**SUPPLEMENTARY INFOREMATION for:**

# Dual-role Catalysis of Iridium in Photo-irradiation Synthesis of 9-Fluorenones through Intramolecular Cyclization via Hydrogen Evolution

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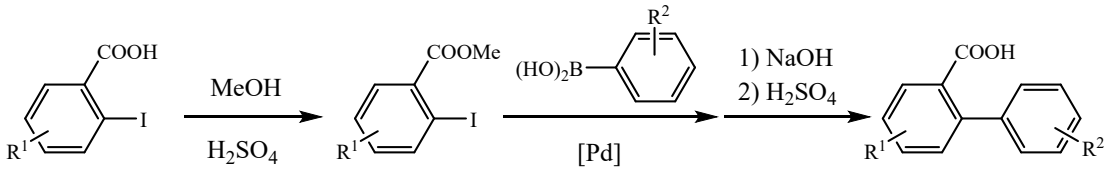
## Contents

# 1. General Considerations

All reaction procedures were carried out using standard Schlenk techniques under inert atmosphere ($N_2$) otherwise specified. Methyl 2-iodobenzoate derivatives, substituted boronic acids, and other inorganic agents were purchased from Aladdin and Macklin and used without further purification. Solvents were used as received. Photoredox catalyst ([$Ir(Fmpbo)_2dtbppy]SbF_6$, [$Ir(FFpbo)_2dtbppy]SbF_6$, [$Ir(NO_2mpbo)_2dtbppy]SbF_6$, [$Ir(dFtbpbo)_2dtbppy]SbF_6$, [$Ir(dFtbpbo)_2ppy]SbF_6$) were prepared in our previous works.[1] NMR spectra were recorded on Bruker 400 NMR spectrometers. $^1H$ NMR chemical shifts were referenced relative to the residual solvent resonances in the deuterated solvent. GC-MS spectra were recorded on a PE680-ST8 spectrometer. HRMS spectra were recorded on a Bruker McriOTOF11 spectrometer. GC spectra for atmosphere analysis were recorded on a Fuli GC-9790 Plus spectrometer with a TCD detector. The light source for visible-light irradiation (SMD 2835 LED, $\lambda_{em}$ 465~467.5 nm, 220V， 5W) was purchased from general commercial sources.

## 2. Preparation of biphenyl carboxylic acids.

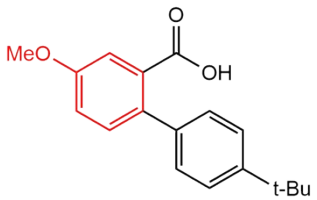



**Preparation of Methyl 2-iodobenzoate derivatives.** [2] The 2-iodobenzoic acid derivatives (1 eq.) were dissolved in 50 mL MeOH in a 100 mL flask. To the stirred solution, 2.3 mL of concentrated $H_2SO_4$ was added dropwise. The mixture was then stirred and heated under 75℃ for 4 hours. After cooled to room temperature, $NaHCO_3$ (3.5 g) was added in batches. The solvent was then condensed in vacuo. The residue was dissolved in 10 mL EtOAc, and washed with saturated aqueous $NaHCO_3$ (3×15 mL). The organic phase was dried over Na2SO4, filtered and the solvent was removed in vacuo to afford a light-yellow oil, which was used in the following step without further purification.

**Preparation of Methyl [1,1′-Biphenyl]-2-carboxylate.** [3] Into a flask filled with a 1.5 mL dioxane solution of methyl 2-iodobenzoate derivatives (0.35 mmol), aryl boronic acid (0.525 mmol, 1.5 eq.), $Pd(PPh_3)_2Cl_2$ (9.8 mg, 4 mol%) was added by 0.5 mL of aqueous potassium carbonate (290.2 mg/mL, 3 eq.). The mixture was then stirred at 100 ℃ under nitrogen protection for 12 hours. After cooled to room temperature, the mixture was washed with brine (5mL) and extracted with EA (5 mLx2). Then the combined organic layers were dried over $Na_2SO_4$ and concentrated. The crude product was purified by column chromatography (PE:EA = 25:1) to afford methyl [1,1′-Biphenyl]-2-carboxylate derivatives as colorless oil.

**Deprotection of Carboxyl Group.** The methyl [1,1′-Biphenyl]-2-carboxylate derivatives was dissolved in 1.5 mL MeOH and aqueous NaOH (50 mg in 1.5 mL $H_2O$) was added. The mixture were heated at 50 ℃ overnight, and condensed in vacuo. The residue was added with 4 mL 1M HCl and stirred rigorously for 30 minutes and then filtered, and washed by water (3×3 mL). The filtered residue was dissolved with EtOAc (15 mL) and dried over $MgSO_4$ and concentrated in vacuo to give the product.

**4'-(*tert*-butyl)-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid.**

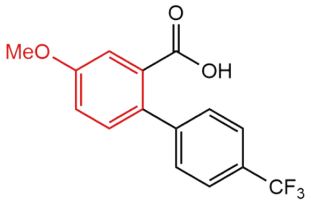



White solid, 97.6 mg, 98%.

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 2.7 Hz, 1H), 7.39 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 1H), 7.24 (s, 1H), 7.10 (dd, *J* = 8.5, 2.8 Hz, 1H), 3.88 (s, 3H), 1.36 (s, *J* = 3.0 Hz, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.67, 158.36, 149.87, 137.57, 135.65, 132.50, 130.06, 128.25, 125.01, 118.32, 115.06, 55.53, 34.49, 31.36.

**4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid.**



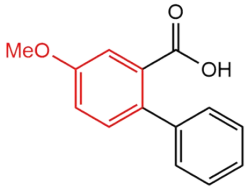

White solid, 97.8 mg, 90%.

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.1 Hz, 2H), 7.52 (d, *J* = 2.7 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.7 Hz, 1H), 7.13 (dd, *J* = 8.5, 2.7 Hz, 1H), 3.89 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 179.08, 159.07, 134.52, 132.27, 132.16, 128.98, 128.46, 124.86, 124.82, 118.49, 115.51, 55.59.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.36.

**4-methoxy-[1,1'-biphenyl]-2-carboxylic acid.** [4] 55.2 mg, 69%.

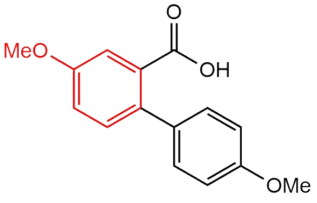



1H NMR (400 MHz, CDCl3) δ 7.46 (d, J = 2.7 Hz, 1H), 7.39 – 7.27 (m, 6H), 7.10 (dd, J = 8.5, 2.7 Hz, 1H), 3.88 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.66, 158.52, 140.75, 135.83, 132.36, 130.12, 128.59, 128.00, 126.99, 118.36, 115.07, 55.55.

HRMS: m/z: 251.06775 ([M+Na] + , calcd. for C14H12O3Na+ : 251.0673)

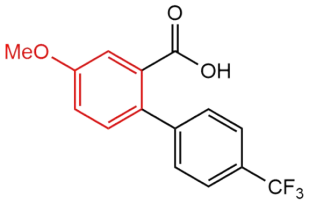
**4,4'-dimethoxy-[1,1'-biphenyl]-2-carboxylic acid.**[5] White solid. 90.2 mg, 99%.




$^1$H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 2.8 Hz, 1H), 7.27 (d, *J* = 8.5 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.09 (dd, *J* = 8.5, 2.8 Hz, 1H), 6.93 – 6.89 (m, 2H), 3.87 (s, 3H), 3.84 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 173.01, 158.79, 158.29, 135.47, 133.09, 132.39, 129.99, 129.69, 118.45, 117.14, 115.02, 113.53, 55.55, 55.22.

**4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid**

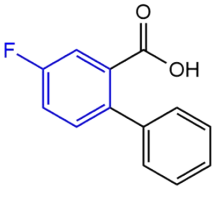



$^1$H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.1 Hz, 2H), 7.52 (d, *J* = 2.7 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.7 Hz, 1H), 7.13 (dd, *J* = 8.5, 2.7 Hz, 1H), 3.89 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 179.08, 159.07, 134.52, 132.27, 132.16, 128.98, 128.46, 124.86, 124.82, 118.49, 115.51, 55.59.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.36.

**4-fluoro-[1,1'-biphenyl]-2-carboxylic acid.** [4] White solid. 64.6 mg. 85%.

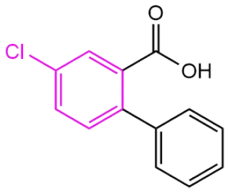


$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, J = 9.1, 2.7 Hz, 1H), 7.41 – 7.32 (m, 4H), 7.27 (m, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.73 (s), 161.49 (d, *J* = 247.9 Hz), 140.04 (s), 139.52 (d, *J* = 3.5 Hz), 132.97 (d, *J* = 7.6 Hz), 130.81 (s), 128.52 (s), 128.12 (s), 127.49 (s), 119.12 (d, *J* = 21.1 Hz), 117.44 (d, *J* = 23.6 Hz).

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -114.65 (td, *J* = 8.4, 5.8 Hz).

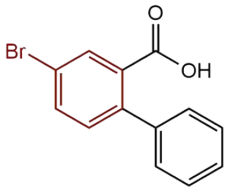
**4-chloro-[1,1'-biphenyl]-2-carboxylic acid.** [4] White solid, 88.1, 99%.




$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 2.1 Hz, 1H), 7.53 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.38 (m, 3H), 7.30 (m, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.63, 141.74, 139.81, 133.29, 132.49, 132.01, 130.66, 130.49, 128.36, 128.16, 127.66.

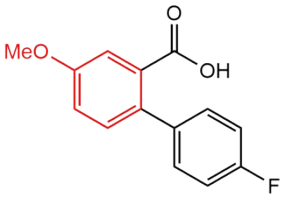
**4-bromo-[1,1'-biphenyl]-2-carboxylic acid.** [6] ivory white solid, 69.8 mg 36%.




$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 2.1 Hz, 1H), 7.69 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.38 (m, 3H), 7.30 (m, 2H), 7.25 (d, *J* = 8.2 Hz, 1H.

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.82, 142.79, 140.27, 135.58, 133.95, 133.26, 131.25, 128.79, 128.69, 128.21, 121.60.

**4'-fluoro-[1,1'-biphenyl]-2-carboxylic acid**

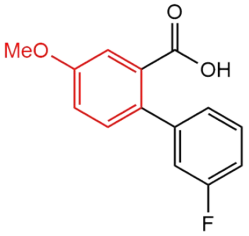



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 2.7 Hz, 1H), 7.28 – 7.22 (m, 3H), 7.10 (dd, *J* = 8.5, 2.7 Hz, 1H), 7.05 (t, *J* = 8.7 Hz, 2H), 3.88 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.37, 163.35, 160.91, 158.63, 136.77, 134.93, 132.39, 130.20, 130.12, 129.91, 118.51, 115.20, 114.97, 114.76, 55.57.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -115.83 – -115.93 (m).

**3'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid**

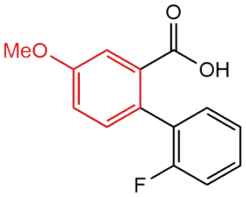



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 2.5 Hz, 1H), 7.32 (dd, *J* = 14.6, 7.9 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.11 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.06 (d, *J* = 7.7 Hz, 1H), 7.05 – 6.98 (m, 2H), 3.88 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.59, 163.61, 161.17, 158.85, 143.05, 134.66, 132.24, 129.41, 129.33, 124.46, 124.43, 118.50, 115.75, 115.53, 115.30, 113.94, 113.74, 55.57.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -72.53 (dd, *J* = 712.5, 6.5 Hz), -113.93 (td, *J* = 9.2, 6.1 Hz).

**2'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid**

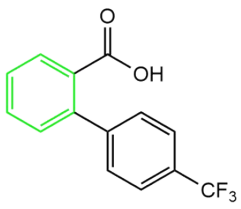



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.37 – 7.28 (m, 3H), 7.23 – 7.14 (m, 2H), 7.08 (t, *J* = 9.0 Hz, 1H), 3.91 (d, *J* = 3.4 Hz, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.60, 159.08, 132.87, 130.57, 129.41, 129.03, 128.95, 123.94, 118.83, 115.42, 115.19, 114.97, 55.59.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -116.17.

**4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid**



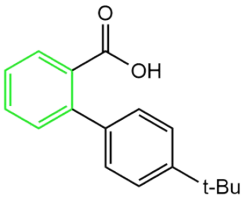

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.7 Hz, 1H), 7.62 (dd, *J* = 14.4, 7.6 Hz, 3H), 7.49

(t, *J* = 7.6 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.05, 144.98, 142.10, 132.25, 131.05, 130.95, 129.28, 128.86, 127.94, 124.90, 124.86.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.42.

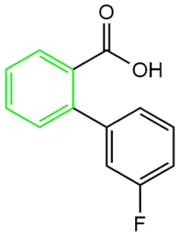
**4'-(*tert*-butyl)-[1,1'-biphenyl]-2-carboxylic acid**




1H NMR (400 MHz, CDCl3) δ 7.89 (d, J = 7.4 Hz, 1H), 7.53 (t, J = 7.3 Hz, 1H), 7.38 (d, J = 5.8 Hz, 4H), 7.27 (d, J = 8.1 Hz, 2H), 6.02 (s, 2H), 1.34 (s, 9H).

13C NMR (101 MHz, CDCl3) δ 173.20, 150.17, 142.87, 137.96, 131.69, 131.19, 130.44, 129.92, 128.16, 126.88, 125.01, 34.50, 31.34.

**3'-fluoro-[1,1'-biphenyl]-2-carboxylic acid**

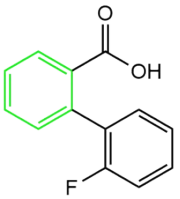



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.34 (dt, *J* = 14.8, 5.3 Hz, 2H), 7.12 – 7.08 (m, 1H), 7.08 – 7.02 (m, 2H).

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -113.77 (td, *J* = 9.1, 6.0 Hz).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.83, 163.62, 161.18, 143.29, 143.21, 142.13, 132.21, 131.01, 130.81, 129.50, 129.41, 129.17, 127.66, 124.30, 124.27, 115.62, 115.41, 114.28, 114.07.

**2'-fluoro-[1,1'-biphenyl]-2-carboxylic acid**

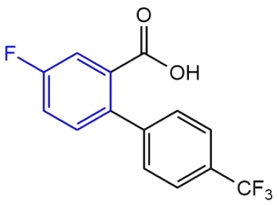



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.61 (td, *J* = 7.6, 1.3 Hz, 1H), 7.47 (td, *J* = 7.7, 1.1 Hz, 1H), 7.38 – 7.27 (m, 3H), 7.20 (dd, *J* = 10.7, 4.2 Hz, 1H), 7.11 – 7.04 (m, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.97, 137.09, 132.53, 131.66, 130.80, 130.34, 130.30, 129.34, 129.25, 127.90, 123.98, 123.94, 115.20, 114.98.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -116.19 (ddd, *J* = 10.1, 7.5, 5.2 Hz).

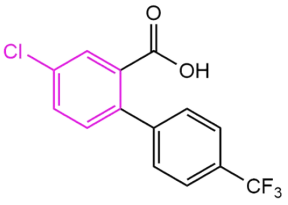
**4-fluoro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid**




$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.72 (dt, *J* = 9.0, 1.6 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.31 (dd, *J* = 6.4, 1.4 Hz, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 171.25, 163.46, 160.98, 144.18, 138.75, 133.31, 133.23, 130.81, 130.74, 130.17, 129.85, 129.25, 125.85, 125.31, 125.28, 123.14, 120.00, 119.79, 118.41, 118.17.

**4-chloro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid**

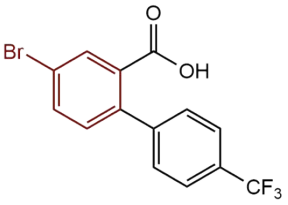



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 2.2 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.56 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.52, 143.69, 140.48, 134.16, 132.36, 132.31, 130.89, 130.44, 129.58, 128.77, 125.02, 124.98.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.50.

**4-bromo-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid**

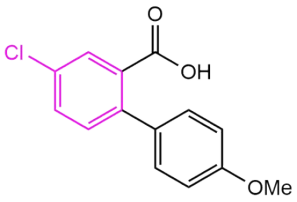


$^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 2.1 Hz, 1H), 7.75 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.57, 143.69, 141.15, 135.46, 133.91, 132.65, 130.35, 129.72, 128.74, 125.05, 122.03.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.52.

**4-chloro-4'-methoxy-[1,1'-biphenyl]-2-carboxylic acid**




$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 2.2 Hz, 1H), 7.51 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 2H), 6.92 (d, *J* = 8.6 Hz, 2H), 3.85 (s, 3H).

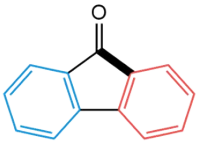
$^{13}$C NMR (101 MHz, $CDCl_3$) δ 172.31, 159.29, 141.37, 132.87, 132.52, 132.06, 132.02, 130.50, 129.57, 113.70, 55.25.

## 3. Synthesis of 9-fluorenones

**General procedure for intramolecular cyclization synthesis of 9-fluorenones.**

Into a 10 mL Schlenk tube equipped with a magnetic stir bar was added photocatalyst (1 mol%), 0.2 mmol of Bpca, $K_2HPO_4$ (7.0 mg, 20 mol%), and $Ph_3P$ (62.9 mg, 1.2 equiv.). The DCM/$H_2O$ (2.0 mL, 4:1 v/v) was added as solvent. The mixture was frozen-degassed and refill with nitrogen for three times. The tube was then set at the center of a 5 W blue light emitting diode (LED) lamp line coil (*d* = 12 cm approx.), and then stirred for 24 h at room temperature. After completion, the mixture was extracted with ethyl acetate (3 × 10 mL). The solvent of organic layer was removed under vacuo. The crude was purified on silica gel chromatography using a mixture of PE/EA (25:1~10:1) to give 9-fluorenone products.

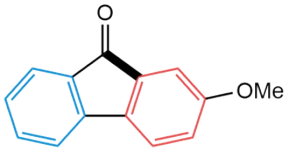
**9*H*-fluoren-9-one (1a)**



$^1$H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 2H).

$^{13}$C NMR (100 MHz, $CDCl_3$): δ 194.08, 144.53, 134.82, 134.24, 129.20, 124.44, 120.43.

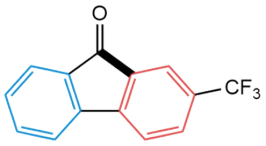
**2-methoxy-9*H*-fluoren-9-one (2a, 1b)**



$^1$H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.2 Hz, 1H), 7.45-7.51 (m, 3H), 7.24-7.32 (m, 2H), 7.04 (d, *J* = 8.0 Hz, 1H), 3.92 (s, 3H).

$^{13}$C NMR (100 MHz, $CDCl_3$): δ 194.20, 161.14, 145.19, 137.30, 136.21, 135.17, 134.60, 128.19, 121.65, 120.62, 119.88, 109.66, 56.05.

**2-(trifluoromethyl)-9*H*-fluoren-9-one (1c)**

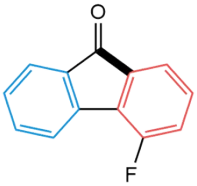


$^1$H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.2 Hz, 1H), 7.61–7.52 (m, 3H), 7.37 (t, *J* = 6.4 Hz, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 192.21, 147.69, 143.32, 135.43, 134.75, 134.59, 131.92, 131.89, 130.53, 125.04, 122.62, 121.54, 121.46, 121.42, 120.79.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.82 (s, 3F).

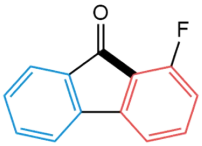
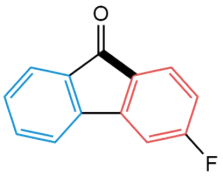
**4-fluoro-9*H*-fluoren-9-one (1d)**



$^1$H NMR (400 MHz, $CDCl_3$) δ 7.70–7.66 (m, 2H), 7.53–7.46 (m, 2H), 7.33–7.24 (m, 2H), 7.20–7.16 (m, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 192.99, 159.37, 156.85, 141.86, 136.96, 135.42, 134.95, 131.14, 131.08, 130.39, 130.24, 129.47, 124.83, 124.38, 124.38, 122.98, 122.86, 120.55, 120.49.

$^{19}$F NMR (376 MHz, CDCl3) δ -119.15 (s, 1F).

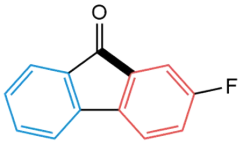



**1-fluoro-9*H*-fluoren-9-one & 3-fluoro-9*H*-fluoren-9-one (1e)**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.70, 7.68, 7.65, 7.63, 7.55, 7.54, 7.51, 7.49, 7.47, 7.46, 7.36, 7.34, 7.32, 7.30, 7.26, 7.17, 7.15, 6.97, 6.94, 6.93.

* This is a mixture.

**2-fluoro-9*H*-fluoren-9-one (1f, 3a)**

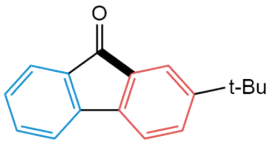


$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, $J$ = 7.2 Hz, 1H), 7.48–7.43 (m, 3H), 7.31–7.24 (m, 2H), 7.13 (t, $J$ = 8.4 Hz, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 192.71, 165.05, 162.56, 114.15, 140.39, 136.60, 136.53, 135.30, 134.56, 129.00, 124.84, 121.90, 121.82, 121.20, 120.39, 122.28, 112.05.

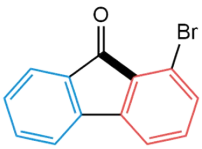
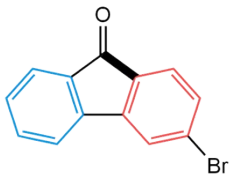
$^{19}$F NMR (376 MHz, $CDCl_3$) δ-111.66 (s, 1F).

**2-(*tert*-butyl)-9*H*-fluoren-9-one (1g)**



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.60 (d, $J$ = 7.5 Hz, 2H), 7.56 (d, $J$ = 8.0 Hz, 1H), 7.43 (dd, $J$ = 7.9, 1.2 Hz, 1H), 7.36 (t, $J$ = 7.5 Hz, 1H), 7.29 (d, $J$ = 7.3 Hz, 1H), 1.39 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 151.37, 145.83, 145.64, 140.06, 137.36, 128.99, 127.34, 126.13, 125.05, 122.13, 119.73, 119.54, 35.01, 31.53.

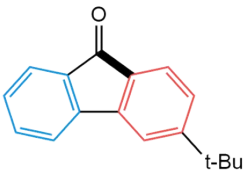



**1-bromo-9*H*-fluoren-9-one & 3-bromo-9*H*-fluoren-9-one (1h)**

1H NMR (400 MHz, CDCl3) δ 7.70, 7.69, 7.64, 7.63, 7.61, 7.55, 7.53, 7.52, 7.50, 7.48, 7.46, 7.45, 7.43, 7.43, 7.41, 7.39, 7.35, 7.34, 7.32, 7.30, 7.29, 7.26.

* This is a mixture.

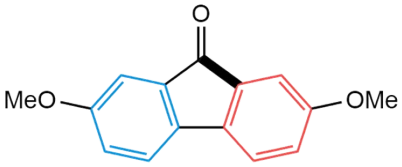
**3-(*tert*-butyl)-9*H*-fluoren-9-one (1i)**



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, $J$ = 7.1 Hz, 1H), 7.59 (d, $J$ = 8.0 Hz, 1H), 7.54 (m, 2H), 7.47 (t, $J$ = 7.6 Hz, 1H), 7.32 (d, $J$ = 8.0 Hz, 1H), 7.29 (d, $J$ = 7.1 Hz, 1H), 1.38 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 193.03, 158.32, 143.88, 133.73, 131.13, 128.20, 125.33, 123.47, 119.35, 116.86, 34.90, 30.44.

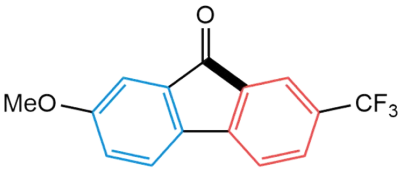
**2,7-dimethoxy-9*H*-fluoren-9-one (2b)**




$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.29 (d, *J* = 8.2 Hz, 2H), 7.16 (d, *J* = 2.5 Hz, 2H), 6.94 (dd, *J* = 8.2, 2.5 Hz, 2H), 3.84 (s, 6H).

$^{13}$C NMR (101 MHz, $CDCl_3$): δ 193.94, 160.12, 137.65, 136.11, 120.68, 120.45, 109.77, 55.87.

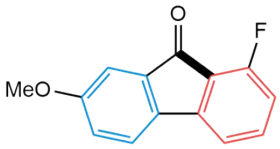
**2-methoxy-7-(trifluoromethyl)-9*H*-fluoren-9-one (2c)**

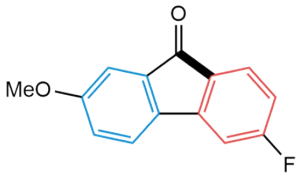



$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.56 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.86 (s, 1H), 3.87 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 192.50, 162.46, 153.68, 148.33, 137.30, 135.69, 134.98, 132.41, 132.08, 130.75, 130.62, 130.58, 127.96, 122.54, 121.89, 120.48, 118.75, 118.71, 118.68, 110.25, 56.12.

$^{19}$F NMR (376 MHz, $CDCl_3$) δ -62.74 (s, 3F).



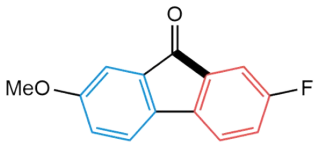




**1-fluoro-7-methoxy-9*H*-fluoren-9-one & 6-fluoro-2-methoxy-9*H*-fluoren-9-one (2e)**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.61, 7.60, 7.59, 7.58, 7.43, 7.42, 7.41, 7.39, 7.37, 7.26, 7.21, 7.19, 7.18, 7.09, 7.01, 6.99, 6.97, 6.88, 6.86, 6.85, 6.84, 6.83, 3.87, 3.85.

* This is a mixture.

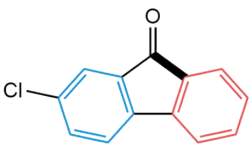
**7-fluoro-2-methoxy-9*H*-fluoren-9-one (2f, 3b)**




$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.33 (m, 2H), 7.29 (dd, *J* = 7.3, 2.5 Hz, 1H), 7.20 (d, *J* = 2.5 Hz, 1H), 7.11 (ddd, *J* = 8.9, 8.1, 2.5 Hz, 1H), 6.99 (dd, *J* = 8.2, 2.5 Hz, 1H), 3.85 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): δ 192.55, 192.54, 163.93, 161.95, 160.66, 160.65, 140.74, 140.71, 136.60, 136.59, 136.47, 136.42, 136.14, 136.12, 121.24, 121.24, 121.07, 120.88, 120.84, 120.78, 120.64, 112.19, 112.00, 109.82, 55.85.

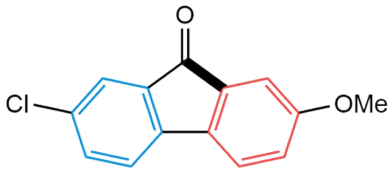
**2-chloro-9*H*-fluoren-9-one (4a)**




$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.29-7.32 (m, 1H), 7.45 (s, 2H), 7.50 (d, *J* = 4.0 Hz, 2H), 7.62 (s, 1H), 7.66 (d, *J* = 7.6 Hz, 1H).

$^{13}$C NMR (100 MHz, $CDCl_3$): δ 192.60, 161.12, 143.20, 136.38, 135.94, 134.43, 133.98, 124.83, 121.65, 120.75, 109.77, 77.31, 77.00, 76.68, 55.93.

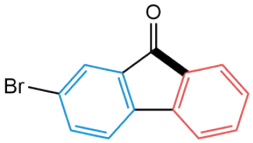
**2-chloro-7-methoxy-9*H*-fluoren-9-one (4b)**




$^{1}$H NMR (400 MHz, $CDCl_3$): δ7.55 (s, 1H), 7.36~7.41 (m,3H), 7.33 (d, J = 7.9 Hz, 1H), 7.20 (s, 1H), 6.99 (d, J = 8.2 Hz, 1H), 3.86 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): δ 192.60, 161.12, 143.20, 136.38, 135.94, 134.43, 133.98, 124.83, 121.65, 120.75, 109.77, 77.31, 77.00, 76.68, 55.93.

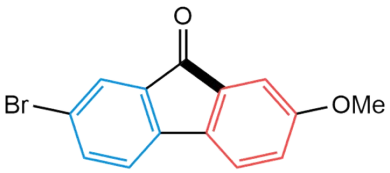
**2-bromo-9*H*-fluoren-9-one (5a)**




$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.31-7.35 (m, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.50-7.51 (m, 2H), 7.61 (d, J = 7.6 Hz, 1H), 7.66 (d, J = 7.6 Hz, 1H), 7.77 (s, 1H).

$^{13}$C NMR (100 MHz, $CDCl_3$): δ 120.72, 121.99, 123.20, 124.86, 127.80, 129.70, 133.95, 135.31, 136.02, 137.36, 143.25, 143.92, 192.63.

**2-bromo-7-methoxy-9*H*-fluoren-9-one (5b)**




$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.55 (d, *J* = 7.9, Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.28 (d, *J* = 7.9, 1H), 7.20 (d, *J* = 2.4 Hz, 1H), 7.00 (d, *J* = 8.2 Hz, 1H), 3.86 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): δ 192.55, 161.22, 143.65, 137.36, 136.38, 136.10, 135.65, 127.70, 121.73, 121.69, 121.13, 120.80, 109.74, 55.93.

# 4. NMR Spectra

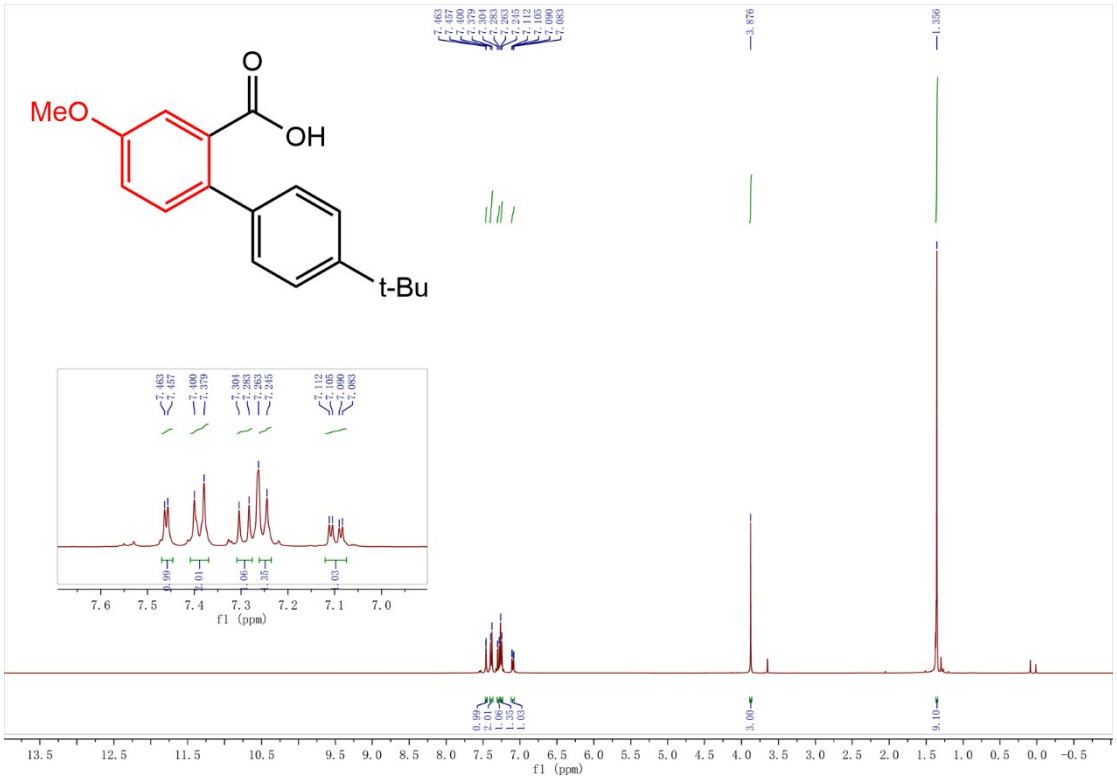



**Figure S1**. $^{1}$H NMR Spectrum of 4'-(*tert*-butyl)-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

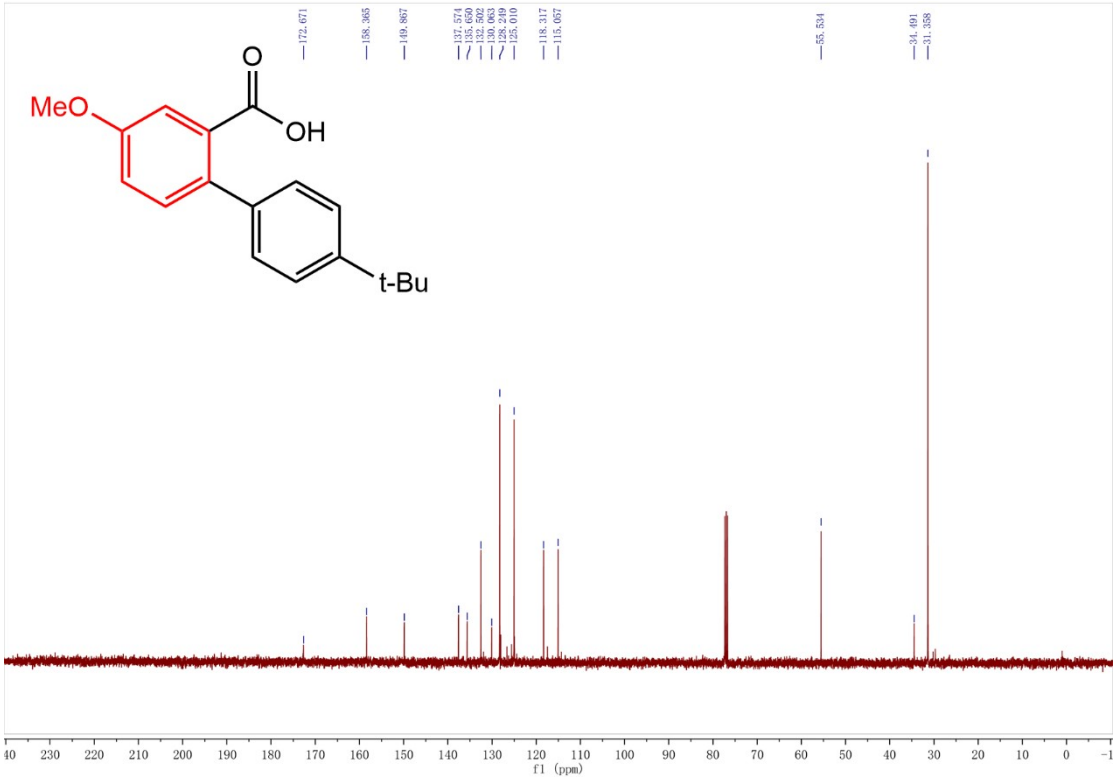



**Figure S2**. $^{13}$C NMR Spectrum of 4'-(*tert*-butyl)-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

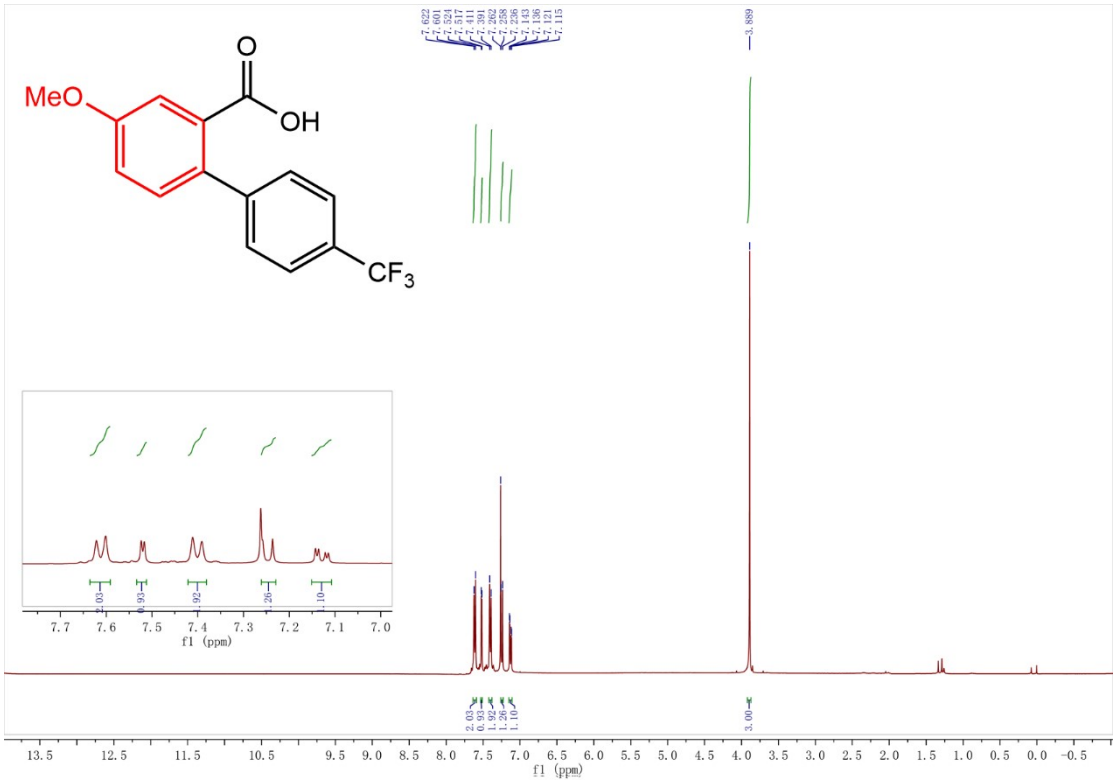



**Figure S3**. [1]H NMR Spectrum of 4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

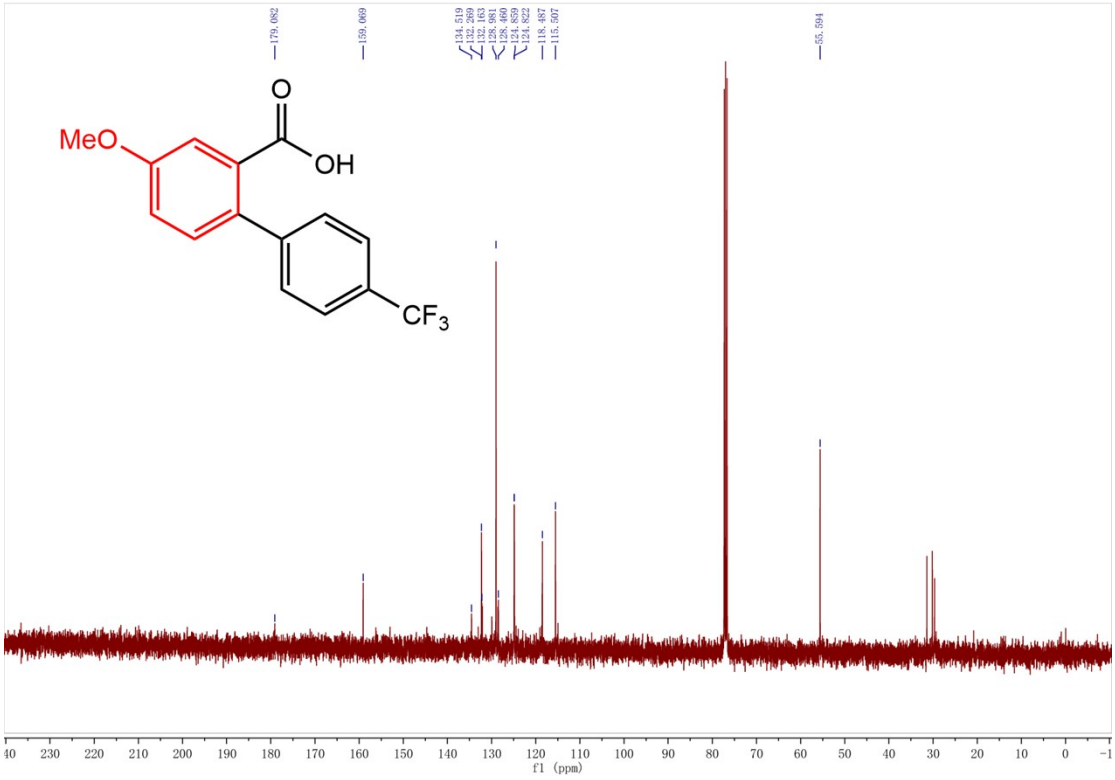



**Figure S4**. [13]C NMR Spectrum of 4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

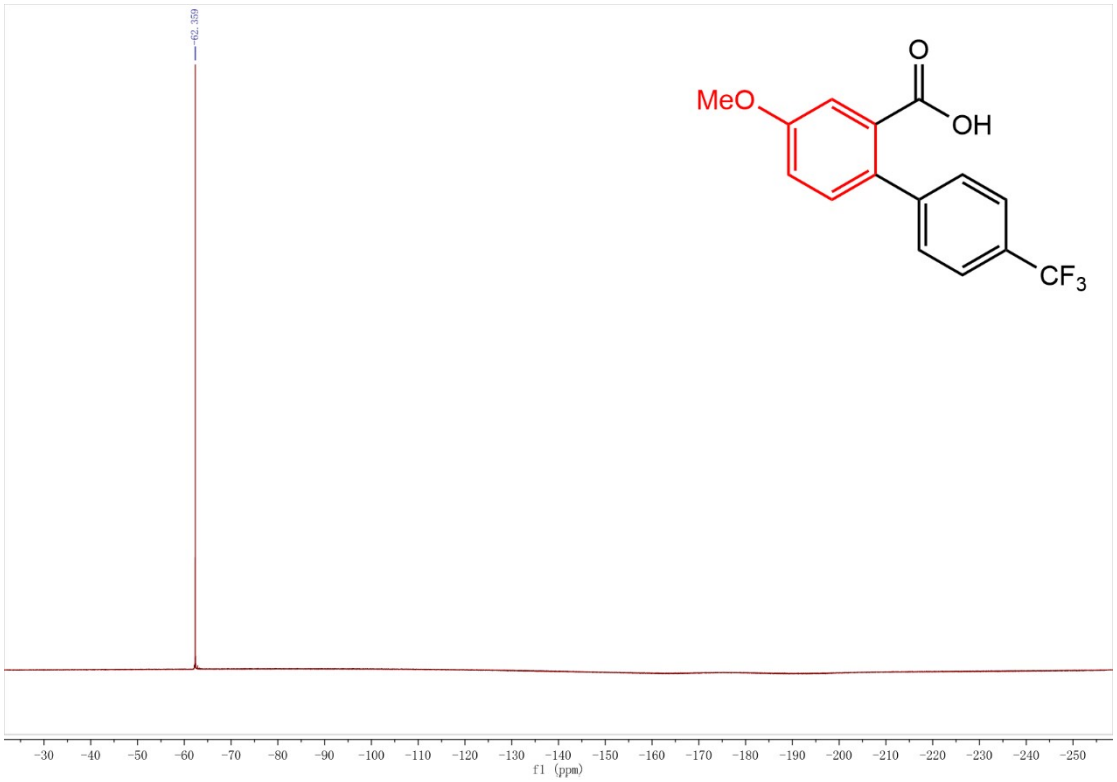



**Figure S5**. $^{19}F$ NMR Spectrum of 4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

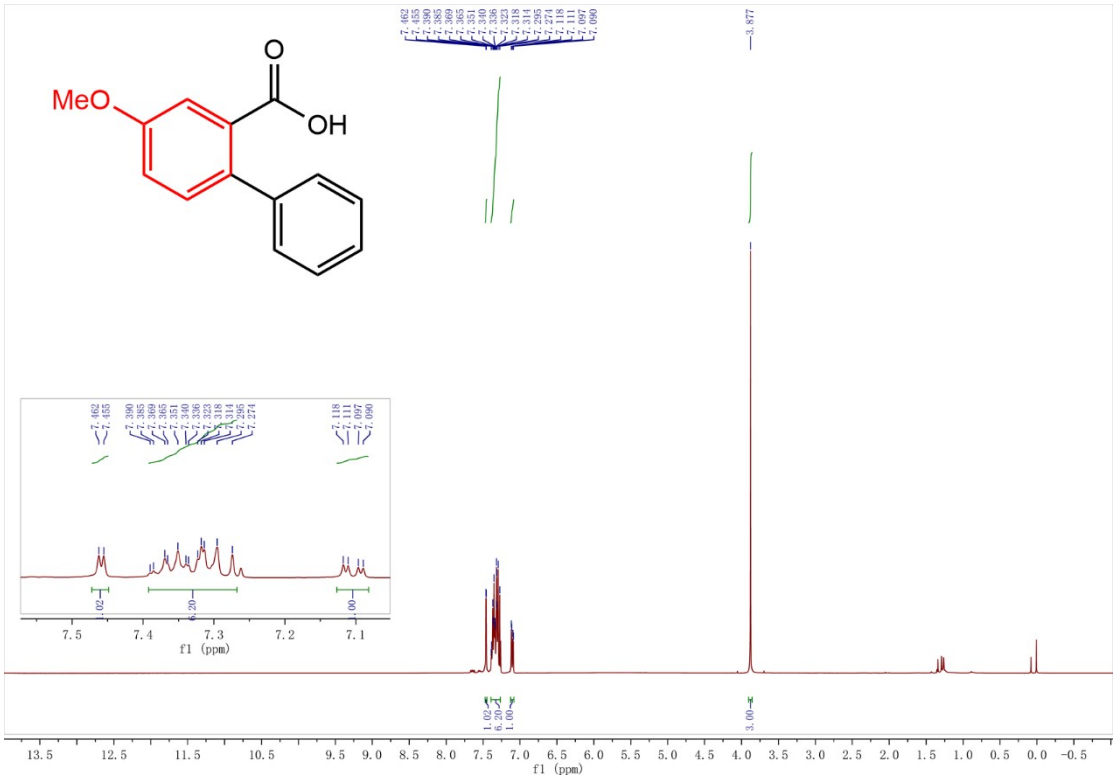



**Figure S6**. $^{1}H$ NMR Spectrum of 4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

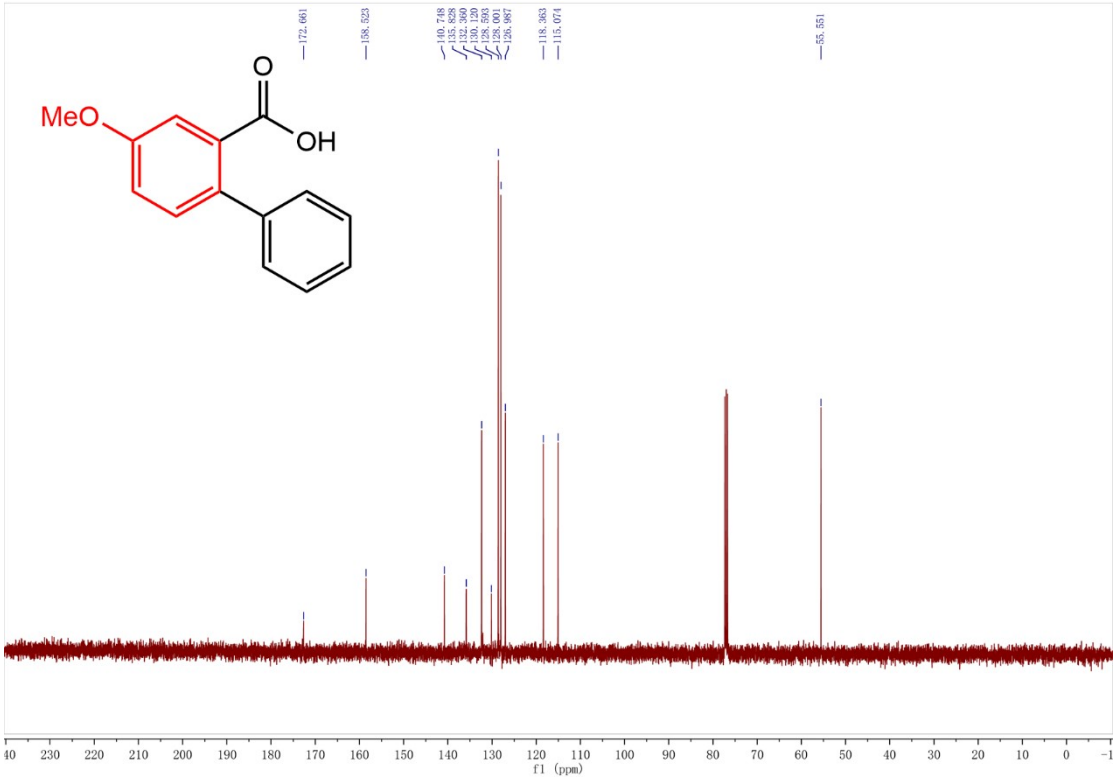



**Figure S7**. $^{13}C$ NMR Spectrum of 4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

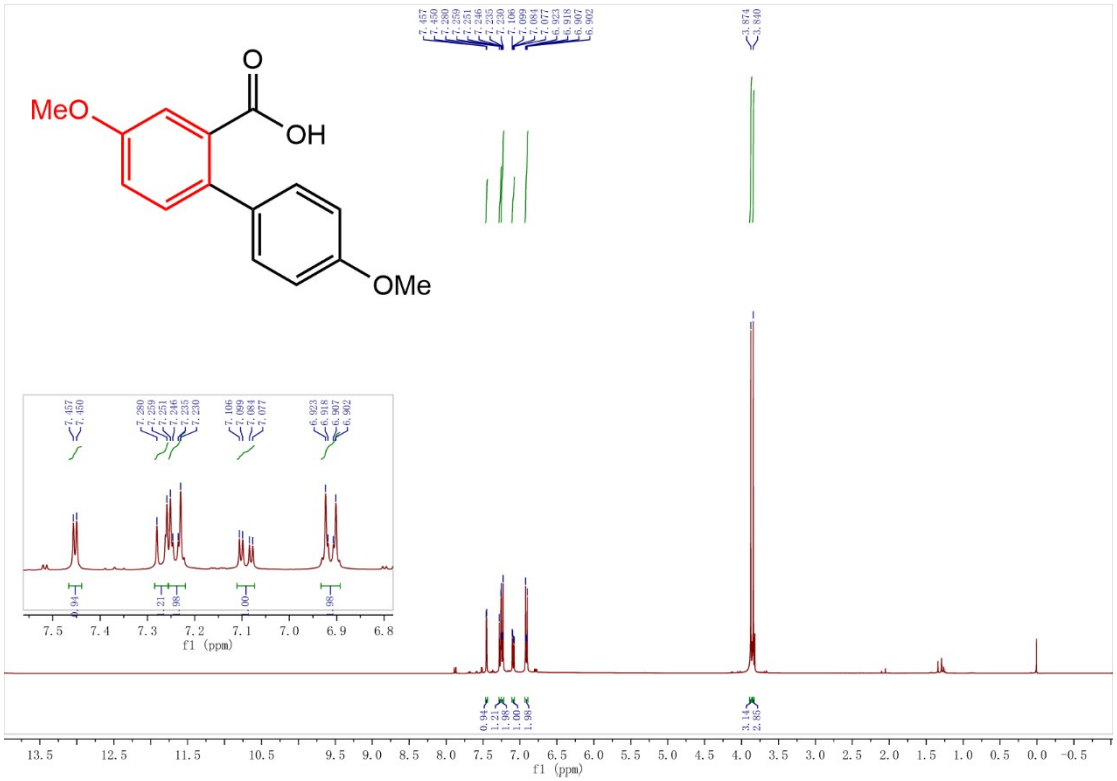



**Figure S8**. $^{1}H$ NMR Spectrum of 4,4'-dimethoxy-[1,1'-biphenyl]-2-carboxylic acid

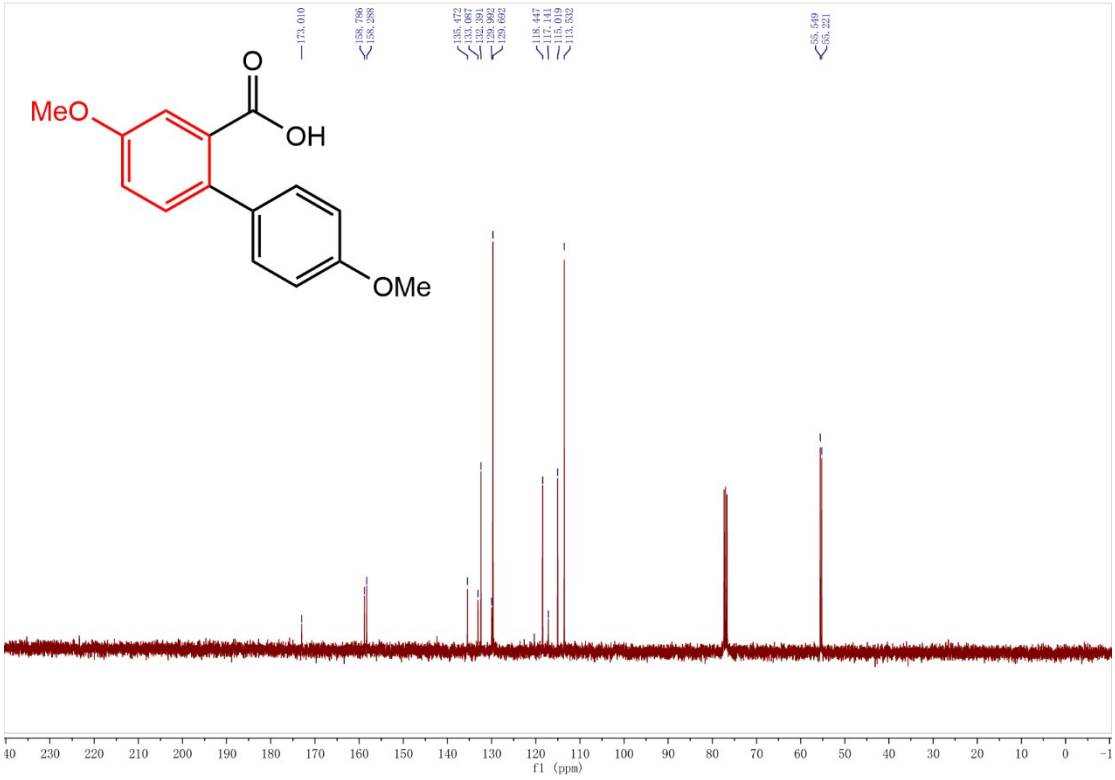



**Figure S9**. $^{13}C$ NMR Spectrum of 4,4'-dimethoxy-[1,1'-biphenyl]-2-carboxylic acid

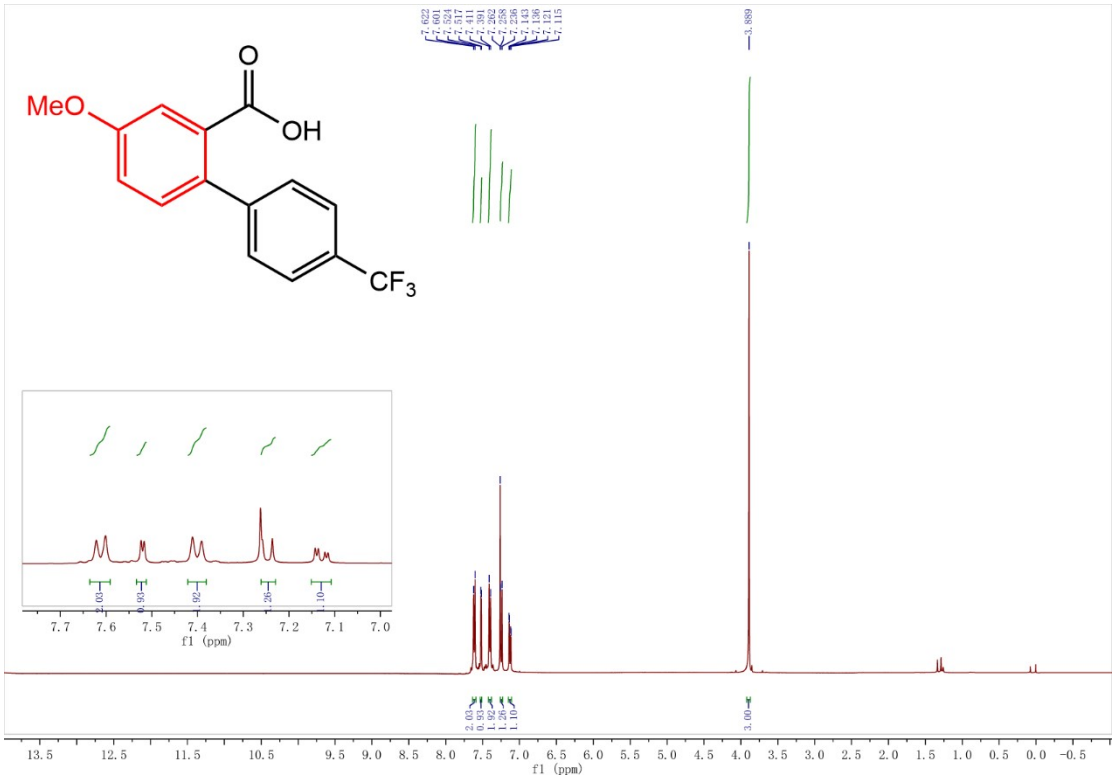



**Figure S10**. $^{1}H$ NMR Spectrum of 4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

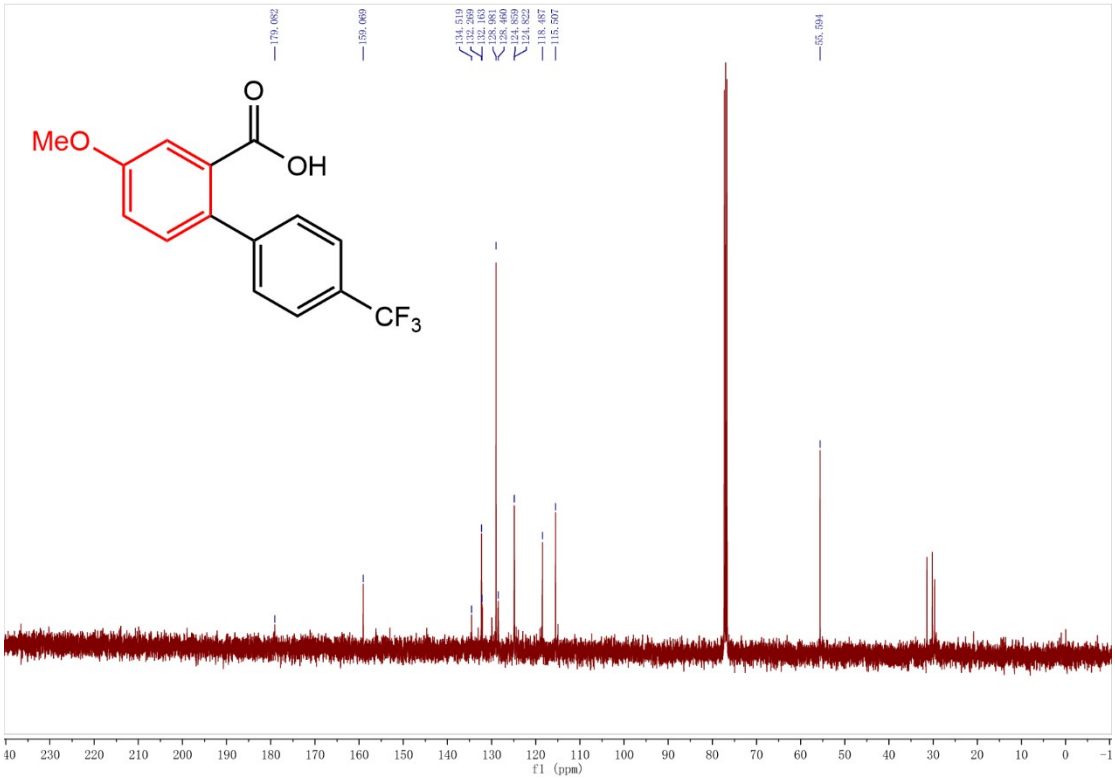



**Figure S11**. $^{13}$C NMR Spectrum of 4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

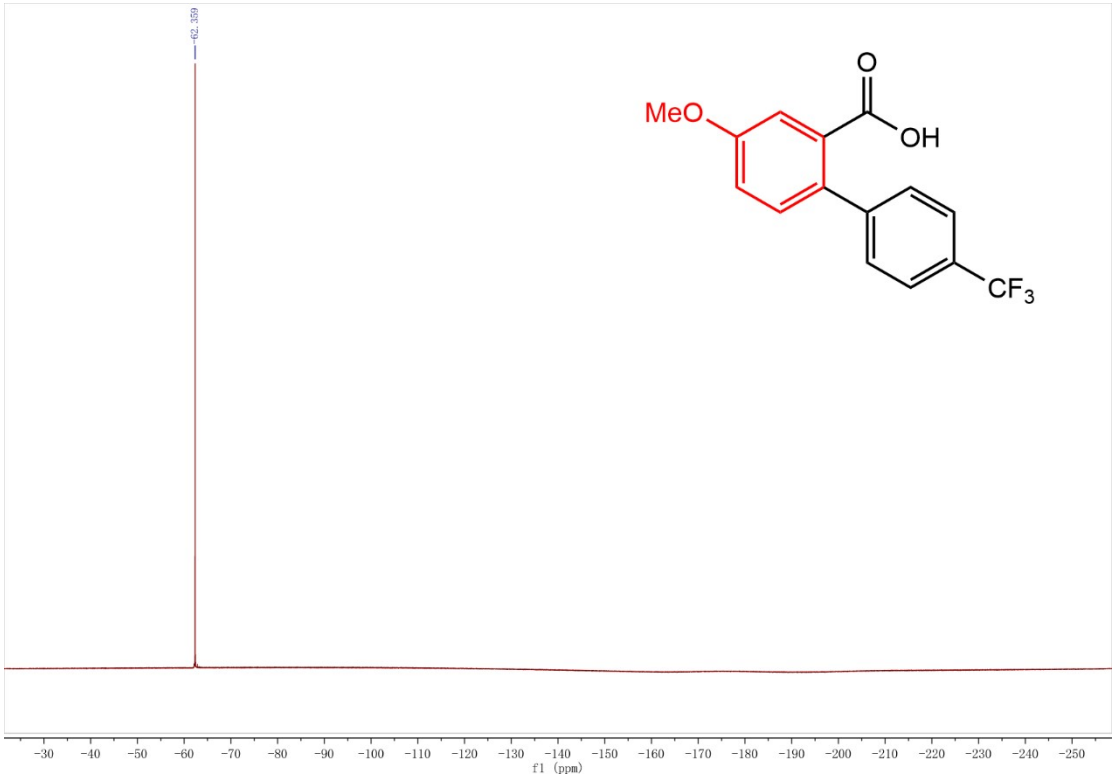



**Figure S12**. $^{19}$F NMR Spectrum of 4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

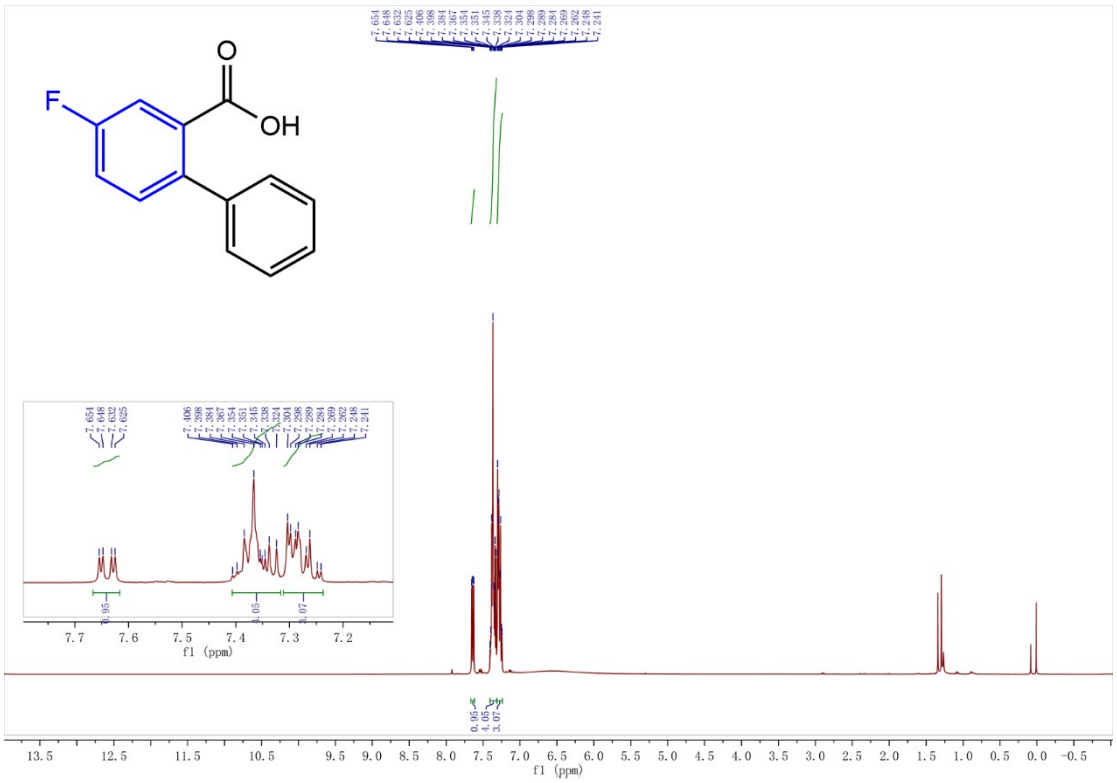



**Figure S13**. $^{1}$H NMR Spectrum of 4-fluoro-[1,1'-biphenyl]-2-carboxylic acid

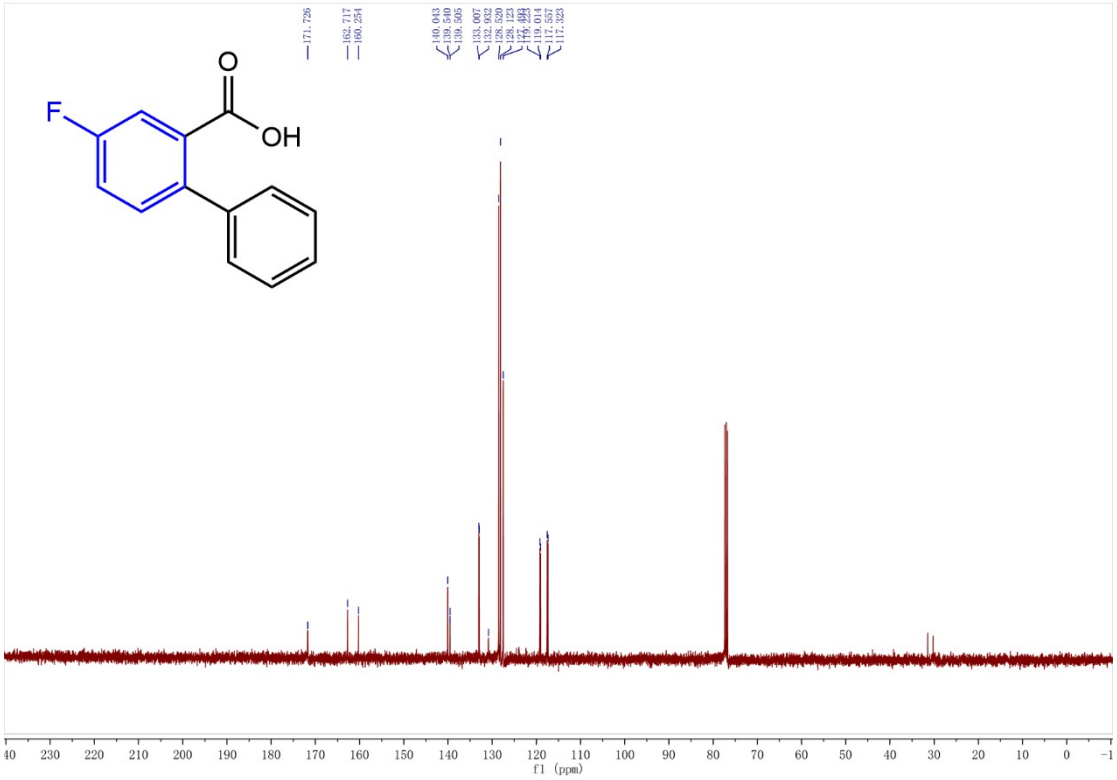



**Figure S14**. $^{13}$C NMR Spectrum of 4-fluoro-[1,1'-biphenyl]-2-carboxylic acid

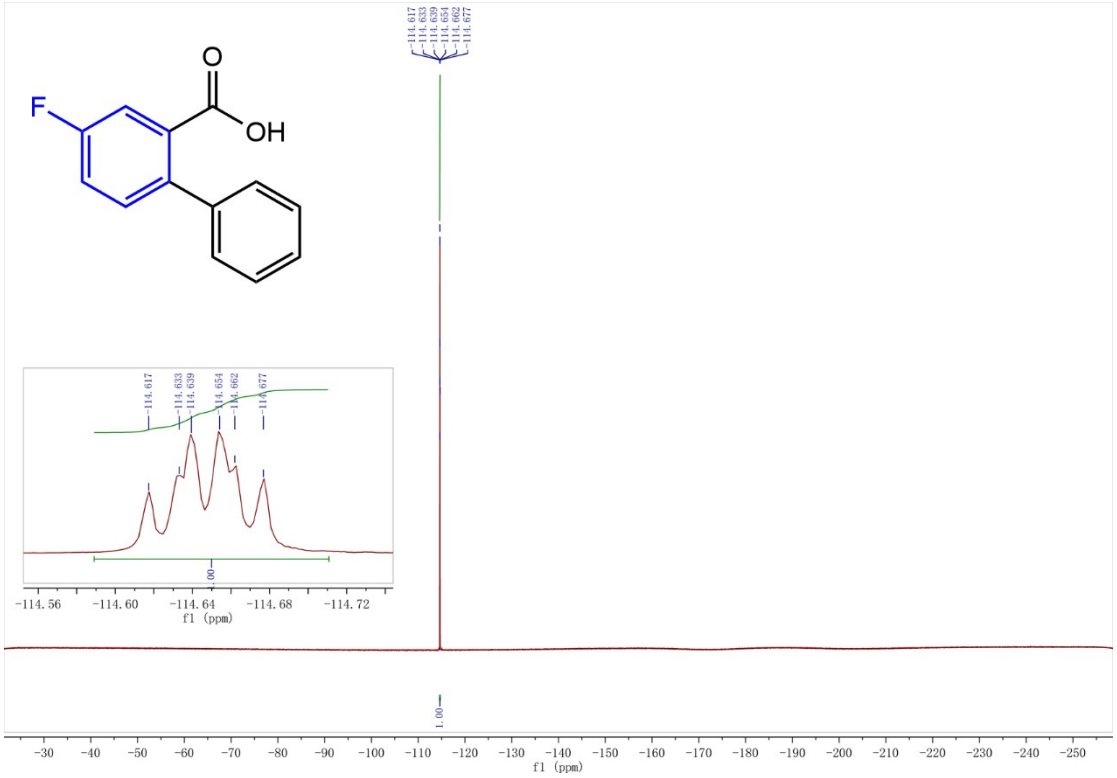



**Figure S15**. $^{19}F$ NMR Spectrum of 4-fluoro-[1,1'-biphenyl]-2-carboxylic acid

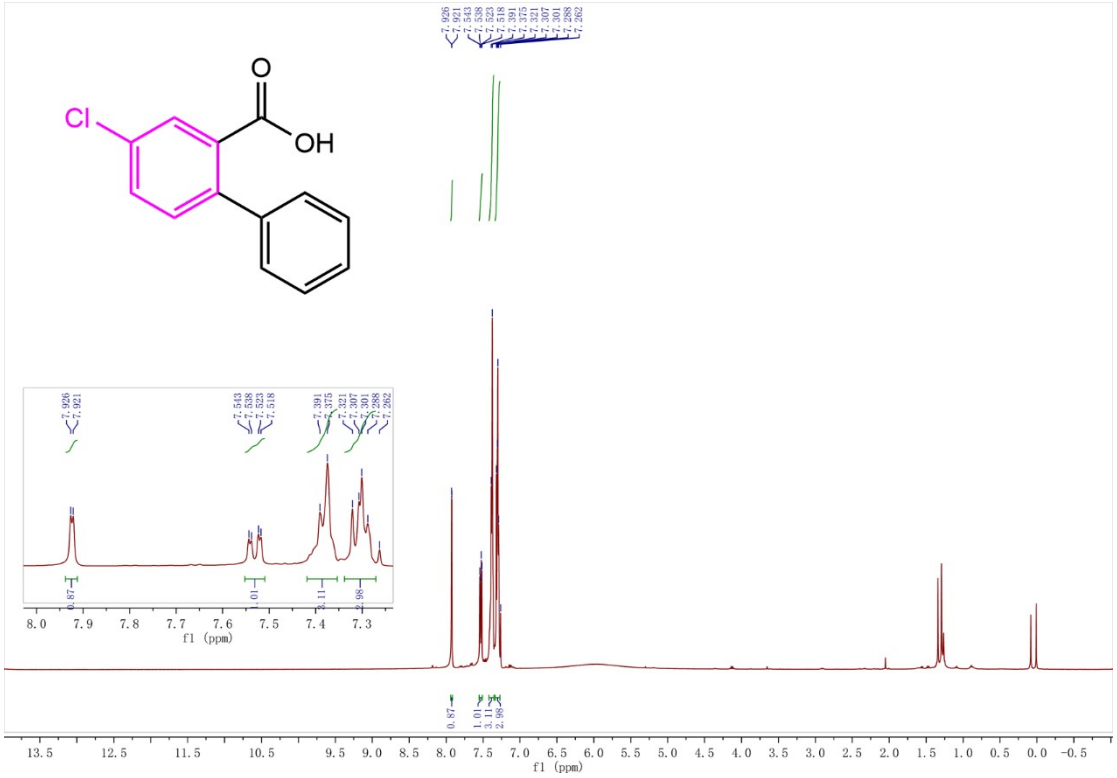



**Figure S16**. $^{1}H$ NMR Spectrum of 4-chloro-[1,1'-biphenyl]-2-carboxylic acid

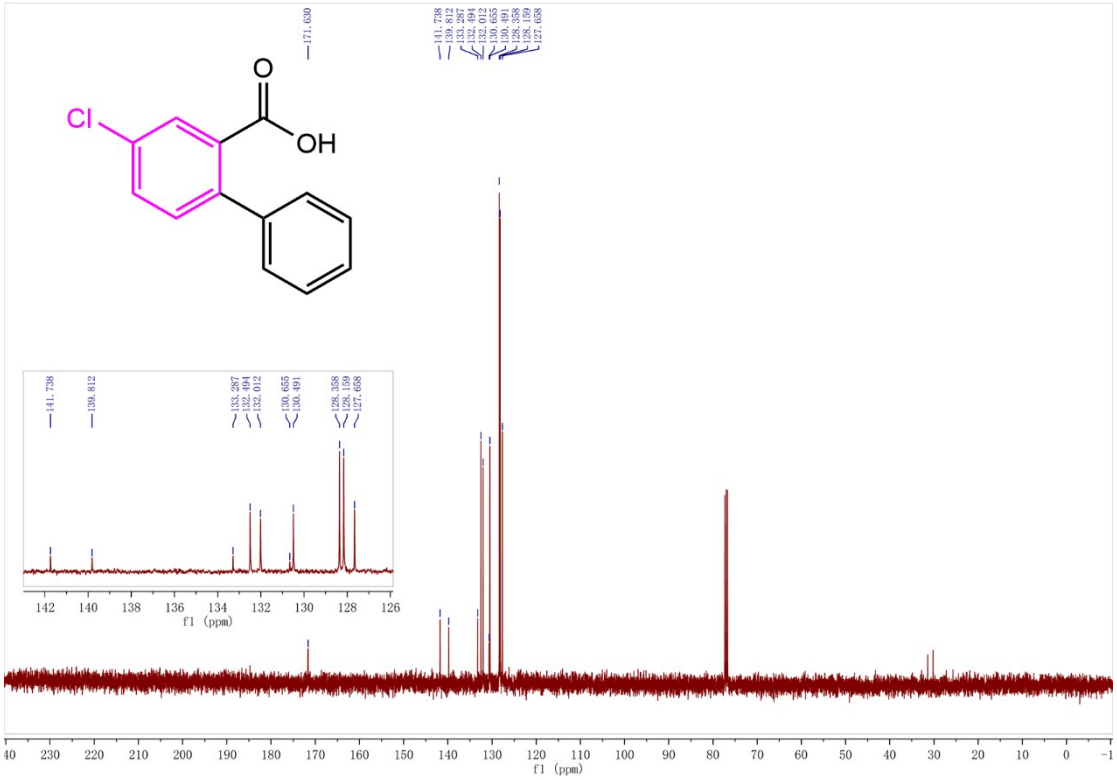



**Figure S17**. $^{13}$C NMR Spectrum of 4-chloro-[1,1'-biphenyl]-2-carboxylic acid

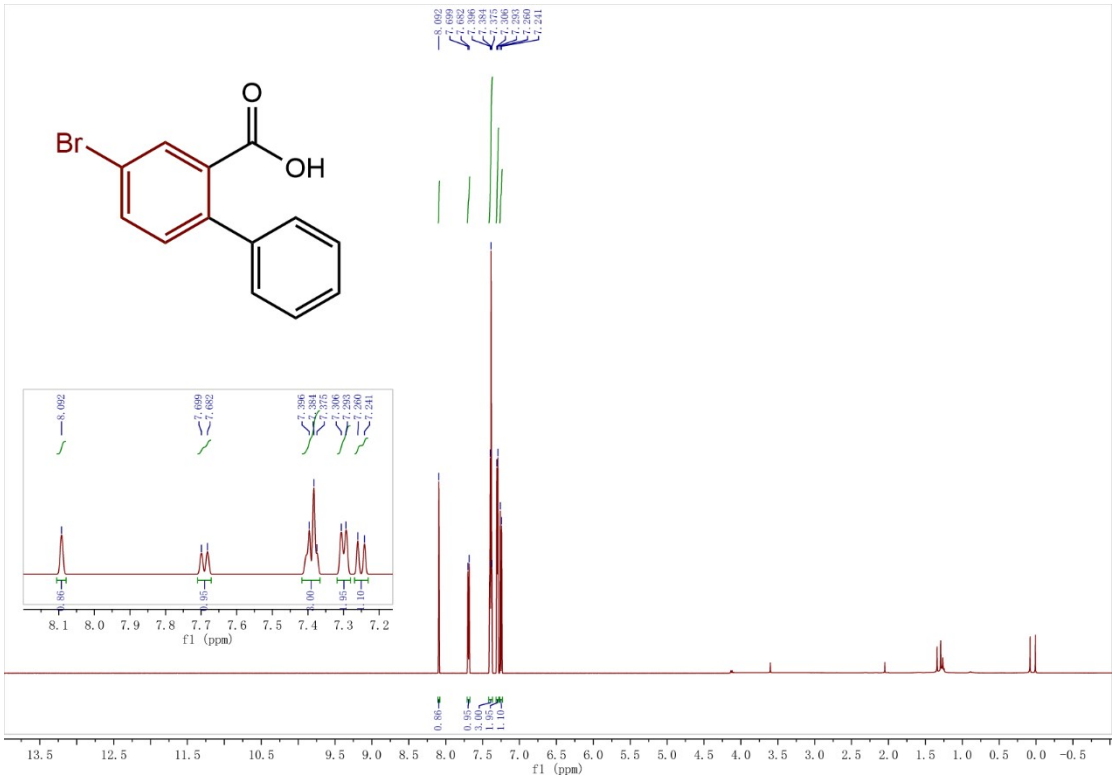



**Figure S18**. $^{1}$H NMR Spectrum of 4-bromo-[1,1'-biphenyl]-2-carboxylic acid

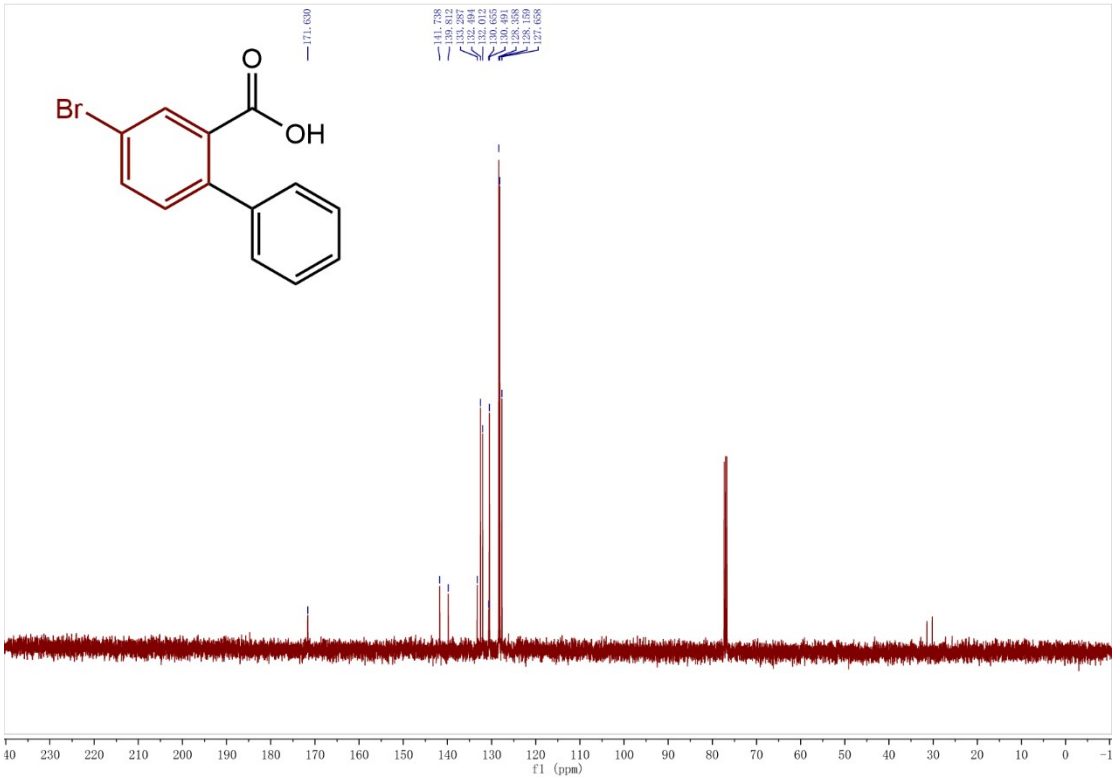



**Figure S19**. $^{13}$C NMR Spectrum of 4-bromo-[1,1'-biphenyl]-2-carboxylic acid

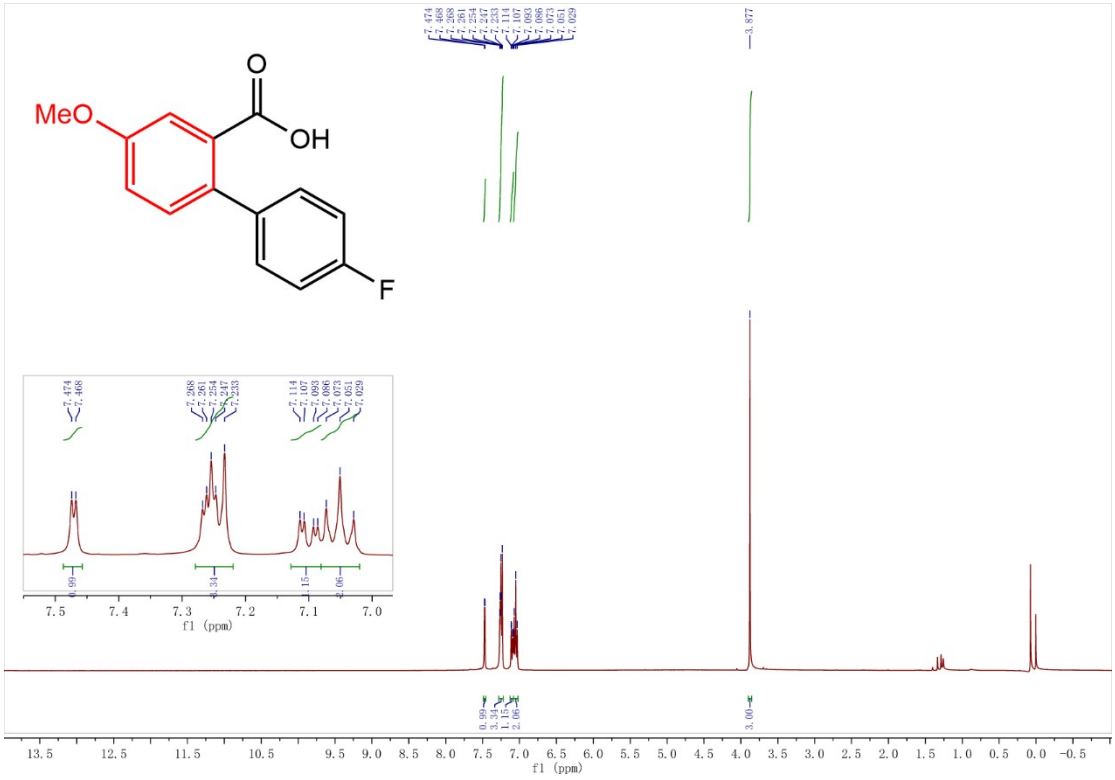



**Figure S20**. $^{1}$H NMR Spectrum of 4'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

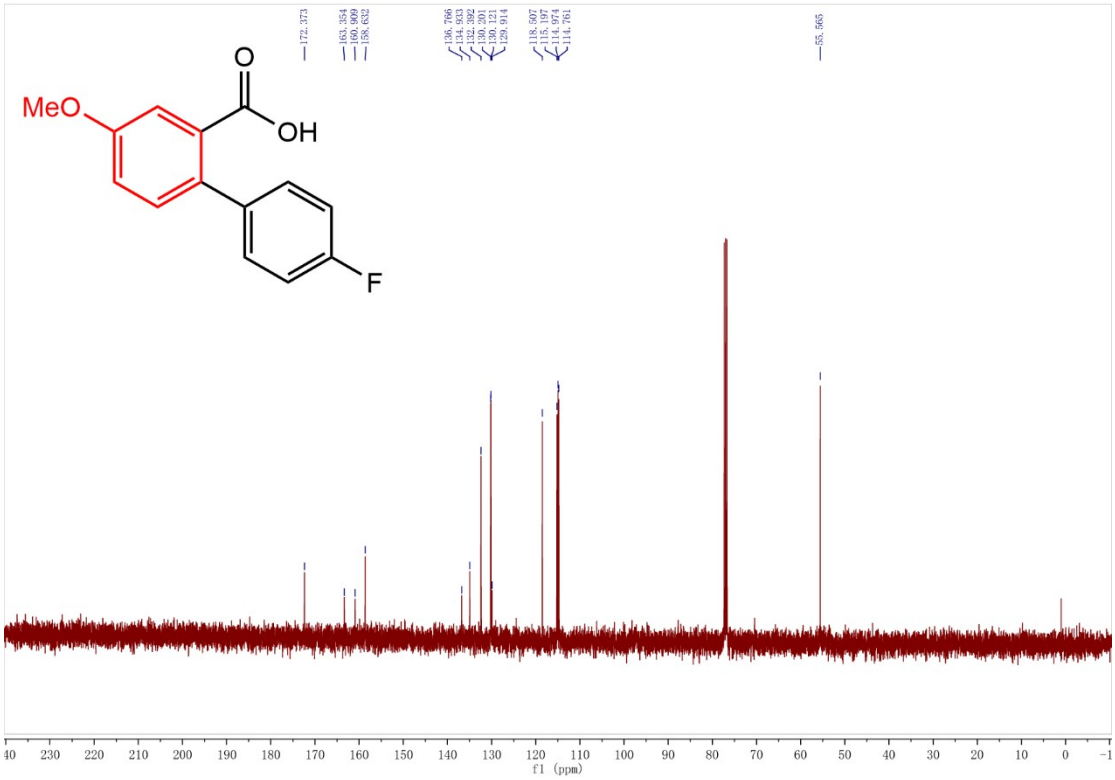



**Figure S21**. $^{13}$C NMR Spectrum of 4'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

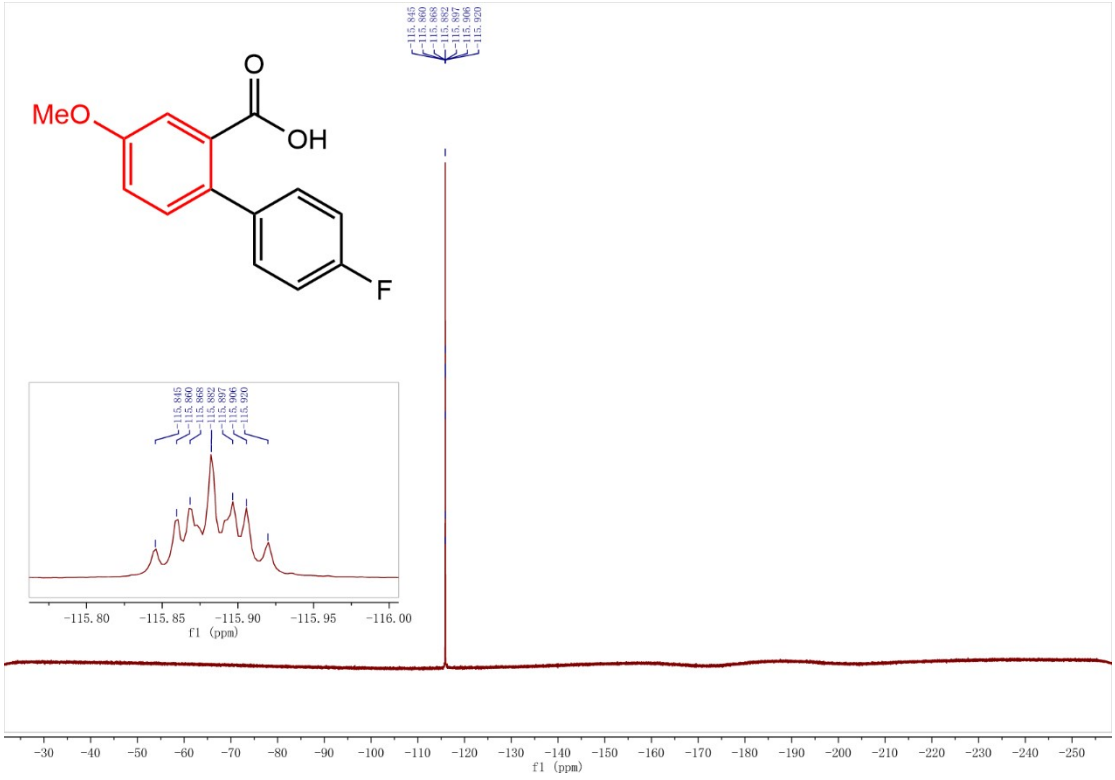



**Figure S22**. $^{19}$F NMR Spectrum of 4'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

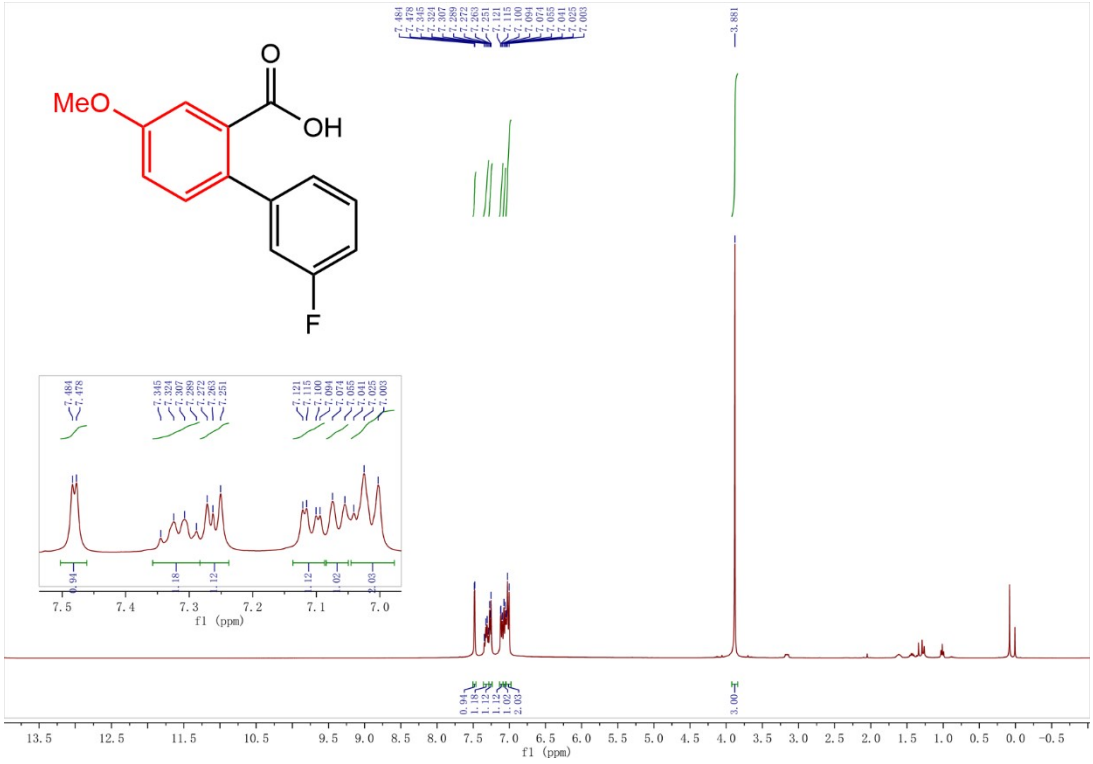



**Figure S23**. $^{1}$H NMR Spectrum of 3'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

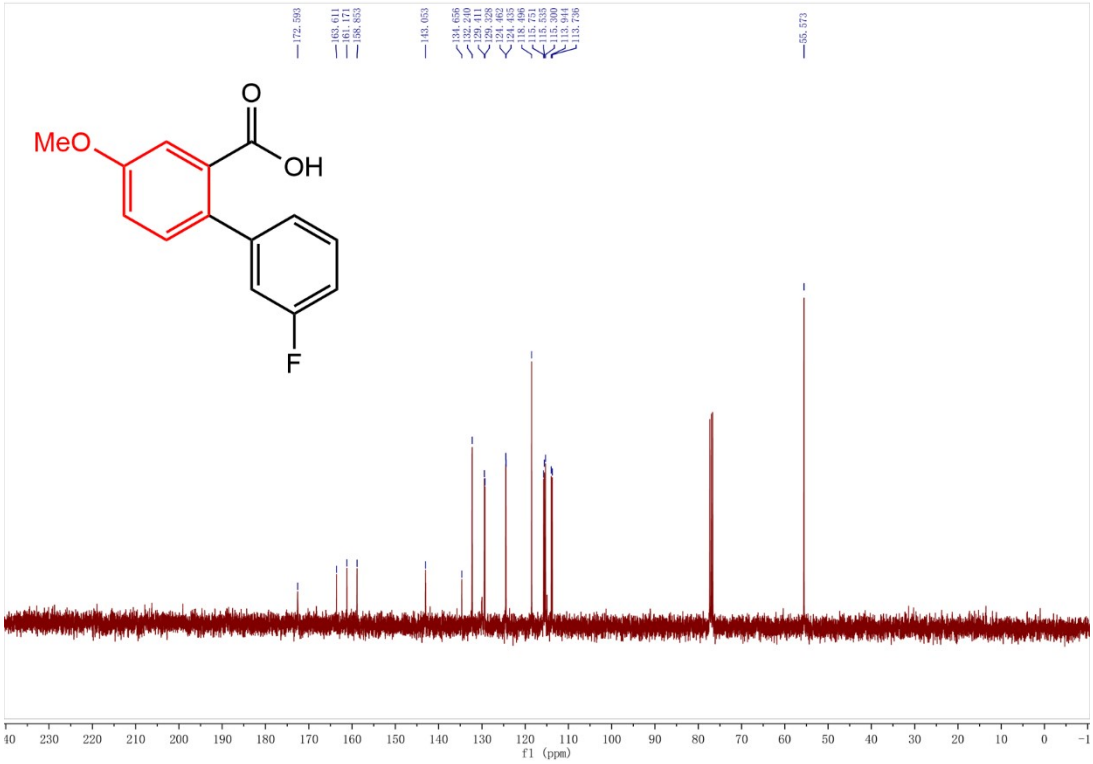



**Figure S24**. $^{13}$C NMR Spectrum of 3'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

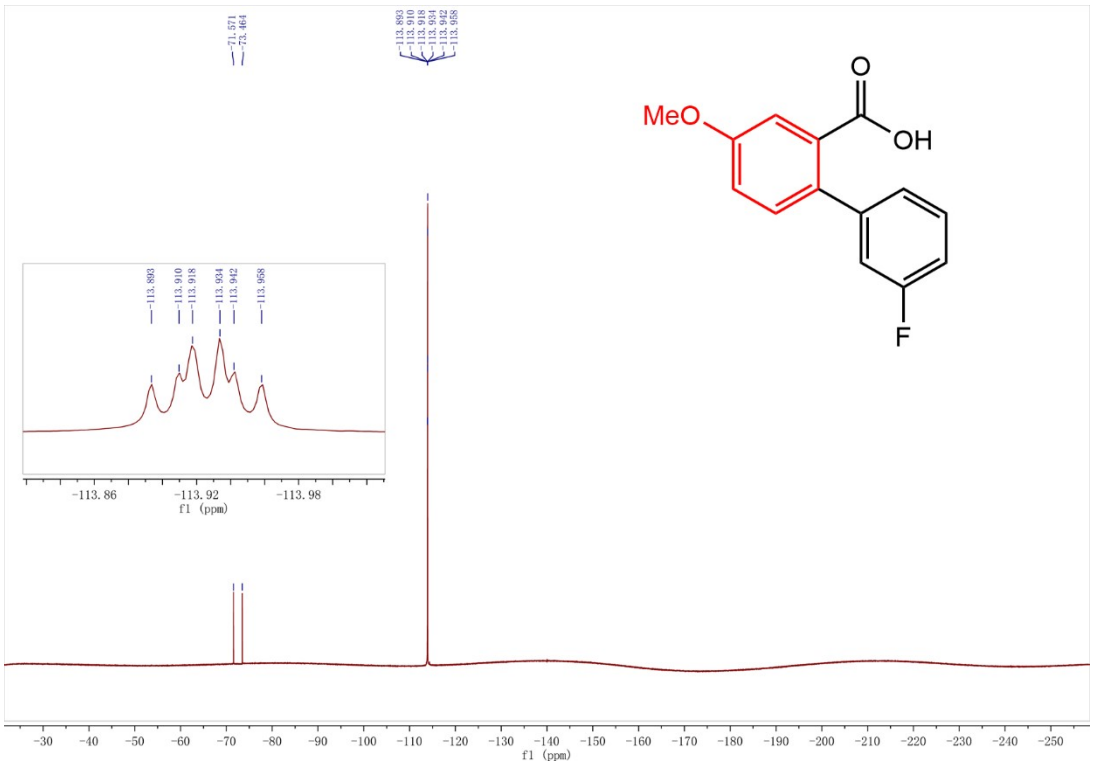



**Figure S25**. $^{19}F$ NMR Spectrum of 3'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

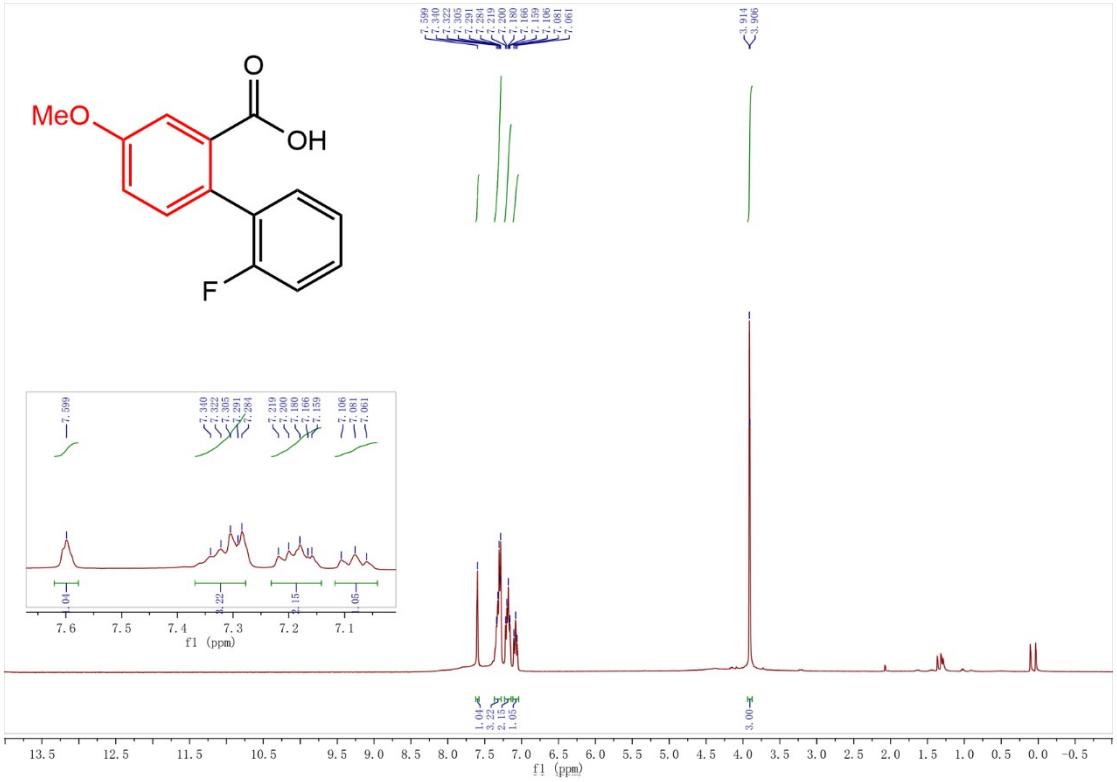



**Figure S26**. $^{1}H$ NMR Spectrum of 2'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

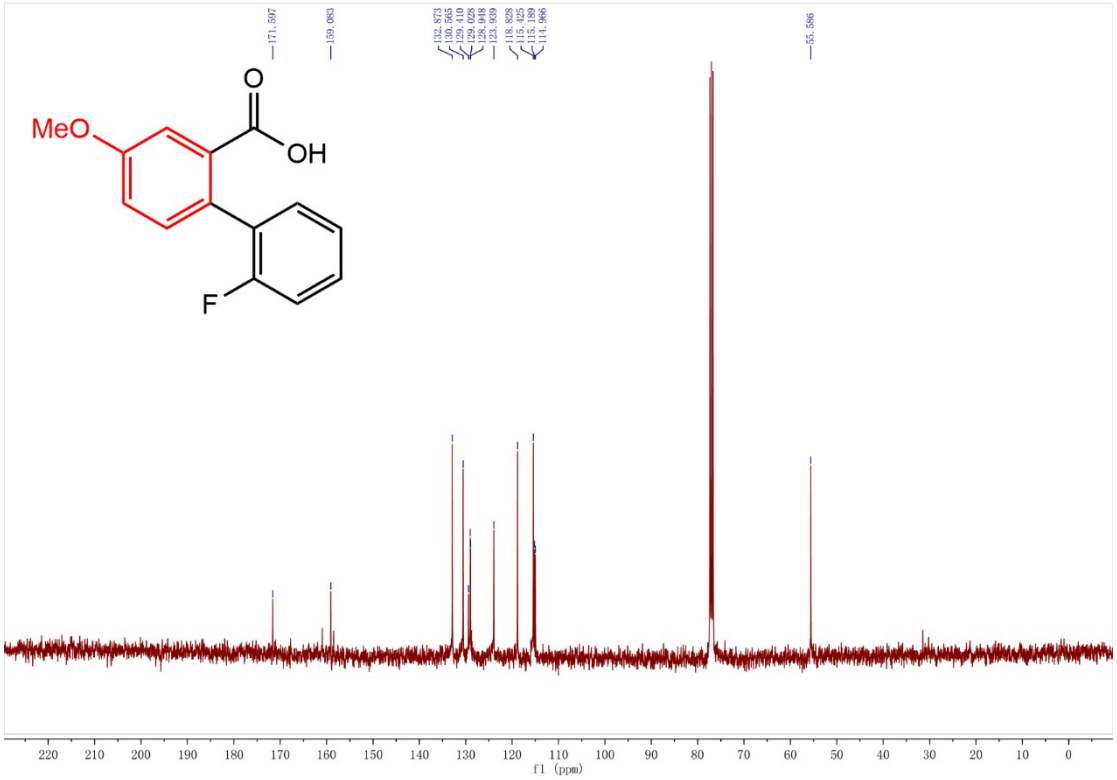



**Figure S27**.[13]C NMR Spectrum of 2'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

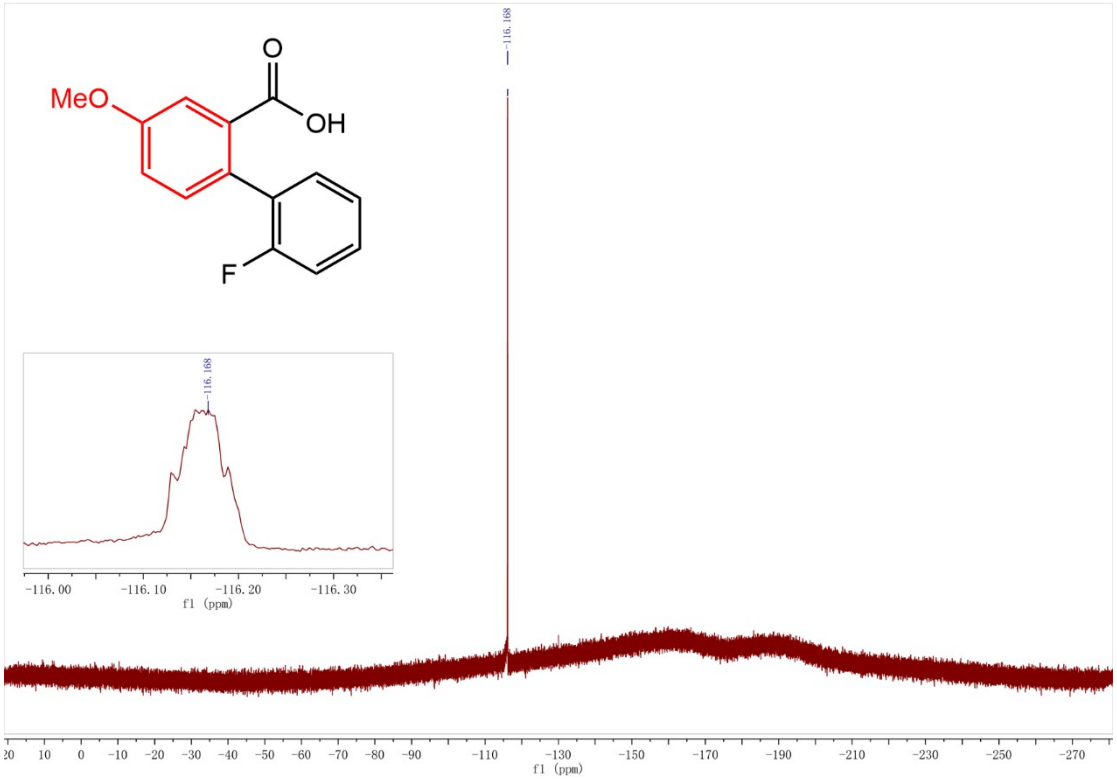



**Figure S28**. [19]F NMR Spectrum of 2'-fluoro-4-methoxy-[1,1'-biphenyl]-2-carboxylic acid

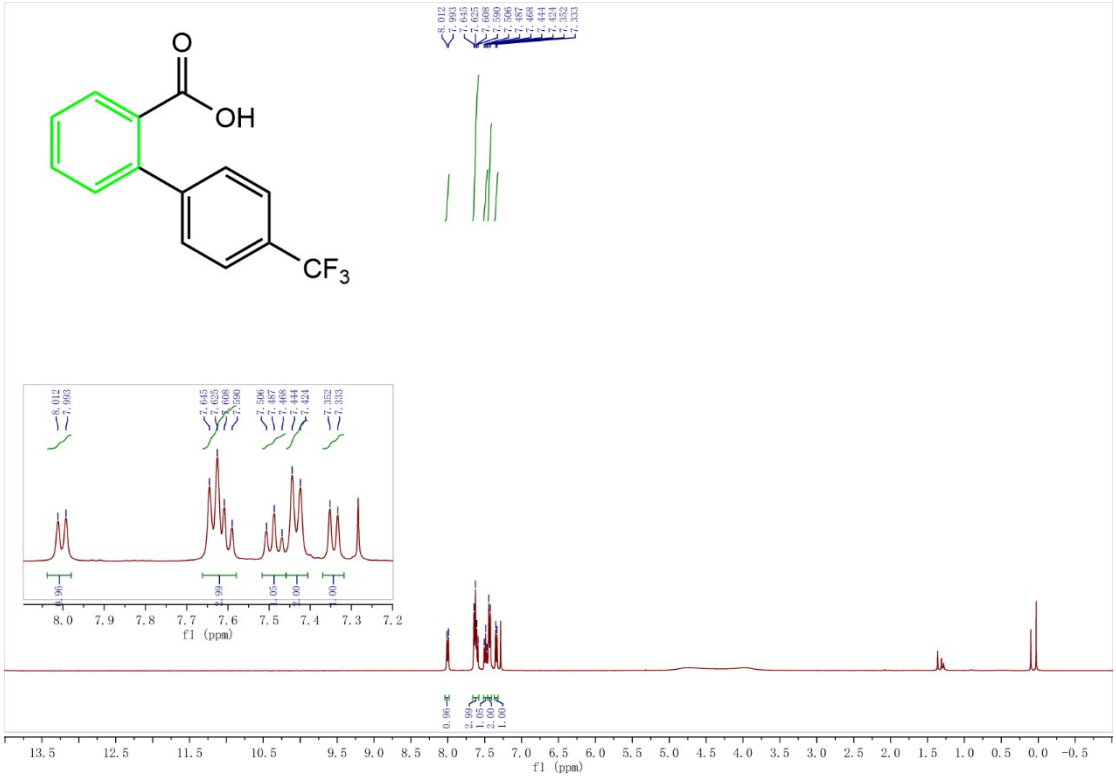



**Figure S29**. $^{1}$H NMR Spectrum of 4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

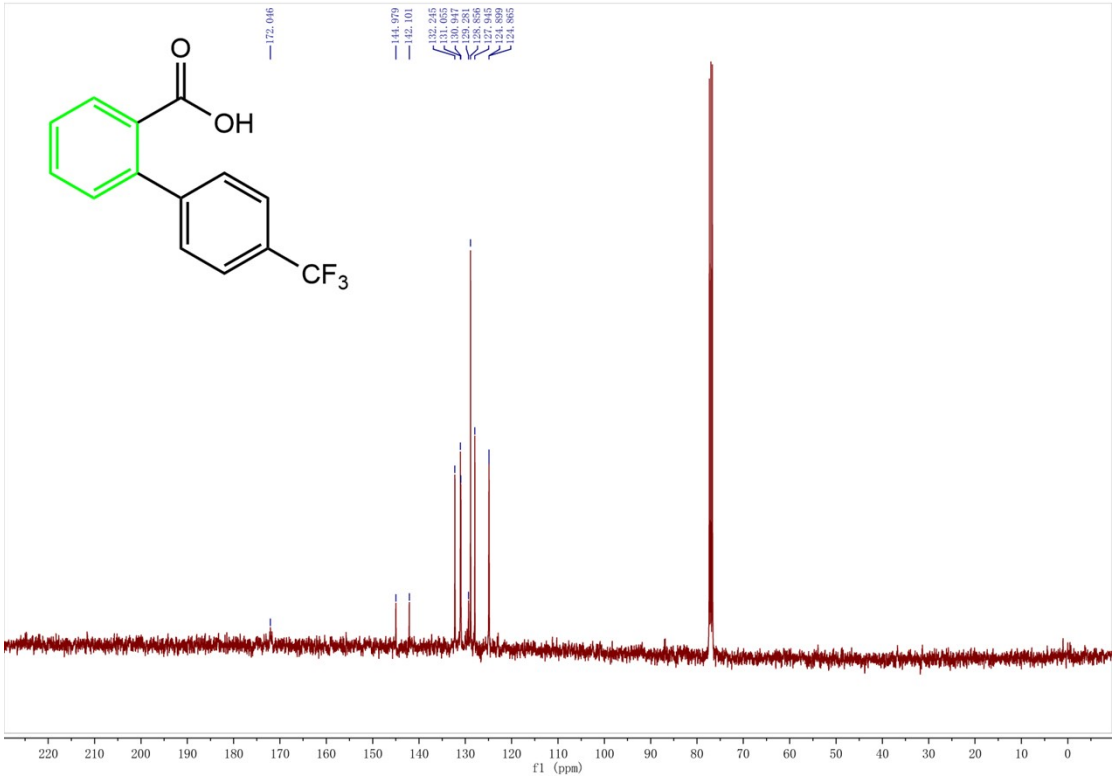



**Figure S30**. $^{13}$C NMR Spectrum of 4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

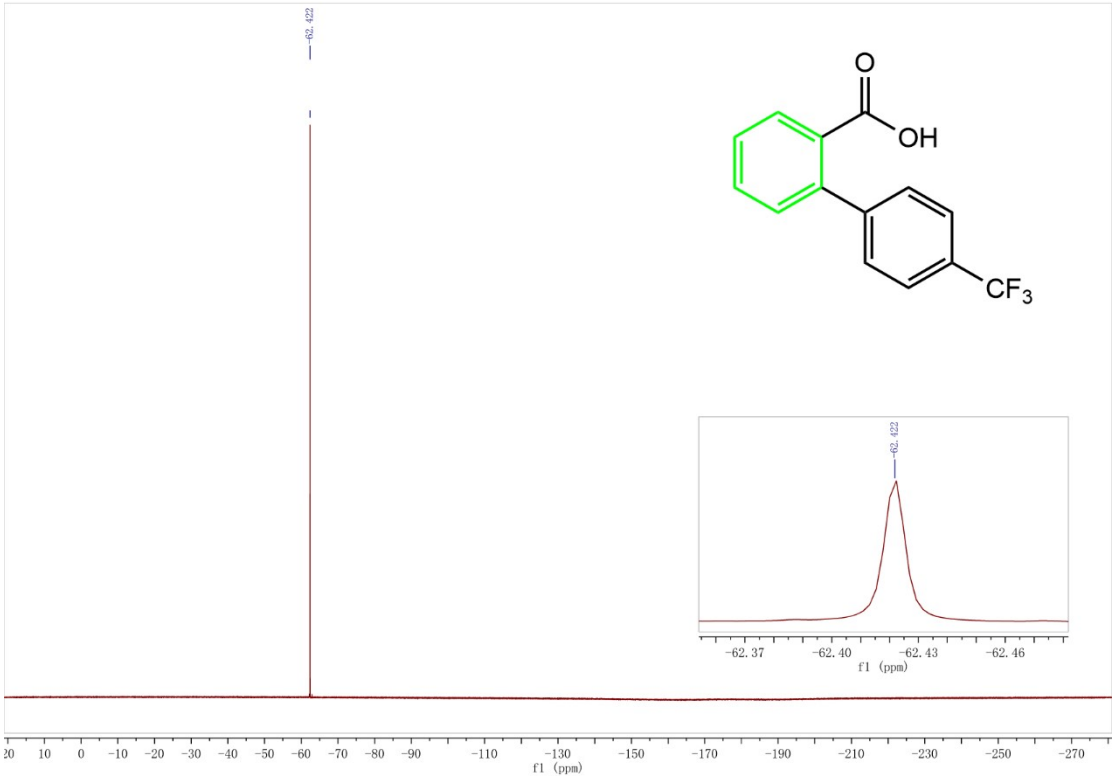



**Figure S31**. $^{19}F$ NMR Spectrum of 4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

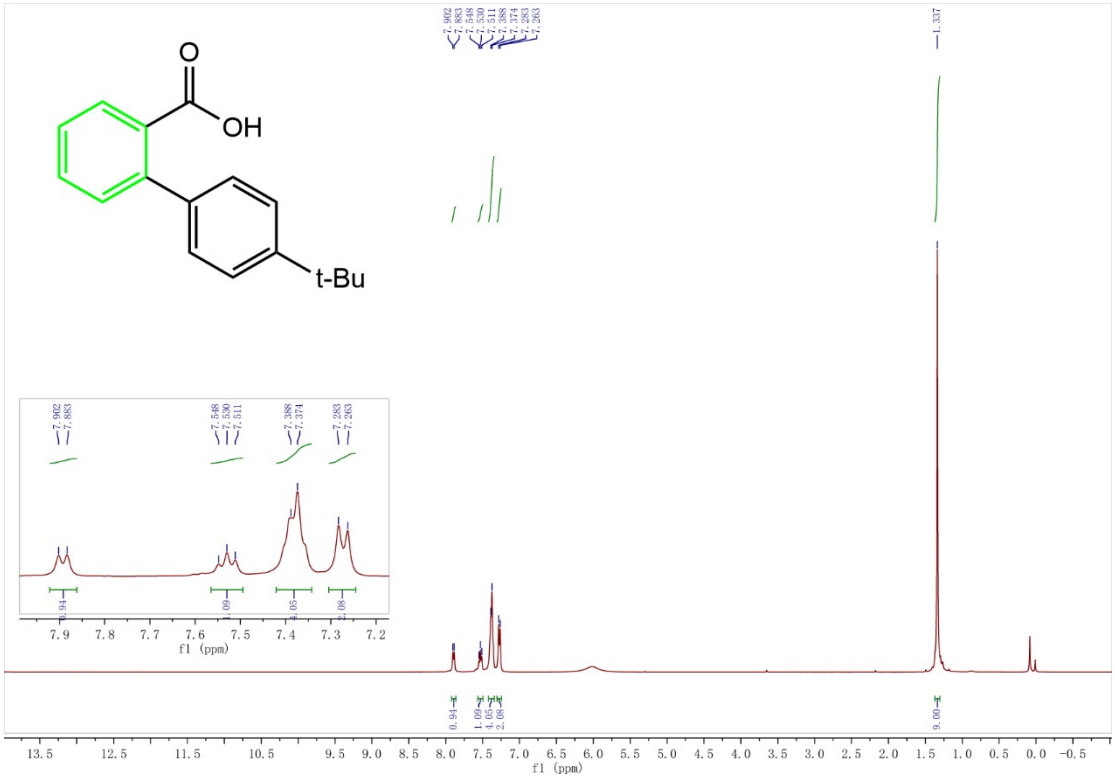



**Figure S32**. $^{1}H$ NMR Spectrum of 4'-(tert-butyl)-[1,1'-biphenyl]-2-carboxylic acid

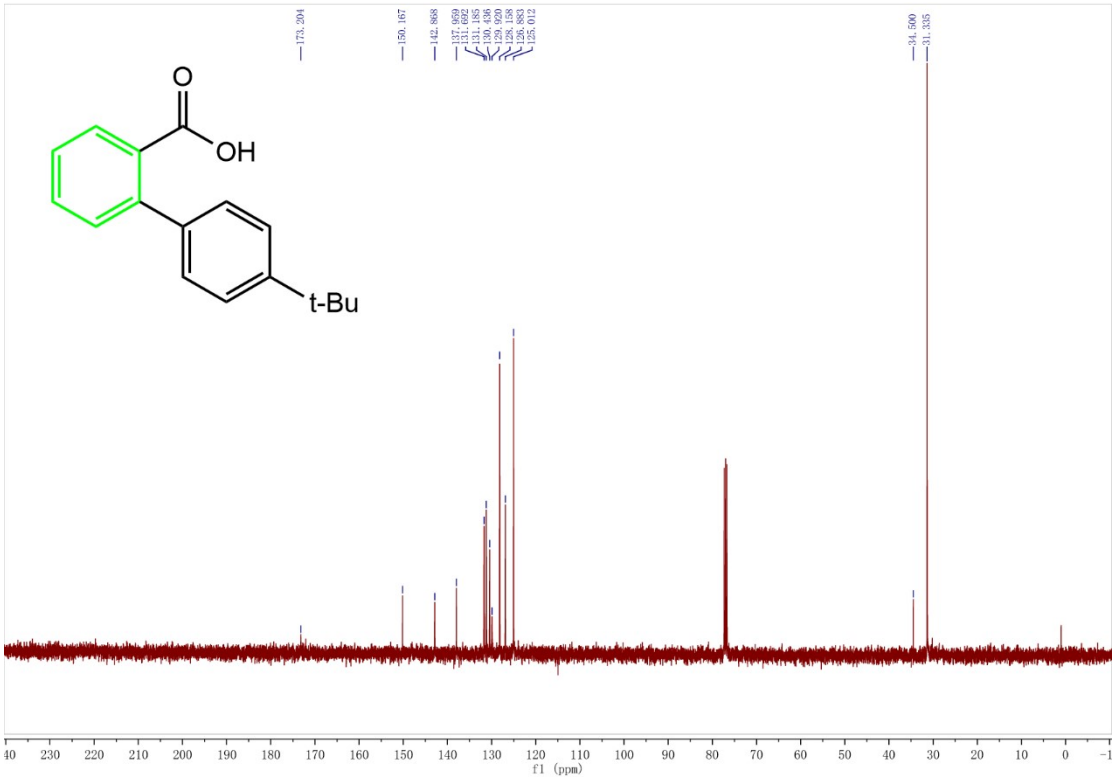



**Figure S33**. $^{13}$C NMR Spectrum of 4'-(tert-butyl)-[1,1'-biphenyl]-2-carboxylic acid

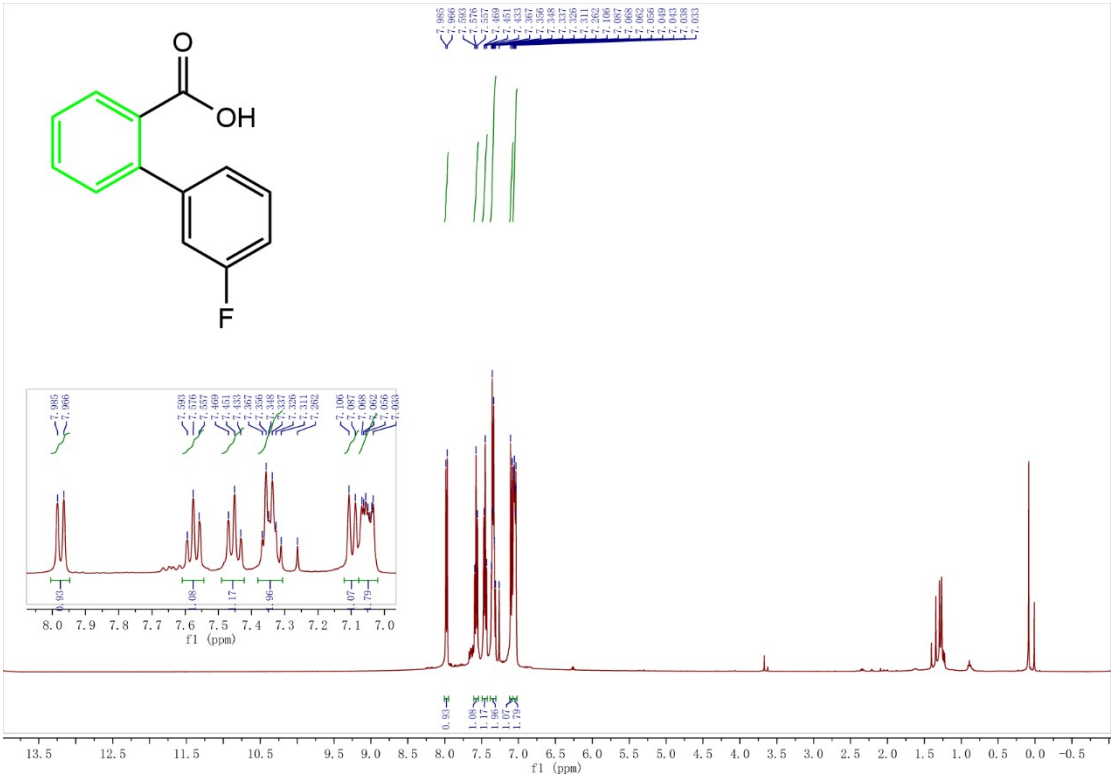



**Figure S34**. $^{1}$H NMR Spectrum of 3'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

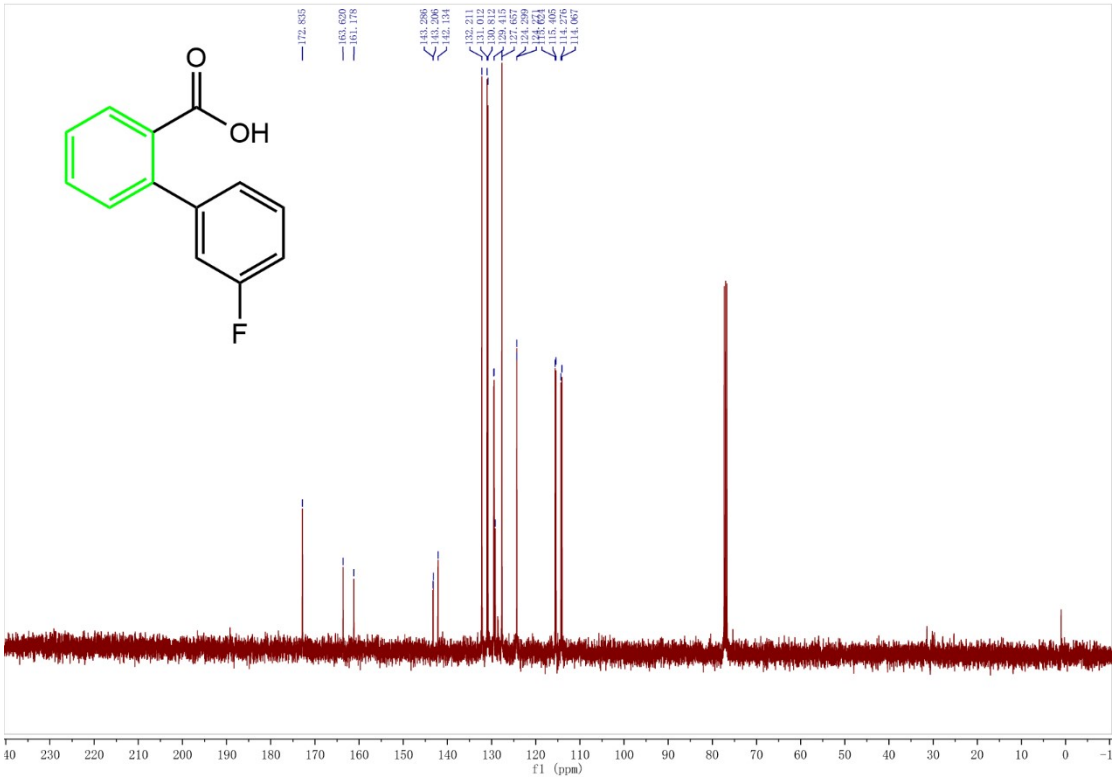



**Figure S35**. $^{13}C$ NMR Spectrum of 3'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

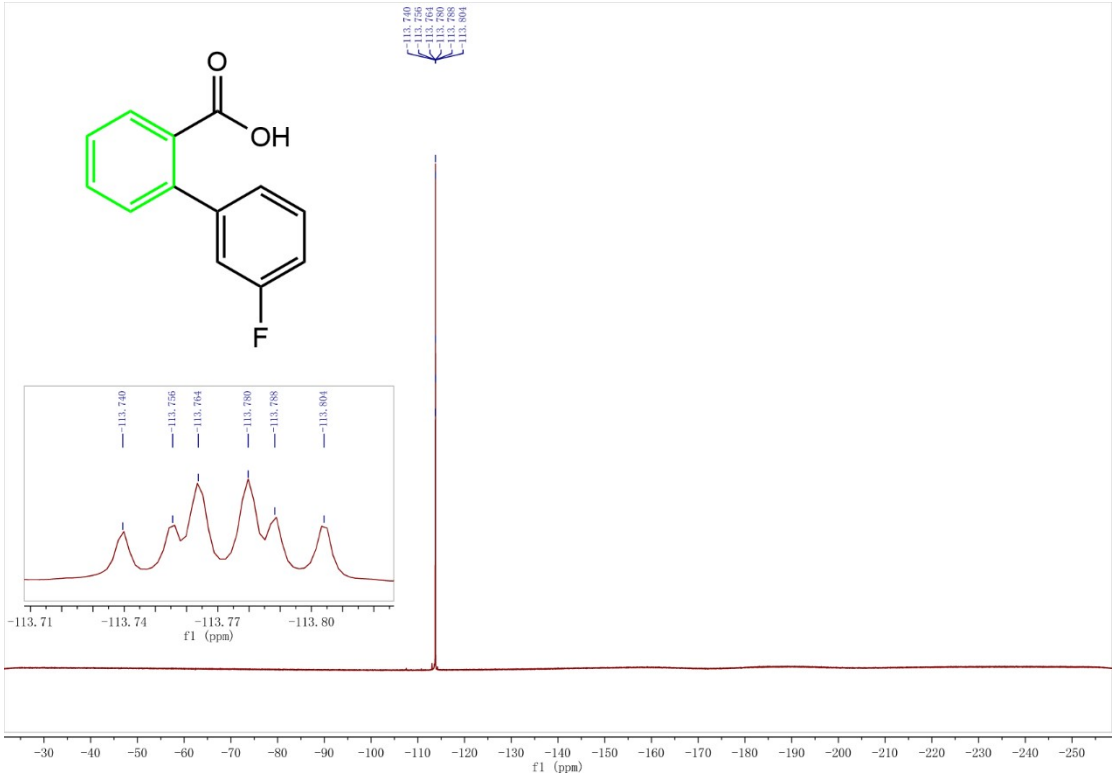



**Figure S36**. $^{19}F$ NMR Spectrum of 3'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

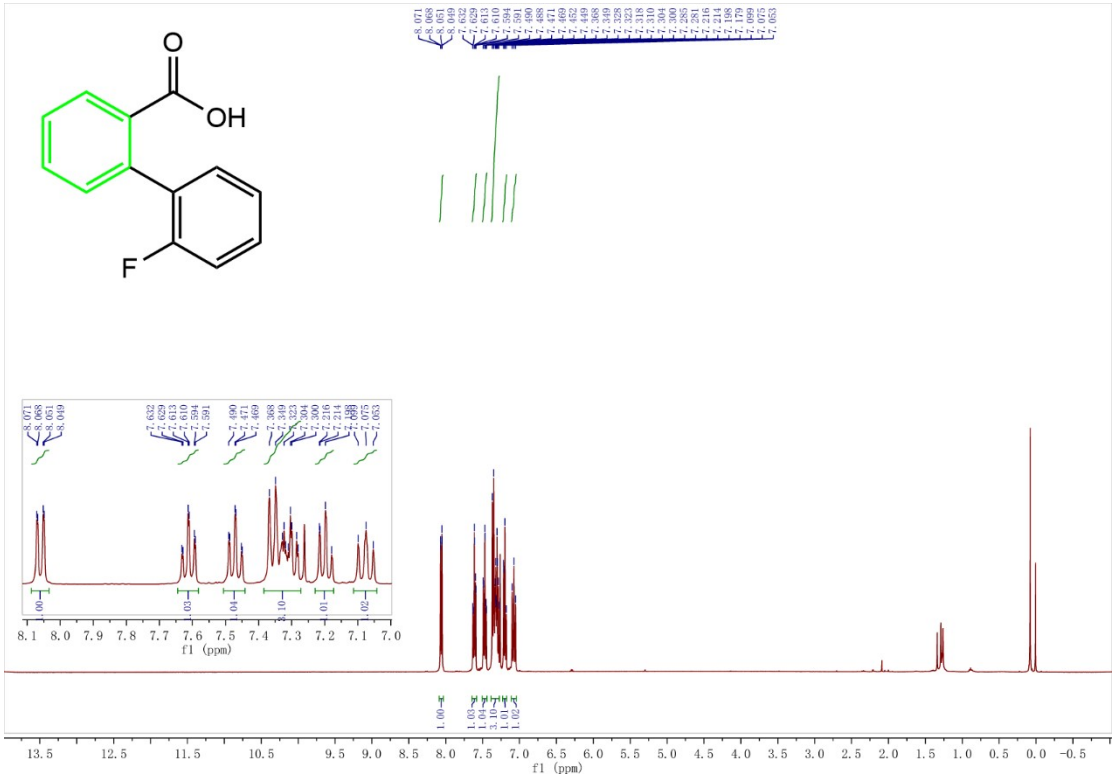



**Figure S37**. [1]H NMR Spectrum of 2'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

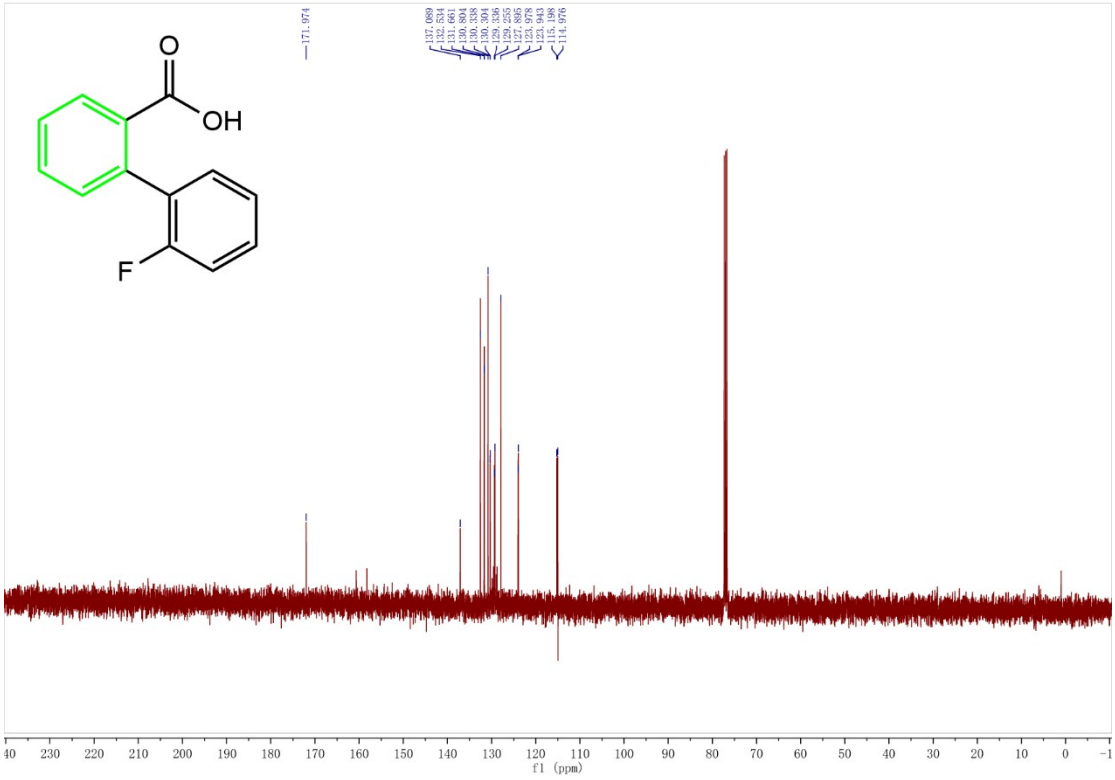



**Figure S38**. [13]C NMR Spectrum of 2'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

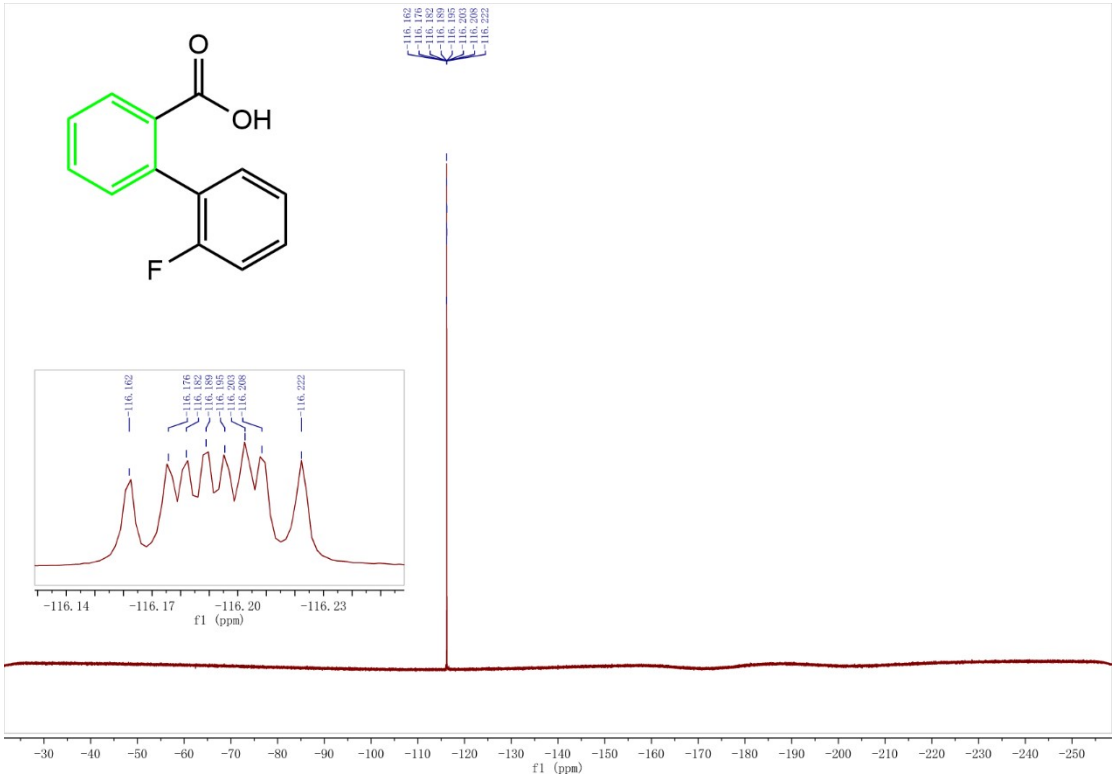



**Figure S39**. $^{19}F$ NMR Spectrum of 2'-fluoro-[1,1'-biphenyl]-2-carboxylic acid

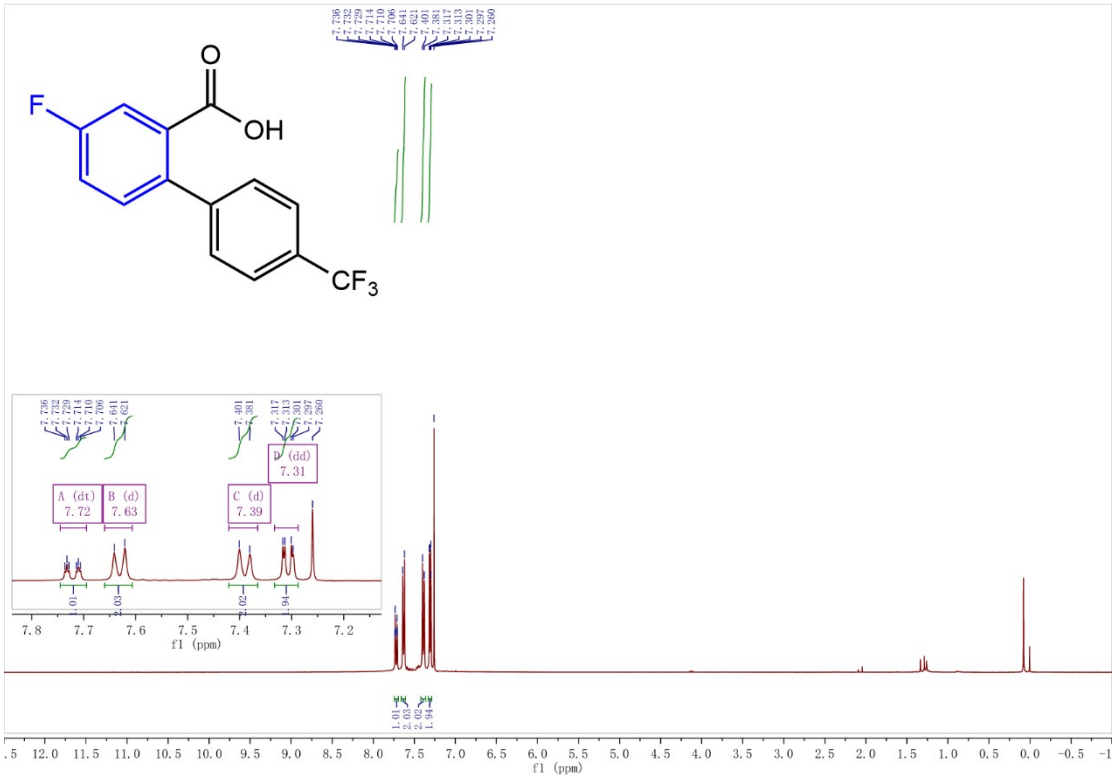



**Figure S40**. $^{1}H$ NMR Spectrum of 4-fluoro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

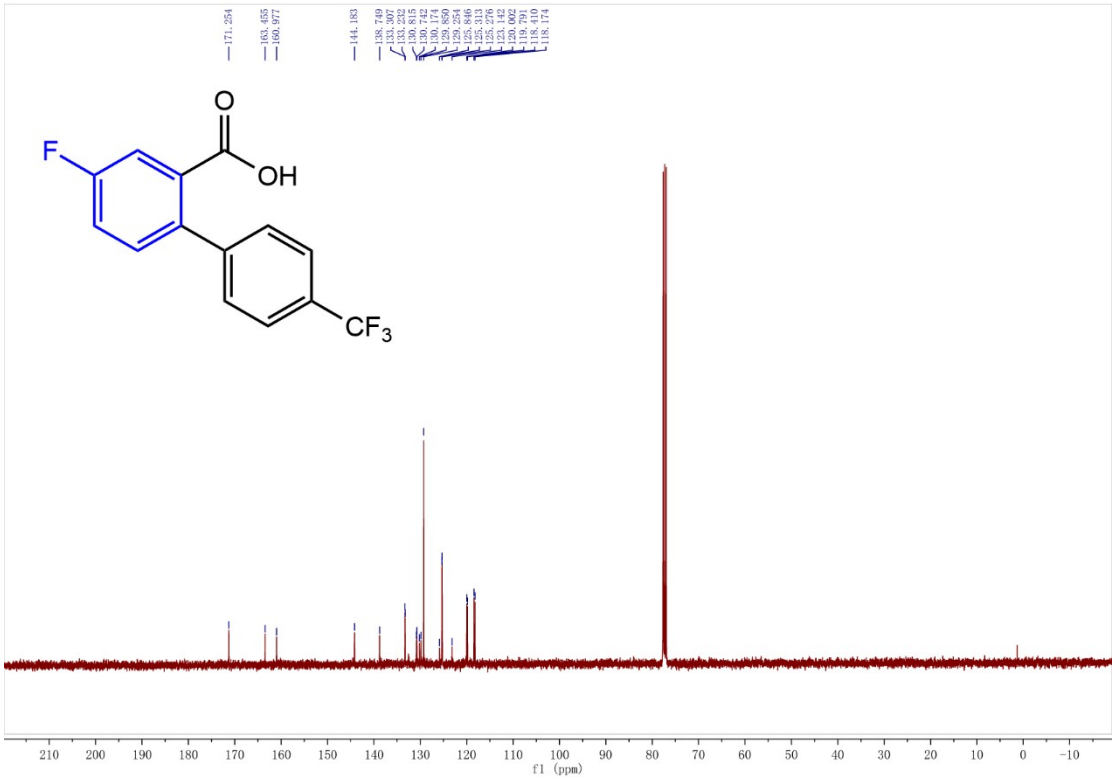



**Figure S41**. $^{13}C$ NMR Spectrum of 4-fluoro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

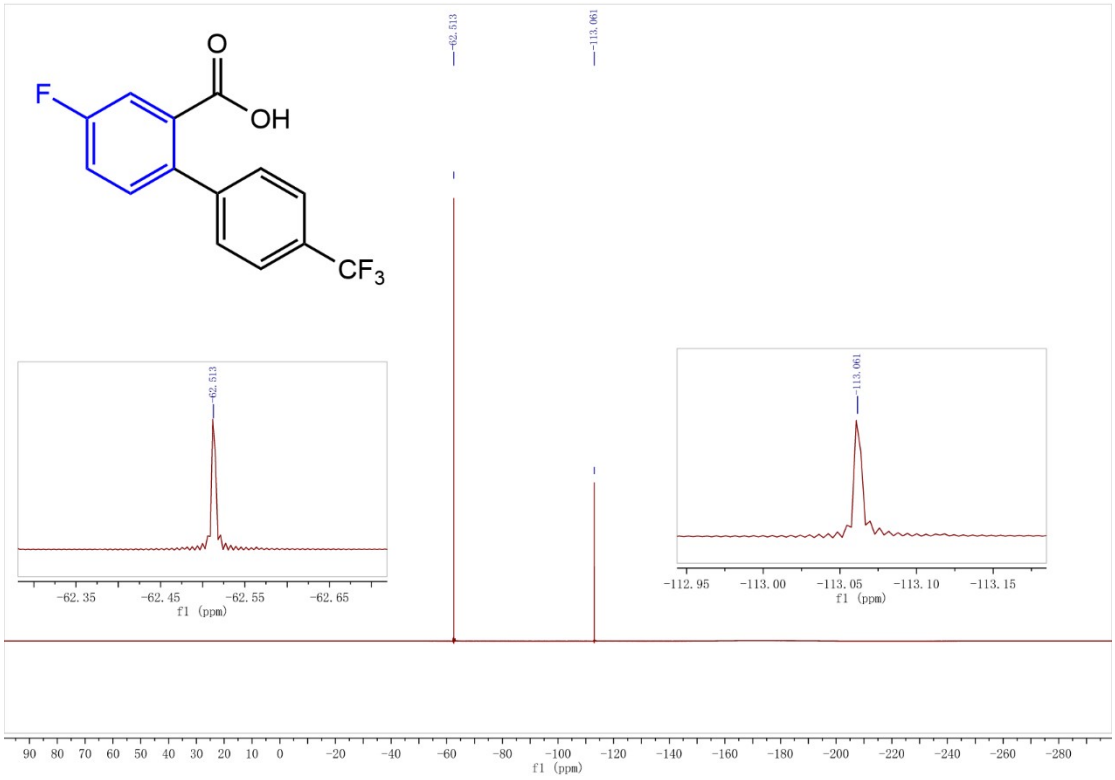



**Figure S42**. $^{19}F$ NMR Spectrum of 4-fluoro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

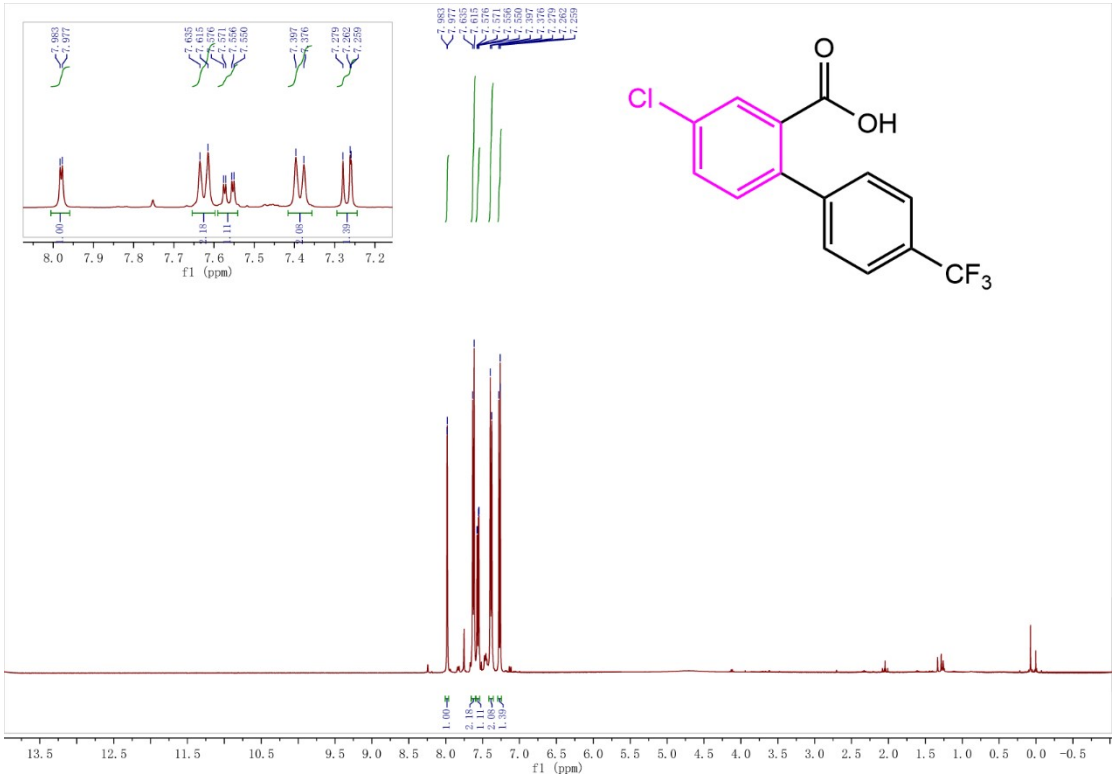



**Figure S43**. [1]H NMR Spectrum of 4-chloro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

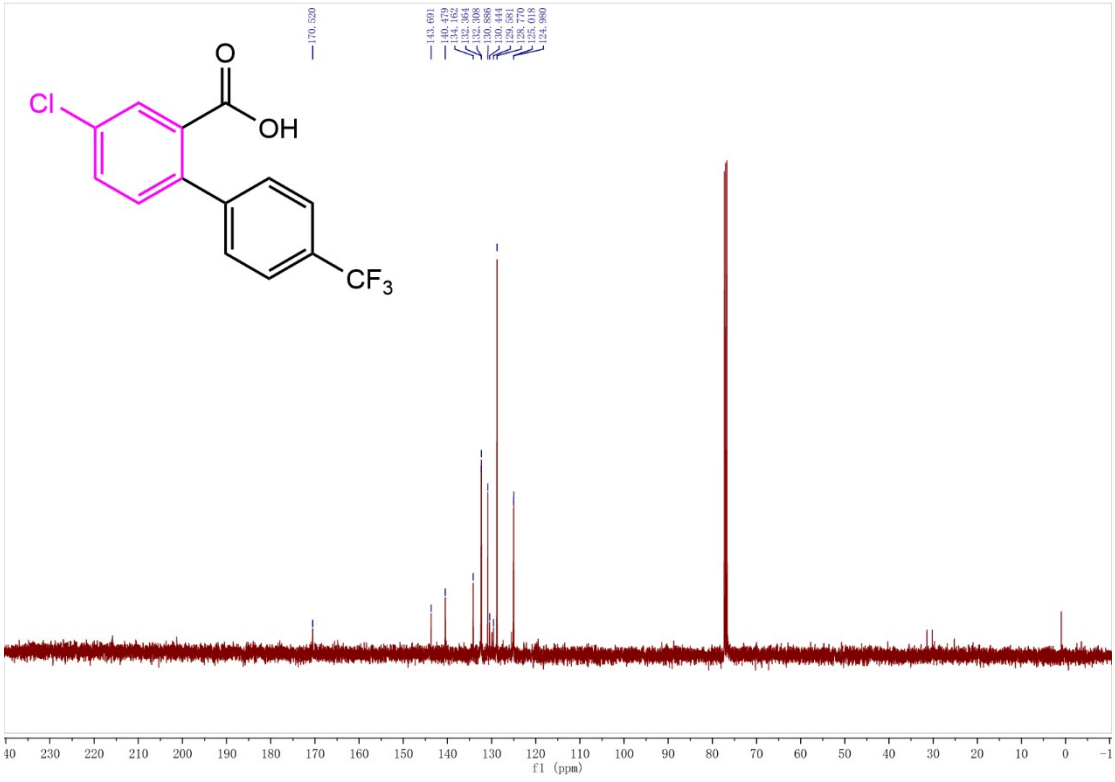



**Figure S44**. [13]C NMR Spectrum of 4-chloro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

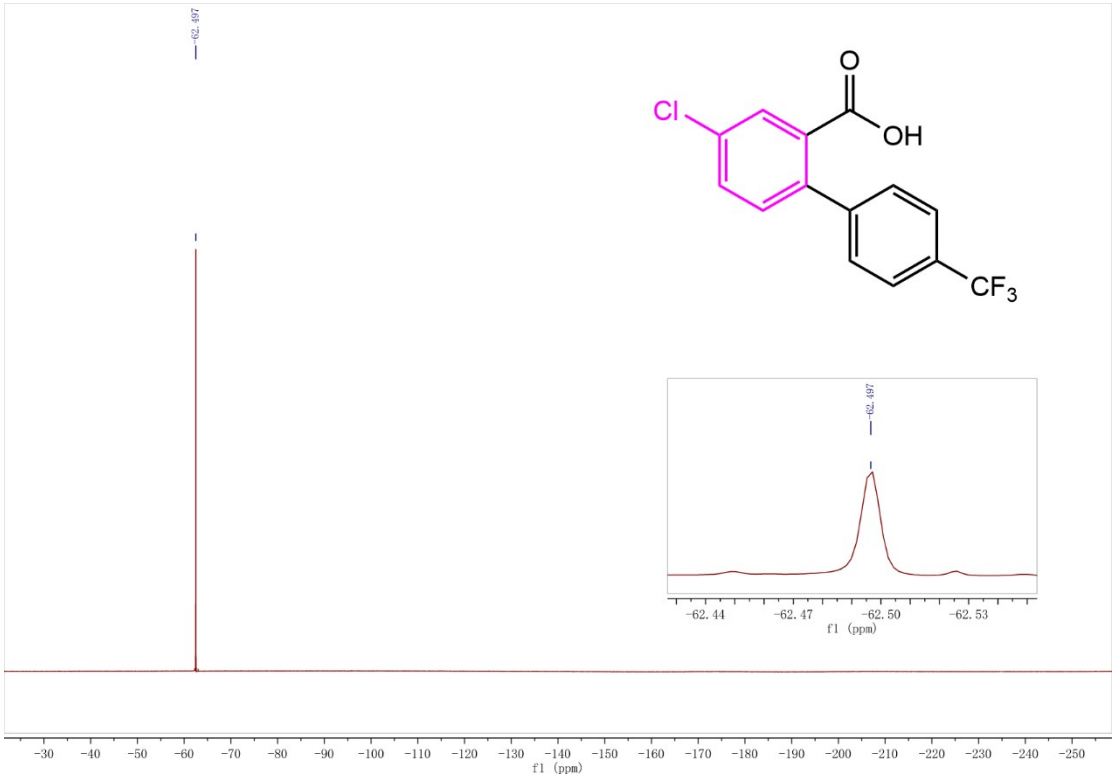



**Figure S45**. [19]F NMR Spectrum of 4-chloro-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

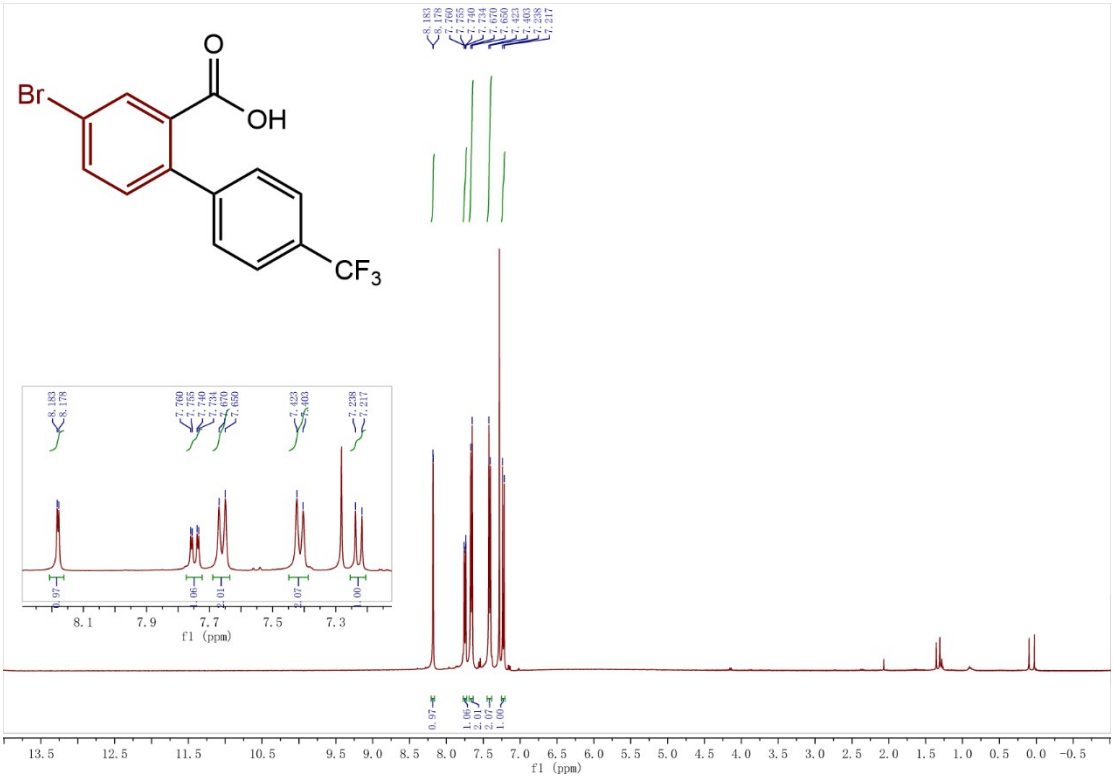



**Figure S46**. [1]H NMR Spectrum of 4-bromo-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

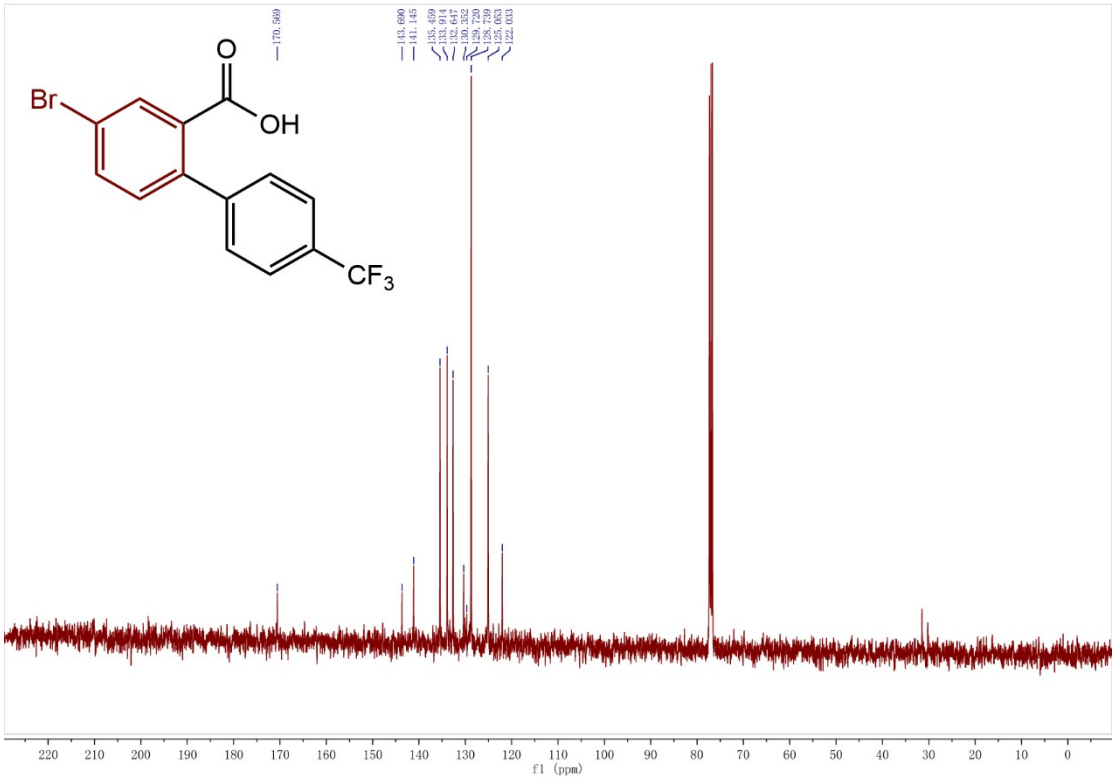



**Figure S47**. $^{13}C$ NMR Spectrum of 4-bromo-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

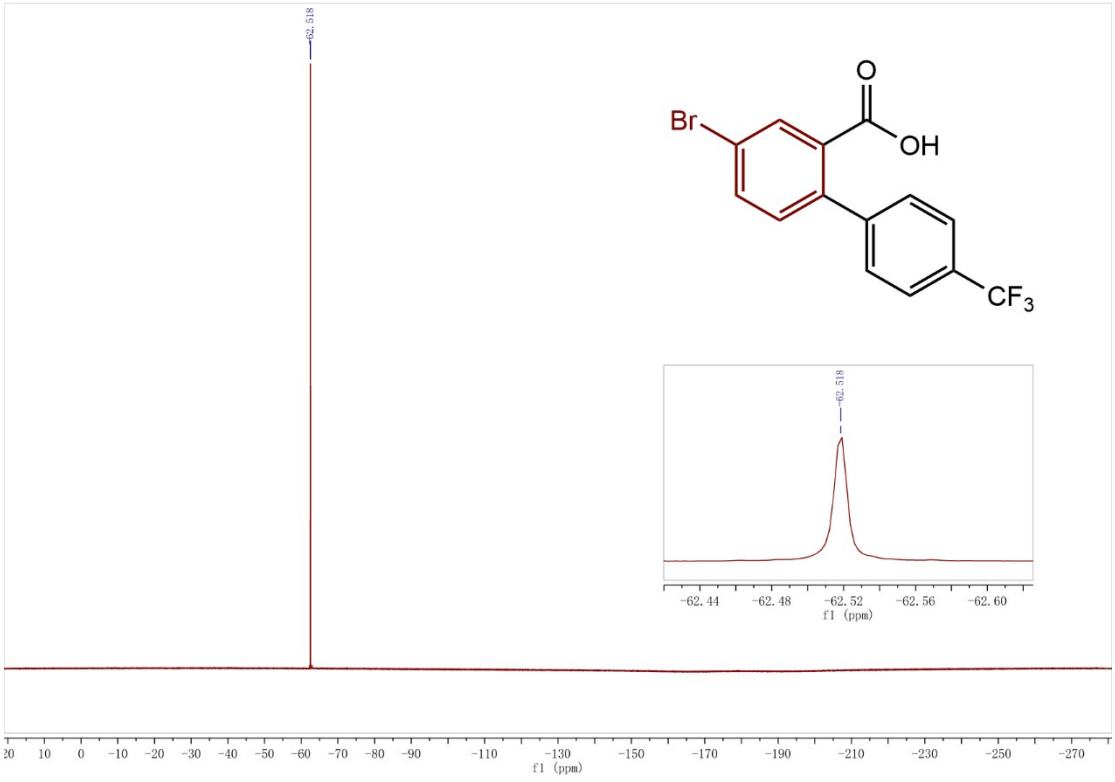



**Figure S48**. $^{19}F$ NMR Spectrum of 4-bromo-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid

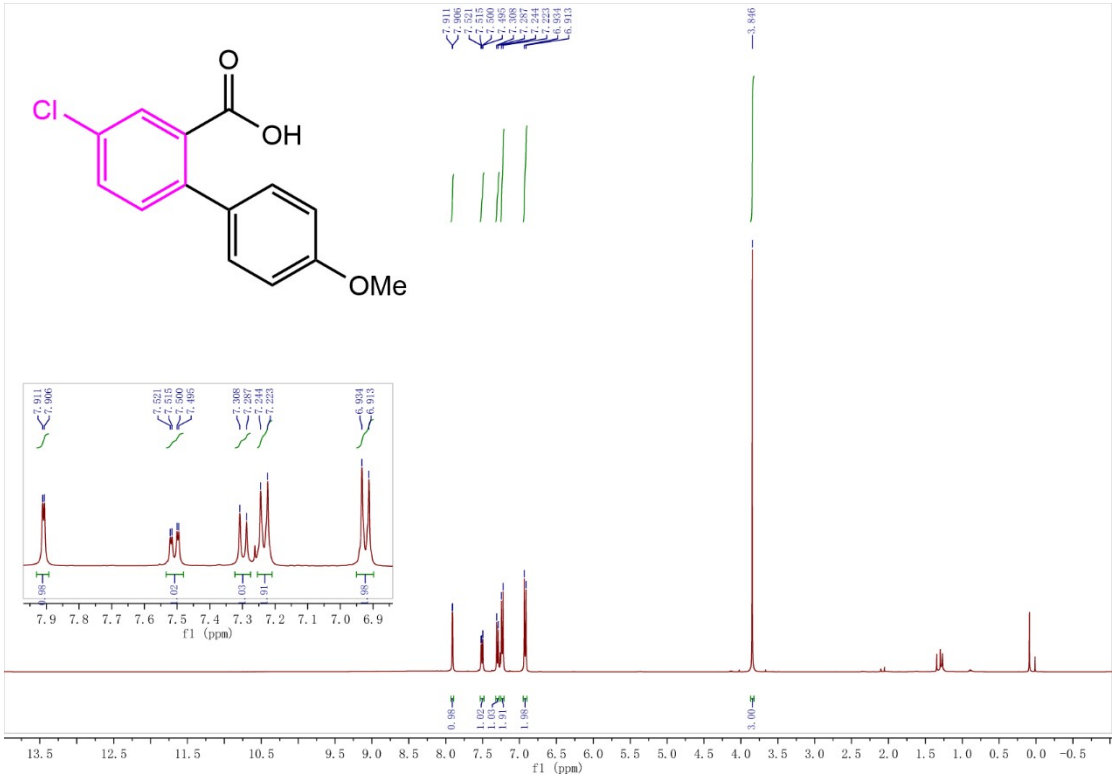



**Figure S49**. $^{1}$H NMR Spectrum of 4-chloro-4'-methoxy-[1,1'-biphenyl]-2-carboxylic acid

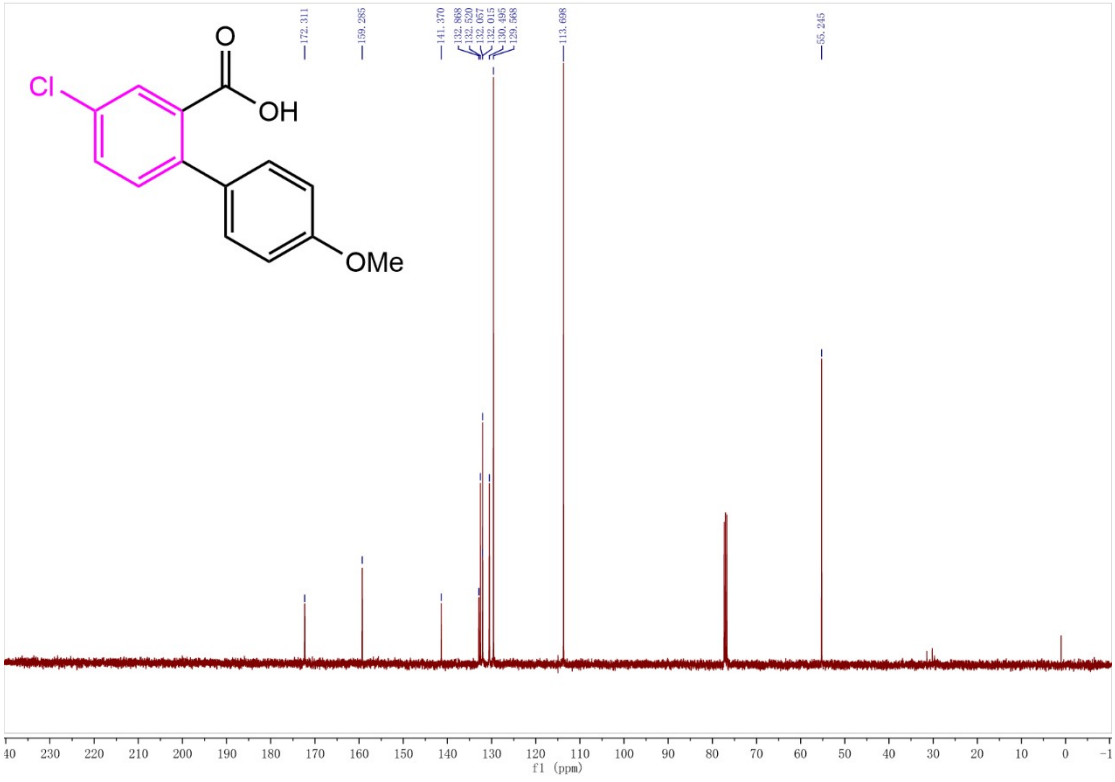



**Figure S50**. $^{13}$C NMR Spectrum of 4-chloro-4'-methoxy-[1,1'-biphenyl]-2-carboxylic acid

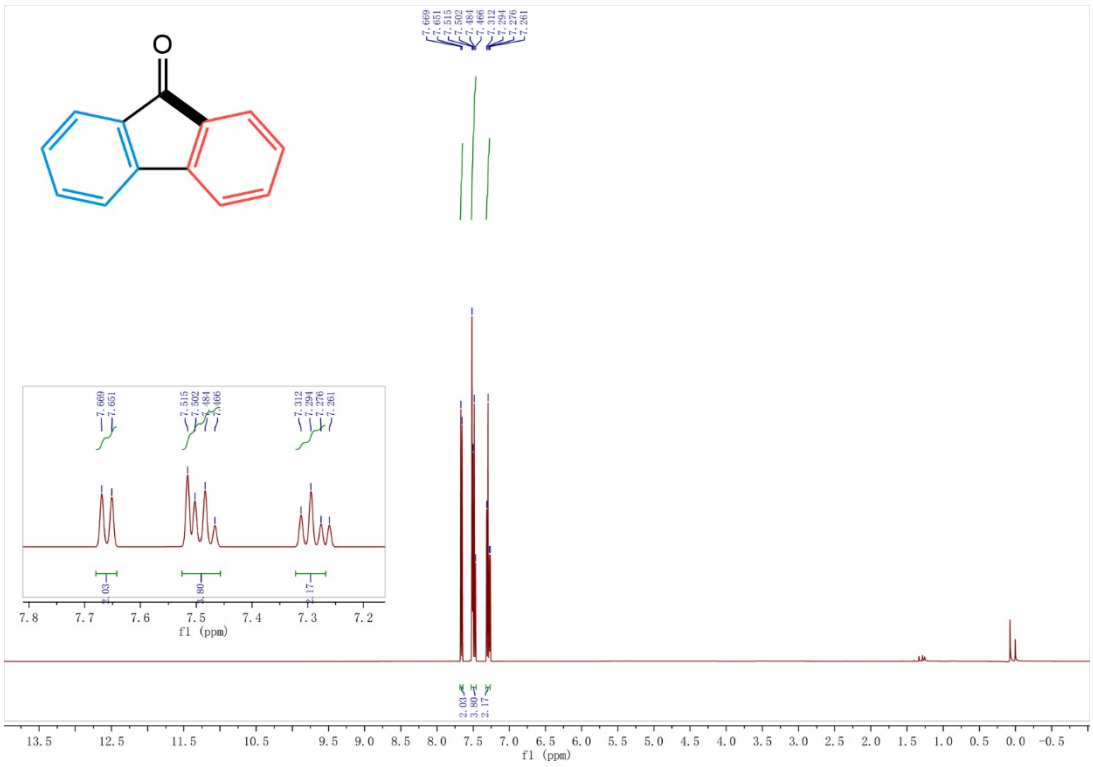


**Figure S51**. $^{1}$H NMR Spectrum of 9*H*-fluoren-9-one (**1a**)

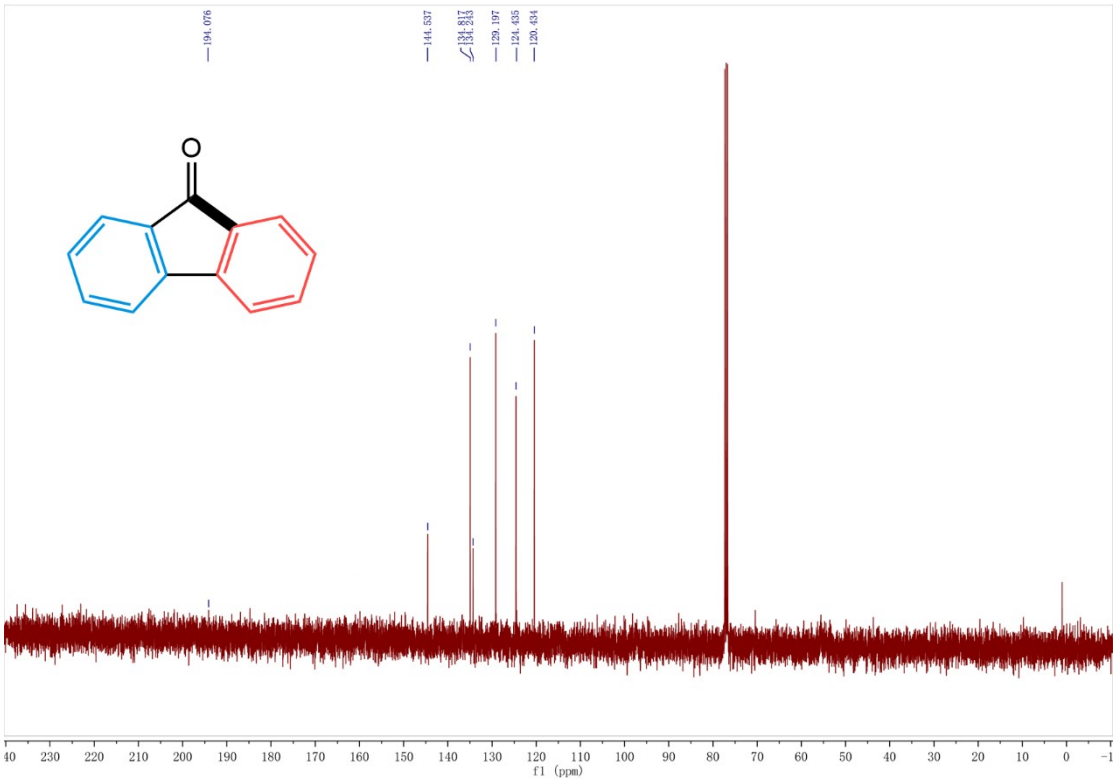


**Figure S52**. $^{13}$C NMR Spectrum of 9*H*-fluoren-9-one (**1a**)

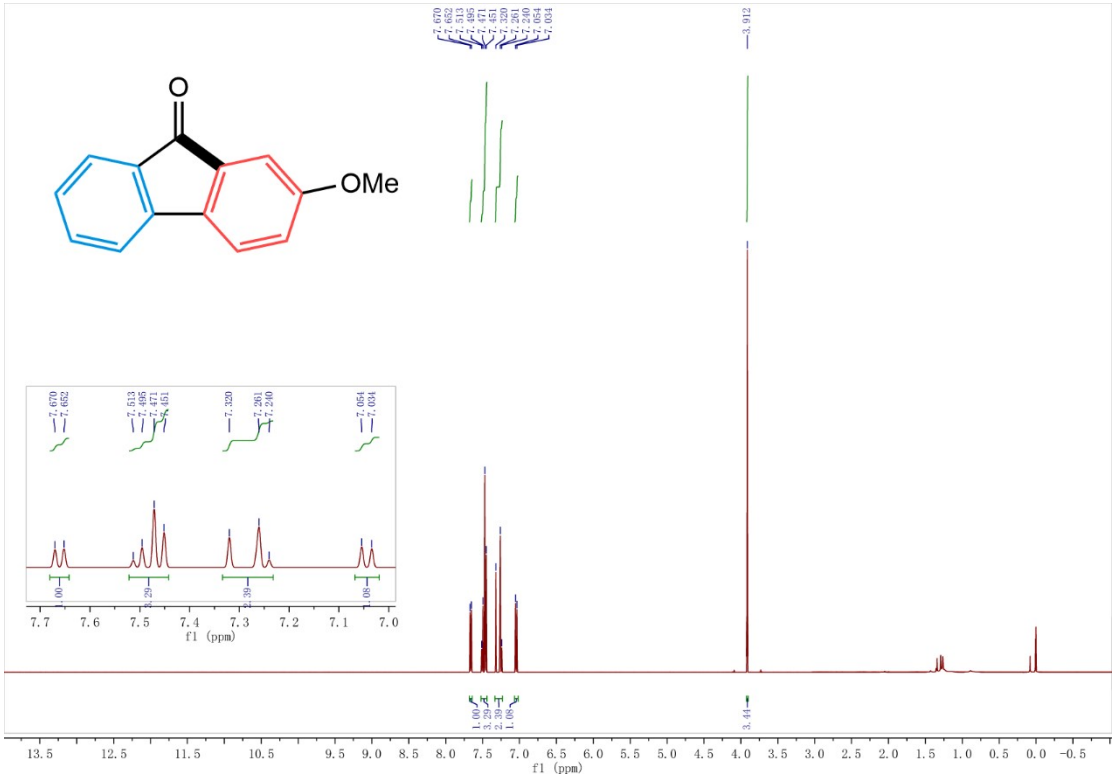



**Figure S53**. [1]H NMR Spectrum of 9*H*-fluoren-9-one 2-methoxy-9H-fluoren-9-one (**2a**, **1b**)

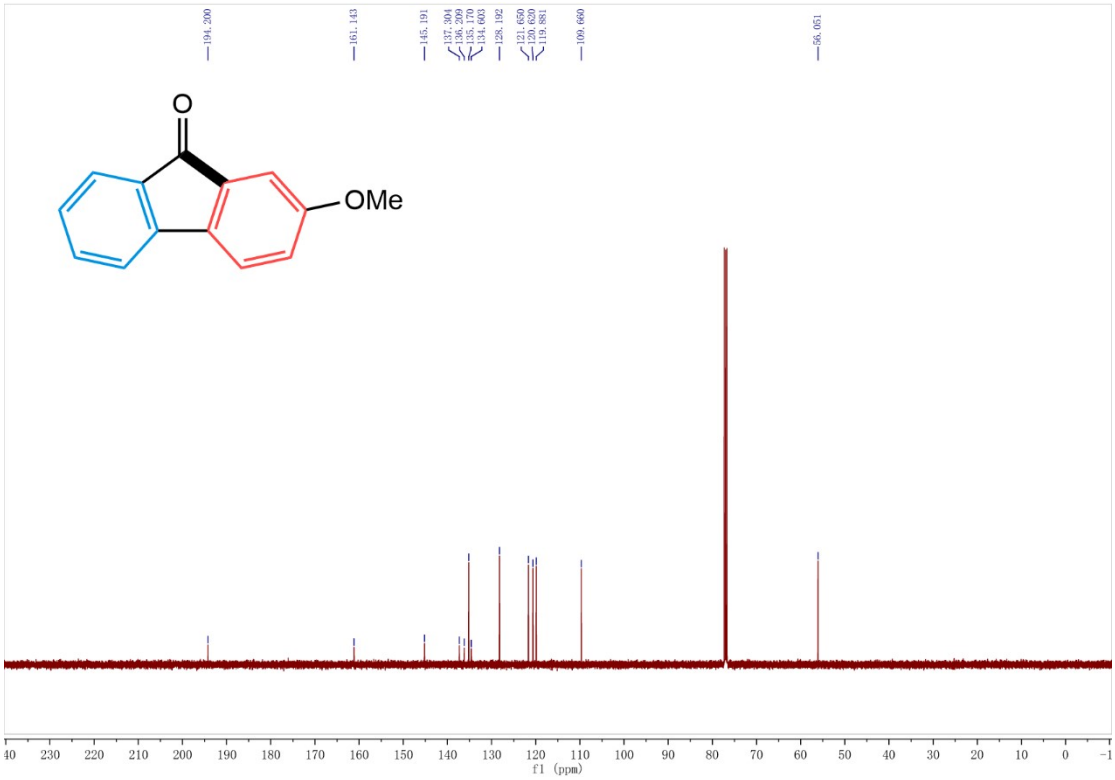



**Figure S54**. [13]C NMR Spectrum of 9*H*-fluoren-9-one 2-methoxy-9H-fluoren-9-one (**2a**, **1b**)

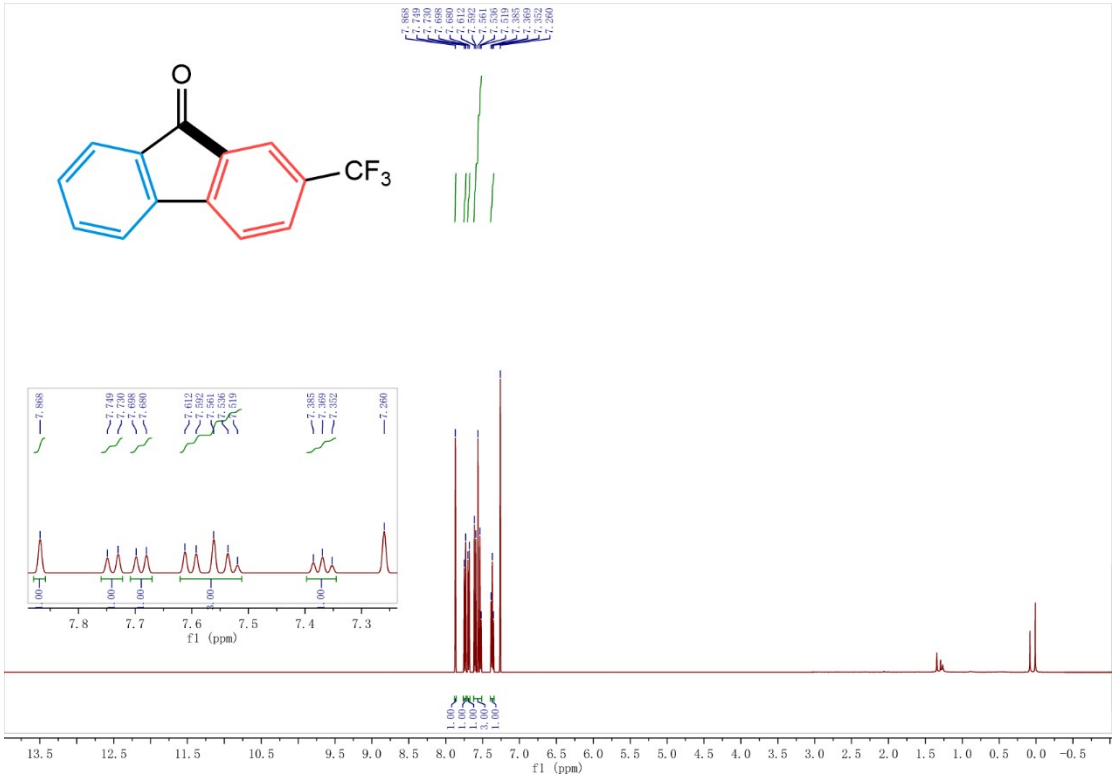



**Figure S55**. $^{1}$H NMR Spectrum of 2-(trifluoromethyl)-9H-fluoren-9-one (**1c**)

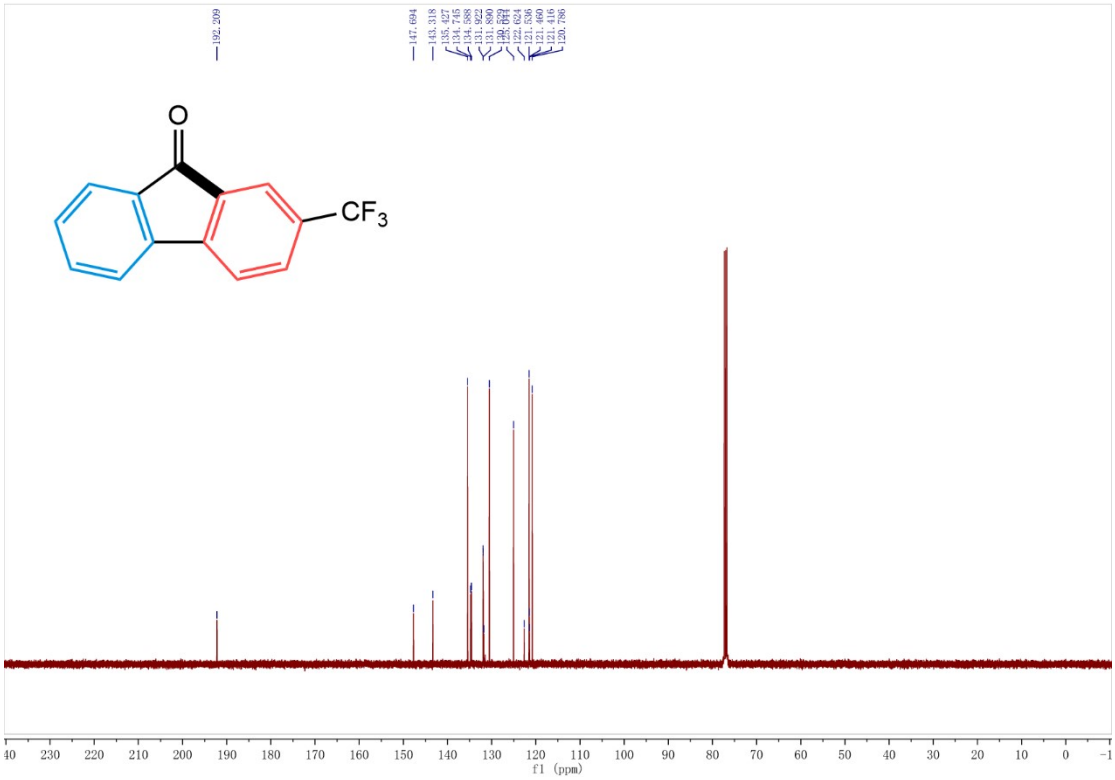



**Figure S56**. $^{13}$C NMR Spectrum of 2-(trifluoromethyl)-9H-fluoren-9-one (**1c**)

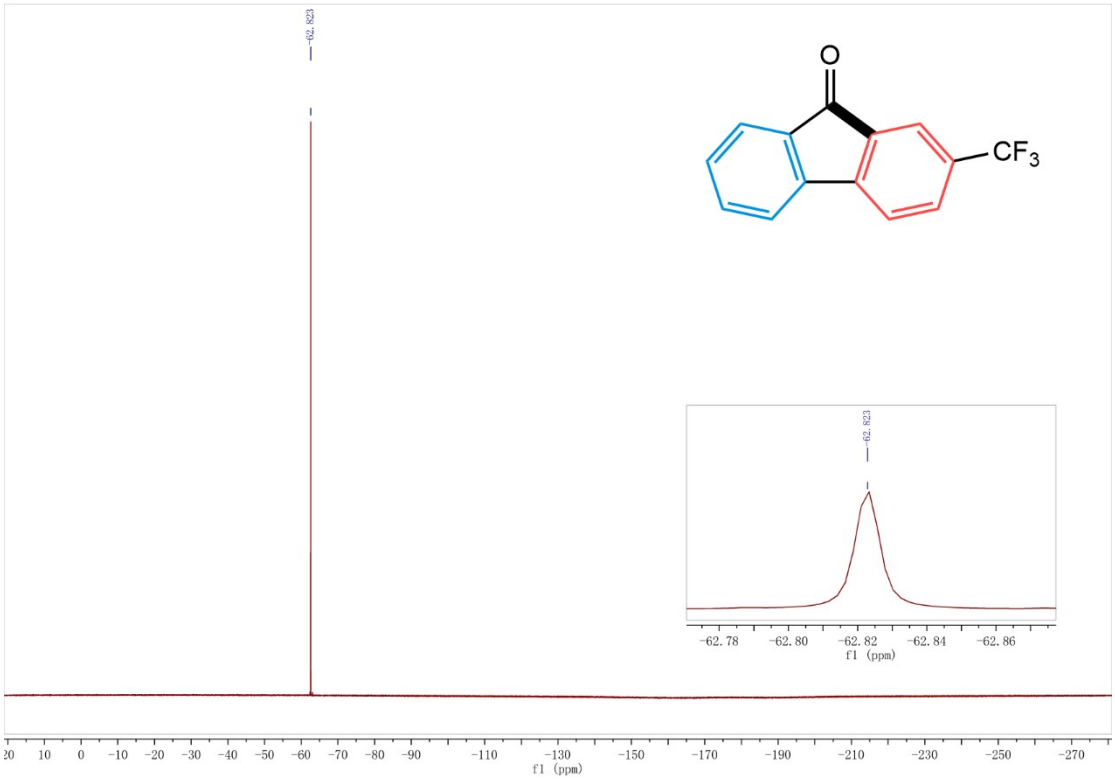



**Figure S57**. $^{19}$F NMR Spectrum of 2-(trifluoromethyl)-9H-fluoren-9-one (**1c**)

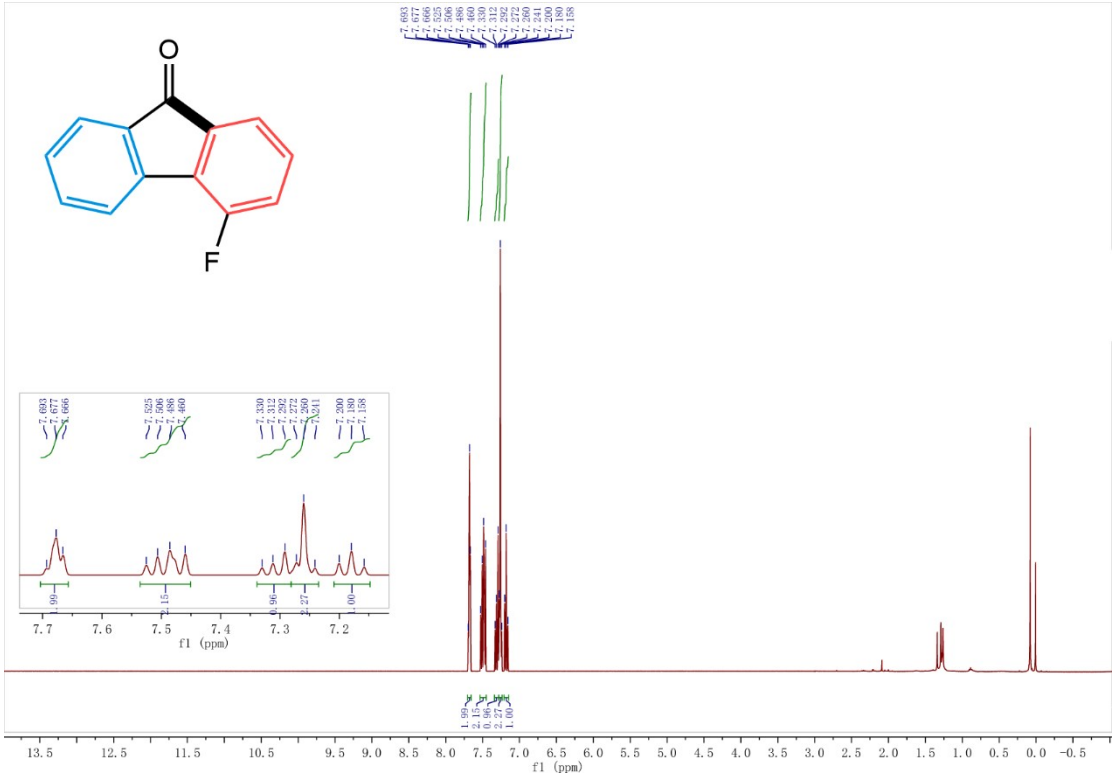



**Figure S58**. $^{1}$H NMR Spectrum of 4-fluoro-9*H*-fluoren-9-one (**1d**)

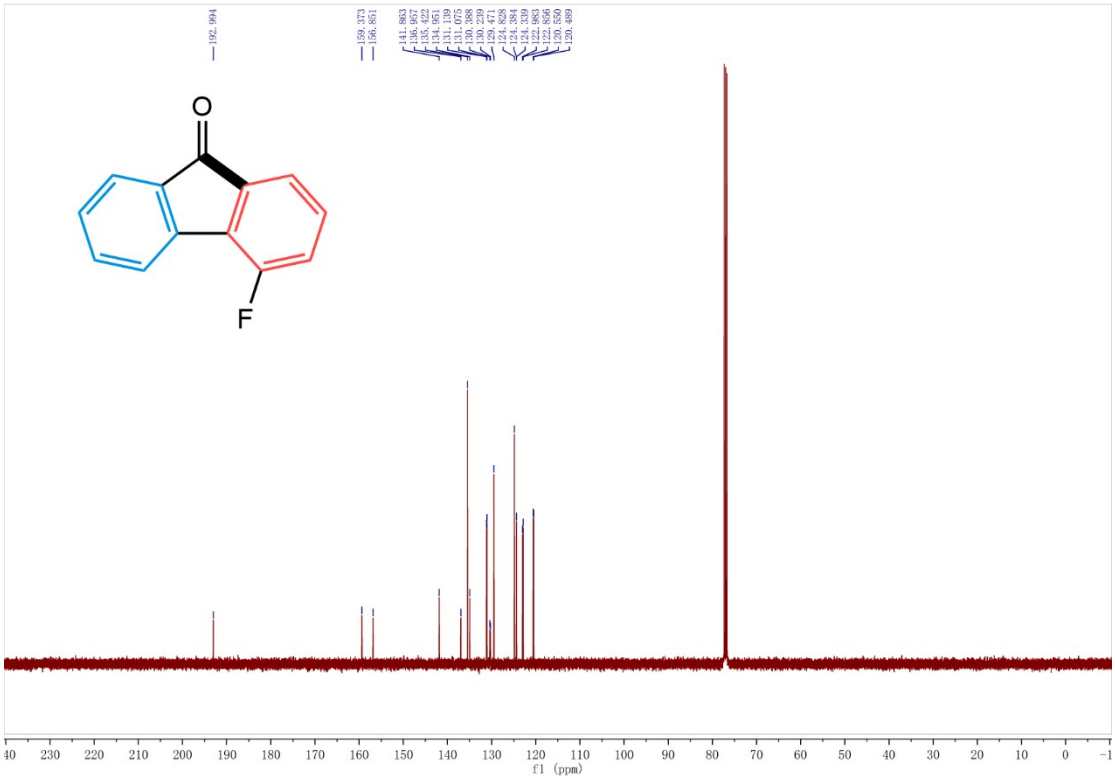



**Figure S59**. $^{13}$C NMR Spectrum of 4-fluoro-9*H*-fluoren-9-one (**1d**)

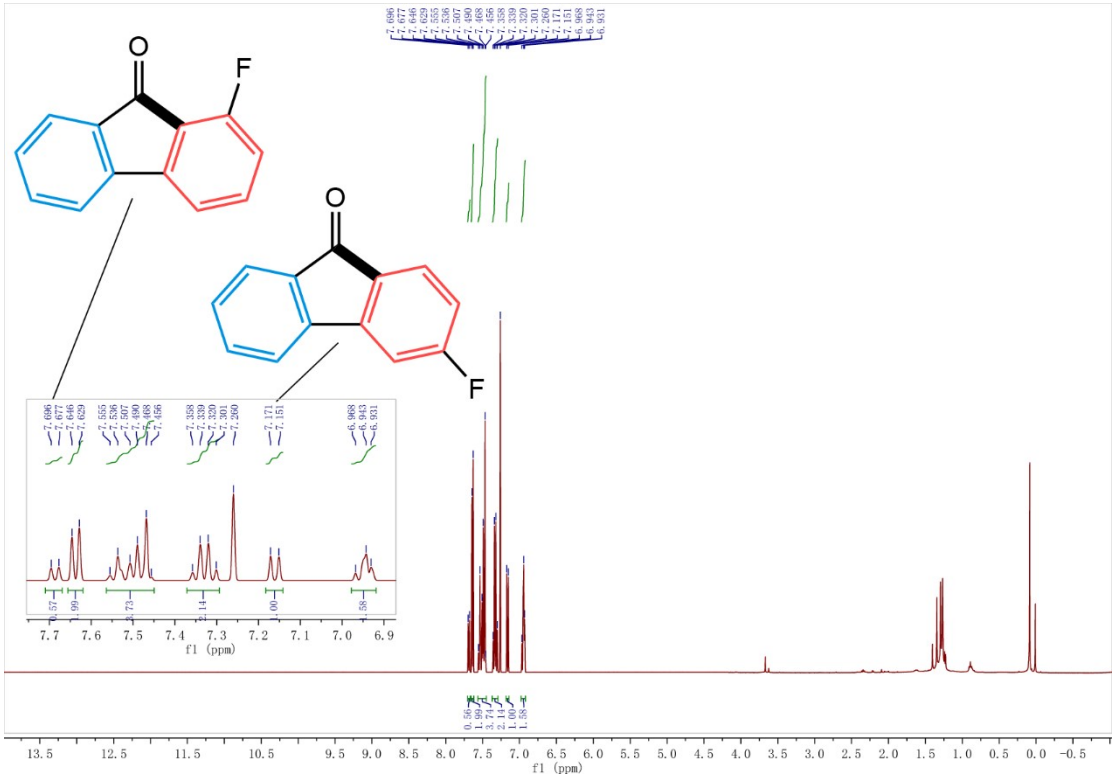



**Figure S60**. $^{1}$H NMR Spectrum of the mixture of 1-fluoro-9H-fluoren-9-one & 3-fluoro-9H-fluoren-9-one (**1e**)

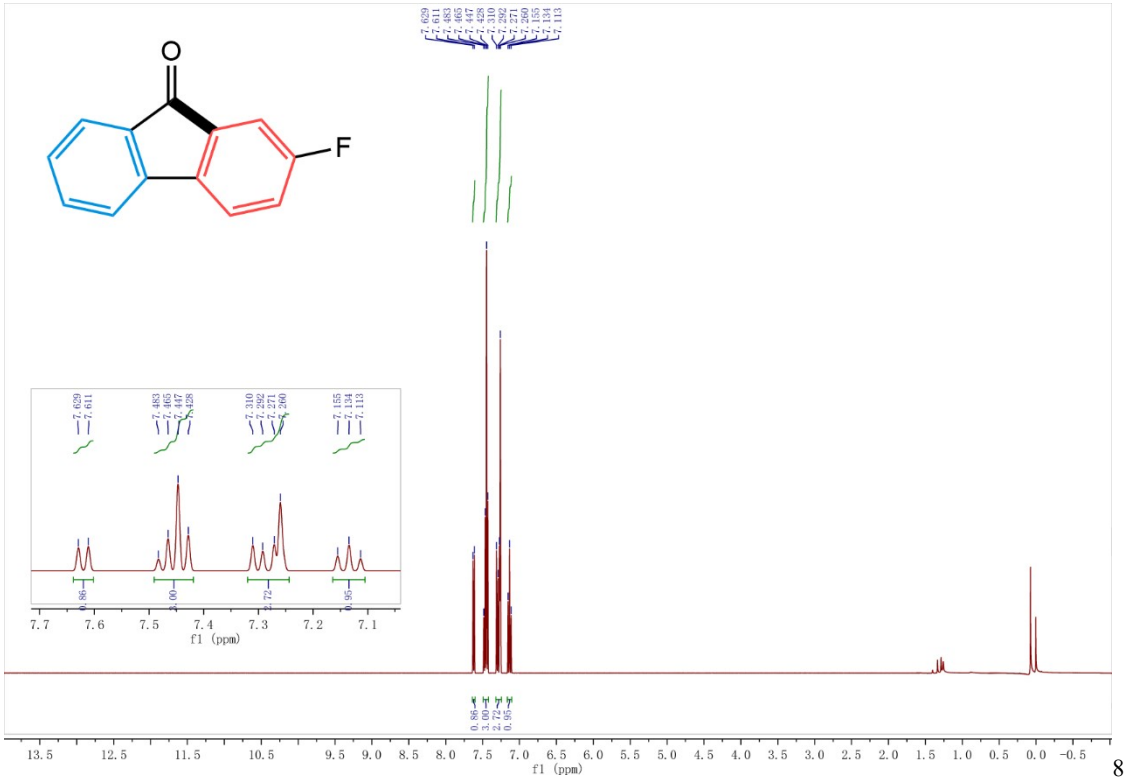



**Figure S61**. $^{1}$H NMR Spectrum of 2-fluoro-9*H*-fluoren-9-one (**1f, 3a**)

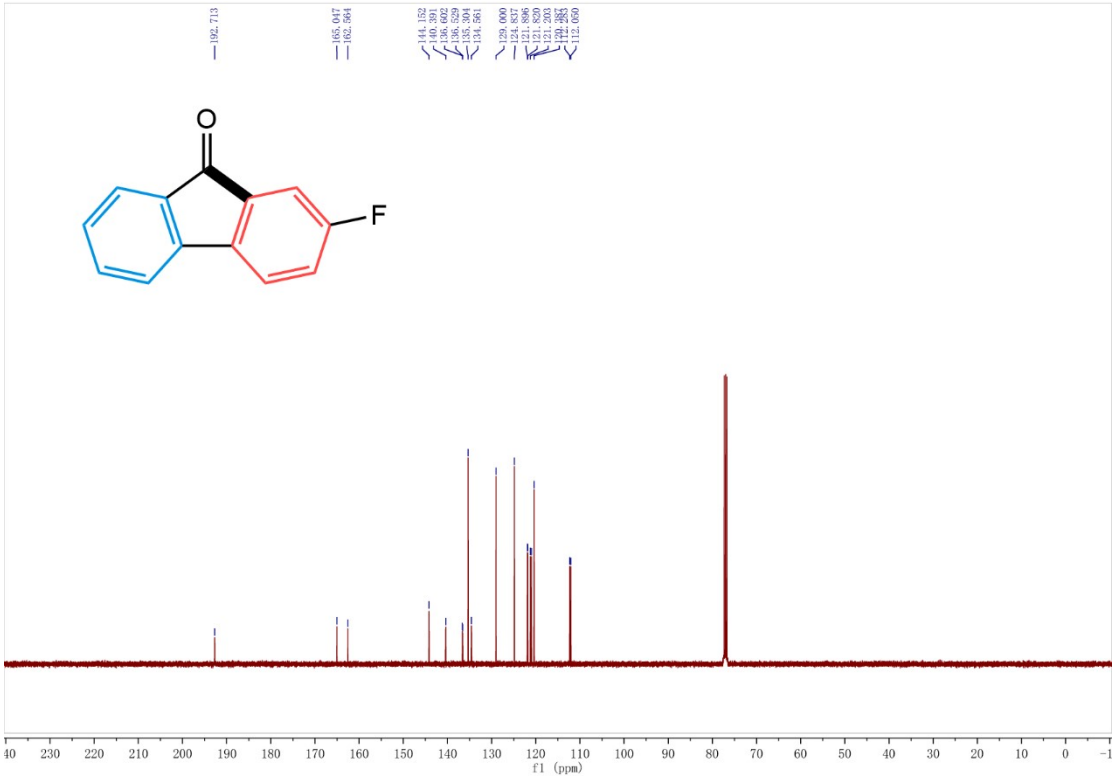



**Figure S62**. $^{13}$C NMR Spectrum of 2-fluoro-9*H*-fluoren-9-one (**1f, 3a**)

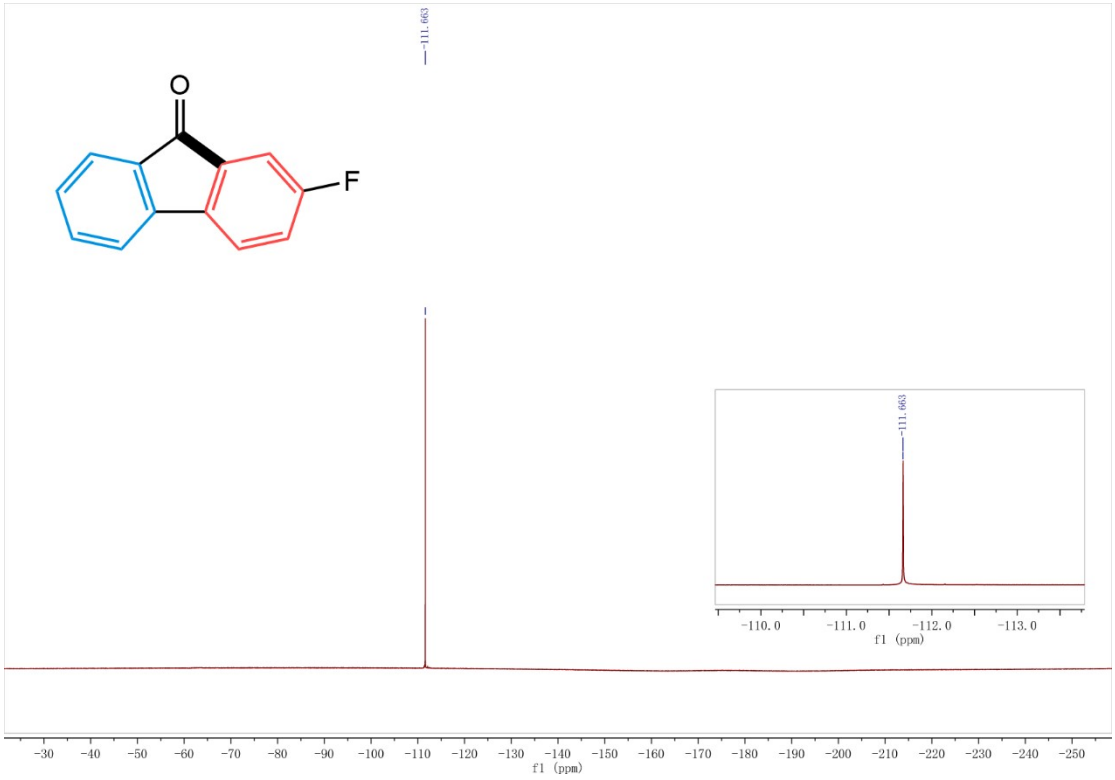



**Figure S63**. $^{19}$F NMR Spectrum of 2-fluoro-9*H*-fluoren-9-one (**1f, 3a**)

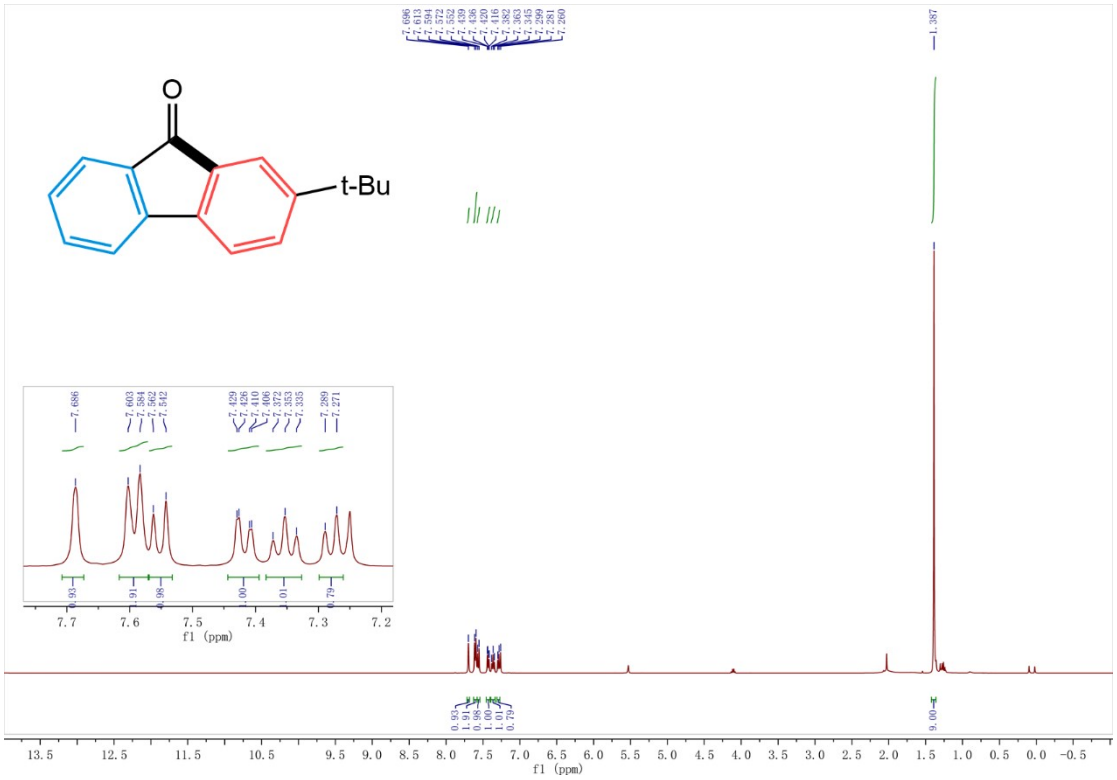



**Figure S64**. $^{1}$H NMR Spectrum of 2-(tert-butyl)-9H-fluoren-9-one (**1g**)

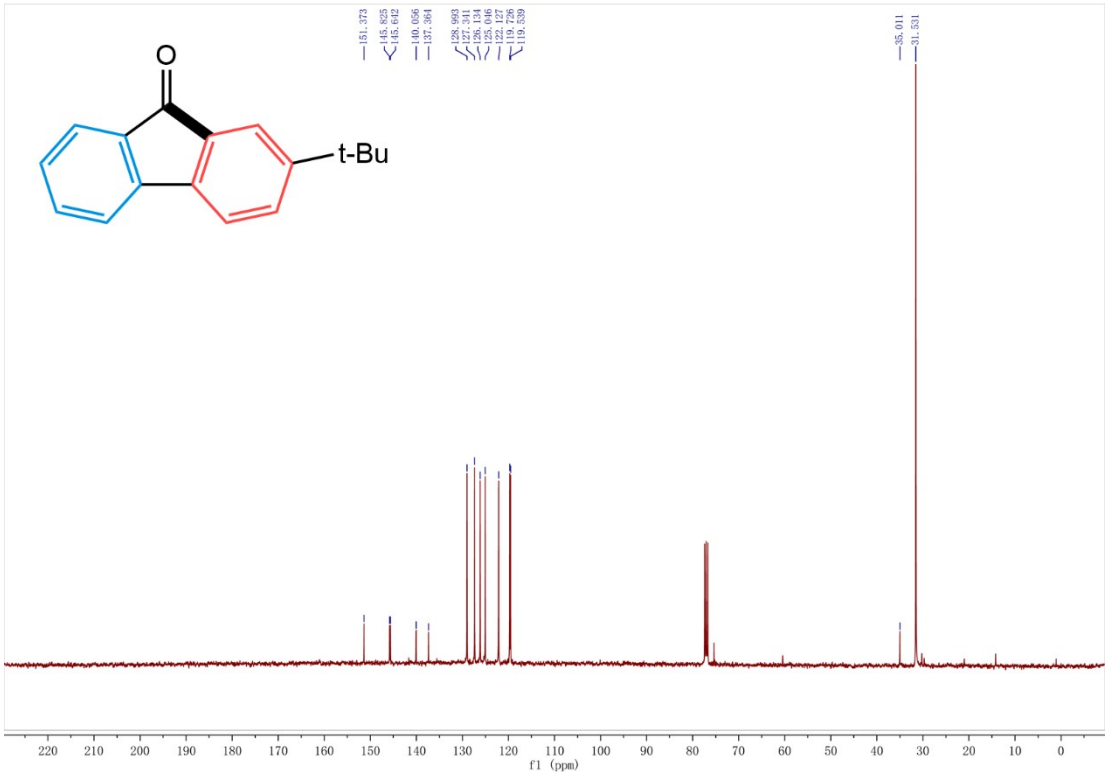



**Figure S65**. $^{13}$C NMR Spectrum of 2-(tert-butyl)-9H-fluoren-9-one (**1g**)

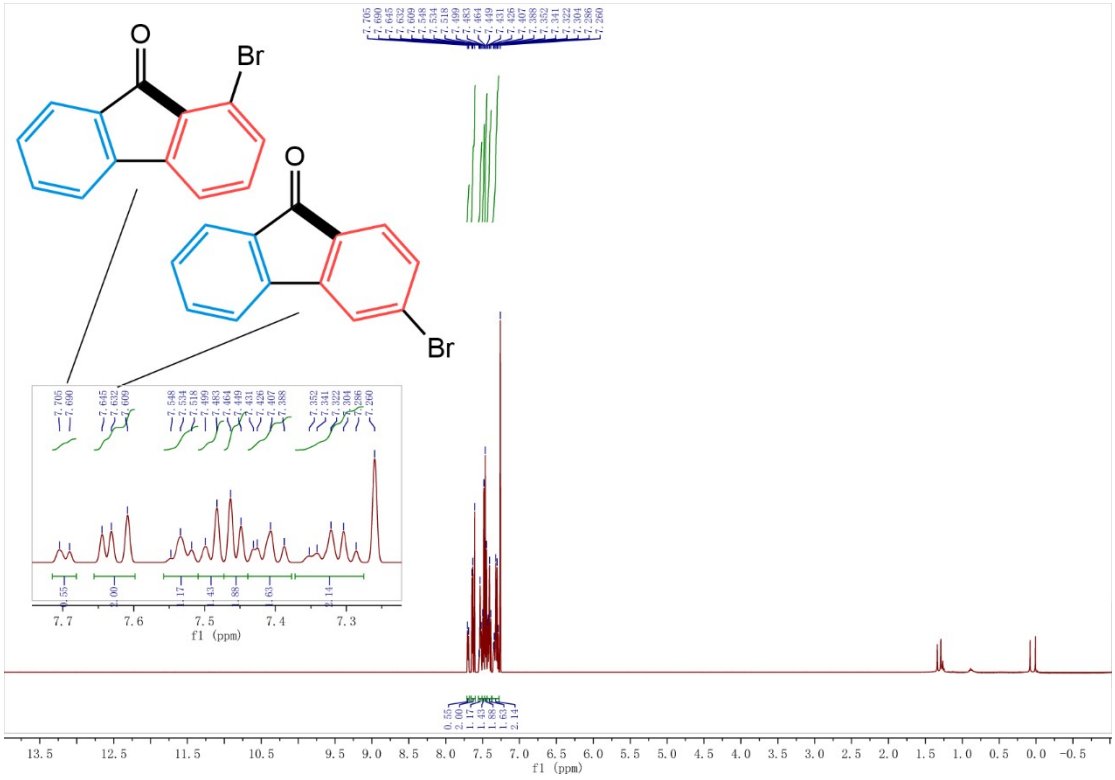



**Figure S66**. $^{1}$H NMR Spectrum of the mixture of 1-bromo-9H-fluoren-9-one & 3-bromo-9H-fluoren-9-one (**1h**)

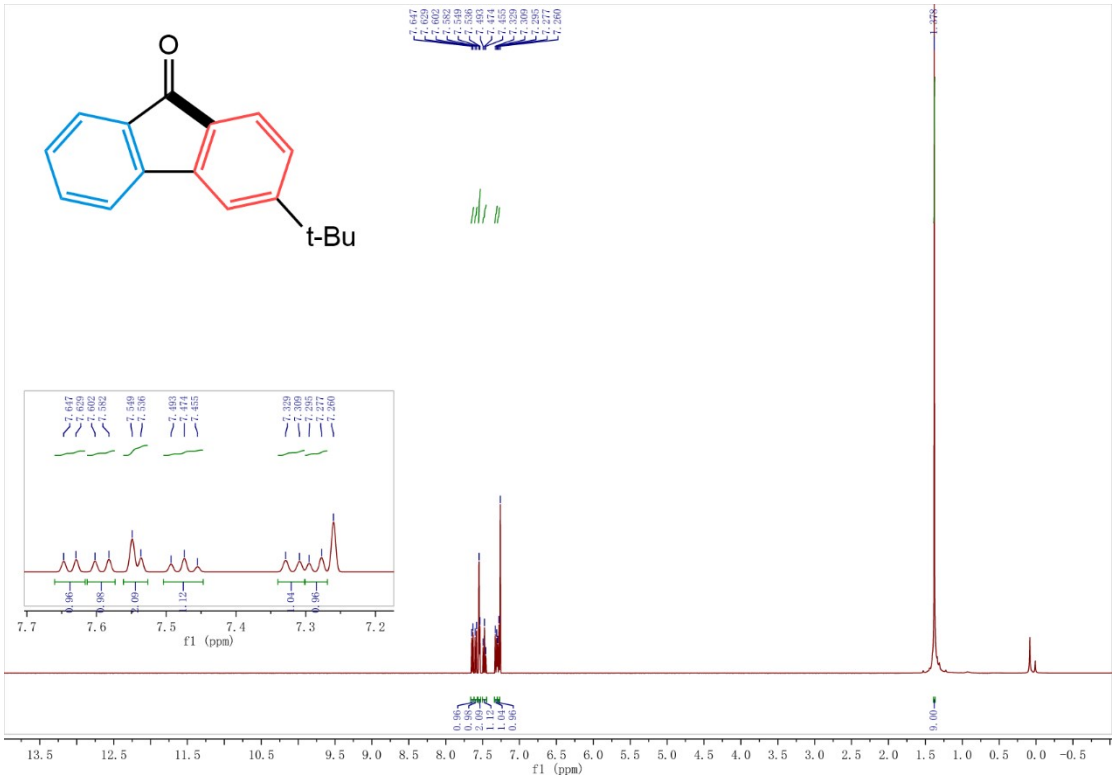



**Figure S67**. [1]H NMR Spectrum of 3-(tert-butyl)-9H-fluoren-9-one (**1i**)

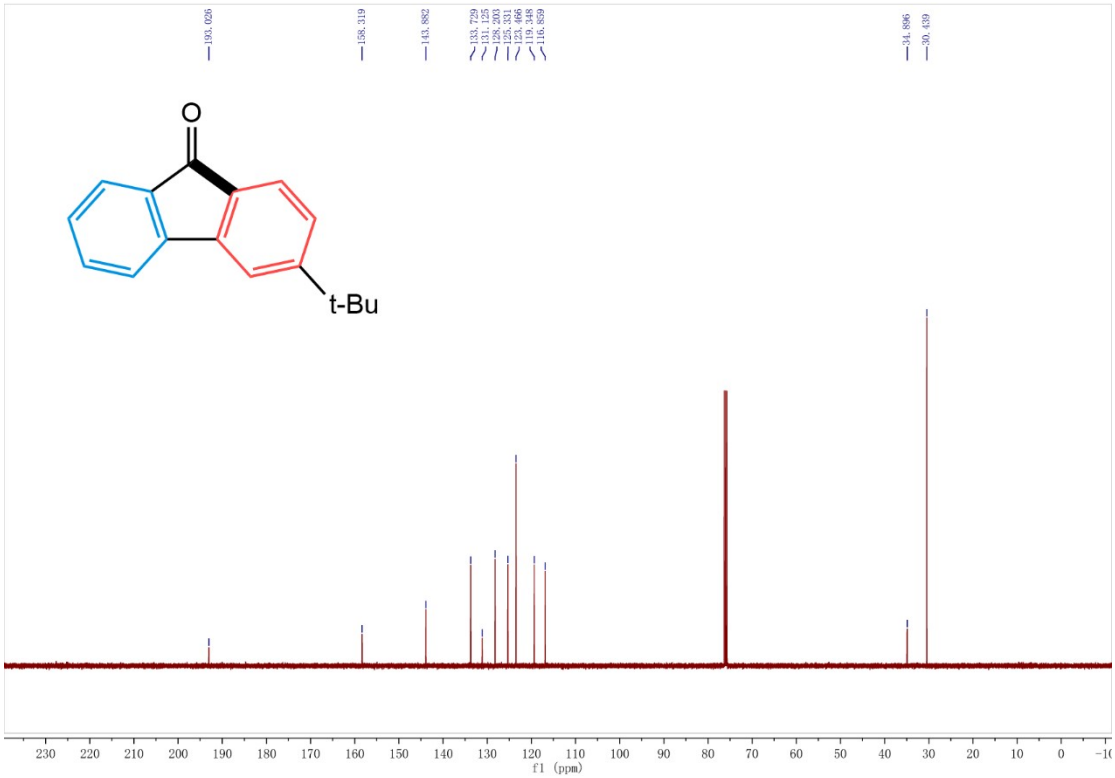



**Figure S68**. [13]C NMR Spectrum of 3-(tert-butyl)-9H-fluoren-9-one (**1i**)

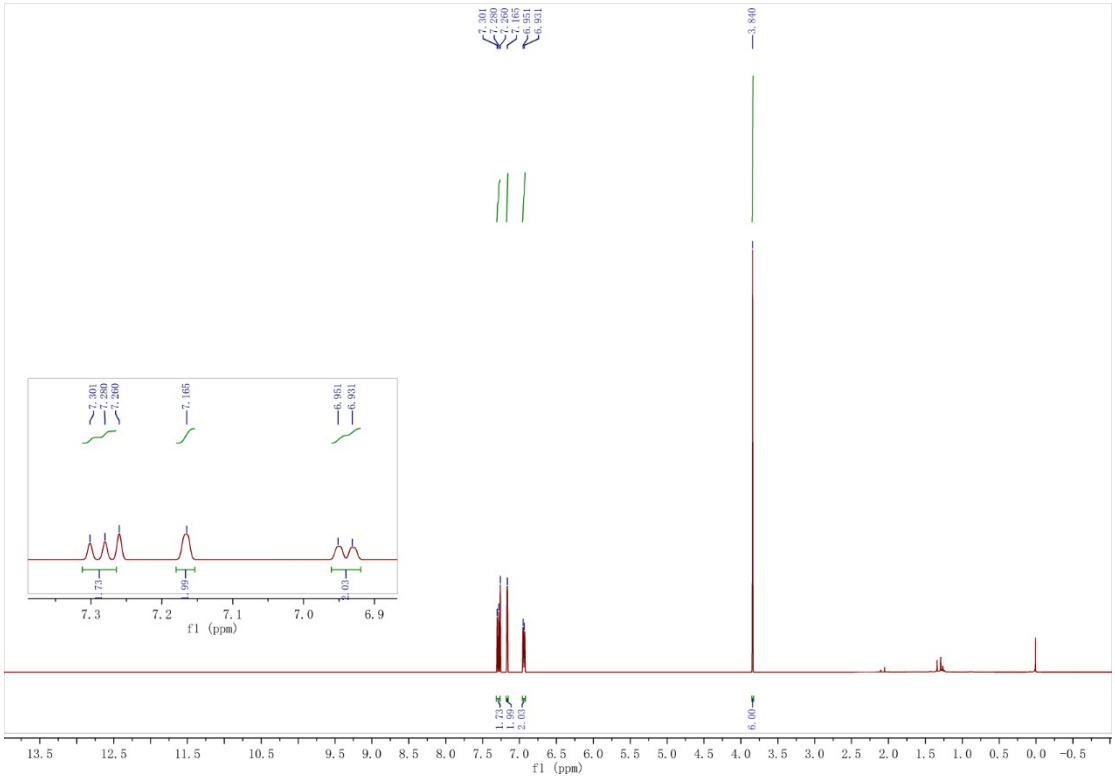


**Figure S69**. [1]H NMR Spectrum of 2,7-dimethoxy-9H-fluoren-9-one (**2b**)

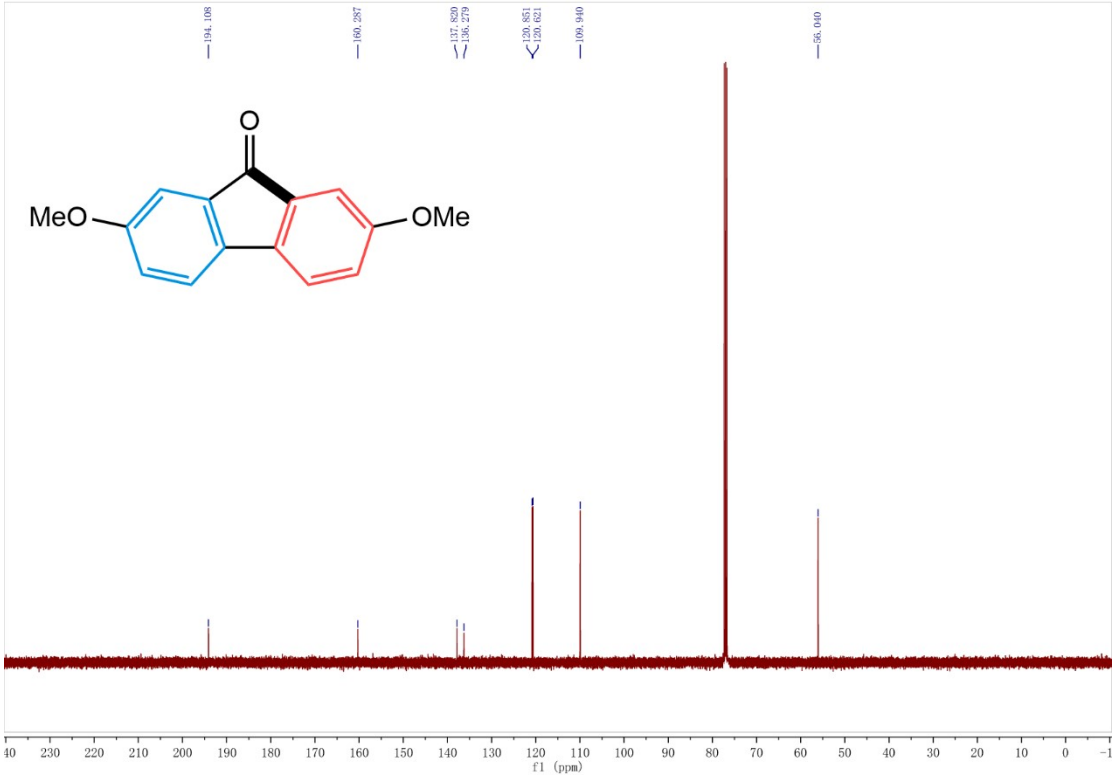



**Figure S70**. [13]C NMR Spectrum of 2,7-dimethoxy-9H-fluoren-9-one (**2b**)

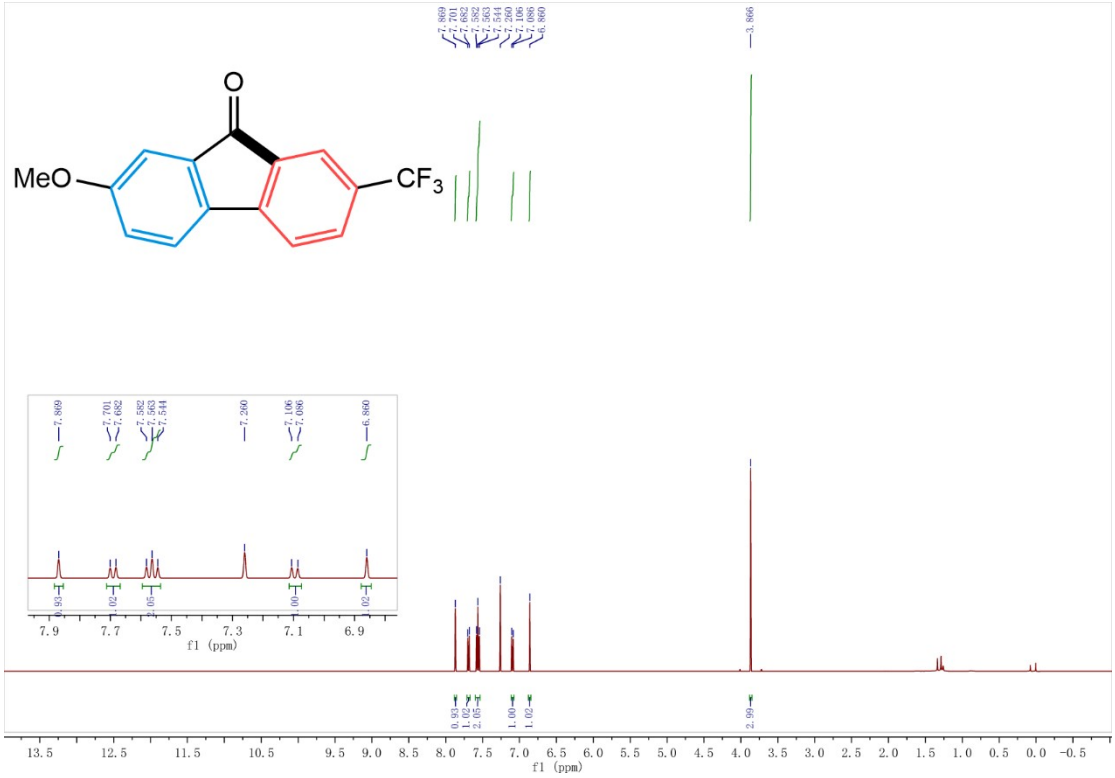



**Figure S71**. [1]H NMR Spectrum of 2-methoxy-7-(trifluoromethyl)-9*H*-fluoren-9-one (**2c**)

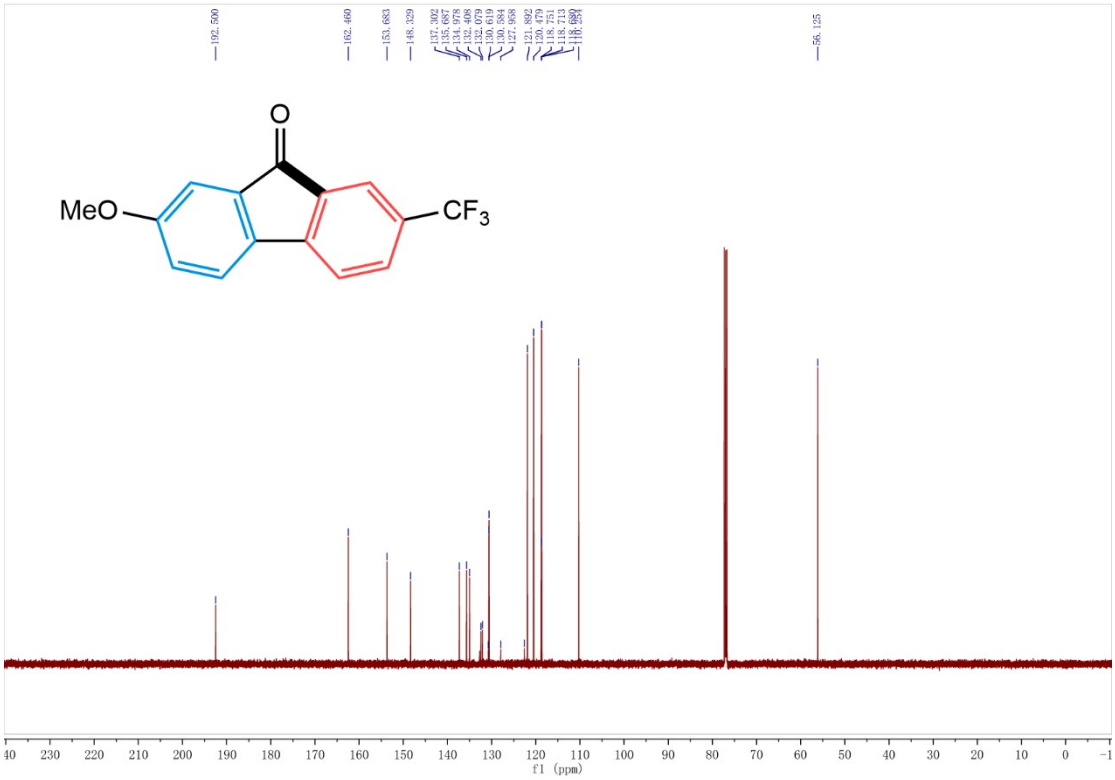



**Figure S72**. [13]C NMR Spectrum of 2-methoxy-7-(trifluoromethyl)-9*H*-fluoren-9-one (**2c**)

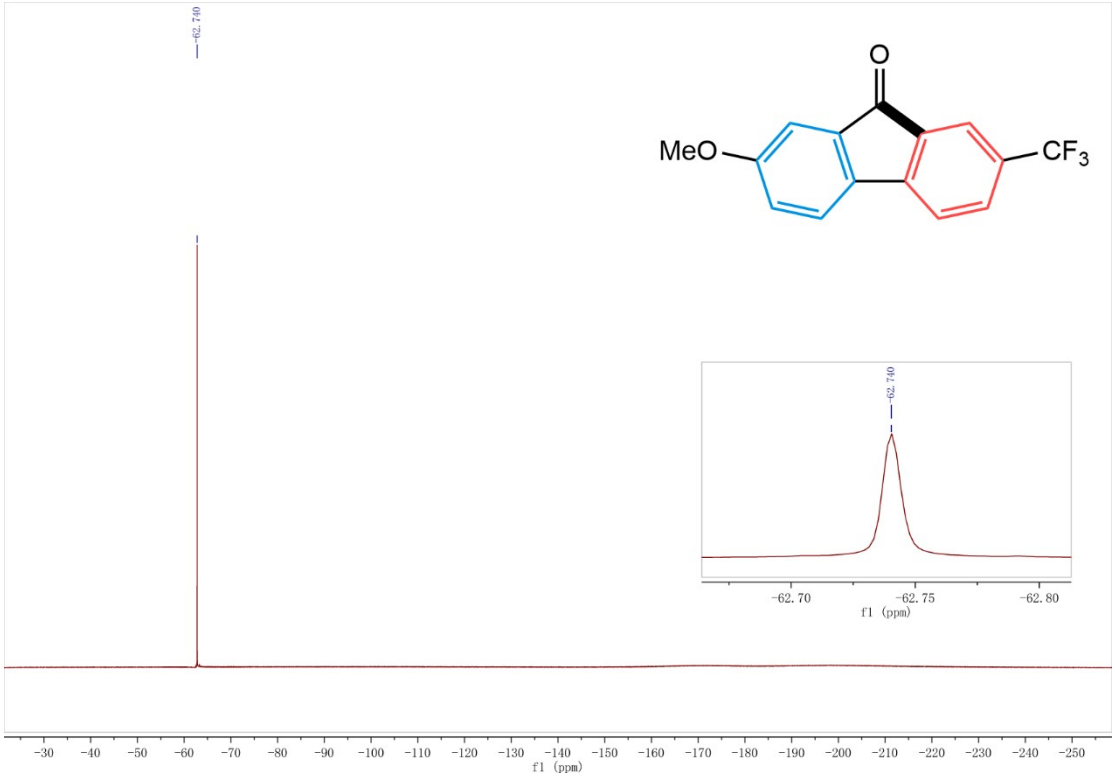



**Figure S73**. [19]F NMR Spectrum of 2-methoxy-7-(trifluoromethyl)-9*H*-fluoren-9-one (**2c**)

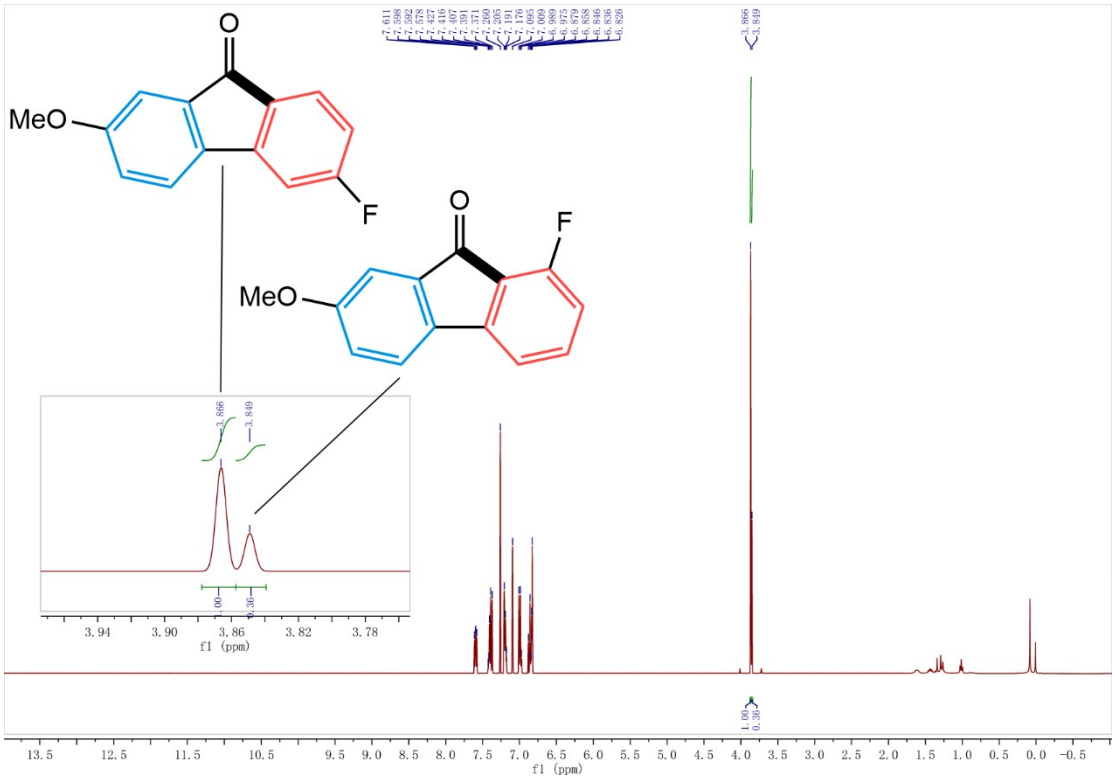



**Figure S74**. [1]H NMR Spectrum of the mixture of 1-fluoro-7-methoxy-9*H*-fluoren-9-one & 6-fluoro-2-methoxy-9*H*-fluoren-9-one (**2e**)

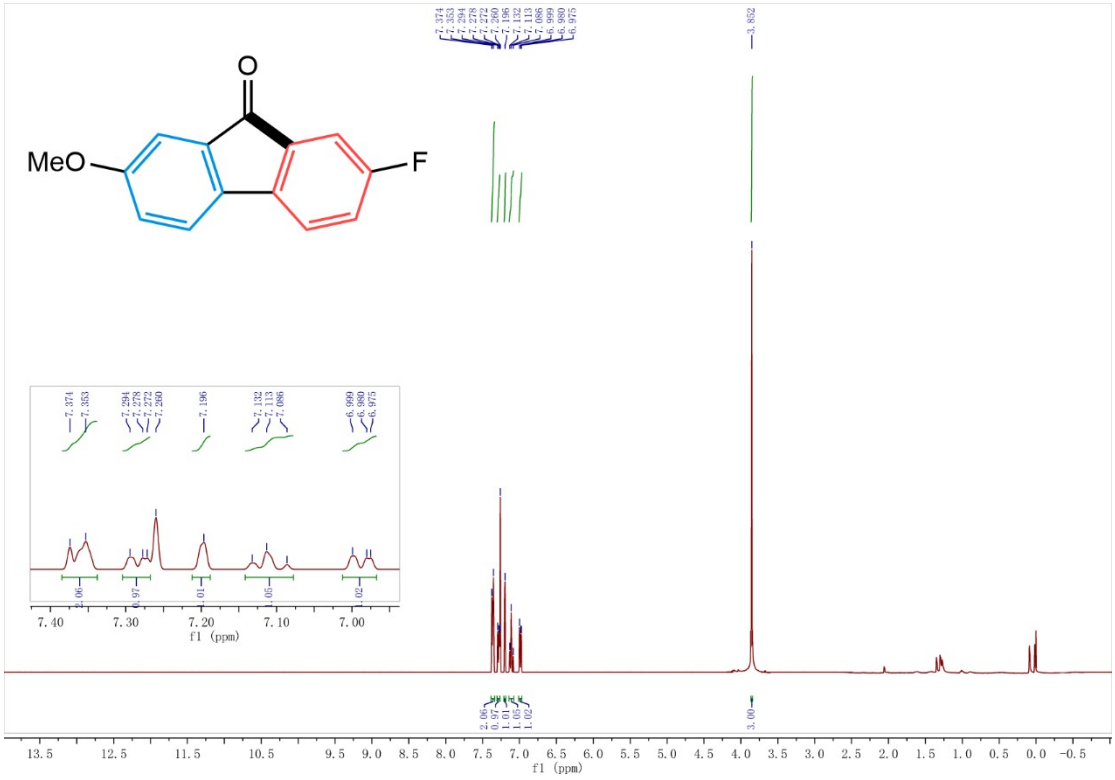



**Figure S75**. [1]H NMR Spectrum of 7-fluoro-2-methoxy-9H-fluoren-9-one (**2f**, **3b**)

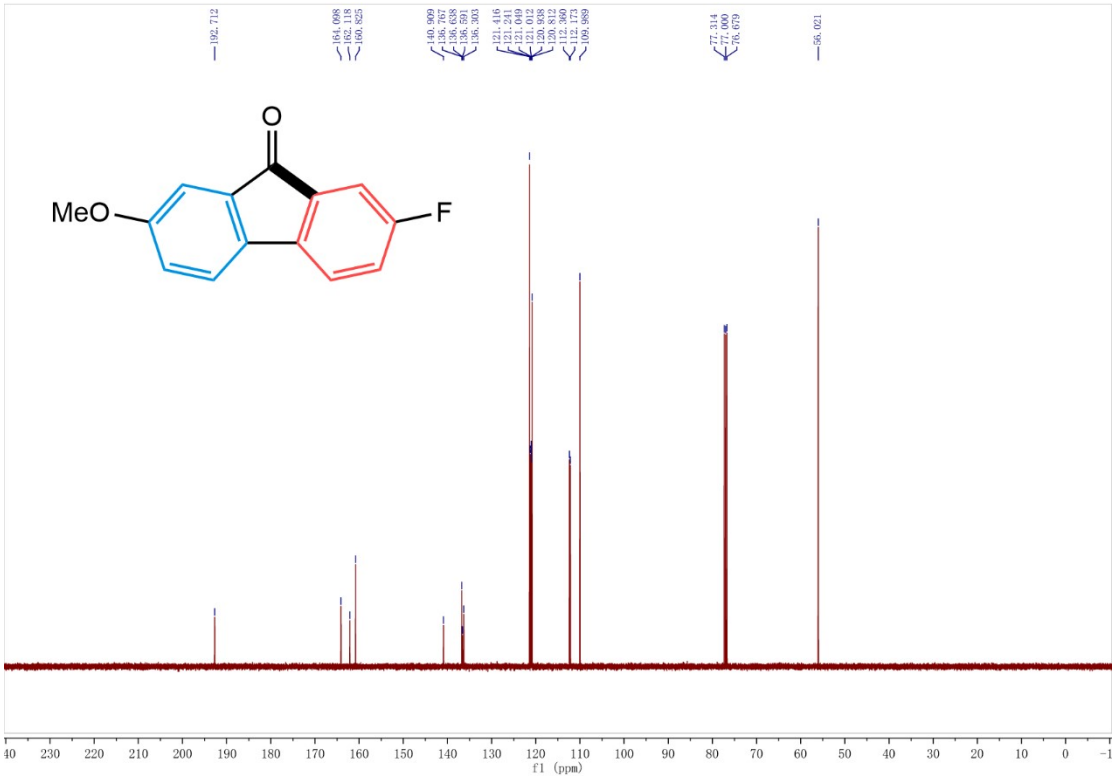



**Figure S76**. [13]C NMR Spectrum of 7-fluoro-2-methoxy-9H-fluoren-9-one (**2f**, **3b**)

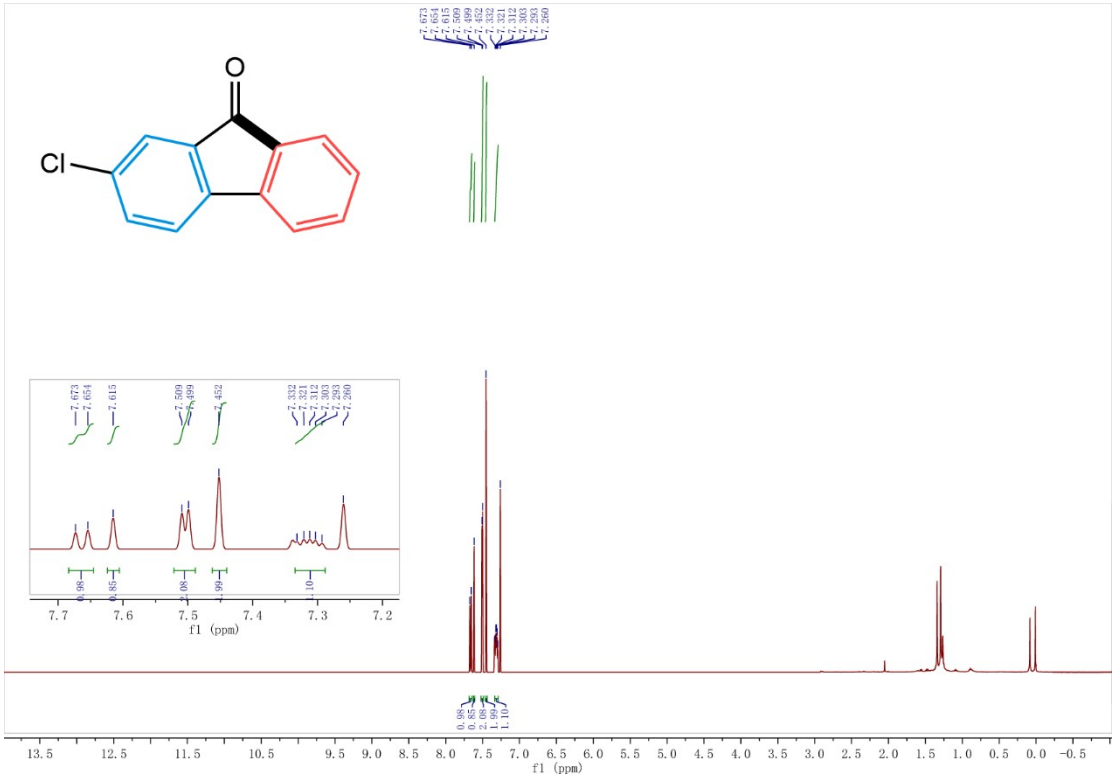



**Figure S77**. $^{1}$H NMR Spectrum of 2-chloro-9H-fluoren-9-one (**4a**)

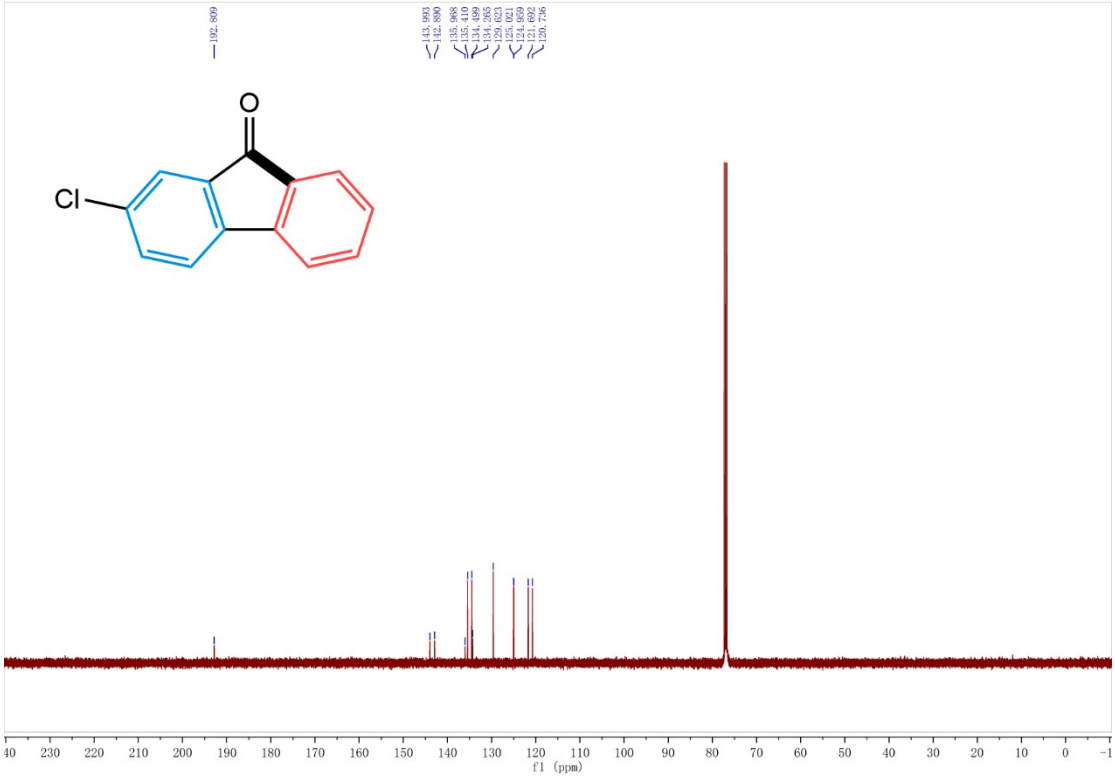



**Figure S78**. $^{13}$C NMR Spectrum of 2-chloro-9H-fluoren-9-one (**4a**)

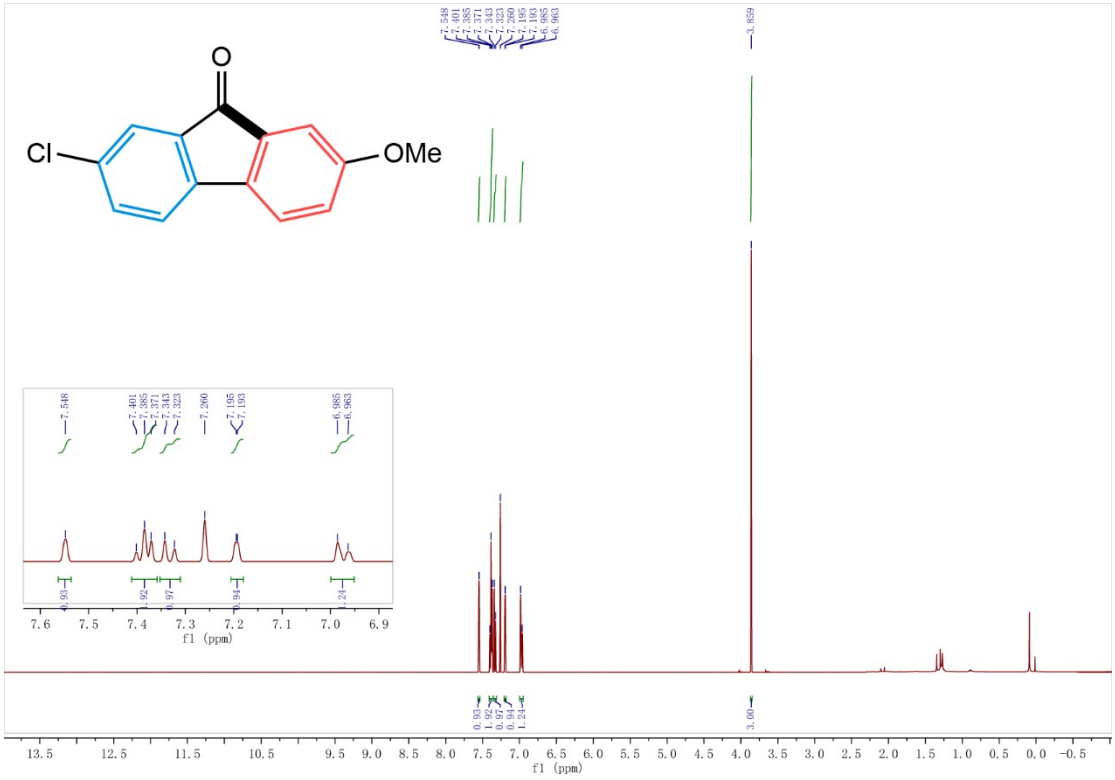



**Figure S79**. $^{1}$H NMR Spectrum of 2-chloro-7-methoxy-9H-fluoren-9-one (**4b**)

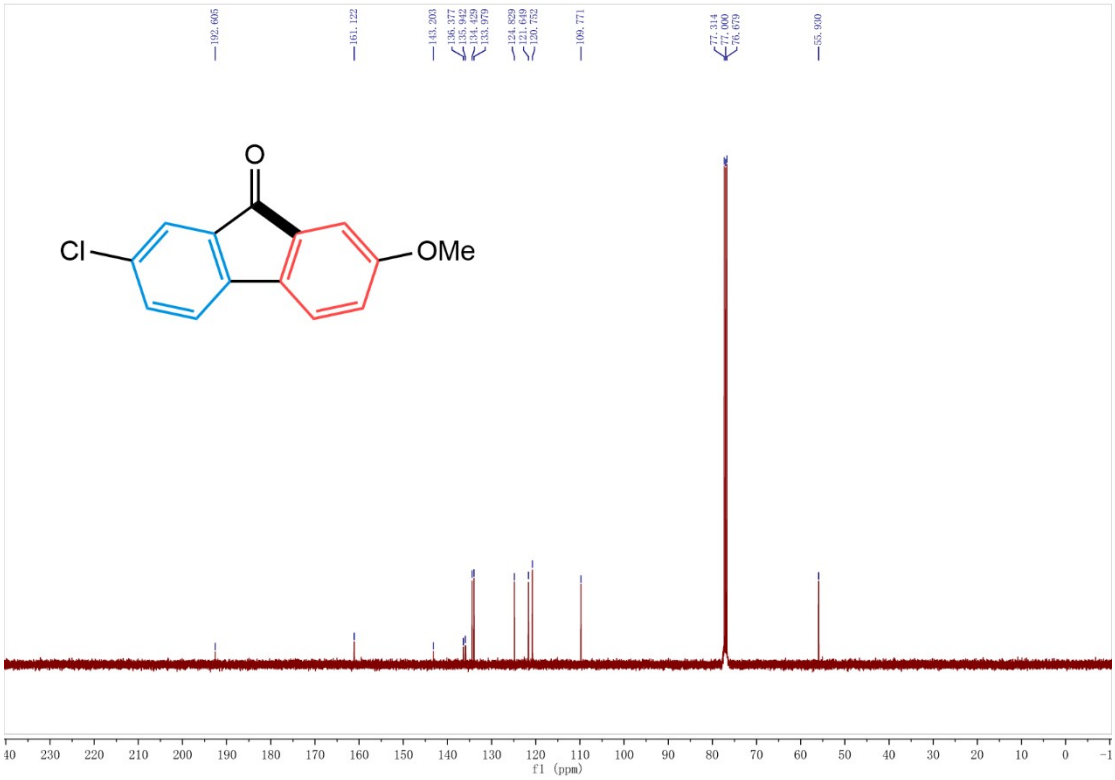



**Figure S80**. $^{13}$C NMR Spectrum of 2-chloro-7-methoxy-9H-fluoren-9-one (**4b**)

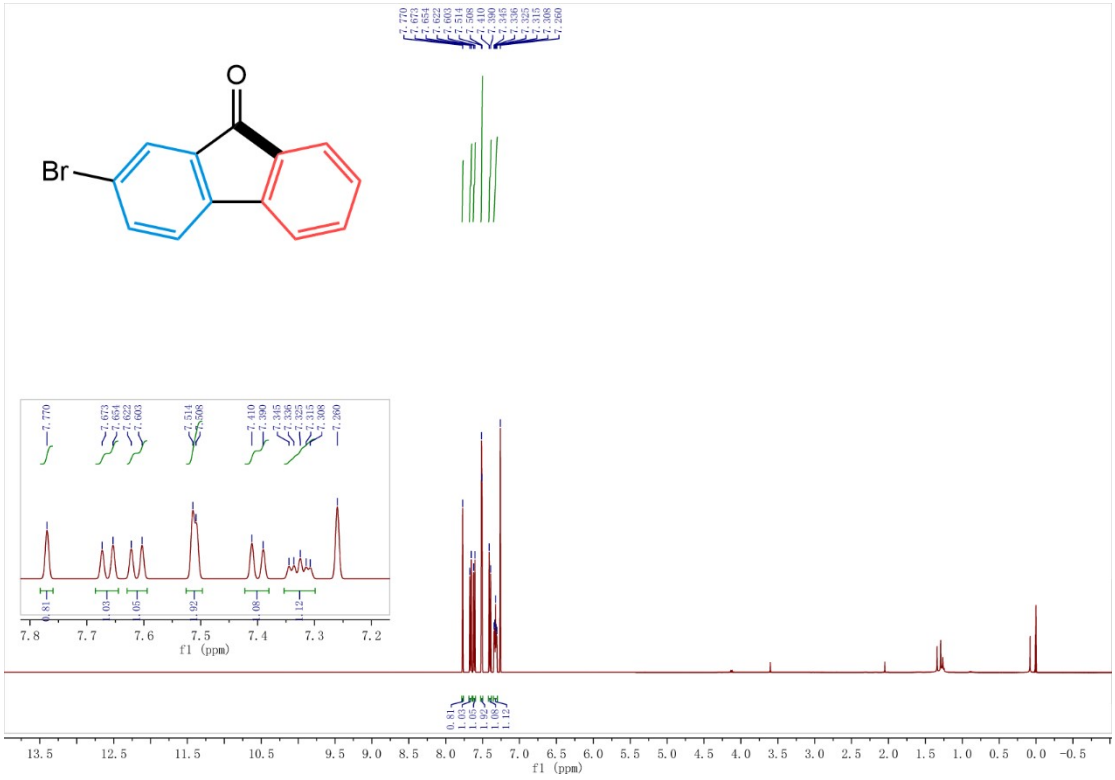



**Figure S81**. $^{1}$H NMR Spectrum of 2-bromo-9H-fluoren-9-one (**5a**)

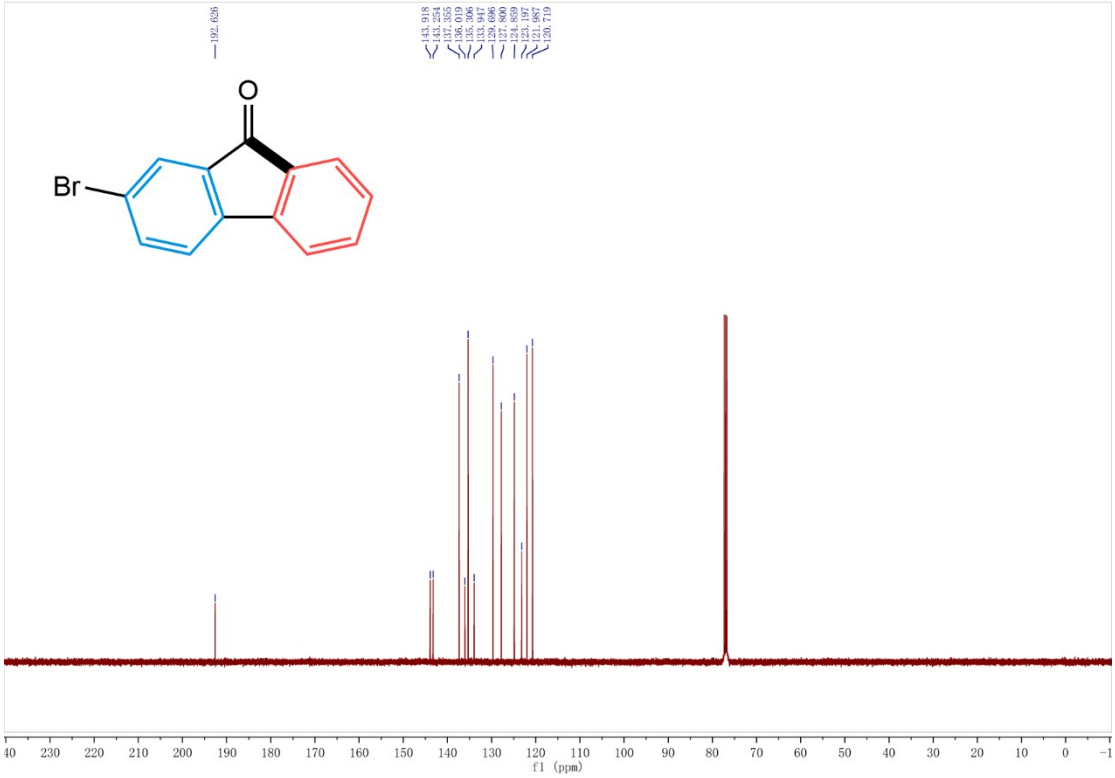



**Figure S82**. $^{13}$C NMR Spectrum of 2-bromo-9H-fluoren-9-one (**5a**)

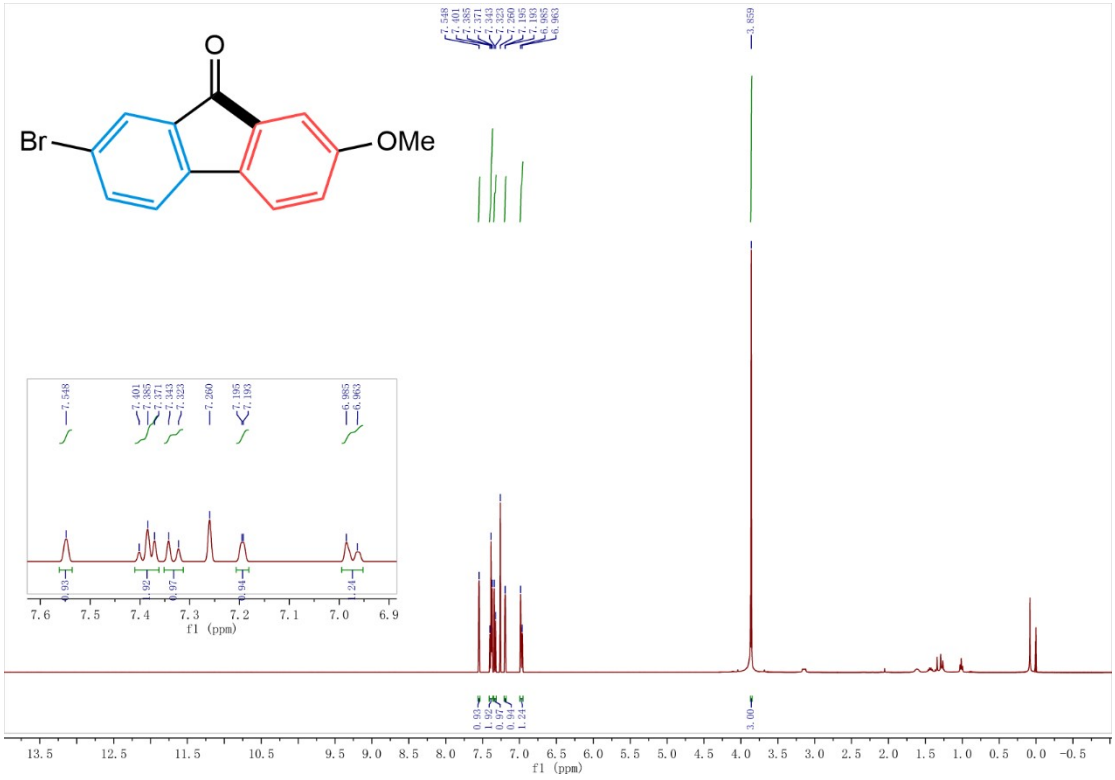



**Figure S83**. $^{1}$H NMR Spectrum of 2-bromo-7-methoxy-9H-fluoren-9-one (**5b**)

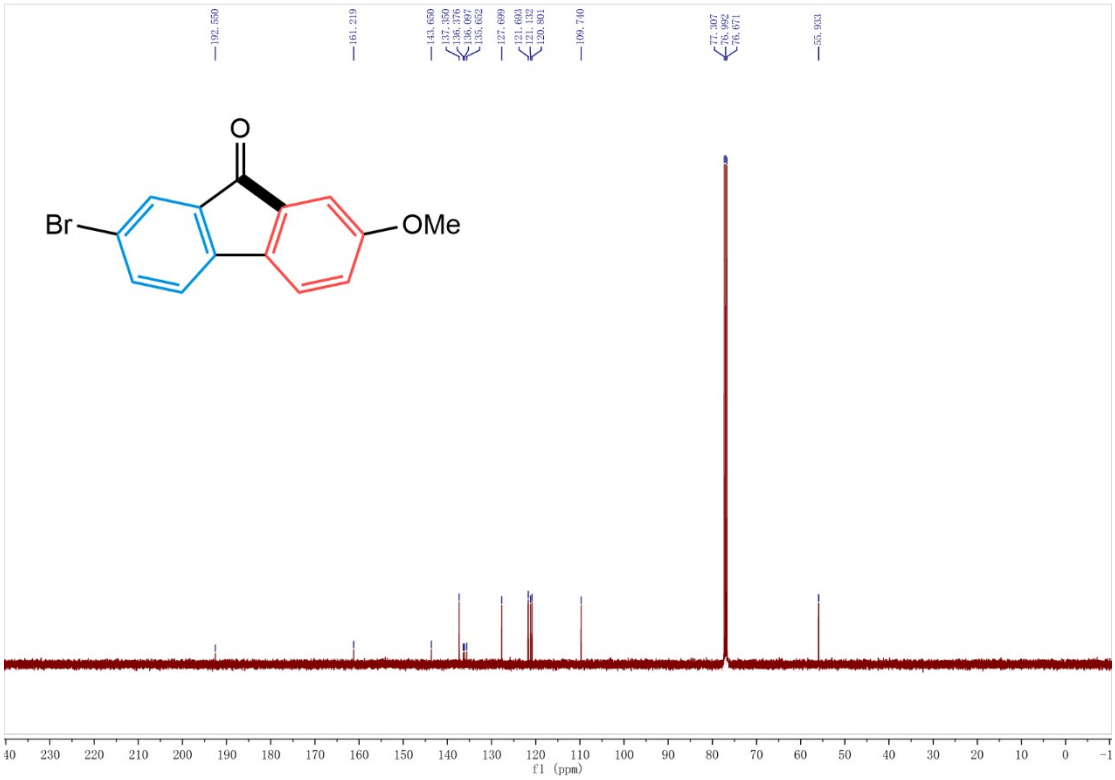



**Figure S84**. $^{13}$C NMR Spectrum of 2-bromo-7-methoxy-9H-fluoren-9-one (**5b**)

# 5. Mechanic Study and DFT Calculation

## 5.1 Detection of hydrogen generation

Conditions: GC-MS spectra were recorded on a FULI GC9790PLUS spectrometer. Column length: 60 m. Inner diameter: 530 μm. Temperature: 70 ℃. Carrier gas: Argon with 20 mL/min flow rate. The volume of the atmosphere above the reaction mixtures is 26.6 mL and the total amount of the gas was 1.088 mmol by estimation (as mentioned in 6.2). The released hydrogen can be quantified by measuring the percentage of the hydrogen in the gas chromatography and the total amount of the gas.

The reaction vessel was sufficiently sealed throughout the experiment and the reaction was conducted as standard. An extra rubber tube was attached to the branch pipe of the Schlenk tube for gas sampling. Right before sampling, the rubber tube was fully vacuumed and clamped with a flat-jaw pinchcock. Then the gas in the reaction system was allowed to flow into the emptied rubber tube by opening the gas valve. The sample is taken by puncture directly on the attached rubber tube with a 250 μL sampler syringe.

Three samples were tested in GC including (a) Hydrogen Standard which is pure hydrogen; (b) atmosphere before reaction; (c) atmosphere after reaction. On the GC spectra, the peaks with retention time 2.3, 2.9 and 3.6 min were attributed to hydrogen, oxygen and nitrogen respectively. The result showed that the atmosphere after the reaction contains 9.01% of hydrogen, which is equivalent to 0.098 mmol.

**Table S1. GC Detection of hydrogen released**

| **Hydrogen Standard** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Peak** | **Comp.** | **Retention Time** | **Type** | **Peak Width** | **Peak Area** | **Peak Height** | **Peak Area** | **Content** | **Amount** |
| **#** | | **[min]** | | **[min]** | **[uV*s]** | **[uV]** | **%** | **[ppm]** | **[mmol]** |
| 1 | $H_2$ | 2.299 | VB | 0.140 | 379739.0 | 47329.22 | 99.7915 | 997915 | N/A |
| 2 | $O_2$ | 2.885 | BB | 0.084 | 793.46 | 143.629 | 0.2085 | 2085 | N/A |
| **Before Reaction** | | | | | | | | | |
| **Peak** | **Comp.** | **Retention Time** | **Type** | **Peak Width** | **Peak Area** | **Peak Height** | **Peak Area** | **Content** | **Amount (26.6 mL)** |
| **#** | | **[min]** | | **[min]** | **[uV*s]** | **[uV]** | **%** | **[ppm]** | **[mmol]** |
| 1 | $O_2$ | 2.910 | BB | 0.142 | 1359.34 | 208.851 | 0.4087 | 4087 | 0.0044 |
| 2 | $N_2$ | 3.647 | VB | 0.261 | 331216.3 | 25909.69 | 99.5913 | 995913 | 1.09 |
| **After Reaction** | | | | | | | | | |
| **Peak** | **Comp.** | **Retention Time** | **Type** | **Peak Width** | **Peak Area** | **Peak Height** | **Peak Area** | **Content** | **Amount (26.6 mL)** |
| **#** | **#** | **[min]** | | **[min]** | **[uV*s]** | **[uV]** | **%** | **[ppm]** | **[mmol]** |
| 1 | $H_2$ | 2.291 | BB | 0.150 | 54102.19 | 7517.196 | 9.0076 | 90076 | 0.098 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 2 | $O_2$ | 2.909 | BB | 0.132 | 964.31 | 166.124 | 0.1605 | 1605 | 0.0017 |
| 3 | $N_2$ | 3.625 | VB | 0.251 | 545564.4 | 42348.09 | 90.8319 | 908319 | 0.99 |

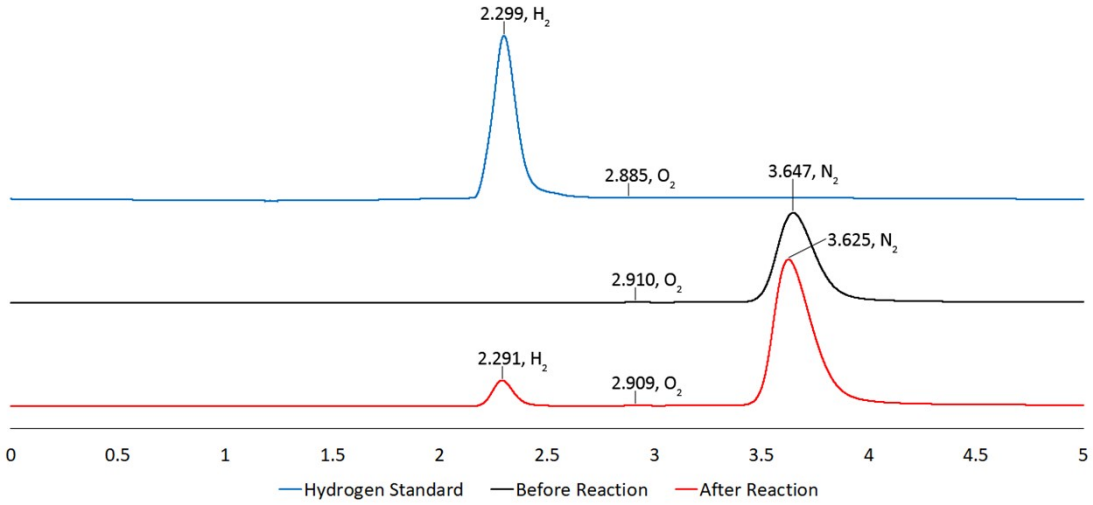
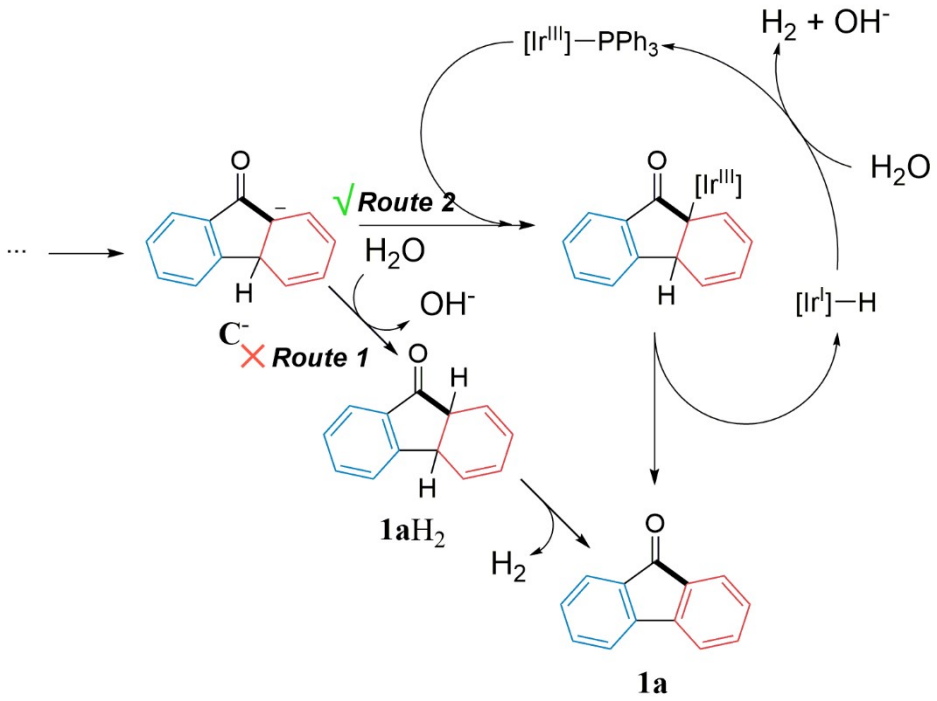



**Figure S85**. Gaseous Spectroscopy of Hydrogen Standard (blue), atmosphere before reaction (black), and atmosphere after reaction (red).




**Scheme S1.** Alternative routes we have envisioned in the early stage of the mechanistic study. The **Route 1** is the direct aromatization-dehydrogenation, and was later proved to be energy unfavored. The **Route 2** is the early hypothesis of the iridium catalyzed dehydrogenation which the DFT calculation was later based on.

## 5.2 Computational details

To shed light on the mechanism of dehydrogenation leading to the production of 9-fluorenone from 9-fluorenone anion, density functional theory (DFT) calculations were then carried out with the Gaussian 09 software package. [7, 8] The geometry optimization and frequency calculations were carried out with M062X method and combined basis set. That is, 6-31G(d,p) for C, H, O, N, F atoms and SDD for Ir atom. [9] Intrinsic reaction coordinate calculations were performed to ensure every TS is connect with corresponding equilibrium structure. Single point energy were calculated at the same level. Truhlar and coworkers' SMD solvation model was employed to consider the solvent effect of dichloromethane (ε=8.93). [10, 11] All discussed Gibbs free energy were calculated with thermal correction.

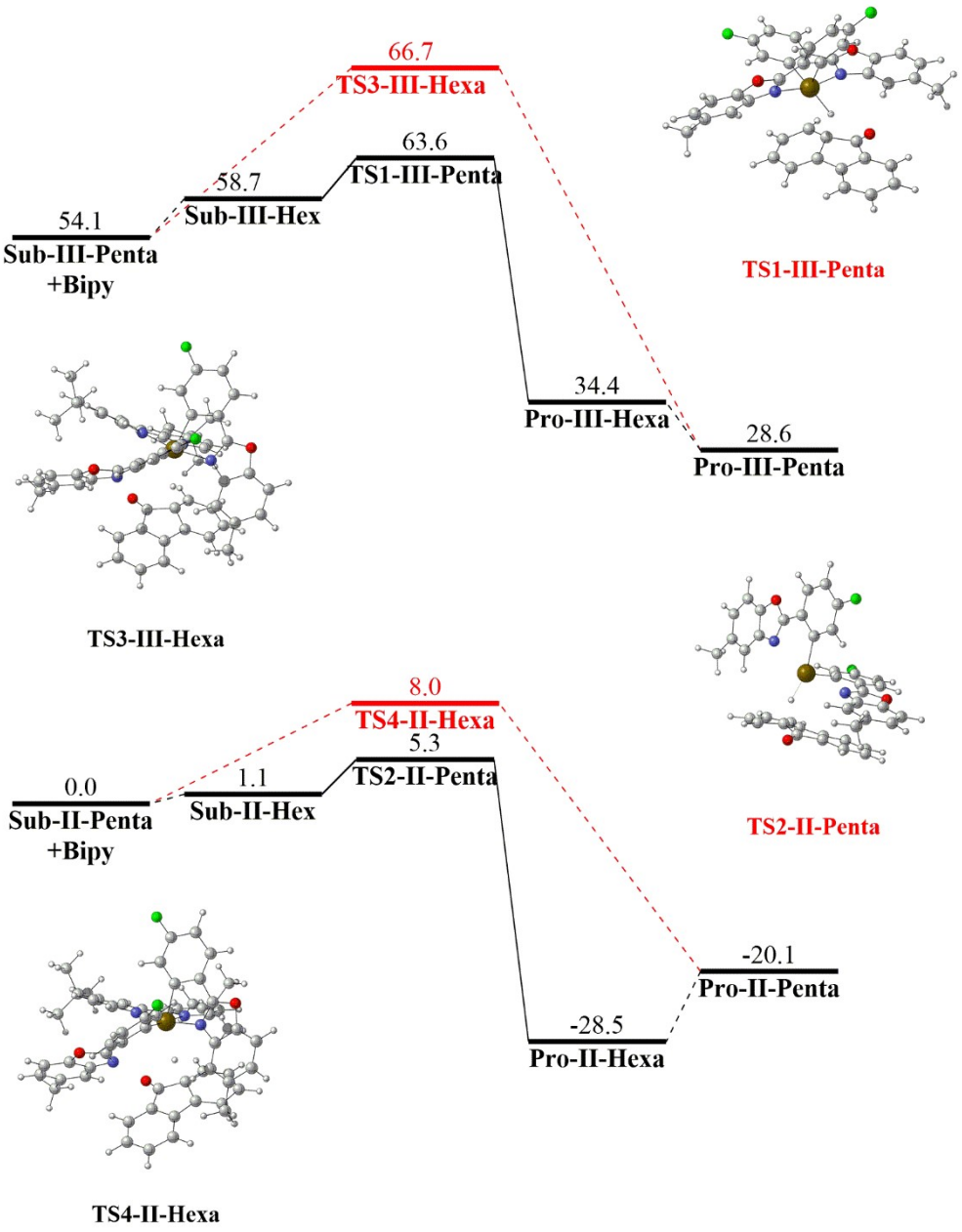



**Figure S85.** Free-energy reaction profiles (kcal mol$^{-1}$) for the reaction of dehydrogenation leading to the production of 9-fluorenone from 9-fluorenone anion, calculated with SMD Model (Dichloromethane) at M06L/6-31G(d,p)/SDD at 298 K.

## 5.3 Optimized structures the imaginary frequencies and coordinates

**Bipyridine**

| | | | |
|---|---|---|---|
| C | 2.61105000 | 2.39367100 | 0.61573100 |
| C | 3.41881300 | 1.28054200 | 0.43942300 |
| C | 2.84163700 | 0.06635000 | 0.05259700 |

| | | | |
|---|---|---|---|
| C | 1.45964400 | 0.06784200 | -0.12147400 |
| C | 0.71806000 | 1.23731900 | 0.08756700 |
| N | 1.28696700 | 2.39785500 | 0.44682400 |
| C | -0.75738900 | 1.24284500 | -0.09266000 |
| C | -1.50907100 | 0.08459600 | 0.10676900 |
| C | -2.89567100 | 0.09361400 | -0.06743800 |
| C | -3.46290900 | 1.31044300 | -0.44355300 |
| C | -2.63986800 | 2.42019300 | -0.61190300 |
| N | -1.31988500 | 2.41357100 | -0.44465800 |
| C | 3.71154700 | -1.16660000 | -0.16753900 |
| C | -3.70619300 | -1.17761600 | 0.16285700 |
| C | 2.88911300 | -2.38913600 | -0.56832500 |
| C | 4.72610800 | -0.86858200 | -1.27970400 |
| C | 4.46537700 | -1.48429600 | 1.13073400 |
| C | -5.19412900 | -0.96270500 | -0.10436300 |
| C | -3.19152100 | -2.27923800 | -0.77317200 |
| C | -3.52640000 | -1.62818400 | 1.61861800 |
| H | 3.05476300 | 3.34221600 | 0.91423100 |
| H | 4.48927900 | 1.36548900 | 0.59860300 |
| H | 0.94951100 | -0.83199600 | -0.44376700 |
| H | -1.01190100 | -0.82698500 | 0.42229800 |
| H | -4.52969000 | 1.41339600 | -0.60376300 |
| H | -3.07748700 | 3.37400800 | -0.90352400 |
| H | 3.55103800 | -3.24807300 | -0.70945500 |
| H | 2.15821900 | -2.66080000 | 0.19948800 |
| H | 2.35130100 | -2.23194000 | -1.50812700 |
| H | 5.36581100 | -1.74005100 | -1.45031200 |
| H | 5.37482200 | -0.02617100 | -1.02440200 |
| H | 4.22390300 | -0.63144700 | -2.22257500 |
| H | 3.77312000 | -1.69458200 | 1.95178800 |
| H | 5.09886200 | -2.36588600 | 0.99220800 |
| H | 5.11156900 | -0.65829700 | 1.43994600 |
| H | -5.73806500 | -1.89593800 | 0.06612300 |
| H | -5.62446700 | -0.20640700 | 0.55877300 |
| H | -5.38439300 | -0.65537100 | -1.13711300 |
| H | -3.76483400 | -3.19931000 | -0.62326500 |
| H | -2.13914200 | -2.51296400 | -0.58930700 |
| H | -3.29277600 | -1.98869100 | -1.82333400 |
| H | -3.87784300 | -0.86337200 | 2.31786500 |
| H | -4.10040200 | -2.54138100 | 1.80417000 |
| H | -2.47997900 | -1.84179100 | 1.85330100 |

**Sub-III-Penta**

| | | | |
|---|---|---|---|
| Ir | -0.51609200 | -0.29568700 | -0.02099800 |
| F | -4.06905500 | -1.42461400 | 3.84797400 |
| N | 1.16678500 | -1.28686500 | 0.64073600 |
| O | 2.11137500 | -2.51342500 | 2.24539100 |
| C | -1.20467100 | -1.07668900 | 1.65679900 |
| C | -2.51074000 | -0.97855100 | 2.15387600 |
| H | -3.29682900 | -0.46605800 | 1.60998400 |
| C | -2.80659800 | -1.54334100 | 3.38175900 |
| C | -1.88408700 | -2.22611100 | 4.17087800 |
| H | -2.19123200 | -2.64418500 | 5.12175500 |
| C | -0.59083400 | -2.34305500 | 3.69536500 |
| H | 0.16009100 | -2.87048400 | 4.27572100 |
| C | -0.25174500 | -1.78087900 | 2.46001100 |
| C | 1.01831100 | -1.85295200 | 1.82599900 |
| C | 3.02541100 | -2.36703500 | 1.22152900 |
| C | 2.43812400 | -1.61753500 | 0.20343900 |
| C | 3.14492500 | -1.31842300 | -0.95504900 |
| H | 2.68999500 | -0.74438800 | -1.75702300 |
| C | 4.46408900 | -1.76366500 | -1.04772900 |
| C | 5.02839100 | -2.50639200 | 0.00796800 |
| H | 6.05609600 | -2.84441700 | -0.08728800 |
| C | 4.32206100 | -2.82880300 | 1.16391800 |
| H | 4.76485900 | -3.40136400 | 1.97025600 |
| C | 5.29532900 | -1.42485300 | -2.24733600 |
| H | 5.91070900 | -2.27049900 | -2.56446800 |
| H | 4.67658500 | -1.11707800 | -3.09238600 |
| H | 5.98068700 | -0.59855900 | -2.02733600 |
| F | -0.05172200 | -5.04103400 | -2.77520100 |
| N | -2.45564100 | 0.36792500 | -0.79505000 |
| O | -3.98858900 | -0.04284500 | -2.37959500 |
| C | -0.99938800 | -1.84525700 | -1.33532600 |
| C | -0.30495100 | -3.03476100 | -1.57659200 |
| H | 0.57812600 | -3.31456900 | -1.00914700 |
| C | -0.74431300 | -3.89938200 | -2.56790100 |
| C | -1.85748400 | -3.65865500 | -3.36496200 |
| H | -2.14553300 | -4.37506000 | -4.12508000 |
| C | -2.57043800 | -2.49376700 | -3.13975600 |
| H | -3.45167600 | -2.27041300 | -3.73360300 |
| C | -2.14582900 | -1.61350600 | -2.13858700 |
| C | -2.84706900 | -0.42320900 | -1.78243900 |
| C | -4.38341200 | 1.08673400 | -1.70268400 |
| C | -3.44818800 | 1.34868900 | -0.70112800 |
| C | -3.66948500 | 2.41421700 | 0.16846200 |
| H | -2.99433500 | 2.62052400 | 0.98509400 |
| C | -4.79773800 | 3.21105800 | -0.02432500 |
| C | -5.69640300 | 2.92343100 | -1.06902800 |
| H | -6.56758200 | 3.55882100 | -1.19888000 |

| | | | |
|---|---|---|---|
| C | -5.51277000 | 1.84600100 | -1.92681400 |
| H | -6.21270900 | 1.60839700 | -2.71902900 |
| C | -5.05970900 | 4.37902300 | 0.87740500 |
| H | -6.03412900 | 4.29570100 | 1.36819800 |
| H | -4.29870100 | 4.46657600 | 1.65508000 |
| H | -5.07175800 | 5.31836100 | 0.31545500 |
| C | -0.43510800 | 3.64926800 | 0.40649800 |
| C | -0.49003700 | 2.50536000 | 1.16949100 |
| C | 1.84067000 | 3.14573900 | -0.26624100 |
| C | 0.78243300 | 3.99974100 | -0.26079700 |
| H | -1.25463800 | 4.36166000 | 0.42612100 |
| H | -1.31963700 | 2.36247600 | 1.85865900 |
| H | 0.90219000 | 5.01272200 | -0.64101700 |
| C | 4.00932800 | 2.38217000 | 0.14009000 |
| C | 5.40158000 | 2.40794900 | 0.13437900 |
| C | 6.04708800 | 3.42496600 | -0.55469800 |
| C | 5.29666200 | 4.42100900 | -1.20167100 |
| C | 3.91028800 | 4.41967300 | -1.17862200 |
| C | 3.24337400 | 3.38713000 | -0.50189700 |
| H | 5.96102600 | 1.63586800 | 0.65674400 |
| H | 7.13093000 | 3.45840600 | -0.59561800 |
| H | 5.81842600 | 5.21376000 | -1.72986900 |
| H | 3.35219900 | 5.20483700 | -1.68009200 |
| C | 3.10512900 | 1.46788700 | 0.85476500 |
| O | 3.38958900 | 0.67024800 | 1.73205900 |
| C | 1.71444100 | 1.74798000 | 0.29119300 |
| H | 1.71450500 | 1.07194400 | -0.59736200 |
| C | 0.48832100 | 1.46463800 | 1.13848600 |
| H | 0.70168700 | 0.99147800 | 2.10204500 |

**Sub-III-Hexa**

| | | | |
|---|---|---|---|
| Ir | -0.06145400 | -0.19191900 | 0.41193900 |
| C | 4.19843500 | 0.09491400 | 1.35817800 |
| C | 2.88199200 | -0.30351200 | 1.30829200 |
| N | 1.88381300 | 0.46497400 | 0.82051900 |
| C | 2.22051200 | 1.71808600 | 0.39962800 |
| C | 3.54194600 | 2.16491600 | 0.42571600 |
| C | 4.57344900 | 1.36010600 | 0.89021600 |
| C | 1.10715900 | 2.56647500 | -0.02081100 |
| N | -0.09454200 | 1.94960000 | -0.04600700 |
| C | -1.18822300 | 2.70452900 | -0.24079700 |
| C | -1.12460900 | 4.05734400 | -0.50743100 |
| C | 0.11583900 | 4.70856800 | -0.56539700 |
| C | 1.23424400 | 3.93143600 | -0.28924900 |
| C | 6.03611700 | 1.77906600 | 0.88423100 |
| C | 6.60887800 | 1.64624300 | 2.30115100 |
| C | 6.21981800 | 3.21808800 | 0.40920200 |
| C | 6.79968300 | 0.84238600 | -0.06341600 |
| C | 0.19060000 | 6.19670000 | -0.87939600 |
| C | -0.57035300 | 6.97193300 | 0.20494800 |
| C | 1.62982600 | 6.70334900 | -0.92998500 |
| C | -0.47125600 | 6.44917700 | -2.24067600 |
| C | -6.85665100 | -0.15771800 | -0.79419200 |
| C | -6.98238000 | -1.38174400 | -0.10605500 |
| C | -6.09152400 | -1.77988100 | 0.88557700 |
| C | -5.06279600 | -0.89714300 | 1.15482800 |
| C | -4.89943200 | 0.32025600 | 0.49713400 |
| C | -5.80632900 | 0.70613200 | -0.48837300 |
| O | -4.03344100 | -1.02656500 | 2.04690200 |
| C | -3.28464400 | 0.11564600 | 1.87058000 |
| N | -3.75299500 | 0.94000800 | 0.98354600 |
| C | -2.14287300 | 0.27020200 | 2.77789100 |
| C | -2.48922800 | 0.39804700 | 4.13260400 |
| C | -1.52909700 | 0.58859900 | 5.11246800 |
| C | -0.21401300 | 0.63291500 | 4.68713200 |
| C | 0.15609900 | 0.47666000 | 3.36472800 |
| C | -0.79415800 | 0.27812700 | 2.34505000 |
| F | 0.76076100 | 0.82106700 | 5.61222900 |
| C | -7.84130900 | 0.19098600 | -1.86995300 |
| C | -3.78832400 | 0.54836900 | -3.34207600 |
| C | -4.54983300 | -0.60986700 | -3.58532100 |
| C | -4.38485600 | -1.77682300 | -2.84620400 |
| C | -3.42922100 | -1.72975700 | -1.85283900 |
| C | -2.66745000 | -0.59689000 | -1.56273600 |
| C | -2.83540200 | 0.55707000 | -2.32297300 |
| O | -3.03228900 | -2.75044800 | -1.01814000 |
| C | -2.04993000 | -2.21398600 | -0.26871400 |
| N | -1.82852000 | -0.93298300 | -0.50244000 |
| C | -1.22282800 | -2.92543400 | 0.64042900 |
| C | -1.46089500 | -4.24437800 | 1.04084900 |
| C | -0.62009300 | -4.84166000 | 1.96217500 |
| C | 0.41301500 | -4.06448000 | 2.46908800 |
| C | 0.66163400 | -2.75721800 | 2.08333900 |
| C | -0.12728700 | -2.13668000 | 1.10556300 |
| F | 1.21868300 | -4.61421500 | 3.40720600 |
| C | -4.02745200 | 1.78051800 | -4.16133900 |
| C | 3.65166300 | -3.48524100 | -2.11057100 |
| C | 4.30902300 | -2.24694500 | -2.30872900 |
| C | 3.36954400 | -1.17062300 | -2.10945300 |
| C | 2.14264300 | -1.75802500 | -1.45560100 |

| | | | |
|---|---|---|---|
| C | 2.23611600 | -3.24597100 | -1.77057100 |
| C | 4.30371500 | -4.69800300 | -2.32064700 |
| C | 5.64009100 | -4.68259800 | -2.69399300 |
| C | 6.30488000 | -3.45900600 | -2.87718200 |
| C | 5.65756700 | -2.24593900 | -2.69640100 |
| C | 3.36996500 | 0.09332800 | -2.60888800 |
| C | 2.15705900 | 0.85405900 | -2.66743500 |
| C | 0.96337600 | 0.25904300 | -2.33666000 |
| C | 0.84918500 | -0.98953200 | -1.64105700 |
| O | 1.33847200 | -4.06880500 | -1.70687400 |
| H | 4.93125600 | -0.60200100 | 1.74982600 |
| H | 2.60036100 | -1.28679900 | 1.65150500 |
| H | 3.75276700 | 3.16039100 | 0.05808300 |
| H | -2.13827900 | 2.18840000 | -0.14539200 |
| H | -2.05018300 | 4.60170500 | -0.66207800 |
| H | 2.21725500 | 4.38255900 | -0.26508000 |
| H | 6.07689400 | 2.29045600 | 3.00767500 |
| H | 7.66274000 | 1.93983800 | 2.30724000 |
| H | 6.55112600 | 0.61986700 | 2.67295100 |
| H | 5.86652700 | 3.35934500 | -0.61677600 |
| H | 5.69447600 | 3.93145600 | 1.05173100 |
| H | 7.28136300 | 3.47892900 | 0.42749300 |
| H | 6.42590300 | 0.92981000 | -1.08803400 |
| H | 7.86354100 | 1.09899100 | -0.06972100 |
| H | 6.71009800 | -0.20548300 | 0.23754600 |
| H | -0.53282800 | 8.04513100 | -0.00522000 |
| H | -0.13096600 | 6.80745300 | 1.19338300 |
| H | -1.62292200 | 6.68010000 | 0.25263900 |
| H | 2.21940400 | 6.18634900 | -1.69328700 |
| H | 1.63587100 | 7.76856400 | -1.17607100 |
| H | 2.14021200 | 6.58780400 | 0.03088400 |
| H | 0.04592800 | 5.91090500 | -3.04081100 |
| H | -1.51908700 | 6.13730800 | -2.24809400 |
| H | -0.44137900 | 7.51635500 | -2.48013500 |
| H | -7.80529600 | -2.04108400 | -0.36776100 |
| H | -6.19202600 | -2.72601100 | 1.40475000 |
| H | -5.68626900 | 1.64700400 | -1.01765000 |
| H | -3.53761400 | 0.36168200 | 4.41604800 |
| H | -1.78196300 | 0.70041900 | 6.15991700 |
| H | 1.22058000 | 0.48529600 | 3.15513100 |
| H | -8.83625700 | 0.38946500 | -1.45751000 |
| H | -7.95719500 | -0.62909300 | -2.58538500 |
| H | -7.53116500 | 1.07902200 | -2.42502800 |
| H | -5.28782700 | -0.59167200 | -4.38214300 |
| H | -4.96233100 | -2.67310000 | -3.04057200 |
| H | -2.23741300 | 1.44146200 | -2.14339400 |
| H | -2.30519500 | -4.79211500 | 0.63338200 |
| H | -0.75759300 | -5.86032000 | 2.30326100 |
| H | 1.46270300 | -2.24508700 | 2.60365300 |
| H | -3.26850000 | 2.54246300 | -3.97285700 |
| H | -5.00321500 | 2.22349500 | -3.93254800 |
| H | -4.02734700 | 1.56001200 | -5.23237400 |
| H | 2.38472400 | -1.83014300 | -0.37534300 |
| H | 3.76695300 | -5.63310800 | -2.18595200 |
| H | 6.17754700 | -5.61286000 | -2.84620500 |
| H | 7.35018500 | -3.46540900 | -3.17210000 |
| H | 6.18986300 | -1.31262900 | -2.85406000 |
| H | 4.25876600 | 0.47990300 | -3.10511500 |
| H | 2.16965800 | 1.84194900 | -3.11750000 |
| H | 0.03745100 | 0.77716100 | -2.58059700 |
| H | 0.00964700 | -1.61802800 | -1.94616300 |

**TS1-III-Penta**

| | | | |
|---|---|---|---|
| Ir | 0.19794600 | -0.33553800 | -0.07671500 |
| F | 4.18713100 | -3.99619600 | -1.05871200 |
| N | -1.44816200 | -1.46401300 | -0.66281100 |
| O | -2.19906000 | -3.39271300 | -1.50353100 |
| C | 1.11867200 | -2.08990100 | -0.68548800 |
| C | 2.46893400 | -2.45175600 | -0.62485300 |
| H | 3.21983400 | -1.80131000 | -0.18593400 |
| C | 2.87547000 | -3.67459100 | -1.13165800 |
| C | 2.01289500 | -4.59844000 | -1.71361300 |
| H | 2.39871900 | -5.53784300 | -2.09054100 |
| C | 0.66915600 | -4.27388600 | -1.77579600 |
| H | -0.04154200 | -4.97193800 | -2.20795600 |
| C | 0.23240800 | -3.04412100 | -1.26908100 |
| C | -1.13107100 | -2.63496900 | -1.19335000 |
| C | -3.28929200 | -2.65577900 | -1.08812300 |
| C | -2.83280000 | -1.45772600 | -0.54405000 |
| C | -3.72650800 | -0.56166200 | 0.03257200 |
| H | -3.37487300 | 0.35776200 | 0.49106900 |
| C | -5.08252200 | -0.87911900 | 0.00423900 |
| C | -5.50887400 | -2.08692600 | -0.58482700 |
| H | -6.57090500 | -2.31365000 | -0.59391900 |
| C | -4.62316800 | -3.00598400 | -1.13782400 |
| H | -4.95546200 | -3.94378100 | -1.56685800 |
| C | -6.09335500 | 0.06914900 | 0.57371600 |
| H | -6.84038100 | -0.45159500 | 1.17892600 |
| H | -5.62209700 | 0.83196500 | 1.19682800 |
| H | -6.63800700 | 0.58761000 | -0.22297600 |

| | | | |
|---|---|---|---|
| F | -2.47123900 | -1.98112600 | 4.38522900 |
| N | 1.99478100 | 0.42015500 | 0.82641000 |
| O | 2.96378300 | 0.97427200 | 2.76993700 |
| C | -0.19881600 | -0.62501500 | 1.89873600 |
| C | -1.28195100 | -1.29607500 | 2.48170900 |
| H | -2.03905700 | -1.79988200 | 1.89078800 |
| C | -1.41328100 | -1.32400300 | 3.85885100 |
| C | -0.52363200 | -0.71532300 | 4.73858800 |
| H | -0.69050500 | -0.77194100 | 5.80736900 |
| C | 0.56790100 | -0.06501000 | 4.19292700 |
| H | 1.30286500 | 0.40615300 | 4.83874200 |
| C | 0.72907200 | -0.02899500 | 2.80314100 |
| C | 1.87321100 | 0.49685300 | 2.14234200 |
| C | 3.88412900 | 1.17759400 | 1.76678600 |
| C | 3.30434200 | 0.81005500 | 0.55172900 |
| C | 4.07743100 | 0.81516700 | -0.60563900 |
| H | 3.67162500 | 0.47142000 | -1.54824400 |
| C | 5.39807000 | 1.25716600 | -0.52044200 |
| C | 5.92578700 | 1.66553800 | 0.71867300 |
| H | 6.95660400 | 2.00420100 | 0.76064700 |
| C | 5.18248700 | 1.62225800 | 1.89408600 |
| H | 5.59971300 | 1.90229800 | 2.85423200 |
| C | 6.24507000 | 1.32329500 | -1.75498000 |
| H | 7.29230600 | 1.09798900 | -1.54071700 |
| H | 5.89499200 | 0.62712200 | -2.52016200 |
| H | 6.21921800 | 2.32656900 | -2.19569800 |
| C | 1.92794600 | 2.46620100 | -2.22834200 |
| C | 1.41874300 | 1.23795200 | -2.60199700 |
| C | -0.16012700 | 3.06430900 | -1.18395400 |
| C | 1.11904900 | 3.40135500 | -1.54215800 |
| H | 2.93795000 | 2.74146900 | -2.51361600 |
| H | 2.02420200 | 0.56760500 | -3.20723000 |
| H | 1.48510700 | 4.41153700 | -1.37637800 |
| C | -2.48005400 | 3.17525500 | -0.91369200 |
| C | -3.71439500 | 3.73228900 | -0.60706900 |
| C | -3.74507800 | 5.00961000 | -0.05738700 |
| C | -2.55258300 | 5.71244100 | 0.14941100 |
| C | -1.31508000 | 5.16682900 | -0.18112200 |
| C | -1.27234000 | 3.87970200 | -0.71675500 |
| H | -4.62700200 | 3.17201300 | -0.79318300 |
| H | -4.69174700 | 5.46730100 | 0.21031400 |
| H | -2.59482200 | 6.71073400 | 0.57485000 |
| H | -0.40392200 | 5.73482900 | -0.01950000 |
| C | -2.17930900 | 1.88092300 | -1.55423000 |
| O | -2.93442300 | 1.13239700 | -2.13859800 |
| C | -0.66967400 | 1.72267500 | -1.43502100 |
| H | -0.79885000 | 1.14888200 | -0.10539400 |
| C | 0.11586200 | 0.81869000 | -2.24094100 |
| H | -0.38390700 | 0.03600700 | -2.80537700 |

**TS3-III-Hexa**

| | | | |
|---|---|---|---|
| C | 3.54085700 | -0.07676700 | -1.93908100 |
| C | 2.17169100 | -0.17720300 | -1.85331900 |
| N | 1.44109100 | 0.50071200 | -0.94396000 |
| C | 2.09007000 | 1.39882400 | -0.15372700 |
| C | 3.47965100 | 1.51910200 | -0.18978100 |
| C | 4.24764400 | 0.76486900 | -1.06796400 |
| C | 1.22784800 | 2.27615600 | 0.63867200 |
| N | -0.10094700 | 2.07224200 | 0.47243900 |
| C | -0.95780300 | 2.92624200 | 1.04780600 |
| C | -0.54099800 | 3.99483200 | 1.81732600 |
| C | 0.82235400 | 4.19752200 | 2.05697900 |
| C | 1.70328300 | 3.31013200 | 1.44251300 |
| C | 5.76736700 | 0.81979900 | -1.11237400 |
| C | 6.22790500 | 1.14672600 | -2.53896300 |
| C | 6.33401700 | 1.86886300 | -0.15893100 |
| C | 6.30298300 | -0.56107900 | -0.70604700 |
| C | 1.27990300 | 5.32879800 | 2.96806600 |
| C | 0.73800400 | 6.66098600 | 2.43413900 |
| C | 0.71187800 | 5.07378400 | 4.37208500 |
| C | 2.80133500 | 5.41625100 | 3.05800000 |
| C | 4.76000600 | -3.42399100 | 1.12481100 |
| C | 4.94417200 | -4.38541800 | 0.11111200 |
| C | 3.99688300 | -4.61485700 | -0.88286400 |
| C | 2.85502500 | -3.83855100 | -0.81650800 |
| C | 2.62870500 | -2.88150600 | 0.17270700 |
| C | 3.59222100 | -2.66125100 | 1.15851400 |
| O | 1.77735100 | -3.83793100 | -1.65046600 |
| C | 0.93594600 | -2.86538000 | -1.12274200 |
| N | 1.39179400 | -2.29602100 | -0.04897200 |
| C | -0.25823500 | -2.60211600 | -1.91391300 |
| C | -0.67001000 | -3.66489500 | -2.74361500 |
| C | -1.72780100 | -3.55167700 | -3.62406400 |
| C | -2.35353000 | -2.31812800 | -3.67801200 |
| C | -1.98239800 | -1.25611500 | -2.88075900 |
| C | -0.93822100 | -1.34086200 | -1.93483500 |
| F | -3.37546000 | -2.14362700 | -4.55126600 |
| C | 5.82877800 | -3.22945700 | 2.15949700 |
| C | -5.32657200 | -1.67170800 | 0.80082600 |
| C | -6.40760300 | -0.85846400 | 0.41014400 |

| | | | |
|---|---|---|---|
| C | -6.24129800 | 0.31905500 | -0.31336100 |
| C | -4.93799600 | 0.65375200 | -0.61115800 |
| C | -3.83798200 | -0.09664200 | -0.19366100 |
| C | -4.01877200 | -1.28769600 | 0.49777000 |
| O | -4.48462000 | 1.70068300 | -1.38863000 |
| C | -3.14766700 | 1.54590200 | -1.42118400 |
| N | -2.70862700 | 0.53920400 | -0.68821000 |
| C | -2.24535500 | 2.25544500 | -2.26813500 |
| C | -2.60393600 | 3.31191700 | -3.11192700 |
| C | -1.65587700 | 3.86675600 | -3.95347300 |
| C | -0.37141600 | 3.33562500 | -3.91877700 |
| C | 0.01328500 | 2.29443900 | -3.08891300 |
| C | -0.92622400 | 1.71337900 | -2.23291300 |
| F | 0.55650000 | 3.87028800 | -4.74284100 |
| C | -5.58748700 | -2.94162000 | 1.55162700 |
| Ir | -0.60886700 | 0.34211000 | -0.74899600 |
| C | -0.16935500 | -2.61470600 | 2.78848700 |
| C | -1.56195600 | -2.61267200 | 3.03972500 |
| C | -2.02747800 | -1.24790800 | 3.15100700 |
| C | -0.93278000 | -0.37046300 | 2.79044000 |
| C | 0.31818700 | -1.21968500 | 2.75498600 |
| C | 0.55224400 | -3.80096200 | 2.72987400 |
| C | -0.12422100 | -5.00742200 | 2.86676400 |
| C | -1.50842800 | -5.01481600 | 3.08780100 |
| C | -2.23278300 | -3.83301600 | 3.18462700 |
| C | -3.23008400 | -0.73576900 | 3.61169100 |
| C | -3.34579100 | 0.63231600 | 3.86794200 |
| C | -2.20460100 | 1.44870500 | 3.76811400 |
| C | -0.99592600 | 0.95753100 | 3.31081200 |
| O | 1.46881400 | -0.81501800 | 2.78504000 |
| H | 4.05433600 | -0.67080100 | -2.68776400 |
| H | 1.61194500 | -0.81501500 | -2.52636800 |
| H | 3.94998500 | 2.22710500 | 0.47986800 |
| H | -2.01262600 | 2.72767100 | 0.88524700 |
| H | -1.28963000 | 4.64885400 | 2.25146500 |
| H | 2.77210300 | 3.42627200 | 1.56663500 |
| H | 5.84230200 | 2.11576900 | -2.87053500 |
| H | 5.90374600 | 0.39136300 | -3.25976200 |
| H | 7.32046200 | 1.18966700 | -2.57803800 |
| H | 6.07012500 | 1.66223700 | 0.88252900 |
| H | 7.42543600 | 1.87224500 | -0.22388200 |
| H | 5.98729100 | 2.87741800 | -0.40542600 |
| H | 6.00236600 | -0.81134200 | 0.31557300 |
| H | 5.93252300 | -1.35080600 | -1.36691100 |
| H | 7.39674100 | -0.56984600 | -0.75060300 |
| H | 1.04875700 | 7.48111400 | 3.08844200 |
| H | -0.35427200 | 6.67049900 | 2.38911000 |
| H | 1.11864800 | 6.87059000 | 1.42982800 |
| H | -0.38182000 | 5.05571100 | 4.37059100 |
| H | 1.06310300 | 4.11919900 | 4.77626700 |
| H | 1.03005300 | 5.86642100 | 5.05632300 |
| H | 3.25852900 | 5.60437500 | 2.08158800 |
| H | 3.08336900 | 6.24231000 | 3.71643300 |
| H | 3.24162900 | 4.50368700 | 3.47091000 |
| H | 5.86273900 | -4.96603000 | 0.10456400 |
| H | 4.14663700 | -5.35547600 | -1.66033800 |
| H | 3.41467000 | -1.92594900 | 1.93759900 |
| H | -0.13827700 | -4.60775300 | -2.68284000 |
| H | -2.05174200 | -4.37315400 | -4.25191000 |
| H | -2.53331100 | -0.33299700 | -3.02382000 |
| H | 5.91600500 | -4.10245400 | 2.81529800 |
| H | 5.62218700 | -2.36339900 | 2.79156700 |
| H | 6.81150900 | -3.08467700 | 1.69979900 |
| H | -7.41450200 | -1.17999200 | 0.65980300 |
| H | -7.08074800 | 0.91803300 | -0.64543400 |
| H | -3.16816700 | -1.90198900 | 0.77569700 |
| H | -3.62123700 | 3.69163100 | -3.10878400 |
| H | -1.88698600 | 4.68514600 | -4.62448200 |
| H | 1.04456500 | 1.95767600 | -3.13494600 |
| H | -5.64793500 | -2.76029300 | 2.63101400 |
| H | -4.79275100 | -3.67280200 | 1.39035200 |
| H | -6.53531900 | -3.39561400 | 1.25273700 |
| H | -0.85031800 | -0.34317000 | 1.28102000 |
| H | 1.62725000 | -3.77616400 | 2.57963300 |
| H | 0.41624400 | -5.94699700 | 2.81007900 |
| H | -2.02237800 | -5.96567500 | 3.19805600 |
| H | -3.29966400 | -3.85894200 | 3.38627000 |
| H | -4.05798700 | -1.40547200 | 3.83589600 |
| H | -4.27963700 | 1.04413400 | 4.23633500 |
| H | -2.26512700 | 2.48409200 | 4.09837900 |
| H | -0.10296100 | 1.57689200 | 3.30675900 |

**Pro-III-Penta**

| | | | |
|---|---|---|---|
| Ir | 0.52870600 | 0.32566800 | -0.37088700 |
| F | 3.09650800 | -0.26689100 | 4.54916700 |
| N | -1.38889400 | 0.66215000 | 0.35972000 |
| O | -2.75401600 | 0.84775000 | 2.11620000 |
| C | 0.83627400 | 0.23718400 | 1.74538700 |
| C | 2.00451400 | 0.02153600 | 2.48142800 |
| H | 2.97344300 | -0.10335800 | 2.00250200 |

| | | | |
|---|---|---|---|
| C | 1.94814300 | -0.05113600 | 3.86568300 |
| C | 0.77469900 | 0.08234400 | 4.59893700 |
| H | 0.80076900 | 0.01324200 | 5.67996200 |
| C | -0.39974900 | 0.31096200 | 3.90051900 |
| H | -1.33957900 | 0.42334300 | 4.43417300 |
| C | -0.35806700 | 0.39088200 | 2.50446300 |
| C | -1.50176700 | 0.62291800 | 1.67750100 |
| C | -3.49729000 | 1.06778600 | 0.97332300 |
| C | -2.65169300 | 0.96186400 | -0.12969000 |
| C | -3.13768200 | 1.15421800 | -1.41715300 |
| H | -2.47756500 | 1.06919600 | -2.27506300 |
| C | -4.49241100 | 1.45097600 | -1.56217500 |
| C | -5.32101100 | 1.53166800 | -0.42496900 |
| H | -6.37549500 | 1.75101900 | -0.56617100 |
| C | -4.84424300 | 1.34238400 | 0.86911500 |
| H | -5.48777900 | 1.40338900 | 1.73863400 |
| C | -5.07582900 | 1.68898400 | -2.92161700 |
| H | -5.24110200 | 2.75770400 | -3.09774500 |
| H | -4.41582200 | 1.32746800 | -3.71296600 |
| H | -6.04685200 | 1.19904800 | -3.03380100 |
| F | -0.19726800 | 5.64139200 | 0.00918100 |
| N | 2.57421400 | 0.20466700 | -0.88380300 |
| O | 4.46236600 | 1.35914100 | -1.21795300 |
| C | 1.00317600 | 2.24506700 | -0.41085100 |
| C | 0.14666800 | 3.32945900 | -0.17002500 |
| H | -0.90701900 | 3.19633500 | 0.04725700 |
| C | 0.65198500 | 4.61533300 | -0.22124800 |
| C | 1.98210200 | 4.92480100 | -0.49515000 |
| H | 2.30527200 | 5.95814100 | -0.51793400 |
| C | 2.84674400 | 3.87267100 | -0.72995200 |
| H | 3.89321800 | 4.06160900 | -0.94927700 |
| C | 2.37100300 | 2.55741300 | -0.68700900 |
| C | 3.14744500 | 1.39442400 | -0.92500800 |
| C | 4.74666800 | 0.02095800 | -1.38084600 |
| C | 3.57471300 | -0.70967500 | -1.17958700 |
| C | 3.58877700 | -2.09579000 | -1.30065800 |
| H | 2.68513900 | -2.67842900 | -1.16740300 |
| C | 4.79647200 | -2.71989200 | -1.61351700 |
| C | 5.95793800 | -1.94564900 | -1.80202000 |
| H | 6.88712700 | -2.45299900 | -2.04458200 |
| C | 5.95835400 | -0.55843100 | -1.69279200 |
| H | 6.85401900 | 0.03260600 | -1.84390600 |
| C | 4.86361400 | -4.20963200 | -1.76234200 |
| H | 5.08903200 | -4.49658400 | -2.79454200 |
| H | 5.65306400 | -4.63892100 | -1.13857900 |
| H | 3.92025100 | -4.68445700 | -1.48518600 |
| C | 0.75585500 | -3.10607500 | 0.95857800 |
| C | 0.12970800 | -3.13911300 | 2.20163300 |
| C | -1.33173800 | -2.61897100 | -0.11245700 |
| C | 0.03436900 | -2.84562900 | -0.21471400 |
| H | 1.82622900 | -3.28229200 | 0.89876400 |
| H | 0.71549100 | -3.34029700 | 3.09255800 |
| H | 0.52802500 | -2.84318300 | -1.18323900 |
| C | -3.60039700 | -2.21040800 | -0.49641100 |
| C | -4.75546600 | -1.94542300 | -1.21098200 |
| C | -4.65871500 | -1.80788200 | -2.59740600 |
| C | -3.42445800 | -1.92467200 | -3.23282700 |
| C | -2.25642200 | -2.18907800 | -2.50959000 |
| C | -2.35364700 | -2.33686700 | -1.13529400 |
| H | -5.70841400 | -1.84367300 | -0.69927200 |
| H | -5.54718400 | -1.60039200 | -3.18498000 |
| H | -3.36695500 | -1.80552100 | -4.31053600 |
| H | -1.30129200 | -2.27286300 | -3.01893400 |
| C | -3.41308800 | -2.38420800 | 0.97032500 |
| O | -4.26269300 | -2.31582800 | 1.84017200 |
| C | -1.95787900 | -2.65119700 | 1.14680200 |
| H | 0.09483400 | 0.30413400 | -2.01588600 |
| C | -1.24307200 | -2.90438300 | 2.30456600 |
| H | -1.74441800 | -2.91571800 | 3.26871700 |

**Pro-III-Hexa**

| | | | |
|---|---|---|---|
| C | 3.53764100 | 1.36908600 | -1.49287400 |
| C | 2.18650400 | 1.12645600 | -1.65702700 |
| N | 1.30483900 | 1.14354700 | -0.64243000 |
| C | 1.76099200 | 1.54374500 | 0.58175900 |
| C | 3.11173200 | 1.79191500 | 0.79597000 |
| C | 4.04818600 | 1.67901000 | -0.23019900 |
| C | 0.73091400 | 1.77576100 | 1.59640400 |
| N | -0.53989800 | 1.58105900 | 1.17423600 |
| C | -1.54418600 | 1.89743100 | 2.00536700 |
| C | -1.33471300 | 2.39583400 | 3.27533200 |
| C | -0.03018900 | 2.55800100 | 3.76106400 |
| C | 1.00229800 | 2.23620300 | 2.88598000 |
| C | 5.52552900 | 1.93014000 | 0.04197000 |
| C | 5.71756900 | 3.40960800 | 0.40258800 |
| C | 5.97968300 | 1.05979100 | 1.22091500 |
| C | 6.38821000 | 1.59742800 | -1.17333000 |
| C | 0.20484600 | 3.04688200 | 5.18451200 |
| C | -0.46300900 | 4.41656800 | 5.36318900 |
| C | -0.42914300 | 2.04302700 | 6.15817300 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.69061200 | 3.17657700 | 5.51085700 | C | -2.95543200 | -3.25419300 | 3.21246500 |
| C | 5.33590300 | -2.57174300 | -0.21712600 | C | -3.36970700 | -2.08650300 | 3.86176600 |
| C | 5.81144400 | -2.55352400 | -1.54382000 | C | -2.50520800 | -1.00605600 | 4.02848400 |
| C | 4.98139800 | -2.30726500 | -2.63434400 | C | -1.19345200 | -1.07407800 | 3.55303200 |
| C | 3.64923600 | -2.08530100 | -2.33831800 | O | 1.54434700 | -1.87488500 | 2.34076500 |
| C | 3.13441500 | -2.10627000 | -1.04162300 | H | 4.17655400 | 1.30376000 | -2.36528700 |
| C | 3.98378800 | -2.34025800 | 0.04097100 | H | 1.77518300 | 0.89288100 | -2.63184900 |
| O | 2.62468500 | -1.79271800 | -3.18483600 | H | 3.43248400 | 2.09307300 | 1.78640200 |
| C | 1.51647000 | -1.64398800 | -2.35093100 | H | -2.54761100 | 1.72876500 | 1.62680800 |
| N | 1.77499800 | -1.83920900 | -1.09344800 | H | -2.19571600 | 2.63518400 | 3.89024200 |
| C | 0.29640600 | -1.27203800 | -3.06958700 | H | 2.03301900 | 2.34638800 | 3.19570800 |
| C | 0.16735500 | -1.88067100 | -4.33365000 | H | 5.14858800 | 3.68515900 | 1.29528200 |
| C | -0.88490700 | -1.60434900 | -5.18709000 | H | 5.39973600 | 4.06401700 | -0.41471700 |
| C | -1.80010300 | -0.66419100 | -4.74732100 | H | 6.77345100 | 3.61399000 | 0.60567000 |
| C | -1.69930600 | -0.03673700 | -3.52336600 | H | 5.81146700 | -0.00109400 | 1.01591900 |
| C | -0.65940200 | -0.31050600 | -2.60840000 | H | 7.04875900 | 1.20516900 | 1.40402000 |
| F | -2.83733000 | -0.33759400 | -5.55982500 | H | 5.45150200 | 1.31107600 | 2.14485700 |
| C | 6.29194900 | -2.84688600 | 0.90625600 | H | 6.27244700 | 0.55228200 | -1.47813000 |
| C | -4.94202200 | -2.34916700 | 0.05901800 | H | 6.15125500 | 2.23086300 | -2.03324400 |
| C | -6.15640800 | -1.65346200 | -0.10678700 | H | 7.44252500 | 1.75778400 | -0.93167100 |
| C | -6.21133100 | -0.31177800 | -0.47246800 | H | -0.30784600 | 4.77851800 | 6.38402300 |
| C | -4.99225400 | 0.30480000 | -0.66270600 | H | -1.54157700 | 4.37215700 | 5.18953700 |
| C | -3.77091700 | -0.34492200 | -0.48764900 | H | -0.04194500 | 5.15711000 | 4.67659800 |
| C | -3.72732000 | -1.68665600 | -0.12190500 | H | -1.50694400 | 1.94672400 | 6.00003400 |
| O | -4.74468600 | 1.59864200 | -1.06957400 | H | 0.01806100 | 1.04961500 | 6.05390900 |
| C | -3.39983800 | 1.68930200 | -1.13706700 | H | -0.27491700 | 2.37279600 | 7.19012500 |
| N | -2.77889200 | 0.57478900 | -0.78629700 | H | 2.19291600 | 3.89436600 | 4.85520100 |
| C | -2.66583900 | 2.83233900 | -1.58262400 | H | 1.81147400 | 3.53053400 | 6.53814800 |
| C | -3.25919000 | 4.03781400 | -1.97952100 | H | 2.21309600 | 2.21859400 | 5.43097800 |
| C | -2.45379900 | 5.07620700 | -2.41581000 | H | 6.86934700 | -2.72988900 | -1.71886500 |
| C | -1.07914900 | 4.86352400 | -2.43562300 | H | 5.35897700 | -2.28403100 | -3.65039800 |
| C | -0.47754300 | 3.67792700 | -2.04421300 | H | 3.59234700 | -2.32560100 | 1.05396300 |
| C | -1.25781300 | 2.60278700 | -1.60403800 | H | 0.91490900 | -2.60369400 | -4.64231200 |
| F | -0.29220500 | 5.88114900 | -2.86262700 | H | -0.99397800 | -2.08596600 | -6.15125400 |
| C | -4.97305500 | -3.80719100 | 0.40479700 | H | -2.45581300 | 0.70670300 | -3.29588300 |
| Ir | -0.69820900 | 0.68699700 | -0.79397500 | H | 6.59273600 | -3.90025500 | 0.92483800 |
| C | 0.36849800 | -3.91842300 | 1.72861800 | H | 5.84795400 | -2.61801300 | 1.87732000 |
| C | -0.94045400 | -4.36586800 | 1.98544000 | H | 7.21115800 | -2.26160900 | 0.80762400 |
| C | -1.66013000 | -3.31241800 | 2.72139700 | H | -7.08721700 | -2.19249400 | 0.04381900 |
| C | -0.79011400 | -2.22347800 | 2.89990000 | H | -7.14952700 | 0.21155100 | -0.61318400 |
| C | 0.53620400 | -2.55702600 | 2.31135200 | H | -2.77545100 | -2.19586300 | -0.00321500 |
| C | 1.27933500 | -4.70975500 | 1.05003400 | H | -4.33794100 | 4.16225000 | -1.94618500 |
| C | 0.86862200 | -5.97049000 | 0.61213300 | H | -2.85967800 | 6.02850100 | -2.73548500 |
| C | -0.42767200 | -6.41559800 | 0.86280100 | H | 0.60808400 | 3.61521700 | -2.09471900 |
| C | -1.34652700 | -5.61970100 | 1.55386600 | H | -5.51985200 | -3.98860600 | 1.33543500 |

| | | | |
|---|---|---|---|
| H | -3.96665700 | -4.21427500 | 0.51491900 |
| H | -5.48202100 | -4.38416800 | -0.37399800 |
| H | -0.51980300 | -0.81278900 | -0.09523300 |
| H | 2.28700700 | -4.35264000 | 0.86043700 |
| H | 1.56079900 | -6.60867100 | 0.07299500 |
| H | -0.73017400 | -7.39859900 | 0.51557100 |
| H | -2.35156600 | -5.98287400 | 1.74609200 |
| H | -3.63829000 | -4.08996000 | 3.09931000 |
| H | -4.38449400 | -2.02134300 | 4.24243600 |
| H | -2.85410400 | -0.11121400 | 4.53456700 |
| H | -0.50056300 | -0.24777500 | 3.68376300 |

**Sub-II-Penta**

| | | | |
|---|---|---|---|
| C | -2.46709300 | -4.81164300 | 0.26629400 |
| C | -3.59202700 | -5.00858000 | -0.55163400 |
| C | -4.14046400 | -3.98986700 | -1.33552000 |
| C | -3.50659300 | -2.76999600 | -1.26651800 |
| C | -2.37976700 | -2.53896800 | -0.47061600 |
| C | -1.85039800 | -3.55639300 | 0.31427400 |
| O | -3.83341100 | -1.59940300 | -1.91857300 |
| C | -2.90416600 | -0.70359900 | -1.50254200 |
| N | -2.02508100 | -1.21428400 | -0.64545100 |
| C | -2.79056800 | 0.65210200 | -1.89001400 |
| C | -3.63724100 | 1.32890900 | -2.78249100 |
| C | -3.38355300 | 2.64965500 | -3.10053600 |
| C | -2.28903300 | 3.26767900 | -2.49393300 |
| C | -1.45336900 | 2.64421200 | -1.58604600 |
| C | -1.66402900 | 1.29369000 | -1.26858800 |
| F | -2.03666700 | 4.56122600 | -2.82170300 |
| C | -1.92468300 | -5.93954600 | 1.09208000 |
| C | 3.75394200 | 3.13526900 | -0.50006700 |
| C | 3.83540500 | 4.16661300 | 0.44535400 |
| C | 2.84921100 | 4.36505900 | 1.42046600 |
| C | 1.79746100 | 3.47696900 | 1.41398700 |
| C | 1.69459100 | 2.42071800 | 0.49962000 |
| C | 2.66244700 | 2.25644200 | -0.48447800 |
| O | 0.69810100 | 3.45964700 | 2.24059400 |
| C | -0.04584000 | 2.39775000 | 1.80923500 |
| N | 0.53469800 | 1.72963400 | 0.79284900 |
| C | -1.29063400 | 1.97863900 | 2.30323100 |
| C | -1.99282100 | 2.53774600 | 3.39168500 |
| C | -3.20894200 | 2.00449200 | 3.77235900 |
| C | -3.71205000 | 0.92247600 | 3.04610700 |
| C | -3.05900100 | 0.35722700 | 1.96408000 |
| C | -1.81072500 | 0.85304200 | 1.56437600 |
| F | -4.91282700 | 0.40109200 | 3.43070400 |
| C | 4.83758300 | 2.94659400 | -1.52021900 |
| Ir | -0.63857100 | 0.17902200 | 0.04790200 |
| C | 6.29086400 | -3.29495400 | 1.35374800 |
| C | 6.80035300 | -2.71299300 | 0.17666200 |
| C | 5.99425600 | -1.99459000 | -0.68867200 |
| C | 4.62856000 | -1.83553100 | -0.38141400 |
| C | 4.12916500 | -2.40669200 | 0.82149500 |
| C | 4.94974600 | -3.14760500 | 1.67191100 |
| C | 3.56636900 | -1.18395500 | -1.08423800 |
| C | 2.35642400 | -1.16813000 | -0.17831800 |
| C | 2.68668800 | -2.15454600 | 0.92445400 |
| C | 3.46330400 | -0.72606200 | -2.36953700 |
| C | 2.19118900 | -0.41696600 | -2.92736000 |
| C | 1.04284000 | -0.81827700 | -2.25624300 |
| C | 1.02274700 | -1.24752200 | -0.89739500 |
| O | 1.90220500 | -2.61969300 | 1.74458700 |
| H | -4.05514300 | -5.99042400 | -0.57164800 |
| H | -5.01217600 | -4.14985200 | -1.95909600 |
| H | -0.98223400 | -3.37770700 | 0.94284100 |
| H | -4.49210600 | 0.81718200 | -3.21517200 |
| H | -4.00621600 | 3.20830100 | -3.78898100 |
| H | -0.64491900 | 3.21785800 | -1.14303500 |
| H | -2.50001200 | -6.85594300 | 0.94853000 |
| H | -0.88230500 | -6.15487500 | 0.83795400 |
| H | -1.94147000 | -5.69742100 | 2.15916700 |
| H | 4.68592000 | 4.84120500 | 0.41410500 |
| H | 2.90626100 | 5.17674000 | 2.13672300 |
| H | 2.56728100 | 1.47125700 | -1.22672000 |
| H | -1.58059500 | 3.38867000 | 3.92694400 |
| H | -3.77555800 | 2.40380300 | 4.60592200 |
| H | -3.53833300 | -0.46825400 | 1.44421500 |
| H | 5.49115500 | 3.81939400 | -1.58273400 |
| H | 5.46655200 | 2.08256700 | -1.27521100 |
| H | 4.42500100 | 2.75872700 | -2.51585700 |
| H | 6.95395400 | -3.85249500 | 2.00722700 |
| H | 7.85408600 | -2.83675500 | -0.05803200 |
| H | 6.41162800 | -1.56125600 | -1.59331600 |
| H | 4.53274700 | -3.59123800 | 2.57252900 |
| H | 2.41322600 | -0.21798300 | 0.39112800 |
| H | 4.34112200 | -0.70184100 | -3.01416700 |
| H | 2.12640400 | -0.05527100 | -3.94858000 |
| H | 0.10784100 | -0.87159900 | -2.81473100 |
| H | 0.43991200 | -2.15340400 | -0.70436300 |

**Sub-II-Hexa**

| | | | |
|---|---|---|---|
| Ir | -0.09116000 | -0.14538000 | 0.45066400 |
| C | 4.18133200 | 0.06260300 | 1.34379200 |
| C | 2.85182200 | -0.28931400 | 1.34465300 |
| N | 1.86298100 | 0.46404400 | 0.82560500 |
| C | 2.21209500 | 1.71814200 | 0.32698600 |
| C | 3.57521500 | 2.09723300 | 0.27700700 |
| C | 4.58171500 | 1.29146500 | 0.75529900 |
| C | 1.14856500 | 2.53993200 | -0.13162400 |
| N | -0.09911400 | 1.95328700 | -0.12582500 |
| C | -1.16654600 | 2.73854200 | -0.32931400 |
| C | -1.08367900 | 4.06928600 | -0.68292400 |
| C | 0.19478400 | 4.67328500 | -0.82961700 |
| C | 1.28972000 | 3.89360500 | -0.53028100 |
| C | 6.06060500 | 1.64171700 | 0.66559200 |
| C | 6.66266500 | 1.67825200 | 2.07674900 |
| C | 6.29463400 | 2.99459400 | -0.00208500 |
| C | 6.77663700 | 0.56162500 | -0.15801300 |
| C | 0.29520300 | 6.12967700 | -1.26673000 |
| C | -0.43306400 | 7.01577600 | -0.24652600 |
| C | 1.74218700 | 6.60408300 | -1.37814900 |
| C | -0.37840300 | 6.28825500 | -2.63703300 |
| C | -6.83339800 | -0.66108800 | -0.61986300 |
| C | -6.61206100 | -1.89372600 | 0.02832400 |
| C | -5.58283400 | -2.08487000 | 0.94472300 |
| C | -4.78315000 | -0.98332300 | 1.18553400 |
| C | -4.97228400 | 0.25470400 | 0.57409500 |
| C | -6.00725700 | 0.42734500 | -0.34346400 |
| O | -3.69131800 | -0.87935000 | 2.00177900 |
| C | -3.25876100 | 0.41532800 | 1.82649600 |
| N | -3.98127100 | 1.12591200 | 1.01508200 |
| C | -2.12279300 | 0.82058100 | 2.66582900 |
| C | -2.47257100 | 1.41845700 | 3.88448500 |
| C | -1.51003100 | 1.77294800 | 4.81746300 |
| C | -0.19733700 | 1.49088500 | 4.48561200 |
| C | 0.17397800 | 0.91404600 | 3.28615900 |
| C | -0.77655300 | 0.56574100 | 2.30663500 |
| F | 0.77617000 | 1.80401600 | 5.38098800 |
| C | -7.94087100 | -0.54033800 | -1.62365000 |
| C | -3.86870300 | 0.54306100 | -3.31579000 |
| C | -4.58646200 | -0.63890900 | -3.57548800 |
| C | -4.37715200 | -1.80726500 | -2.84919700 |
| C | -3.43105200 | -1.73532200 | -1.84824600 |
| C | -2.70993100 | -0.57864100 | -1.54212600 |
| C | -2.91476000 | 0.57406400 | -2.29732500 |
| O | -3.02053900 | -2.74392300 | -1.01021900 |
| C | -2.07468900 | -2.17408000 | -0.23051800 |
| N | -1.87927600 | -0.88519100 | -0.46568200 |
| C | -1.27816600 | -2.86125800 | 0.71968400 |
| C | -1.53513900 | -4.16888500 | 1.14735100 |
| C | -0.73166800 | -4.74270100 | 2.11566000 |
| C | 0.28555400 | -3.95384600 | 2.64073200 |
| C | 0.55195300 | -2.65880300 | 2.23158400 |
| C | -0.19964200 | -2.05758600 | 1.20893900 |
| F | 1.05449900 | -4.48673800 | 3.62392500 |
| C | -4.15772900 | 1.77843500 | -4.11491100 |
| C | 3.56332500 | -3.73057300 | -1.75720100 |
| C | 4.26878200 | -2.53466300 | -2.06054500 |
| C | 3.37658900 | -1.41596100 | -1.96933600 |
| C | 2.10694900 | -1.90224200 | -1.31107200 |
| C | 2.15310800 | -3.41497200 | -1.47798300 |
| C | 4.17487700 | -4.97990800 | -1.84929400 |
| C | 5.51329200 | -5.05071800 | -2.20593500 |
| C | 6.22518800 | -3.87032400 | -2.49360900 |
| C | 5.62370600 | -2.62485800 | -2.43221100 |
| C | 3.44194200 | -0.18365400 | -2.55800100 |
| C | 2.27098500 | 0.61217100 | -2.70637000 |
| C | 1.03985900 | 0.09954400 | -2.34611200 |
| C | 0.85689300 | -1.09455000 | -1.59004300 |
| O | 1.22589300 | -4.20316400 | -1.35447000 |
| H | 4.90221600 | -0.62587300 | 1.76987900 |
| H | 2.54923800 | -1.24071100 | 1.75924500 |
| H | 3.81174800 | 3.05108200 | -0.17879100 |
| H | -2.13261300 | 2.26075800 | -0.19095200 |
| H | -1.99684800 | 4.63195000 | -0.84154100 |
| H | 2.28622500 | 4.31652500 | -0.56996300 |
| H | 6.17613400 | 2.43859100 | 2.69578100 |
| H | 7.73062500 | 1.91590900 | 2.03056700 |
| H | 6.56076200 | 0.71708600 | 2.58822300 |
| H | 5.90680300 | 3.01466800 | -1.02556800 |
| H | 5.82476400 | 3.81226600 | 0.55327600 |
| H | 7.36714800 | 3.20500400 | -0.05251400 |
| H | 6.38195000 | 0.52194700 | -1.17793300 |
| H | 7.84934300 | 0.77461400 | -0.21864400 |
| H | 6.65856000 | -0.43270600 | 0.28193900 |
| H | -0.38260800 | 8.06701400 | -0.54909100 |
| H | 0.01942700 | 6.92989800 | 0.74629300 |
| H | -1.48933800 | 6.74816200 | -0.15496200 |
| H | 2.31039200 | 6.01452300 | -2.10427800 |
| H | 1.76740200 | 7.64675000 | -1.70867600 |

| | | | |
|---|---|---|---|
| H | 2.26503000 | 6.55186600 | -0.41829700 |
| H | 0.11705000 | 5.67363400 | -3.39524300 |
| H | -1.43195500 | 5.99616200 | -2.60782400 |
| H | -0.33245800 | 7.33114900 | -2.96773900 |
| H | -7.26468900 | -2.72917900 | -0.21015600 |
| H | -5.40464500 | -3.04161400 | 1.42311900 |
| H | -6.15304200 | 1.37977300 | -0.84531400 |
| H | -3.52171900 | 1.59968200 | 4.10368900 |
| H | -1.76011800 | 2.23661400 | 5.76425600 |
| H | 1.23376800 | 0.74748300 | 3.12649700 |
| H | -8.92577300 | -0.60299900 | -1.14861700 |
| H | -7.89883700 | -1.34533000 | -2.36414400 |
| H | -7.89320600 | 0.41020200 | -2.15974100 |
| H | -5.32553900 | -0.63849000 | -4.37176600 |
| H | -4.92270200 | -2.72170700 | -3.05280500 |
| H | -2.34781900 | 1.47689700 | -2.11107600 |
| H | -2.36407900 | -4.72756900 | 0.72191800 |
| H | -0.88474000 | -5.75171900 | 2.47888500 |
| H | 1.34150400 | -2.13312300 | 2.75778800 |
| H | -3.42341000 | 2.56330600 | -3.92241300 |
| H | -5.14519700 | 2.18415200 | -3.86643700 |
| H | -4.16299000 | 1.57473500 | -5.18939800 |
| H | 2.31668700 | -1.88727600 | -0.22049200 |
| H | 3.60123900 | -5.87863700 | -1.63671800 |
| H | 6.01769200 | -6.00993300 | -2.26386300 |
| H | 7.27226500 | -3.94195100 | -2.77510300 |
| H | 6.19335100 | -1.73004800 | -2.66685900 |
| H | 4.36456000 | 0.13591800 | -3.04151900 |
| H | 2.33715100 | 1.57943100 | -3.19565200 |
| H | 0.14435200 | 0.65034100 | -2.63172000 |
| H | -0.02008300 | -1.69336800 | -1.84462600 |

**TS2-II-Penta**

| | | | |
|---|---|---|---|
| C | -6.04658500 | 1.04625500 | -1.82574800 |
| C | -6.78518400 | 0.78874600 | -0.65417900 |
| C | -6.18044000 | 0.45509800 | 0.55616100 |
| C | -4.80150600 | 0.38980100 | 0.54236800 |
| C | -4.03189200 | 0.63651600 | -0.59612900 |
| C | -4.65369200 | 0.96756100 | -1.79919600 |
| O | -3.94665600 | 0.08300200 | 1.56526400 |
| C | -2.69431900 | 0.14462500 | 0.99751500 |
| N | -2.69797700 | 0.47324000 | -0.27000900 |
| C | -1.55665900 | -0.19456700 | 1.81060300 |
| C | -1.75136800 | -0.63482500 | 3.12960300 |
| C | -0.69202800 | -1.06403300 | 3.90924400 |
| C | 0.57245900 | -1.04712400 | 3.32940500 |
| C | 0.81350500 | -0.60541900 | 2.04685300 |
| C | -0.24732000 | -0.15911500 | 1.22560000 |
| F | 1.61841200 | -1.49260700 | 4.07147000 |
| C | -6.76751400 | 1.40546300 | -3.09085400 |
| C | 6.37819200 | -0.28890900 | -0.71641000 |
| C | 7.00092500 | 0.85344300 | -0.17420600 |
| C | 6.28805800 | 1.99089400 | 0.19778700 |
| C | 4.92186000 | 1.93380400 | 0.00451500 |
| C | 4.26691400 | 0.82470100 | -0.53051500 |
| C | 4.99598700 | -0.30394600 | -0.89979300 |
| O | 3.97506500 | 2.88032200 | 0.28441200 |
| C | 2.78489800 | 2.29816100 | -0.08984300 |
| N | 2.91025300 | 1.09600600 | -0.58462300 |
| C | 1.57139000 | 3.05580300 | 0.11959000 |
| C | 1.67689200 | 4.40312600 | 0.50551200 |
| C | 0.54941900 | 5.17166700 | 0.73447200 |
| C | -0.68269500 | 4.55279600 | 0.57486400 |
| C | -0.82222500 | 3.22933900 | 0.20311500 |
| C | 0.30312900 | 2.42343000 | -0.05356300 |
| F | -1.80065400 | 5.29008000 | 0.79314700 |
| C | 7.20753200 | -1.48185400 | -1.08928500 |
| Ir | 0.09605200 | 0.43802800 | -0.60539700 |
| C | -1.52705100 | -2.89219300 | -0.55664900 |
| C | -0.56613200 | -3.43425600 | 0.33937200 |
| C | 0.73986500 | -3.35800100 | -0.25698900 |
| C | 0.61356400 | -2.63251200 | -1.51106000 |
| C | -0.86526200 | -2.49481400 | -1.81170900 |
| C | -2.88569600 | -2.89593700 | -0.24671100 |
| C | -3.29602800 | -3.39036200 | 0.98353200 |
| C | -2.34874800 | -3.89958800 | 1.88921600 |
| C | -0.99717800 | -3.92849500 | 1.58096100 |
| C | 1.98424400 | -3.80449800 | 0.17103300 |
| C | 3.08138000 | -3.72120600 | -0.68549100 |
| C | 2.89482400 | -3.26600300 | -2.00981300 |
| C | 1.67985800 | -2.78991500 | -2.45617200 |
| O | -1.38217000 | -2.18953200 | -2.88269700 |
| H | -7.86895000 | 0.85180200 | -0.69898600 |
| H | -6.75916400 | 0.25669600 | 1.45133100 |
| H | -4.06714400 | 1.15618100 | -2.69372900 |
| H | -2.75771300 | -0.65933000 | 3.53653200 |
| H | -0.82588500 | -1.41506600 | 4.92573300 |
| H | 1.83379400 | -0.62406900 | 1.67239200 |
| H | -6.07723800 | 1.51060600 | -3.93004700 |
| H | -7.31042100 | 2.35086200 | -2.98756700 |

| | | | |
|---|---|---|---|
| H | -7.50884600 | 0.64682200 | -3.36030700 |
| H | 8.07899100 | 0.84285600 | -0.03865600 |
| H | 6.77624500 | 2.86302900 | 0.61813200 |
| H | 4.49310200 | -1.17382900 | -1.31042800 |
| H | 2.65869400 | 4.85032800 | 0.62335300 |
| H | 0.60830000 | 6.21321000 | 1.02775200 |
| H | -1.82562700 | 2.82434500 | 0.10849400 |
| H | 7.93962800 | -1.23625500 | -1.86551500 |
| H | 6.58720400 | -2.29909000 | -1.46418100 |
| H | 7.77471400 | -1.85968400 | -0.23268800 |
| H | 0.58302000 | -1.27600500 | -1.12070400 |
| H | -3.60500800 | -2.49895700 | -0.95901200 |
| H | -4.34783300 | -3.37872600 | 1.25433300 |
| H | -2.68463600 | -4.27486500 | 2.85228400 |
| H | -0.28134800 | -4.32618100 | 2.29573300 |
| H | 2.08910100 | -4.26890700 | 1.15019600 |
| H | 4.05592200 | -4.07885800 | -0.36786600 |
| H | 3.73100700 | -3.32033900 | -2.70502400 |
| H | 1.54616500 | -2.45900900 | -3.48297000 |

**TS4-II-Hexa**

| | | | |
|---|---|---|---|
| C | 3.59475200 | -0.09326500 | -1.82637900 |
| C | 2.23053000 | -0.21826400 | -1.74428900 |
| N | 1.46357400 | 0.45209500 | -0.85896700 |
| C | 2.08264500 | 1.42284400 | -0.07803800 |
| C | 3.49211000 | 1.54155900 | -0.10106000 |
| C | 4.27704200 | 0.79230800 | -0.94725800 |
| C | 1.22080200 | 2.28906800 | 0.65251000 |
| N | -0.12949800 | 2.06308000 | 0.48749000 |
| C | -0.99662500 | 2.94313200 | 1.00449100 |
| C | -0.61771500 | 4.04230200 | 1.74562600 |
| C | 0.75737100 | 4.24123500 | 2.03773500 |
| C | 1.65356300 | 3.35718300 | 1.47710200 |
| C | 5.79609400 | 0.88321200 | -0.99299400 |
| C | 6.24428900 | 1.25761700 | -2.41234600 |
| C | 6.34272000 | 1.92465700 | -0.01957100 |
| C | 6.38315900 | -0.48673100 | -0.62508600 |
| C | 1.17031100 | 5.37980200 | 2.96209200 |
| C | 0.69149400 | 6.71443100 | 2.37565600 |
| C | 0.50685500 | 5.16471200 | 4.33048700 |
| C | 2.68271400 | 5.44832400 | 3.15930800 |
| C | 4.76955700 | -3.45877800 | 1.11886800 |
| C | 5.02696700 | -4.29580100 | 0.01544800 |
| C | 4.10436700 | -4.48696300 | -1.01079900 |
| C | 2.91042200 | -3.80280600 | -0.88176200 |
| C | 2.61155400 | -2.97176200 | 0.19920200 |
| C | 3.55024000 | -2.78626100 | 1.21484800 |
| O | 1.85025100 | -3.77084400 | -1.73601800 |
| C | 0.94504700 | -2.90475700 | -1.12487400 |
| N | 1.34669500 | -2.43694600 | 0.01503900 |
| C | -0.24724900 | -2.62649000 | -1.91420700 |
| C | -0.65020400 | -3.67496900 | -2.76527500 |
| C | -1.70661500 | -3.54923900 | -3.64746800 |
| C | -2.33319100 | -2.31491500 | -3.67656300 |
| C | -1.96468700 | -1.26742100 | -2.86066700 |
| C | -0.92070700 | -1.36094900 | -1.91009700 |
| F | -3.35460100 | -2.12627000 | -4.55289400 |
| C | 5.81367500 | -3.29759400 | 2.18461800 |
| C | -5.38133400 | -1.60103100 | 0.68829500 |
| C | -6.43979600 | -0.77798100 | 0.25952400 |
| C | -6.23556600 | 0.40146400 | -0.45398600 |
| C | -4.91931600 | 0.72514600 | -0.70452000 |
| C | -3.84305500 | -0.03826000 | -0.25031300 |
| C | -4.06008700 | -1.22689200 | 0.43488200 |
| O | -4.42678000 | 1.76440300 | -1.46702700 |
| C | -3.08798700 | 1.58698900 | -1.45690000 |
| N | -2.68798300 | 0.57638200 | -0.70738400 |
| C | -2.15213000 | 2.26690300 | -2.29072500 |
| C | -2.46752200 | 3.32234800 | -3.15423600 |
| C | -1.49073800 | 3.83770700 | -3.98844400 |
| C | -0.22193500 | 3.27035300 | -3.92451500 |
| C | 0.12153900 | 2.23513400 | -3.07136800 |
| C | -0.84733200 | 1.68925000 | -2.22176200 |
| F | 0.73159800 | 3.76673500 | -4.74842500 |
| C | -5.67692100 | -2.86883900 | 1.43131900 |
| Ir | -0.58844000 | 0.33075100 | -0.72328000 |
| C | -0.23364600 | -2.68377000 | 2.81939800 |
| C | -1.63403500 | -2.66685300 | 3.04418000 |
| C | -2.08624700 | -1.30036800 | 3.12327400 |
| C | -0.97011500 | -0.43884000 | 2.77398300 |
| C | 0.26835900 | -1.29590400 | 2.78302800 |
| C | 0.47411400 | -3.88139300 | 2.78630500 |
| C | -0.21563200 | -5.08000100 | 2.92525700 |
| C | -1.60575100 | -5.07224600 | 3.12012800 |
| C | -2.31863700 | -3.88191200 | 3.18806700 |
| C | -3.30107800 | -0.76795900 | 3.53231300 |
| C | -3.41743200 | 0.60484900 | 3.75314200 |
| C | -2.26428700 | 1.41137100 | 3.66495300 |
| C | -1.04598000 | 0.90513800 | 3.26034400 |
| O | 1.42882900 | -0.90577500 | 2.83606900 |

| | | | |
|---|---|---|---|
| H | 4.12944700 | -0.69142400 | -2.55601100 |
| H | 1.69573500 | -0.88595100 | -2.41062100 |
| H | 3.94526400 | 2.26954300 | 0.56083800 |
| H | -2.04741400 | 2.72789700 | 0.82813900 |
| H | -1.38152500 | 4.70114300 | 2.14269900 |
| H | 2.71623200 | 3.47215600 | 1.65160800 |
| H | 5.84020000 | 2.22959600 | -2.71265000 |
| H | 5.92079800 | 0.51966000 | -3.15148100 |
| H | 7.33641600 | 1.31823500 | -2.46359200 |
| H | 6.07804800 | 1.69316600 | 1.01656500 |
| H | 7.43470600 | 1.95440700 | -0.08085700 |
| H | 5.97323800 | 2.92966800 | -0.24625300 |
| H | 6.09445900 | -0.77422300 | 0.39026100 |
| H | 6.03711400 | -1.27204700 | -1.30374800 |
| H | 7.47732400 | -0.46129100 | -0.67290300 |
| H | 0.96273800 | 7.54207600 | 3.03929100 |
| H | -0.39403700 | 6.73736200 | 2.24631600 |
| H | 1.14777400 | 6.90453500 | 1.39907500 |
| H | -0.58443800 | 5.16315900 | 4.25673100 |
| H | 0.81158000 | 4.21021700 | 4.77188900 |
| H | 0.79164400 | 5.96288700 | 5.02408500 |
| H | 3.21064500 | 5.61485700 | 2.21520600 |
| H | 2.93336700 | 6.27798700 | 3.82695700 |
| H | 3.07780800 | 4.53297700 | 3.61010000 |
| H | 5.98657100 | -4.80293700 | -0.04034900 |
| H | 4.31553200 | -5.12486900 | -1.86176800 |
| H | 3.31964400 | -2.12888800 | 2.04808500 |
| H | -0.11480700 | -4.61718900 | -2.71913200 |
| H | -2.02745400 | -4.35836500 | -4.29248000 |
| H | -2.51312600 | -0.34131900 | -2.99530300 |
| H | 5.86350000 | -4.17818400 | 2.83498400 |
| H | 5.60602500 | -2.43522000 | 2.82156600 |
| H | 6.81149800 | -3.16806300 | 1.75513700 |
| H | -7.45823300 | -1.09022600 | 0.47129500 |
| H | -7.05734300 | 1.00856200 | -0.81455500 |
| H | -3.22399900 | -1.84625600 | 0.74341300 |
| H | -3.47291900 | 3.73250700 | -3.17088700 |
| H | -1.68710900 | 4.65179800 | -4.67552000 |
| H | 1.14464900 | 1.87111700 | -3.08670500 |
| H | -5.75038900 | -2.68966900 | 2.51024000 |
| H | -4.89157800 | -3.61270000 | 1.28140300 |
| H | -6.62689800 | -3.30728900 | 1.11640700 |
| H | -0.85185400 | -0.41989500 | 1.26090000 |
| H | 1.55138000 | -3.87076600 | 2.64595600 |
| H | 0.31629100 | -6.02544300 | 2.88465100 |
| H | -2.13192100 | -6.01670000 | 3.22887900 |
| H | -3.39091000 | -3.89646000 | 3.36361300 |
| H | -4.14188300 | -1.42743500 | 3.74104400 |
| H | -4.35975100 | 1.03294700 | 4.07986900 |
| H | -2.32779100 | 2.45782100 | 3.95943700 |
| H | -0.15770100 | 1.53101200 | 3.24987700 |

**Pro-II-Penta**

| | | | |
|---|---|---|---|
| C | -1.92573700 | -4.13791700 | 3.61729200 |
| C | -3.30567600 | -4.28341900 | 3.37778700 |
| C | -3.96406600 | -3.59868200 | 2.35756700 |
| C | -3.17983000 | -2.76240700 | 1.58806800 |
| C | -1.80952500 | -2.58675100 | 1.79169400 |
| C | -1.16802000 | -3.28046300 | 2.81783700 |
| O | -3.54750900 | -1.97848500 | 0.53275600 |
| C | -2.37668400 | -1.35617000 | 0.13733800 |
| N | -1.33258300 | -1.68842100 | 0.85494600 |
| C | -2.45686400 | -0.42649900 | -0.95767200 |
| C | -3.70562300 | -0.20277100 | -1.56637400 |
| C | -3.86210400 | 0.73263800 | -2.57275400 |
| C | -2.72648400 | 1.44876200 | -2.94628300 |
| C | -1.48516900 | 1.24460700 | -2.39078000 |
| C | -1.27523600 | 0.27829400 | -1.37007800 |
| F | -2.86616500 | 2.40472400 | -3.90798600 |
| C | -1.28161800 | -4.91316500 | 4.72879900 |
| C | 4.96613900 | 1.22209100 | 2.22713800 |
| C | 6.07059500 | 0.38966000 | 1.95651500 |
| C | 6.01965600 | -0.65094500 | 1.03060500 |
| C | 4.81199100 | -0.82208300 | 0.38496500 |
| C | 3.69754100 | -0.01789100 | 0.62678400 |
| C | 3.76152100 | 1.01832200 | 1.55375500 |
| O | 4.46917600 | -1.75625800 | -0.56606000 |
| C | 3.16930800 | -1.48172200 | -0.85931100 |
| N | 2.67129000 | -0.46758500 | -0.18191400 |
| C | 2.38016100 | -2.19987800 | -1.81128000 |
| C | 2.86719000 | -3.28794700 | -2.54536800 |
| C | 2.03808600 | -3.93232700 | -3.44965700 |
| C | 0.73837300 | -3.45126900 | -3.57788300 |
| C | 0.23941900 | -2.37858000 | -2.86169600 |
| C | 1.04412900 | -1.68945000 | -1.93430000 |
| F | -0.07837700 | -4.08102000 | -4.46484900 |
| C | 5.09427200 | 2.32574700 | 3.23454500 |
| Ir | 0.56823400 | -0.02606000 | -0.70126900 |
| C | -1.70799400 | 2.58052400 | 1.91510500 |
| C | -2.24404200 | 3.10270200 | 0.72426800 |

| | | | |
|---|---|---|---|
| C | -1.23693700 | 3.97638100 | 0.10120500 |
| C | -0.10430200 | 4.01462400 | 0.93264100 |
| C | -0.34364800 | 3.14300600 | 2.11828700 |
| C | -2.42688400 | 1.70280800 | 2.70732600 |
| C | -3.71357100 | 1.34310200 | 2.30005500 |
| C | -4.25381200 | 1.86956200 | 1.12807600 |
| C | -3.52577900 | 2.75536400 | 0.32762700 |
| C | -1.24258100 | 4.67483100 | -1.09739600 |
| C | -0.10630400 | 5.41302400 | -1.44232200 |
| C | 1.01073100 | 5.45551800 | -0.60841000 |
| C | 1.01877600 | 4.74904500 | 0.59563100 |
| O | 0.40057200 | 2.96440400 | 3.06596600 |
| H | -3.87621200 | -4.95591800 | 4.01246400 |
| H | -5.02676900 | -3.71854000 | 2.17892800 |
| H | -0.10311200 | -3.15563700 | 2.98912900 |
| H | -4.56954800 | -0.76626100 | -1.22764200 |
| H | -4.81690400 | 0.92379200 | -3.04803100 |
| H | -0.65483700 | 1.84794900 | -2.75211500 |
| H | -0.22147200 | -4.67127400 | 4.82458400 |
| H | -1.36155200 | -5.99262900 | 4.56367700 |
| H | -1.75894600 | -4.70825200 | 5.69221200 |
| H | 6.99818300 | 0.56598200 | 2.49384100 |
| H | 6.87502500 | -1.28623400 | 0.83193700 |
| H | 2.89212400 | 1.64044400 | 1.74358000 |
| H | 3.89032200 | -3.62821800 | -2.40839000 |
| H | 2.36811700 | -4.77788400 | -4.04136200 |
| H | -0.79256100 | -2.08168900 | -3.04018600 |
| H | 5.44435100 | 1.94936500 | 4.20050600 |
| H | 4.13939100 | 2.82951400 | 3.39806700 |
| H | 5.81812300 | 3.08108200 | 2.91131800 |
| H | 0.48392900 | 1.30068500 | 0.37128400 |
| H | -1.99163500 | 1.29815600 | 3.61669100 |
| H | -4.29692100 | 0.64860700 | 2.89673900 |
| H | -5.25475100 | 1.57788000 | 0.82368800 |
| H | -3.95729900 | 3.14867700 | -0.58790400 |
| H | -2.09907200 | 4.64087300 | -1.76462100 |
| H | -0.09222600 | 5.96152700 | -2.37912700 |
| H | 1.87891500 | 6.03572000 | -0.90379200 |
| H | 1.88692400 | 4.75864700 | 1.24909800 |

**Pro-II-Hexa**

| | | | |
|---|---|---|---|
| C | -3.66710200 | -1.90232900 | -0.42678700 |
| C | -2.31325100 | -1.86847700 | -0.70497800 |
| N | -1.40260800 | -1.30585500 | 0.10791100 |
| C | -1.83911500 | -0.83429000 | 1.31864400 |
| C | -3.19706600 | -0.83153900 | 1.63197700 |
| C | -4.15324900 | -1.34799300 | 0.76260200 |
| C | -0.79526700 | -0.44264900 | 2.25778500 |
| N | 0.47564100 | -0.63412200 | 1.81891300 |
| C | 1.48729600 | -0.37637900 | 2.65900700 |
| C | 1.29525900 | 0.06970700 | 3.95076100 |
| C | -0.00568200 | 0.29170200 | 4.43169700 |
| C | -1.04616100 | 0.02962600 | 3.55040800 |
| C | -5.63187700 | -1.31027700 | 1.13170400 |
| C | -5.84137800 | -2.01641300 | 2.47794800 |
| C | -6.07546500 | 0.15403800 | 1.25169800 |
| C | -6.49841700 | -1.99844100 | 0.07895200 |
| C | -0.22261400 | 0.78998200 | 5.85526500 |
| C | 0.33228000 | -0.25555000 | 6.83262800 |
| C | 0.53340100 | 2.11099900 | 6.05143900 |
| C | -1.69948900 | 1.02086500 | 6.16563600 |
| C | -5.03331200 | 2.38882500 | -1.64522900 |
| C | -5.66403100 | 1.54699500 | -2.58166300 |
| C | -4.97576300 | 0.56560900 | -3.29475200 |
| C | -3.62361800 | 0.46739100 | -3.02776400 |
| C | -2.96250200 | 1.28882400 | -2.11195200 |
| C | -3.66443500 | 2.25924600 | -1.39988200 |
| O | -2.71057800 | -0.40704800 | -3.53501300 |
| C | -1.52017600 | -0.07702300 | -2.88248100 |
| N | -1.62756900 | 0.92177000 | -2.06371600 |
| C | -0.38890400 | -0.93174900 | -3.25069500 |
| C | -0.32926700 | -1.25134700 | -4.61996400 |
| C | 0.64955200 | -2.07571000 | -5.14673500 |
| C | 1.56151700 | -2.59648500 | -4.24573900 |
| C | 1.52120000 | -2.32264300 | -2.89457100 |
| C | 0.55056400 | -1.47543000 | -2.31641300 |
| F | 2.53197000 | -3.42664600 | -4.71126600 |
| C | -5.83564700 | 3.42221200 | -0.90946000 |
| C | 5.03822200 | 1.55943200 | -1.15669500 |
| C | 6.20731400 | 0.81081300 | -0.91131500 |
| C | 6.17895500 | -0.51701200 | -0.49496800 |
| C | 4.92301700 | -1.06524300 | -0.33646900 |
| C | 3.74563800 | -0.35376300 | -0.56383600 |
| C | 3.78430700 | 0.97534000 | -0.97326100 |
| O | 4.59238000 | -2.34857500 | 0.04494700 |
| C | 3.24171900 | -2.37591300 | 0.03269700 |
| N | 2.69571900 | -1.22245600 | -0.31462100 |
| C | 2.42999200 | -3.51362300 | 0.33620300 |
| C | 2.94491700 | -4.76455800 | 0.70042000 |
| C | 2.07023800 | -5.80570800 | 0.96359300 |

| | | | |
|---|---|---|---|
| C | 0.70774500 | -5.54785200 | 0.85152500 |
| C | 0.18393200 | -4.31592100 | 0.49435900 |
| C | 1.03380600 | -3.23869600 | 0.21314700 |
| F | -0.14747900 | -6.56957000 | 1.11024600 |
| C | 5.15919800 | 2.97637000 | -1.63004400 |
| Ir | 0.61810700 | -1.17291900 | -0.26820500 |
| C | 0.02757800 | 4.47887700 | -0.89062000 |
| C | 1.38036500 | 4.93492300 | -0.86675600 |
| C | 1.97244200 | 4.49983100 | 0.38470500 |
| C | 0.97562700 | 3.77807700 | 1.10670600 |
| C | -0.27397600 | 3.76145200 | 0.34862300 |
| C | -0.78082100 | 4.75888400 | -1.99725400 |
| C | -0.25501700 | 5.48214000 | -3.06049900 |
| C | 1.07556000 | 5.93487400 | -3.03331000 |
| C | 1.89467600 | 5.66113700 | -1.93832000 |
| C | 3.24357800 | 4.66811900 | 0.92647100 |
| C | 3.53480100 | 4.11225100 | 2.17299600 |
| C | 2.55551300 | 3.39295600 | 2.88026500 |
| C | 1.27888900 | 3.22870900 | 2.35474600 |
| O | -1.36703200 | 3.25176200 | 0.69882900 |
| H | -4.32472800 | -2.36430500 | -1.15302700 |
| H | -1.92141300 | -2.30248400 | -1.61717000 |
| H | -3.50538400 | -0.42260100 | 2.58710400 |
| H | 2.48572300 | -0.53200900 | 2.26196600 |
| H | 2.16336400 | 0.25103300 | 4.57528100 |
| H | -2.07176100 | 0.18527500 | 3.85838700 |
| H | -5.29600700 | -1.52577600 | 3.28879300 |
| H | -5.51393900 | -3.05984300 | 2.43627600 |
| H | -6.90280700 | -2.00864000 | 2.74486500 |
| H | -5.97448800 | 0.67218000 | 0.29406400 |
| H | -7.12550000 | 0.20704700 | 1.55778000 |
| H | -5.48306800 | 0.70138900 | 1.99100100 |
| H | -6.41432900 | -1.51455400 | -0.89881000 |
| H | -6.23711200 | -3.05443000 | -0.04085300 |
| H | -7.54921200 | -1.95193500 | 0.37864700 |
| H | 0.19834800 | 0.08337800 | 7.86476000 |
| H | 1.40067100 | -0.43024200 | 6.67711800 |
| H | -0.18337400 | -1.21469900 | 6.72421000 |
| H | 1.60858200 | 1.99293500 | 5.89193000 |
| H | 0.17325100 | 2.88367200 | 5.36577700 |
| H | 0.39065000 | 2.47633900 | 7.07331200 |
| H | -2.28585100 | 0.10076400 | 6.08161600 |
| H | -1.80806800 | 1.38512100 | 7.19103200 |
| H | -2.14346400 | 1.76905500 | 5.50204600 |
| H | -6.73260600 | 1.66037500 | -2.74512100 |
| H | -5.47536500 | -0.08533200 | -4.00377500 |
| H | -3.14173500 | 2.86878900 | -0.66473400 |
| H | -1.06782800 | -0.82001100 | -5.28814900 |
| H | 0.70871900 | -2.30792700 | -6.20325200 |
| H | 2.26532300 | -2.81394500 | -2.27621500 |
| H | -5.77879700 | 4.39961900 | -1.40201400 |
| H | -5.46929200 | 3.56137600 | 0.11092300 |
| H | -6.89321400 | 3.15127600 | -0.85658700 |
| H | 7.17033000 | 1.29130100 | -1.05872600 |
| H | 7.08318600 | -1.08542900 | -0.31227400 |
| H | 2.86459900 | 1.52670600 | -1.14671800 |
| H | 4.01730800 | -4.92154300 | 0.77867300 |
| H | 2.41400900 | -6.79307000 | 1.24804700 |
| H | -0.89930000 | -4.21882700 | 0.43830500 |
| H | 5.74036800 | 3.58343900 | -0.92900200 |
| H | 4.18024200 | 3.44237800 | -1.75171100 |
| H | 5.67672200 | 3.02653200 | -2.59362000 |
| H | 0.58103300 | 0.44755700 | -0.58877700 |
| H | -1.80844600 | 4.40414900 | -2.02308900 |
| H | -0.87460300 | 5.69951800 | -3.92620300 |
| H | 1.46870200 | 6.49803900 | -3.87464700 |
| H | 2.92428700 | 6.01271800 | -1.92635400 |
| H | 4.00652600 | 5.22547300 | 0.38768900 |
| H | 4.52546200 | 4.23571700 | 2.60104700 |
| H | 2.80116300 | 2.96499700 | 3.84898200 |
| H | 0.51902800 | 2.67257100 | 2.89945800 |

# 6. Miscellaneous

## 6.1 Solubility of Bpca Salts

The estimation of the solubility of BpcaNa and BpcaK in DCM was performed as follow. Into 10 mL of 0.1 M aqueous NaOH/KOH was added by 297 mg of Bpca (1.5 mmol). The mixture was stirred under 80 ºC for 12 hours and then filtered to obtain a clear solution. The solution was then dried under vacuum to yield BpcaNa and BpcaK as white, hygroscopic powder. Into a flask equipped with magnetic stir bar and 100 mg of salt was added by 25.0 mL of DCM. The flask was then sealed with glass stoppers and stirred under room temperature for 1 hour to form saturated solutions. The solution was then filtered and dried in vacuo. The residues were afforded in 41.0 mg for BpcaNa and 27.4 mg for BpcaK. The estimated solubility in DCM of BpcaNa is 0.00745 mol/L and 0.00463 for BpcaK.

## 6.2 Analysis of the Ratio of Oxygen to $PPh_3$

The inner volume of the vessels used in the reaction was estimated by the weight of the water to fill. The 10 mL Schlenk tube has total volume of 28.6 mL. The volume of the atmosphere above the reaction mixtures is 26.6 mL, and the amount of the gas was 1.09 mmol by estimation. The dissolution of oxygen in the reaction solution is also taken into account: $2.31\times10^{-4}$ mmol (<1 mol%) in 0.4 mL $H_2O$ and $3.96\times10^{-3}$ mmol (0.020 eq.) in 1.6 mL DCM. [12]

**Table S2**. The amount of oxygen in selective reactions

| Key Conditions | Oxygen | $PPh_3$ | $n(O_2)/n(PPh_3)$ | Yield of fluorenone |
|---|---|---|---|---|
| In $O_2$, $PPh_3$ 3 eq. | 5.47 eq. | 3.0 eq. | 1.82 | 0% |
| In air | 1.22 eq. | 1.2 eq. | 1.02 | 25% |
| In air, $PPh_3$ 3 eq. | 1.22 eq. | 3.0 eq. | 0.41 | 59% |
| In $N_2$, $PPh_3$ 1.5 eq. | 0.21 eq. | 1.5 eq. | 0.14 | 81% |
| Freeze-pump-refill with $N_2$ | <0.1% | 1.2 eq. | ≈ 0 | 85% |

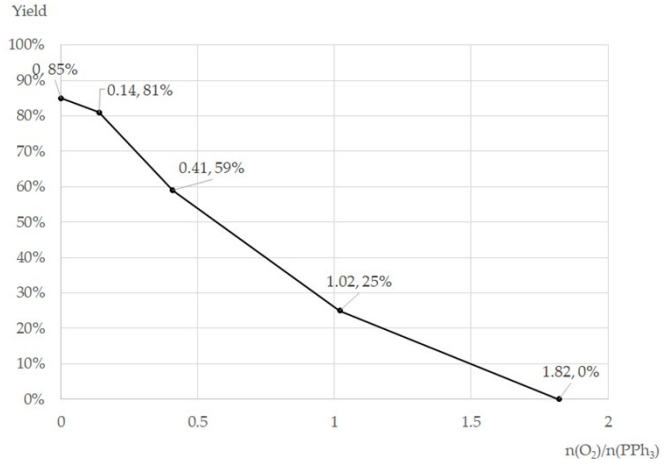



**Figure S86.** The relation between the ratio of $O_2/PPh_3$ molar and the yield

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