300
C	-1.67638600	4.92200000	1.02984200
H	-3.48894200	3.83627800	1.33493000
C	-0.34463700	4.89156200	0.62166800
H	1.28000100	3.68947200	-0.11545300
H	-2.12277000	5.86059200	1.35404400
H	0.24427000	5.80713200	0.62316100
H	1.52967400	-0.92432600	-1.93980900
H	-4.89481400	2.41791600	0.49305600

C	-0.18631100	1.15854800	-0.18006600
C	0.98866400	0.62917300	-0.58510900
C	2.24596800	1.40542800	-0.69589300
C	2.71751500	1.79386600	-1.95266700
C	2.99000000	1.73370500	0.44173800
C	3.89513300	2.52599500	-2.06801100
H	2.14274200	1.53538300	-2.84275300
C	4.17080100	2.45805400	0.32432300
H	2.62938200	1.41983100	1.42154700
C	4.62245100	2.86130400	-0.92978000
H	4.24506200	2.83596600	-3.05160600
H	4.74118600	2.70912000	1.21733800
H	5.54512800	3.43252500	-1.02007700

TS_6

C	2.88738800	-1.49661100	-0.52886200
C	2.31858900	-2.75911200	-0.76235800
C	4.25991200	-1.38742500	-0.38463400
C	3.07631500	-3.90357300	-0.87729500
C	5.03987400	-2.54891800	-0.50637500
H	4.72140000	-0.42931900	-0.15831800
C	4.46776200	-3.78939700	-0.75502100
H	2.59331800	-4.86459000	-1.05278100
H	6.12088300	-2.47065200	-0.39586300
H	5.09881700	-4.67218000	-0.84293400
C	0.83625900	-2.60930200	-0.79440000
O	0.02463600	-3.51869900	-0.87643800
C	0.57414000	-1.16113400	-0.63247400
C	-0.73606500	-0.54691500	-0.48082100
C	-1.86163300	-1.08068300	-1.33083900
C	-1.62370700	-1.43871900	-2.66234400
C	-3.17736100	-1.15963000	-0.86233000
C	-2.65502900	-1.86742000	-3.48953300
H	-0.60865300	-1.36997600	-3.05439700
C	-4.21529200	-1.58132500	-1.68724100
H	-3.40699000	-0.86294800	0.16242200
C	-3.95819300	-1.94054800	-3.00606700
H	-2.43909400	-2.13926300	-4.52216300
H	-5.23025400	-1.62831700	-1.29443500
H	-4.76820400	-2.27262100	-3.65374900
C	1.77745200	-0.50852600	-0.45687200
C	1.78616400	0.89389700	-0.21343900
C	2.77013200	1.84930200	-0.04927000
O	4.12642900	1.68056700	-0.10050000
C	4.65938900	1.92286100	-1.39162400
H	5.74758900	1.81512800	-1.31976900
H	4.27065500	1.19854900	-2.12507000
C	2.16379000	3.13023100	0.16242300
C	0.74951500	2.98093500	0.12123600
C	2.75327300	4.38012500	0.38582000
C	-0.06144800	4.10840100	0.29714300
C	1.93037000	5.47970100	0.56086900
H	3.83853000	4.47349100	0.42841300
C	0.53340700	5.34404600	0.51414400
H	-1.14701400	4.03178400	0.26341700
H	2.36778100	6.46183300	0.73784500
H	-0.09517800	6.22301300	0.65113100
H	4.41900700	2.93878000	-1.74035100
C	0.47963600	1.57292300	-0.11691600
C	-0.70300500	0.90656200	-0.31043600
C	-1.98275100	1.66276700	-0.36892300
C	-2.74595600	1.90824100	0.77414200
C	-2.44097100	2.13832700	-1.60058800
C	-3.94415700	2.61227600	0.69059700
H	-2.38725700	1.55912900	1.74346400
C	-3.63712700	2.84092200	-1.68579800
H	-1.84987600	1.94633100	-2.49616200
C	-4.39279700	3.07949300	-0.54050200
H	-4.52529100	2.80128200	1.59229100
H	-3.98175000	3.20457100	-2.65260000
H	-5.32961600	3.63044300	-0.60789200
H	-1.01649500	-0.95718300	0.81919100
N	-1.44362300	-1.37560900	2.06284700
H	-2.28621800	-0.79685100	2.13677300
C	-1.92890900	-2.79475600	1.97918900
C	-3.12186700	-2.99008700	2.89937100
C	-0.84732600	-3.82217700	2.24727400
H	-2.25326100	-2.91683800	0.93488800
H	-3.93708300	-2.29250900	2.65809400
H	-3.51941300	-4.00811200	2.79981900
H	-2.84626800	-2.84436300	3.95418800
H	0.00463200	-3.71785200	1.56779600
H	-0.48918400	-3.79425900	3.28541700
H	-1.27159200	-4.81936300	2.07536400
C	-0.56916000	-1.02436600	3.22438200
C	-0.88240200	0.38527600	3.69059400
C	0.90452600	-1.14328900	2.87886100
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H	-0.28025100	0.63174500	4.57375000
H	-0.63212100	1.12079500	2.91134500
H	1.17822300	-2.13107100	2.49243000
H	1.18684900	-0.39049400	2.12967900
H	1.50561700	-0.95877600	3.77881700

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C	-1.78687000	2.00799000	-0.96169000
C	-1.21770700	3.26827400	-0.70311100
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C	-1.96654300	4.42315500	-0.62728900
C	-3.93367500	3.09797300	-1.06012300
H	-3.64239200	0.97032100	-1.36268100
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H	-3.97258000	5.22756700	-0.74531300
C	0.24888300	3.10418400	-0.49574100
O	1.02279700	4.00828400	-0.23540600
C	0.50567100	1.64290800	-0.62108800
C	1.69972600	0.95382700	-0.34739800
C	2.96946900	1.68211100	-0.09092100
C	3.56194000	2.44179100	-1.10474000
C	3.61824800	1.60159700	1.14433100
C	4.76845100	3.09705100	-0.89232500
H	3.06115200	2.51520400	-2.07049800
C	4.82580400	2.25710500	1.36089600
H	3.16647000	1.01633200	1.94536100
C	5.40647100	3.00543800	0.34206700
H	5.21443000	3.68223000	-1.69570800
H	5.31474100	2.18203900	2.33153100
H	6.35340400	3.51722200	0.50895000
C	-0.71374300	0.99487600	-0.90055100

C	-0.75882200	-0.41195000	-0.94918300
C	-1.78391100	-1.37152300	-1.13103200
O	-3.08564200	-1.13571200	-1.55826000
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H	-4.25217500	-0.92468500	-3.21588800
H	-2.60052000	-0.25149000	-3.38503500
C	-1.21931900	-2.66965500	-1.03434800
C	0.17411600	-2.54613800	-0.71855500
C	-1.80478200	-3.93920400	-1.19685300
C	0.94719200	-3.71196900	-0.58316000
C	-1.01601500	-5.06363300	-1.05049200
H	-2.86467500	-4.02318100	-1.44235200
C	0.35546100	-4.95338100	-0.74758100
H	2.01223400	-3.65146900	-0.36460300
H	-1.45680500	-6.05262800	-1.17877700
H	0.95890700	-5.85471300	-0.64807300
H	-2.85166700	-2.02121400	-3.43004000
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C	1.65831900	-0.45655700	-0.32863900
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C	3.00041700	-1.84553300	1.26191400
C	3.91424900	-1.38712500	-0.91496700
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C	5.04142400	-2.13889900	-0.59814700
H	3.82801100	-0.90967000	-1.89120000
C	5.15126700	-2.74394200	0.65047600
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H	5.83900100	-2.25180500	-1.33125400
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H	-6.15392100	-0.30528300	2.01888100

TS_7

C	-1.57408700	2.24645000	-0.83685000
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C	-1.55379100	4.66384700	-0.48915000
C	-3.61560500	3.50902800	-0.97459500
H	-3.49488700	1.36747700	-1.30359000
C	-2.93666000	4.69087800	-0.69569300
H	-0.98905700	5.56945200	-0.26882700
H	-4.69151900	3.53781700	-1.14569400
H	-3.48119500	5.63188600	-0.64152200
C	0.54415100	3.16613300	-0.34422500
O	1.39084800	3.99949100	-0.07827300
C	0.68291100	1.68855800	-0.48529900
C	1.81255100	0.89457500	-0.24532000
C	3.13828400	1.50556800	0.03509200
C	3.78997500	2.24514700	-0.95600200
C	3.77672100	1.32705500	1.26512100
C	5.04876700	2.78619300	-0.72744300
H	3.29627200	2.39309700	-1.91676500
C	5.03583000	1.87036700	1.49752100
H	3.27757200	0.75550800	2.04755700
C	5.67711700	2.59921600	0.50104600
H	5.54229100	3.35748300	-1.51267900
H	5.51768400	1.72250700	2.46317500
H	6.66462000	3.02210400	0.68098300
C	-0.58622700	1.14680600	-0.77694900
C	-0.73381400	-0.23778100	-0.88045200
C	-1.88822200	-1.09558500	-1.01560800
O	-3.05643200	-0.73911100	-1.70473300
C	-2.86564400	-0.61777500	-3.10079100
H	-3.83738900	-0.37307800	-3.54705700
H	-2.14976900	0.18485100	-3.34023700
C	-1.39121900	-2.44892000	-1.06532100
C	0.00188600	-2.45251200	-0.77345800
C	-2.07057200	-3.64525000	-1.32422300
C	0.68835900	-3.67395100	-0.72333300
C	-1.36776200	-4.83925100	-1.27672000
H	-3.13355300	-3.62344900	-1.57067200
C	0.00242200	-4.85423700	-0.97437600
H	1.75566400	-3.70850300	-0.51187500
H	-1.88164500	-5.77803400	-1.48346600
H	0.53763900	-5.80233200	-0.94577500
H	-2.49636800	-1.55933600	-3.53628600
C	0.41832700	-1.06609700	-0.62579600
C	1.66048800	-0.50863700	-0.28518500
C	2.80776200	-1.39998200	0.03192600
C	2.83810900	-2.09331600	1.24559200
C	3.86007500	-1.57268700	-0.86946600
C	3.89463700	-2.94355200	1.55141000
H	2.01274700	-1.96704000	1.94878500
C	4.91506800	-2.42827000	-0.56807200
H	3.84547200	-1.03041300	-1.81502200
C	4.93491400	-3.11629000	0.64174000
H	3.90493800	-3.47631800	2.50140700
H	5.72684600	-2.55710500	-1.28263600
H	5.76200500	-3.78456600	0.87709400
H	-2.46306700	-0.74609100	0.38975600
N	-3.11025800	-0.19614300	1.23447300
H	-3.16390400	0.76097000	0.86498000
C	-4.48919200	-0.77598100	1.16919300
C	-5.47661300	0.08518700	1.93160900
C	-4.47641800	-2.22441800	1.61122400
H	-4.72915100	-0.74225700	0.09684700
H	-5.45847900	1.12446200	1.57194700
H	-6.49475300	-0.29886600	1.79008800
H	-5.27655300	0.09070600	3.01210900
H	-3.75287900	-2.81286400	1.03022400

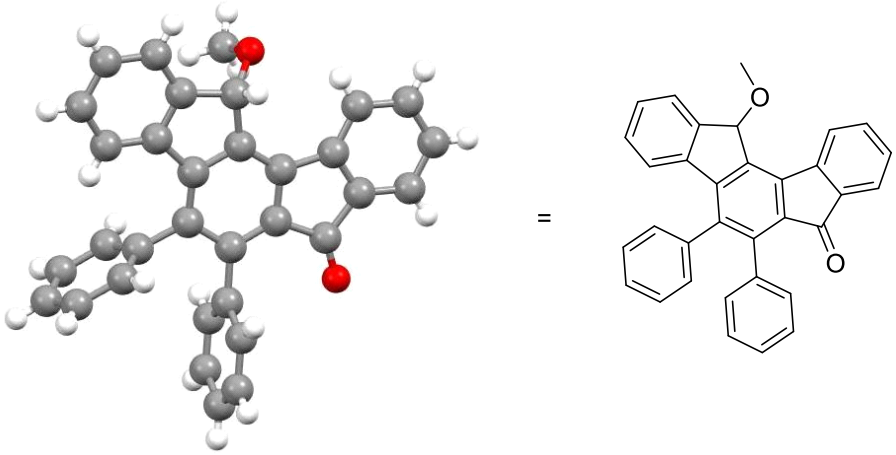
H	-4.23819300	-2.33194900	2.67832500
H	-5.46959000	-2.66245500	1.45302800
C	-2.42149600	-0.15798500	2.56881300
C	-1.96628100	1.26111000	2.85053800
C	-1.26081100	-1.13621800	2.58646100
H	-3.16208400	-0.45637800	3.32425400
H	-2.80644600	1.97043400	2.82888200
H	-1.49552000	1.32252700	3.83912200
H	-1.22154900	1.58260700	2.10712400
H	-1.57501500	-2.15807700	2.33755100
H	-0.48893400	-0.82957300	1.86478900
H	-0.80493900	-1.15307000	3.58462200
C	-3.29624500	0.23267900	-1.11432800
C	-3.06096000	0.89620800	1.18839300
C	-4.65697800	0.51603900	-1.05558700
H	-2.85162800	-0.13939600	-2.03760700
C	-4.42210300	1.17435600	1.24967900
H	-2.42760600	1.05222400	2.06291100
C	-5.22223100	0.98906500	0.12523000
H	-5.27879100	0.36552300	-1.93680000
H	-4.85931900	1.53948300	2.17786200
H	-6.28768600	1.20936900	0.17053800

3aa

C	3.13793900	-0.84040500	-0.14890500
C	3.05392600	-2.23859000	-0.08402400
C	4.37917700	-0.22129400	-0.19006700
C	4.17973200	-3.04055900	-0.07199500
C	5.52013600	-1.03056100	-0.18302900
H	4.46471200	0.86403600	-0.20060200
C	5.42930200	-2.42000300	-0.12795700
H	4.07884500	-4.12395900	-0.01781600
H	6.50236400	-0.56111600	-0.21597400
H	6.33720600	-3.02062500	-0.12193000
C	1.62407900	-2.64871100	-0.01908200
O	1.21151800	-3.78879600	0.06676500
C	0.84647500	-1.37131900	-0.07156200
C	-0.53145400	-1.16873400	-0.02730100
C	-1.47911100	-2.31261600	0.03785700
C	-2.24800300	-2.53786200	1.18133600
C	-1.63822700	-3.15732500	-1.06295100
C	-3.15730700	-3.58914000	1.22414100
H	-2.12645500	-1.88544200	2.04590700
C	-2.55286000	-4.20254100	-1.02395900
H	-1.03478400	-2.98876000	-1.95526100
C	-3.31496200	-4.42119100	0.12038900
H	-3.74648800	-3.75691900	2.12450300
H	-2.66832000	-4.85211000	-1.89037000
H	-4.03036700	-5.24167100	0.15195800
C	1.76383700	-0.29987800	-0.14800600
C	1.28410200	0.99018700	-0.20905100
C	2.03006200	2.29448500	-0.38700900
O	3.08228700	2.56038100	0.51405700
C	2.72091200	2.48971100	1.87360300
H	1.88614900	3.16791800	2.11337000
H	2.44254900	1.46717500	2.17465600
C	0.91015700	3.30513200	-0.36749700
C	-0.33918800	2.67033200	-0.28257800
C	1.02303100	4.68234900	-0.44081400
C	-1.50316700	3.44000500	-0.32744800
C	-0.14208000	5.44754300	-0.45798800
H	2.00657200	5.15040500	-0.48317600
C	-1.38926600	4.82559900	-0.41508800
H	-2.48855700	2.98118300	-0.29311200
H	-0.07983100	6.53318300	-0.51382200
H	-2.29356100	5.43152100	-0.44588700
H	2.51935200	2.30111700	-1.37612800
H	3.59917200	2.79747600	2.45028500
C	-0.11089100	1.21681400	-0.16837600
C	-1.02257300	0.16010600	-0.05948900
C	-2.48425400	0.42623500	0.00511800

X. Crystal structural data of products 3aa

The compound **3aa** was dissolved in $CHCl_3$ to make saturated solution in small via and placed in closed bottle with another solvent as n-hexane. The unit cell parameters and intensity data were collected at 296(2) K on a Rigaku synergy diffractometer using Mo-K_α（λ= 0.71073 Å) radiation from a graphite monochromator. The structures were solved by direct methods and refined on F2 by full-matrix least squares procedures using SHELXTL software. All non-hydrogen atoms were refined anisotropically. All H atoms were located from a difference map and refined isotropically. CIF files of **3aa** (CCDC 2242086) can be obtained from the Cambridge Crystallographic Data Centre using the corresponding deposition numbers. Copies of the data can be obtained, free of charge, on application to the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [e-mail: deposit@ccdc.cam.ac.uk].



ORTEP plot of the crystal structure of **3aa (CCDC 2242086)**

Crystal data and structure refinement for **3aa**

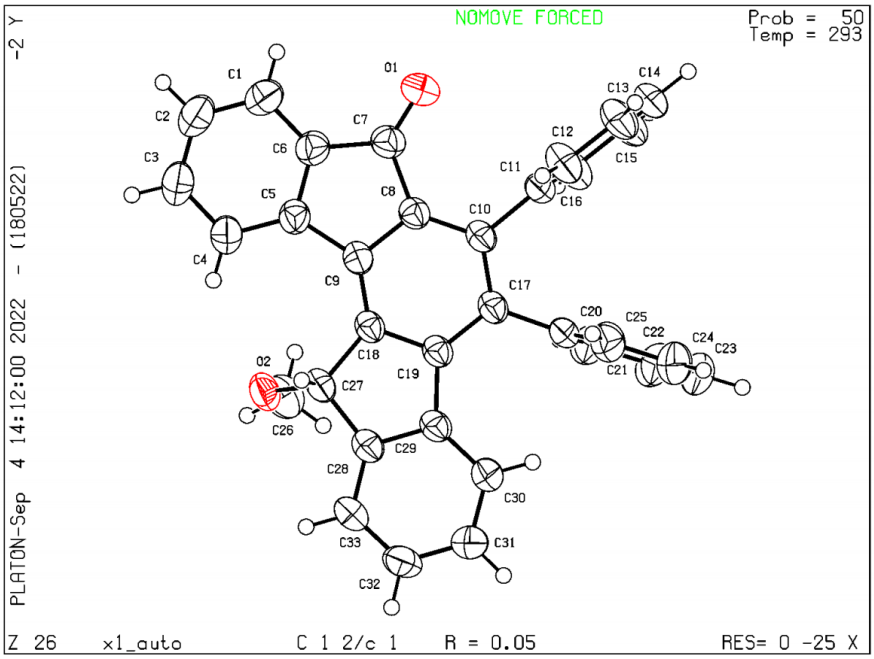
Bond precision	C-C = 0.0026 A	Wavelength=1.54184
Cell	a=22.2806(4)	b=10.11806(12) c=22.3649(4)
	alpha=90	beta=108.7377(18) gamma=90
Temperature	293 K	
	Calculated	Reported
Volume	4774.64(14)	4774.64(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C_{33} H_{22} O_2	C_{33} H_{22} O_2
Sum formula	C_{33} H_{22} O_2	C_{33} H_{22} O_2
Mr	450.51	450.50
Dx,g cm^{-3}	1.253	1.253
Z	8	8

Mu (mm^{-1})	0.601	0.601
F000	1888.0	1888.0
F000’	1893.34	
h,k,lmax	26,12,26	26,11,26
Nref	4378	4281
T_{min}, T_{max}	0.965, 0.976	0.554, 1.000
T_{min}’	0.965	

Data completeness= 0.978 Theta(max)= 68.178

R(reflections)= 0.0488(3514) wR2(reflections)=0.1412 (4281)

S = 1.057 Npar= 317



XI. References

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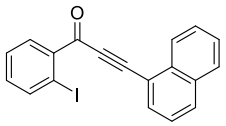
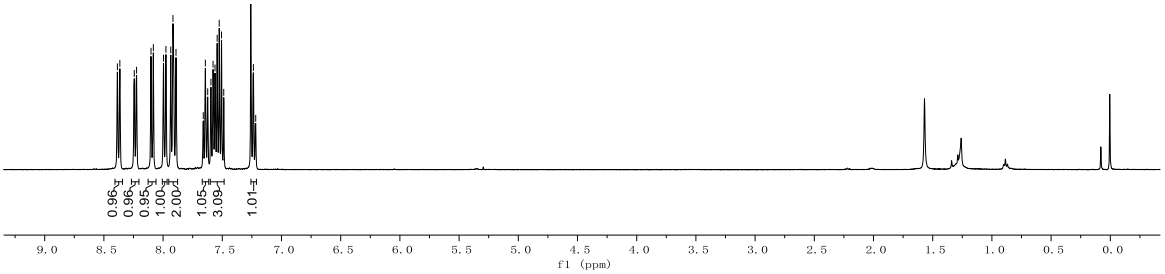
XII. NMR Spectra of Compounds

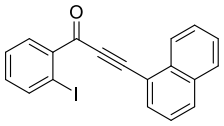
^{1}H NMR of **1f** (400 MHz, $CDCl_3$)



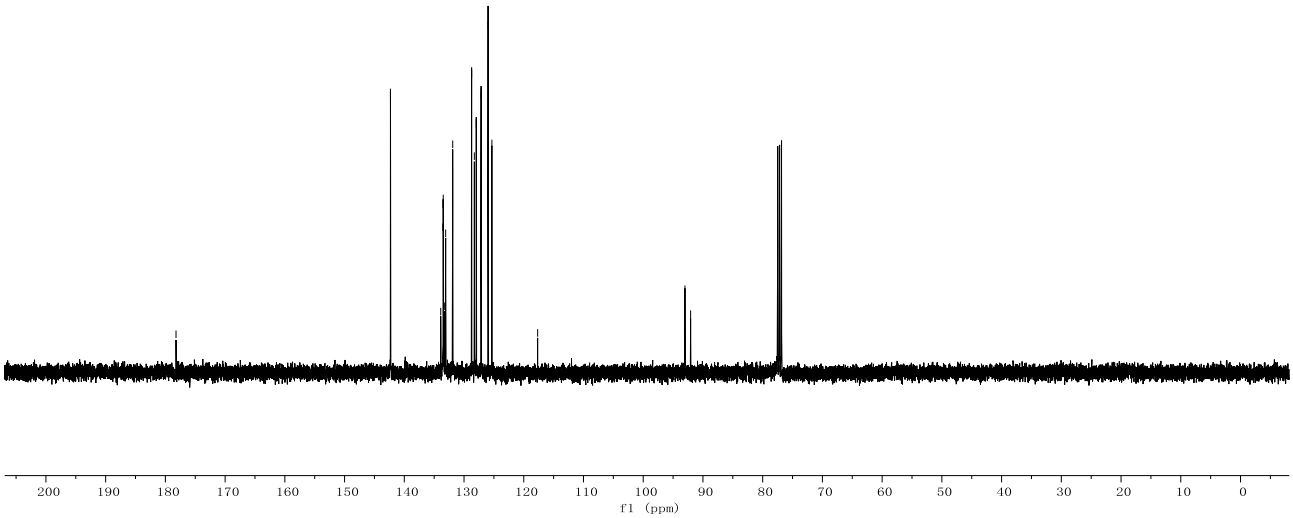
1f



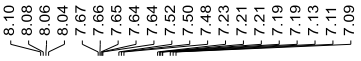
^{13}C NMR of **1f** (100 MHz, $CDCl_3$)

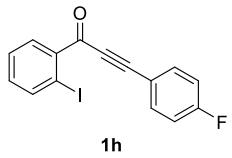


1f

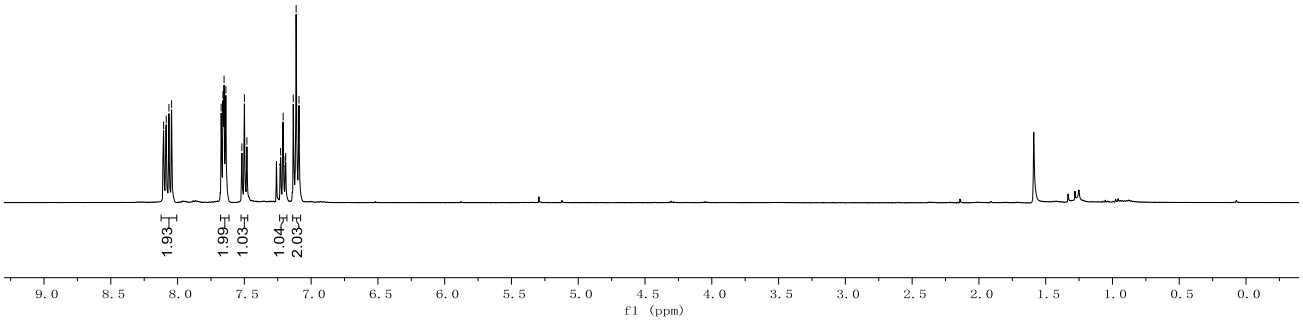


^{1}H NMR of **1h** (400 MHz, $CDCl_3$)

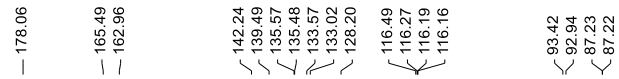


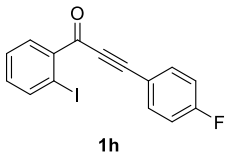


1h

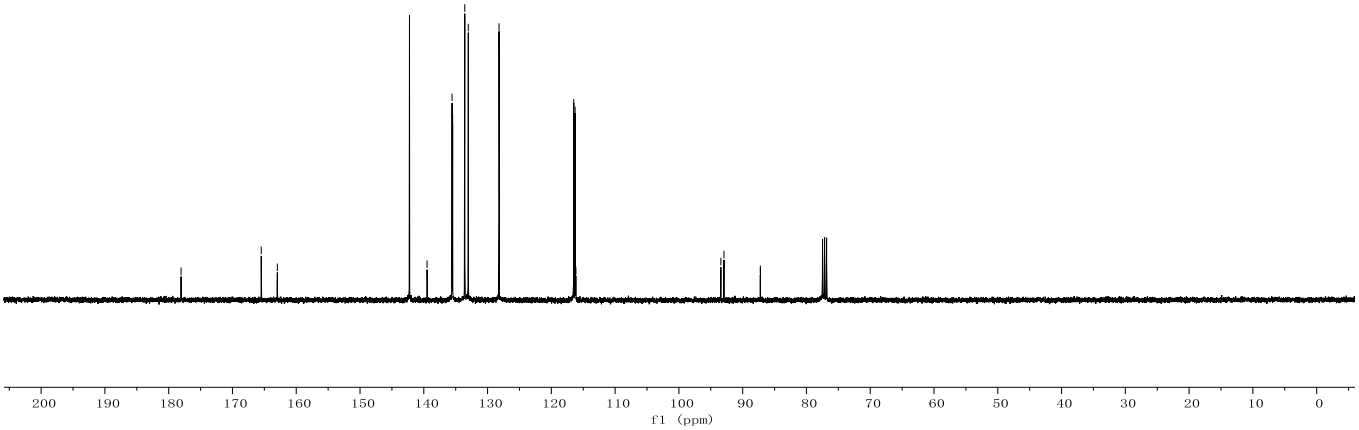


^{13}C NMR of **1h** (100 MHz, $CDCl_3$)

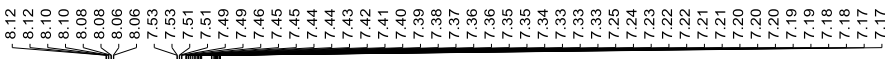


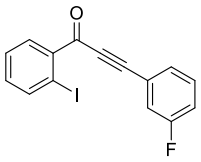


1h

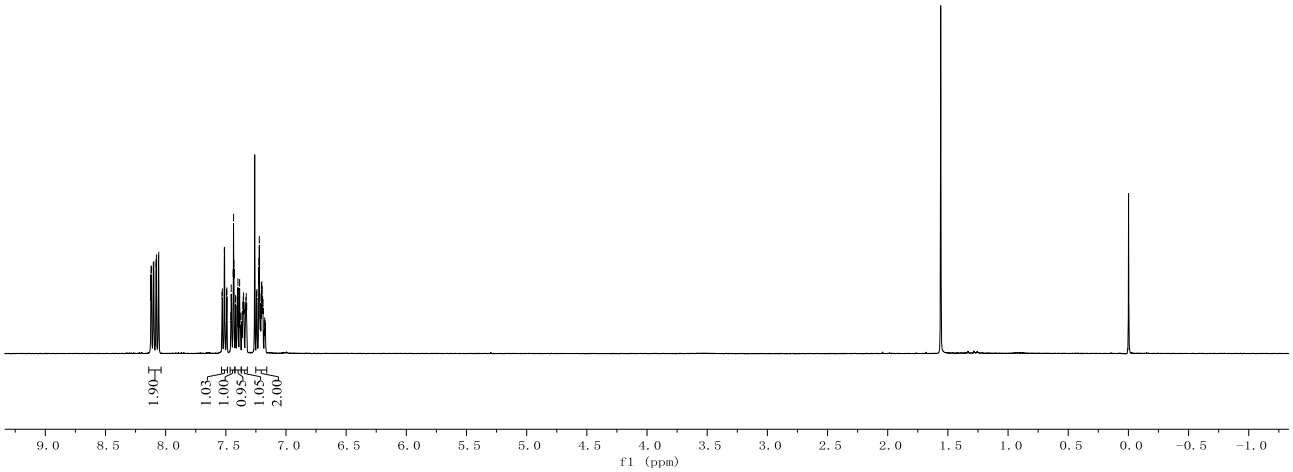


^{1}H NMR of **1i** (400 MHz, $CDCl_3$)

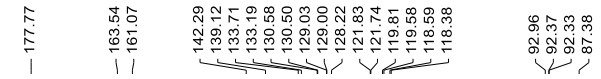


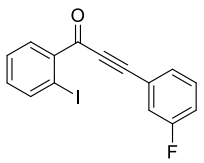


1i

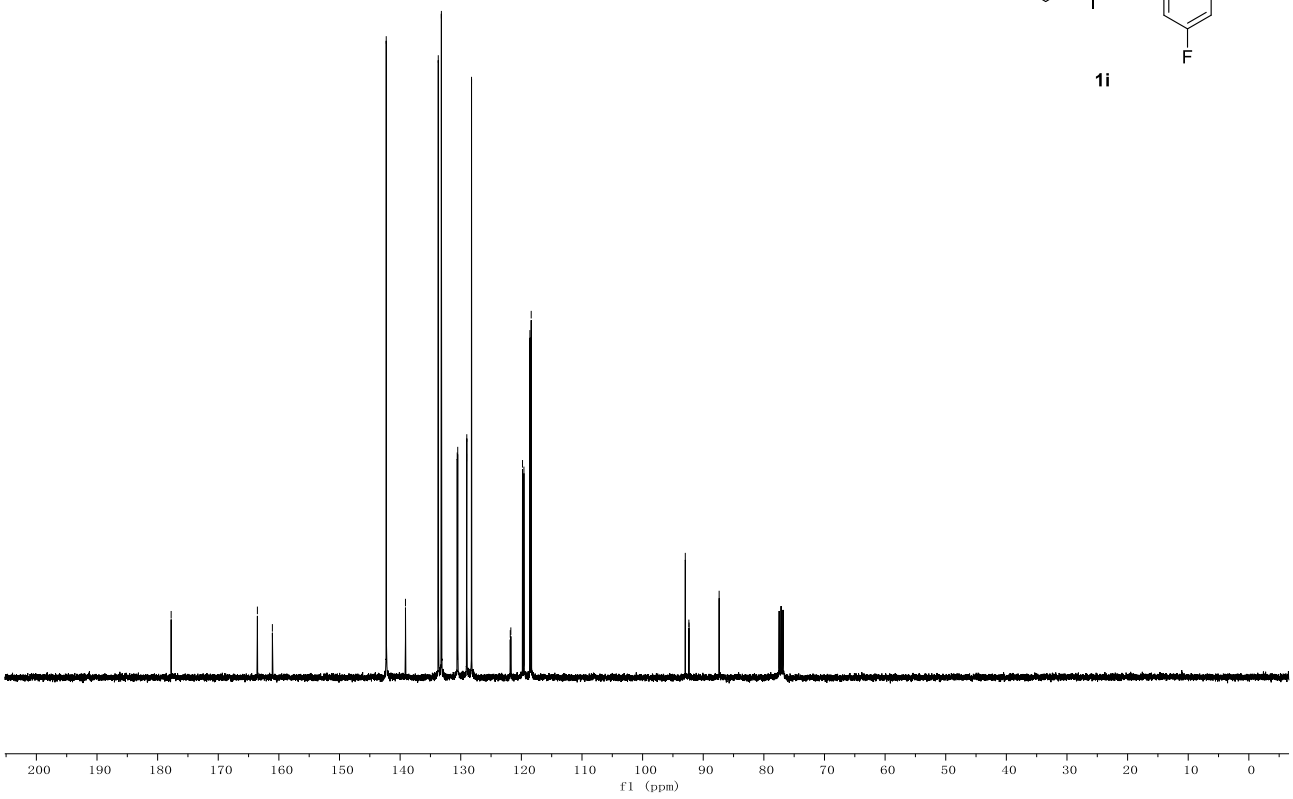


^{13}C NMR of **1i** (100 MHz, $CDCl_3$)

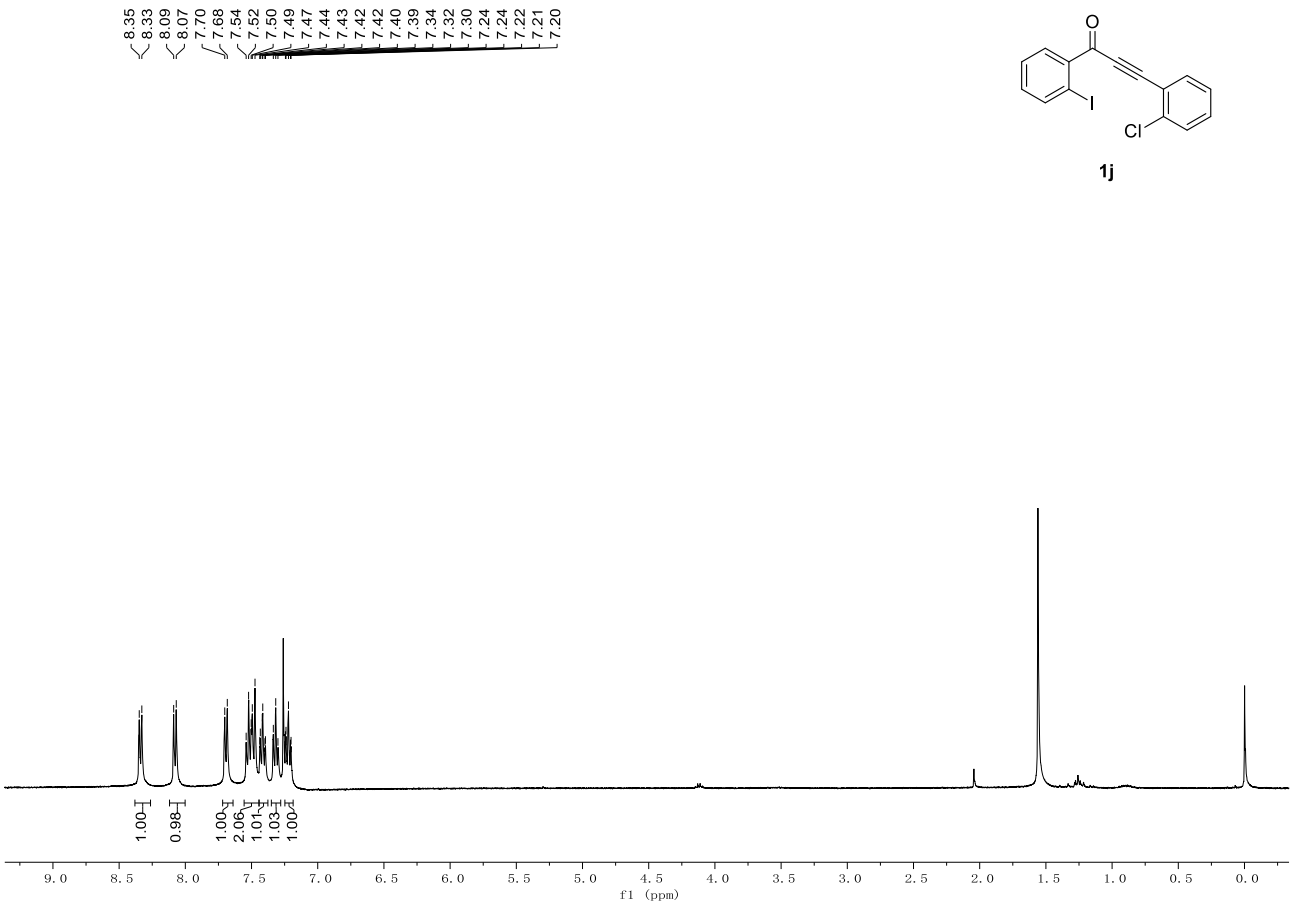




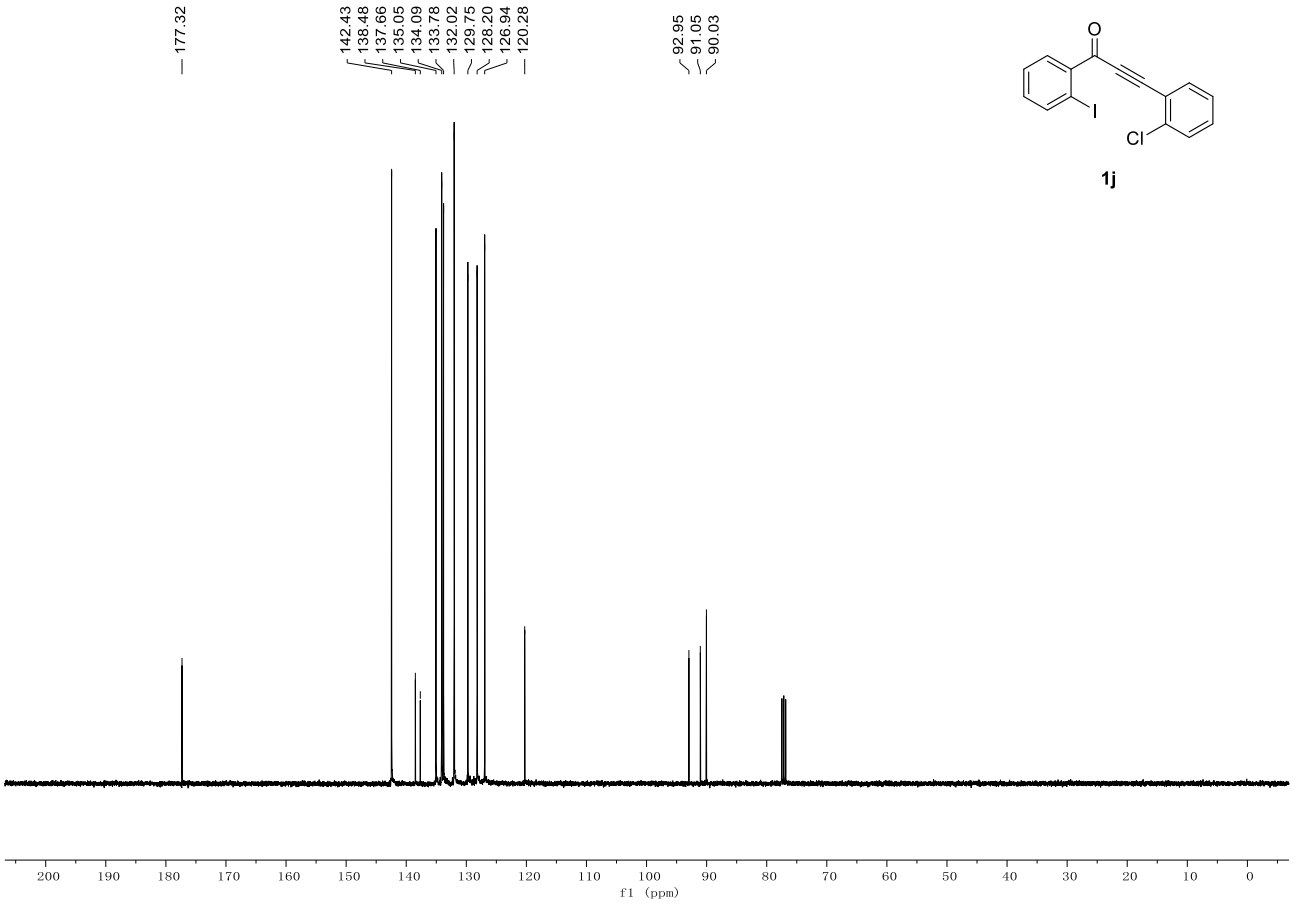
1i



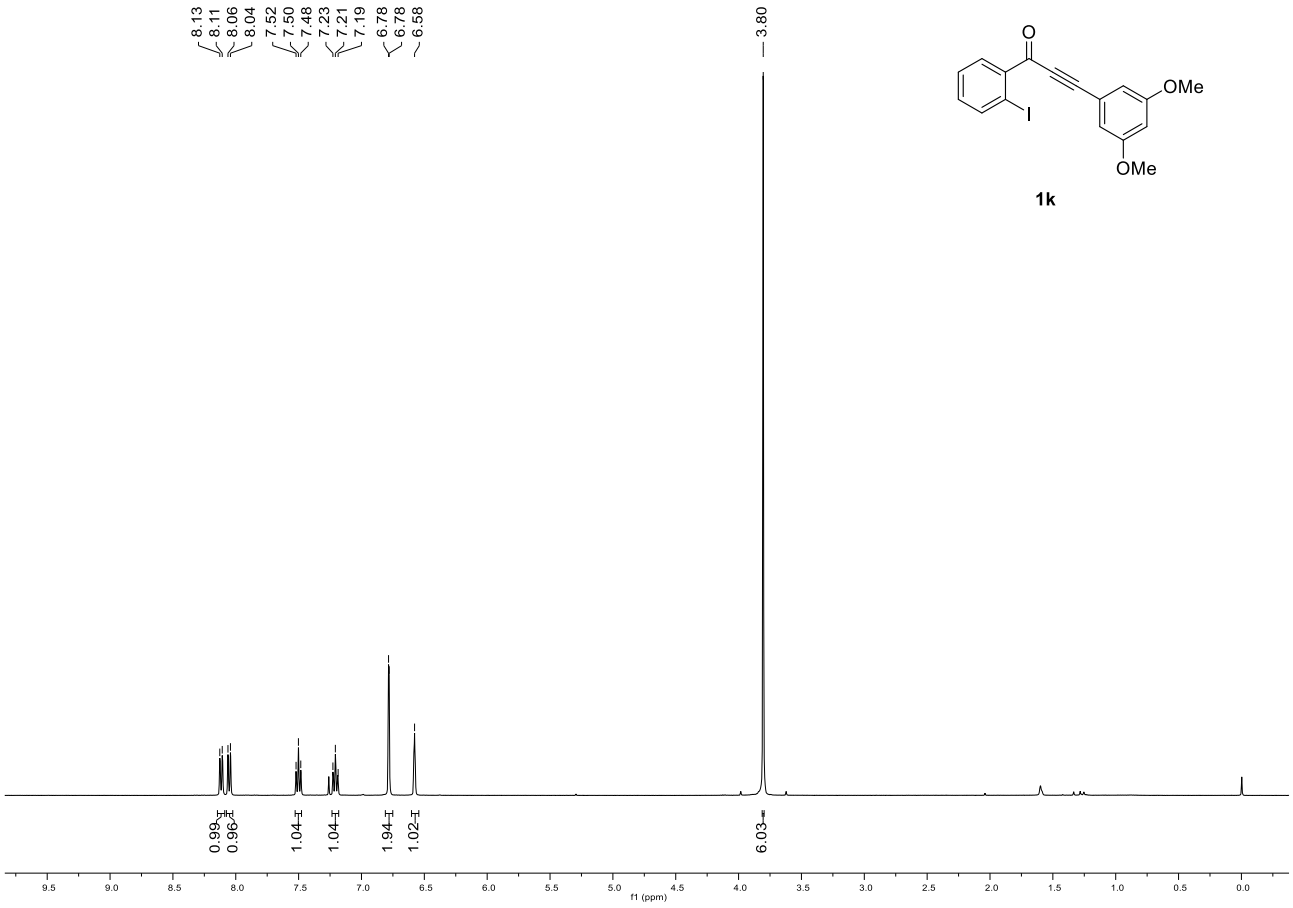
^{1}H NMR of **1j** (400 MHz, $CDCl_3$)



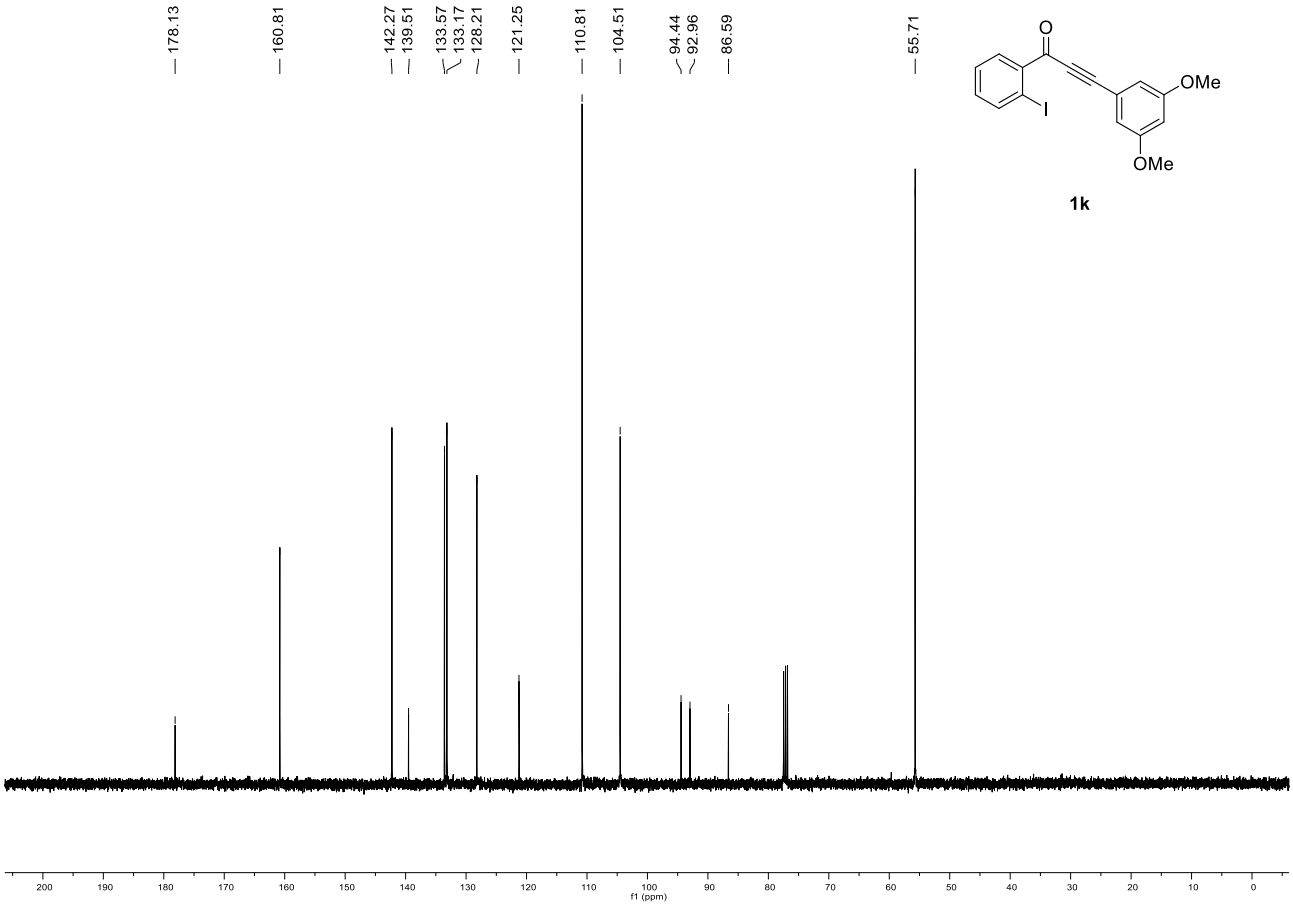
^{13}C NMR of **1j** (100 MHz, $CDCl_3$)



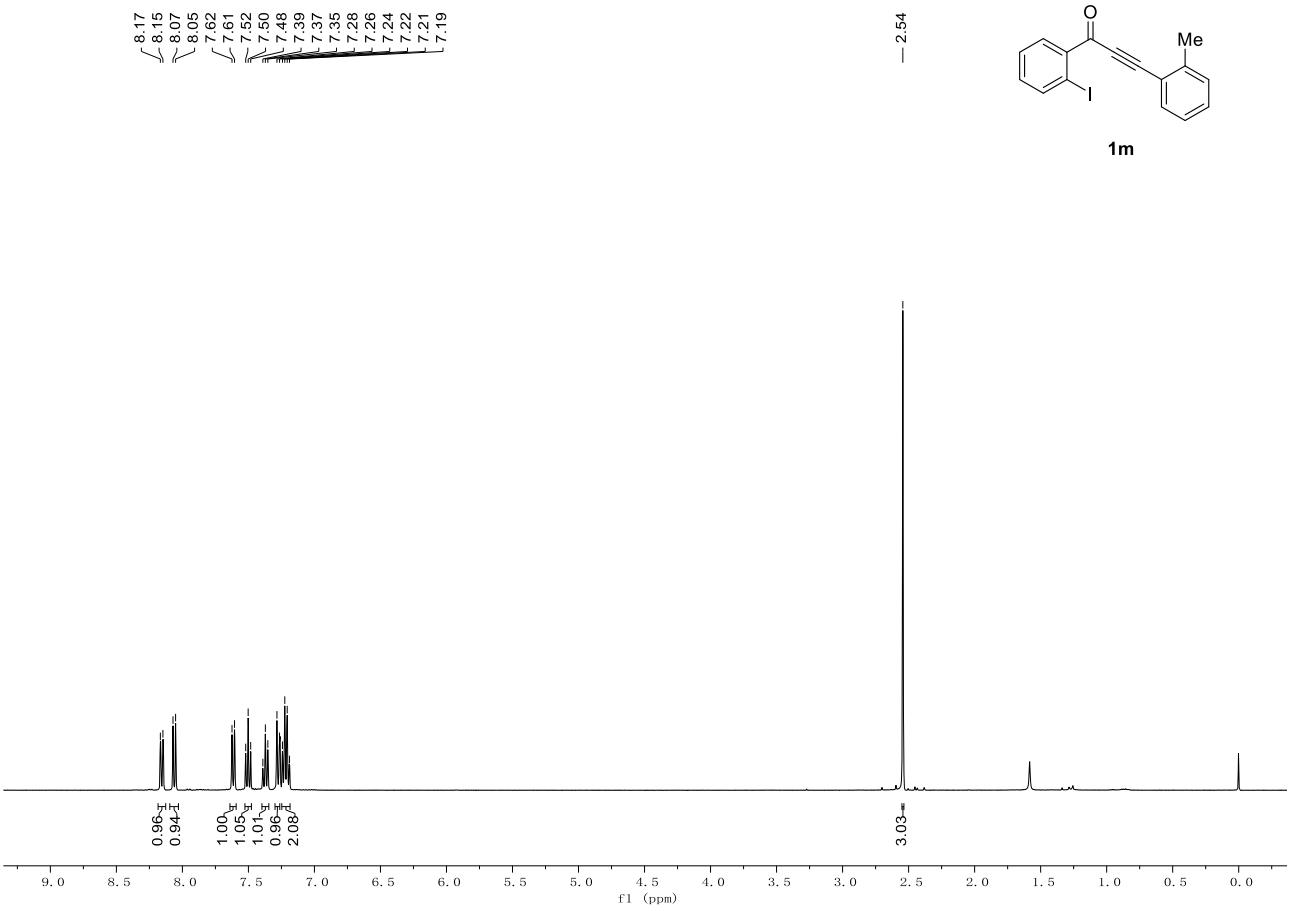
^{1}H NMR of **1k** (400 MHz, $CDCl_3$)



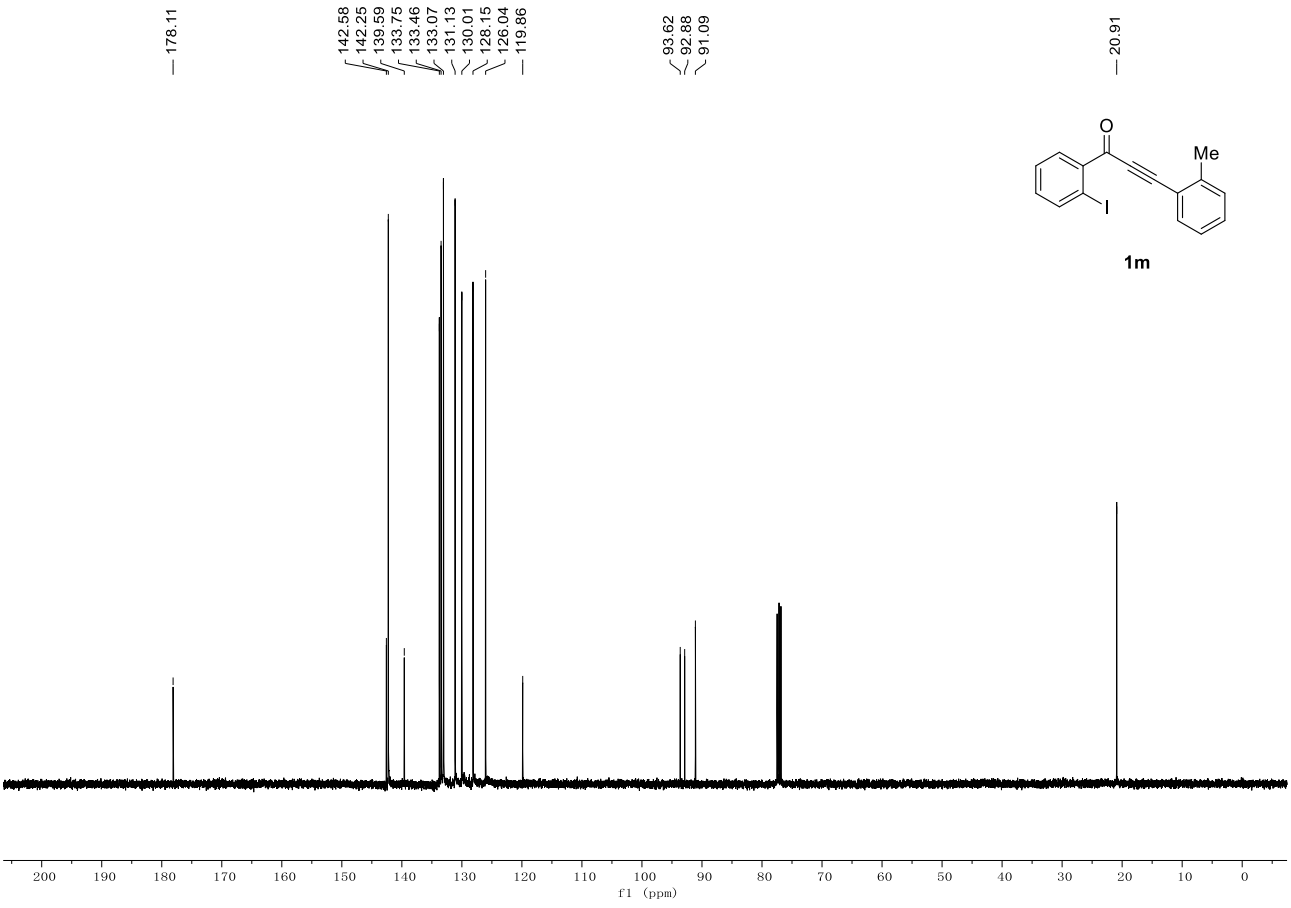
^{13}C NMR of **1k** (100 MHz, $CDCl_3$)



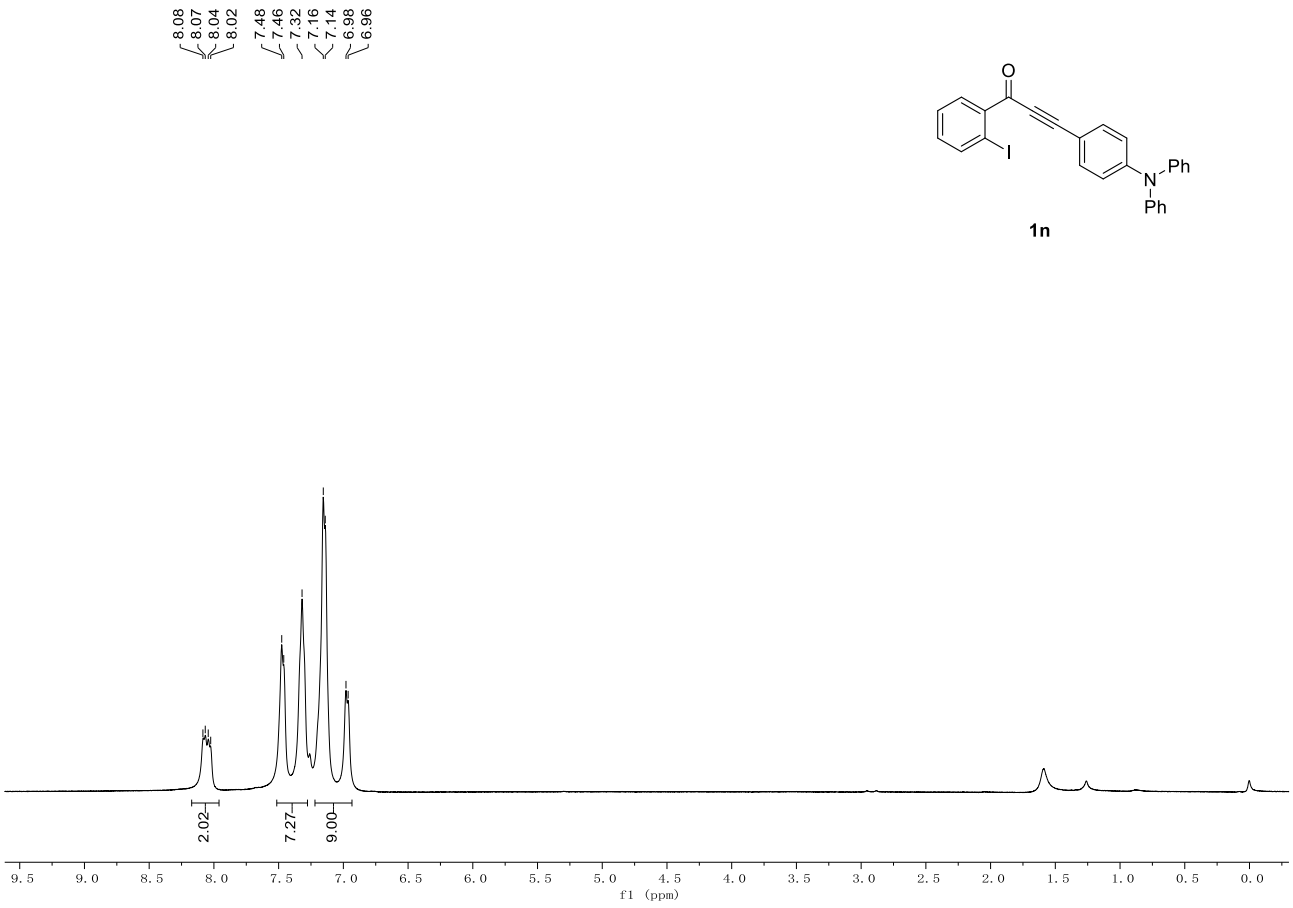
^{1}H NMR of **1m** (400 MHz, $CDCl_3$)



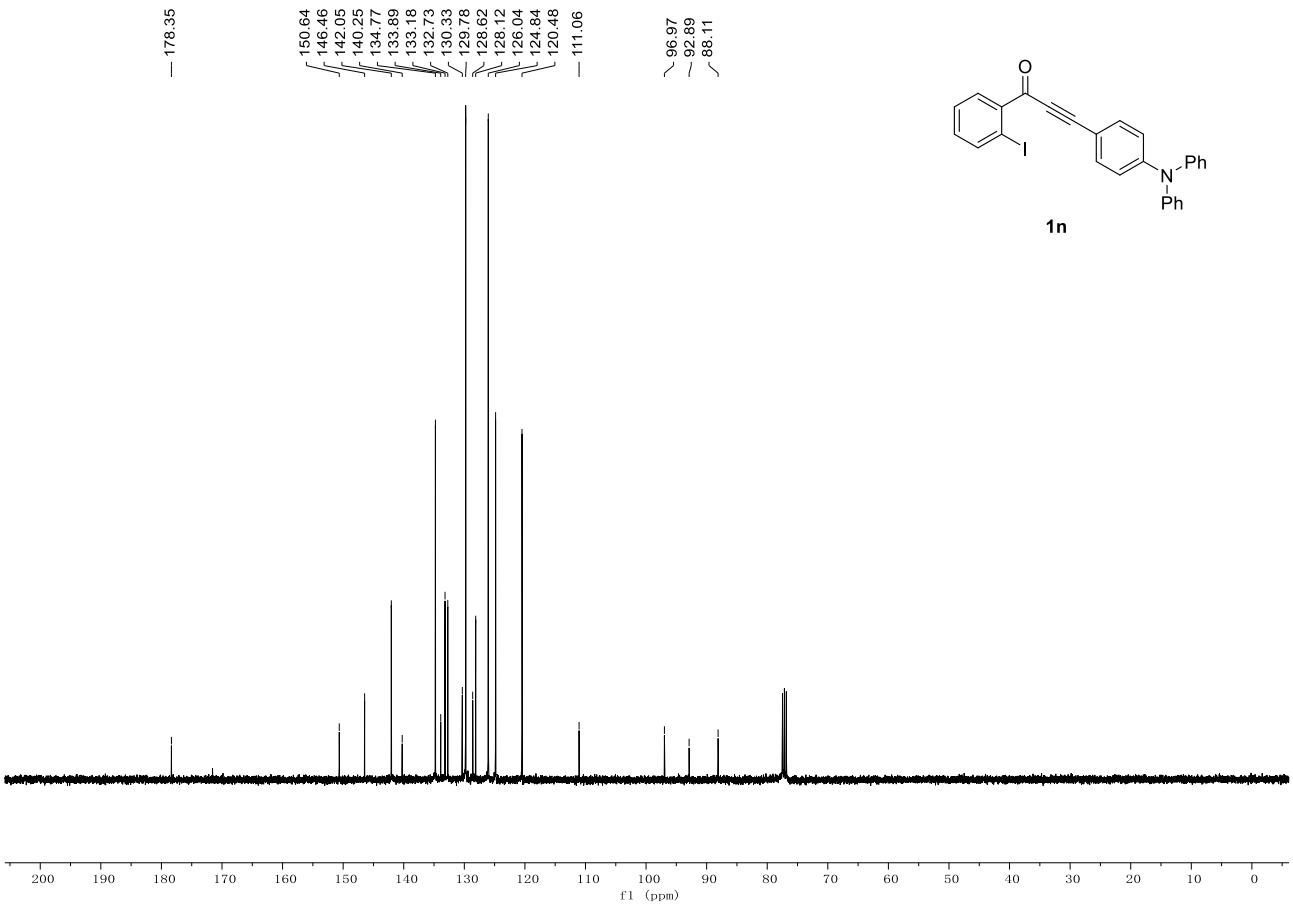
^{13}C NMR of **1m** (100 MHz, $CDCl_3$)



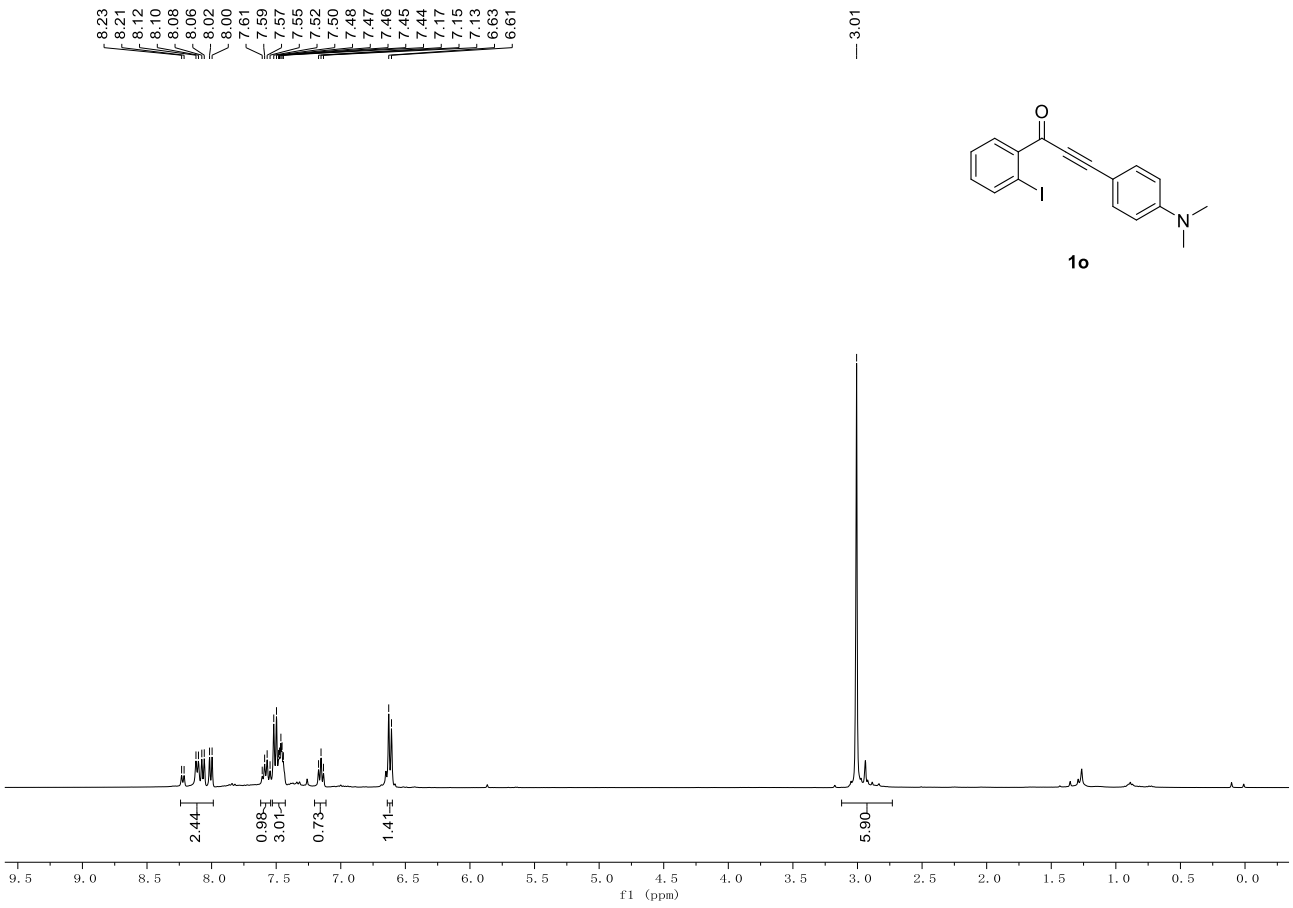
^{1}H NMR of **1n** (400 MHz, $CDCl_3$)



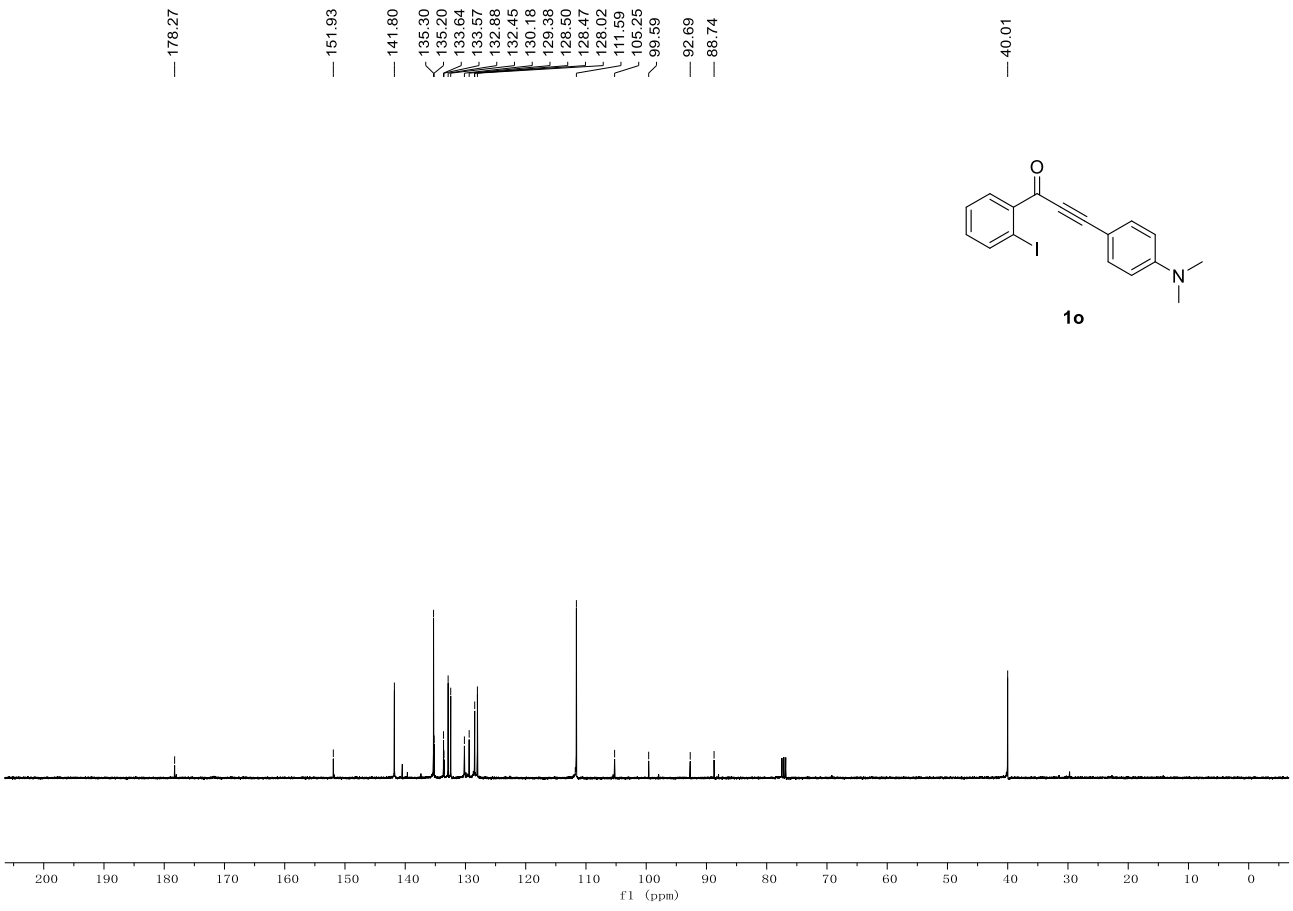
^{13}C NMR of **1n** (100 MHz, $CDCl_3$)



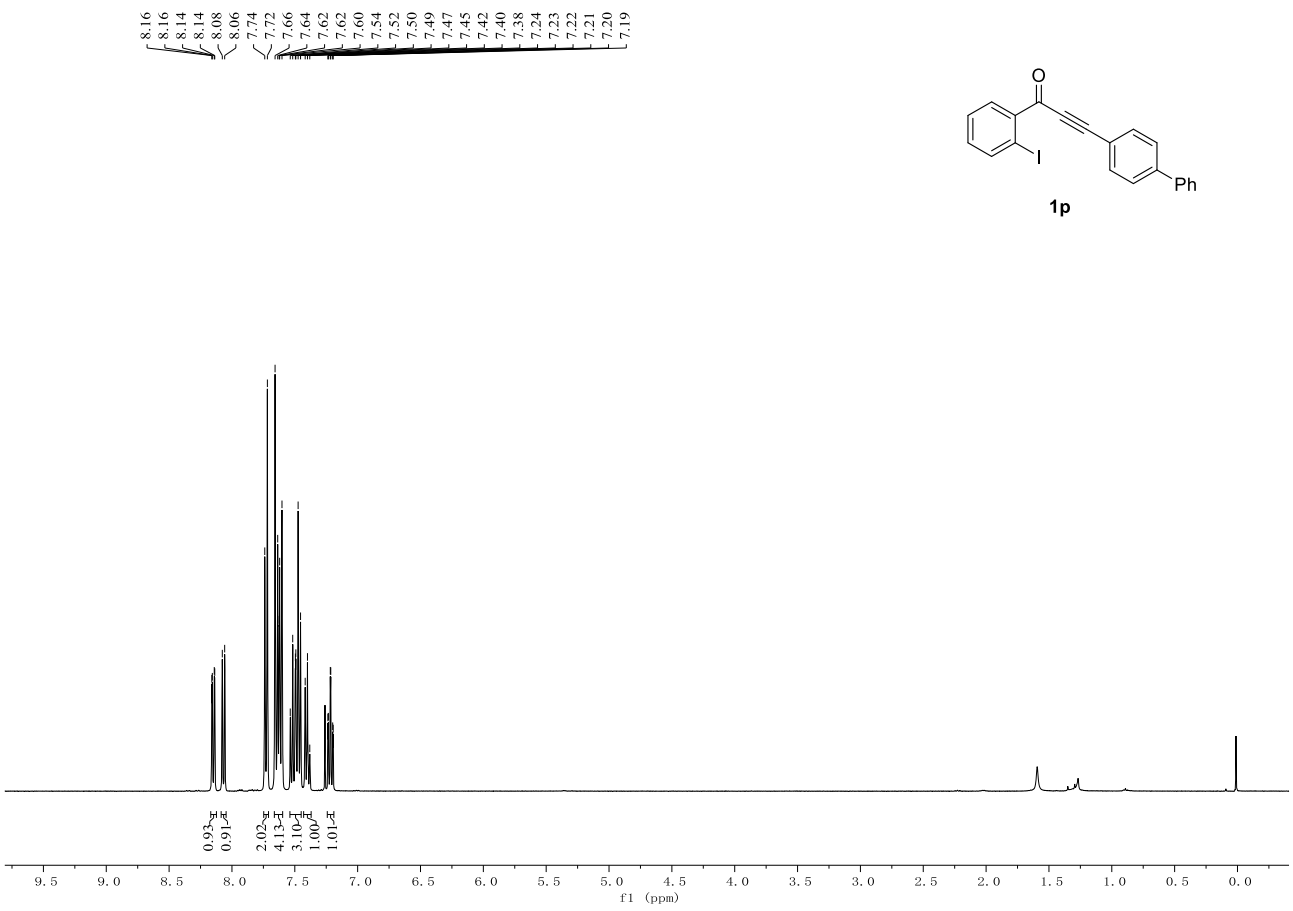
^{1}H NMR of **1o** (400 MHz, $CDCl_3$)



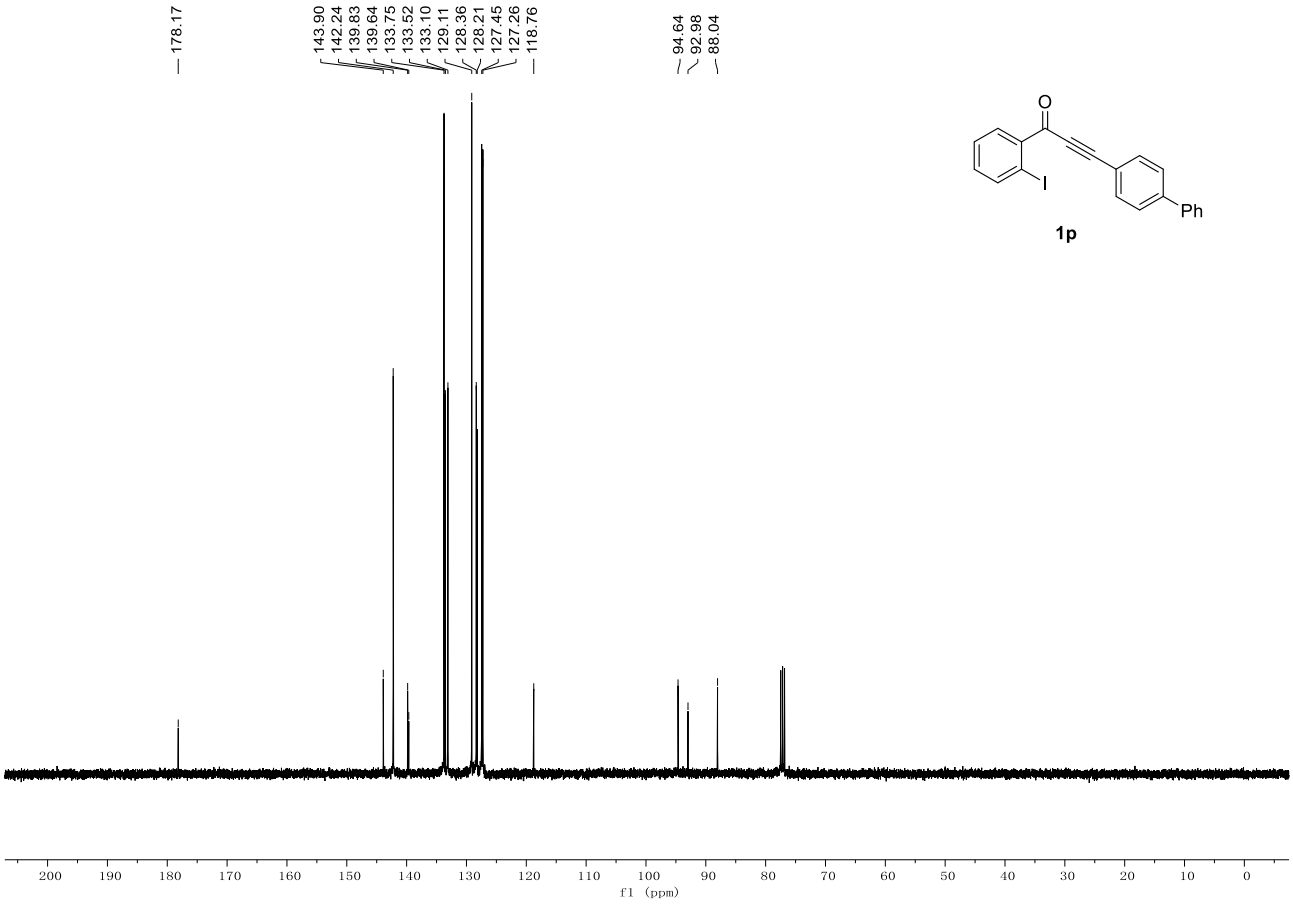
^{13}C NMR of **1o** (100 MHz, $CDCl_3$)



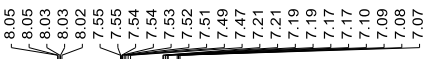
^{1}H NMR of **1p** (400 MHz, $CDCl_3$)

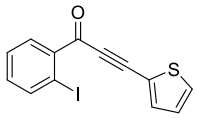


^{13}C NMR of **1p** (100 MHz, $CDCl_3$)

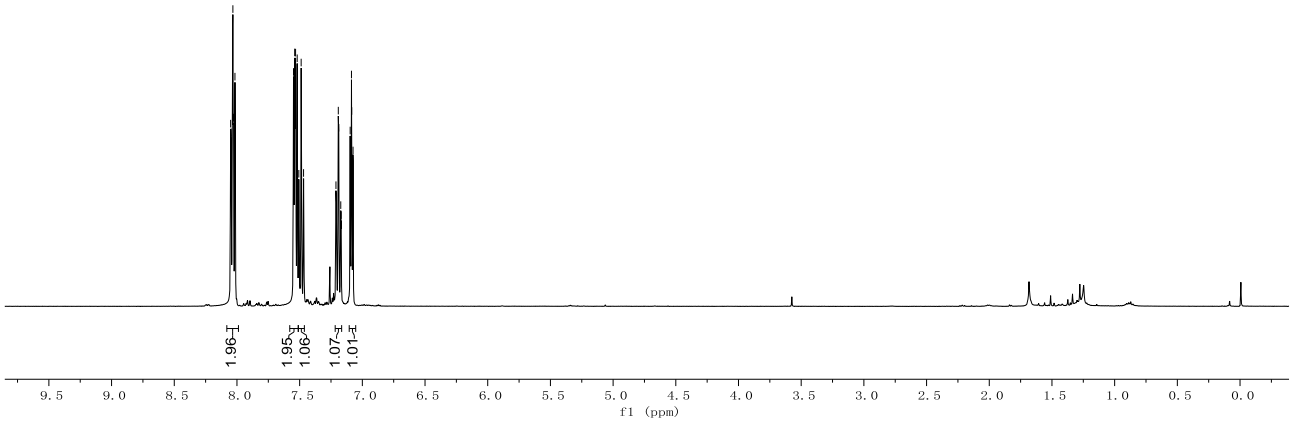


^{1}H NMR of **1r** (400 MHz, $CDCl_3$)

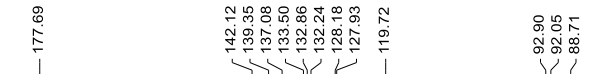


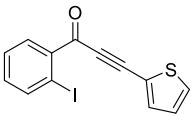


1r

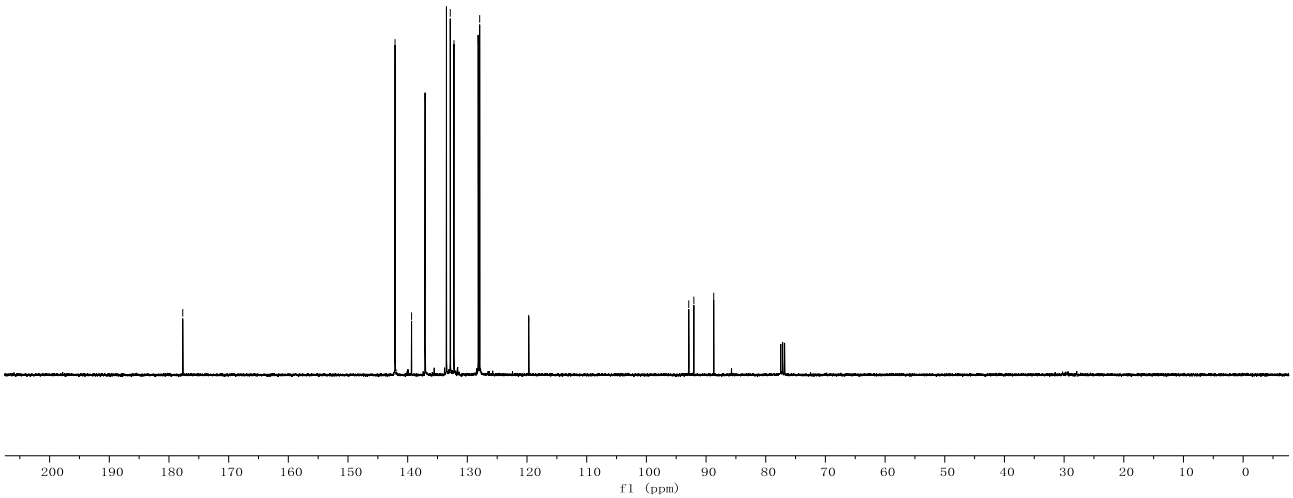


^{13}C NMR of **1r** (100 MHz, $CDCl_3$)

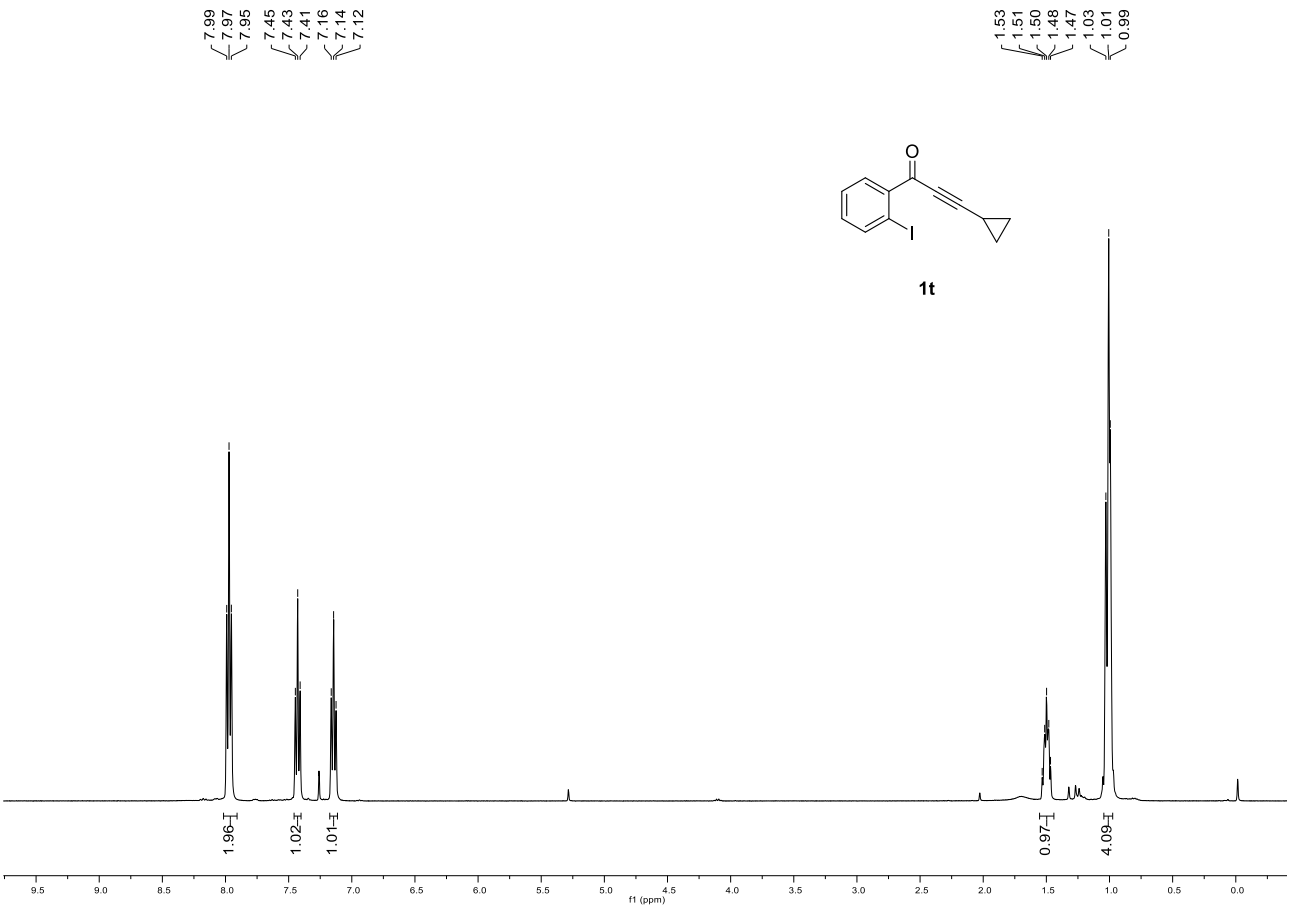




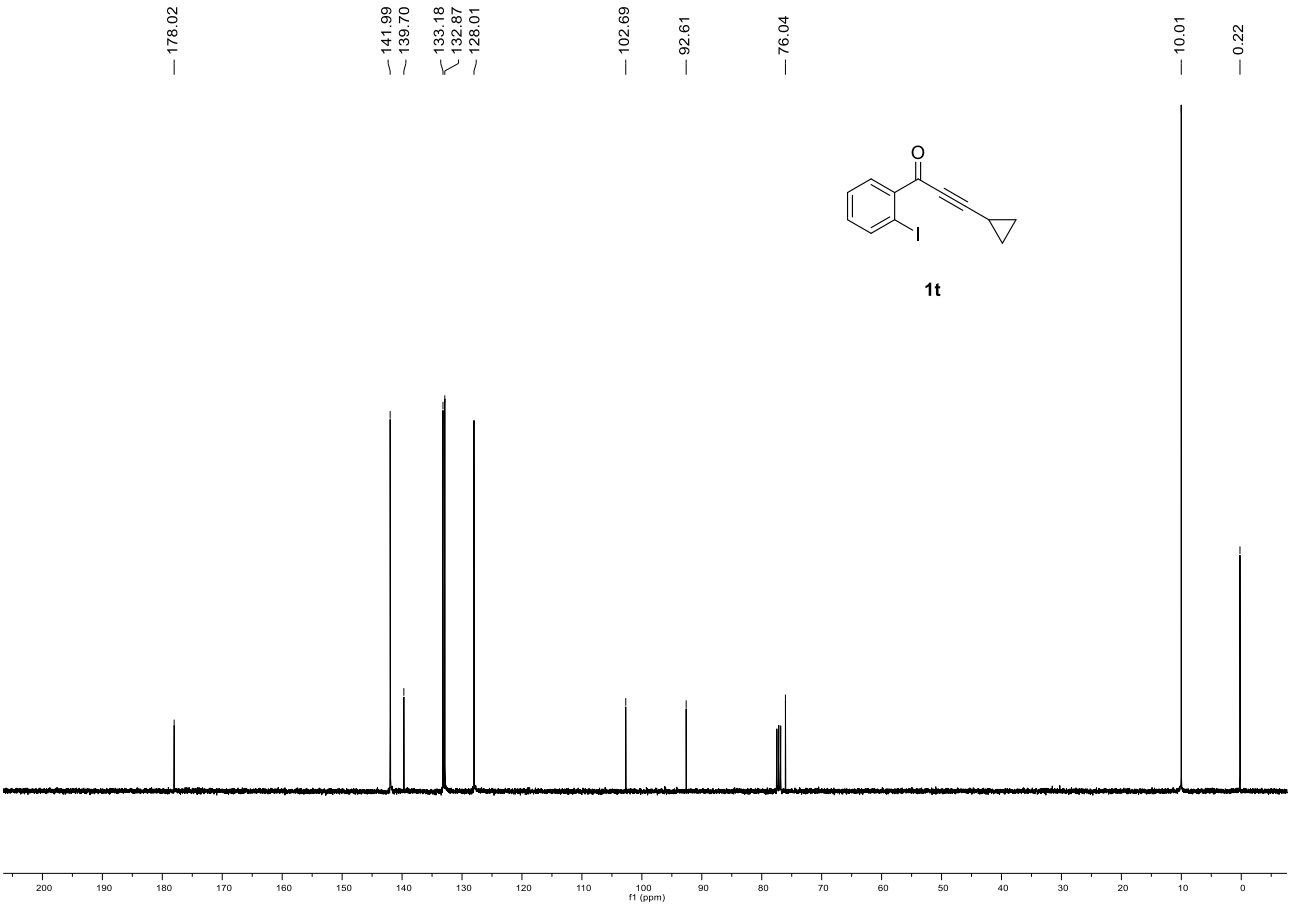
1r



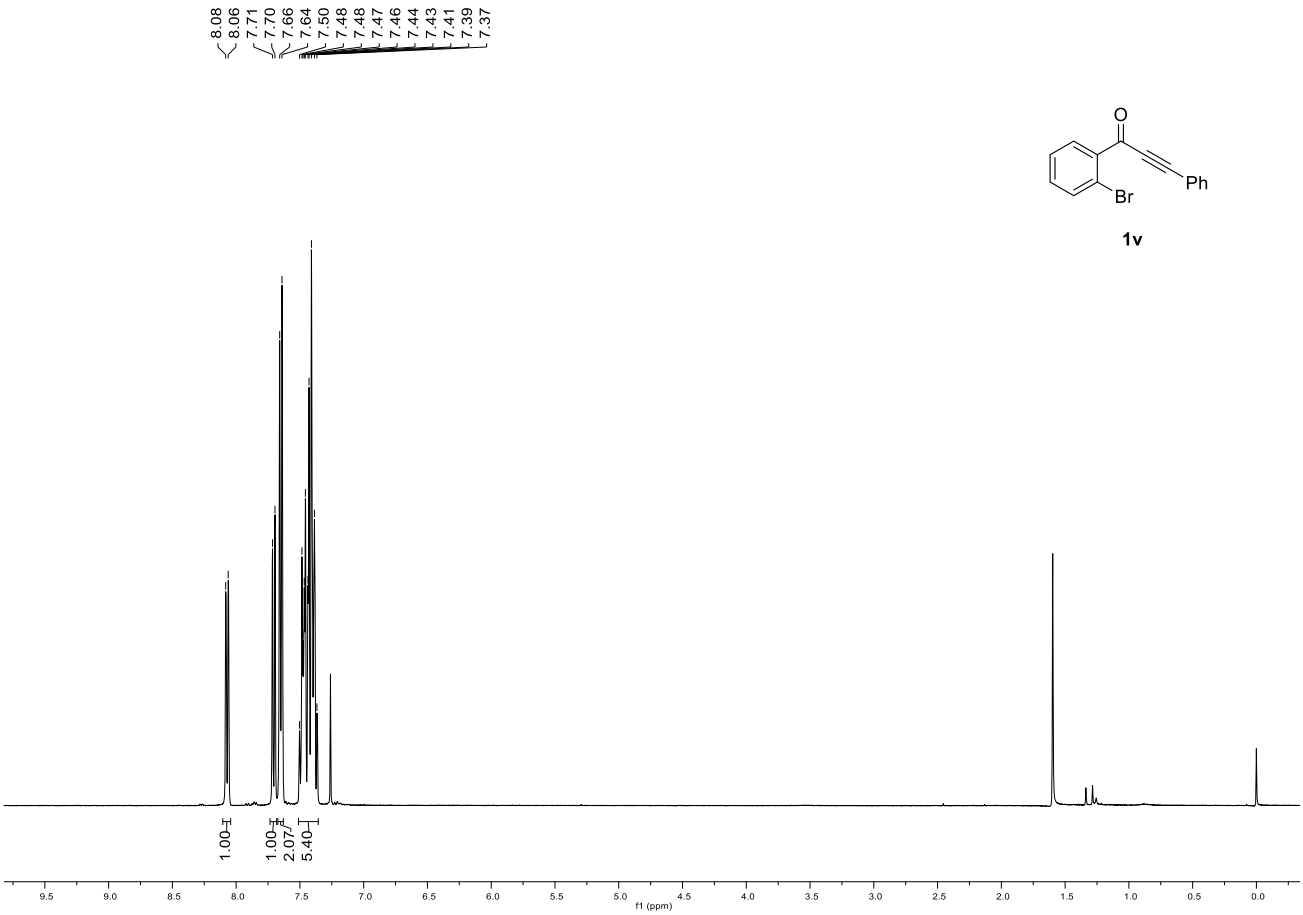
^{1}H NMR of **1t** (400 MHz, $CDCl_3$)



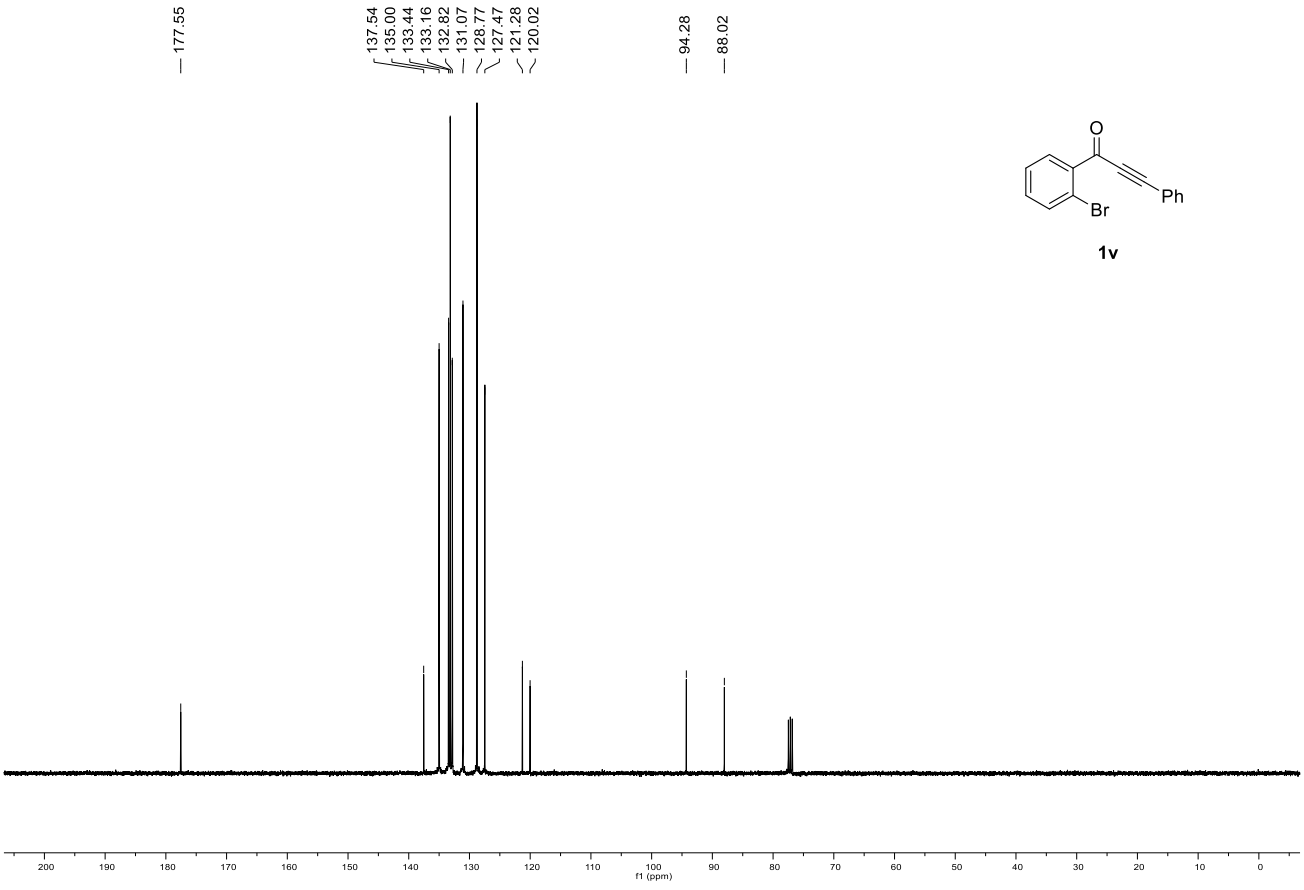
^{13}C NMR of **1t** (100 MHz, $CDCl_3$)



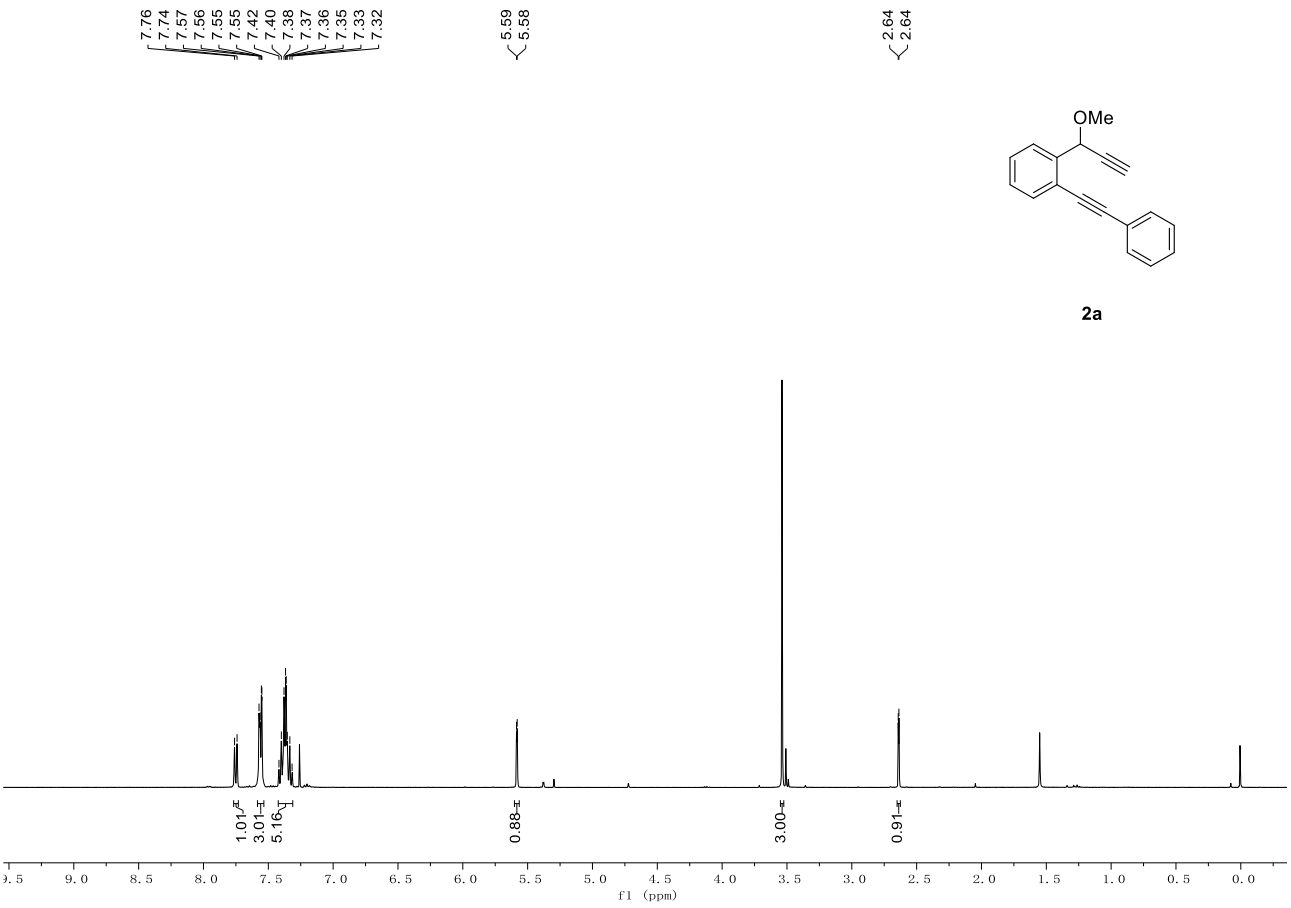
^{1}H NMR of **1v** (400 MHz, $CDCl_3$)



^{13}C NMR of **1v** (100 MHz, $CDCl_3$)

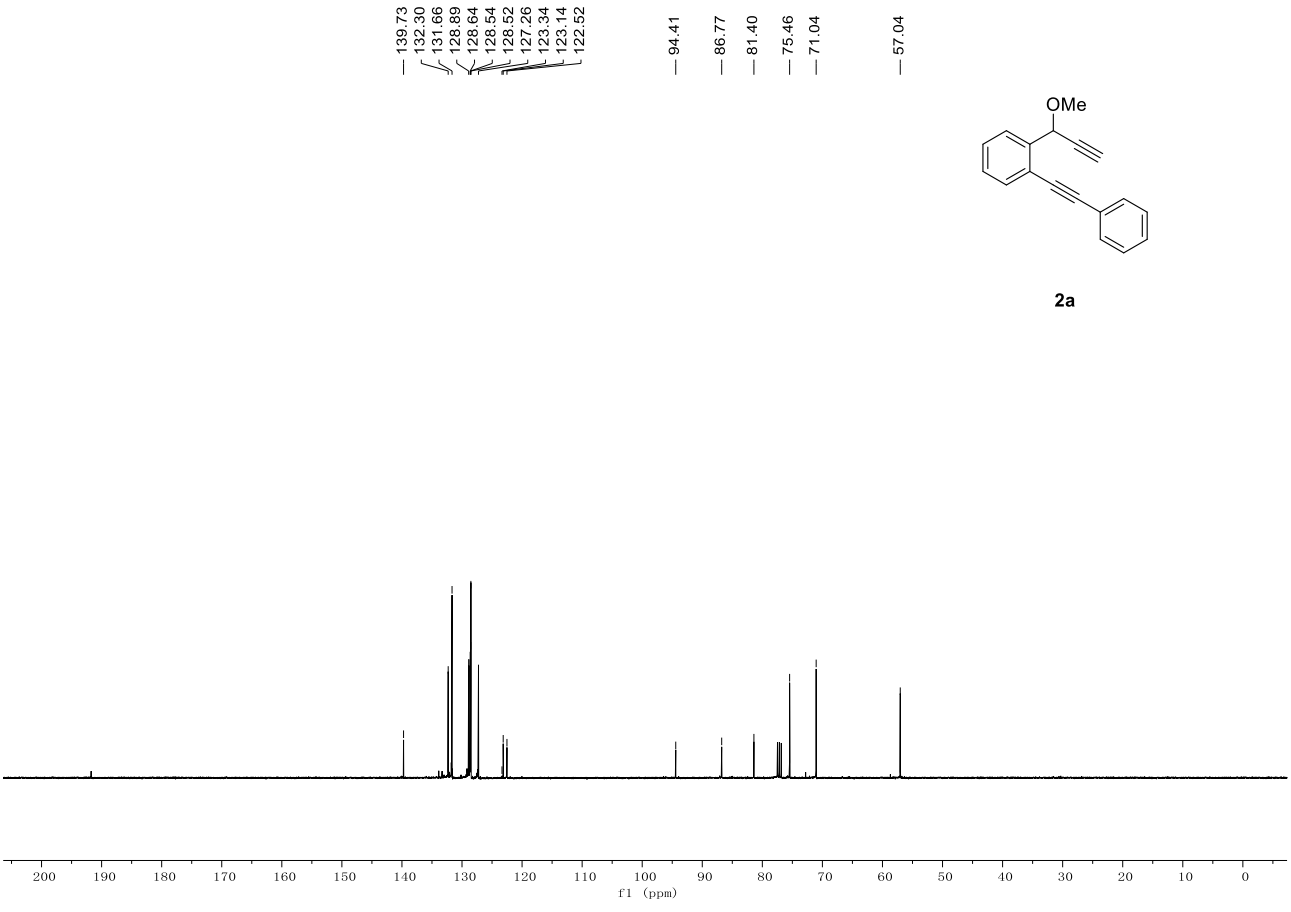


^{1}H NMR of **2a** (400 MHz, $CDCl_3$)



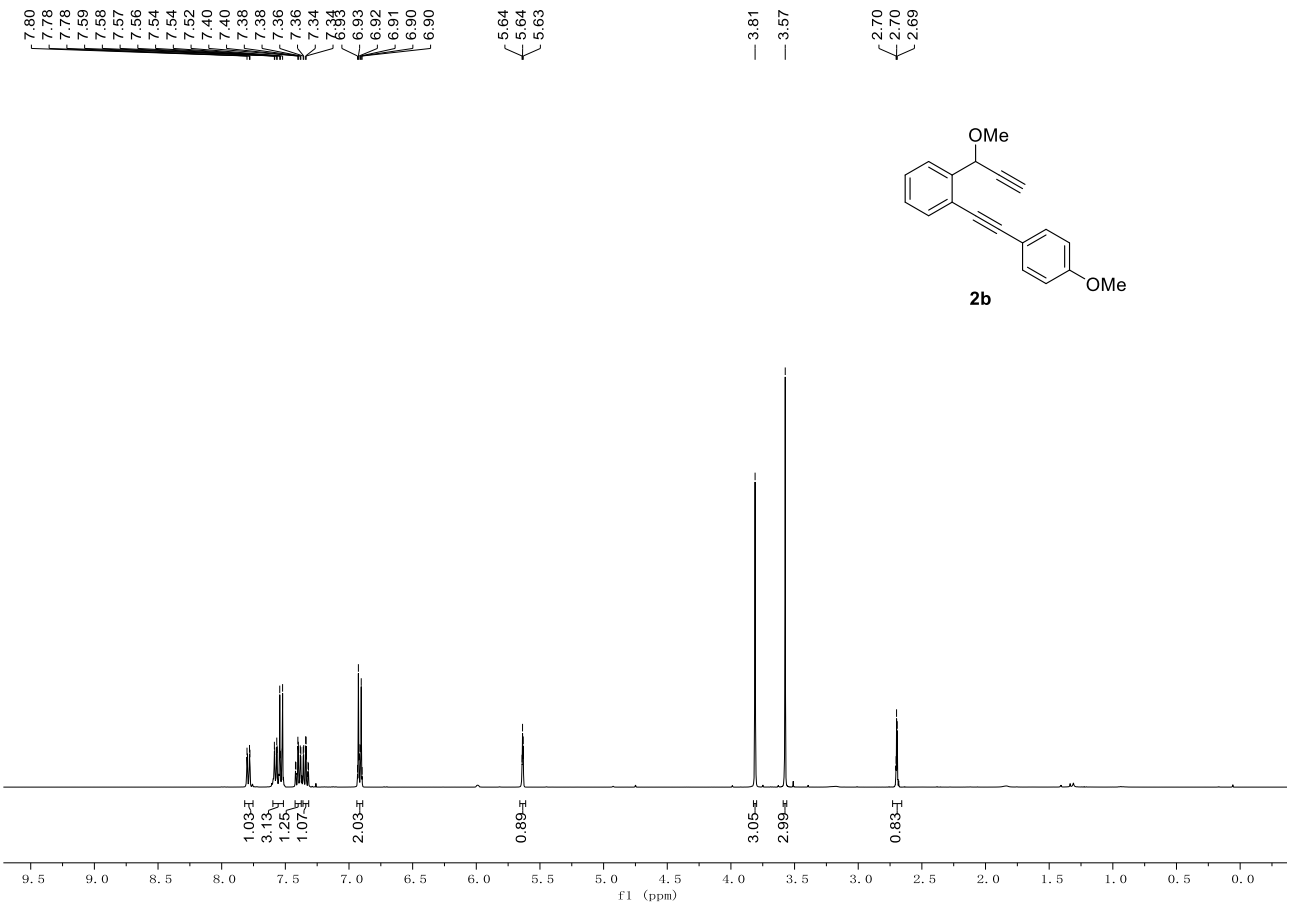
2a

^{13}C NMR of **2a** (100 MHz, $CDCl_3$)

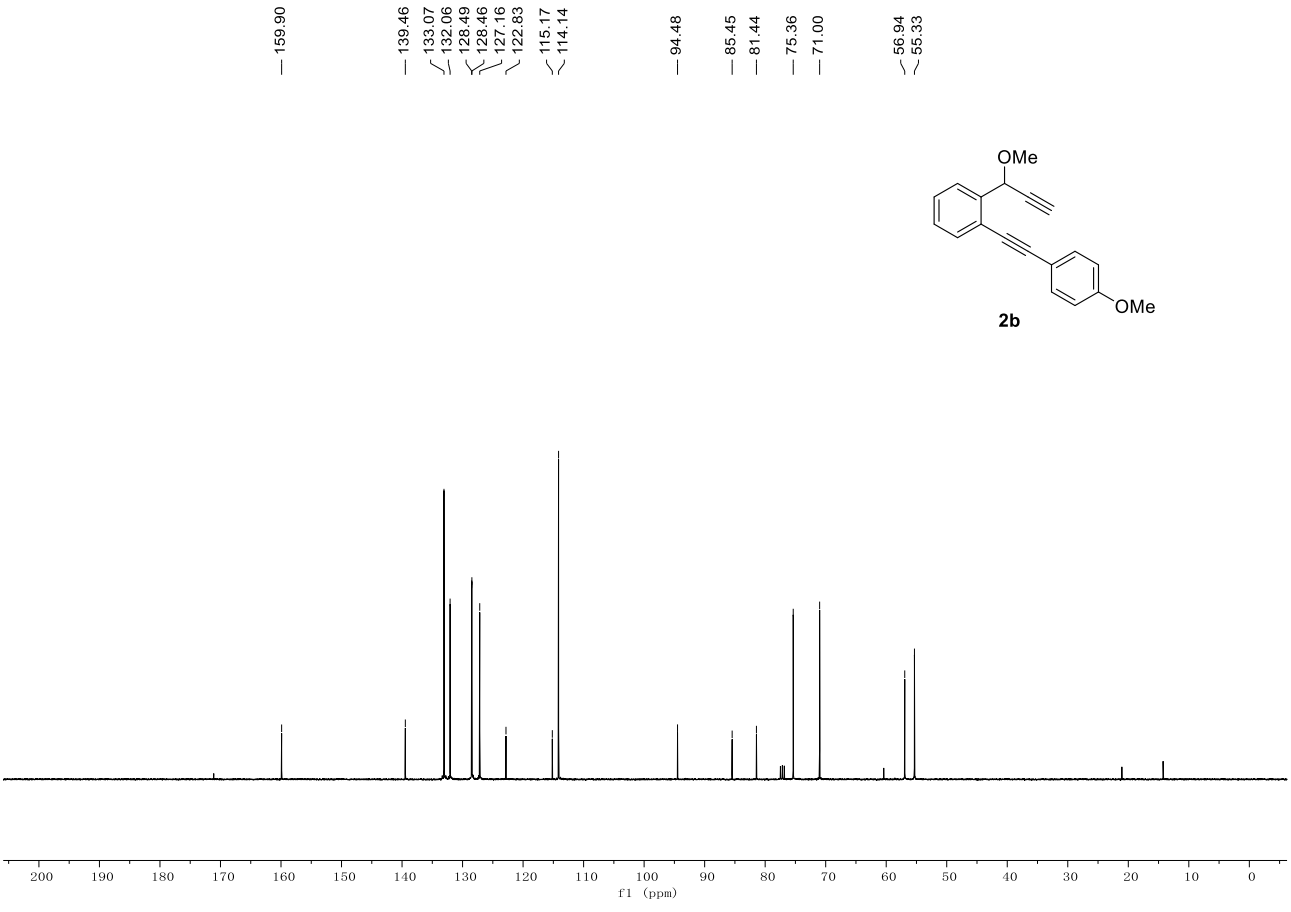


2a

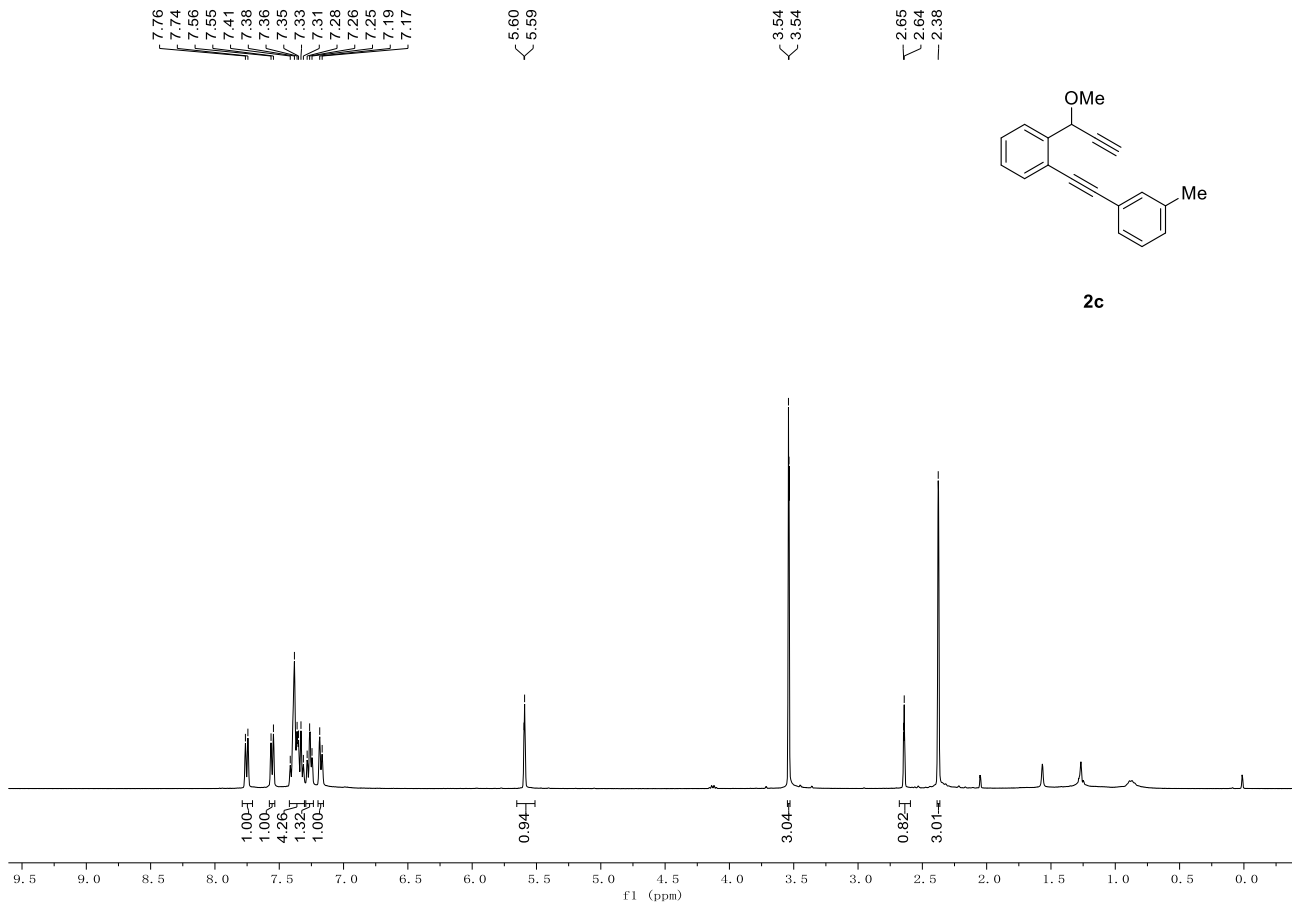
^{1}H NMR of **2b** (400 MHz, $CDCl_3$)



^{13}C NMR of **2b** (100 MHz, $CDCl_3$)

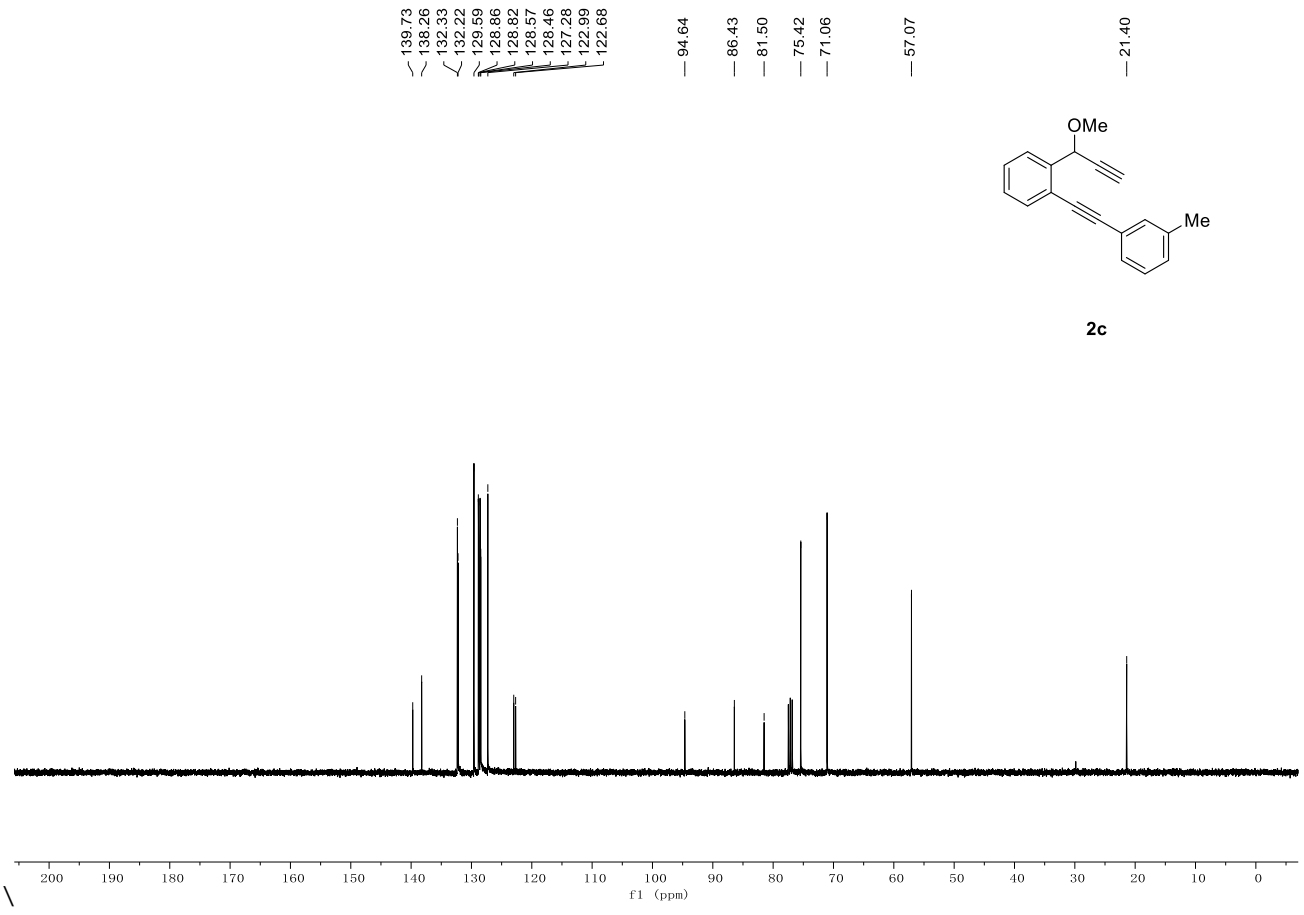


^{1}H NMR of **2c** (400 MHz, $CDCl_3$)



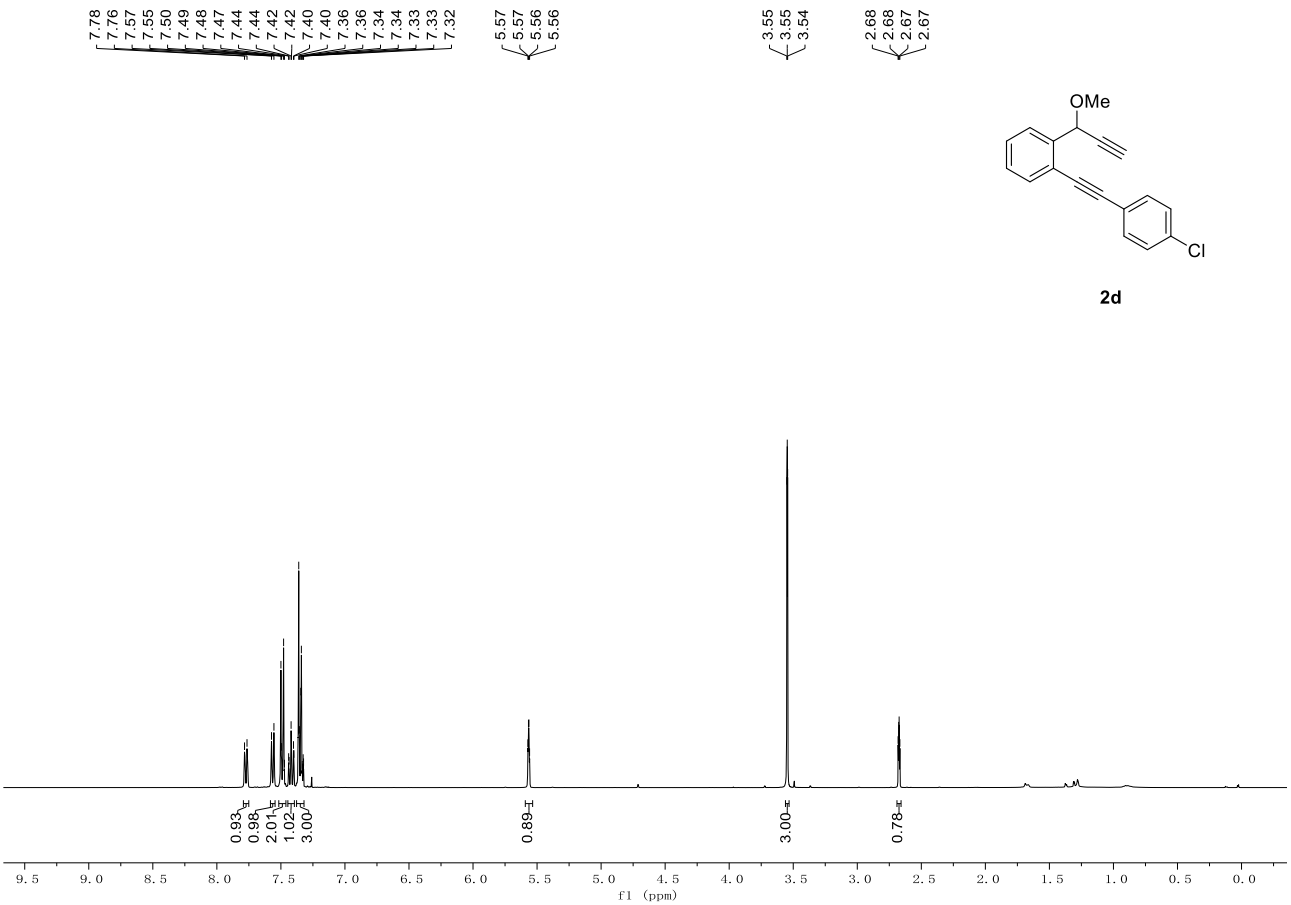
2c

^{13}C NMR of **2c** (100 MHz, $CDCl_3$)

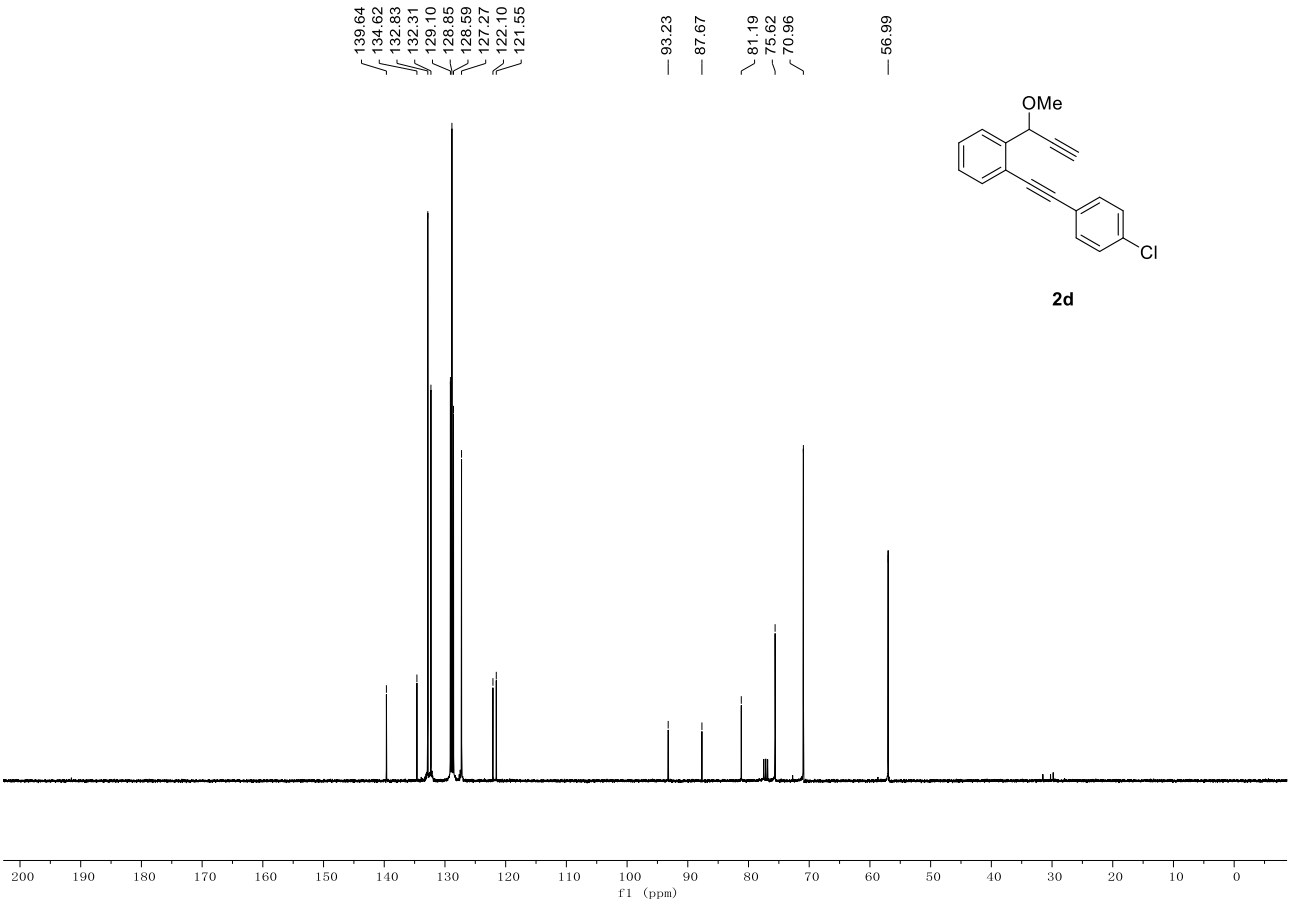


2c

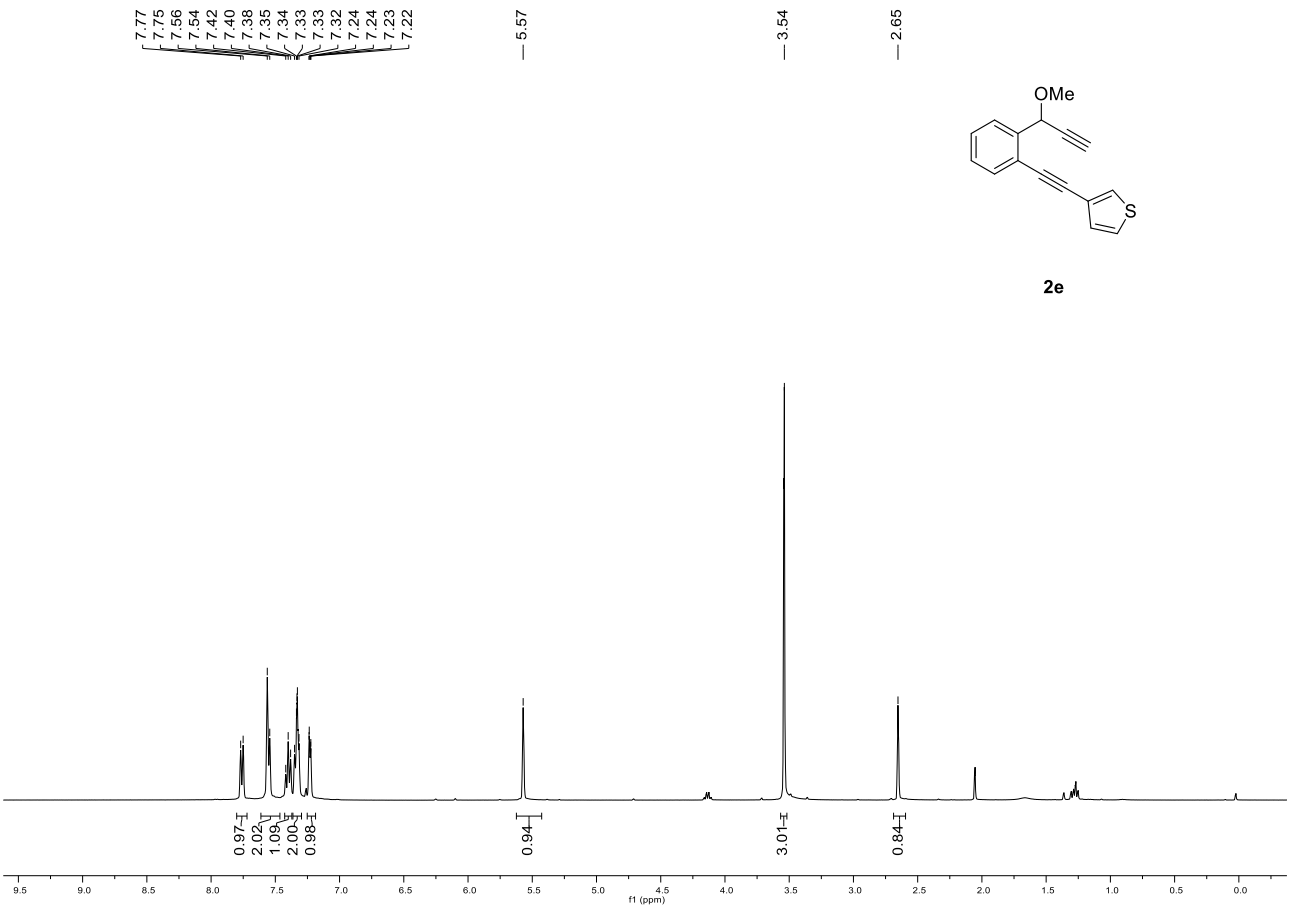
^{1}H NMR of **2d** (400 MHz, $CDCl_3$)



^{13}C NMR of **2d** (100 MHz, $CDCl_3$)

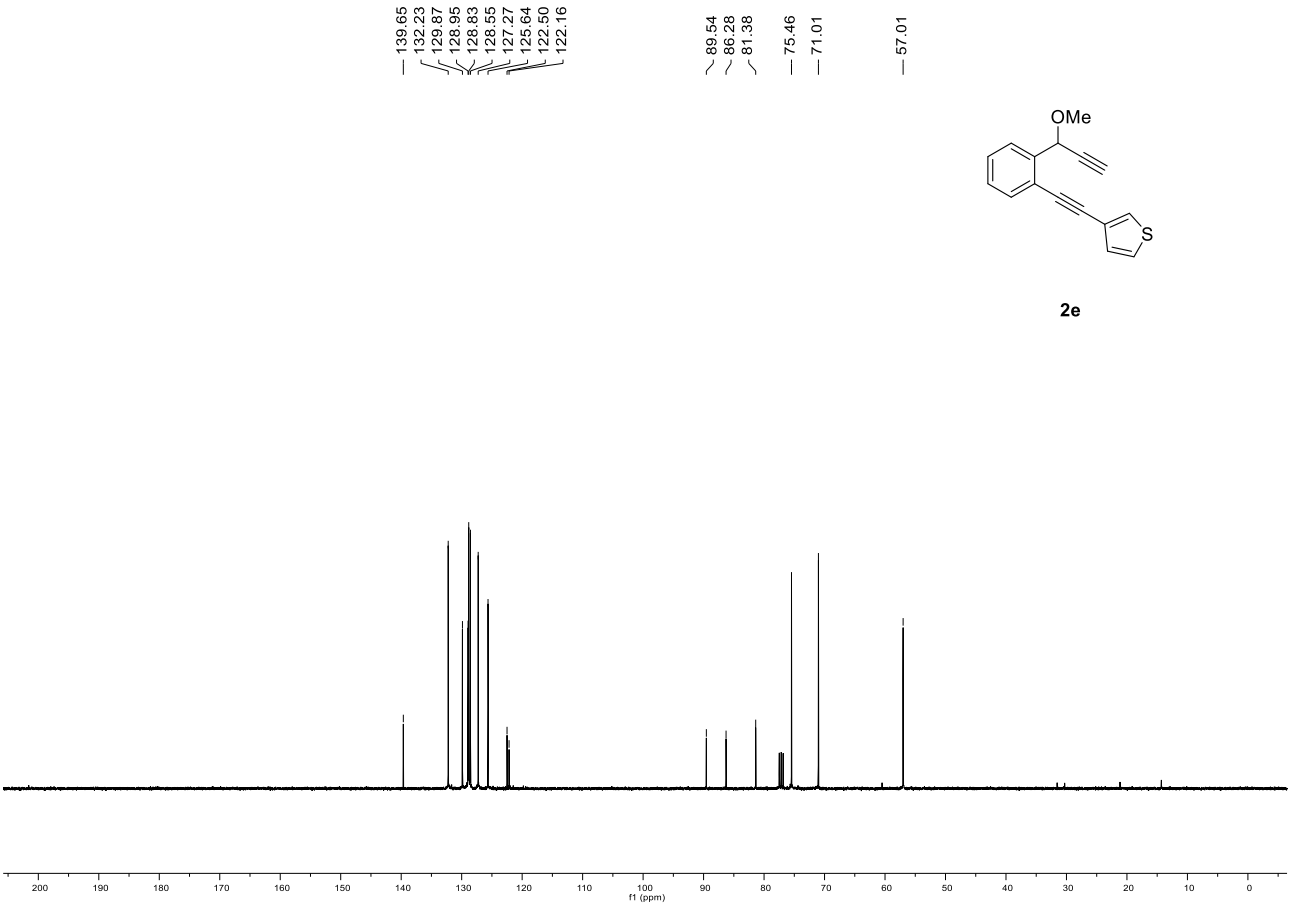


^{1}H NMR of **2e** (400 MHz, $CDCl_3$)



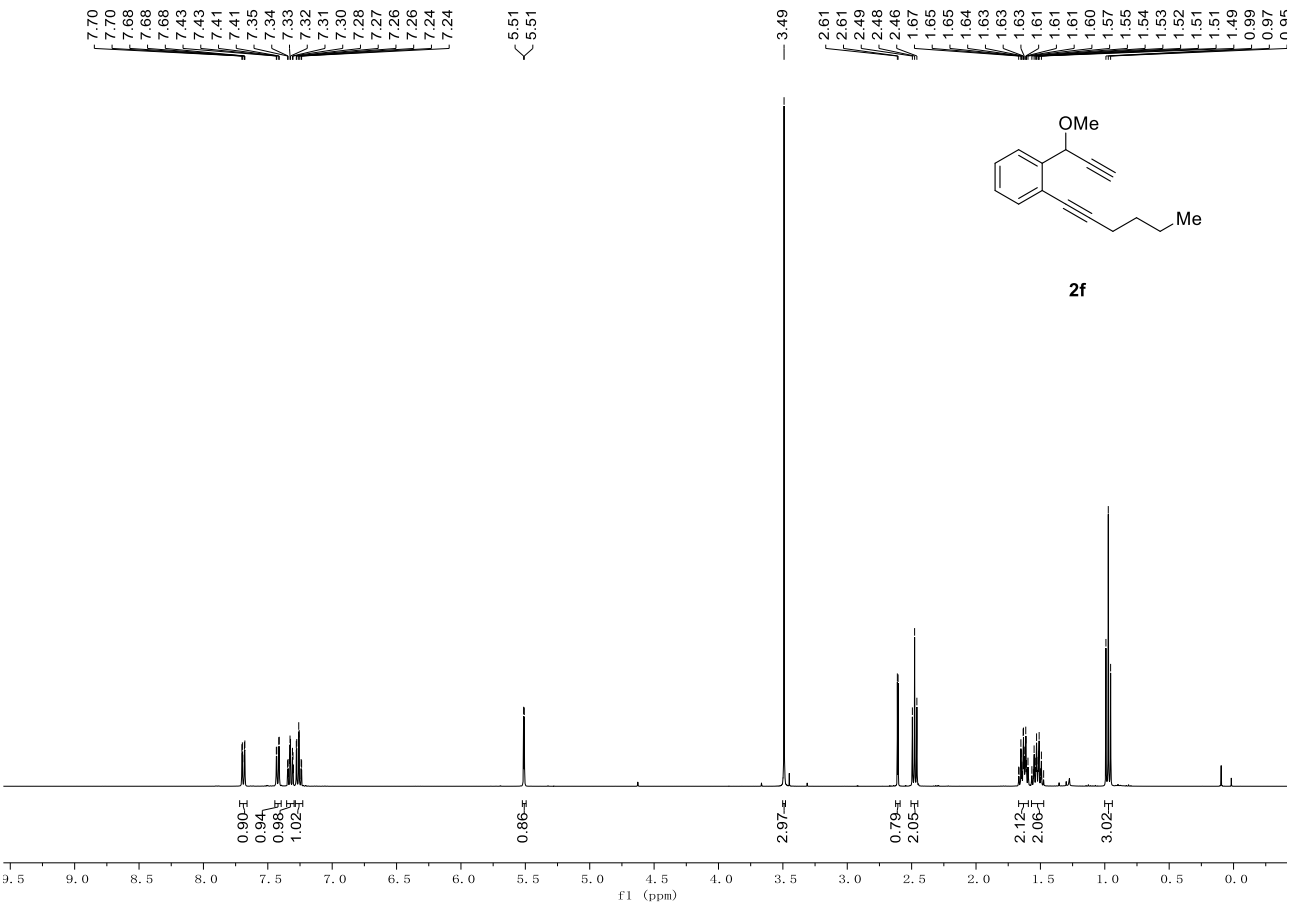
2e

^{13}C NMR of **2e** (100 MHz, $CDCl_3$)

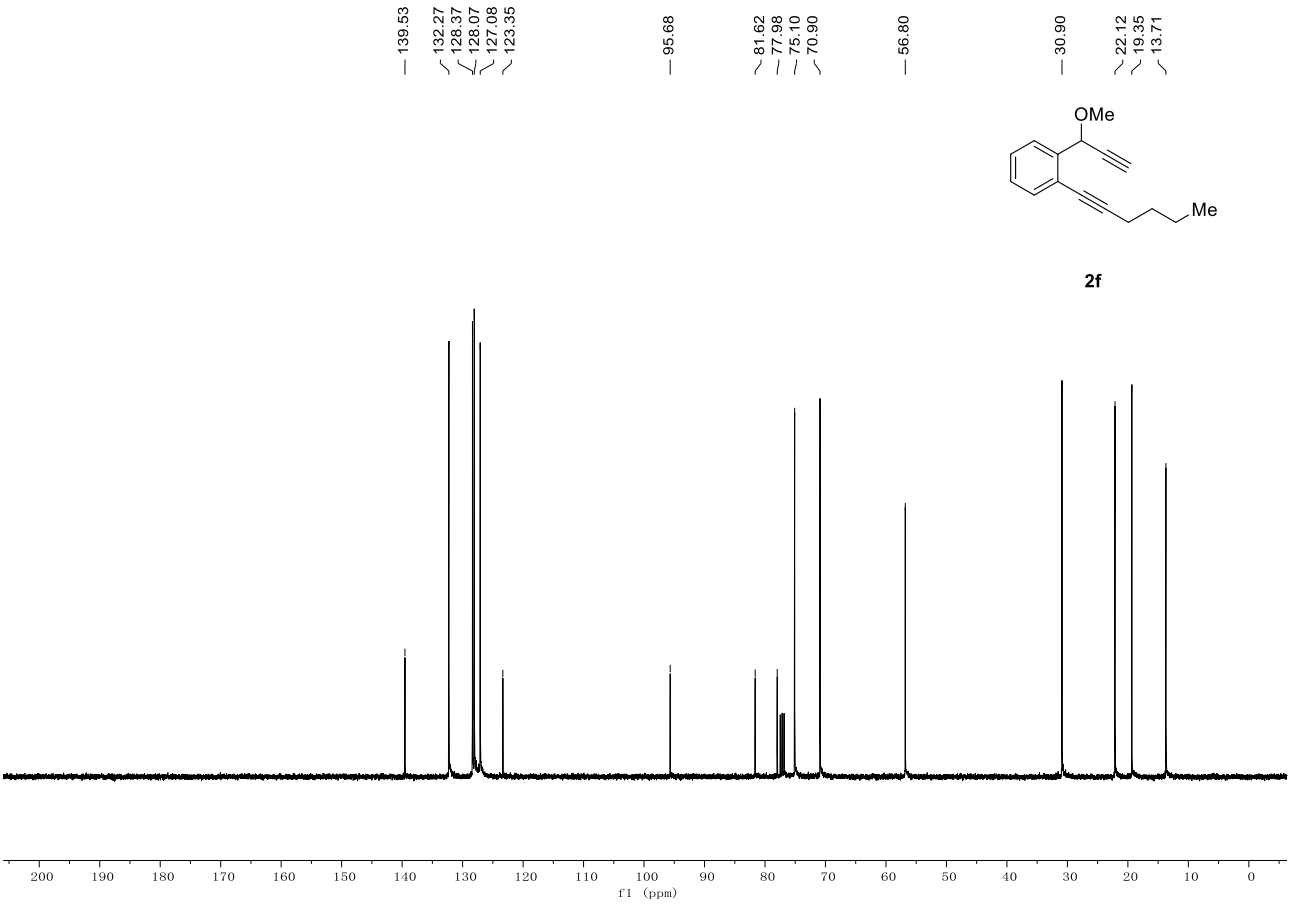


2e

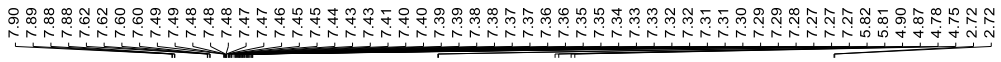
^{1}H NMR of **2f** (400 MHz, $CDCl_3$)

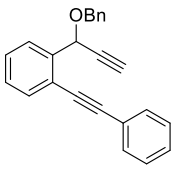


^{13}C NMR of **2f** (100 MHz, CDCl3)

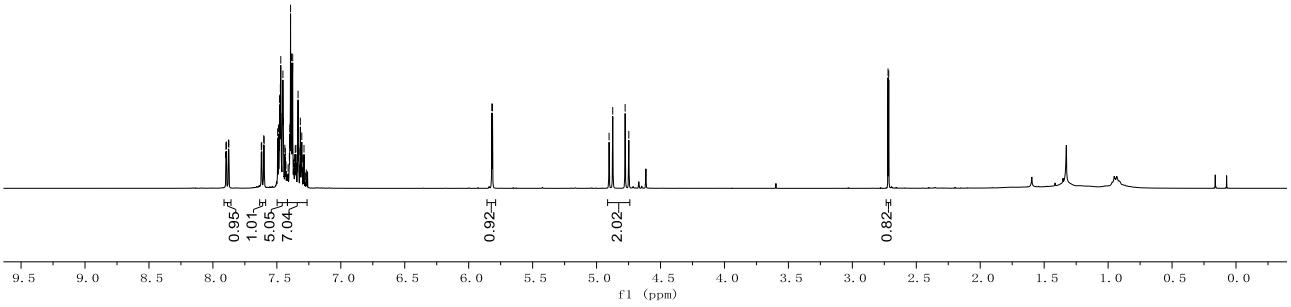


^{1}H NMR of **2g** (400 MHz, $CDCl_3$)

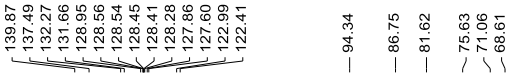


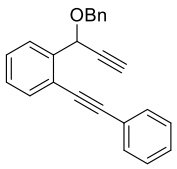


2g

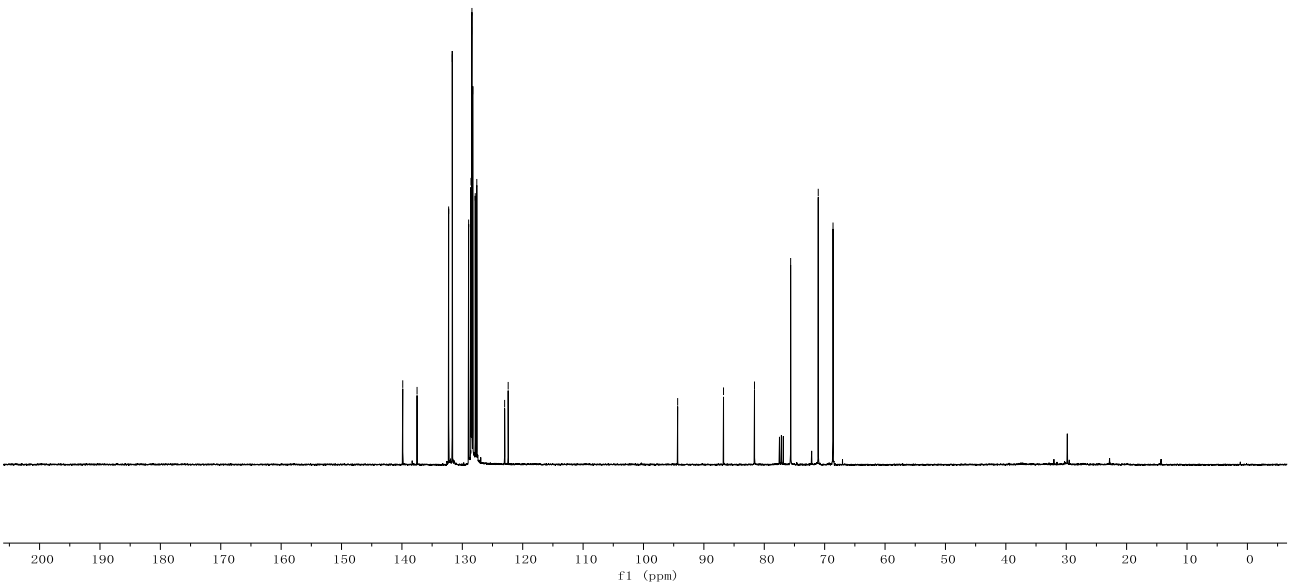


^{13}C NMR of **2g** (100 MHz, $CDCl_3$)

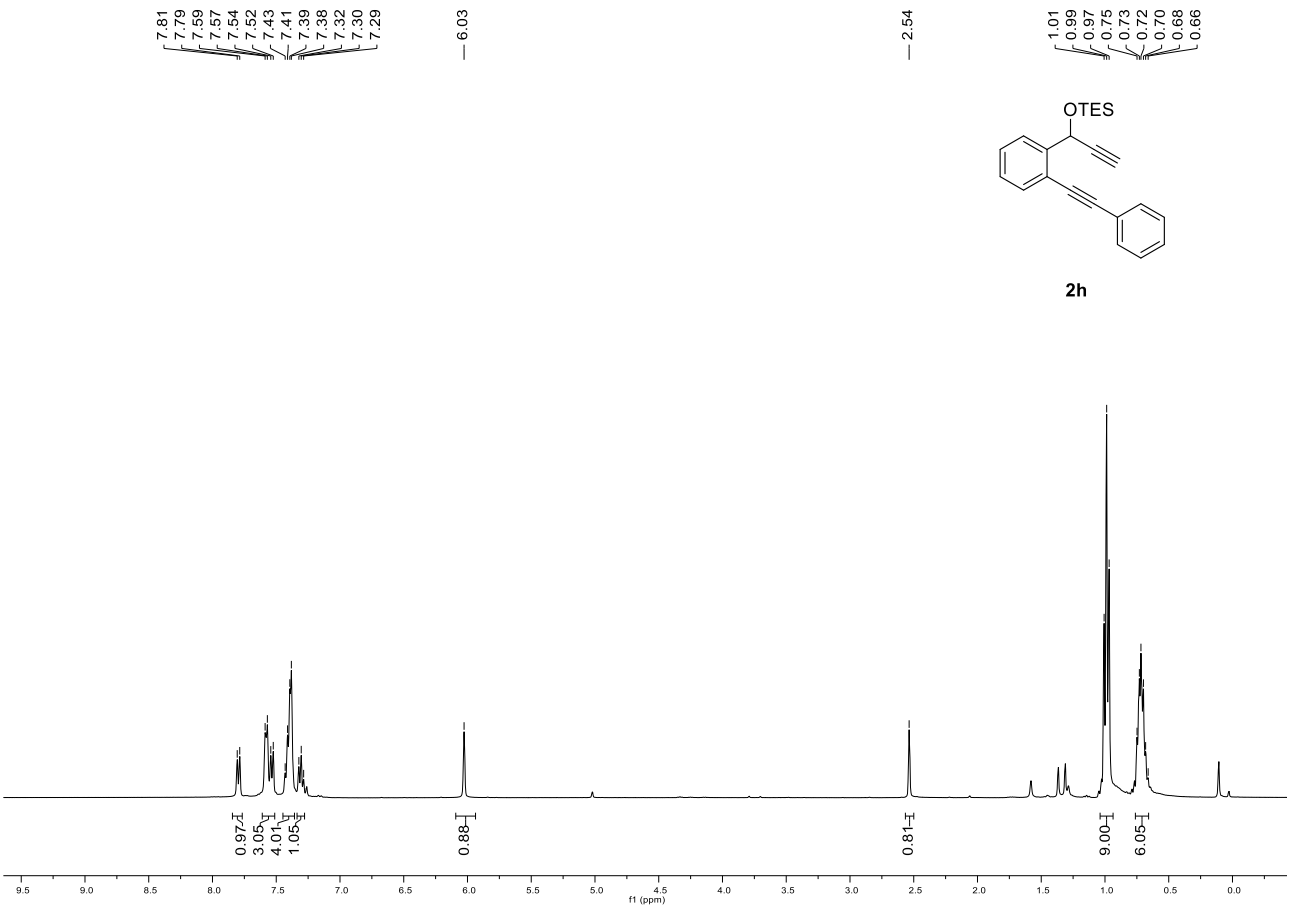




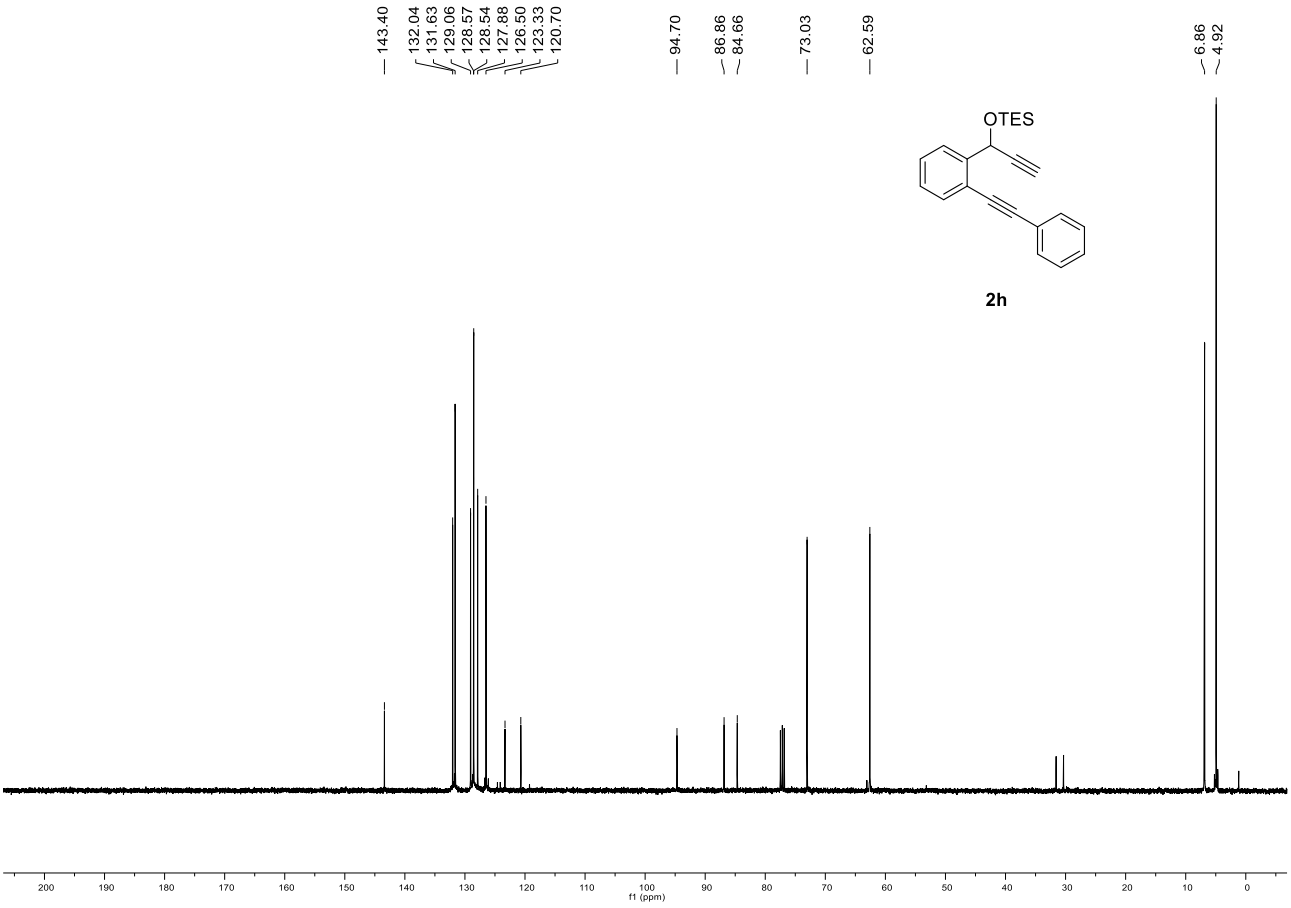
2g



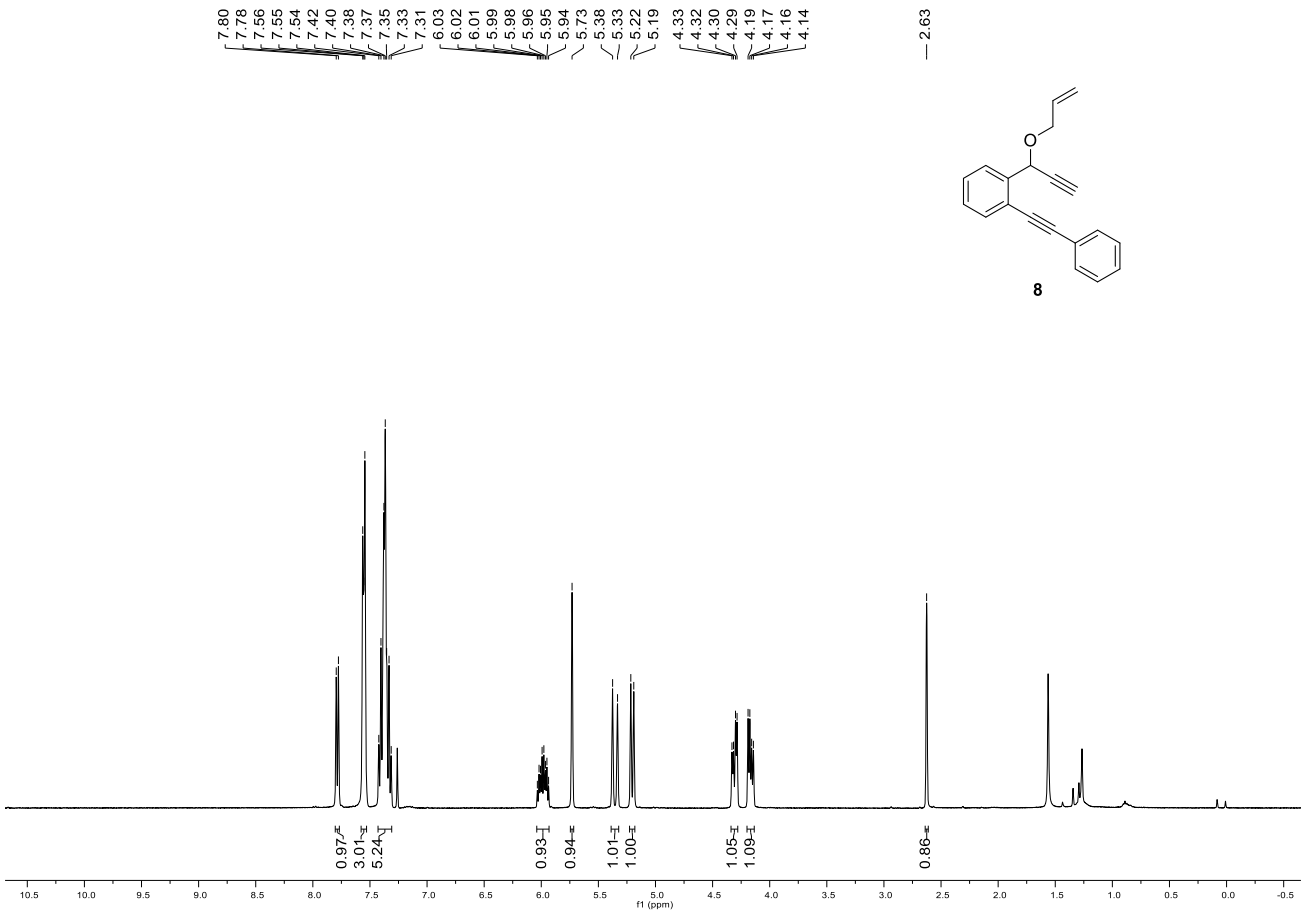
^{1}H NMR of **2h** (400 MHz, $CDCl_3$)



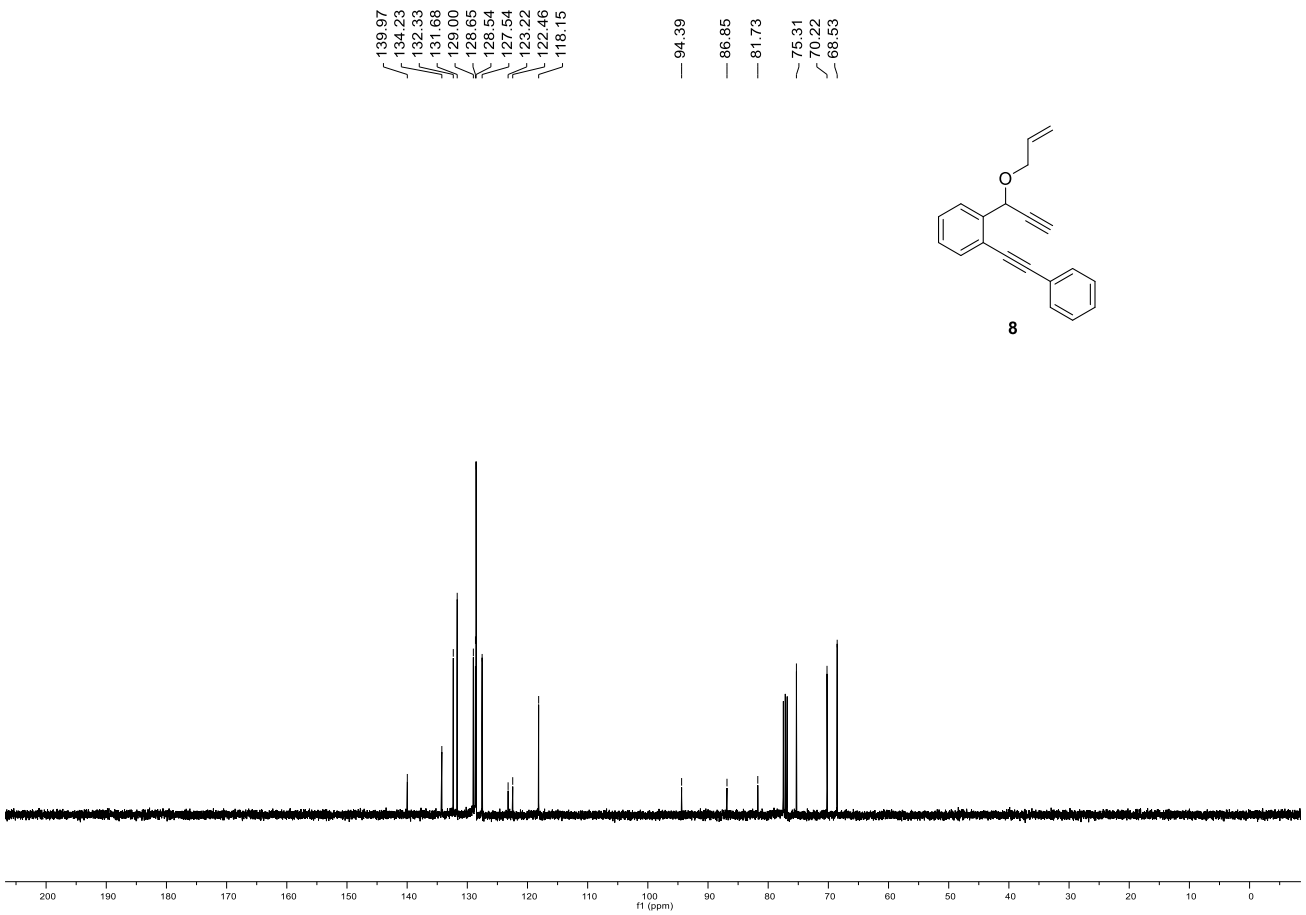
^{13}C NMR of **2h** (100 MHz, $CDCl_3$)



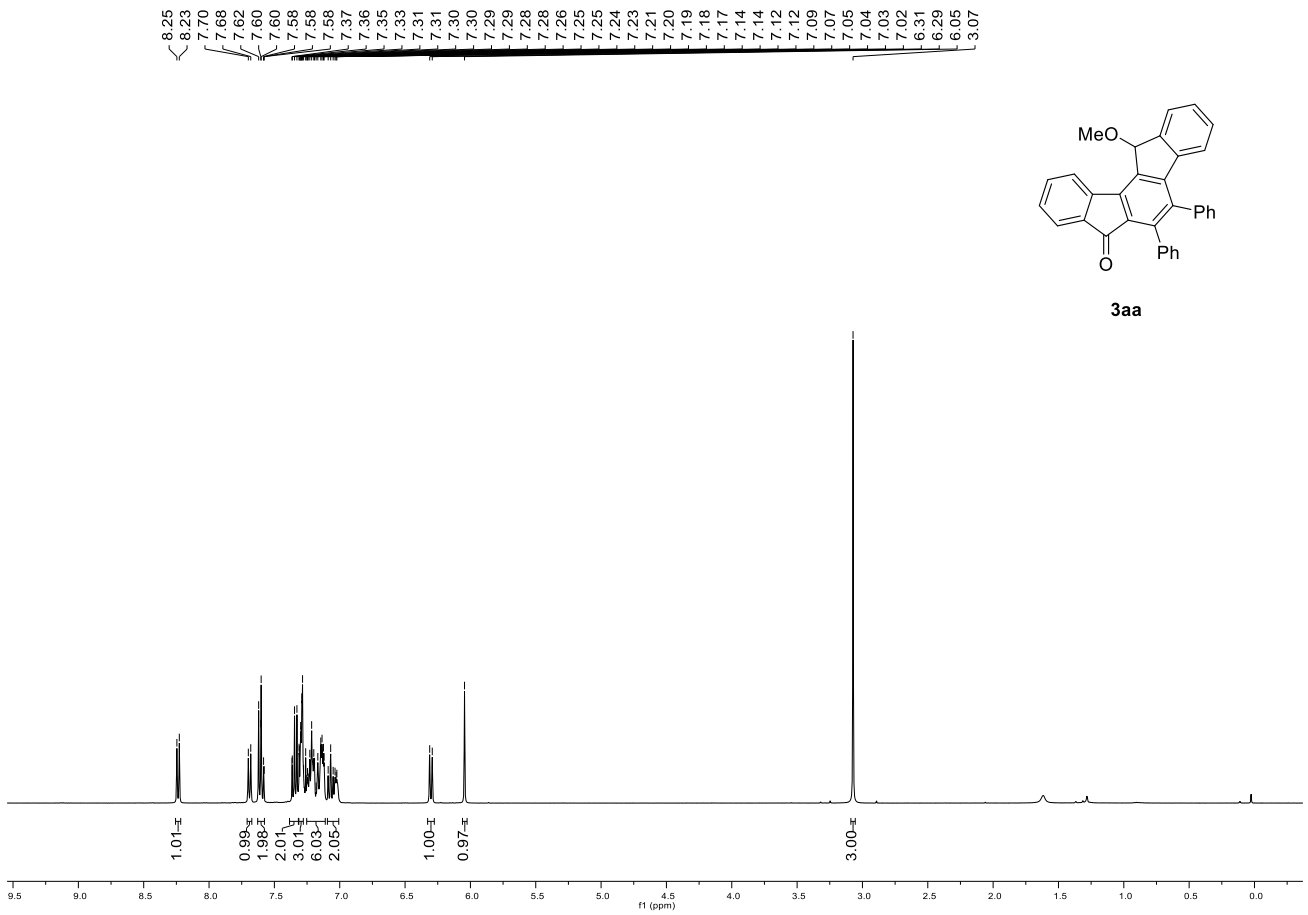
^{1}H NMR of **8** (400 MHz, $CDCl_3$)



^{13}C NMR of **8** (100 MHz, $CDCl_3$)

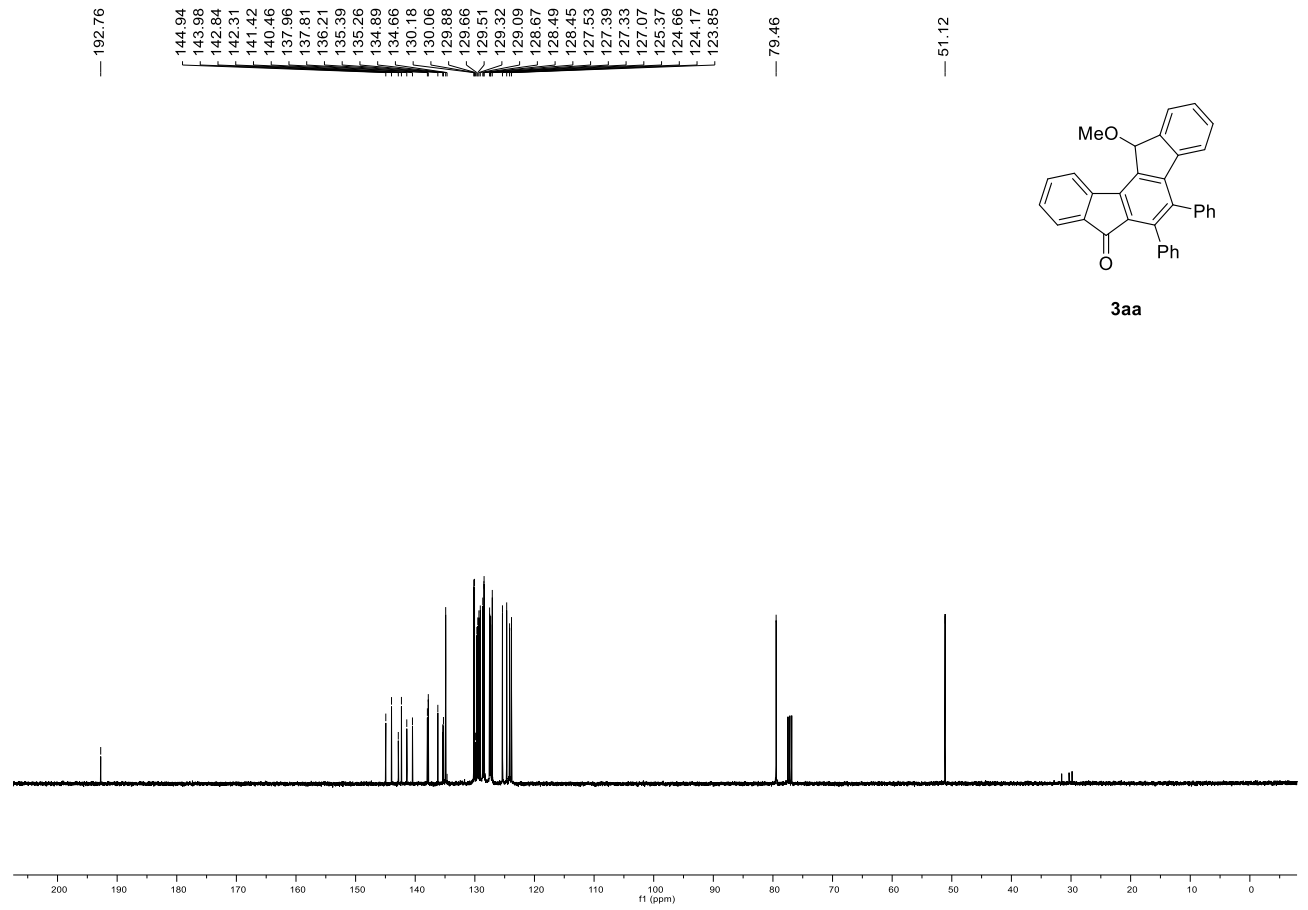


^{1}H NMR of **3aa** (400 MHz, $CDCl_3$)



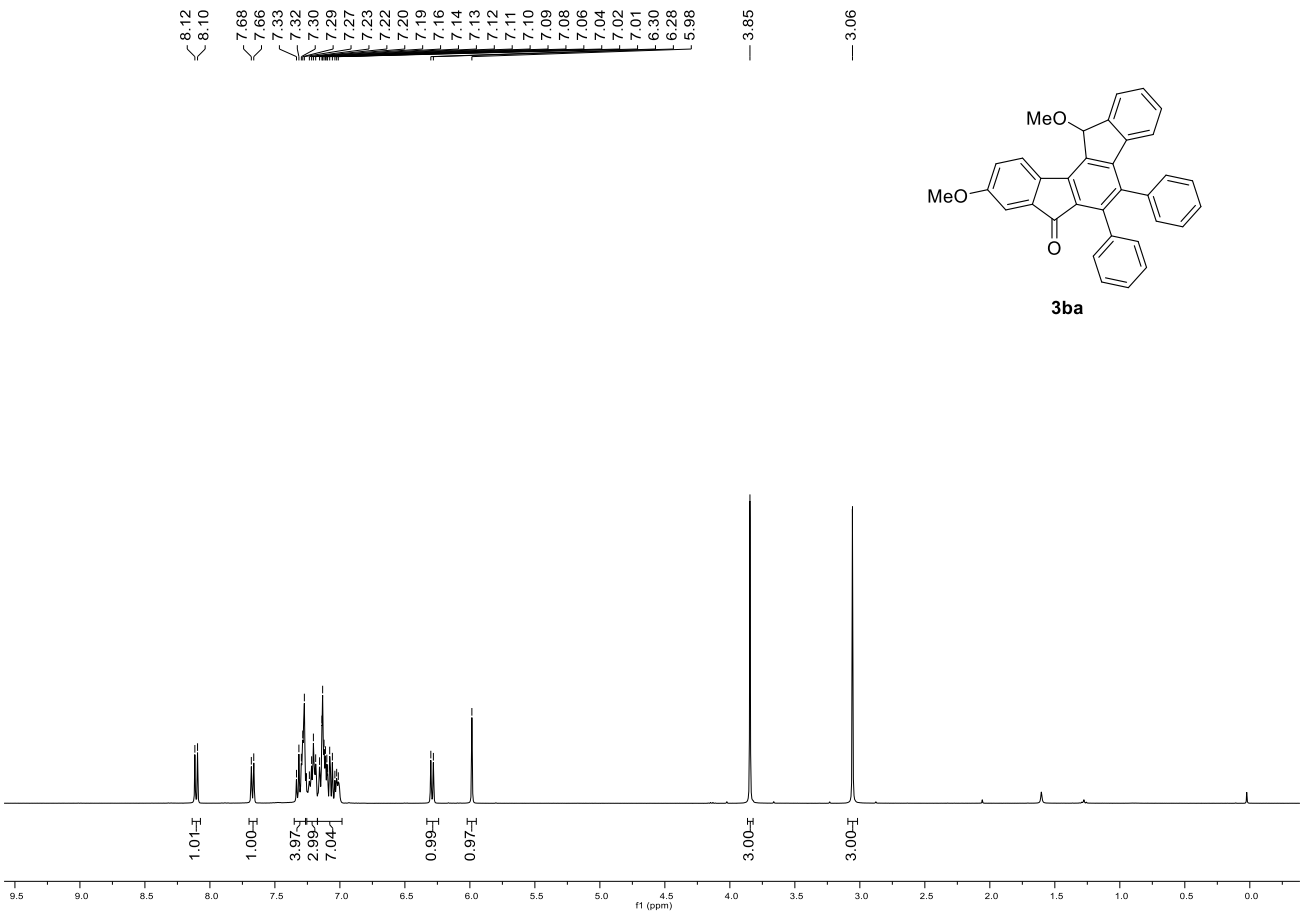
3aa

^{13}C NMR of **3aa** (100 MHz, $CDCl_3$)

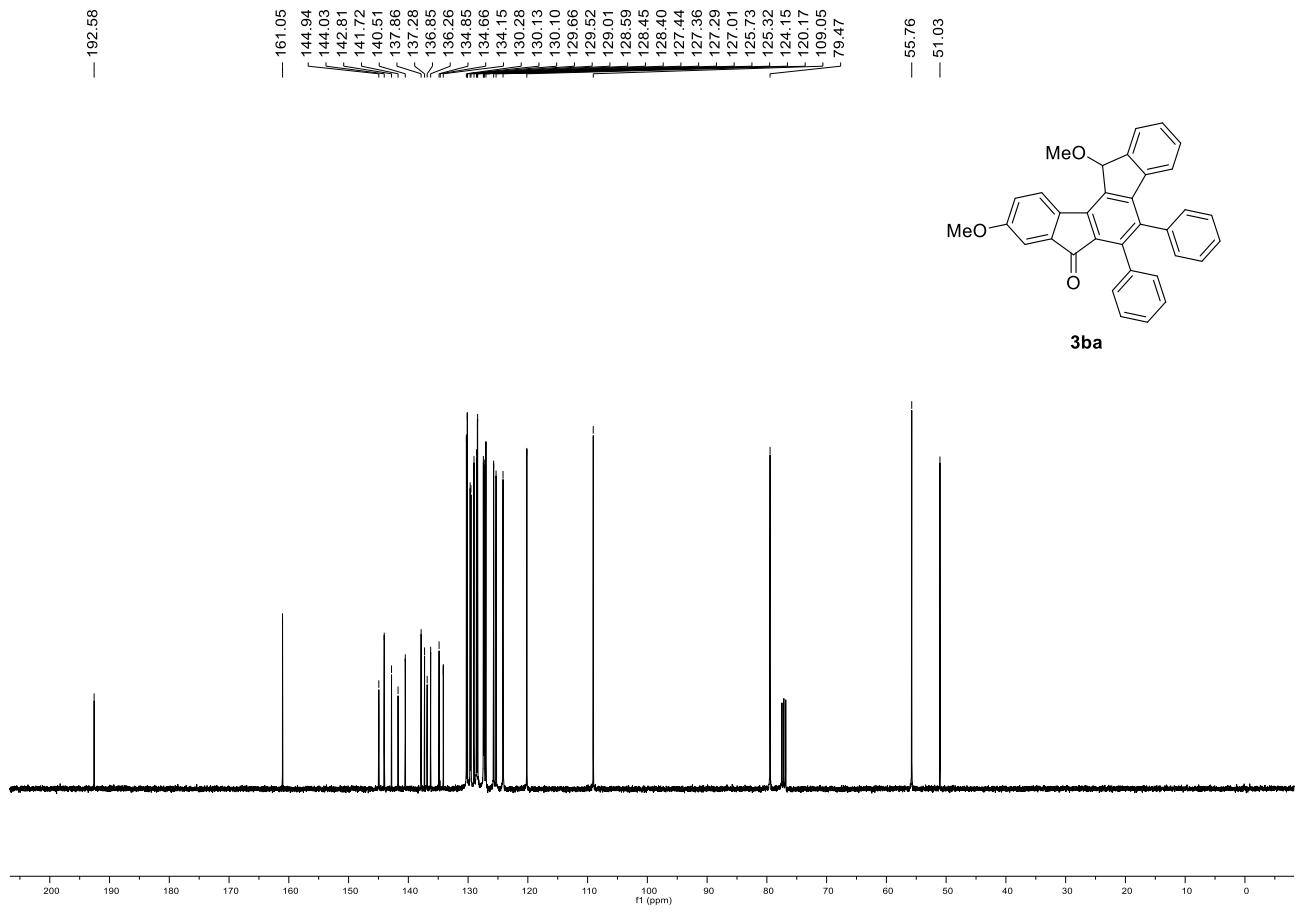


3aa

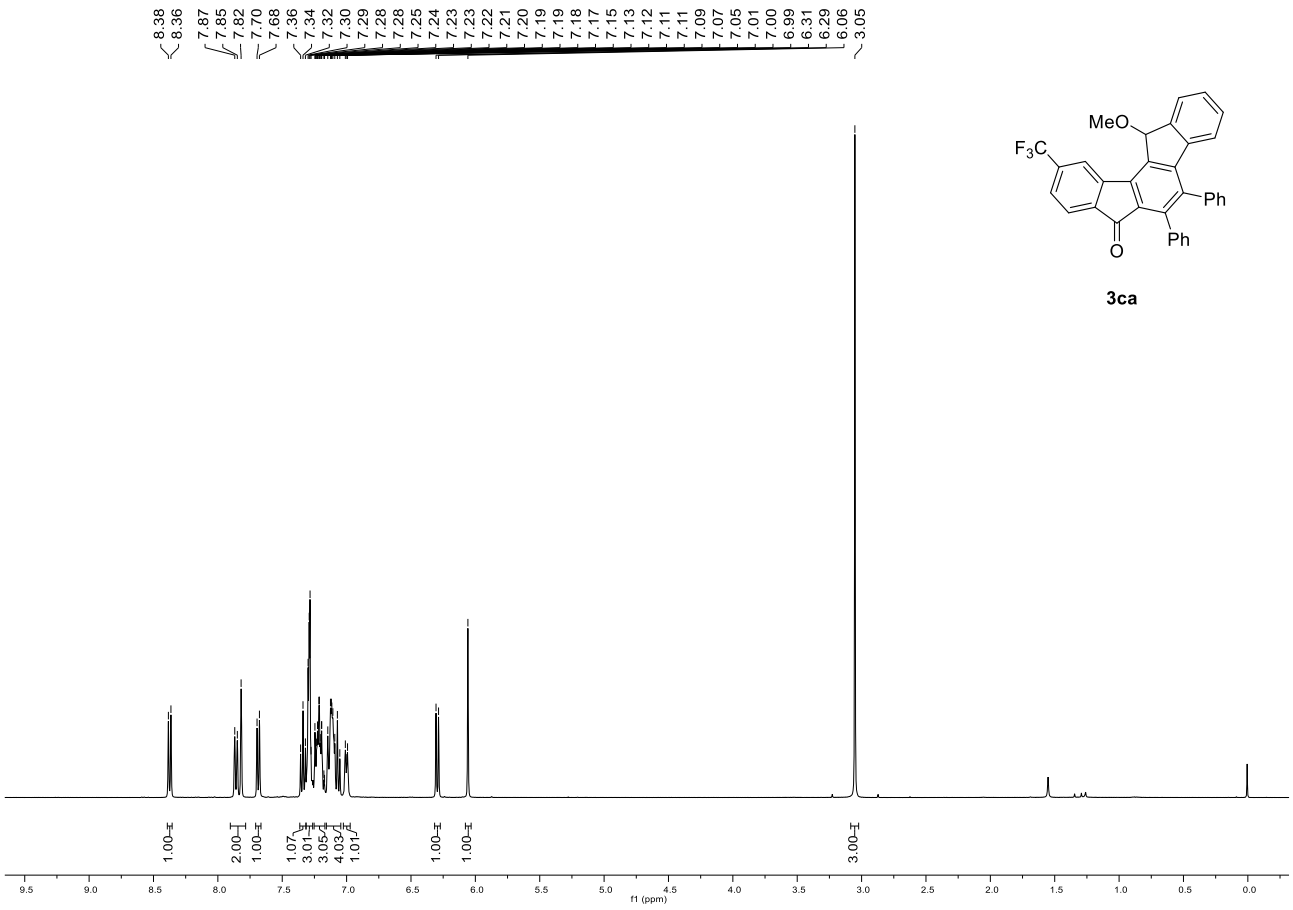
^{1}H NMR of **3ba** (400 MHz, $CDCl_3$)



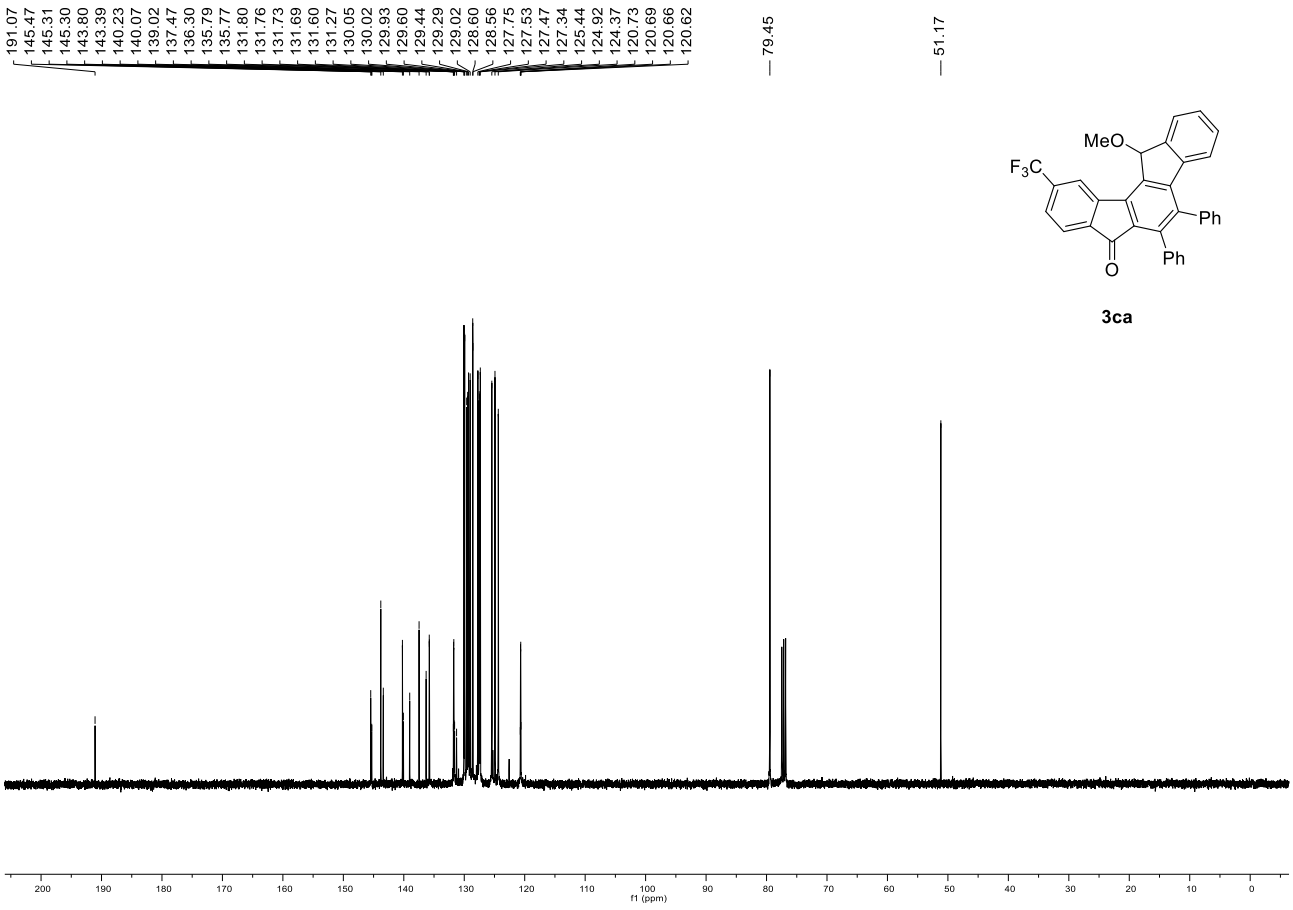
^{13}C NMR of **3ba** (100 MHz, $CDCl_3$)



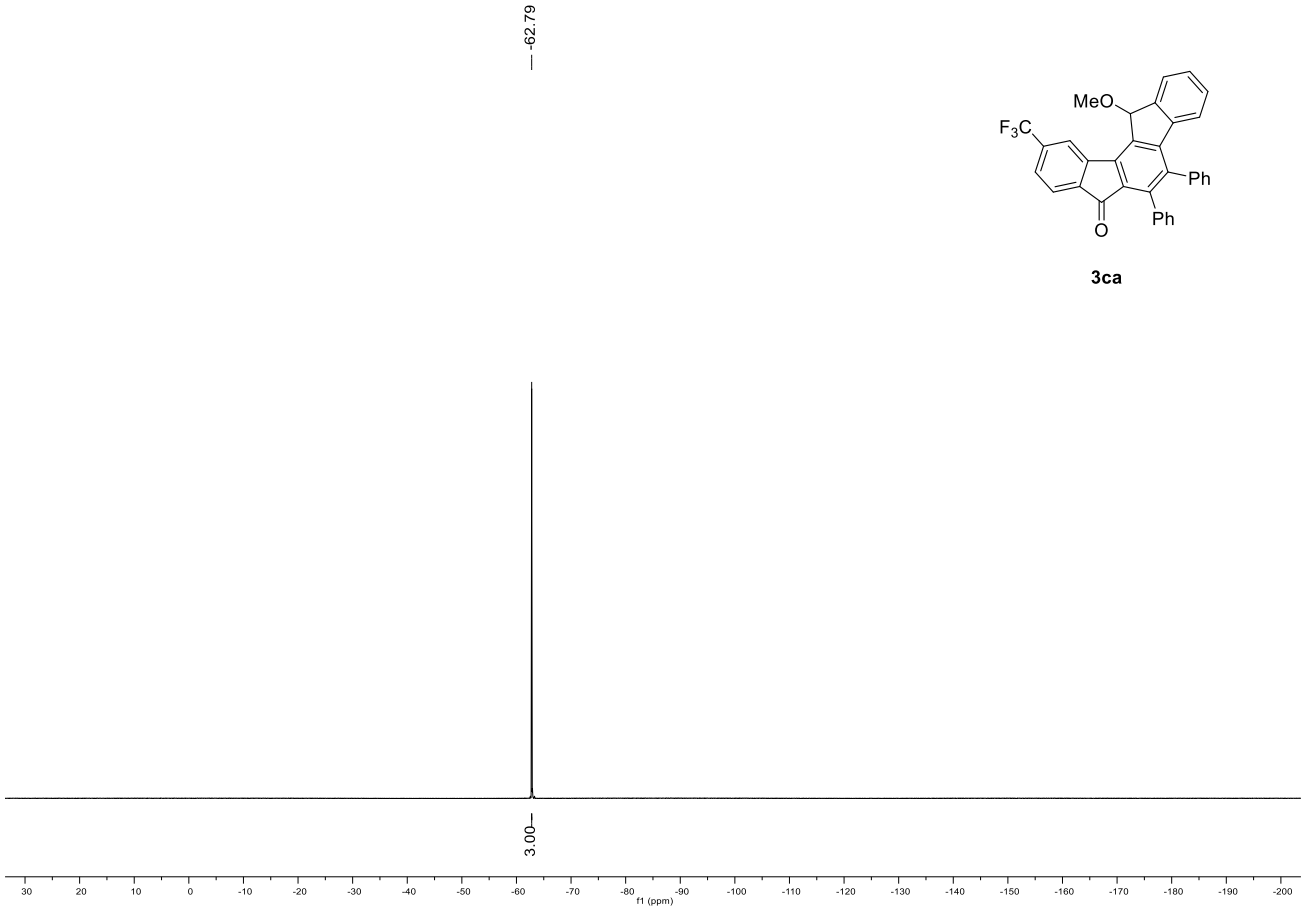
^{1}H NMR of **3ca** (400 MHz, $CDCl_3$)



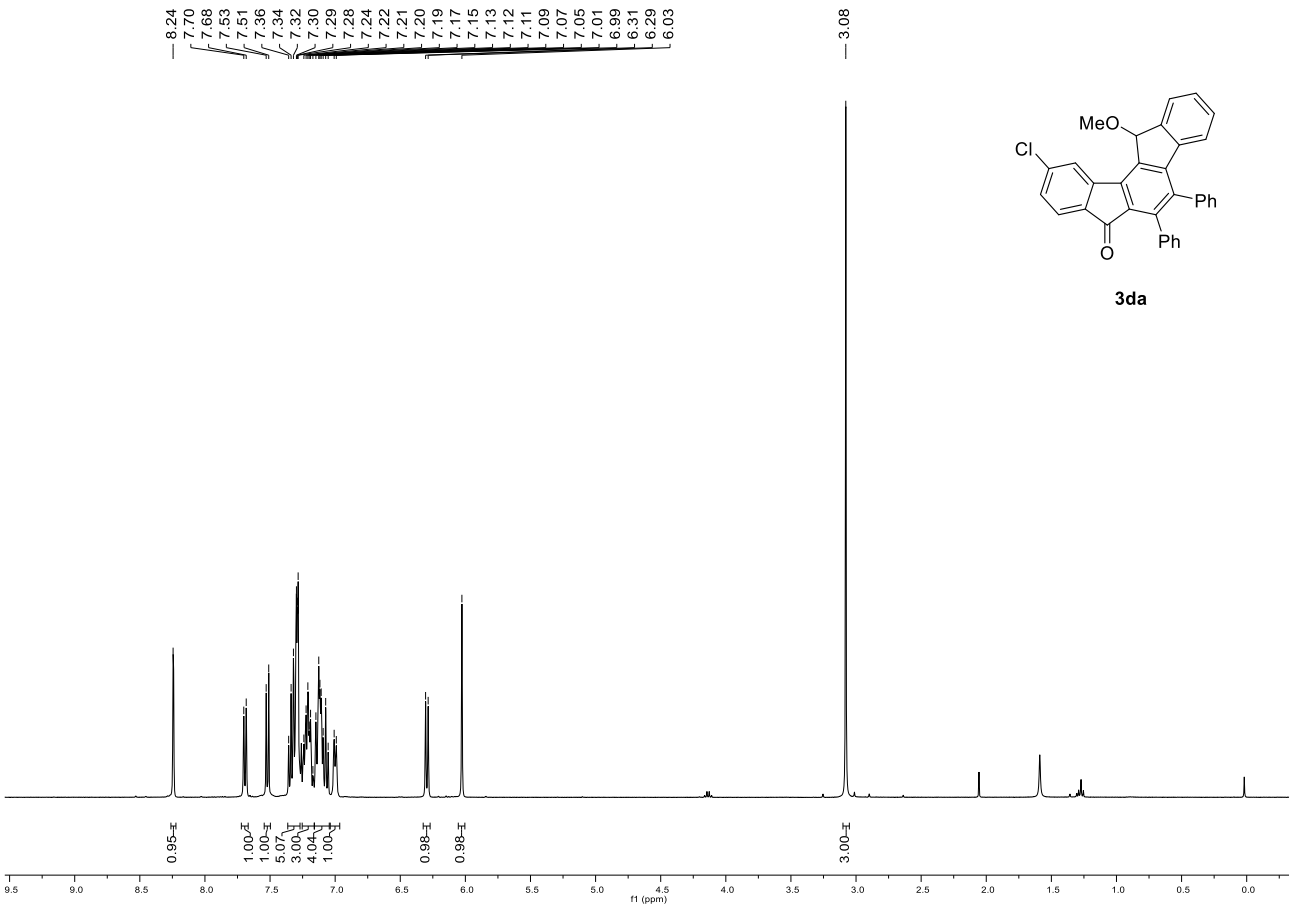
^{13}C NMR of **3ca** (100 MHz, $CDCl_3$)



^{19}F NMR of **3ca** (376 MHz, $CDCl_3$)

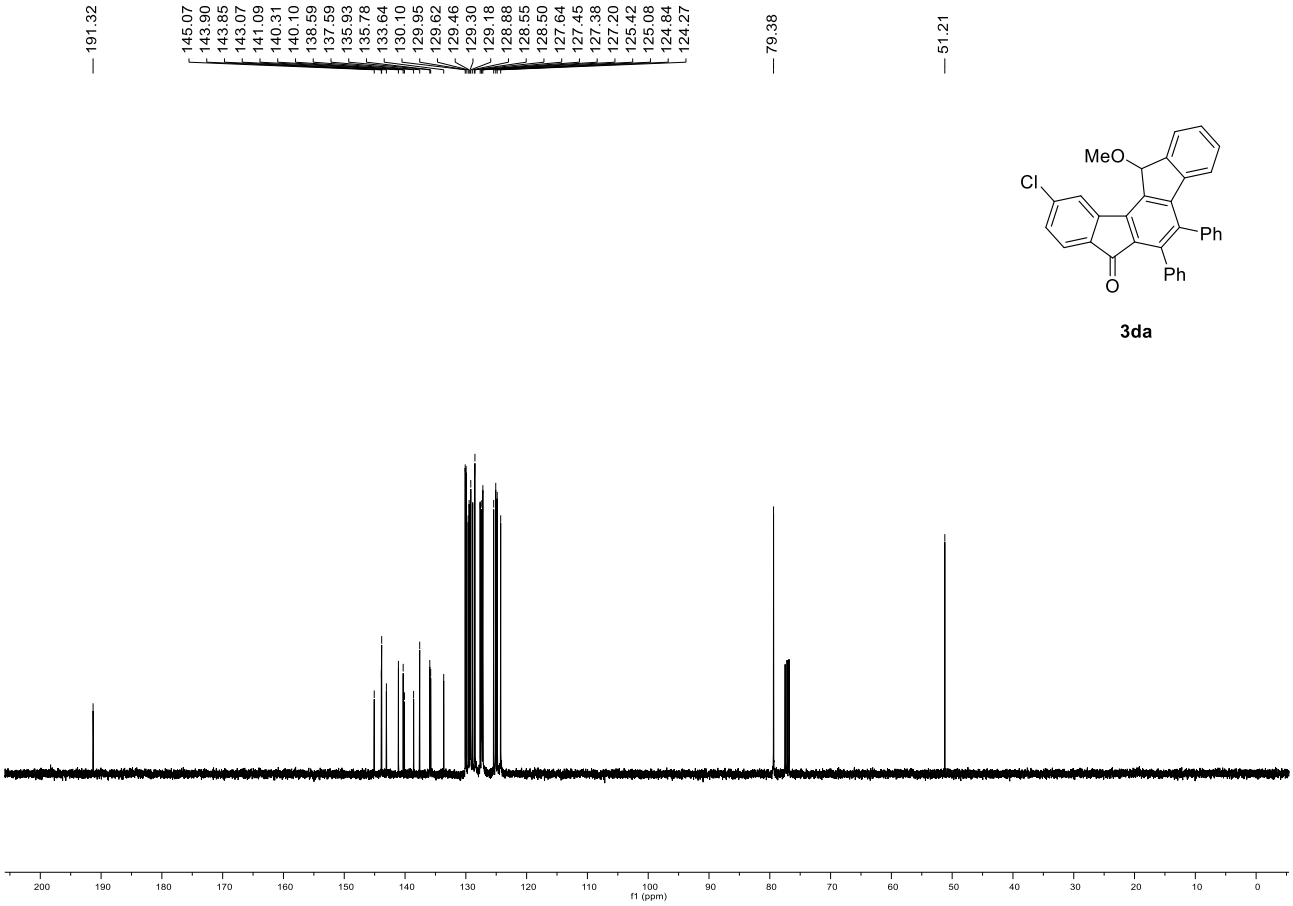


^{1}H NMR of **3da** (400 MHz, $CDCl_3$)



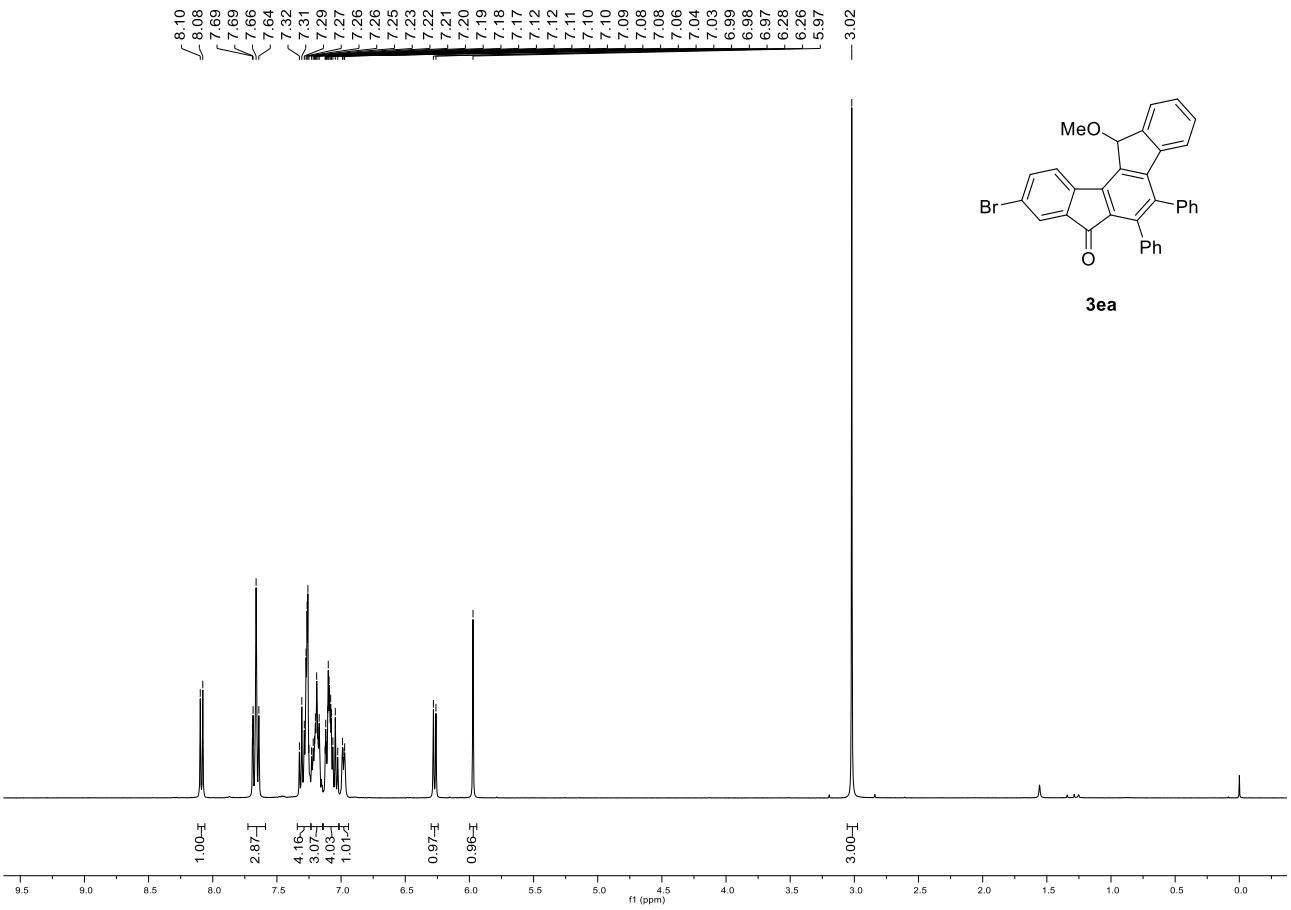
3da

^{13}C NMR of **3da** (100 MHz, $CDCl_3$)



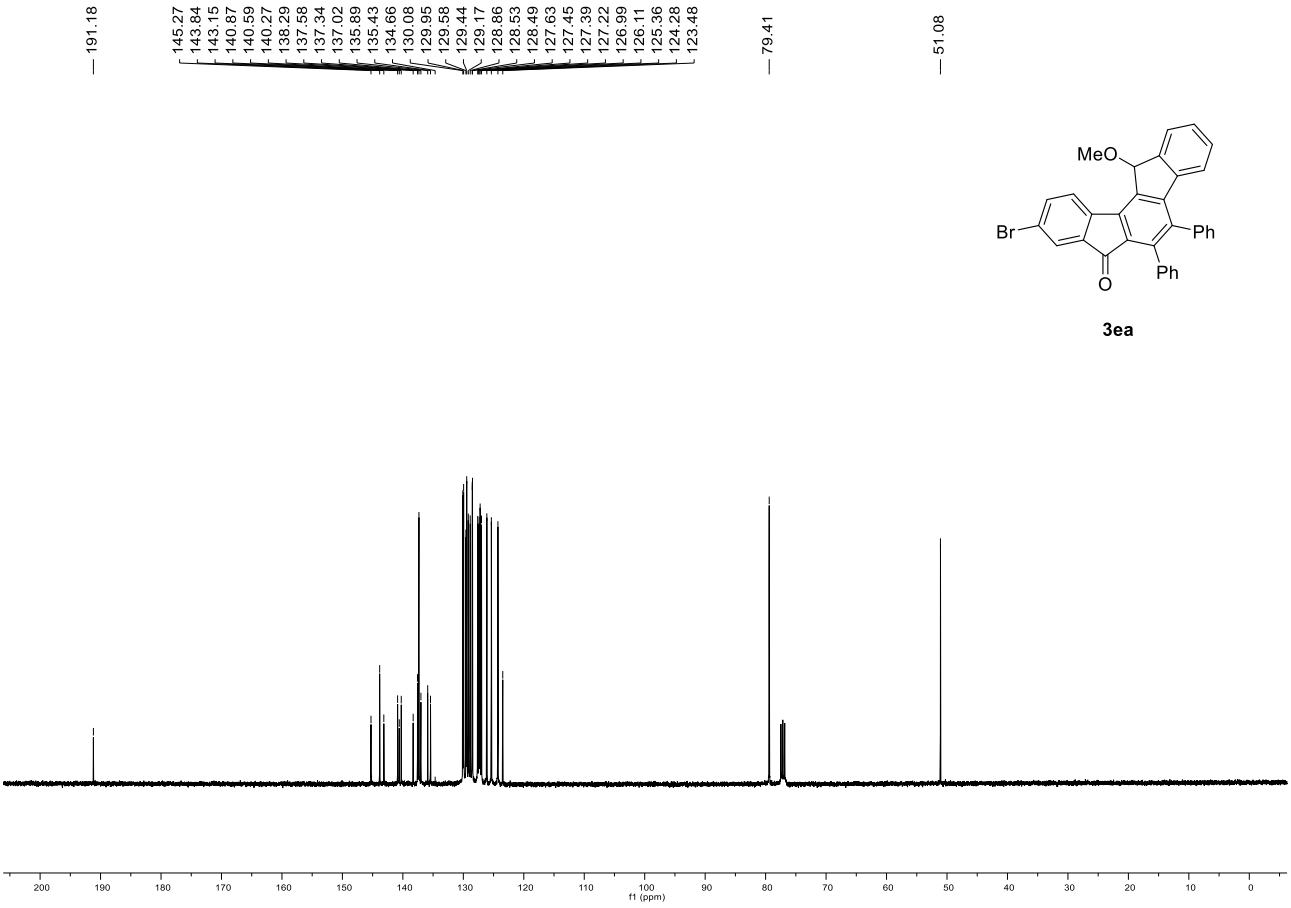
3da

^{1}H NMR of **3ea** (400 MHz, $CDCl_3$)



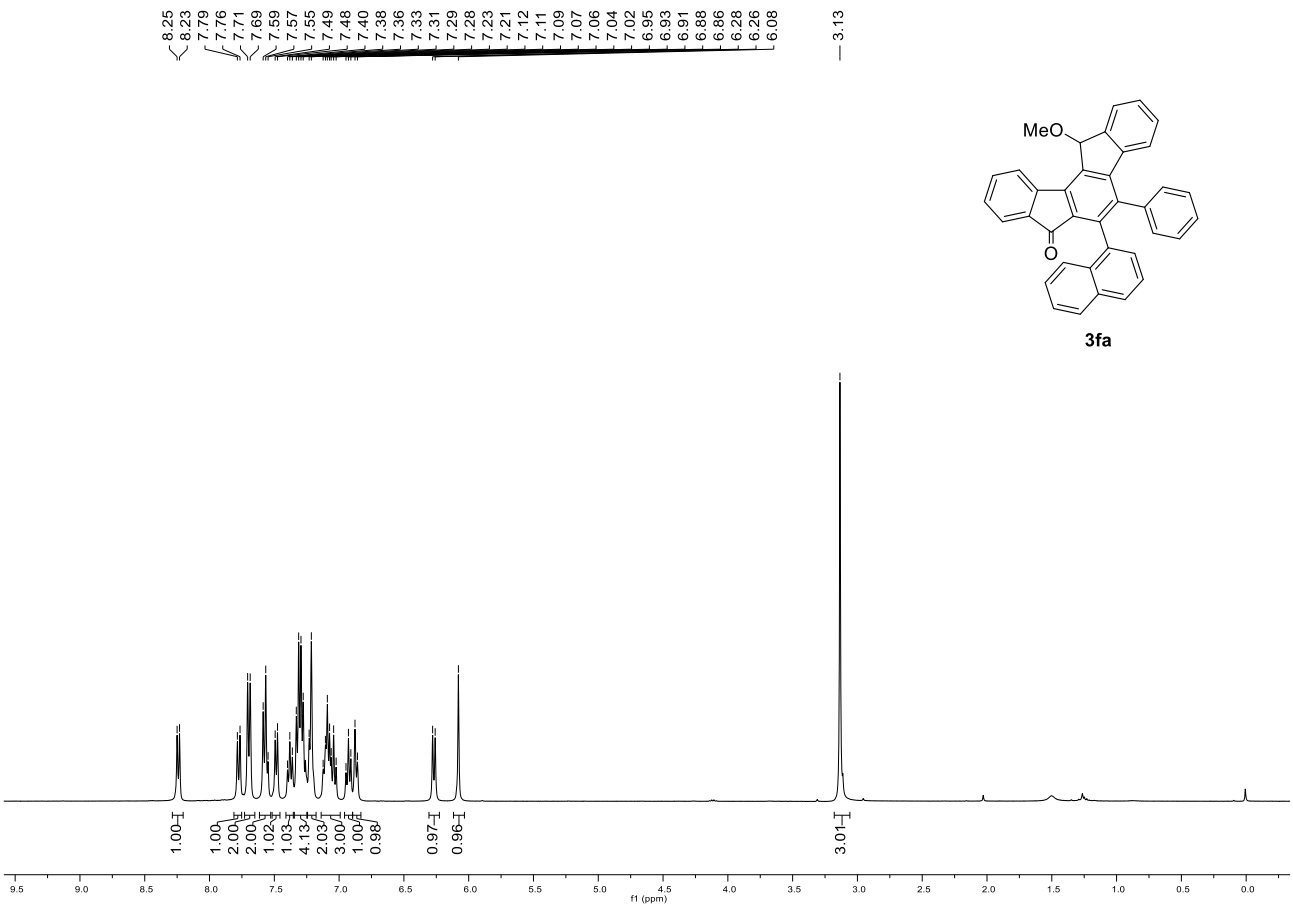
3ea

^{13}C NMR of **3ea** (100 MHz, $CDCl_3$)

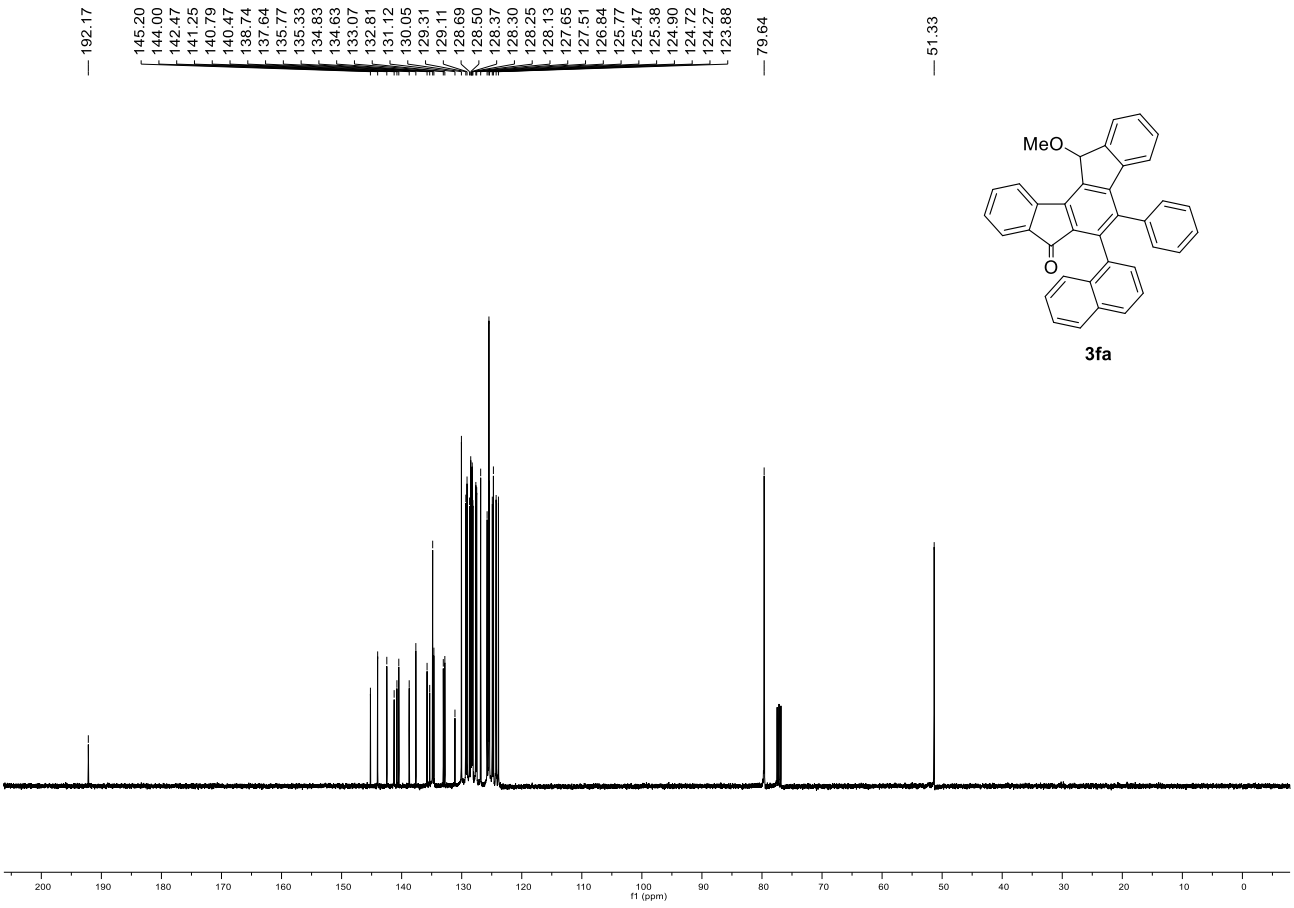


3ea

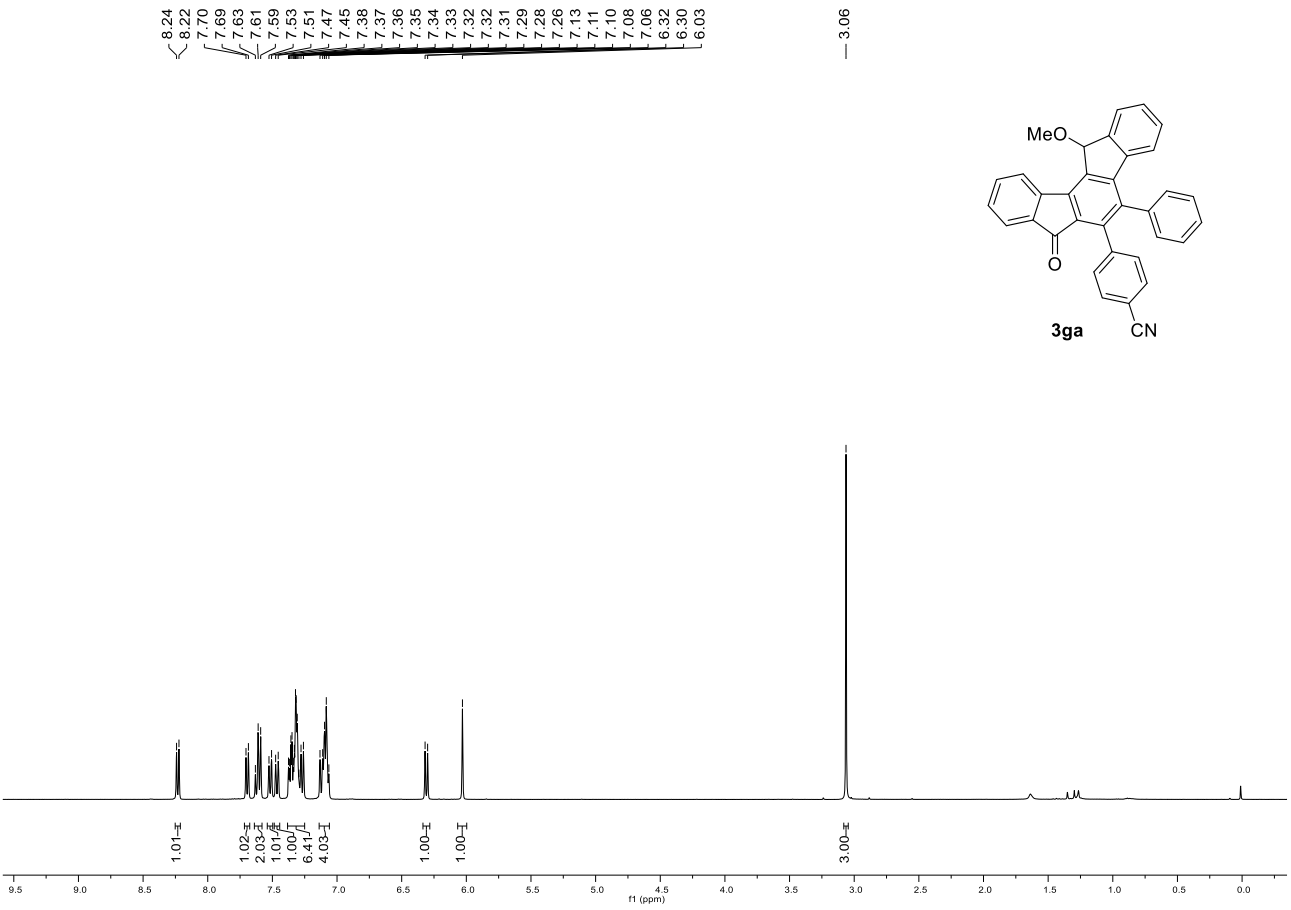
^{1}H NMR of **3fa** (400 MHz, $CDCl_3$)



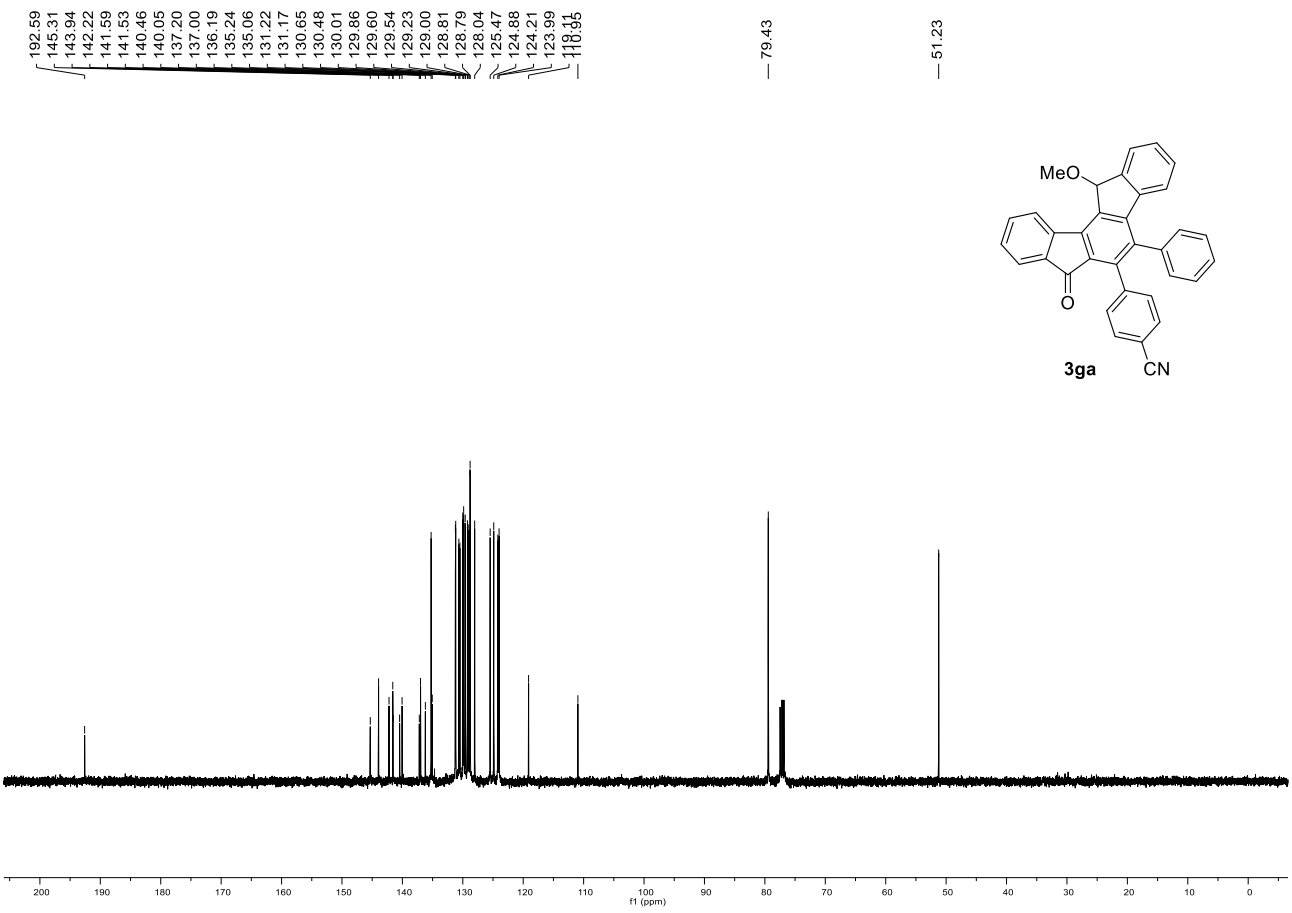
^{13}C NMR of **3fa** (100 MHz, $CDCl_3$)



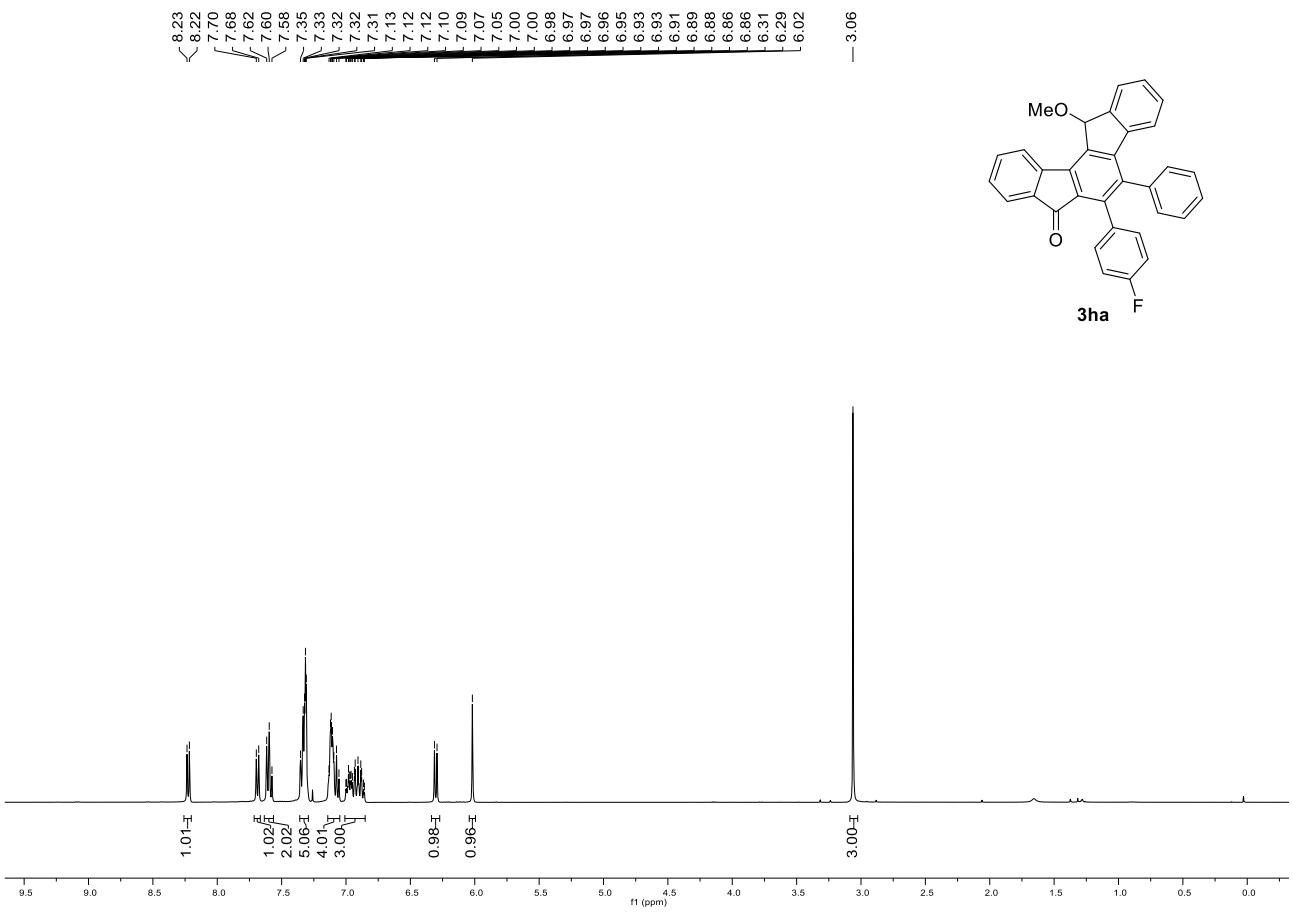
^{1}H NMR of **3ga** (400 MHz, $CDCl_3$)



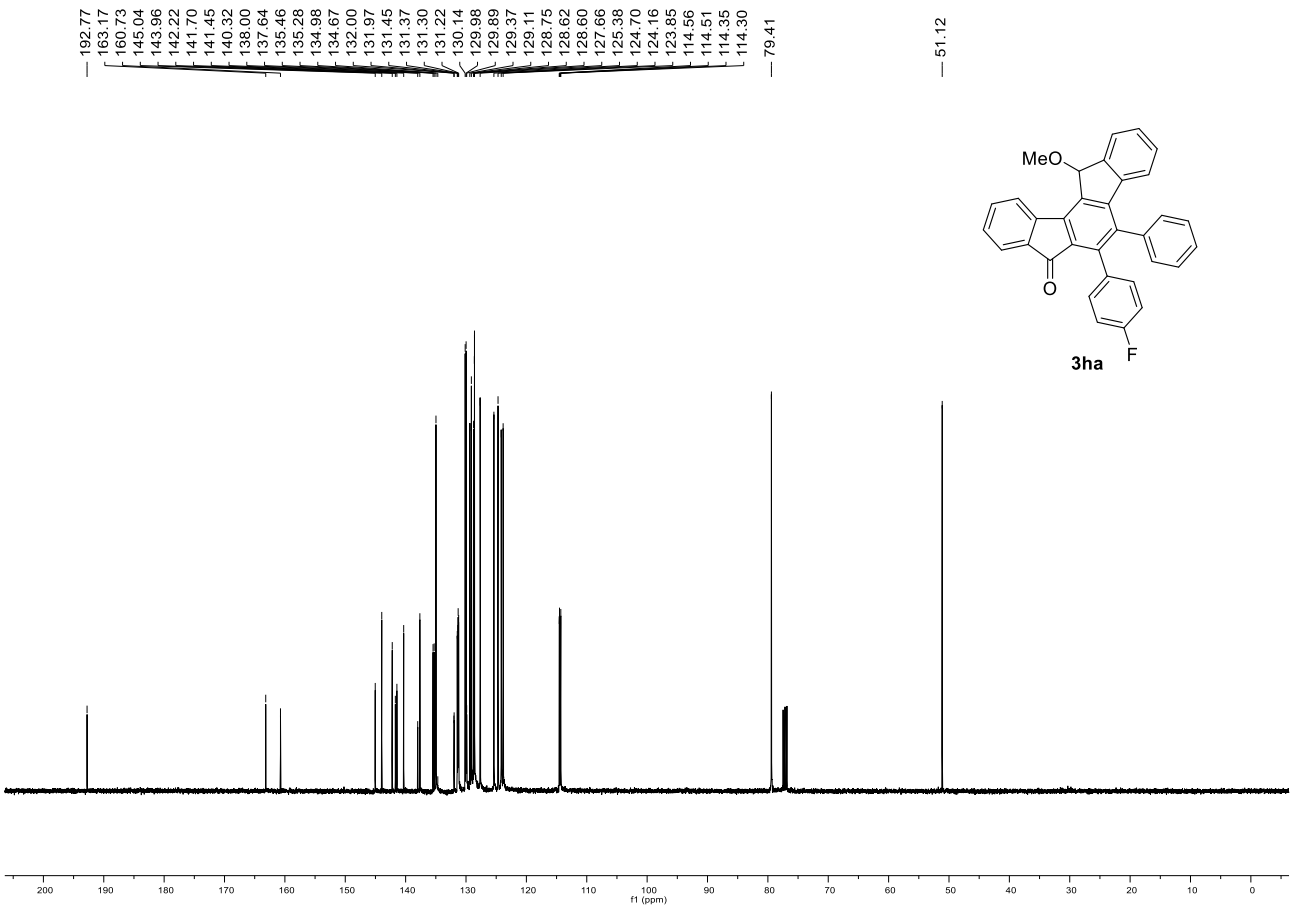
^{13}C NMR of **3ga** (100 MHz, $CDCl_3$)



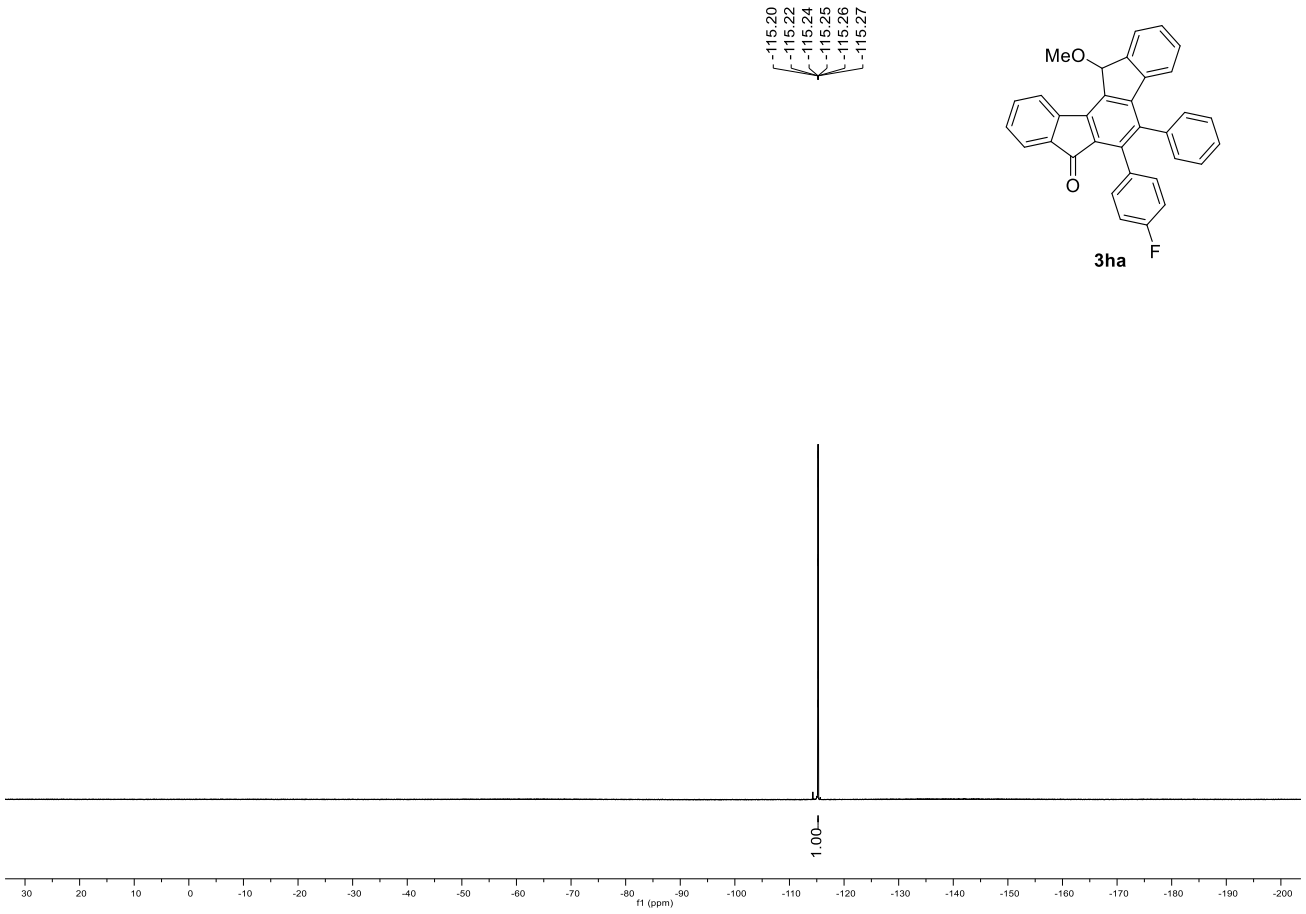
^{1}H NMR of **3ha** (400 MHz, $CDCl_3$)



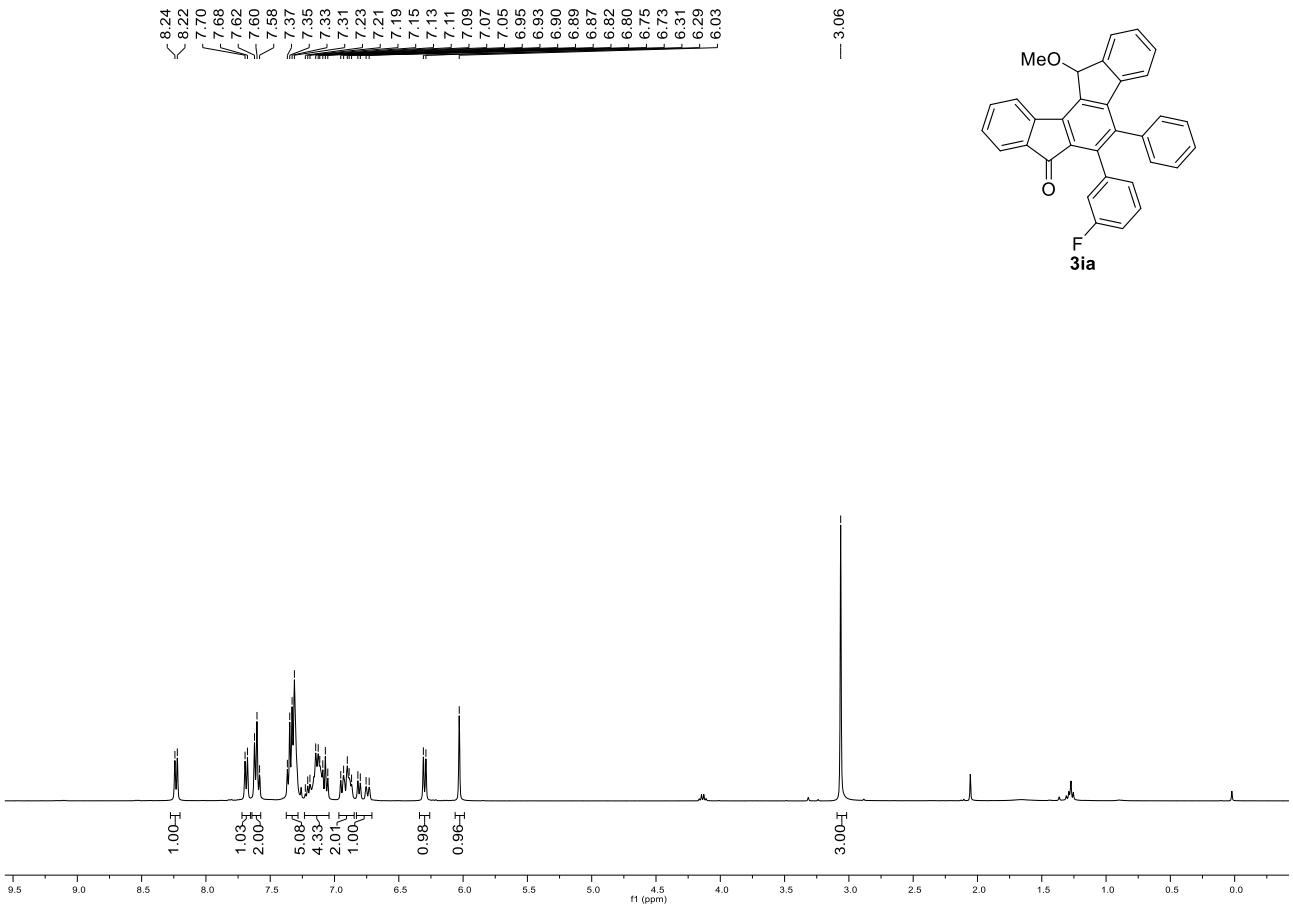
^{13}C NMR of **3ha** (100 MHz, $CDCl_3$)



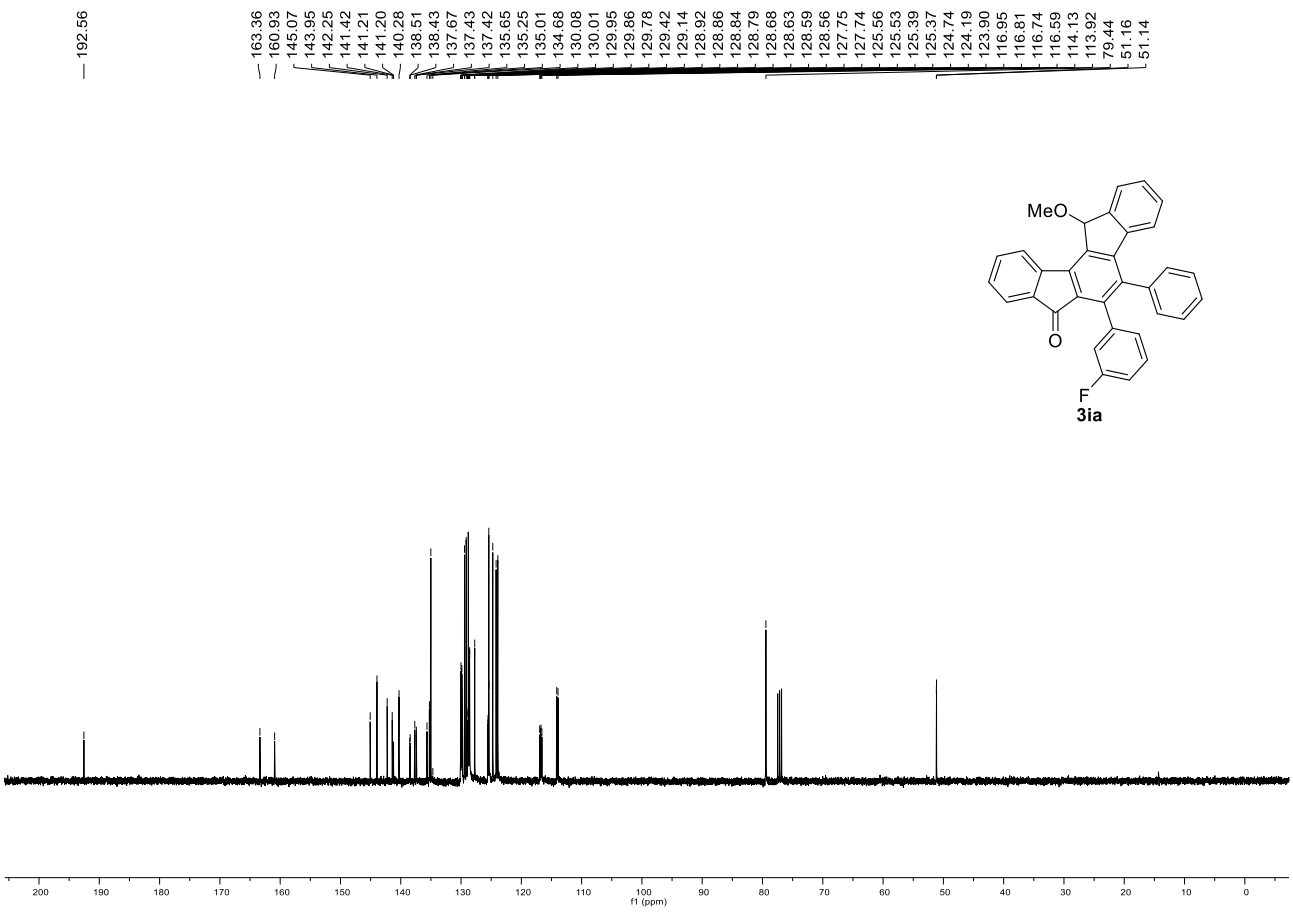
^{19}F NMR of **3ha** (376 MHz, $CDCl_3$)



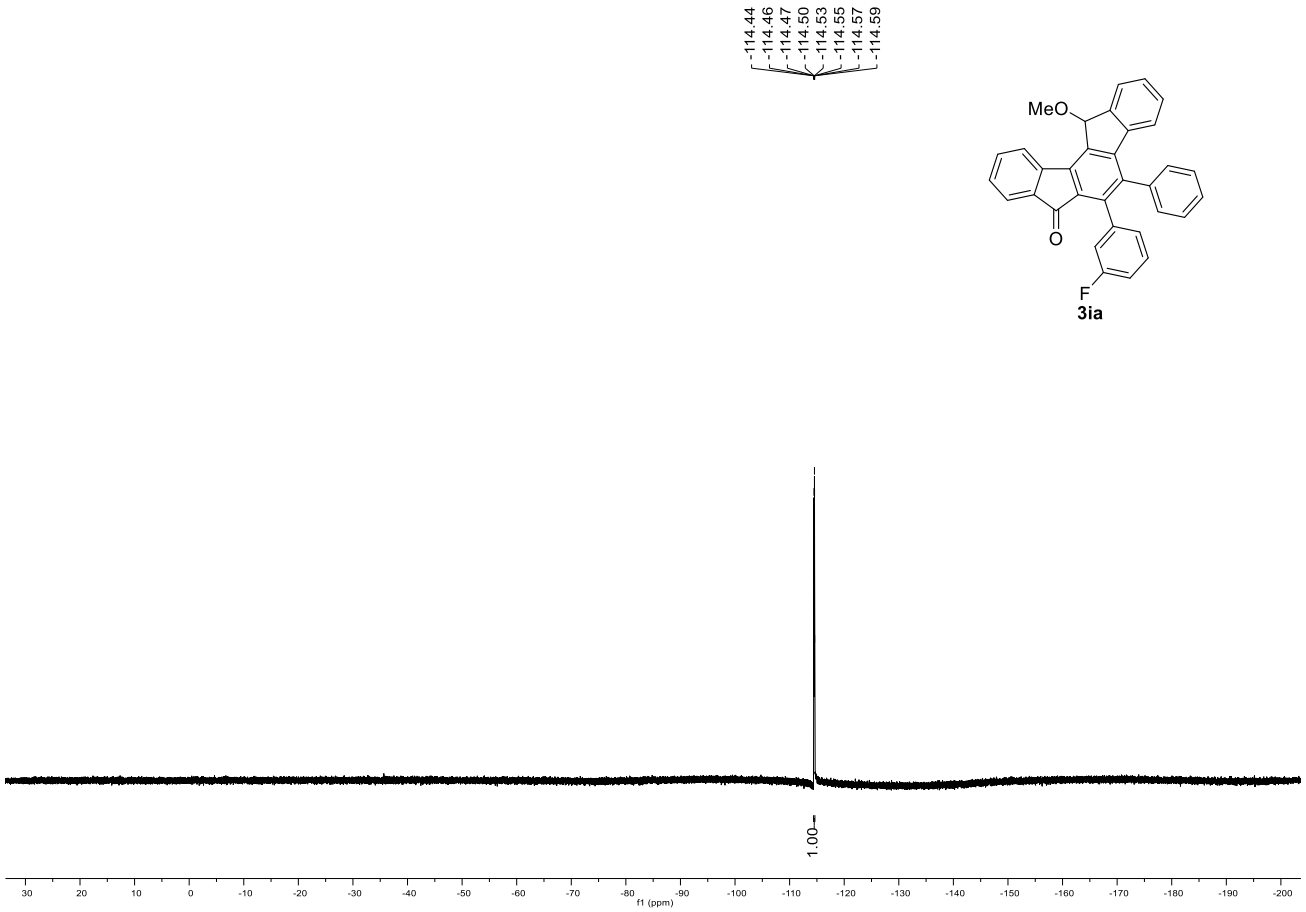
^{1}H NMR of **3ia** (400 MHz, $CDCl_3$)



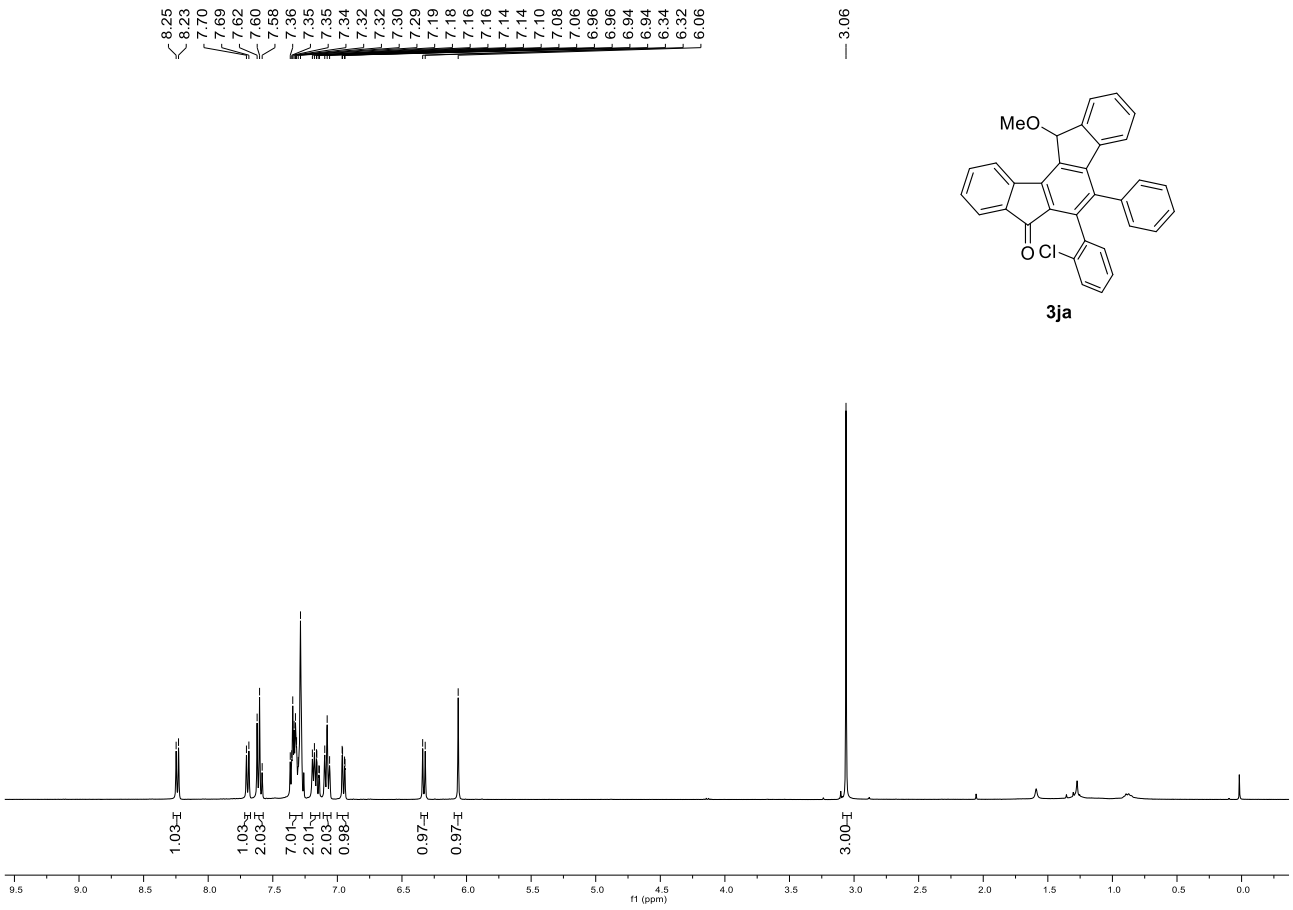
^{13}C NMR of **3ia** (100 MHz, $CDCl_3$)



^{19}F NMR of **3ia** (376 MHz, $CDCl_3$)

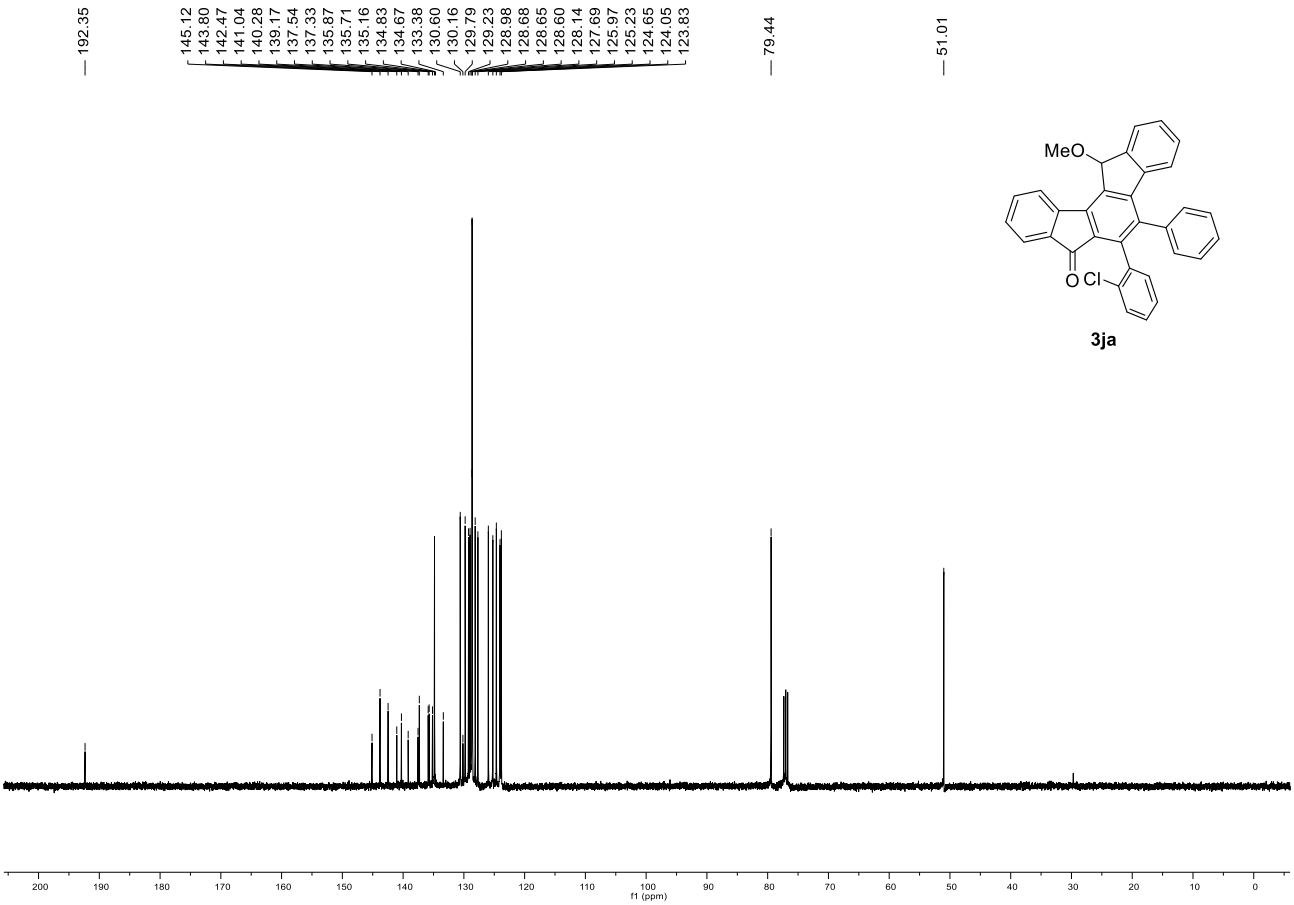


^{1}H NMR of **3ja** (400 MHz, $CDCl_3$)



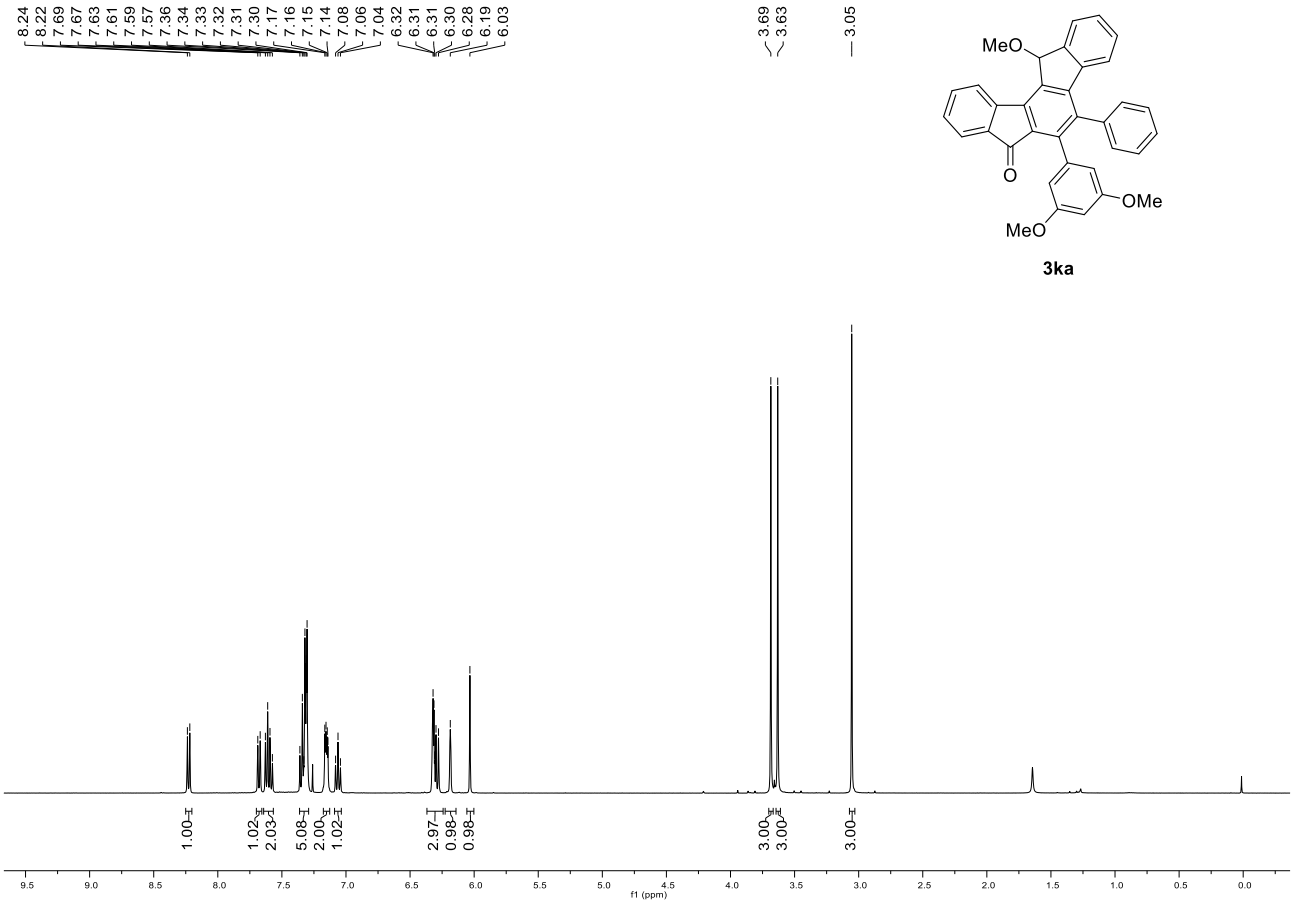
3ja

^{13}C NMR of **3ja** (100 MHz, $CDCl_3$)

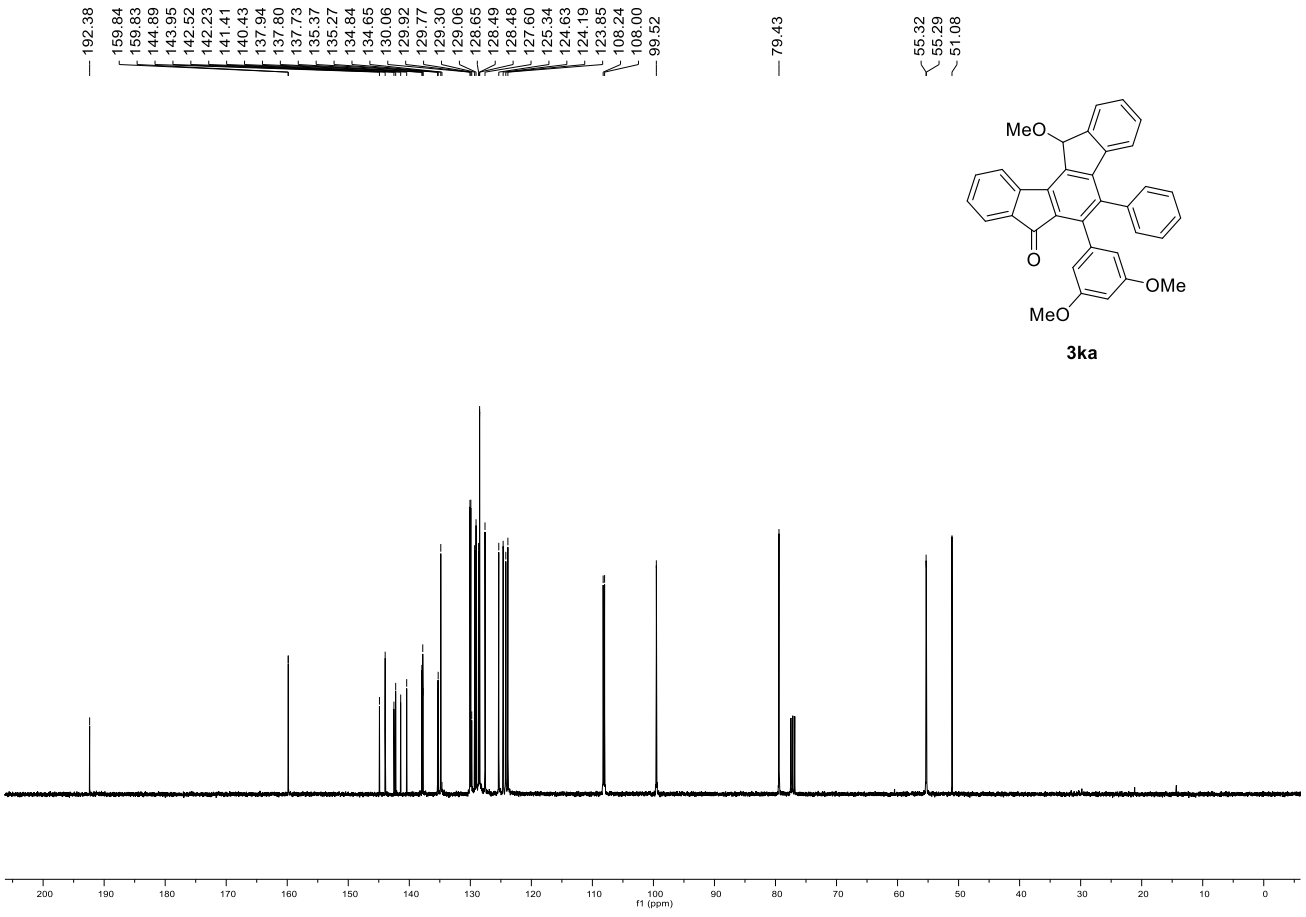


3ja

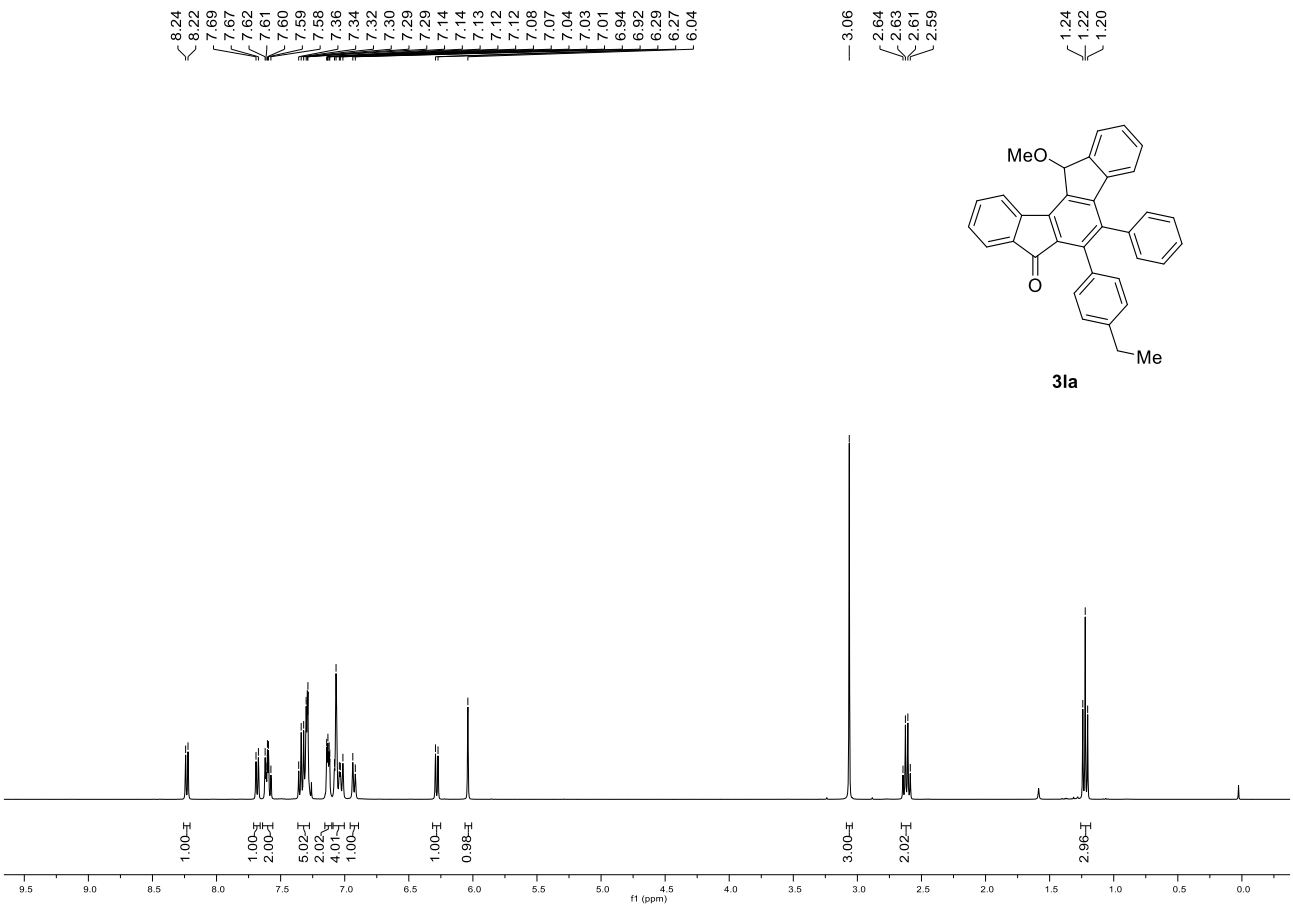
^{1}H NMR of **3ka** (400 MHz, $CDCl_3$)



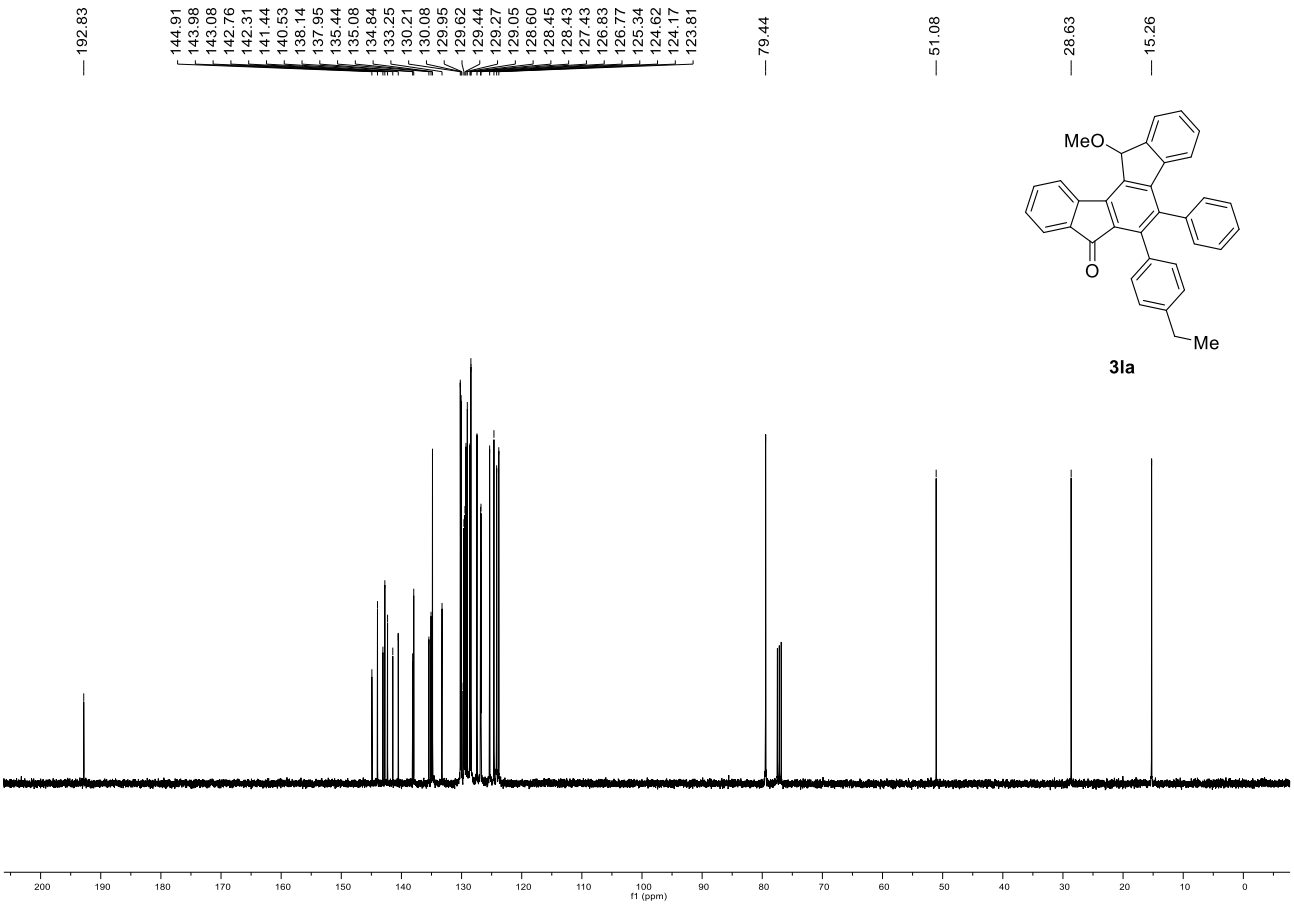
^{13}C NMR of **3ka** (100 MHz, $CDCl_3$)



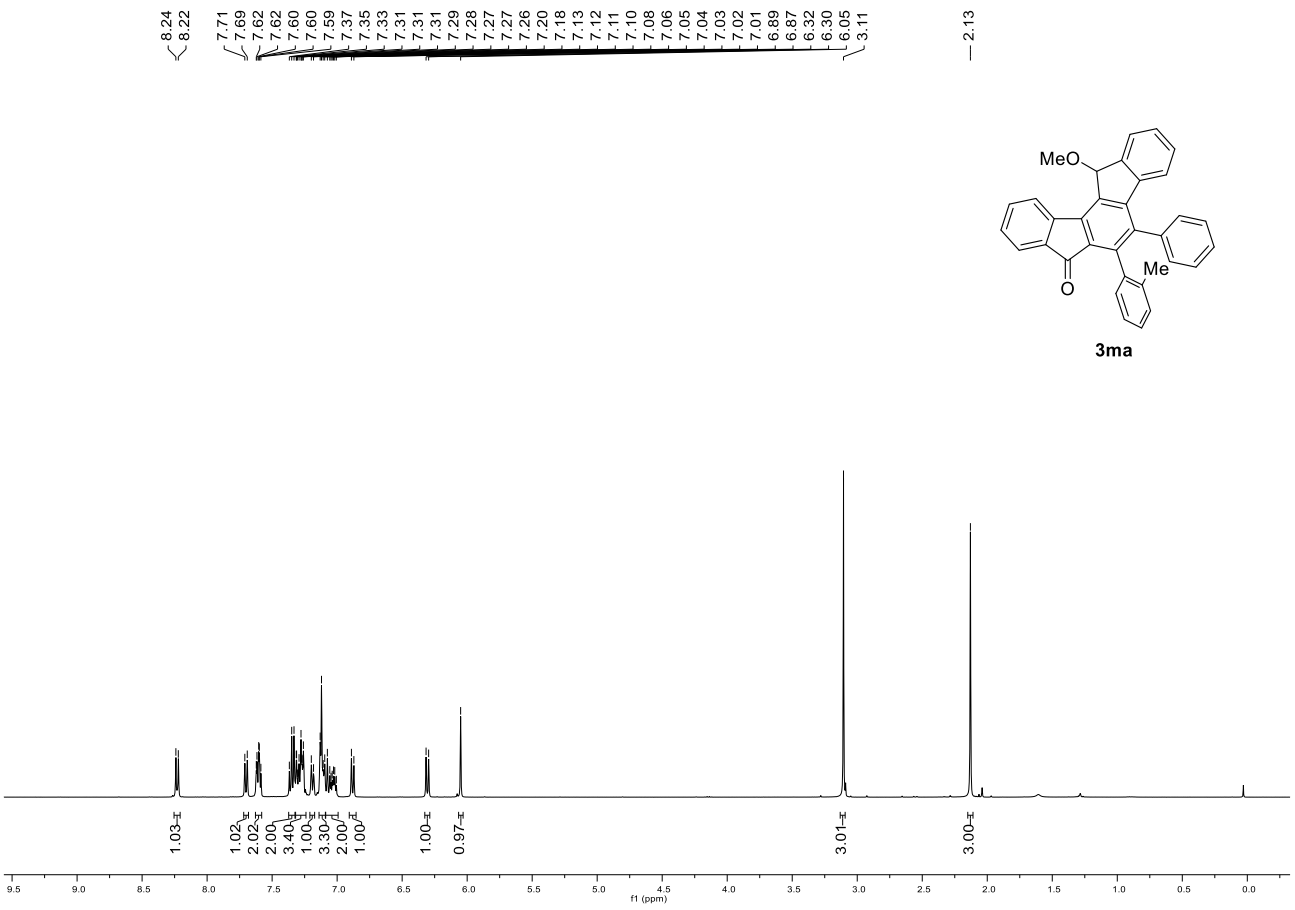
^{1}H NMR of **3la** (400 MHz, $CDCl_3$)



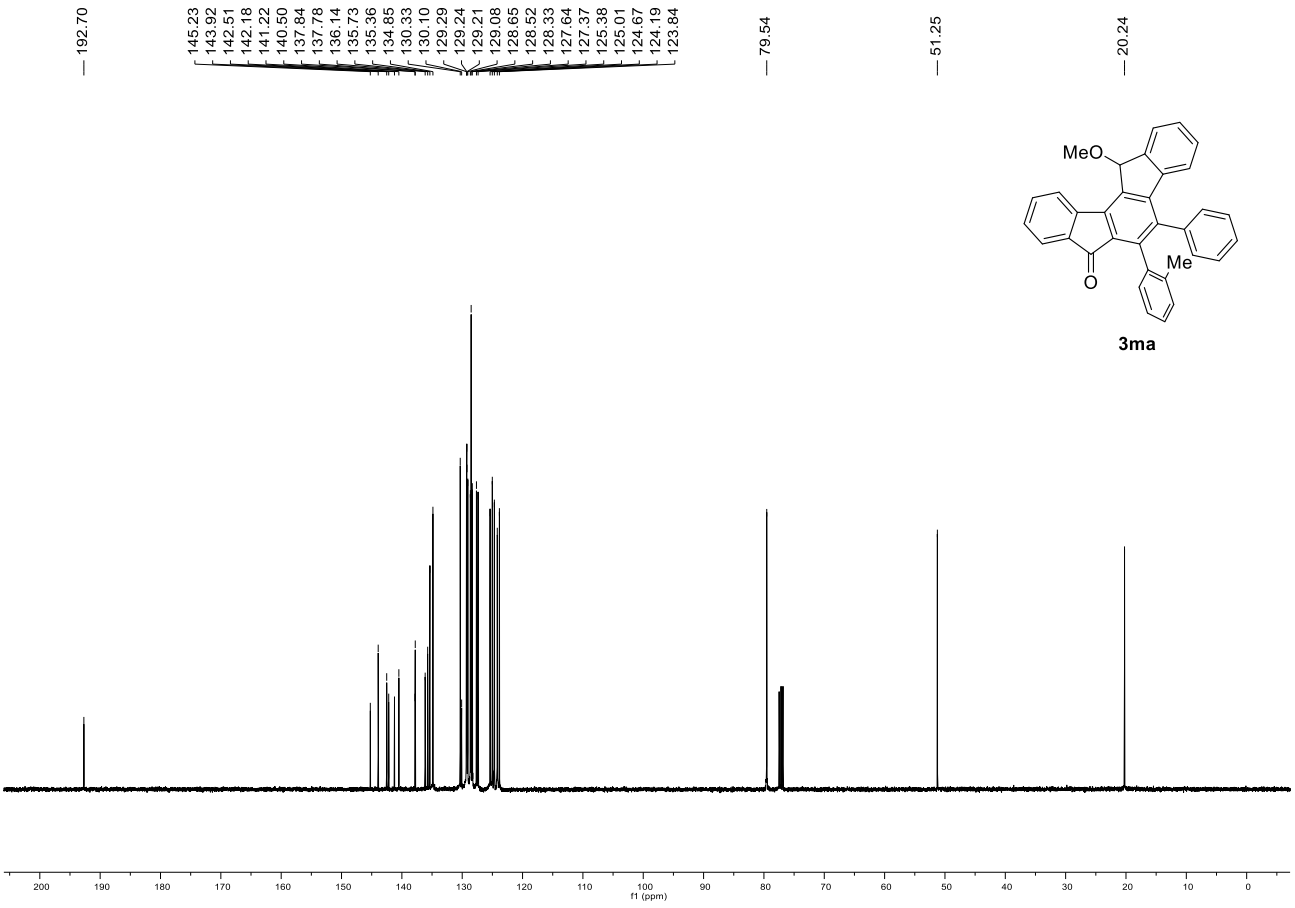
^{13}C NMR of **3la** (100 MHz, $CDCl_3$)



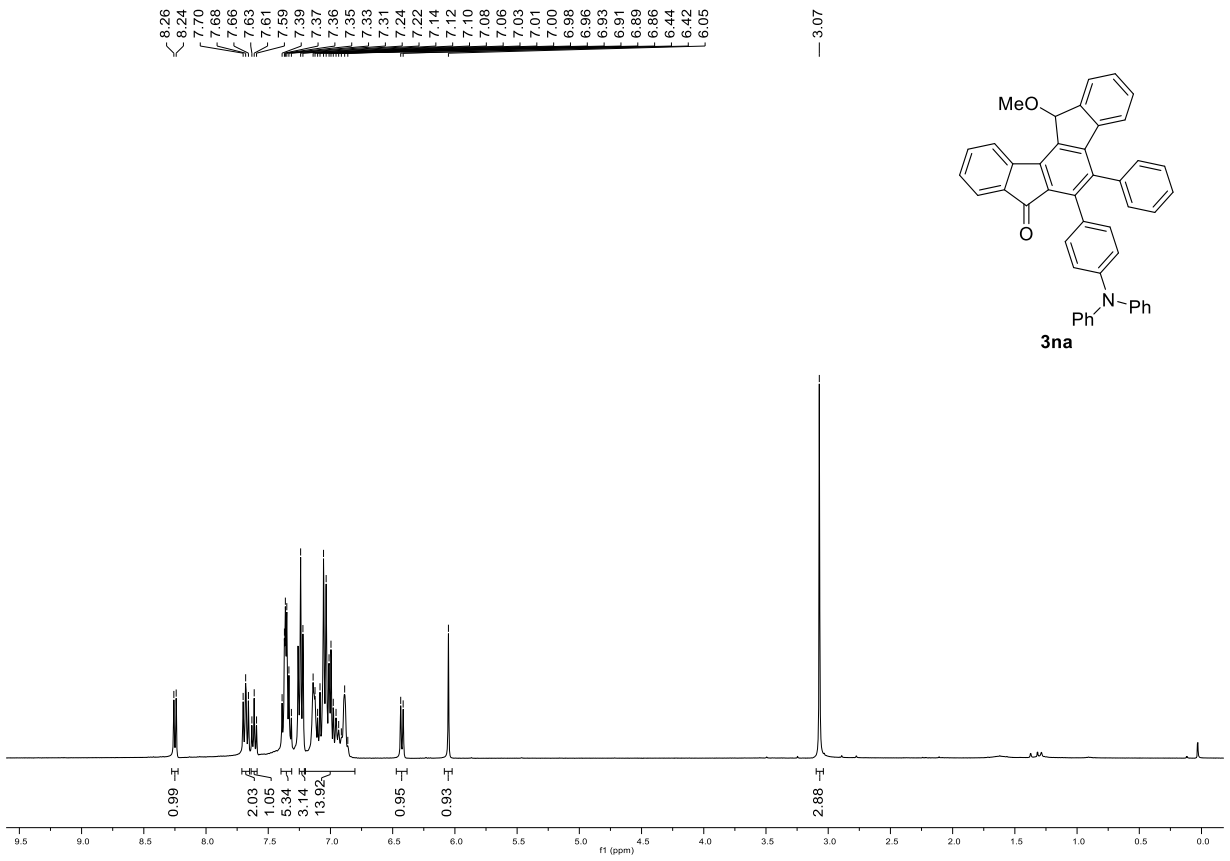
^{1}H NMR of **3ma** (400 MHz, $CDCl_3$)



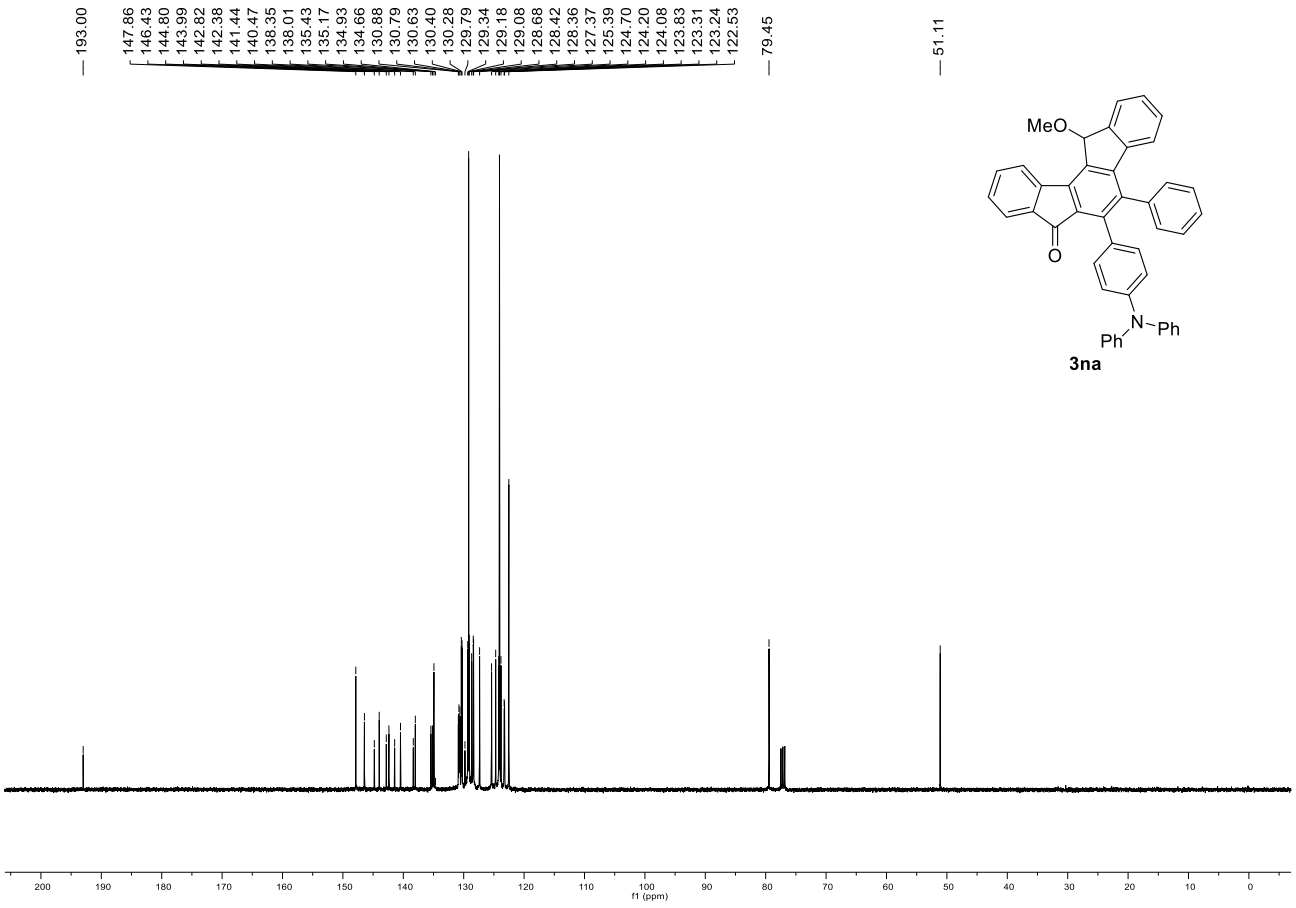
^{13}C NMR of **3ma** (100 MHz, $CDCl_3$)



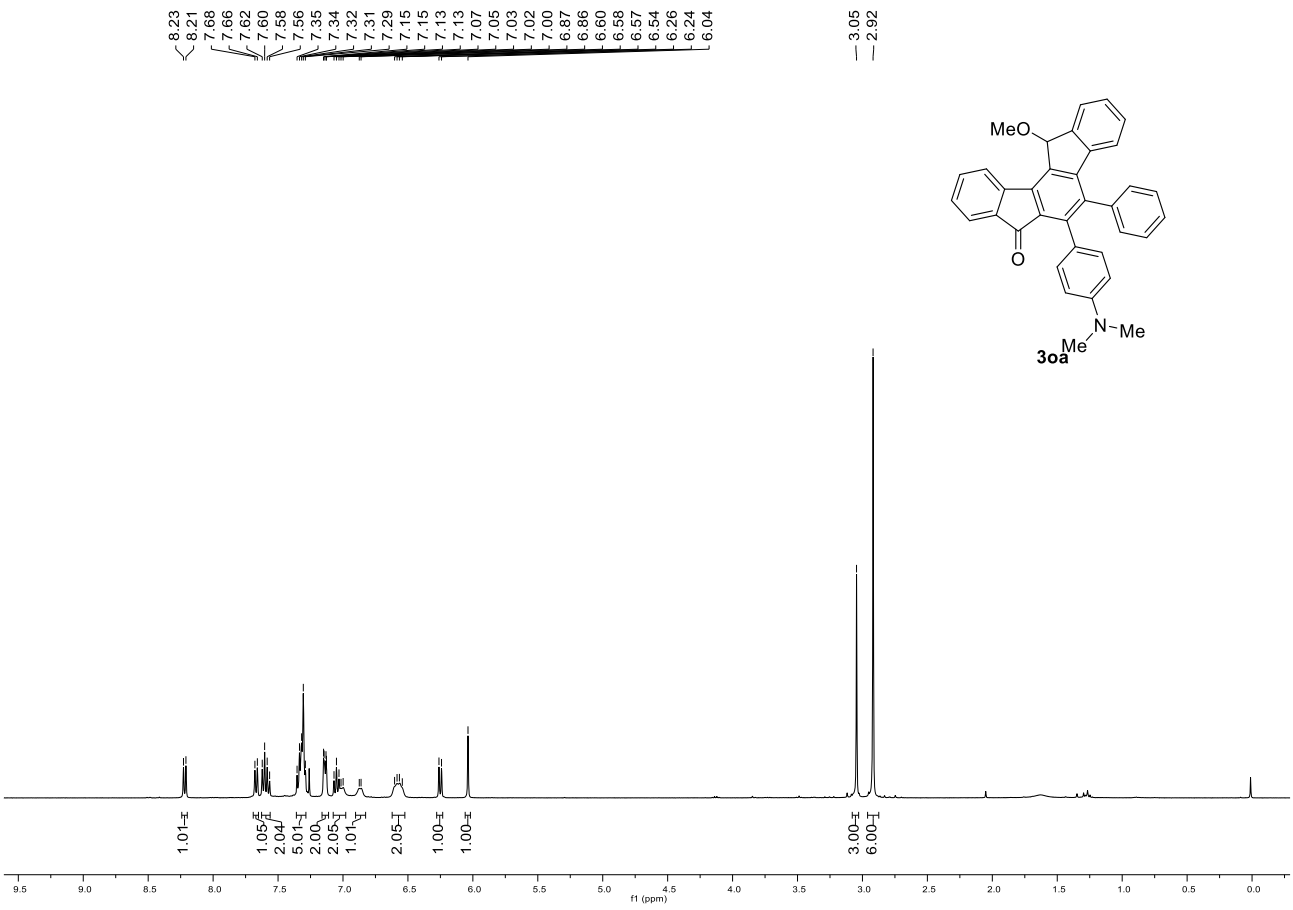
^{1}H NMR of **3na** (400 MHz, $CDCl_3$)



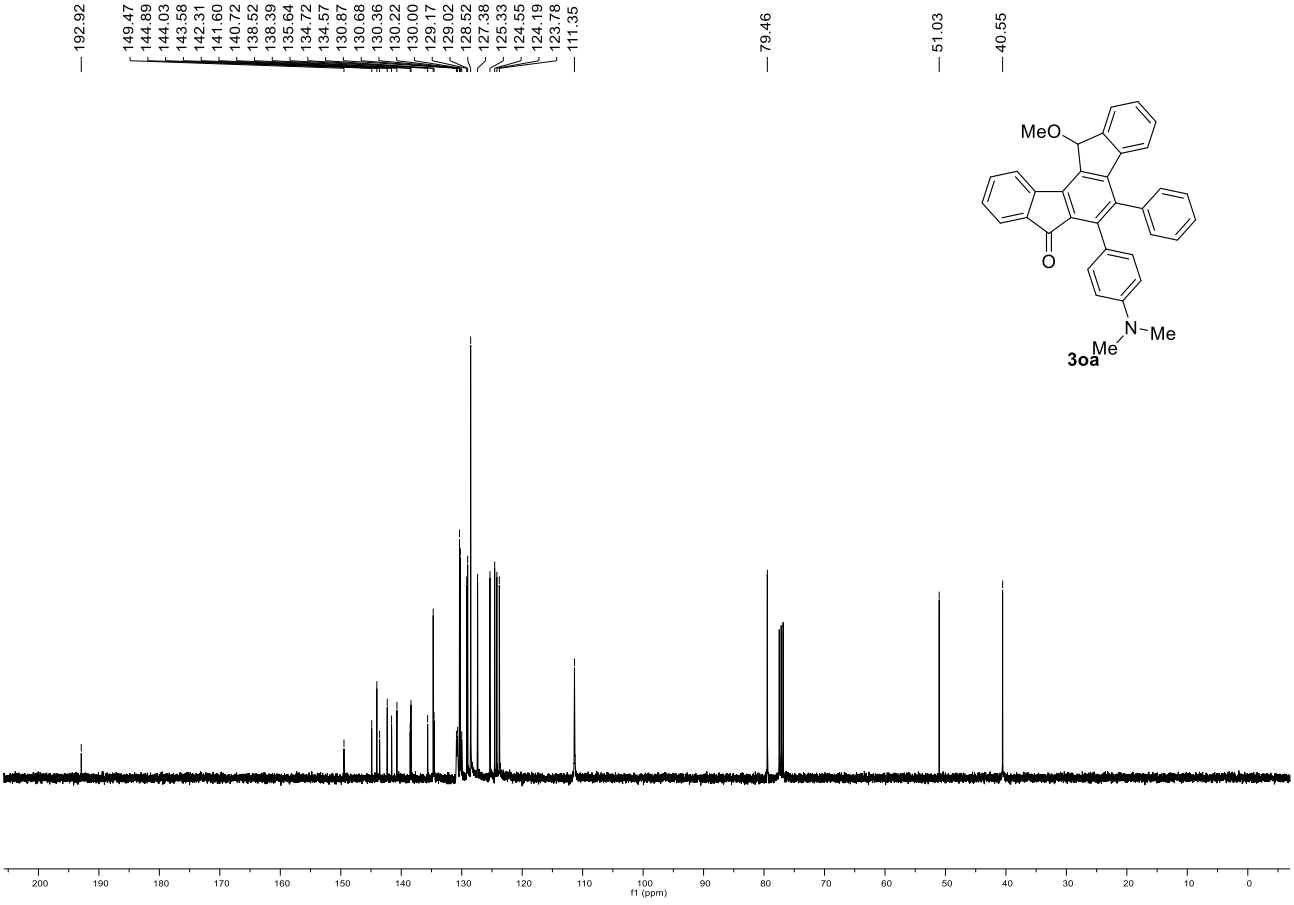
^{13}C NMR of **3na** (100 MHz, $CDCl_3$)



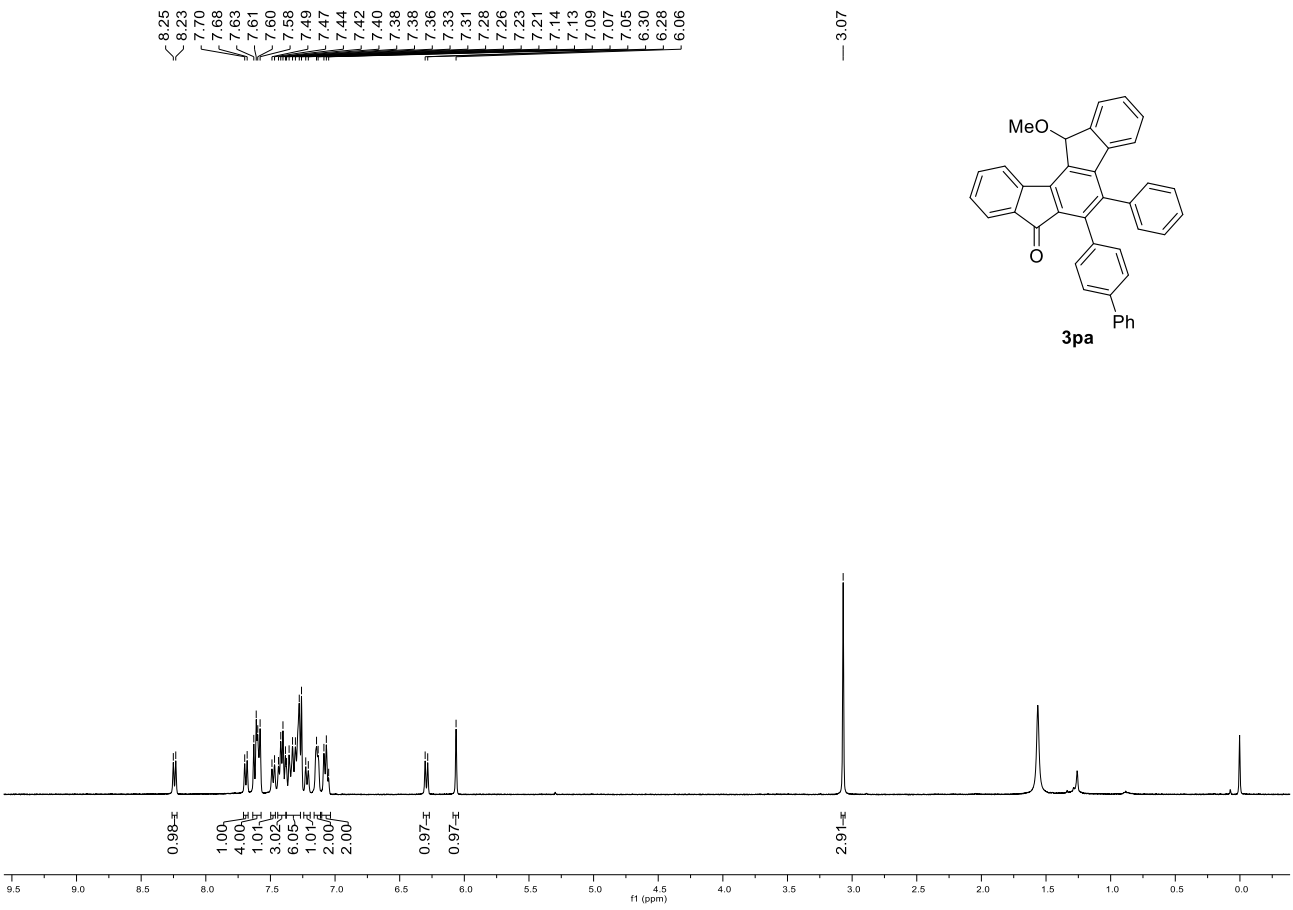
^{1}H NMR of **3oa** (400 MHz, $CDCl_3$)



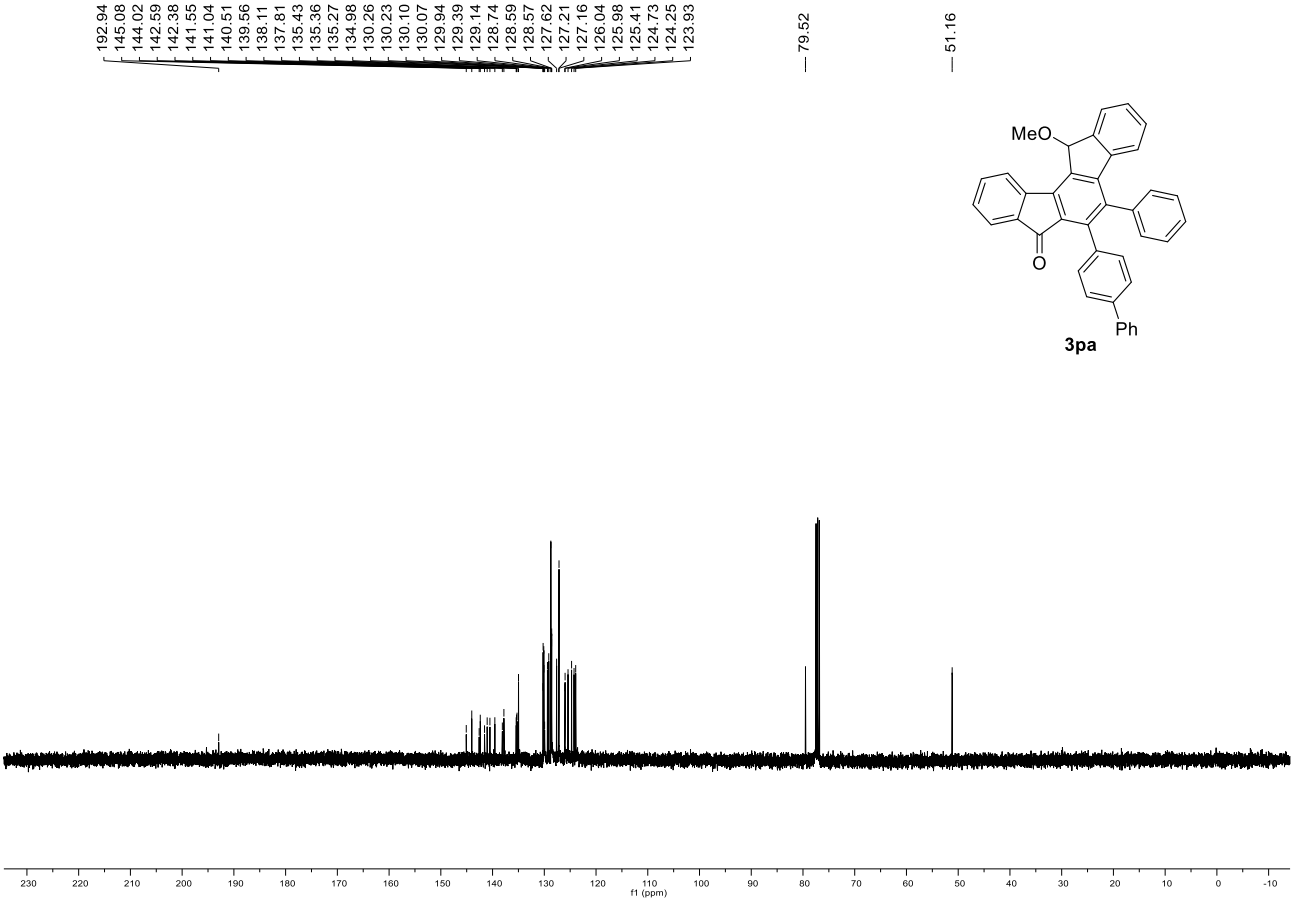
^{13}C NMR of **3oa** (100 MHz, $CDCl_3$)



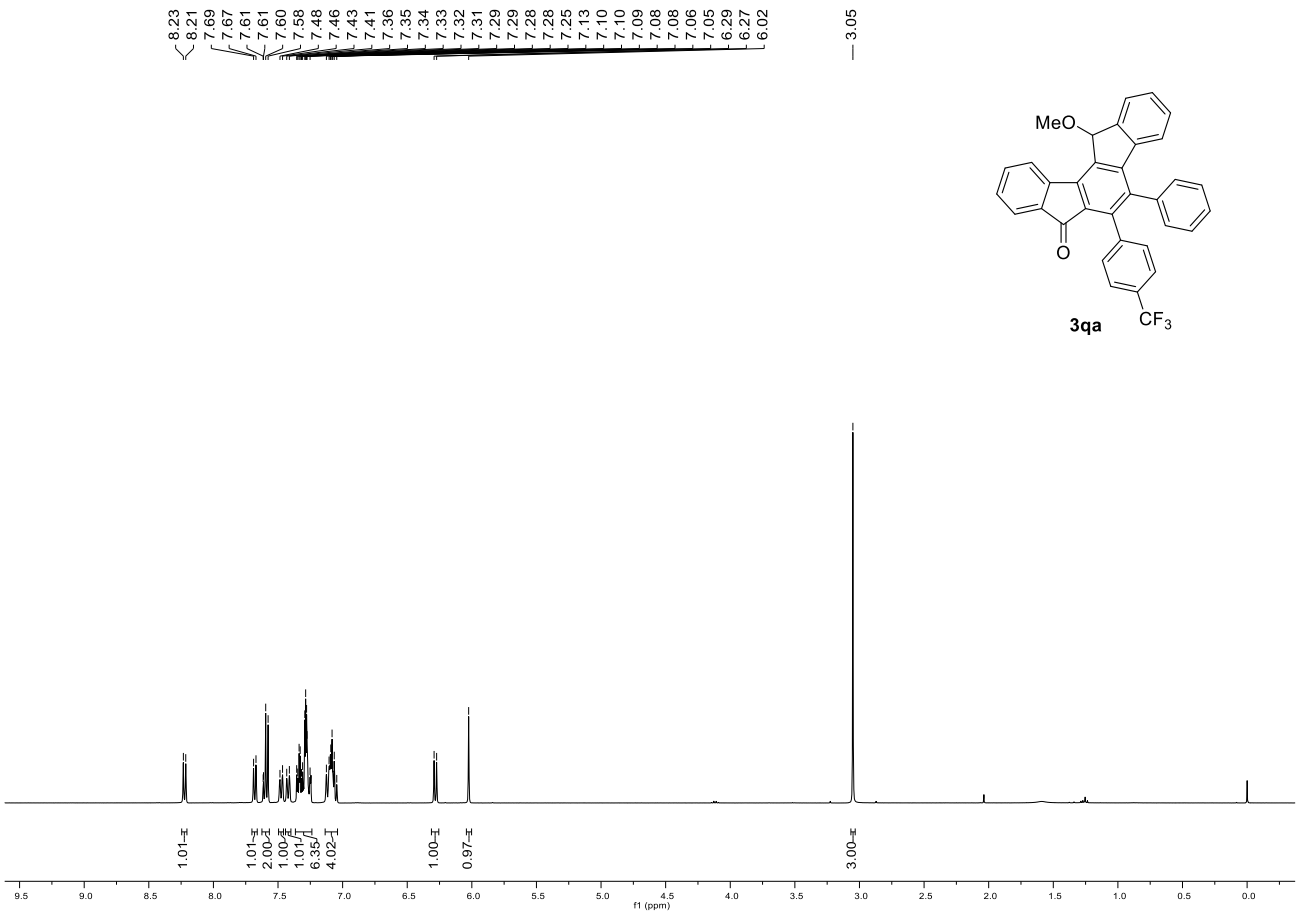
^{1}H NMR of **3pa** (400 MHz, $CDCl_3$)



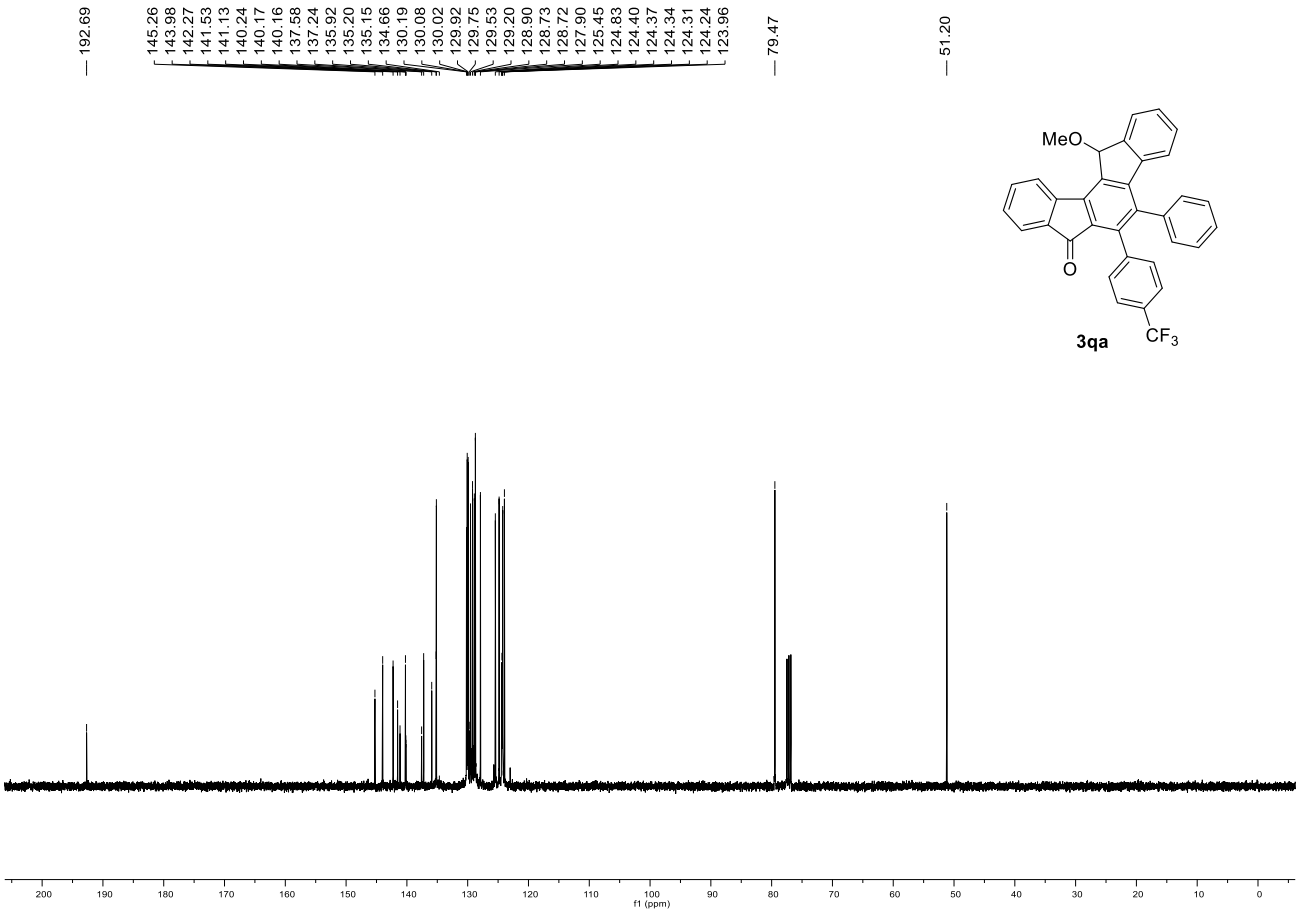
^{13}C NMR of **3pa** (100 MHz, $CDCl_3$)



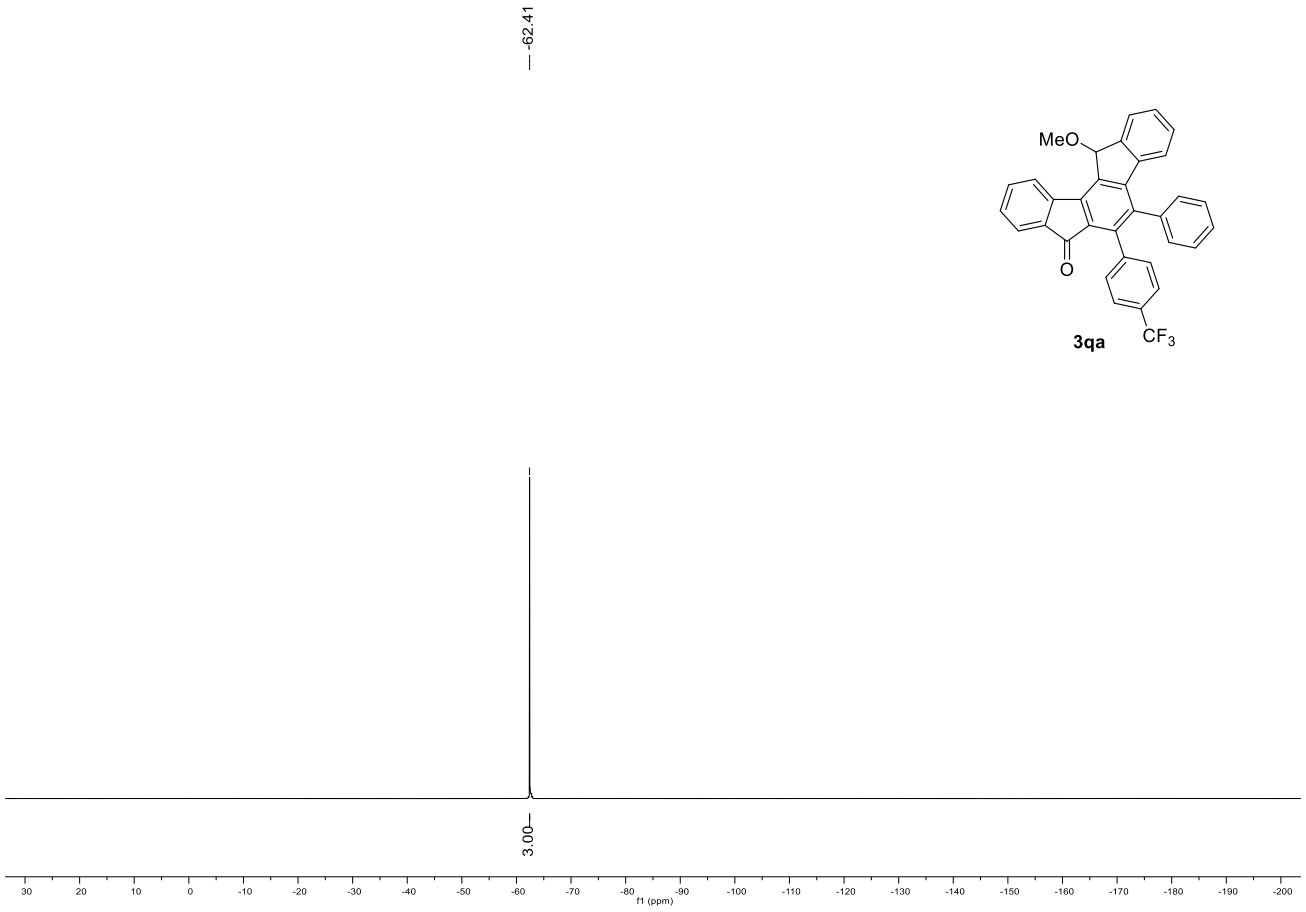
^{1}H NMR of **3qa** (400 MHz, $CDCl_3$)



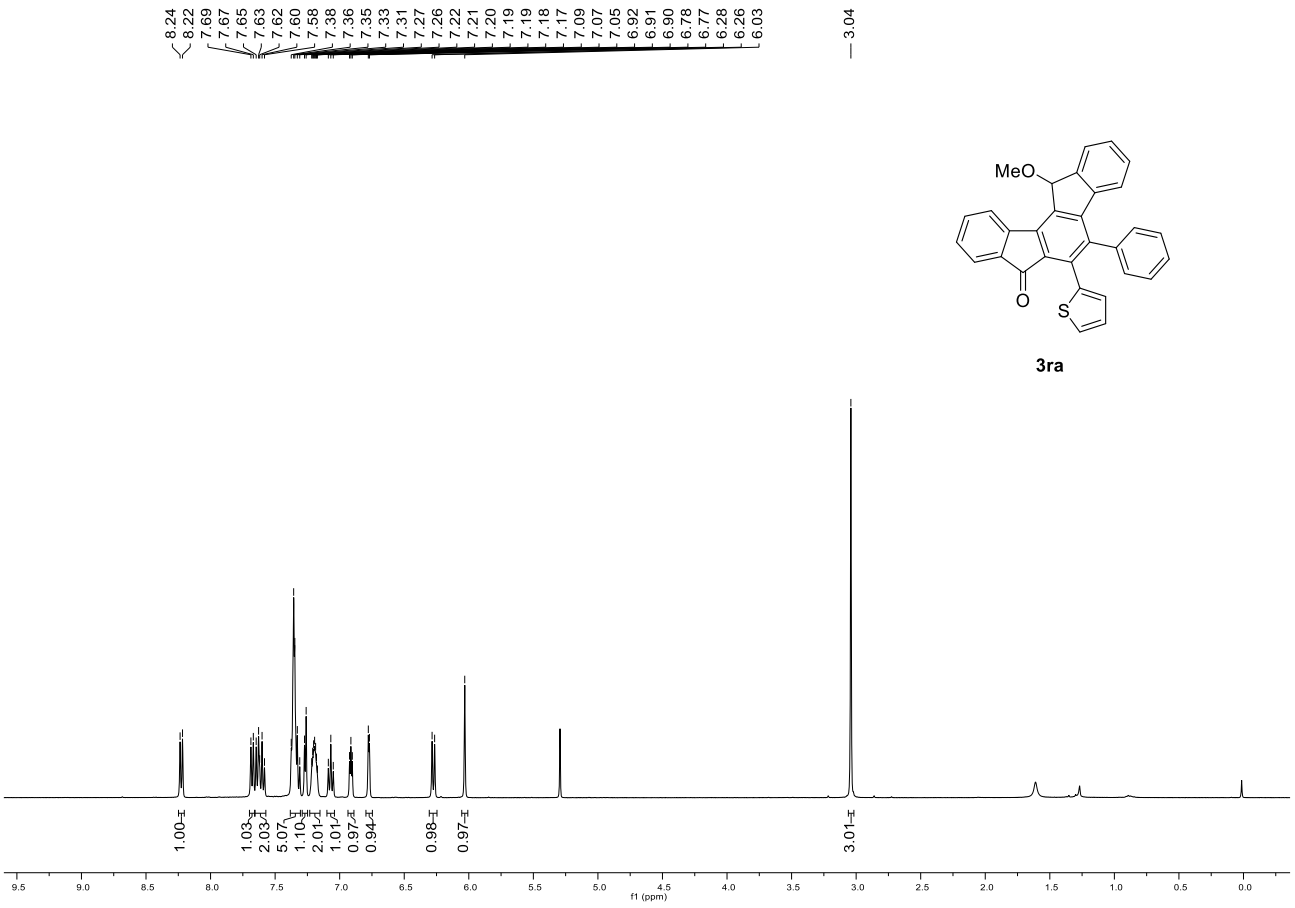
^{13}C NMR of **3qa** (100 MHz, $CDCl_3$)



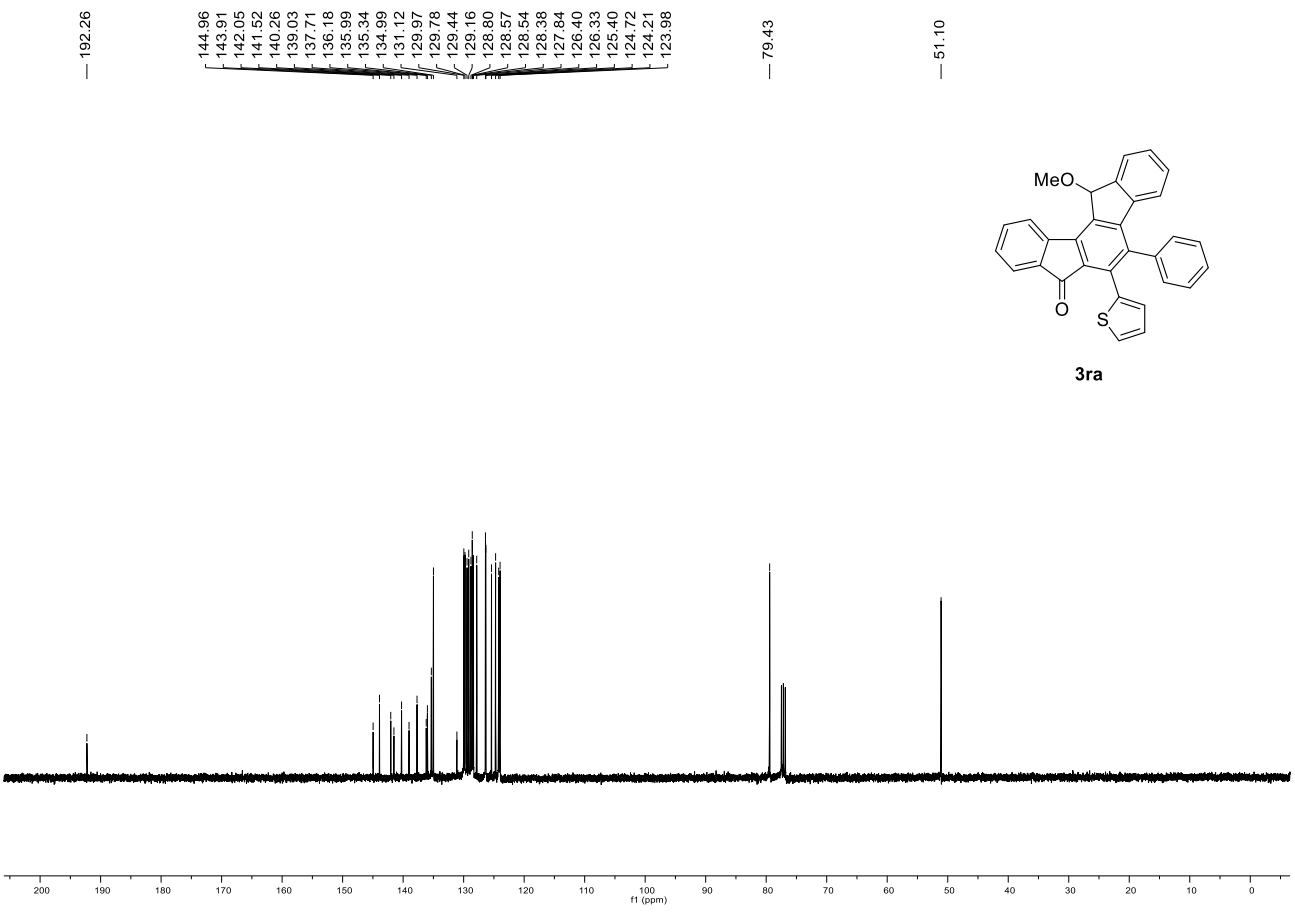
^{19}F NMR of **3qa** (376 MHz, $CDCl_3$)



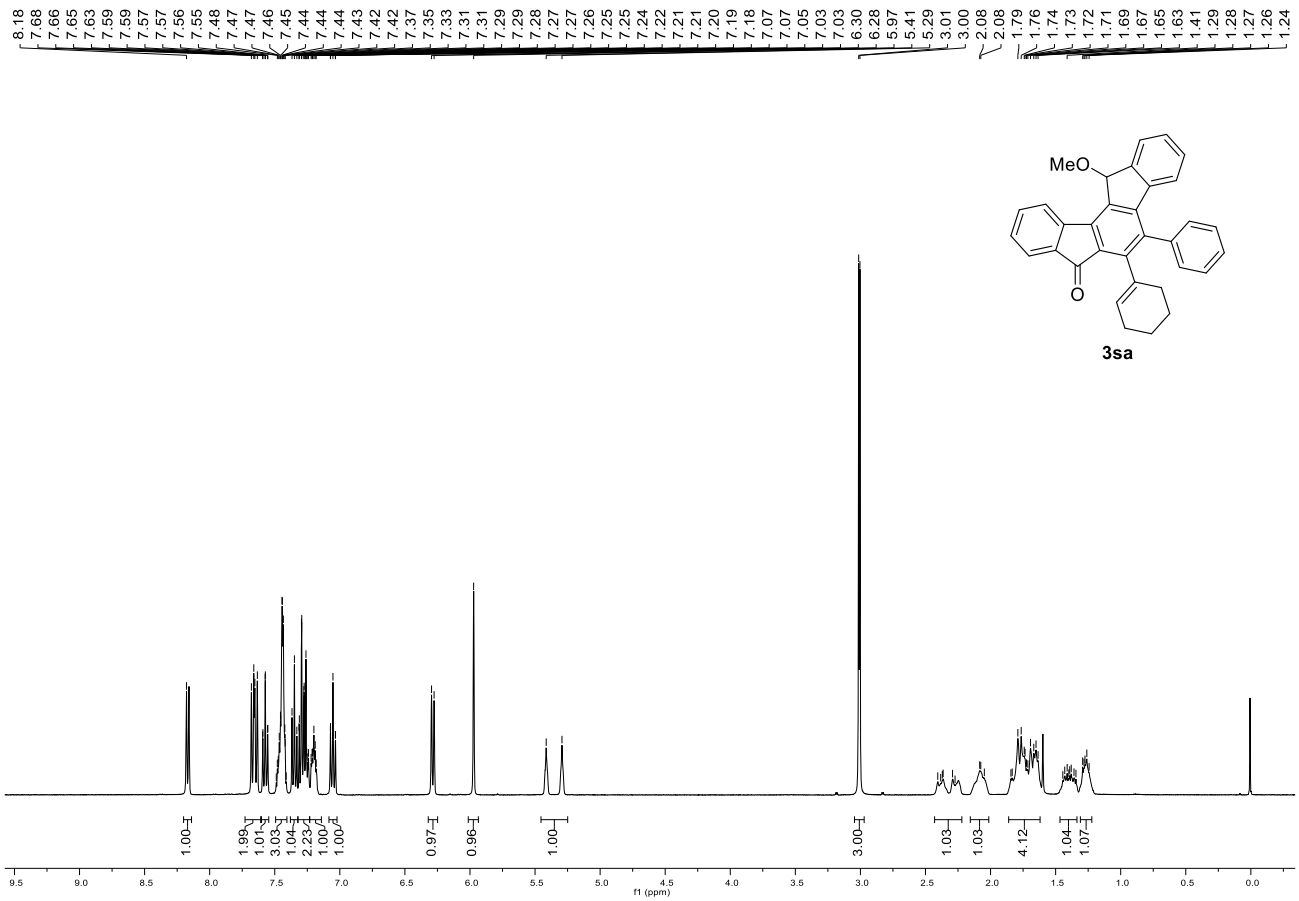
^{1}H NMR of **3ra** (400 MHz, $CDCl_3$)



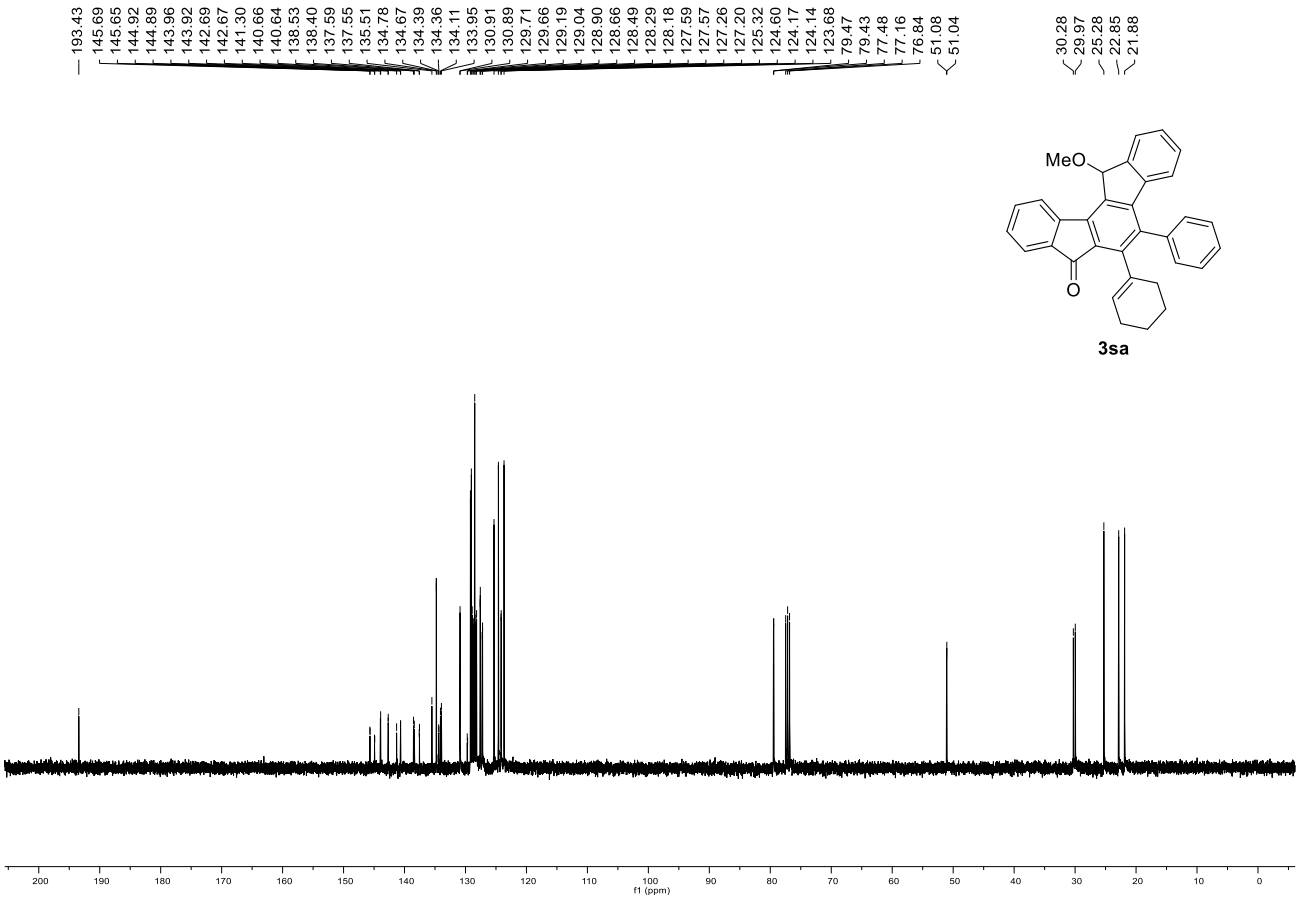
^{13}C NMR of **3ra** (100 MHz, $CDCl_3$)



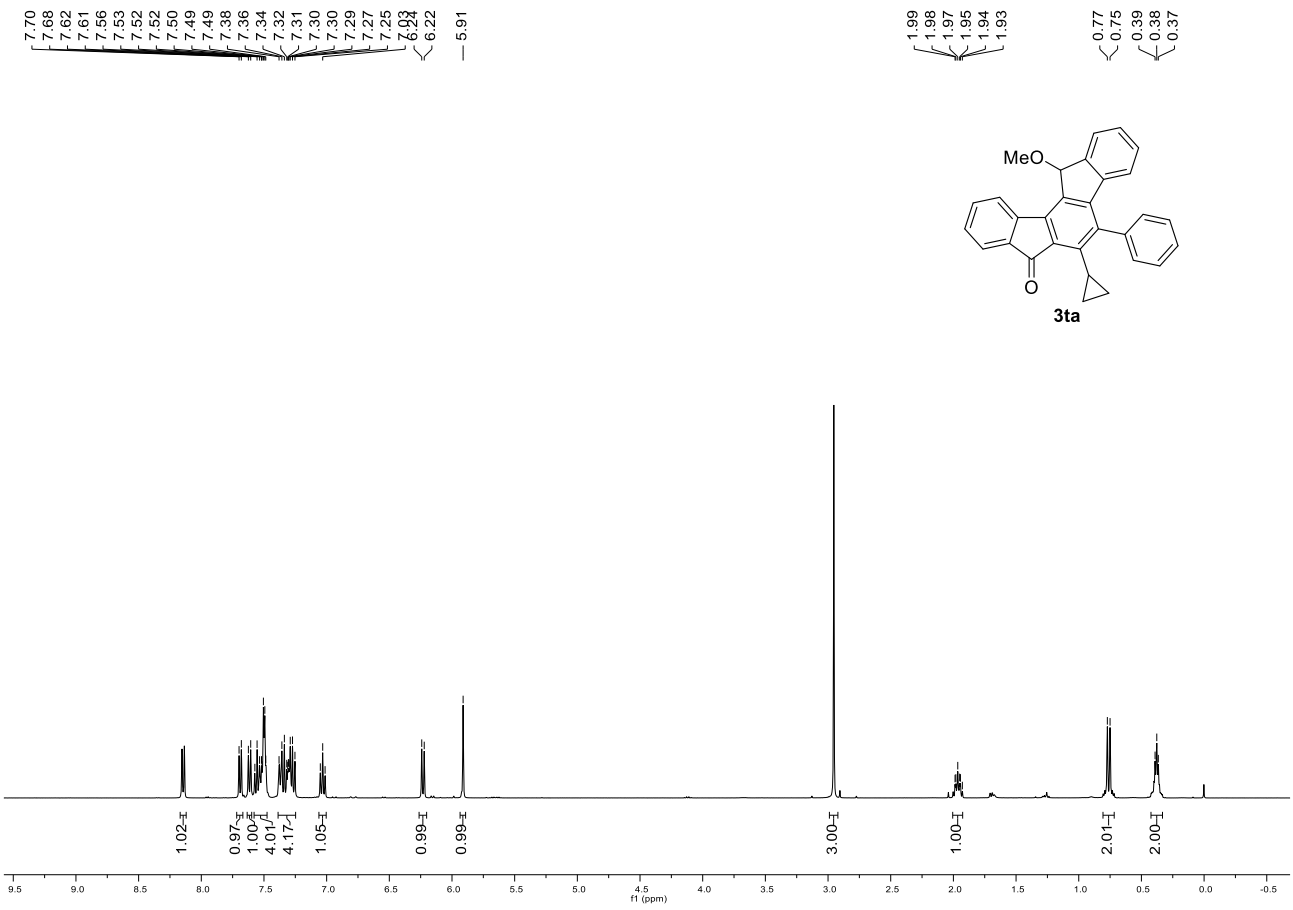
^{1}H NMR of **3sa** (400 MHz, $CDCl_3$)



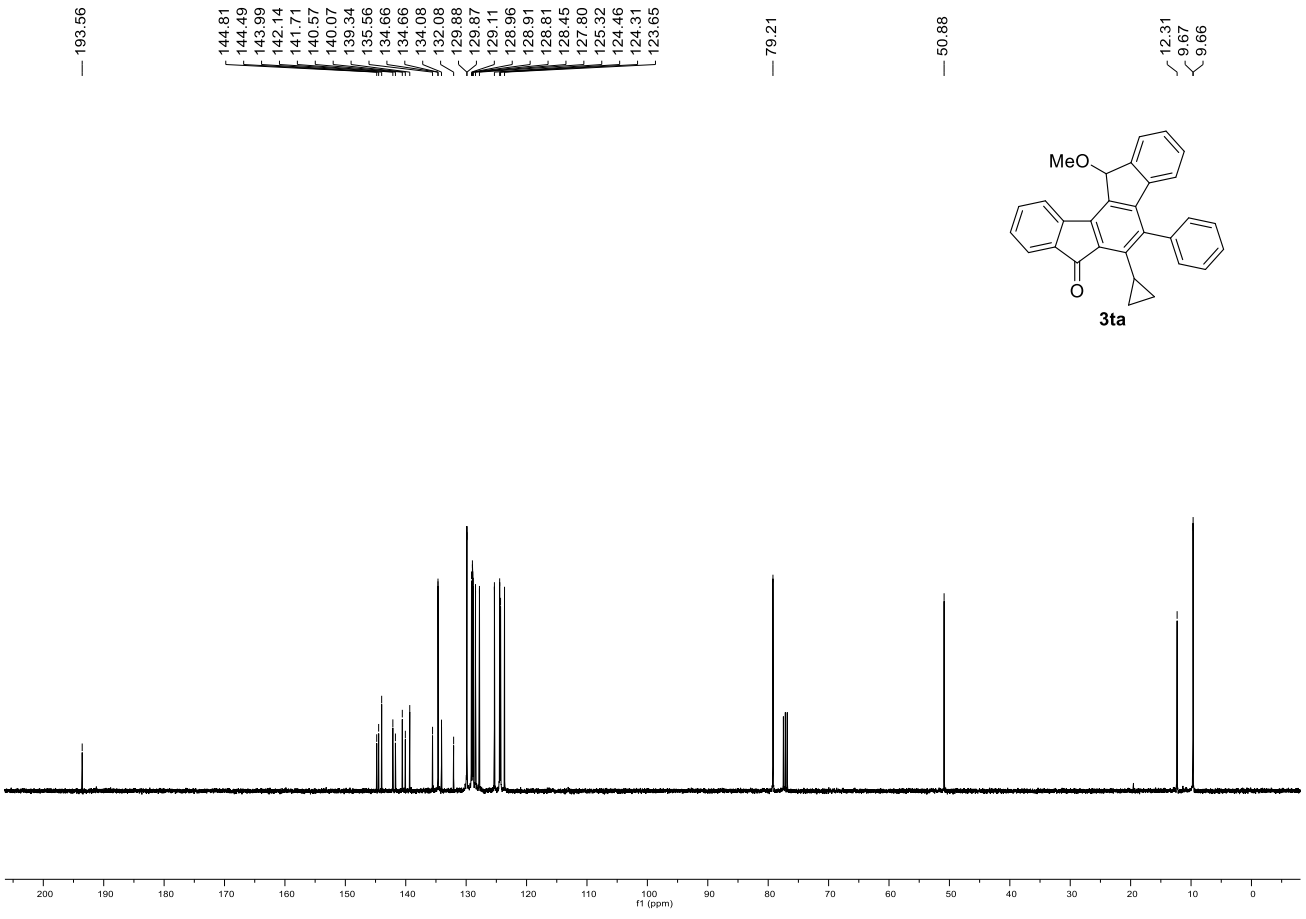
^{13}C NMR of **3sa** (100 MHz, $CDCl_3$)



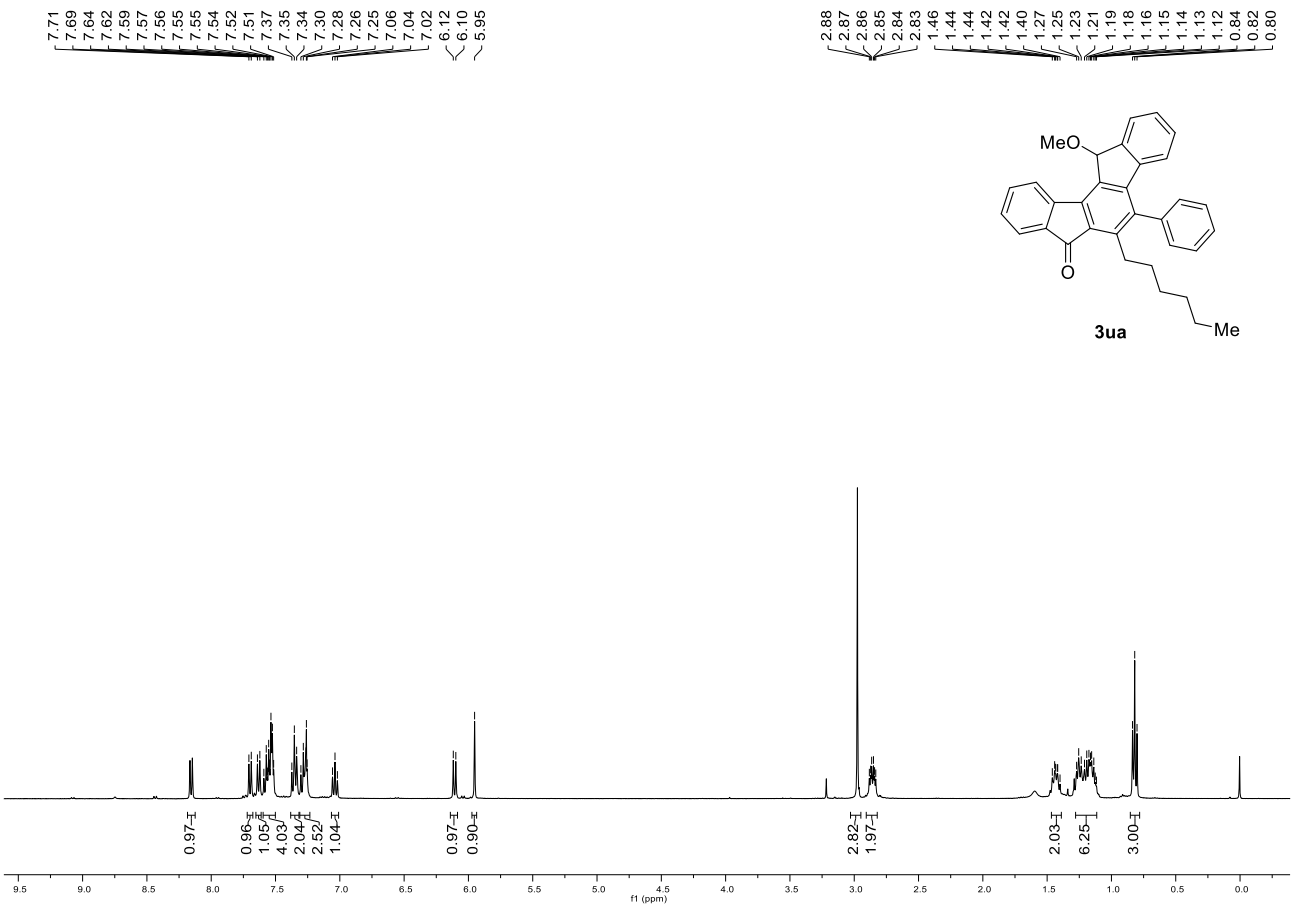
^{1}H NMR of **3ta** (400 MHz, $CDCl_3$)



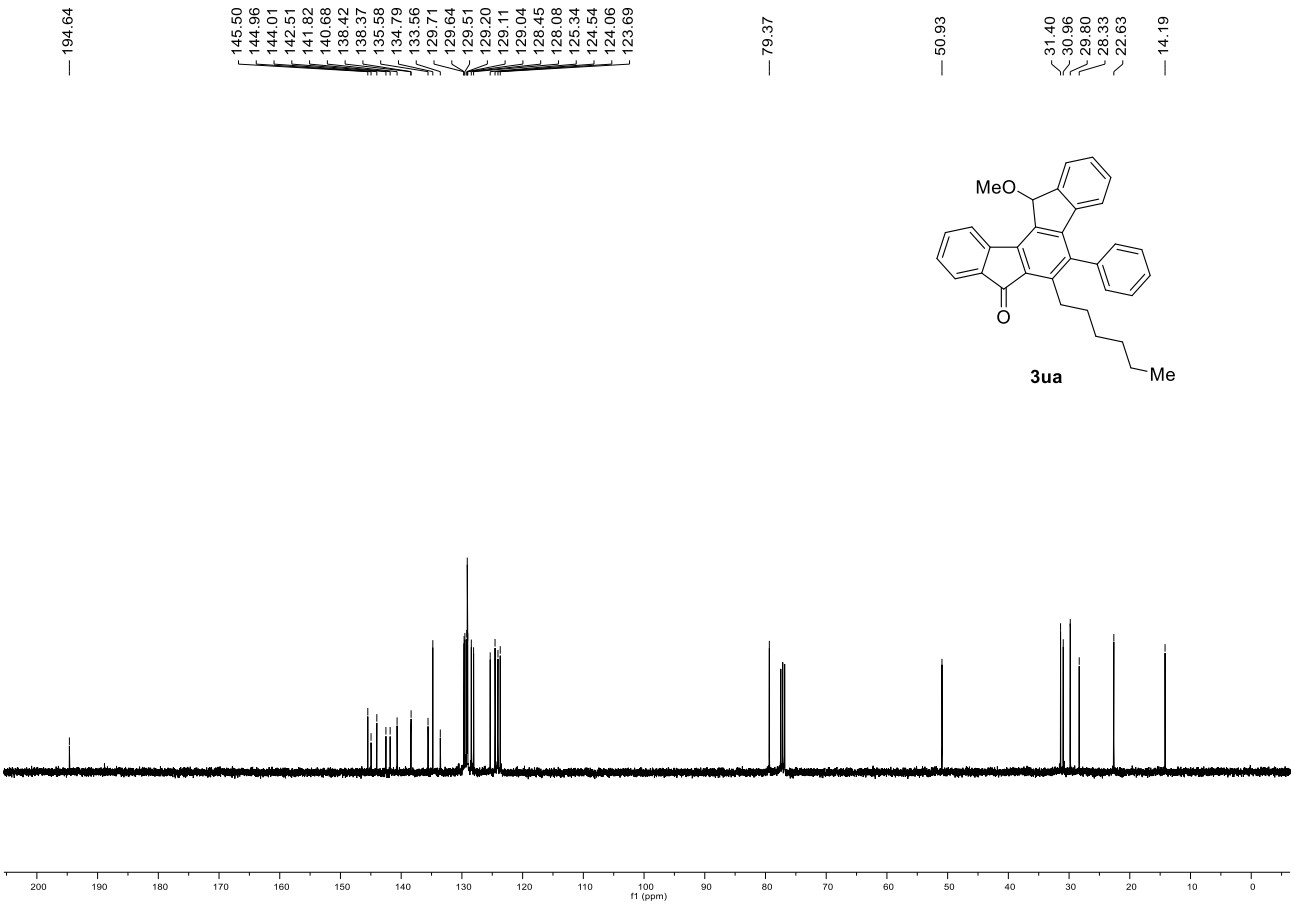
^{13}C NMR of **3ta** (100 MHz, $CDCl_3$)



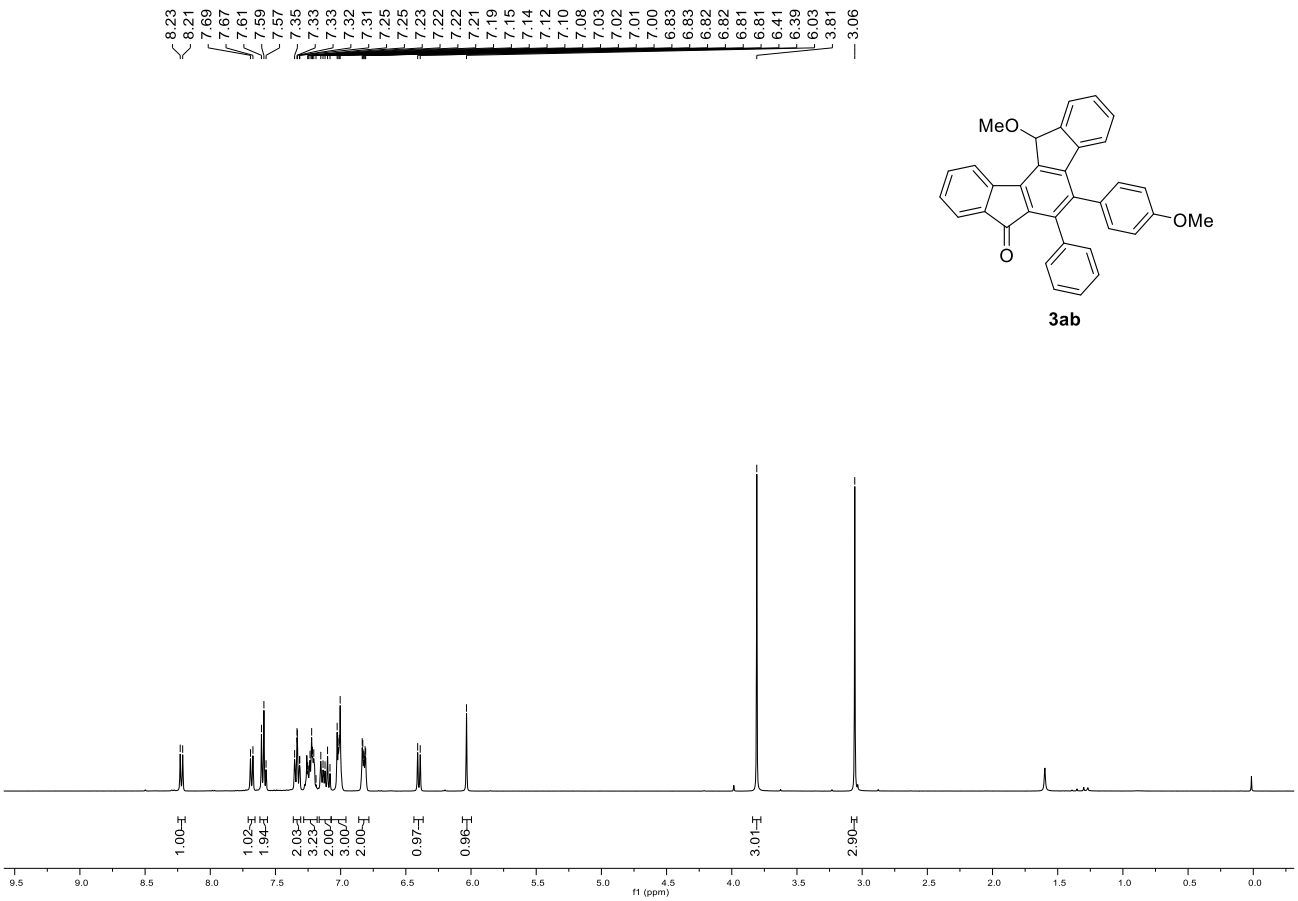
^{1}H NMR of **3ua** (400 MHz, $CDCl_3$)



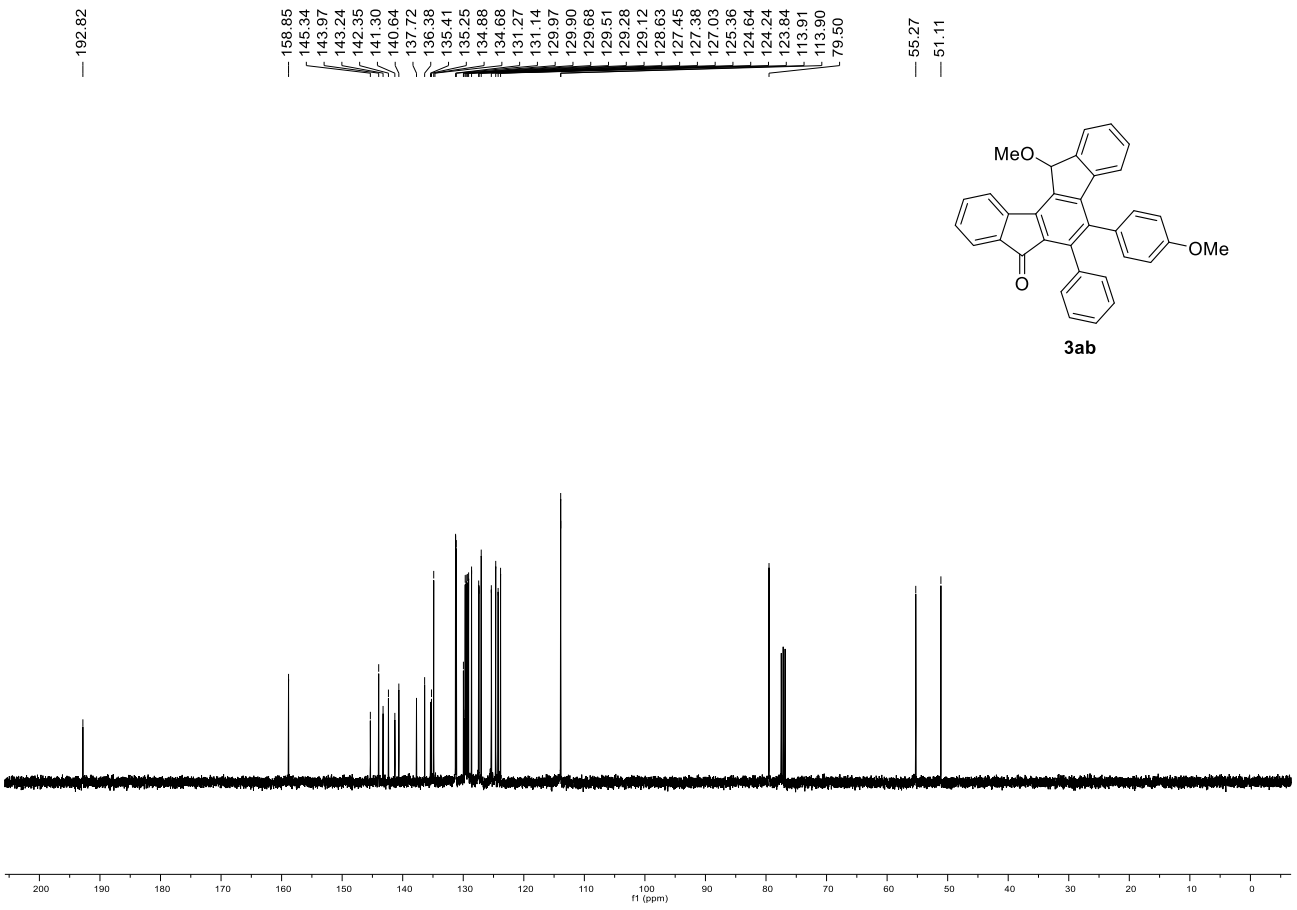
^{13}C NMR of **3ua** (100 MHz, $CDCl_3$)



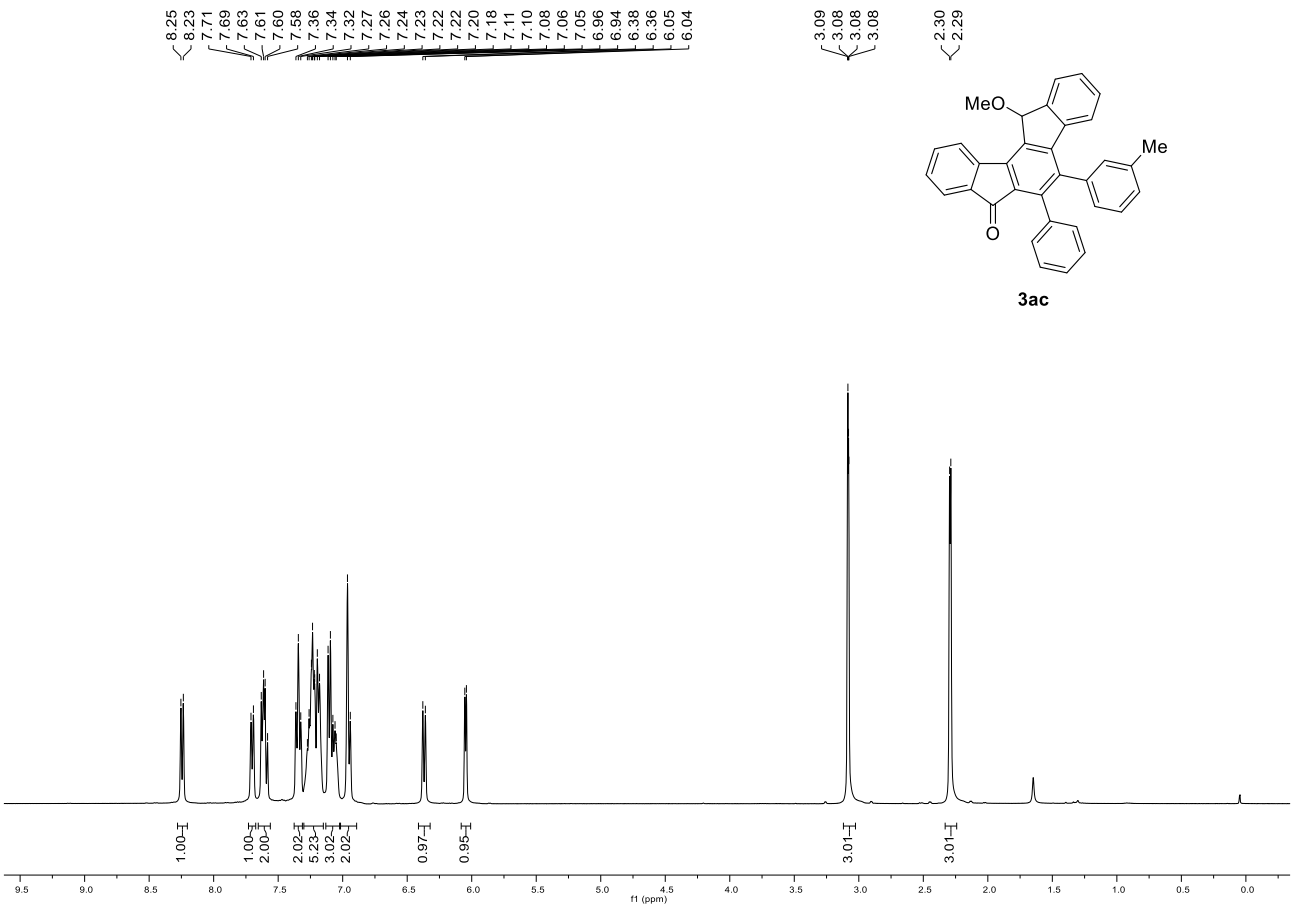
^{1}H NMR of **3ab** (400 MHz, $CDCl_3$)



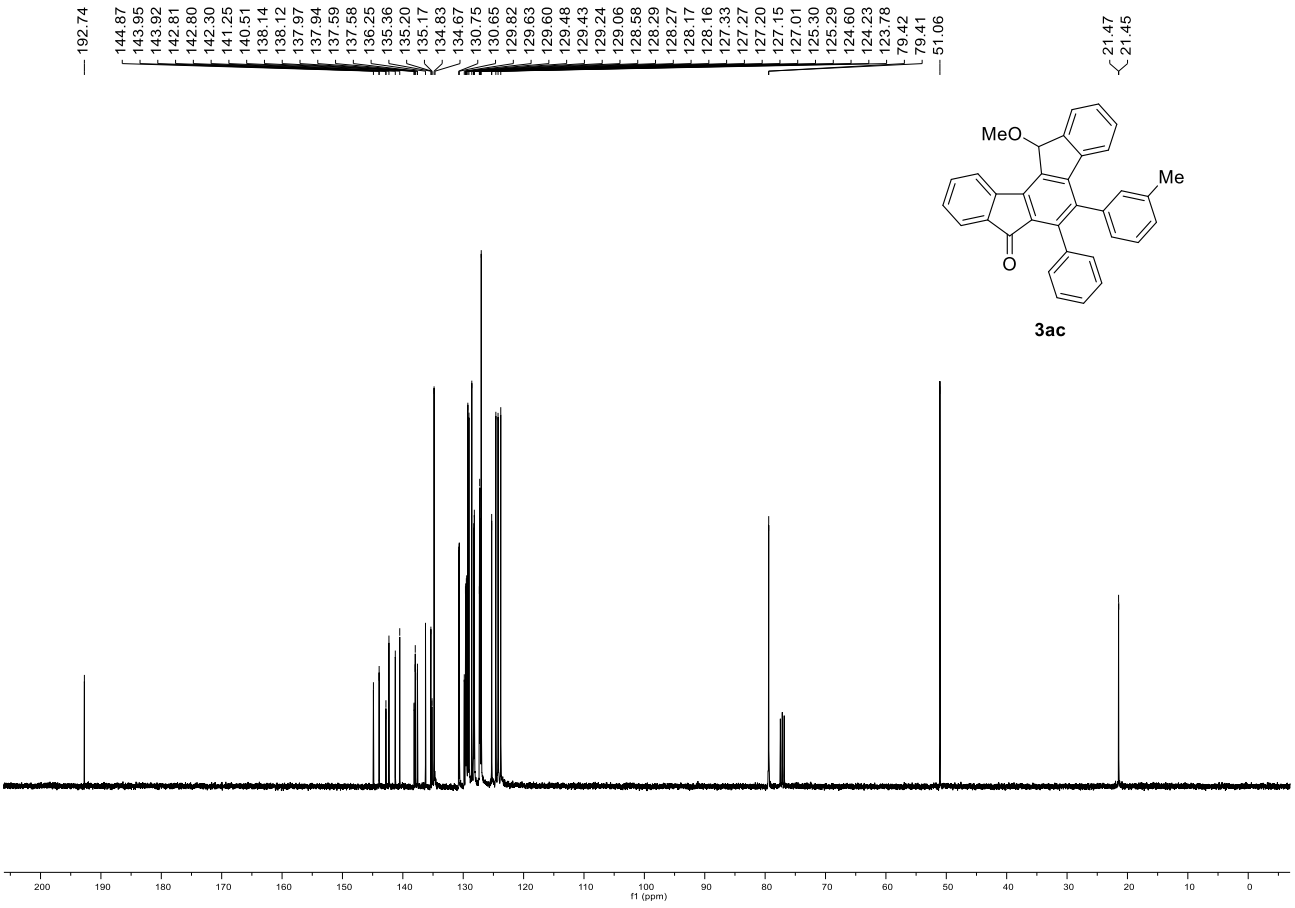
^{13}C NMR of **3ab** (100 MHz, $CDCl_3$)



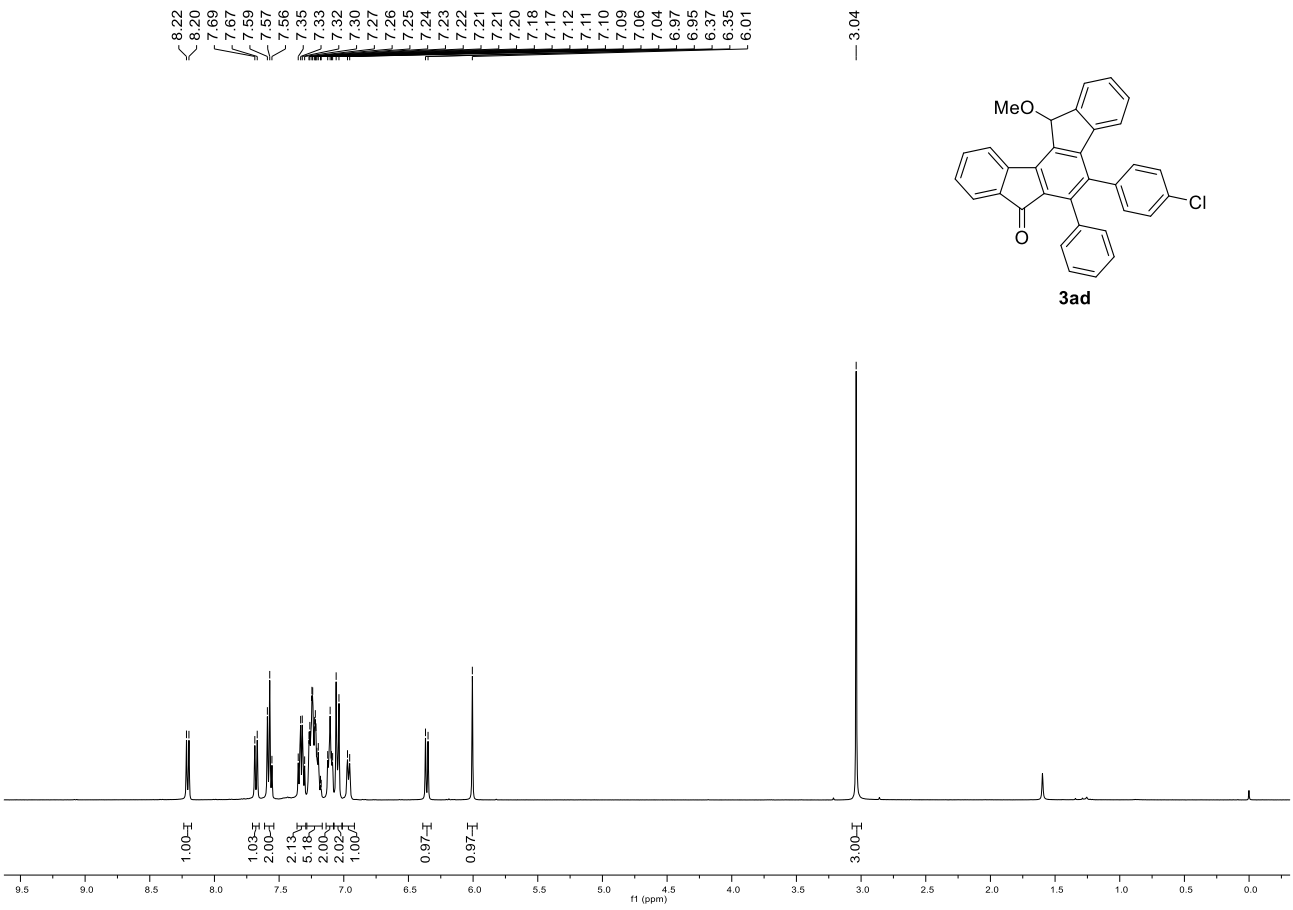
^{1}H NMR of **3ac** (400 MHz, $CDCl_3$)



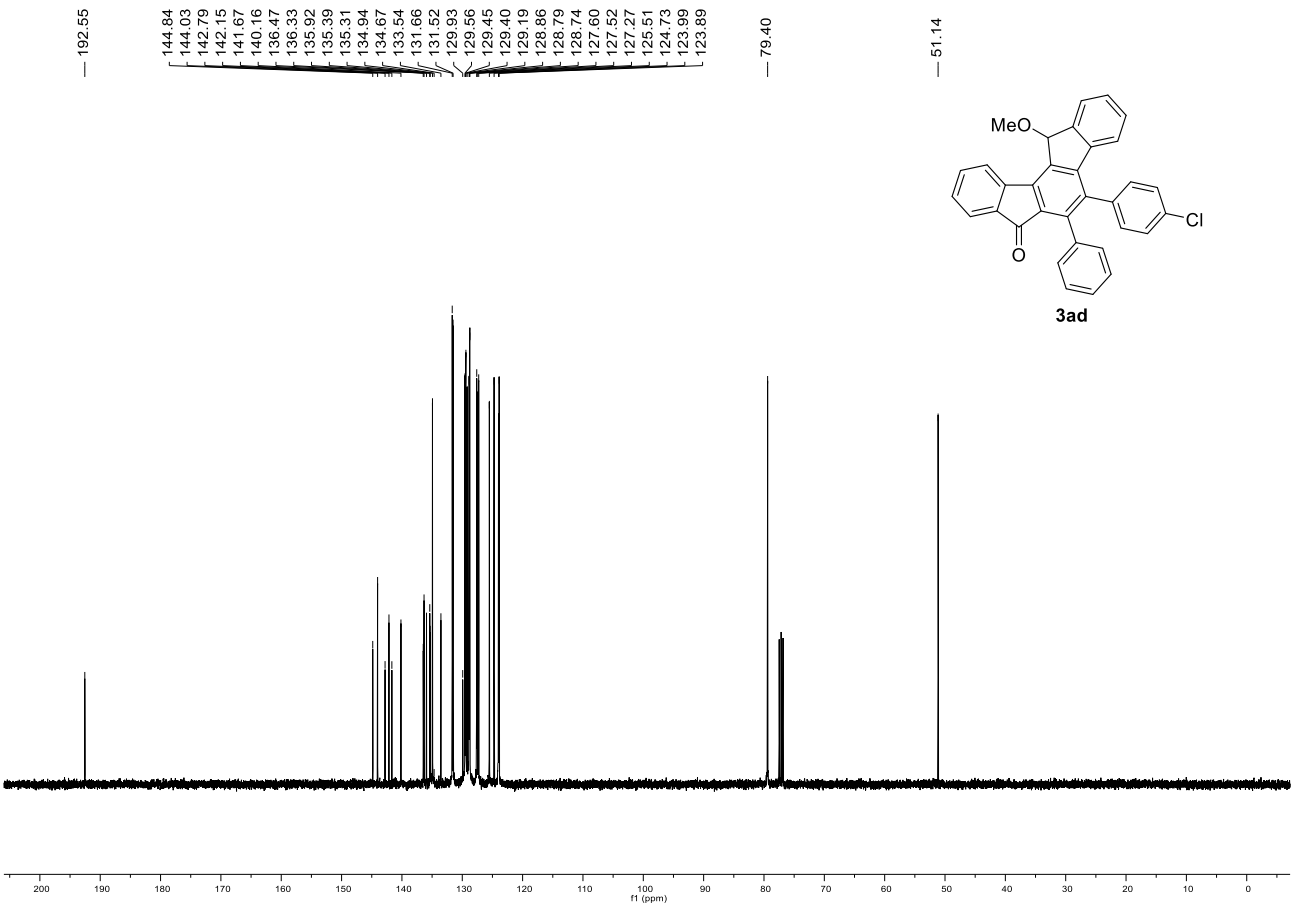
^{13}C NMR of **3ac** (100 MHz, $CDCl_3$)



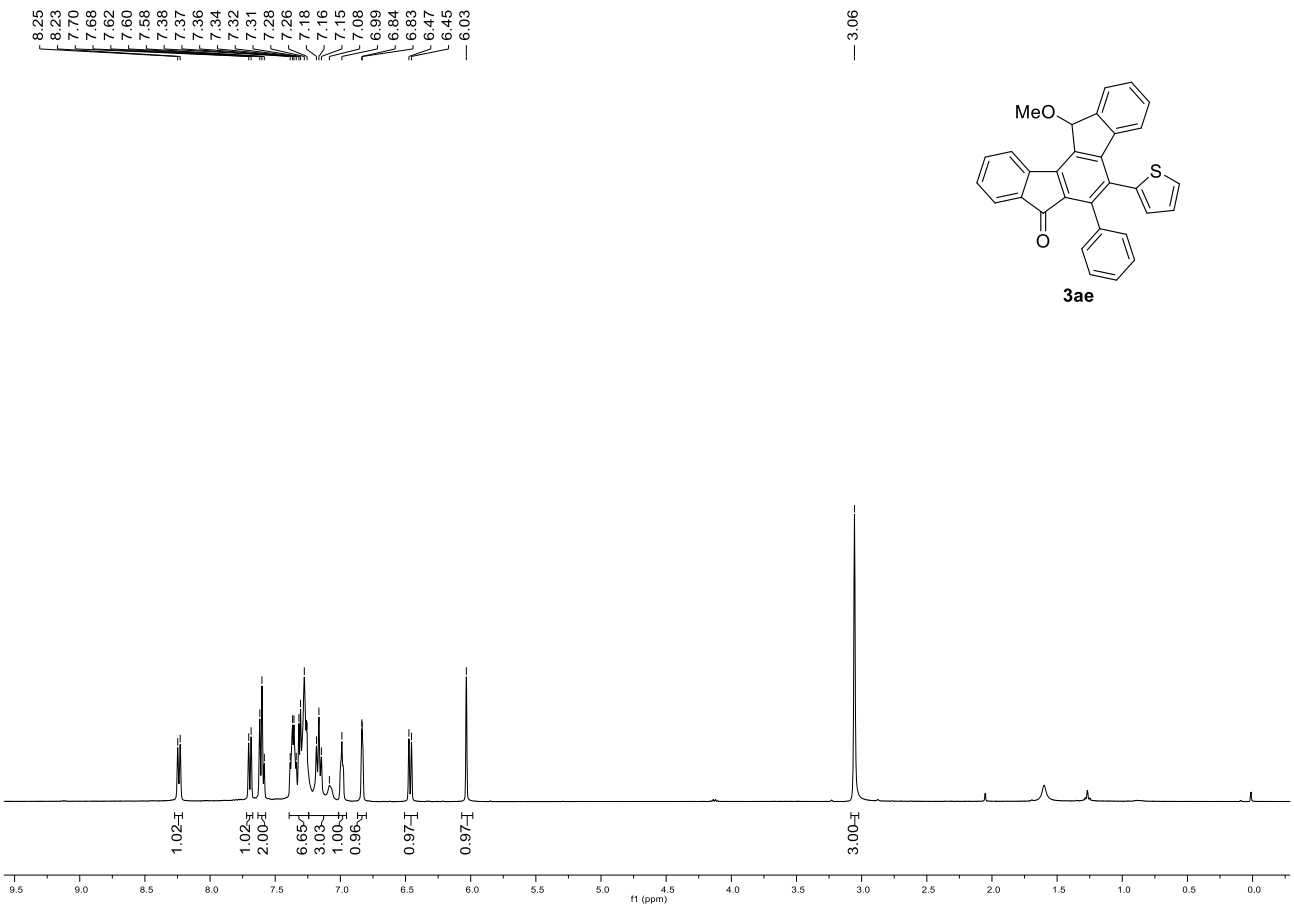
^{1}H NMR of **3ad** (400 MHz, $CDCl_3$)



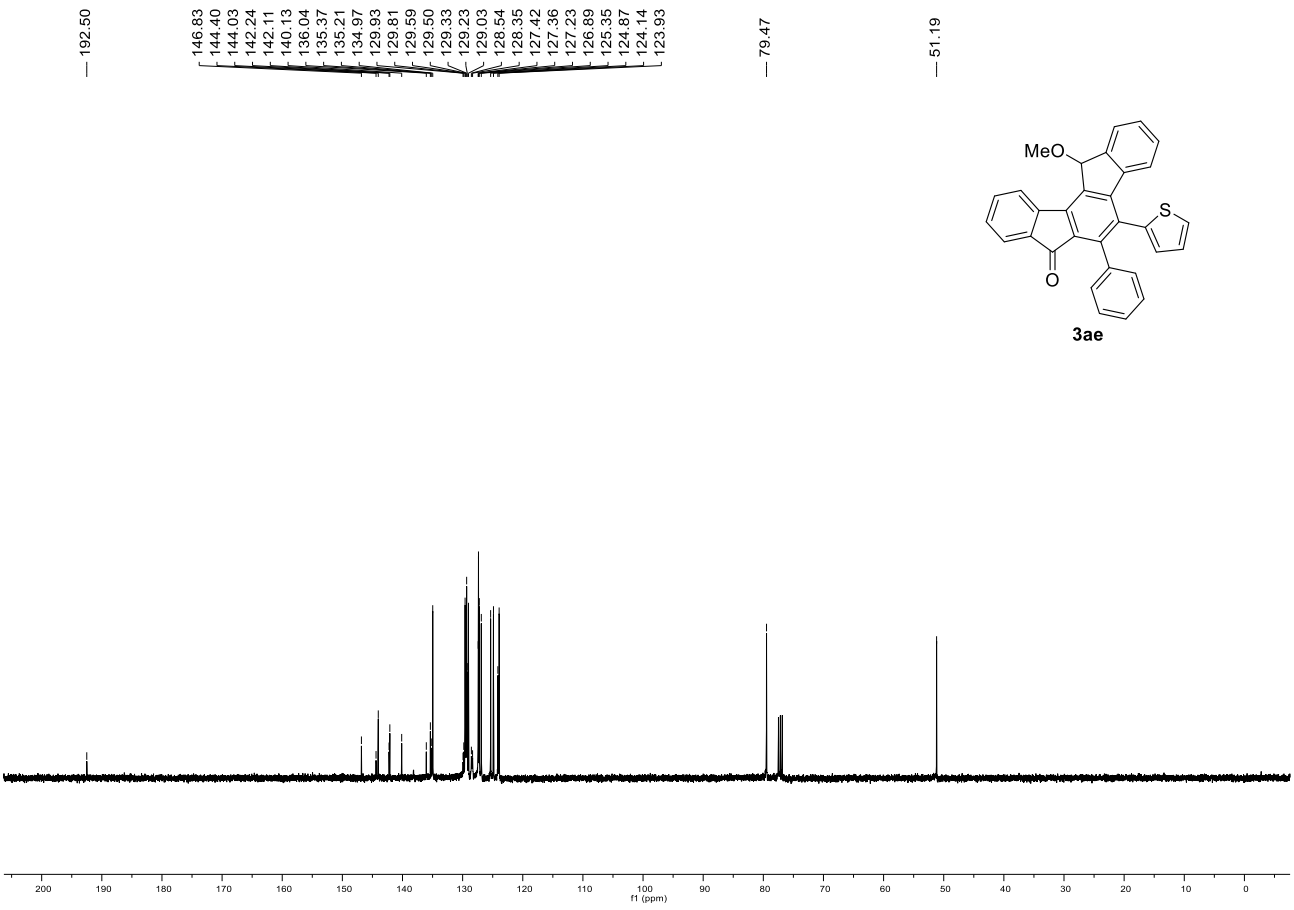
^{13}C NMR of **3ad** (100 MHz, $CDCl_3$)



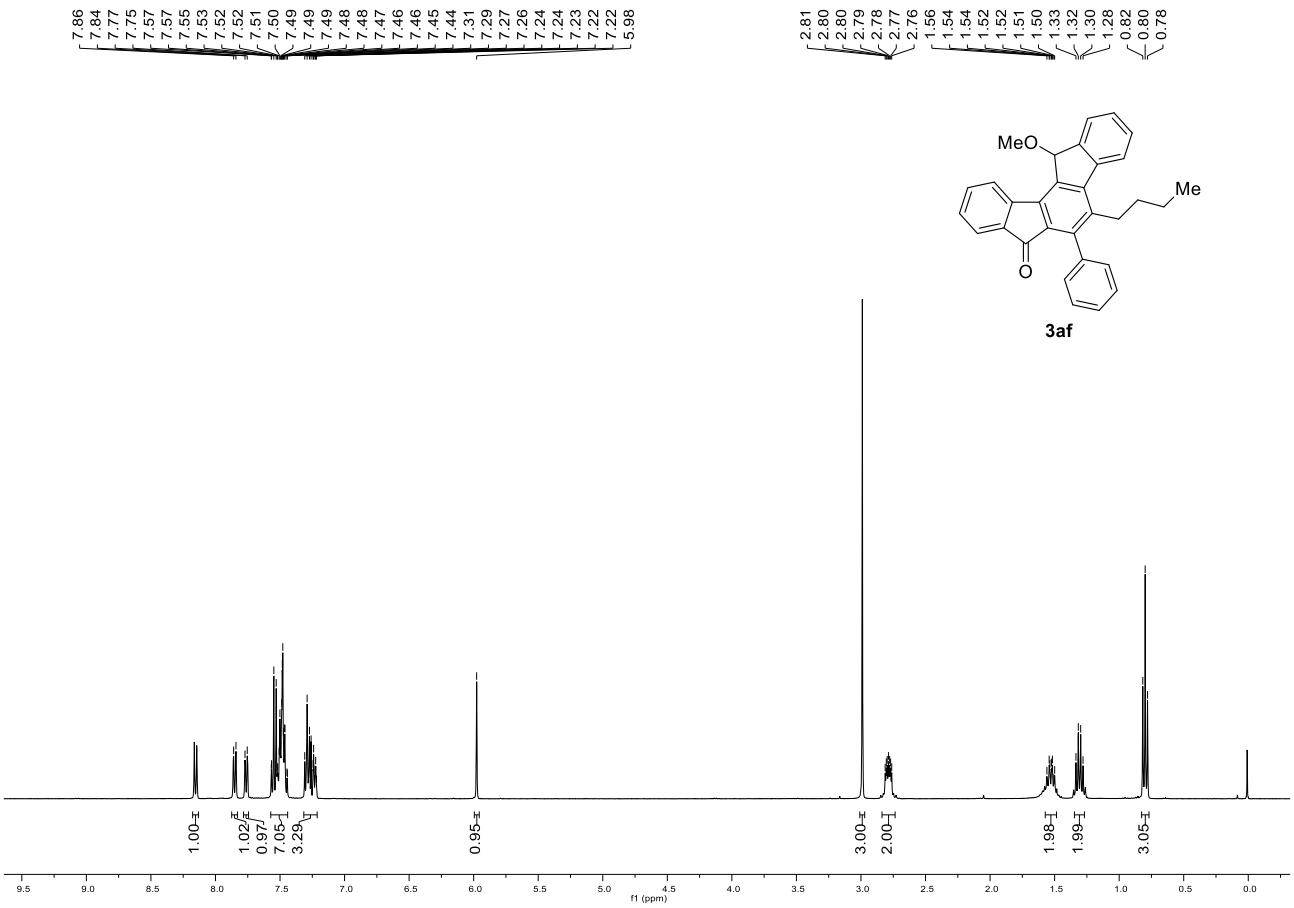
^{1}H NMR of **3ae** (400 MHz, $CDCl_3$)



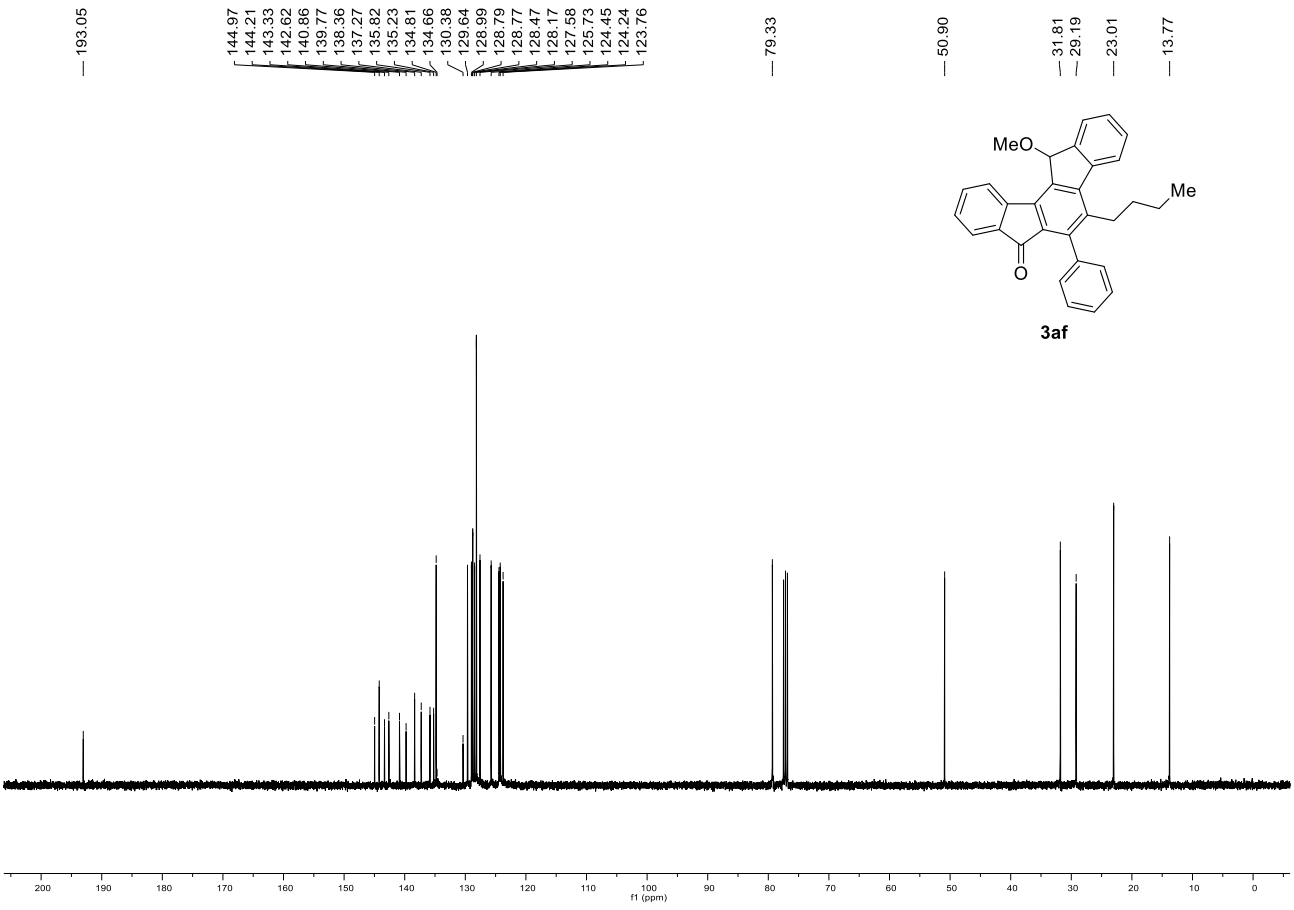
^{13}C NMR of **3ae** (100 MHz, $CDCl_3$)



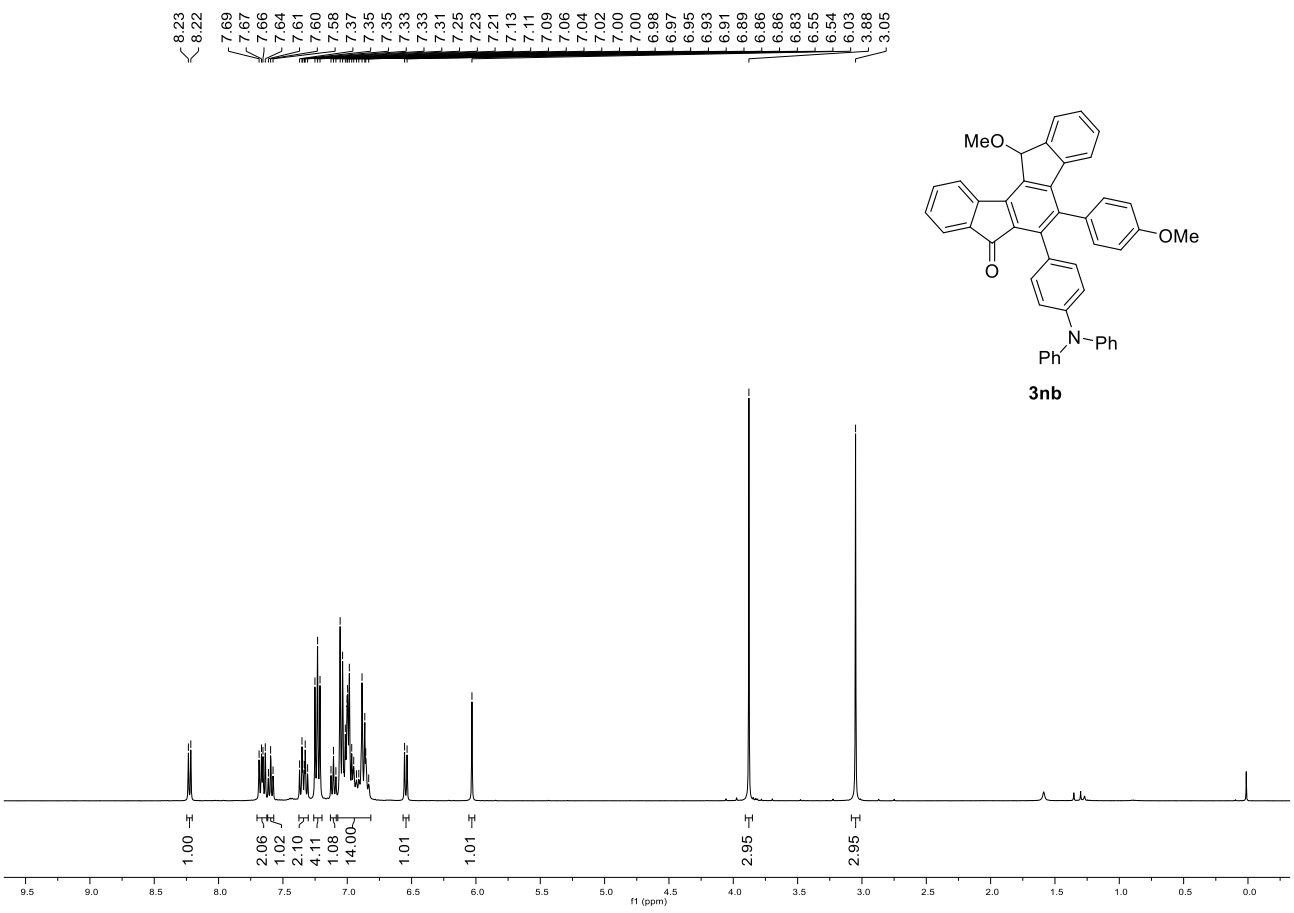
^{1}H NMR of **3af** (400 MHz, $CDCl_3$)



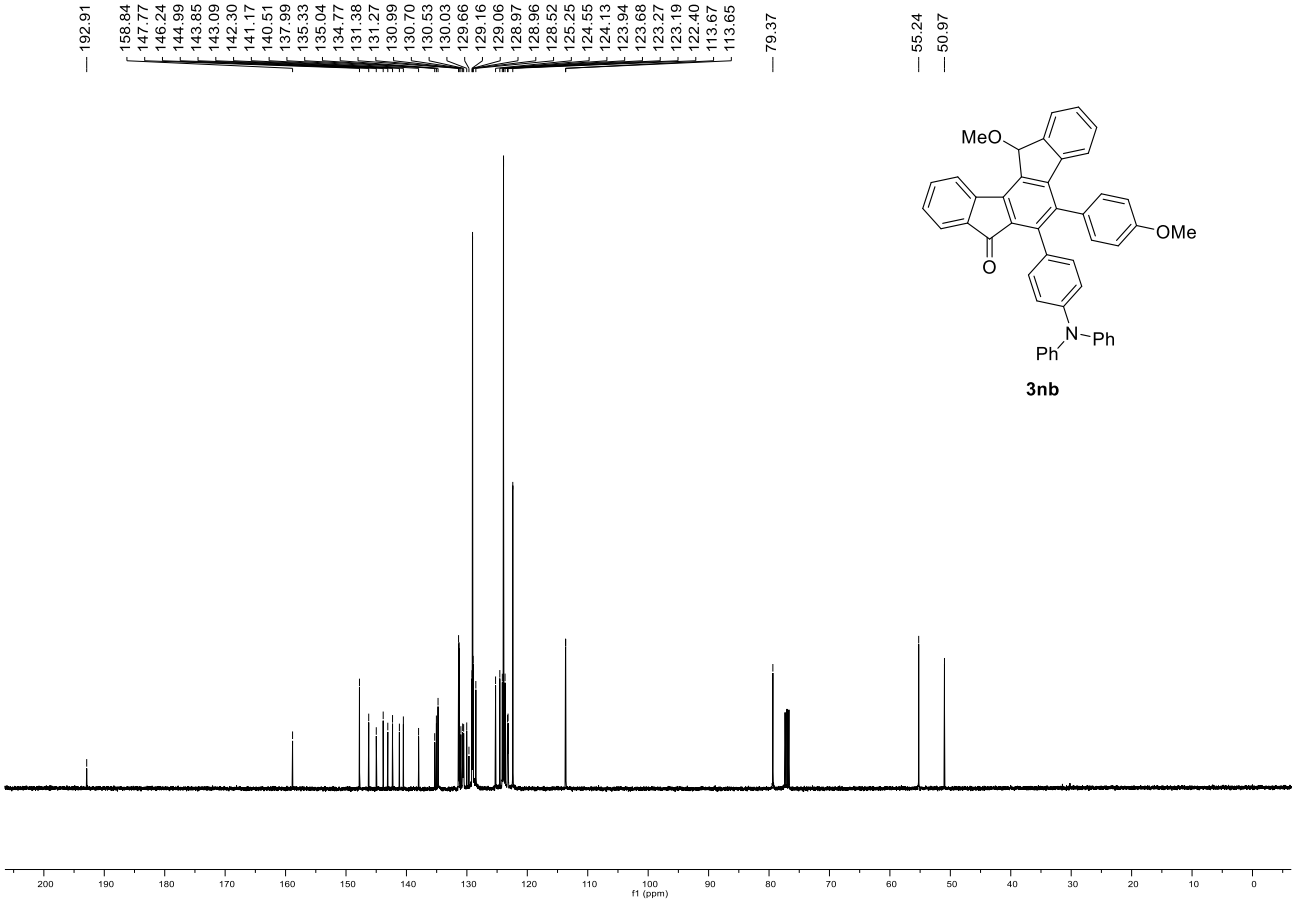
^{13}C NMR of **3af** (100 MHz, $CDCl_3$)



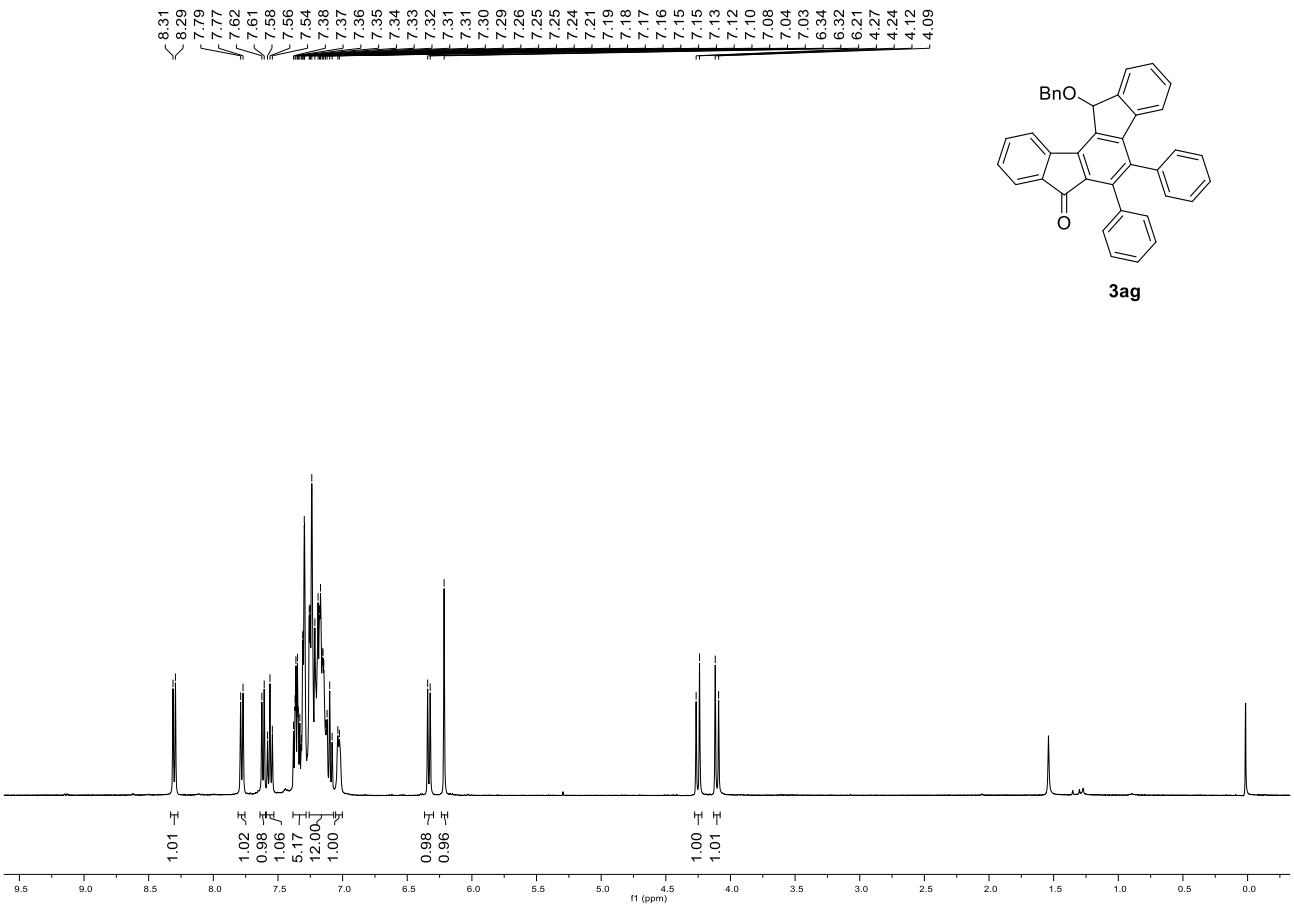
^{1}H NMR of **3nb** (400 MHz, $CDCl_3$)



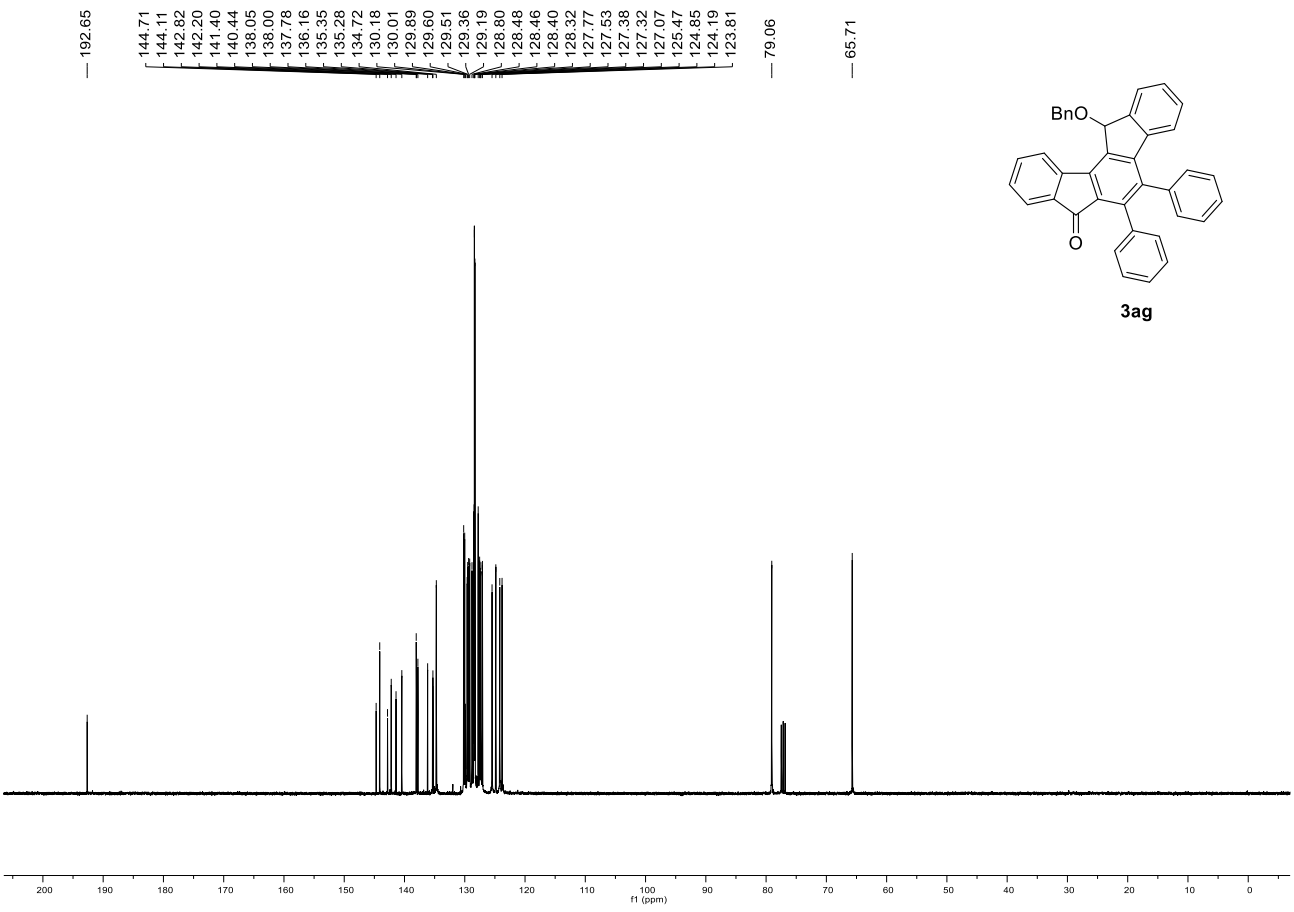
^{13}C NMR of **3nb** (100 MHz, $CDCl_3$)



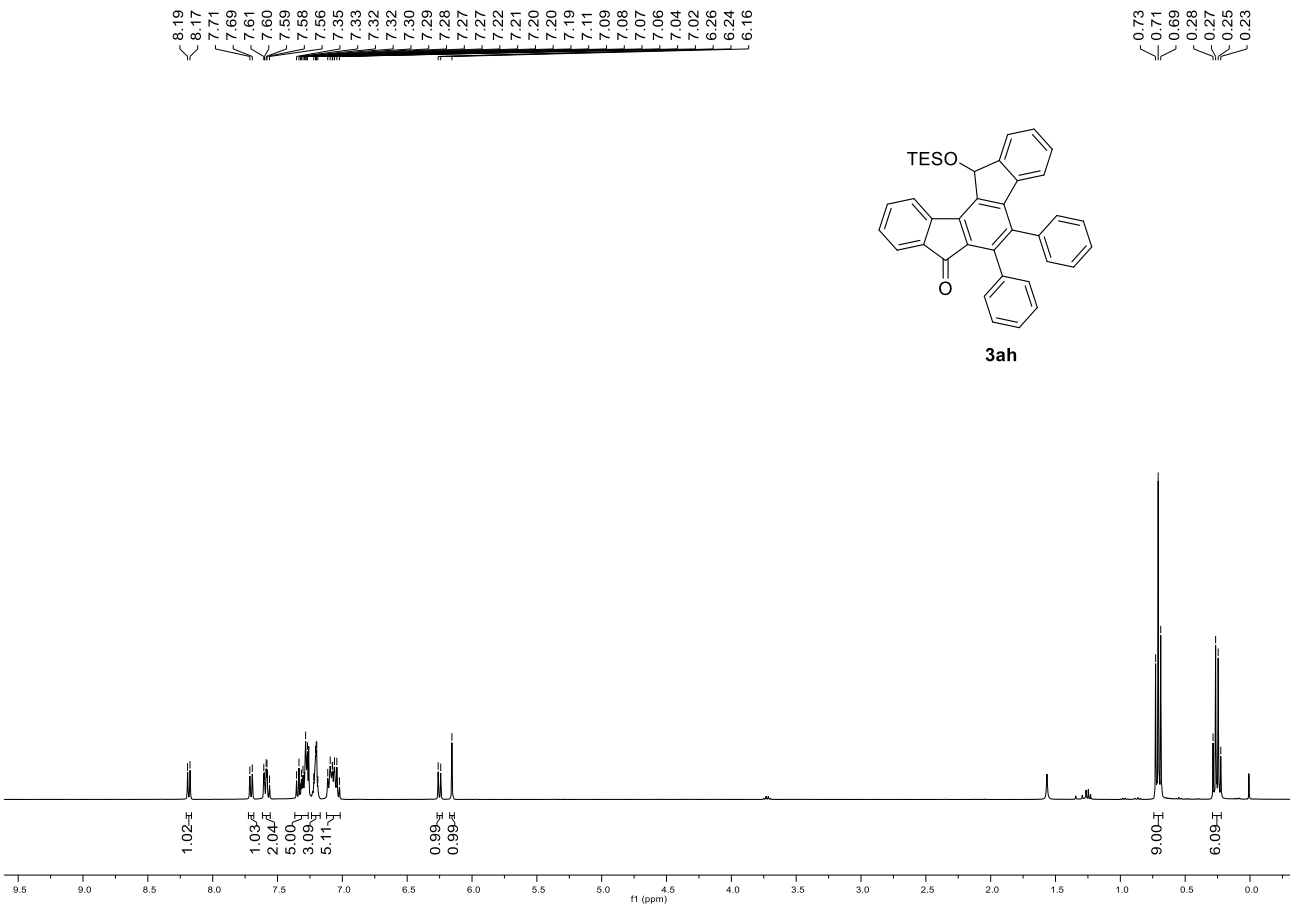
^{1}H NMR of **3ag** (400 MHz, $CDCl_3$)



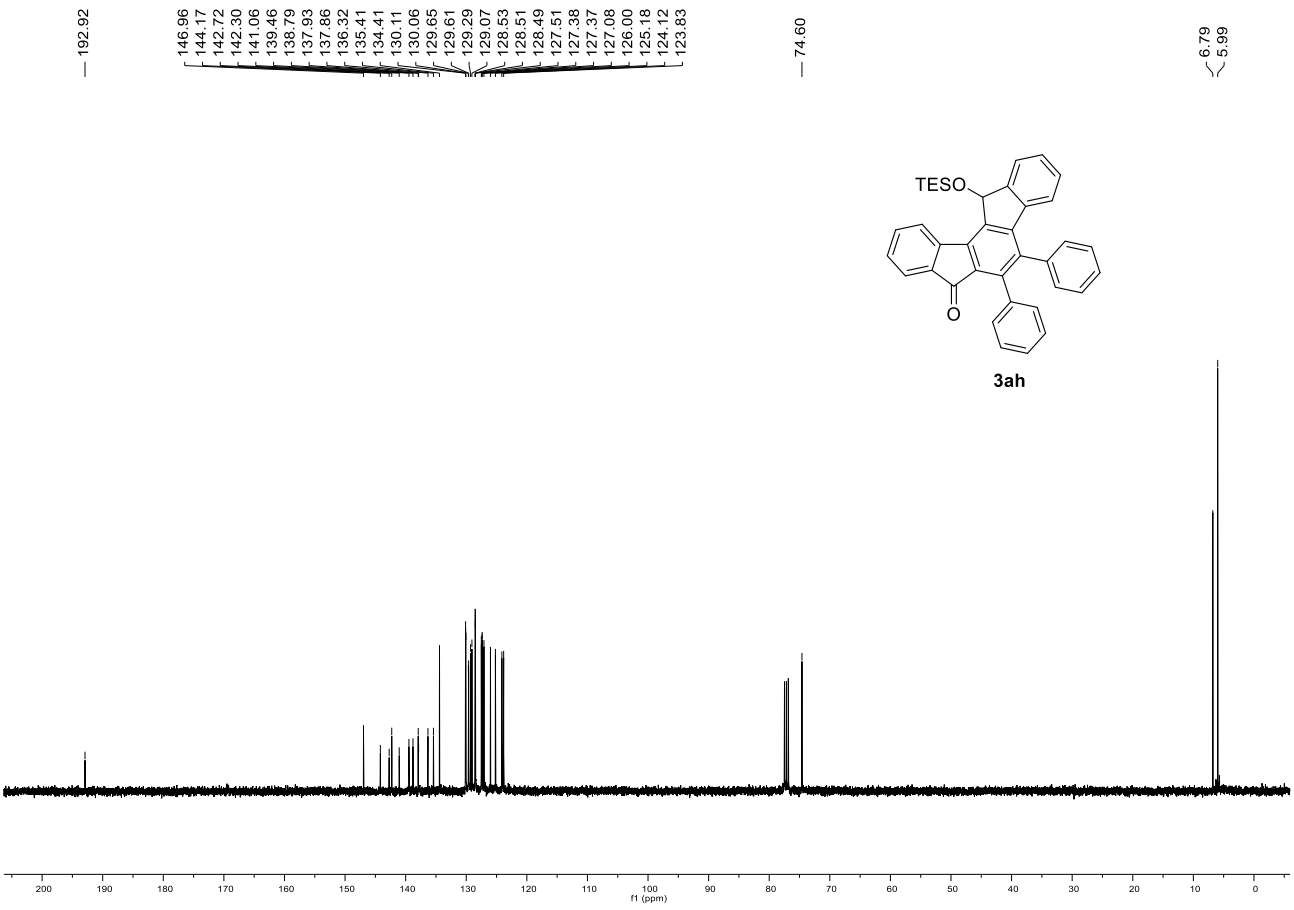
^{13}C NMR of **3ag** (100 MHz, $CDCl_3$)



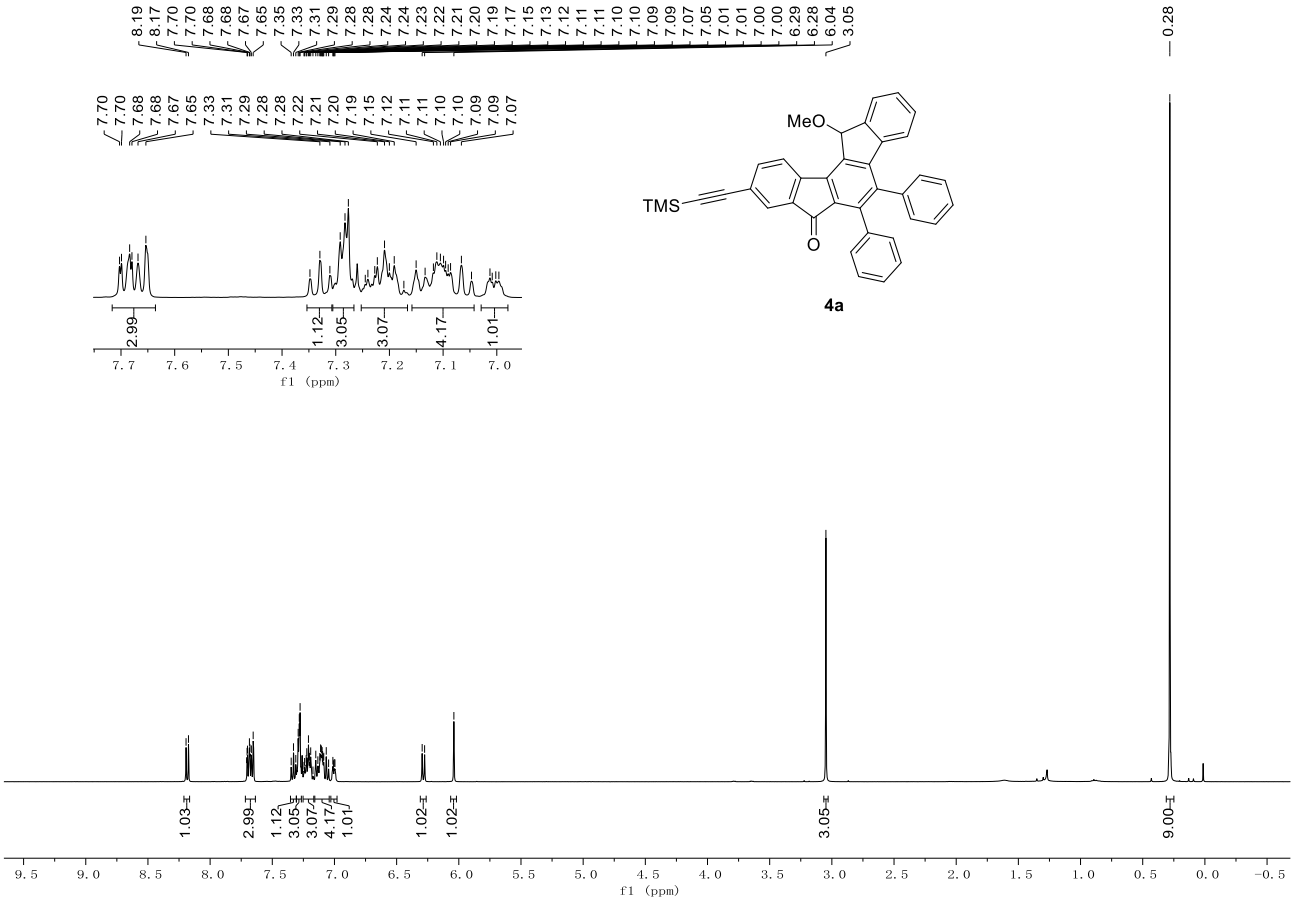
^{1}H NMR of **3ah** (400 MHz, $CDCl_3$)



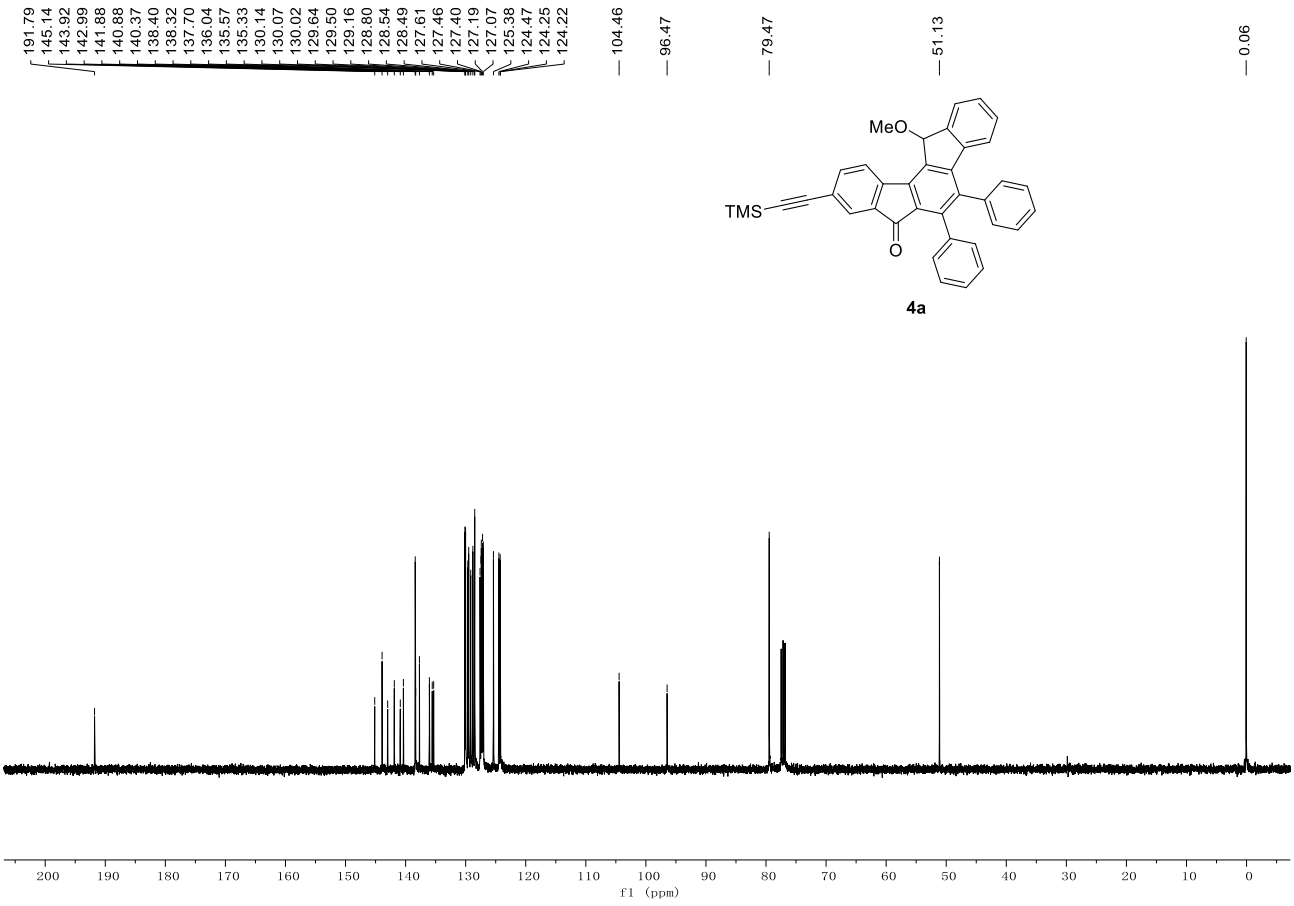
^{13}C NMR of **3ah** (100 MHz, $CDCl_3$)



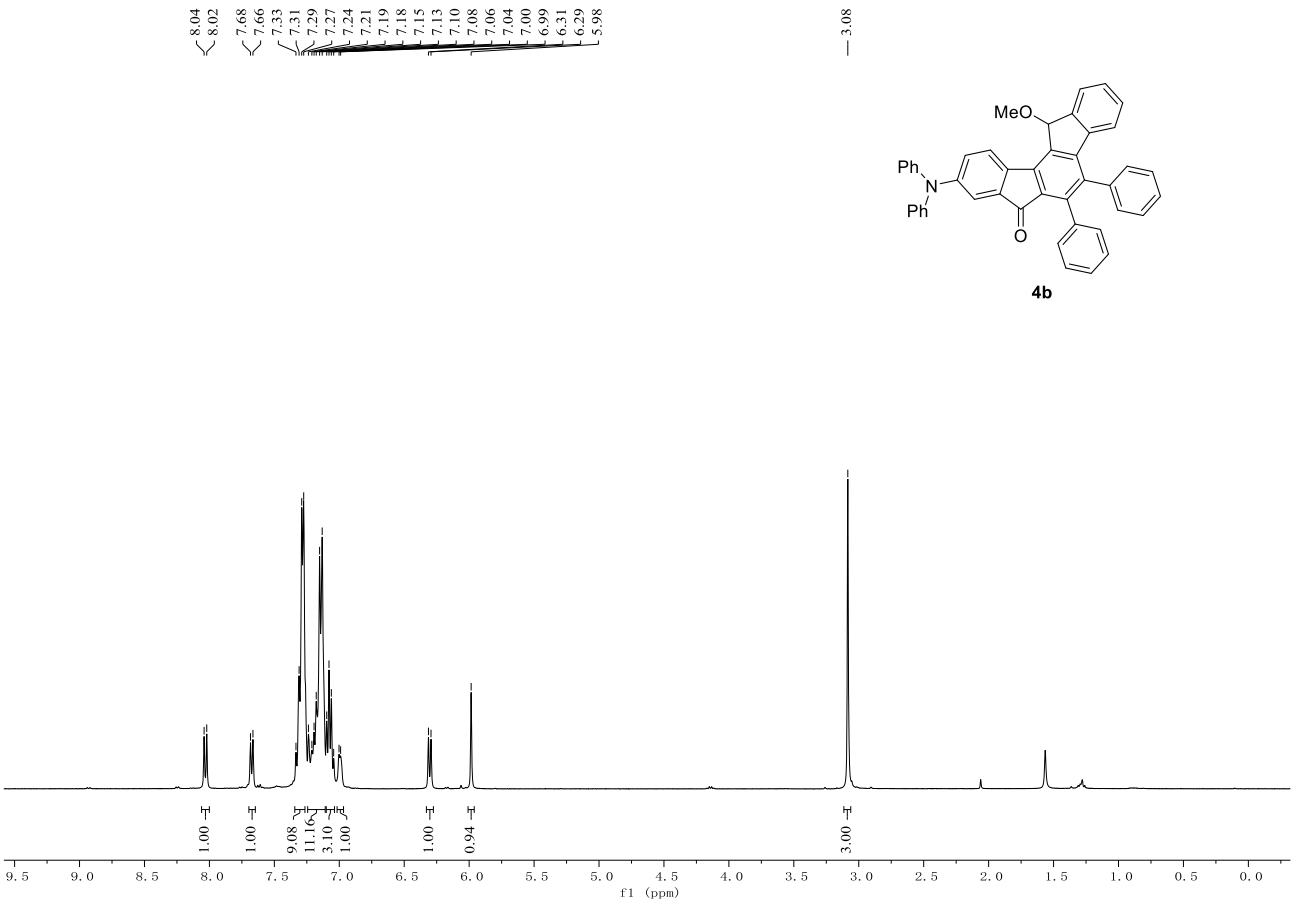
^{1}H NMR of **4a** (400 MHz, $CDCl_3$)



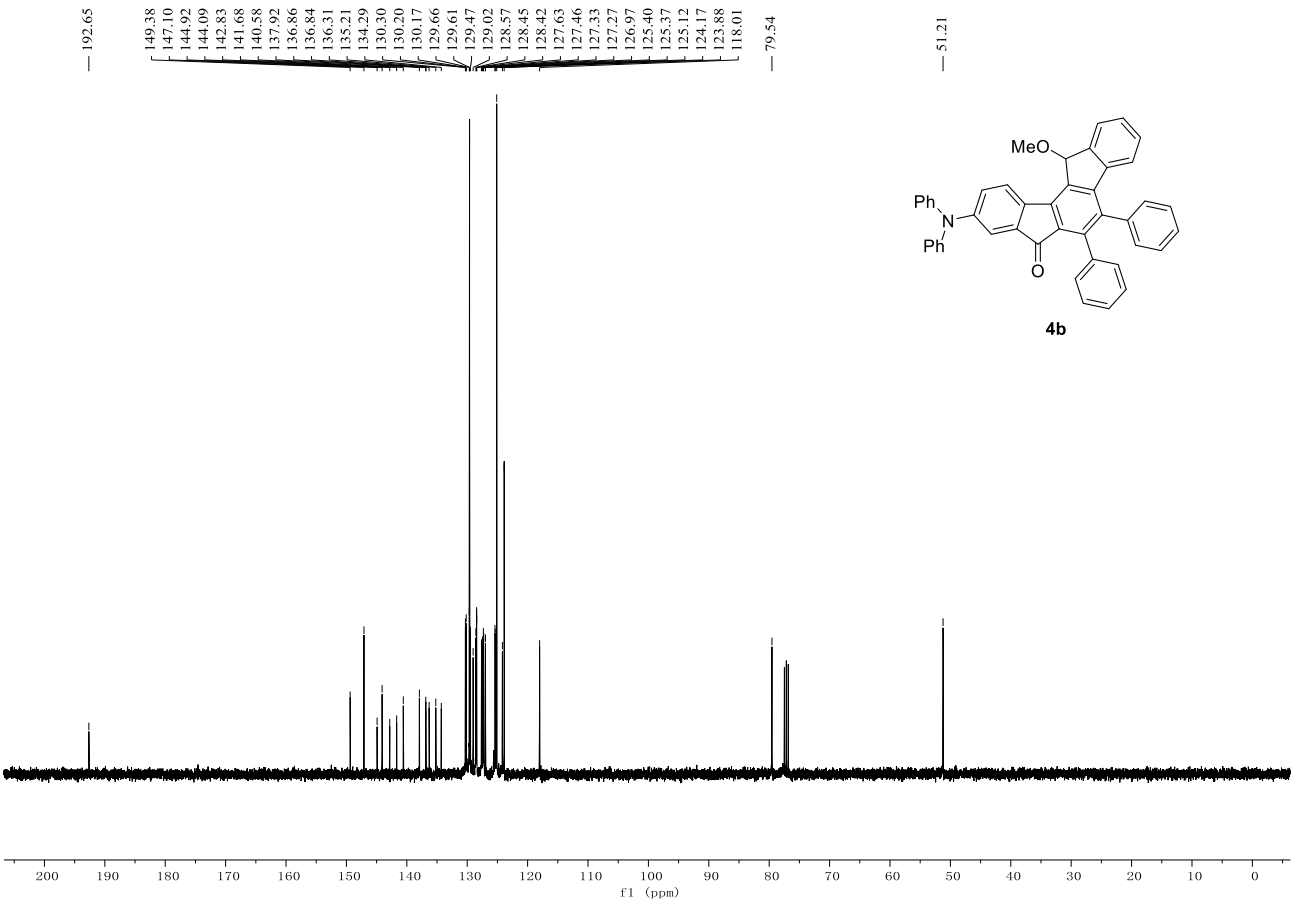
^{13}C NMR of **4a** (100 MHz, $CDCl_3$)



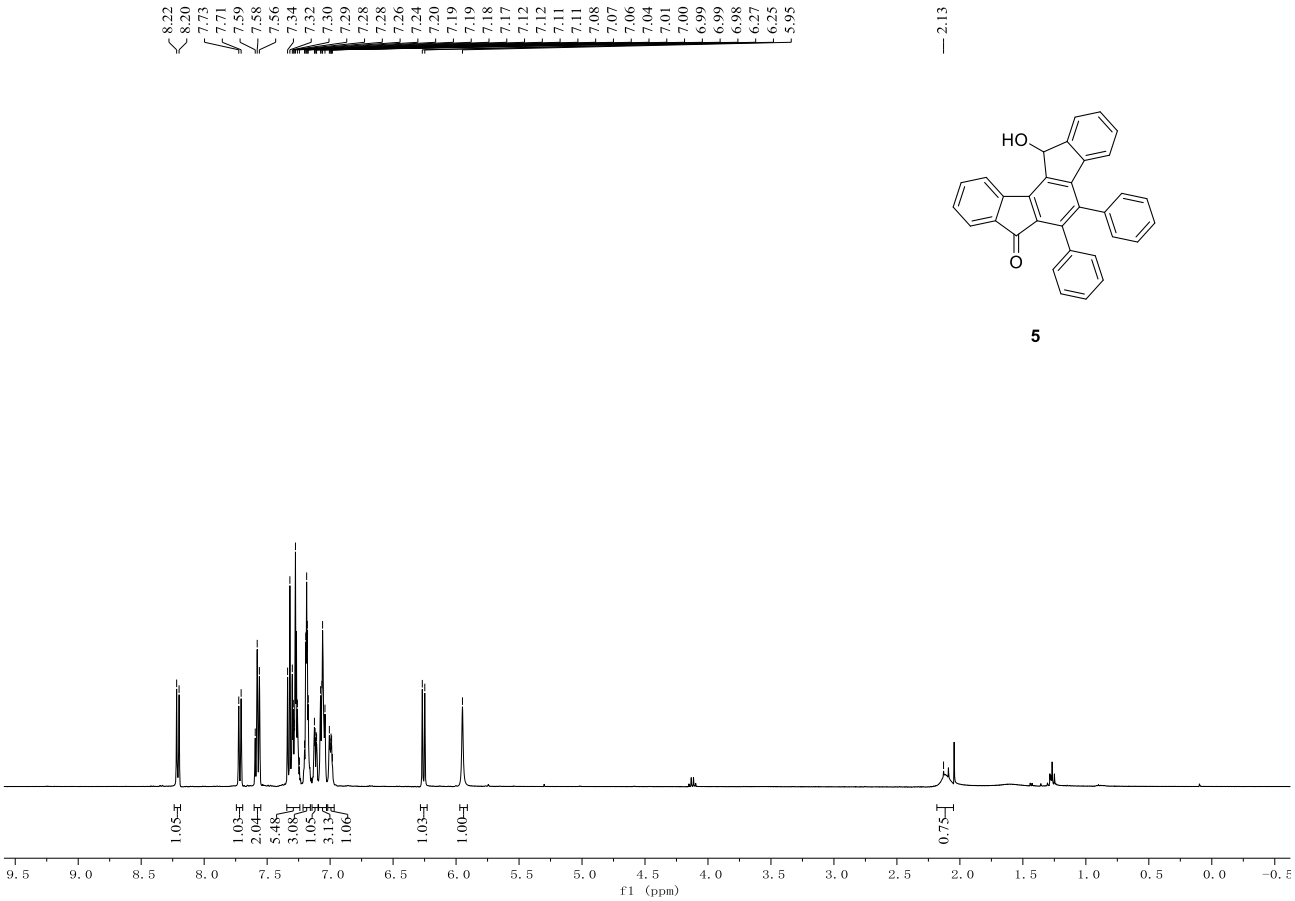
^{1}H NMR of **4b** (400 MHz, $CDCl_3$)



^{13}C NMR of **4b** (100 MHz, $CDCl_3$)

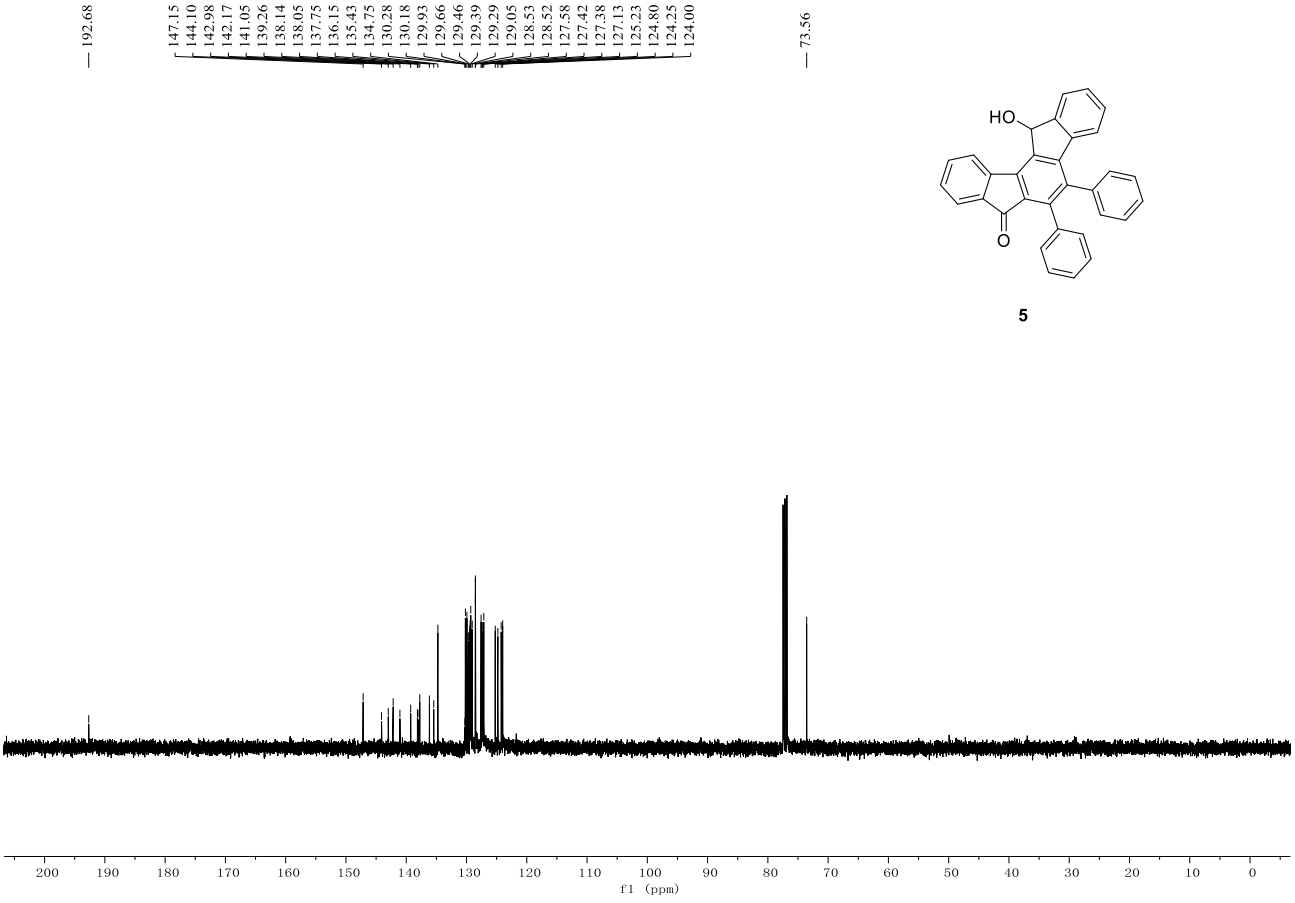


^{1}H NMR of **5** (400 MHz, $CDCl_3$)



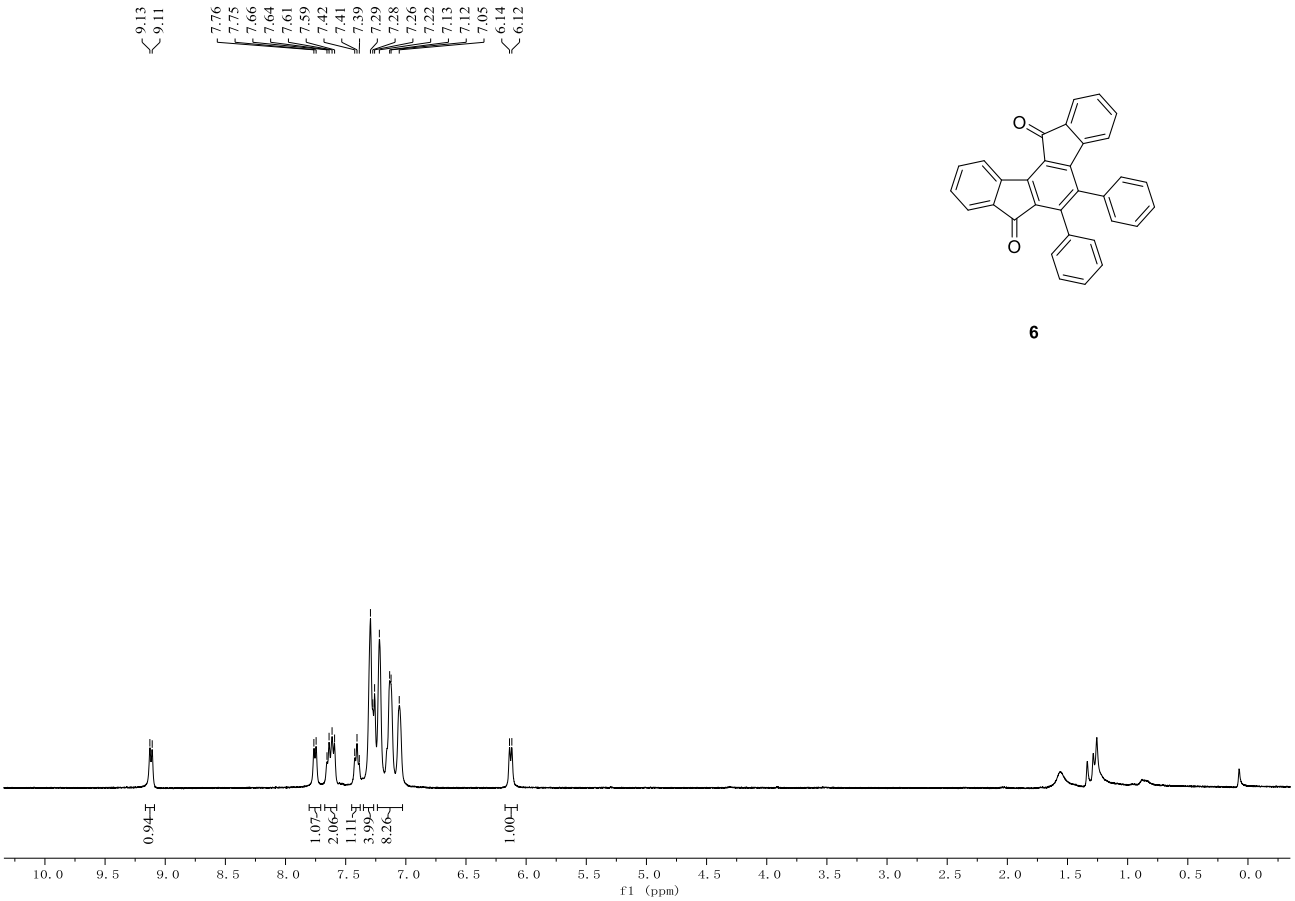
5

^{13}C NMR of **5** (100 MHz, $CDCl_3$)



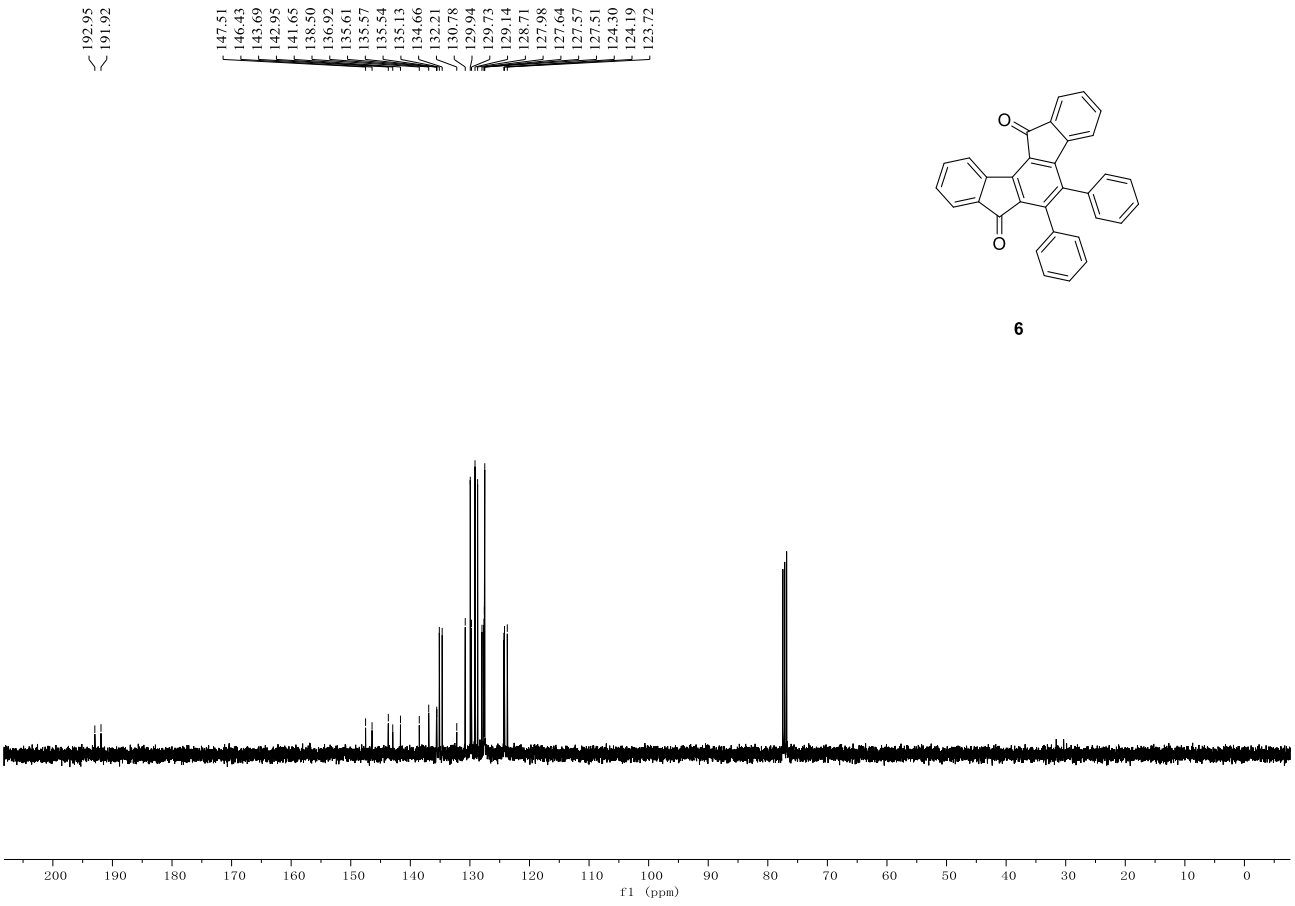
5

^{1}H NMR of **6** (400 MHz, $CDCl_3$)



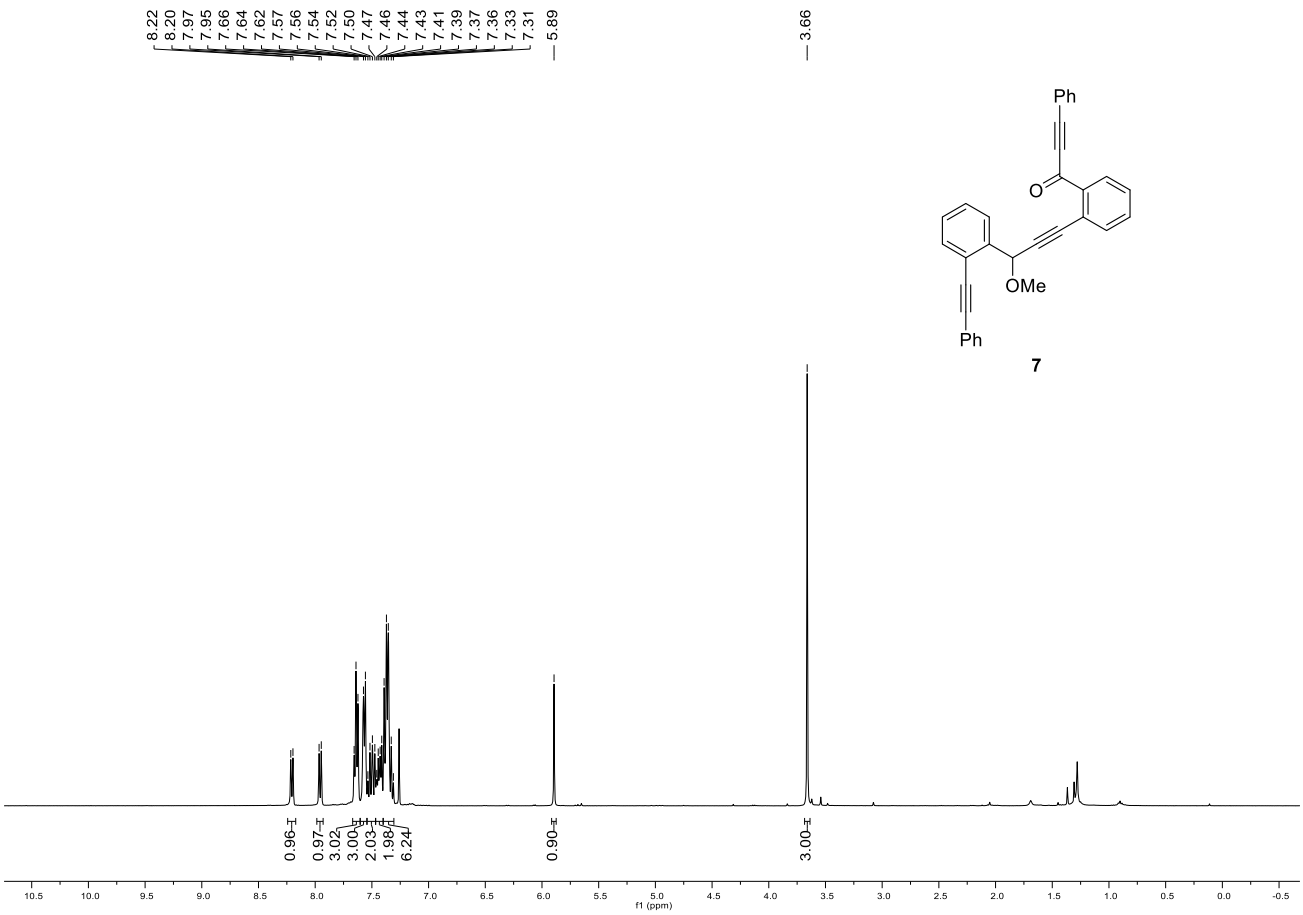
6

^{13}C NMR of **6** (100 MHz, $CDCl_3$)

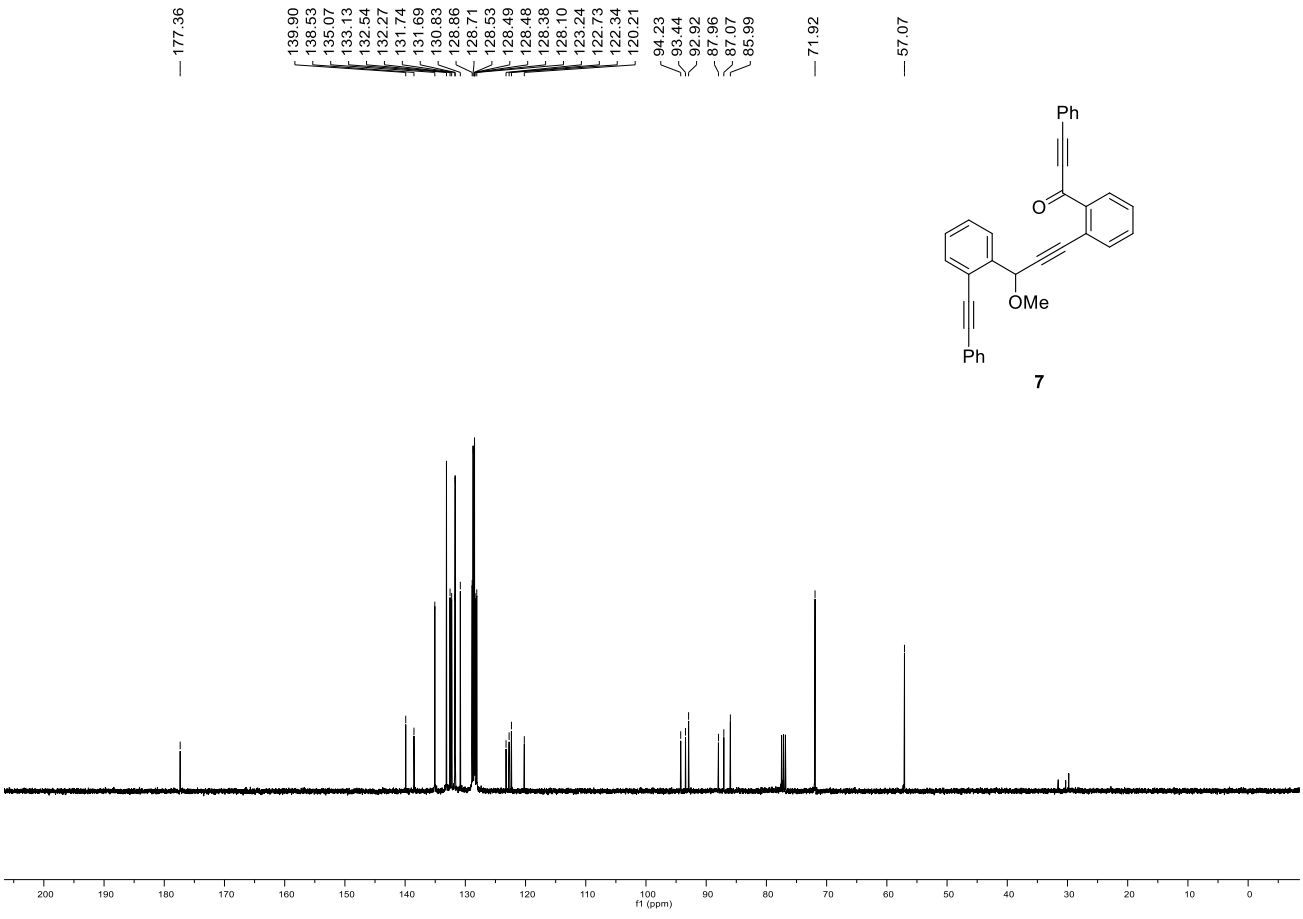


6

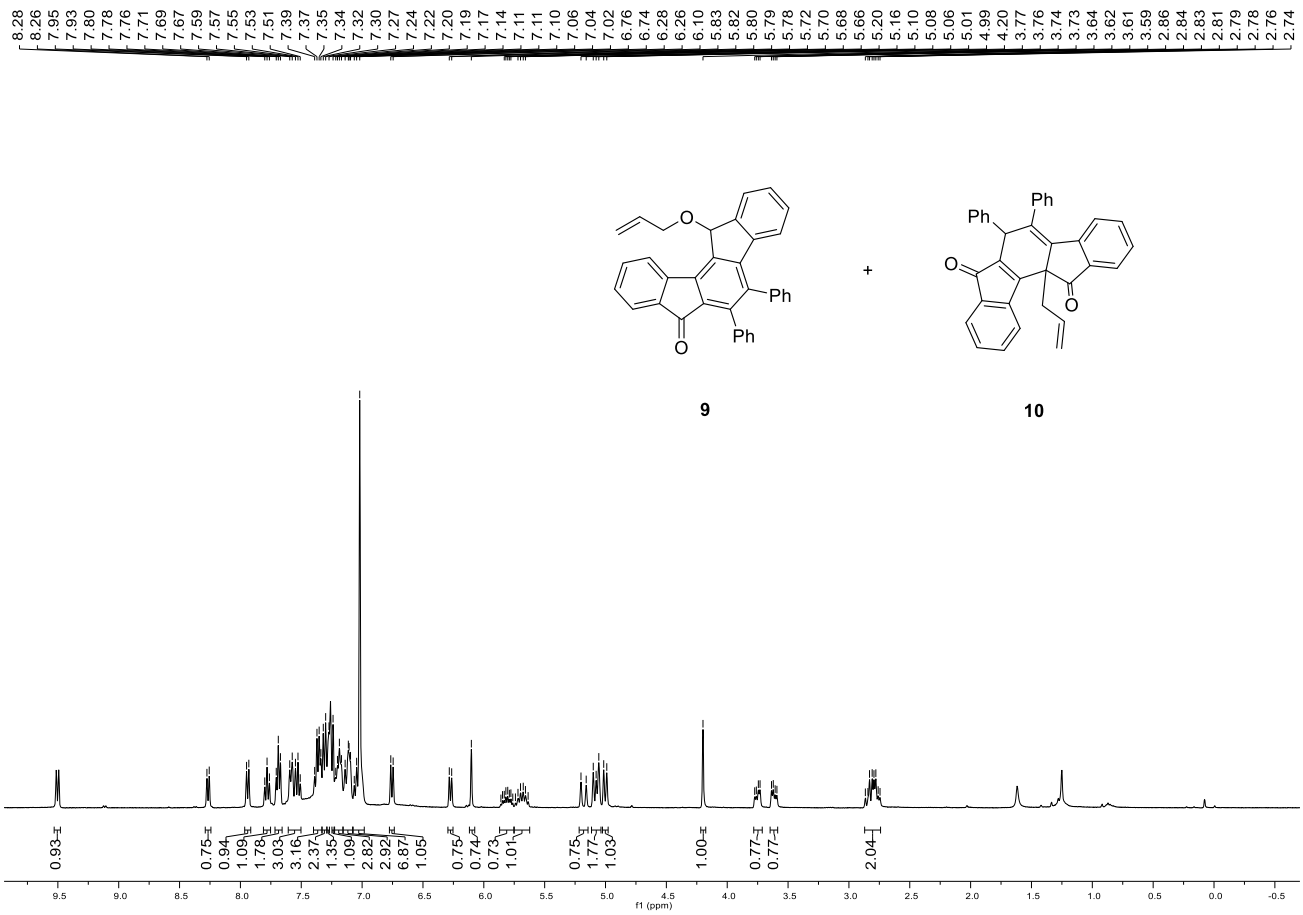
^{1}H NMR of **7** (400 MHz, $CDCl_3$)



^{13}C NMR of **7** (100 MHz, $CDCl_3$)



^{1}H NMR of **9 and 10** (400 MHz, $CDCl_3$)



^{13}C NMR of **9 and 10** (100 MHz, $CDCl_3$)