Supporting Information

Benzofuranone-Based Spiropyrans: Synthesis, Temperature-Dependent Photochromic Properties, and DFT Calculations

Xincheng Zhou[a], Zhichao Chang[a], Yongchun Hu[a], Jianming Zhong[a], Jiaying Liao[a], Chunying Rong[c,], and Wang Zhou[a,b,]**

[a] *Key Laboratory of Chemical Biology and Traditional Chinese Medicine, Ministry of Education of China, Changsha 410081, China*

[b] *Key Laboratory of the Assembly and Application of Organic Functional Molecules of Hunan Province, Changsha 410081, China*

[c] *Key Laboratory of Light Energy Conversion Materials of Hunan Province College, Hunan Normal University, Changsha 410081, China*

Email: rongchunying@aliyun.com; wzhou@hunnu.edu.cn

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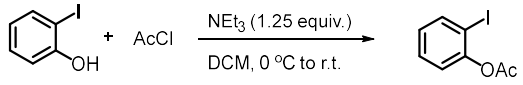
1. General Remarks

^{1}H NMR spectra were recorded on a Bruker AVIII-500 spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) or solvent peak in $CDCl_3$ (δ = 7.26 ppm) and in DMSO-d_6 (δ = 2.49 ppm). ^{13}C NMR spectra were obtained by using the same NMR spectrometers and calibrated with $CDCl_3$ (δ = 77.00 ppm) or DMSO-d_6 (39.50 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), and integration. Mass spectra were recorded using a Bruker APEX IV Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. IR spectra were recorded on a Nexus Thermo Nicolet Fourier Transform Infrared Spectrometer. Single-crystal X-Ray diffraction were collected on an Agilent Supernova X-Ray diffractometer equipped with a large area CCD detector. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. Compounds **5a** and **5n** were prepared according to literature.[1]

2. Preparation of Starting Materials and Analytical Data

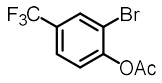
Scheme *S1*. Typical Procedure A for the synthesis of 2-iodophenyl acetate



1a

2-Iodophenyl acetate (**1a**): Acetyl chloride (1.28 mL, 18 mmol) was added to a mixture of 2-iodophenol (3.30 g, 15 mmol), NEt_3 (2.60 mL, 18.75 mmol) in DCM (20 mL) at 0 °C, and then the reaction mixture was stirred at room temperature. The reaction was monitored by TLC. After completion, the reaction mixture was quenched with water (5 mL) and extracted with CH_2Cl_2 (2×20 mL). The organic layer was washed with brine, dried over Na_2SO_4, filtered and evaporated to dryness in vacuo. Subsequent purification by flash column chromatography (PE/EA = 50/1) afforded the **1a** (3.85 g, 98 %) as a colorless oil.[2]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.83 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.37 (td, *J* = 8.0, 1.5 Hz, 1H), 7.10 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.98 (td, *J* = 7.5, 1.5 Hz, 1H), 2.37 (s, 3H).



1b

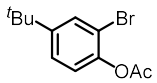
2-Bromo-4-(trifluoromethyl)phenyl acetate (**1b**): The reaction of acetyl chloride (0.26 mL, 3.6 mmol), 2-bromo-4-(trifluoromethyl)phenol (0.41 mL, 3 mmol), and N Et_3 (0.52 mL, 3.75 mmol) in DCM (5 mL) under **typical procedure A** afforded **1b** (764.1 mg, 90%) as a pale-yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89 (d, *J* = 2.0 Hz, 1H), 7.60 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.26 (d, *J* = 8.3, 1H), 2.38 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.0, 151.0, 130.7 (q, J_{C-F} = 3.7 Hz), 129.6 (q, J_{C-F} = 33.6 Hz), 125.7 (q, J_{C-F} = 3.7 Hz), 124.2, 122.9 (q, J_{C-F} = 273.3 Hz), 116.8, 20.7.

^{19}F NMR (471 MHz, $CDCl_3$)**:** δ -62.4.

HRMS (ESI) m/z: calcd for $C_9H_7BrF_3O_2^+$ $(M+H)^+$ 282.9576, found 282.9564.

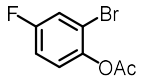


1c

2-Bromo-4-(tert-butyl)phenyl acetate (**1c**): The reaction of acetyl chloride (0.26 mL, 3.6 mmol), 2-bromo-4-(*tert*-butyl)phenol (0.51 mL, 3 mmol), and NEt_3 (0.52 mL, 3.75 mmol) in DCM (5 mL) under **typical procedure A** afforded **1c** (610.4 mg, 75%) as a colorless oil.[3]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.59 (d, *J* = 2.3 Hz, 1H), 7.33 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.04 (d, *J* = 8.5 Hz, 1H), 2.35 (s, 3H), 1.31 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.8, 150.7, 145.7, 130.3, 125.6, 122.9, 115.6, 34.6, 31.2, 20.8.



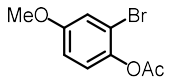
1d

2-Bromo-4-fluorophenyl acetate (**1d**): The reaction of acetyl chloride (0.26 mL, 3.6 mmol), 2-bromo-4-fluorophenol (573.0 mg, 3 mmol), and NEt_3 (0.52 mL, 3.75 mmol) in DCM (5 mL) under **typical procedure A** afforded **1d** (600.4 mg, 86%) as a pale-yellow oil.[4]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (dd, J = 7.5, 3.0 Hz, 1H), 7.14-7.08 (m, 1H), 7.07-7.01 (m, 1H), 2.35 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.6, 159.9 (d, J_{C-F} = 249.6 Hz), 144.5 (d, J_{C-F} = 3.4 Hz), 124.4 (d, J_{C-F} = 8.8 Hz), 120.3 (d, J_{C-F} = 26.3 Hz), 116.5 (d, J_{C-F} = 10.0 Hz), 115.4 (d, J_{C-F} = 23.2 Hz), 20.7.

^{19}F NMR (471 MHz, $CDCl_3$): δ -114.4.



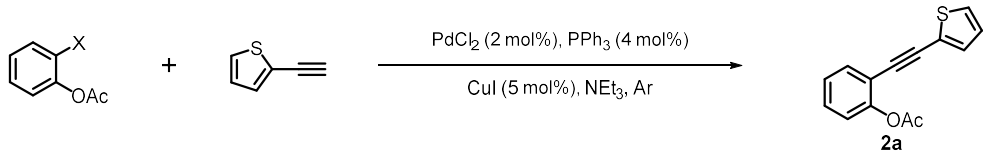
1e

2-Bromo-4-methoxyphenyl acetate (**1e**): The reaction of acetyl chloride (0.26 mL, 3.6 mmol), 2-bromo-4-methoxyphenol (609.0 mg, 3 mmol), NEt_3 (0.52 mL, 3.75 mmol) in DCM (5 mL) under **typical procedure A** afforded **1e** (718.8 mg, 98%) as a pale-yellow oil.[4]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.13 (d, J = 3.0 Hz, 1H), 7.03 (d, J = 9.0 Hz, 1H), 6.90-6.81 (m, 1H), 3.79 (s, 3H), 2.33 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 169.0, 157.8, 141.8, 123.8, 118.1, 116.3, 114.2, 55.8, 20.7.

Scheme *S2*. Typical Procedure B for the synthesis of 2-(thiophen-2-ylethynyl)phenyl acetate

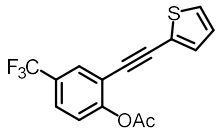


2a

2-(Thiophen-2-ylethynyl)phenyl acetate (**2a**): To an oven-dried tube under an argon atmosphere, 2-iodophenyl acetate (1.05 g, 4 mmol), $PdCl_2$ (14.2 mg, 0.08 mmol, 2.0 mol%), PPh_3 (42.0 mg, 0.16 mmol, 4.0 mol%), CuI (38.1 mg, 0.2 mmol, 5.0 mol%), 2-ethynylthiophene (0.40 mL, 4 mmol), and NEt_3 (10 mL) were added. The reaction mixture was heated to 45 °C and allowed to stir for 20 h. The reaction mixture was cooled down to room temperature, filtered through a celite pad, and washed with EA. The combined filtrate was concentrated in vacuo, and the residue was purified by silica gel column chromatography (PE/EA = 50/1) to afford **2a** (582.8 mg, 60%) as a yellow solid.[5]

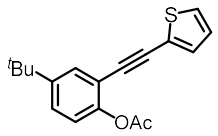
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.54-7-7.50 (m, 1H), 7.38-7.32 (m, 1H), 7.32-7.28 (m,

1H), 7.27-7.18 (m, 2H), 7.11 (d, J = 8.0 Hz, 1H), 7.02-6.99 (m, 1H), 2.37 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 168.9, 151.4, 132.6, 132.1, 129.6, 127.6, 127.2, 125.9, 122.8, 122.3, 117.1, 87.9, 87.3, 20.8.
IR (neat): ν_{max} = 1763, 1365, 1180 cm^{-1}.
HRMS (ESI) m/z: calcd for $C_{14}H_{11}O_2S^+$ $(M+H)^+$ 243.0474, found 243.0470.



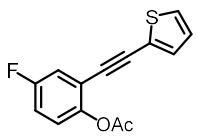
2b

2-(Thiophen-2-ylethynyl)-4-(trifluoromethyl)phenyl acetate (**2b**): The reaction of 2-bromo-4-(trifluoromethyl)phenyl acetate (657.2 mg, 2.3 mmol), $PdCl_2$ (20.4 mg, 0.115 mmol), PPh_3 (60.3 mg, 2.76 mmol), CuI (21.9 mg, 0.115 mmol), 2-ethynylthiophene (0.28 mL, 2.76 mmol) in NEt_3 (5 mL) under **typical procedure B** (80 °C for 13 h) afforded **2b** (316.4 mg, 44%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84-7.81 (m, 1H), 7.63-7.59 (m, 1H), 7.38-7.34 (m, 1H), 7.32-7.29 (m, 1H), 7.28-7.24 (m, 1H), 7.05-7.02 (m, 1H), 2.40 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 168.4, 153.6, 132.7 (q, J_{C-F} = 2.0 Hz), 129.8 (q, J_{C-F} = 21.0 Hz), 128.6, 128.3 (q, J_{C-F} = 7.2 Hz), 127.3 (q, J_{C-F} = 8.8 Hz), 126.3 (q, J_{C-F} = 20.8 Hz), 123.4 (q, J_{C-F} = 273.0 Hz), 123.0, 122.0, 118.2, 88.9, 86.6, 20.8 (q, J_{C-F} = 2.3 Hz).
^{19}F NMR (471 MHz, $CDCl_3$): δ -62.5.
IR (neat): ν_{max} = 1768, 1333, 1168, 1121, 1095, 1068 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{15}H_{10}F_3O_2S^+$ $(M+H)^+$ 311.0348, found 311.0340.



2c

4-(*Tert*-butyl)-2-(thiophen-2-ylethynyl)phenyl acetate (**2c**): The reaction of 2-bromo-4-(tert-butyl)phenyl acetate (590.0 mg, 2.18 mmol), $PdCl_2$ (19.5 mg, 0.11 mmol), PPh_3 (57.7 mg, 0.22 mmol), CuI (21.0 mg, 0.11 mmol), and 2-ethynylthiophene (0.26 mL, 2.62 mmol) in NEt_3 (5 mL) under **typical procedure B** (80 °C for 23 h) afforded **2c** (323.5 mg, 50%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.56 (d, J = 2.0 Hz, 1H), 7.38 (dd, J = 8.5, 2.5 Hz, 1H), 7.31-7.25 (m, 2H), 7.08-6.98 (m, 2H), 2.37 (s, 3H), 1.33 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 169.2, 149.0, 148.8, 132.0, 129.7, 127.5, 127.1, 126.9, 123.0, 121.6, 116.2, 88.5, 86.7, 34.5, 31.2, 20.9.
IR (neat): ν_{max} = 1763, 1493, 1360, 1190 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{18}H_{19}O_2S^+$ $(M+H)^+$ 299.1100, found 299.1097.



2d

4-Fluoro-2-(thiophen-2-ylethynyl)phenyl acetate (**2d**): The reaction of 2-bromo-4-fluorophenyl acetate (536.0 mg, 2.3 mmol), $PdCl_2$ (20.4 mg, 0.115 mmol), PPh_3 (60.3 mg, 2.76 mmol), CuI (21.9 mg, 0.115 mmol), 2-ethynylthiophene (0.28 mL, 2.76 mmol) in NEt_3 (5 mL) under **typical procedure B** (80 ºC for 18 h) afforded **2d** (302.7 mg, 51%) as a yellow solid.

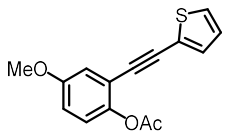
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34 (d, *J* = 5.0 Hz, 1H), 7.28 (d, *J* = 5.0 Hz, 1H), 7.24 (dd, *J* = 8.0, 2.5 Hz, 1H), 7.11-7.00 (m, 3H), 2.37 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.9, 159.7 (d, J_{C-F} = 246.1 Hz), 147.4 (d, J_{C-F} = 3.0 Hz), 132.5, 128.1, 127.3 (d, J_{C-F} = 7.7 Hz), 123.6 (d, J_{C-F} = 9.1 Hz), 122.2, 118.8 (d, J_{C-F} = 24.8 Hz), 118.5 (d, J_{C-F} = 10.1 Hz), 116.4 (d, J_{C-F} = 23.3 Hz), 88.3, 86.9 (d, J_{C-F} = 2.8 Hz), 20.7.

^{19}F NMR (471 MHz, $CDCl_3$): δ -116.3.

IR (neat): ν_{max} = 1763, 1487, 1169, 729 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{14}H_{10}FO_2S^+$ $(M+H)^+$ 261.0380, found 261.0375.



2e

4-Methoxy-2-(thiophen-2-ylethynyl)phenyl acetate (**2e**): The reaction of 2-bromo-4-methoxyphenyl acetate (473.8 mg, 1.9 mmol), $PdCl_2$ (17.7 mg, 0.1 mmol), PPh_3 (52.5 mg, 0.2 mmol), CuI (19.0 mg, 0.1 mmol), 2-ethynylthiophene (0.23 mL, 2.3 mmol) in NEt_3 (5 mL) under **typical procedure B** (80 ºC for 12 h) afforded **2e** (248.0 mg, 47%) as a yellow oil.

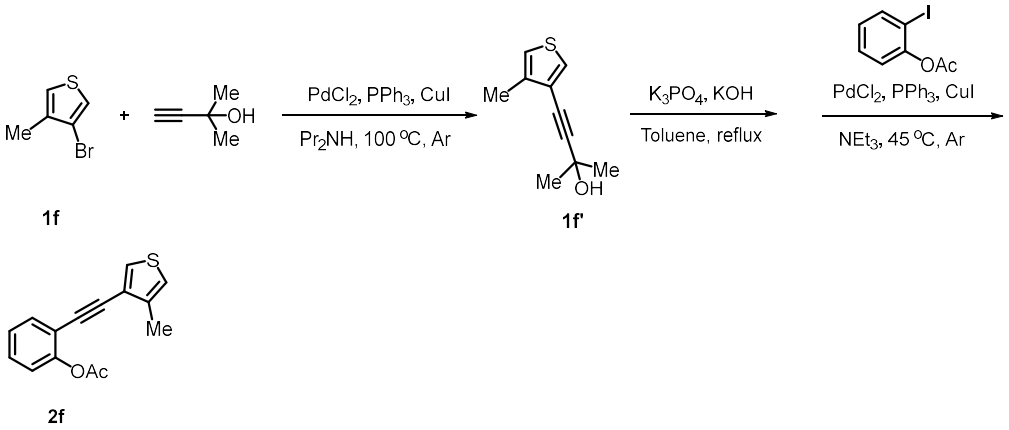
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33-7.30 (m, 1H), 7.28-7.25 (m, 1H), 7.06-6.99 (m, 3H), 6.90 (dd, *J* = 9.0, 3.0 Hz, 1H), 3.81 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 169.4, 157.0, 145.0, 132.2, 127.7, 127.2, 123.0, 122.7, 117.5, 116.5, 115.9, 88.0, 87.2, 55.7, 20.8.

IR (neat): ν_{max} = 1763, 1493, 1174, 1036 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{15}H_{13}O_3S^+$ $(M+H)^+$ 273.0580, found 273.0575.

Scheme *S3*. Synthesis of 2-((4-methylthiophen-3-yl)ethynyl)phenyl acetate



2-Methyl-4-(4-methylthiophen-3-yl)but-3-yn-2-ol (**1f'**): To an oven-dried tube under an argon atmosphere, $PdCl_2$ (71.0 mg, 0.4 mmol), PPh_3 (210.0 mg, 0.8 mmol), CuI (76.2 mg, 0.4 mmol), 3-bromo-4-methylthiophene (0.45 mL, 4 mmol), 2-methylbut-3-yn-2-ol (0.59 mL, 6 mmol), and dipropylamine (6 mL) were added. The reaction mixture was stirred at 100 °C, and the progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was cooled down to room temperature. Dipropylamine was removed under reduced pressure. Water was added to the reaction mixture, and then it was extracted with ethyl acetate. After drying of the combined organic phase over Na_2SO_4 and removal of ethyl acetate, subsequent purification of the residue by flash column chromatography (PE/EA = 10/1) afforded **1f'** (407.4 mg, 57%) as a yellow oil.[6]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (d, *J* = 3.0 Hz, 1H), 6.90-6.86 (m, 1H), 2.27-2.25 (m, 3H), 2.22 (bs, 1H), 1.62 (s, 6H).

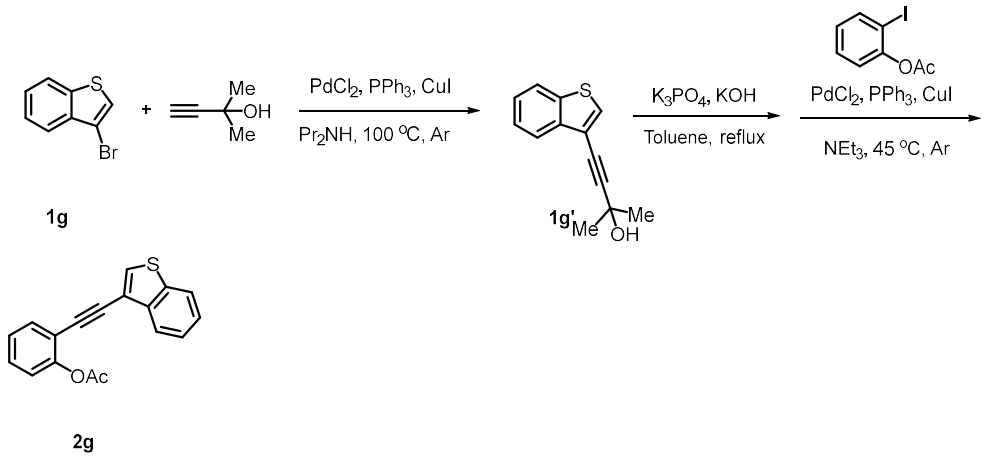
^{13}C NMR (126 MHz, $CDCl_3$): δ 139.0, 128.4, 123.0, 120.5, 95.6, 76.9, 65.7, 31.5, 14.7.

HRMS (ESI) m/z calcd for $C_{10}H_{13}OS^+$ $(M+H)^+$ 181.0682, found 181.0680.

2-((4-Methylthiophen-3-yl)ethynyl)phenyl acetate (**2f**): The reactions were carried under a nitrogen atmosphere. A flask was charged with the protected acetylenes (**1f'**, 407.4 mg, 2.26 mmol), KOH (126.8 mg, 2.26 mmol), K_3PO_4 (479.7 mg, 2.26 mmol), and toluene (5 mL). Then the flask was immersed into a preheated oil bath. The suspensions were stirred vigorously at reflux temperature until complete conversion, as monitored by TLC. The mixtures were then allowed to cool to room temperature and filtered through a pad of celite, which was washed several times with toluene. After evaporation of the organic phase to dryness the desired crude products were obtained. The crude product required no further processing and was directly used for the next reaction. To another oven-dired tube under an argon atmosphere, $PdCl_2$ (8.0 mg, 0.045 mmol), PPh_3 (23.7 mg, 0.090 mmol), CuI (21.5 mg, 0.113 mmol), 2-iodophenyl acetate (594.5 mg, 2.26 mmol), the crude product of the above synthesis (2.26 mmol) and NEt_3 (5 mL) were added. The resulting mixture was heated to 45 °C and allowed to stir for 12 h. The reaction mixture was cooled down to room temperature, filtered through a celite pad, and washed with EA. The combined filtrate was concentrated in vacuo, and the residue was purified by silica gel column chromatography (PE/EA = 50/1) to afford

2f (268.8 mg, 46%) as a yellow oil.[7]
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.47 (d, *J* = 3.5 Hz, 1H), 7.36 (td, *J* = 8.0, 2.0 Hz, 1H), 7.24 (td, *J* = 7.5, 1.5 Hz, 1H), 7.13 (d, *J* = 8.0, 1H), 6.97-6.91 (m, 1H), 2.36 (s, 3H), 2.35 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 168.8, 151.2, 138.9, 133.1, 129.3, 128.9, 125.9, 123.4, 122.3, 120.7, 117.4, 88.8, 85.8, 20.9, 14.8.
IR (neat): ν_{max} = 2913, 1757, 1625, 1190 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{15}H_{13}O_2S^+$ $(M+H)^+$ 257.0631, found 257.0624.

Scheme *S4*. Synthesis of 2-(benzo[*b*]thiophen-3-ylethynyl)phenyl acetate



4-(Benzo[*b*]thiophen-3-yl)-2-methylbut-3-yn-2-ol (**1g'**): To an oven-dried tube under an argon atmosphere, $PdCl_2$ (17.7 mg, 0.1 mmol), PPh_3 (52.5 mg, 0.2 mmol), CuI (19.0 mg, 0.1 mmol), 3-bromobenzo[*b*]thiophene (0.13 mL, 1.0 mmol), 2-methylbut-3-yn-2-ol (0.15 mL, 1.5 mmol), dipropylamine (2.0 mL) were added. The reaction mixture was stirred at 100 °C, and the progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was cooled down to room temperature. Diethylamine was removed under reduced pressure, water was added to the reaction mixture, and then it was extracted with ethyl acetate. After drying of the extract over Na_2SO_4 and removal of ethyl acetate, a brown slurry was obtained. Subsequent purification by flash column chromatography (PE/EA = 10/1) afforded **1g'** (185.3 mg, 86%) as a yellow oil.[6]
^{1}H NMR (500 MHz, DMSO-d_6): δ 6.96 (d, *J* = 8.0 Hz, 1H), 6.89 (s, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.51-6.30 (m, 2H), 4.61 (s, 1H), 0.47 (s, 6H).
^{13}C NMR (126 MHz, DMSO-d_6): δ 139.2, 138.7, 131.0, 125.7, 125.4, 123.5, 122.8, 117.6, 99.1, 74.5, 64.3, 32.1.

2-(Benzo[*b*]thiophen-3-ylethynyl)phenyl acetate (**2g**): The reactions were carried under a nitrogen atmosphere. A flask was charged with the protected acetylenes (**1g'**, 149.3 mg, 0.7 mmol), KOH (39.3 mg, 0.7 mmol), K_3PO_4 (148.6 mg, 0.7 mmol), and toluene (2.0 mL). Then the flask was immersed into a preheated oil bath. The suspensions were stirred vigorously at reflux temperature until complete conversion, as monitored by TLC. The mixtures were then allowed to cool to room temperature and filtered through a plug of celite, which was washed several times with toluene. After

evaporation of the organic phase to dryness the desired crude products were obtained. The crude product required no further processing and was directly used for the next reaction. To another oven-dired tube under an argon atmosphere, $PdCl_2$ (2.5 mg, 0.014 mmol), PPh_3 (7.4 mg, 0.028 mmol), CuI (6.7 mg, 0.035 mmol), 2-iodophenyl acetate (184.2 mg, 0.7 mmol), the crude product of the above synthesis (0.7 mmol) and NEt_3 (2.0 mL) were added. The resulting mixture was heated to 45 °C and allowed to stir for 14 h. The reaction mixture was cooled down to room temperature, filtered through a celite pad, and washed with EA. The combined filtrate was concentrated in vacuo, and the residue was purified by silica gel column chromatography (PE/EA = 50/1) to afford **2g** (106.4 mg, 52%) as a yellow oil.

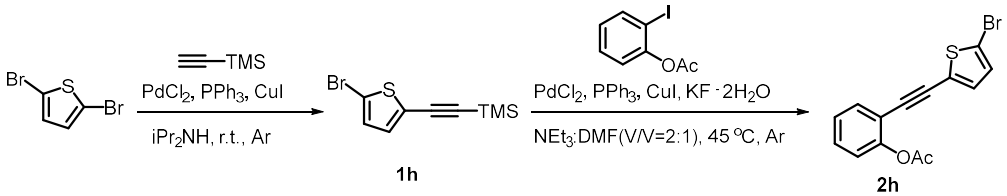
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.70 (s, 1H), 7.66 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.53-7.46 (m, 1H), 7.46-7.36 (m, 2H), 7.33-7.24 (m, 1H), 7.18 (dd, *J* = 8.0, 1.0 Hz, 1H), 2.38 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.9, 151.5, 139.0, 138.8, 133.1, 130.2, 129.6, 126.0, 125.1, 124.8, 122.8, 122.6, 122.3, 118.0, 117.2, 87.7, 86.6, 20.9.

IR (neat): ν_{max} = 2923, 1757, 1179, 761 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{18}H_{13}O_2S^+$ $(M+H)^+$ 293.0631, found 293.0624.

Scheme *S5*. Synthesis of 2-((5-bromothiophen-2-yl)ethynyl)phenyl acetate



((5-Bromothiophen-2-yl)ethynyl)trimethylsilane (**1h**): To an oven-dried tube, 2,5-dibromothiophene (2.42 g, 10 mol), $PdCl_2$ (44.3 mg, 0.25 mmol), PPh_3 (131.2 mg, 0.5 mmol), CuI (47.6 mg, 0.25 mmol), ethynyltrimethylsilane (1.41 mL, 10 mmol) and diisopropylamine (15 mL) were added. The mixture was stirred at room temperature overnight under nitrogen atmosphere. After removal of the solvent under reduce pressure, the residue was purified by column with petroleum ether as the mobile-phase to afford **1h** (797.0 mg, 31%) as a yellow oil.[8]

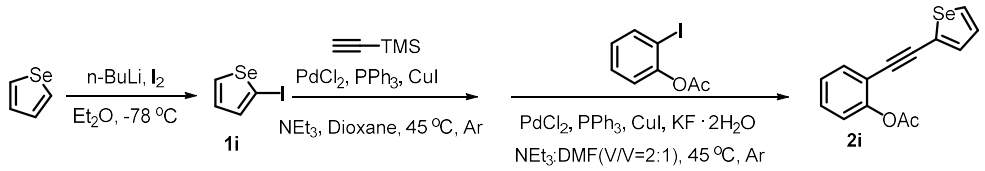
^{1}H NMR (500 MHz, $CDCl_3$): δ 6.96 (d, *J* = 4.0 Hz, 1H), 6.90 (d, *J* = 4.0 Hz, 1H), 0.24 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 132.9, 129.8, 125.0, 113.1, 100.1, 96.4, -0.3.

2-((5-Bromothiophen-2-yl)ethynyl)phenyl acetate (**2h**): To an oven-dried tube under an argon atmosphere, 2-iodophenyl acetate (789.2 mg, 3 mmol), $PdCl_2$ (10.7 mg, 0.06 mmol), PPh_3 (31.5 mg, 0.12 mmol), CuI (28.6 mg, 0.15 mmol), ((5-bromothiophen-2-yl)ethynyl)trimethylsilane (770.0 mg, 3 mmol), $KF{\cdot}2H_2O$ (494.2 mg, 5.25 mmol), DMF (3 mL) and NEt_3 (6 mL) were added. The reaction mixture was heated to 45 °C and allowed to stir for 13 h. After completion, the reaction mixture was quenched with water (20 mL) and extracted with ethyl acetate (3×20 mL). The organic layer was washed with brine, dried over Na_2SO_4, filtered and evaporated to dryness in vacuo. Subsequent purification by flash column chromatography (PE/EA = 20/1) afforded **2h** (307.0 mg,

32 %) as a yellow oil.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.54 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.38 (td, *J* = 8.0, 1.0 Hz, 1H), 7.24 (td, *J* = 7.0, 1.5 Hz, 1H), 7.13 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.00 (d, *J* = 3.8, 1H), 6.96 (d, *J* = 3.8, 1H), 2.36 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 168.8, 151.4, 132.6, 132.4, 130.2, 129.9, 126.0, 124.5, 122.4, 116.7, 113.6, 89.0, 86.2, 20.8.
IR (neat): ν_{max} = 1763, 1419, 1180 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{14}H_{10}BrO_2S^+$ $(M+H)^+$ 320.9579, found 320.9573.

Scheme *S6*. Synthesis of 2-(selenophen-2-ylethynyl)phenyl acetate

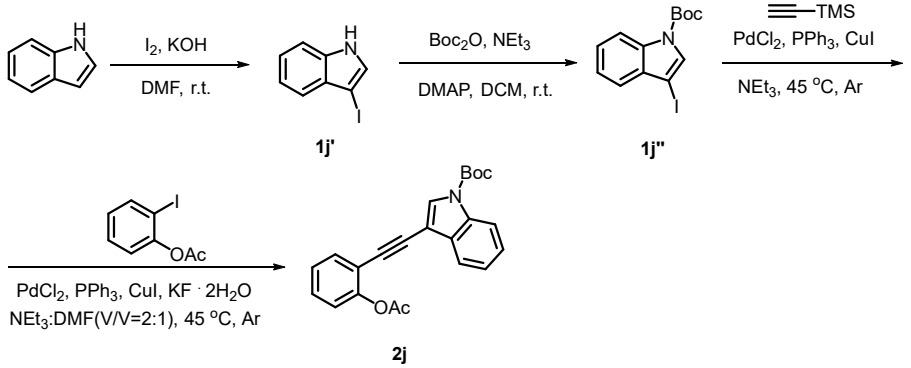


2-Iodoselenophene (**1i**): To a solution of selenophene (1.31 g, 10 mmol) in anhydrous ether (26 mL) was added dropwise a hexane solution of *n*-BuLi (2.5 M solution, 4.0 mL, 10 mmol) with stirring at room temperature under argon atmosphere, and then the reaction mixture was refluxed for 10 min. After being cooled to -78 °C, to this was added dropwise a solution of iodine (2.54 g, 10 mmol) in anhydrous ether (26 mL) over a period of 20 min. The solution was allowed to warm to 0 °C and stirred for 1 h. After being warmed to room temperature, the reaction mixture was then poured into ice water and extracted with ether. The combined ether extracts were washed successively with saturated aqueous $NaHSO_3$ and brine, and dried over Na_2SO_4. Solvent evaporation afforded an oily product which was chromatographed on silica gel by eluting with pentane to give 2-iodothiophene (**1i**) (1.86 g, 72%) as a colorless oil.[9]
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 (dd, *J* = 6.0, 1.0 Hz, 1H), 7.52 (dd, *J* = 4.0, 1.0 Hz, 1H), 6.97 (dd, *J* = 6.0, 4.0 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 140.0, 137.1, 131.3.

2-(Selenophen-2-ylethynyl)phenyl acetate (**2i**): To an oven-dried tube under an argon atmosphere, 2-iodoselenophene (1.28 g, 5 mmol), $PdCl_2$ (8.9 mg, 0.05 mmol), PPh_3 (26.2 mg, 0.1 mmol), CuI (19.0 mg, 0.1 mmol), ethynyltrimethylsilane (1.06 mL, 7.5 mmol), dioxane (8 mL) and NEt_3 (8 mL) were added. The mixture was stirred at 45 °C overnight. After evaporation of the organic phase to dryness the desired crude products were obtained. The crude product required no further processing and was directly used for the next reaction. To another oven-dried tube under an argon atmosphere, $PdCl_2$ (17.7 mg, 0.1 mmol), PPh_3 (52.4 mg, 0.2 mmol), CuI (38.1 mg, 0.2 mmol), 2-iodophenyl acetate (1.32 g, 5 mmol), the crude product of the above synthesis (5 mmol), $KF{\cdot}2H_2O$ (823.6 mg, 8.75 mmol), DMF (6 mL) and NEt_3 (12 mL) were added. The resulting mixture was heated to 45 °C and allowed to stir for 13 h. The reaction mixture was cooled down to room temperature, filtered through a celite pad, and washed with EA. The combined filtrate was concentrated in vacuo, and the residue was purified by silica gel column chromatography (PE/EA = 50/1) to afford **2i** (977.8 mg, 72%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 5.5 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.45

(d, *J* = 4.0 Hz, 1H), 7.41-7.33 (m, 1H), 7.29-7.21 (m, 2H), 7.13 (d, *J* = 8.0 Hz, 1H), 2.38 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 168.9, 151.2, 134.4, 133.6, 132.5, 129.63, 129.59, 127.0, 126.0, 122.3, 117.2, 89.7, 89.5, 20.9.
IR (neat): ν_{max} = 2929, 1763, 1371, 1174 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{14}H_{11}O_2Se^+$ $(M+H)^+$ 290.9919, found 290.9911.

Scheme *S7*. Synthesis of *tert*-butyl 3-((2-acetoxyphenyl)ethynyl)-1*H*-indole-1-carboxylate



3-Iodo-1*H*-indole (1j'): A solution of I_2 (2.54 g, 10 mmol) in DMF (12 mL) was added dropwise to a solution of 1*H*-indole (1.17 g, 10 mmol) and KOH (1.40 g, 25 mmol) in DMF (12 mL) at room temperature and stirred for 1 h. The reaction mixture was poured into ice and water (100 mL) containing ammonia (0.5%) and sodium metabisulphite (0.1% aqueous solution). The precipitate was filtered, washed with cold water and dried under vacuum. The compound was obtained as orange solid (2.34 g, 96%).[10]
^{1}H NMR (500 MHz, DMSO-d_6): δ 11.44 (s, 1H), 7.45 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 1H), 7.13-6.89 (m, 2H).
^{13}C NMR (126 MHz, DMSO-d_6): δ 136.3, 130.1, 129.8, 122.7, 120.4, 120.2, 112.4, 56.4.

***Tert*-butyl 3-iodo-1*H*-indole-1-carboxylate (1j")**: 3-Iodo-1*H*-indole (931.7 mg, 3.9 mmol) was dissolved in CH_2Cl_2 (10 mL), treated with Boc_2O (936.3 mg, 4.29 mmol), NEt_3 (1.64 mL, 11.7 mmol), and DMAP (23.9 mg, 0.195 mmol) and stirred at room temperature for 1 h. The solution was then washed twice with sodium metabisulphite (5% aqueous solution), dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography (petroleum ether). The compound was obtained as orange oil (957.8 mg, 72%).[10]
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.73 (s, 1H), 7.45-7.35 (m, 2H), 7.32-7.28 (m, 1H), 1.67 (s, 9H) ppm.

***Tert*-butyl 3-((2-acetoxyphenyl)ethynyl)-1*H*-indole-1-carboxylate (2j)**: To an oven-dried tube under an argon atmosphere, tert-butyl 3-iodo-1H-indole-1-carboxylate (892.3 mg, 2.6 mmol), $PdCl_2$ (9.2 mg, 0.052 mmol), PPh_3 (27.3 mg, 0.104 mmol), CuI (19.8 mg, 0.104 mmol), ethynyltrimethylsilane (0.55 mL, 3.9 mmol) and NEt_3 (10 mL) were added. The mixture was stirred at 45 °C overnight. After evaporation of the organic phase to dryness the desired crude products were obtained. The crude product required

no further processing and was directly used for the next reaction. To another oven-dried tube under an argon atmosphere, $PdCl_2$ (9.3 mg, 0.052 mmol), PPh_3 (27.3 mg, 0.104 mmol), CuI (24.8 mg, 0.13 mmol), 2-iodophenyl acetate (683.9 mg, 2.6 mmol), the crude product of the above synthesis (2.6 mmol), $KF{\cdot}2H_2O$ (428.3 mg, 4.55 mmol), DMF (3 mL) and NEt_3 (6 mL) were added. The resulting mixture was heated to 45 °C and allowed to stir for 13 h. The reaction mixture was cooled down to room temperature, filtered through a celite pad, and washed with EA. The combined filtrate was concentrated in vacuo, and the residue was purified by silica gel column chromatography (PE/EA = 50/1) to afford **2j** (724.9 mg, 74%) as a yellow oil.

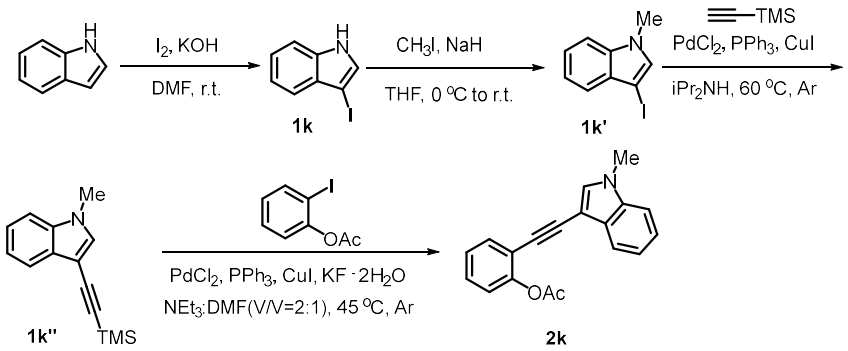
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.0 Hz, 1H), 7.83 (s, 1H), 7.72 (d, *J* = 7.0 Hz, 1H), 7.62 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.42-7.23 (m, 4H), 7.15 (d, *J* = 7.0 Hz, 1H), 2.37 (s, 3H), 1.69 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.0, 151.4, 133.0, 130.4, 129.4, 128.9, 126.0, 125.3, 123.3, 122.3, 119.9, 117.5, 115.3, 103.1, 87.6, 86.1, 84.5, 28.1, 21.0.

IR (neat): ν_{max} = 1731, 1450, 1371, 1153 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{23}H_{22}NO_4^+$ $(M+H)^+$ 376.1543, found 376.1535.

Scheme *S8*. Synthesis of 2-((1-methyl-1*H*-indol-3-yl)ethynyl)phenyl acetate



3-Iodo-1-methyl-1*H*-indole (1k`): To a solution of 3-iodo-1*H*-indole (2.19 g, 9 mmol) in THF (20 mL) at 0 °C was added NaH (542.3 mg, 60 % dispersion in mineral oil, 13.5 mmol). The heterogeneous mixture was stirred at 0 °C for 15 minutes and at room temperature for 1h. The mixture was then cooled to 0 °C, treated with iodomethane (0.75 mL, 12.06 mmol), and allowed to warm to room temperature. After 30 minutes, the reaction mixture was cooled to 0 °C, quenched with saturated NH_4Cl (10 mL), and extracted with EA (3 × 20 mL). The organic layers were combined, washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The resulting oil was purified by flash chromatography (PE/EA = 50/1) to provide 3-iodo-1-methyl-1*H*-indole (2.31 g, 100 % yield) as a colorless oil.[11]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.0 Hz, 1H), 7.33-7.27 (m, 2H), 7.23-7.18 (m, 1H), 7.15 (s, 1H), 3.81 (s, 3H).

2-((1-Methyl-1*H*-indol-3-yl)ethynyl)phenyl acetate (**2k**): To an oven-dried tube under an argon atmosphere, 3-iodo-1-methyl-1*H*-indole (2.31 g, 9 mmol), $PdCl_2$ (31.9 mg, 0.18 mmol), PPh_3 (94.4 mg, 0.36 mmol), CuI (68.6 mg, 0.36 mmol), ethynyltrimethylsilane (1.91 mL, 13.5 mmol) and *i*-Pr_2NH (15 mL) were added. The

mixture was stirred at 60 ºC for 15 h. After evaporation of the organic phase to dryness the desired crude products were obtained. The crude product required no further processing and was directly used for the next reaction. To another oven-dried tube under an argon atmosphere, $PdCl_2$ (31.9 mg, 0.18 mmol), PPh_3 (94.4 mg, 0.36 mmol), CuI (68.6 mg, 0.36 mmol), 2-iodophenyl acetate (2.37 g, 9 mmol), the crude product of the above synthesis (9 mmol), $KF{\cdot}2H_2O$ (1.48 g, 15.75 mmol), DMF (10 mL) and NEt_3 (20 mL) were added. The resulting mixture was heated to 45 ºC and allowed to stir for 17 h. The reaction mixture was cooled down to room temperature, filtered through a celite pad, and washed with EA. The combined filtrate was concentrated in vacuo, and the residue was purified by silica gel column chromatography (PE/EA = 10/1) to afford **2k** (1.58 g, 60%) as a yellow solid.

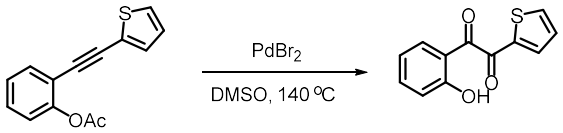
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.38-7.28 (m, 4H), 7.28-7.19 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 1H), 3.80 (s, 3H), 2.39 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 169.1, 151.1, 136.2, 132.6, 132.4, 129.0, 128.6, 125.9, 122.7, 122.1, 120.5, 119.9, 118.3, 109.6, 96.6, 88.2, 85.7, 33.1, 21.0.

IR (neat): ν_{max} = 2918, 2203, 1752, 1466, 1190 cm^{-1}.

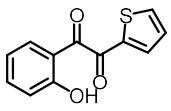
HRMS (ESI) m/z calcd for $C_{19}H_{16}NO_2^+$ $(M+H)^+$ 290.1176, found 290.1170.

Scheme *S9*. Typical Procedure C for the synthesis of 1-(2-hydroxyaryl)-2-arylethane-1,2-diones



2a 3a

To a vial equipped with a condenser was added 2-(thiophen-2-ylethynyl)phenyl acetate (200.0 mg, 0.83 mmol), $PdBr_2$ (22.0 mg, 0.083 mmol), and DMSO (4.0 mL). The mixture was stirred at 140 °C under air and the progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was cooled down to room temperature, and water (10 mL) was added. The resulting mixture was extracted with ethyl acetate (3×10 mL). The combined organic layers were concentrated in vacuo and the residue was purified by column chromatography on silica gel or preparative thin-layer chromatography (petroleum ether : ethyl acetate = 20:1) to obtain the desired products 1-(2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3a**). Substrates **3b**–**3k** were synthesized according to the similar procedures.[10]



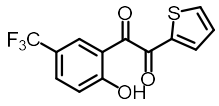
3a

1-(2-Hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (3a): yellow solid, 107.4 mg, 56%.[1]

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.38 (s, 1H), 7.89-7.86 (m, 1H), 7.80-7.76 (m, 1H), 7.68-7.63 (m, 1H), 7.60-7.53 (m, 1H), 7.24-7.18 (m, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.94-6.89 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 196.7, 183.6, 163.7, 139.6, 138.2, 137.4, 137.0, 132.6,

128.9, 119.7, 118.6, 116.33.



3b

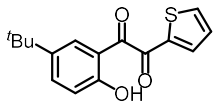
1-(2-Hydroxy-5-(trifluoromethyl)phenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3b**): The reaction of 2-(thiophen-2-ylethynyl)-4-(trifluoromethyl)phenyl acetate (450 mg, 1.45 mmol), $PdBr_2$ (38.6 mg, 0.145 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3b** (193.8 mg, 45%) as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.70 (s, 1H), 8.02-8.00 (m, 1H), 7.94-7.90 (m, 1H), 7.87-7.83 (m, 1H), 7.81-7.76 (m, 1H), 7.25-7.16 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 195.7, 182.3, 166.0, 139.0, 138.1, 137.3, 134.4 (q, J_{C-F} = 3.4 Hz), 130.1 (q, J_{C-F} =4.0 Hz), 129.1, 123.4 (q, J_{C-F} =272.2 Hz), 122.2 (q, J_{C-F} = 33.8 Hz), 119.7, 115.6.

^{19}F NMR (471 MHz, $CDCl_3$): δ -64.4.

IR (neat): ν_{max} = 2923, 1635, 1413, 1323, 1296, 1190, 1121 cm^{-1}.



3c

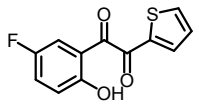
1-(5-(*Tert*-butyl)-2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3c**): The reaction of 4-(*tert*-butyl)-2-(thiophen-2-ylethynyl)phenyl acetate (298.0 mg, 1 mmol), $PdBr_2$ (26.6 mg, 0.1 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3c** (186.5 mg, 65%) as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.29 (s, 1H), 7.87 (d, J = 5.0 Hz, 1H), 7.80 (d, J = 5.0 Hz, 1H), 7.67-7.58 (m, 2H), 7.24-7.17 (m, 1H), 7.02 (d, J = 8.5 Hz, 1H), 1.24 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 196.6, 183.8, 161.8, 142.4, 139.7, 137.2, 136.9, 136.3, 128.9, 128.2, 118.2, 115.6, 34.1, 31.1.

IR (neat): ν_{max} = 2918, 1651, 1631, 1413, 1185 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{16}H_{17}O_3S^+$ $(M+H)^+$ 289.0893, found 289.0885.



3d

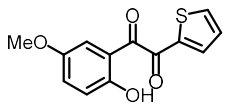
1-(5-Fluoro-2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3d**): The reaction of 4-fluoro-2-(thiophen-2-ylethynyl)phenyl acetate (272.7 mg, 1.05 mmol), $PdBr_2$ (28.0 mg, 0.105 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3d** (176.6 mg, 67%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.20 (s, 1H), 7.90 (dd, J = 4.5, 1.0 Hz, 1H), 7.82 (dd, J = 4.5, 1.0 Hz, 1H), 7.40 (dd, J = 8.5, 3.0 Hz, 1H), 7.36-7.28 (m, 1H), 7.24-7.21 (m, 1H), 7.05 (dd, J = 8.0, 4.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 195.5 (d, J_{C-F} = 3.0 Hz), 182.7, 160.1, 155.0 (d, J_{C-F} = 240.5 Hz), 139.2, 137.8, 137.2, 129.0, 126.2 (d, J_{C-F} = 24.1 Hz), 120.1 (d, J_{C-F} = 7.2 Hz), 117.1 (d, J_{C-F} = 23.9 Hz), 115.6 (d, J = 6.9 Hz).

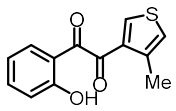
^{19}F NMR (471 MHz, $CDCl_3$): δ -122.7.

IR (neat): ν_{max} = 2918, 1652, 1632, 1473, 1409, 1237, 1157 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{12}H_8FO_3S^+$ $(M+H)^+$ 251.0173, found 251.0165.



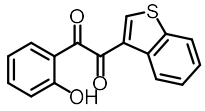
3e

1-(2-Hydroxy-5-methoxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3e**): The reaction of 4-methoxy-2-(thiophen-2-ylethynyl)phenyl acetate (223.0 mg, 0.82 mmol), $PdBr_2$ (21.8 mg, 0.082 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3e** (92.9 mg, 43%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 11.13 (s, 1H), 7.88 (d, *J* = 4.0 Hz, 1H), 7.81 (d, *J* = 4.0 Hz, 1H), 7.24-7.18 (m, 2H), 7.10 (d, *J* = 3.0 Hz, 1H), 7.02 (d, *J* = 9.0 Hz, 1H), 3.73 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 195.9, 183.5, 158.6, 152.1, 139.5, 137.4, 137.1, 129.0, 127.2, 119.7, 115.5, 113.4, 55.9.
IR (neat): ν_{max} = 2918, 1651, 1636, 1587, 1484, 1405, 1253, 1169 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{13}H_{11}O_4S^+$ $(M+H)^+$ 263.0373, found 263.0366.



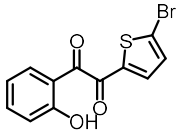
3f

1-(2-Hydroxyphenyl)-2-(4-methylthiophen-3-yl)ethane-1,2-dione (**3f**): The reaction of 2-((4-methylthiophen-3-yl)ethynyl)phenyl acetate (238.0 mg, 0.93 mmol), $PdBr_2$ (24.8 mg, 0.093 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3f** (46.7 mg, 20%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 11.42 (s, 1H), 8.05 (d, *J* = 3.0 Hz, 1H), 7.61-7.49 (m, 2H), 7.12-6.99 (m, 2H), 6.97-6.83 (m, 1H), 2.58 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 198.3, 186.8, 163.6, 140.1, 139.5, 138.0, 135.2, 132.5, 123.8, 119.6, 118.6, 116.4, 16.3.
IR (neat): ν_{max} = 2922, 1667, 1630, 1438, 1206 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{13}H_{11}O_3S^+$ $(M+H)^+$ 247.0423, found 247.0418.



3g

1-(Benzo[*b*]thiophen-3-yl)-2-(2-hydroxyphenyl)ethane-1,2-dione (**3g**): The reaction of 2-(benzo[b]thiophen-3-ylethynyl)phenyl acetate (129.0 mg, 0.44 mmol), $PdBr_2$ (11.7 mg, 0.044 mmol) in DMSO (2.0 mL) under **typical procedure C** afforded **3g** (69.0 mg, 56%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 11.48 (s, 1H), 8.86 (d, *J* = 8.0 Hz, 1H), 8.38 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 7.75-7.44 (m, 4H), 7.09 (d, *J* = 8.5 Hz, 1H), 7.02-6.79 (m, 1H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 196.1, 186.1, 164.1, 155.6, 155.3, 138.3, 132.7, 126.5, 125.2, 123.6, 122.7, 119.7, 118.7, 118.6, 116.1, 111.8.
IR (neat): ν_{max} = 2923, 1651, 1626, 1487, 1457, 1206, 1143 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{16}H_{11}O_3S^+$ $(M+H)^+$ 283.0423, found 283.0420.



3h

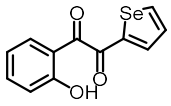
1-(5-Bromothiophen-2-yl)-2-(2-hydroxyphenyl)ethane-1,2-dione (**3h**): The reaction of 2-((5-bromothiophen-2-yl)ethynyl)phenyl acetate (307.0 mg, 0.96 mmol), $PdBr_2$ (25.6 mg, 0.096 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3h** (144.7 mg, 49%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.32 (s, 1H), 7.68 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.64-7.48 (m, 2H), 7.18 (d, *J* = 4.0 Hz, 1H), 7.07 (d, *J* = 8.5 Hz, 1H), 6.97-6.86 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 195.8, 182.1, 163.9, 140.8, 138.4, 137.2, 132.6, 132.1, 127.1, 119.7, 118.7, 116.2.

IR (neat): ν_{max} = 2921, 1653, 1629, 1402 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{12}H_8BrO_3S^+$ $(M+H)^+$ 310.9372, found 310.9366.



3i

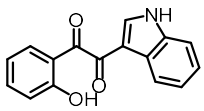
1-(2-Hydroxyphenyl)-2-(selenophen-2-yl)ethane-1,2-dione (**3i**): The reaction of 2-(selenophen-2-ylethynyl)phenyl acetate (578.0 mg, 2 mmol), $PdBr_2$ (53.0 mg, 0.2 mmol) in DMSO (5.0 mL) under **typical procedure C** afforded **3i** (360.1 mg, 64%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.38 (s, 1H), 8.62 (dd, *J* = 5.5, 1.0 Hz, 1H), 8.13-7.90 (m, 1H), 7.65 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.62-7.52 (m, 1H), 7.45 (dd, *J* = 5.5, 4.0 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 1H), 6.96-6.85 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 196.9, 184.8, 163.6, 145.5, 143.8, 139.8, 138.2, 132.7, 131.6, 119.7, 118.6, 116.4.

IR (neat): ν_{max} = 2924, 1650, 1628, 1227, 1203, 1156 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{12}H_9O_3Se^+$ $(M+H)^+$ 280.9711, found 280.9710.



3j

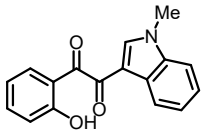
1-(2-Hydroxyphenyl)-2-(1H-indol-3-yl)ethane-1,2-dione (**3j**): The reaction of tert-butyl 3-((2-acetoxyphenyl)ethynyl)-1H-indole-1-carboxylate (112.5 mg, 0.3 mmol), $PdBr_2$ (8.0 mg, 0.03 mmol) in DMSO (2.0 mL) under **typical procedure C** (10 parallel reactions) afforded **3j** (245.4 mg, 31%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.63 (s, 1H), 8.95 (s, 1H), 8.46 (d, *J* = 6.5 Hz, 1H), 7.90 (d, *J* = 3.0 Hz, 1H), 7.80 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.58-7.51 (m, 1H), 7.50-7.44 (m, 1H), 7.43-7.34 (m, 2H), 7.06 (d, *J* = 8.5 Hz, 1H), 6.89 (t, *J* = 8.0 Hz, 1H).

^{13}C NMR (126 MHz, DMSO-d_6): δ 196.2, 188.7, 160.4, 137.3, 137.14, 137.08, 131.4, 125.7, 124.1, 123.0, 121.5, 120.8, 120.1, 117.8, 113.1, 112.6.

IR (neat): ν_{max} = 3217, 2922, 1635, 1605, 1578, 1439, 1237 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{16}H_{12}NO_3^+$ $(M+H)^+$ 266.0812, found 266.0804.



3k

1-(2-Hydroxyphenyl)-2-(1-methyl-1H-indol-3-yl)ethane-1,2-dione (**3k**): The reaction of 2-((1-methyl-1H-indol-3-yl)ethynyl)phenyl acetate (86.7 mg, 0.3 mmol), $PdBr_2$ (8.0 mg, 0.03 mmol) in DMSO (2.0 mL) under **typical procedure C** (5 parallel reactions) afforded **3k** (136.0 mg, 32%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 11.67 (s, 1H), 8.50-8.40 (m, 1H), 7.80 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.75 (s, 1H), 7.59-7.49 (m, 1H), 7.46-7.33 (m, 3H), 7.06 (d, *J* = 7.5 Hz, 1H), 6.92-6.84 (m, 1H), 3.83 (s, 3H).

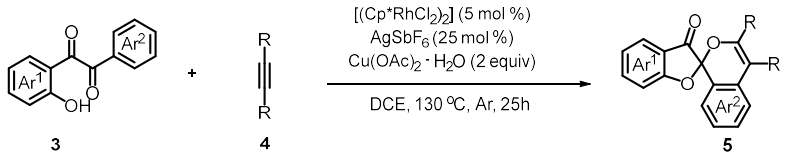
^{13}C NMR (126 MHz, $CDCl_3$): δ 198.8, 185.5, 163.6, 139.5, 137.7, 137.6, 133.0, 126.1, 124.4, 123.6, 122.5, 119.4, 118.4, 116.7, 112.6, 110.1, 33.8.

IR (neat): ν_{max} = 2918, 2160, 1970, 1620, 1528, 1457, 1086 cm^{-1}.

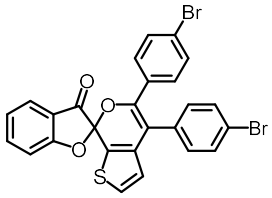
HRMS (ESI) m/z calcd for $C_{17}H_{14}NO_3^+$ $(M+H)^+$ 280.0968, found 280.0964.

3. Preparation Products 5 and Analytical Data

Scheme *S10*. Typical Procedure D for the synthesis of benzofuranone-based spiropyrans



To an oven-dried vial, ethane-1,2-dione (**3**, 0.1 mmol), alkyne (**4**, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mm), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), DCE (1.0 mL) were added successively. The vial was charged with Ar and sealed immediately. The resulting mixture was stirred at 130 °C and the progress of the reaction was monitored by TLC. After the completion of the reaction (25 h), the mixture was cooled down to room temperature, filtered through a celite pad, and washed with ethyl acetate. The filtrate was concentrated in vacuo and the residue was purified by column chromatography on silica gel or preparative thin-layer chromatography (petroleum ether : ethyl acetate = 50:1) to obtain the products.[1]



5b

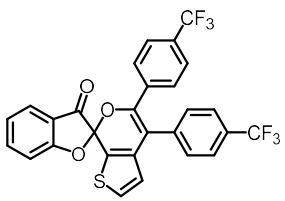
4',5'-Bis(4-bromophenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5b**): The reaction of 1-(2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3a**, 23.2 mg, 0.1 mmol), 1,2-bis(4-bromophenyl)ethyne (67.2 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5b** (29.2 mg, 57%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 5.3 Hz, 1H), 7.32-7.24 (m, 2H), 7.24-7.14 (m, 3H), 7.13-7.00 (m, 3H), 6.78 (d, *J* = 5.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 194.9, 169.8, 145.1, 140.1, 138.7, 134.7, 132.2, 132.10, 132.05, 131.0, 130.6, 127.7, 125.7, 123.7, 123.2, 122.8, 121.9, 120.5, 118.0, 113.5, 112.5, 102.5.

IR (neat): ν_{max} = 1731, 1604, 1482, 1455, 1004, 877 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{26}H_{14}Br_2O_3SNa^+$ $(M+Na)^+$ 586.8923, found 586.8923.



5c

4',5'-Bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5c**): The reaction of 1-(2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3a**, 23.2 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5c** (33.4 mg, 62%) as a yellow solid.

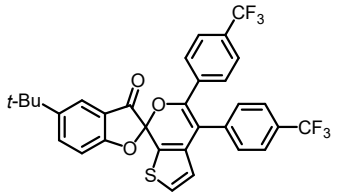
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, *J* = 7.5 Hz, 1H), 7.79-7.72 (m, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.42-7.38 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 8.5 Hz, 1H), 6.77 (d, *J* = 5.0 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 194.7, 169.8, 145.0, 140.2, 139.4, 138.2, 136.5, 130.8, 130.4 (q, $J_{C\text{-}F}$ = 32.6 Hz), 130.1 (q, $J_{C\text{-}F}$ = 32.8 Hz), 129.4, 128.0, 126.1 (q, $J_{C\text{-}F}$ = 272.5 Hz), 126.0 (q, $J_{C\text{-}F}$ = 3.8 Hz), 125.8, 124.8 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.9 (q, $J_{C\text{-}F}$ = 272.5 Hz), 123.6, 123.3, 121.1, 117.9, 113.5, 113.4, 102.3.

^{19}F NMR (471 MHz, $CDCl_3$): δ -62.6, -62.9.

IR (neat): ν_{max} = 2925, 1737, 1615, 1319, 1115, 1064 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{28}H_{14}F_6O_3SNa^+$ $(M+Na)^+$ 567.0460, found 567.0461.



5d

3-(*Tert*-butyl)-4',5'-bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5d**): The reaction of 1-(5-(tert-butyl)-2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3c**, 28.8 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5d** (20.0 mg, 33%) as a yellow solid.

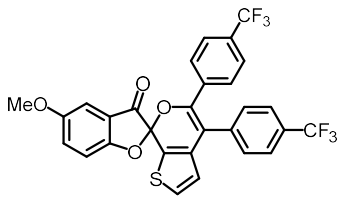
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.88-7.78 (m, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.44-7.36 (m, 3H), 7.31 (d, *J* = 8.5 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 1H), 6.77 (d, *J* = 5.5 Hz, 1H), 1.37 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 197.3, 168.2, 146.7, 145.1, 139.5, 138.3, 138.1, 136.6, 130.8, 130.3 (q, $J_{C\text{-}F}$ = 33.3 Hz), 130.0 (q, $J_{C\text{-}F}$ = 32.9 Hz), 129.4, 127.9, 125.9 (q, $J_{C\text{-}F}$ = 3.4 Hz), 124.8 (q, $J_{C\text{-}F}$ = 3.8 Hz), 124.0 (q, $J_{C\text{-}F}$ = 272.4 Hz), 123.7 (q, $J_{C\text{-}F}$ = 272.4 Hz), 123.6, 121.6, 121.3, 117.4, 113.3, 112.9, 102.7, 34.7, 31.3.

^{19}F NMR (471 MHz, $CDCl_3$): δ -62.5, -62.8.

IR (neat): ν_{max} = 1742, 1620, 1487, 1323, 1126, 1063 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{32}H_{22}F_6O_3SNa^+$ $(M+Na)^+$ 623.1086, found 623.1085.



5e

5-Methoxy-4',5'-bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5e**): The reaction of 1-(2-hydroxy-5-methoxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3e**, 26.2 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5e** (16.6 mg, 29%) as a yellow solid.

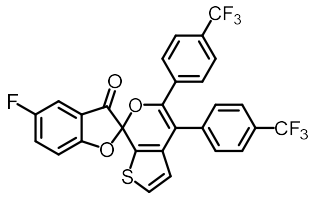
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.65 (d, J = 8.5 Hz, 2H), 7.46-7.35 (m, 6H), 7.31 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 3.0 Hz, 1H), 7.02 (d, J = 9.0 Hz, 1H), 6.76 (d, J = 5.0 Hz, 1H), 3.86 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 195.1, 165.3, 155.8, 145.1, 139.5, 138.1, 136.6, 130.8, 130.4 (q, $J_{C\text{-}F}$ = 32.8 Hz), 130.1 (q, $J_{C\text{-}F}$ = 32.6 Hz), 130.0, 129.4, 127.9, 126.0 (q, $J_{C\text{-}F}$ = 3.8 Hz), 124.8 (q, $J_{C\text{-}F}$ = 3.8 Hz), 124.0 (q, $J_{C\text{-}F}$ = 273.0 Hz), 123.7 (q, $J_{C\text{-}F}$ = 272.2 Hz), 123.6, 121.4, 117.8, 114.5, 113.3, 105.3, 103.0, 56.0.

^{19}F NMR (471 MHz, $CDCl_3$): δ -62.5, -62.8.

IR (neat): ν_{max} = 1731, 1493, 1317, 1126, 1068 cm^{-1}.

HRMS (ESI) m/z calcd for $C_{29}H_{16}F_6O_4SNa^+$ $(M+Na)^+$ 597.0566, found 597.0565.



5f

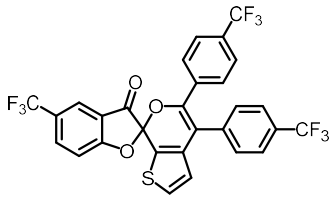
4-Fluoro-4',5'-bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5f**): The reaction of 1-(5-fluoro-2-hydroxyphenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3d**, 25.0 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5f** (27.3 mg, 49%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.66 (d, J = 8.0 Hz, 2H), 7.51-7.38 (m, 7H), 7.31 (d, J = 8.5 Hz, 2H), 7.09-7.04 (m, 1H), 6.77 (d, J = 5.0 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 194.3 (d, $J_{C\text{-}F}$ = 2.6 Hz), 166.0, 158.3 (d, $J_{C\text{-}F}$ = 245.8 Hz), 145.0, 139.3, 138.2, 136.4, 130.8, 130.5 (q, $J_{C\text{-}F}$ = 32.9 Hz), 130.2 (q, $J_{C\text{-}F}$ = 32.3 Hz), 129.4, 128.1, 127.7 (d, $J_{C\text{-}F}$ = 25.7 Hz), 126.0 (q, $J_{C\text{-}F}$ = 4.0 Hz), 124.9 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.9 (q, $J_{C\text{-}F}$ = 272.8 Hz), 123.70 (q, $J_{C\text{-}F}$ = 273.0 Hz), 123.69, 120.8, 118.4 (d, $J_{C\text{-}F}$ = 8.1 Hz), 114.8 (d, $J_{C\text{-}F}$ = 7.6 Hz), 113.4, 110.8 (d, $J_{C\text{-}F}$ = 24.1 Hz), 103.4.

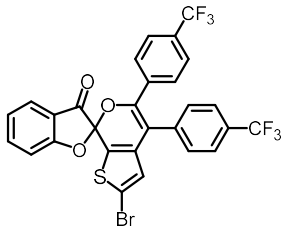
^{19}F NMR (471 MHz, $CDCl_3$): δ -62.5, -62.8, -118.4.

IR (neat): ν_{max} = 1742, 1487, 1329, 1126, 1063 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{28}H_{13}F_7O_3SNa^+$ $(M+Na)^+$ 585.0366, found 585.0367.



5g

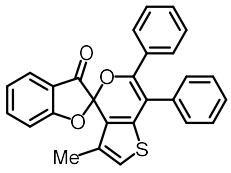
2-(Trifluoromethyl)-4',5'-bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5d**): The reaction of 1-(2-hydroxy-5-(trifluoromethyl)phenyl)-2-(thiophen-2-yl)ethane-1,2-dione (**3b**, 30.0 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 ºC for 25 h) afforded **5g** (14.5 mg, 24%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 8.04-7.95 (m, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.48-7.39 (m, 5H), 7.31 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 1H), 6.79 (d, *J* = 5.0 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 193.4, 171.1, 145.0, 139.1, 138.5, 136.8, 136.2, 130.8, 130.6 (q, J_{C-F} = 32.8 Hz), 130.3 (q, J_{C-F} = 32.5 Hz), 129.3, 128.5, 126.05 (q, J_{C-F} = 3.7 Hz), 126.01 (q, J_{C-F} = 34.1 Hz), 124.9 (q, J_{C-F} = 3.9 Hz), 123.9 (q, J_{C-F} = 272.4 Hz), 123.8, 123.7 (q, J_{C-F} = 272.8 Hz), 123.6 (q, J_{C-F} = 4.0 Hz), 123.4 (q, J_{C-F} = 272.5 Hz), 120.3, 118.1, 114.3, 113.6, 103.6.
^{19}F NMR (471 MHz, $CDCl_3$): δ -62.1, -62.5, -62.9.
IR (neat): ν_{max} = 1747, 1625, 1323, 1116, 1063 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{29}H_{13}F_9O_3SNa^+$ $(M+Na)^+$ 635.0334, found 635.0331.



5h

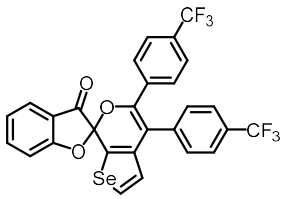
2'-Bromo-4',5'-bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one (**5h**): The reaction of 1-(5-bromothiophen-2-yl)-2-(2-hydroxyphenyl)ethane-1,2-dione (**3h**, 31.0 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 ºC for 25 h) afforded **5h** (22.6 mg, 36%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 7.5 Hz, 2H), 7.48-7.36 (m, 4H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 5.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 194.7, 169.8, 145.0, 140.2, 139.4, 138.2, 136.6, 130.8, 130.4 (q, J_{C-F} = 32.6 Hz), 130.1 (q, J_{C-F} = 32.9 Hz), 129.4, 128.0, 126.0 (q, J_{C-F} = 3.8 Hz), 125.8, 124.8 (q, J_{C-F} = 4.3 Hz), 124.7 (q, J_{C-F} = 272.7 Hz), 123.7 (q, J_{C-F} = 276.1 Hz), 123.6, 123.3, 121.2, 117.9, 113.5, 113.4, 102.4.
^{19}F NMR (471 MHz, $CDCl_3$): δ -64.8, -65.2.
IR (neat): ν_{max} = 1731, 1610, 1317, 1121, 1069 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{28}H_{14}BrF_6O_3S^+$ $(M+H)^+$ 622.9746, found 622.9730.



5i

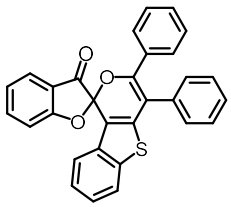
3'-Methyl-6',7'-diphenyl-3*H*-spiro[benzofuran-2,4'-thieno[3,2-*c*]pyran]-3-one (**5i**): The reaction of 1-(2-hydroxyphenyl)-2-(4-methylthiophen-3-yl)ethane-1,2-dione (**3f**, 24.7 mg, 0.1 mmol), diphenylacetylene (35.6 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1.0 mL) under **typical procedure D** (130 °C for 25 h) afforded **5i** (23.6 mg, 53%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86-7.80 (m, 1H), 7.76-7.69 (m, 1H), 7.41-7.31 (m, 5H), 7.24-7.04 (m, 7H),6.84-6.81 (m, 1H), 1.90 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 196.0, 170.2, 144.8, 142.5, 139.7, 135.9, 133.9, 133.2, 130.1, 129.0, 128.8, 128.3, 127.9, 127.6, 125.4, 122.9, 121.4, 121.2, 118.8, 113.2, 111.9, 103.1, 15.0.
IR (neat): ν_{max} = 1736, 1609, 1455, 1189, 883 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{27}H_{18}O_3SNa^+$ $(M+Na)^+$ 445.0869, found 445.0869.



5j

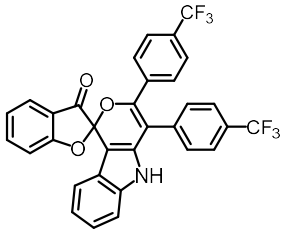
4',5'-Bis(4-(trifluoromethyl)phenyl)-3*H*-spiro[benzofuran-2,7'-selenopheno[2,3-*c*]pyran]-3-one (**5j**): The reaction of 1-(2-hydroxyphenyl)-2-(selenophen-2-yl)ethane-1,2-dione (**3i**, 27.9 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5j** (13.7 mg, 23%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (d, J = 5.5 Hz, 1H), 7.84 (d, J = 7.0 Hz, 1H), 7.79-7.71 (m, 1H), 7.66 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.3 Hz, 2H), 7.23 (t, J = 7.5 Hz, 1H), 7.09 (d, J = 8.5 Hz, 1H), 6.99 (d, J = 5.5 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 195.2, 169.7, 145.1, 140.3, 140.2, 139.7, 136.6, 133.1, 131.0, 130.2 (q, J_{C-F} = 32.5 Hz), 130.0 (q, J_{C-F} = 32.6 Hz), 129.2, 126.6, 125.9 (q, J_{C-F}

= 3.7 Hz), 125.8, 125.0, 124.8 (q, J_{C-F} = 3.7 Hz), 123.9 (q, J_{C-F} = 272.8 Hz), 123.7 (q, J_{C-F} = 274.6 Hz), 123.3, 117.7, 114.3, 113.5, 103.6.
^{19}F NMR (471 MHz, $CDCl_3$): δ -62.5, -62.8.
IR (neat): ν_{max} = 1736, 1614, 1317, 1120, 1063 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{28}H_{14}F_6O_3SeNa^+$ $(M+Na)^+$ 614.9905, found 614.9904.



5k

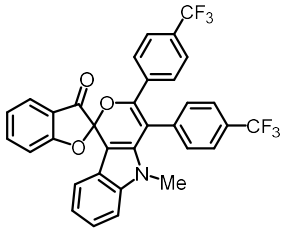
3',4'-Diphenyl-3*H*-spiro[benzofuran-2,1'-benzo[4,5]thieno[3,2-*c*]pyran]-3-one (**5k**): The reaction of 1-(benzo[*b*]thiophen-3-yl)-2-(2-hydroxyphenyl)ethane-1,2-dione (**3g**, 28.2 mg, 0.1 mmol), diphenylacetylene (35.6 mg, 0.2 mmol), [(Cp*$RhCl_2$)$_2$] (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5k** (38.1 mg, 83%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.0 Hz, 1H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.48-7.38 (m, 5H), 7.32-7.10 (m, 9H), 7.07 (d, *J* = 8.5 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 195.5, 170.4, 147.2, 143.2, 140.0, 139.2, 135.8, 135.2, 132.9, 130.1, 129.2, 129.0, 128.8, 128.2, 127.7, 125.5, 125.1, 124.3, 123.2, 122.6, 120.9, 118.6, 115.3, 113.4, 111.8, 103.1.
IR (neat): ν_{max} = 1736, 1604, 1461, 1180, 872, 755, 734 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{30}H_{18}O_3SNa^+$ $(M+Na)^+$ 481.0869, found 481.0870.



5l

3',4'-Bis(4-(trifluoromethyl)phenyl)-3*H*,5'*H*-spiro[benzofuran-2,1'-pyrano[4,3-*b*]indol]-3-one (**5l**): The reaction of 1-(2-hydroxyphenyl)-2-(1*H*-indol-3-yl)ethane-1,2-dione (**3j**, 26.5 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), [(Cp*$RhCl_2$)$_2$] (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCE (1 mL) under **typical procedure D** (130 °C for 25 h) afforded **5l** (14.8 mg, 26%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.81-7.75 (m, 1H), 7.68 (d, *J* = 7.5 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.38-7.30 (m, 4H), 7.30-7.26 (m, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.12 (t, *J* = 7.0 Hz, 1H), 7.08-6.98 (m, 2H), 6.95 (d, *J* = 8.0 Hz, 1H).
^{13}C NMR (126 MHz, DMSO-d_6): δ 195.7, 169.9, 146.6, 141.5, 138.1, 137.4, 137.2, 134.7, 131.8, 130.0, 129.4 (q, J_{C-F} = 32.9 Hz), 129.3 (q, J_{C-F} = 32.0 Hz), 126.7 (q, J_{C-F}

= 4.0 Hz), 125.8, 125.6 (q, J_{C-F} = 4.0 Hz), 124.6 (q, J_{C-F} = 272.8 Hz), 124.2 (q, J_{C-F} = 273.7 Hz), 124.1, 123.3, 122.8, 121.4, 117.9, 117.7, 113.6, 113.0, 110.0, 105.1, 98.4.
^{19}F NMR (471 MHz, DMSO-d_6): δ -61.1, -61.4 .
IR (neat): ν_{max} = 3321, 1725, 1609, 1317, 1105, 1063 cm^{-1}.
HRMS (ESI) m/z: calcd for $C_{32}H_{17}F_6NO_3Na^+$ $(M+Na)^+$ 600.1005, found 600.1008.



5m

5'-Methyl-3',4'-bis(4-(trifluoromethyl)phenyl)-3*H*,5'*H*-spiro[benzofuran-2,1'-pyrano[4,3-*b*]indol]-3-one (**5m**)**:** The reaction of 1-(2-hydroxyphenyl)-2-(1-methyl-1H-indol-3-yl)ethane-1,2-dione (**3k**, 27.9 mg, 0.1 mmol), 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (62.8 mg, 0.2 mmol), [(Cp*$RhCl_2$)$_2$] (3.2 mg, 0.005 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), $Cu(OAc)_2{\cdot}H_2O$ (40.0 mg, 0.2 mmol), in DCM (1 mL) under **typical procedure D** (130 ºC for 25 h) afforded **5m** (15.3 mg, 26%) as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.83-7.48 (m, 5H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.29-7.19 (m, 3H), 7.10-6.92 (m, 3H), 3.11 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$): δ 195.9, 170.1, 147.8, 140.0, 139.4, 138.2, 137.2, 134.5, 132.0, 130.8 (q, J_{C-F} = 32.9 Hz), 130.2 (q, J_{C-F} = 32.5 Hz), 129.2, 126.1 (q, J_{C-F} = 3.8 Hz), 125.4, 124.8 (q, J_{C-F} = 3.8 Hz), 123.8 (q, J_{C-F} = 272.8 Hz), 123.7 (q, J_{C-F} = 270.9 Hz), 123.2, 122.9, 122.0, 121.3, 118.42, 118.35, 113.3, 109.7, 109.6, 104.7, 99.4, 32.2.
^{19}F NMR (471 MHz, $CDCl_3$): δ -62.5, -62.8.
IR (neat): ν_{max} = 1736, 1609, 1323, 1126 cm^{-1}.
HRMS (ESI) m/z calcd for $C_{33}H_{19}F_6NO_3Na^+$ $(M+Na)^+$ 614.1161, found 614.1160.

4. Photochromic Properties of Benzofuranone-Based Spiropyrans 5a–5n

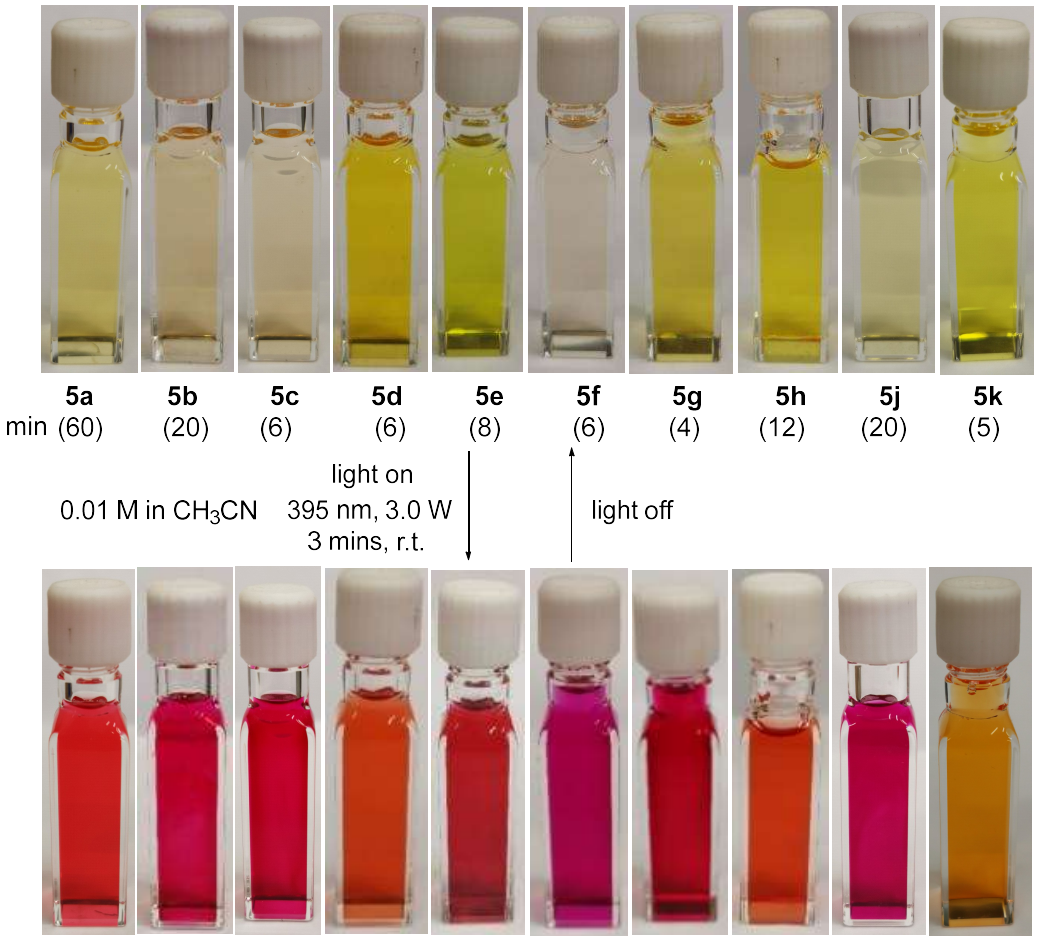


Figure *S1.* Photochromic behaviors of compounds **5a**–**h** and **5j**–**k** in acetonitrile (0.01 M) at room temperature. Number in parentheses refers to the time needed for reverse isomerization from the photostationary state to the original state in the absence of light.

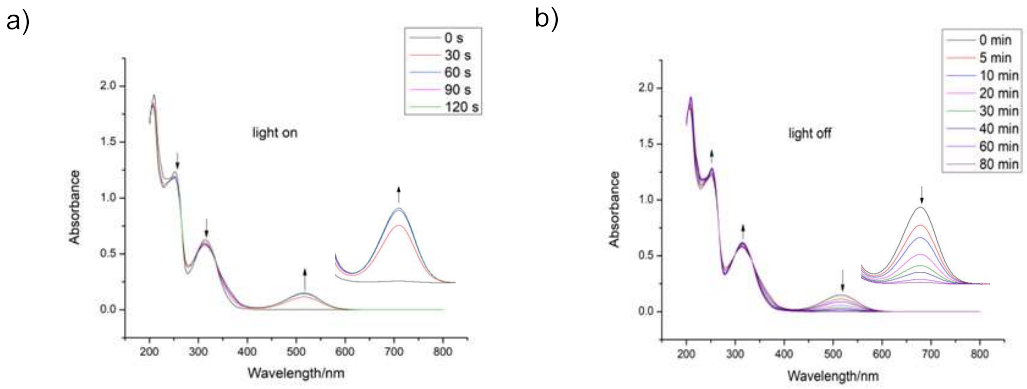


Figure *S2.* a) Time-dependent ultraviolet-visible absorption spectra of **5a** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

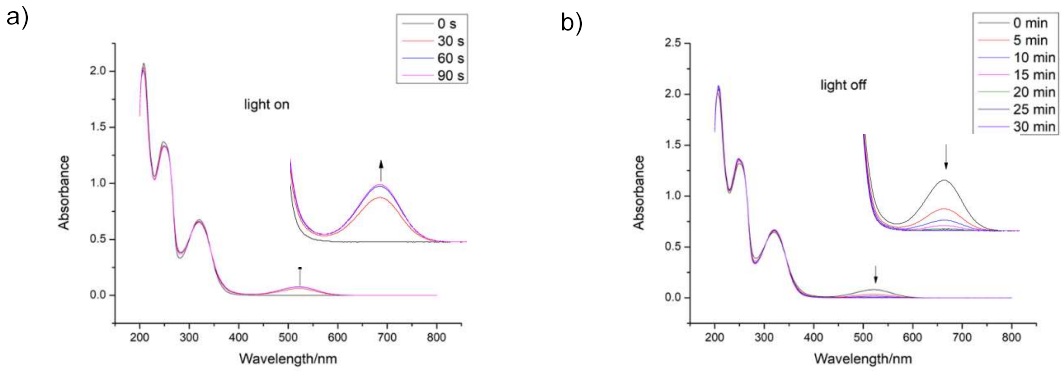


Figure *S3.* a) Time-dependent ultraviolet-visible absorption spectra of **5b** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

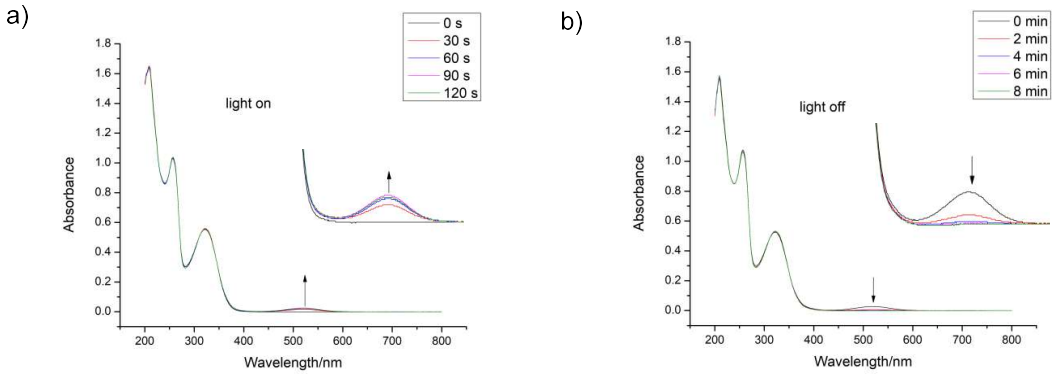


Figure *S4.* a) Time-dependent ultraviolet-visible absorption spectra of **5c** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

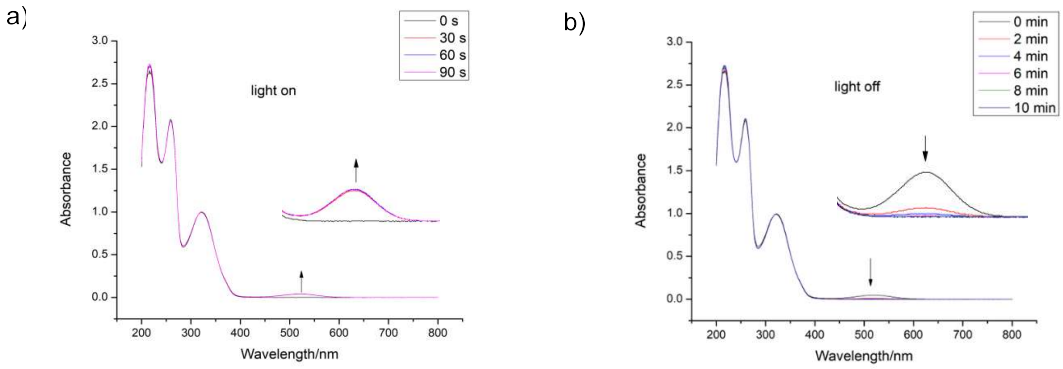


Figure *S5.* a) Time-dependent ultraviolet-visible absorption spectra of **5d** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

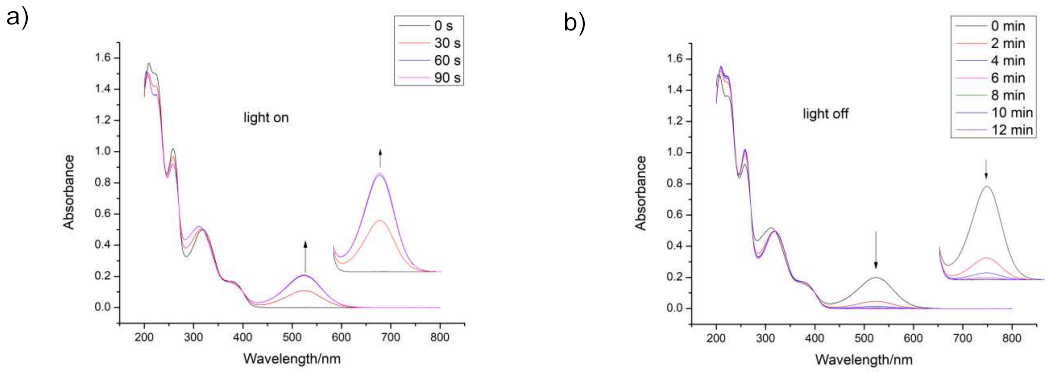


Figure *S6.* a) Time-dependent ultraviolet-visible absorption spectra of **5e** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

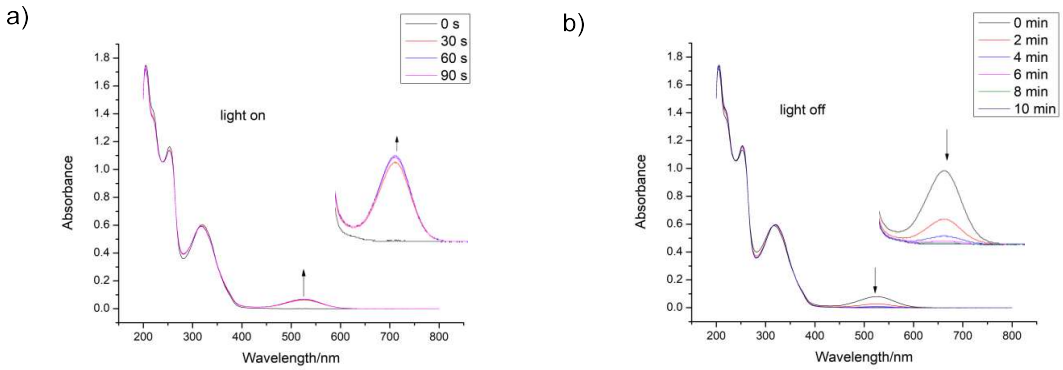


Figure *S7.* a) Time-dependent ultraviolet-visible absorption spectra of **5f** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

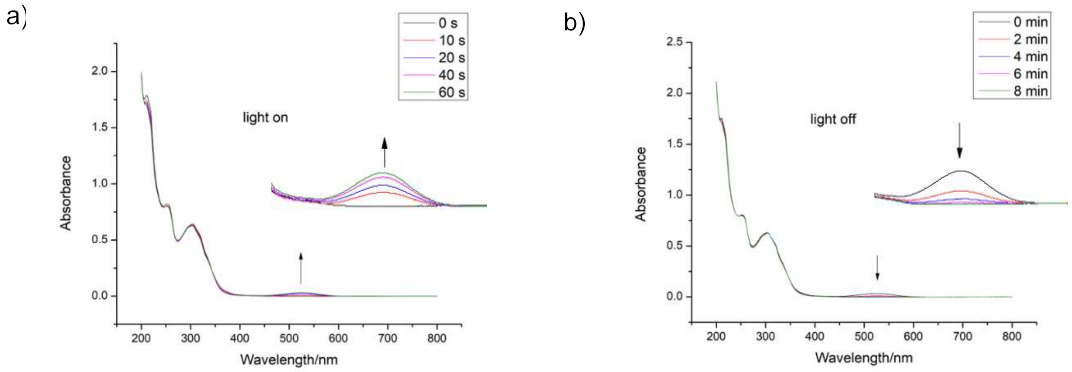


Figure *S8.* a) Time-dependent ultraviolet-visible absorption spectra of **5g** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

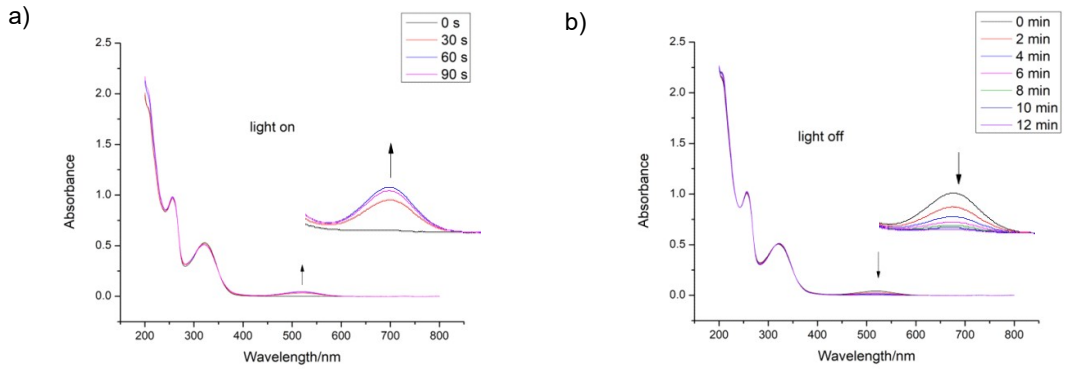


Figure *S9.* a) Time-dependent ultraviolet-visible absorption spectra of **5h** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

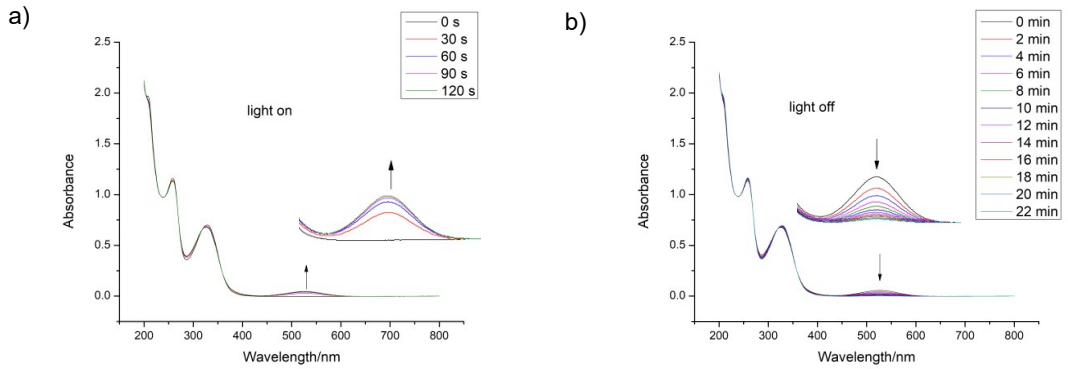


Figure *S10.* a) Time-dependent ultraviolet-visible absorption spectra of **5i** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm. b) The spectral changes after the light was switched off.

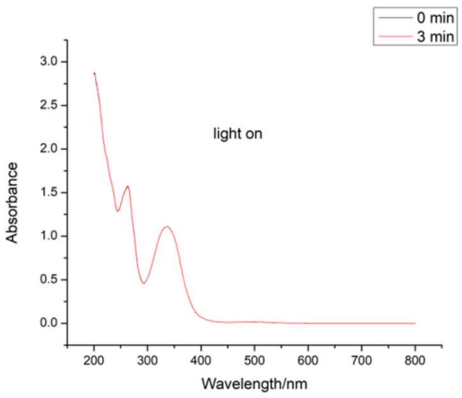


Figure *S11.* Time-dependent ultraviolet-visible absorption spectra of **5k** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm.

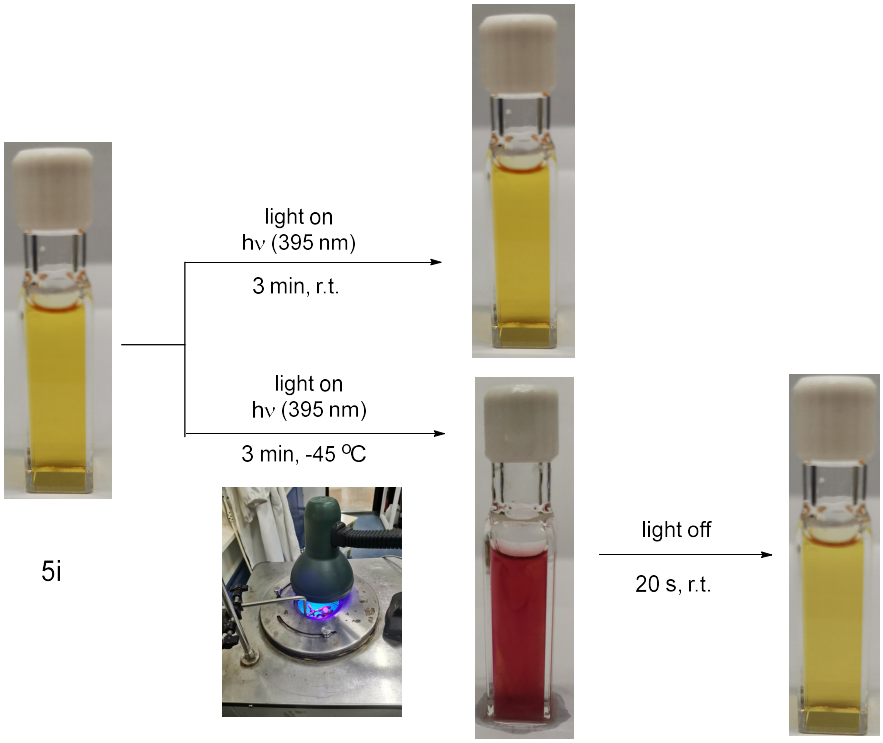


Figure *S12.* Photoswitchability of **5i** in acetonitrile (0.01 M).

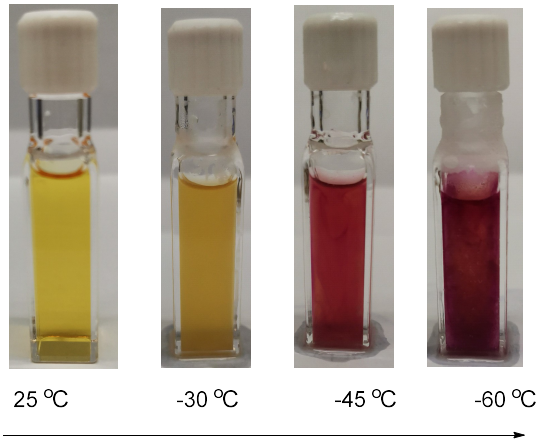


Figure *S13.* Photoswitchability of **5i** in acetonitrile (0.01 M) at different temperatures.

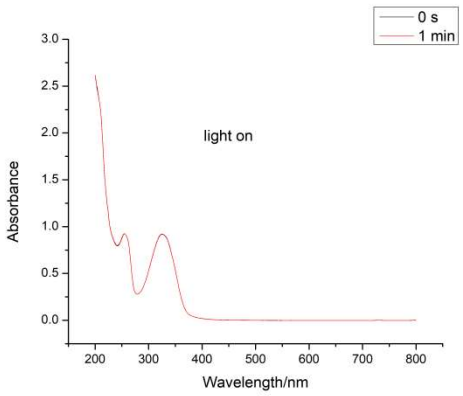


Figure *S14.* Time-dependent ultraviolet-visible absorption spectra of **5i** in acetonitrile (4×10^{-5} M) under photoirradiation at 395 nm.

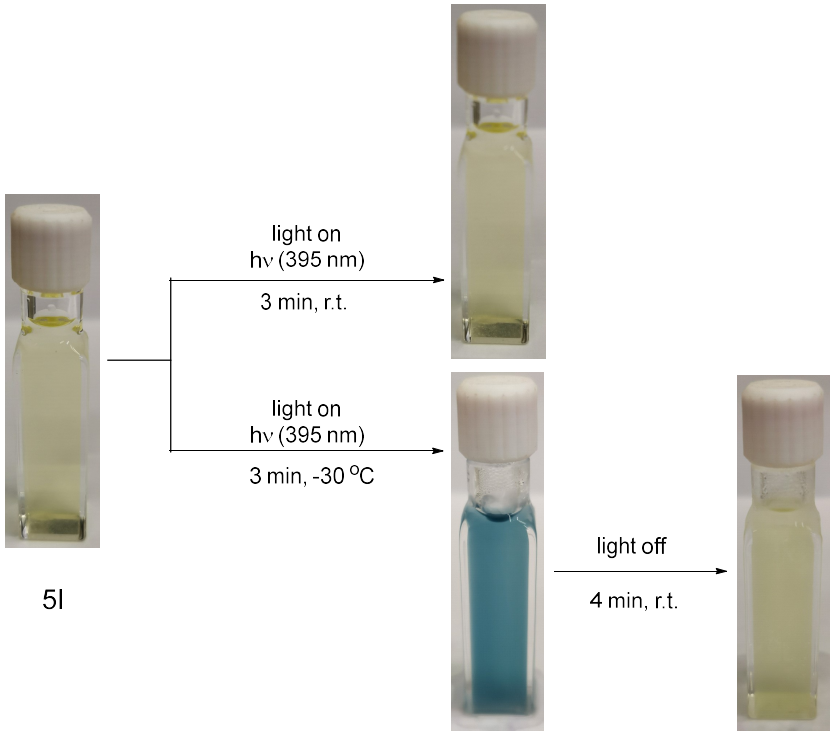


Figure *S15.* Photoswitchability of **5l** in acetonitrile (0.01 M).

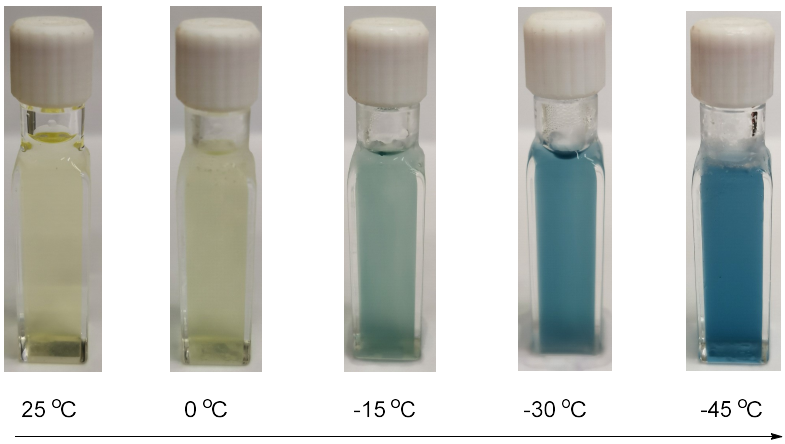


Figure *S16.* Photoswitchability of **5l** (acetonitrile, 0.01 M) at different temperatures.

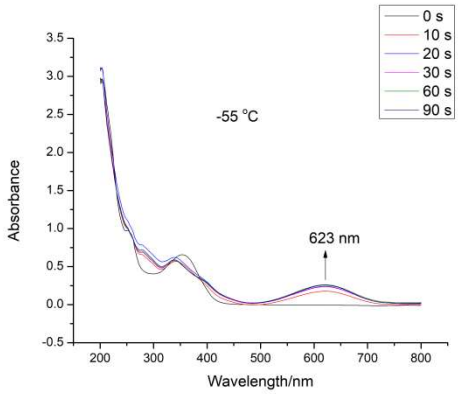


Figure *S17.* Time-dependent ultraviolet-visible absorption spectra of **5l** in ethanol

(4×10^{-5} M) under photoirradiation at 395 nm.

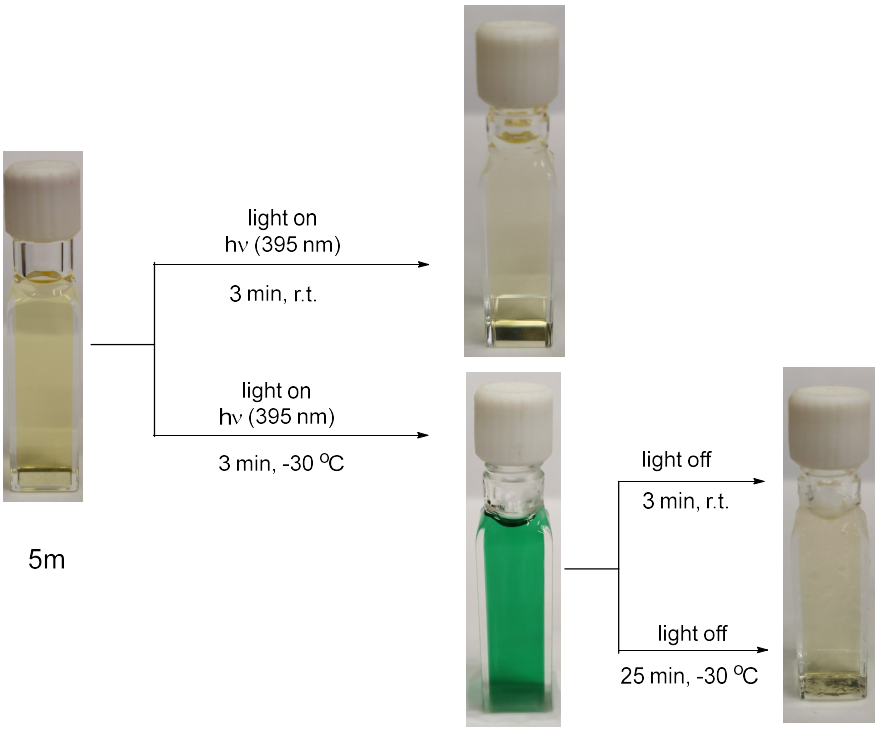


Figure *S18.* Photoswitchability of **5m** in acetonitrile (0.01 M).

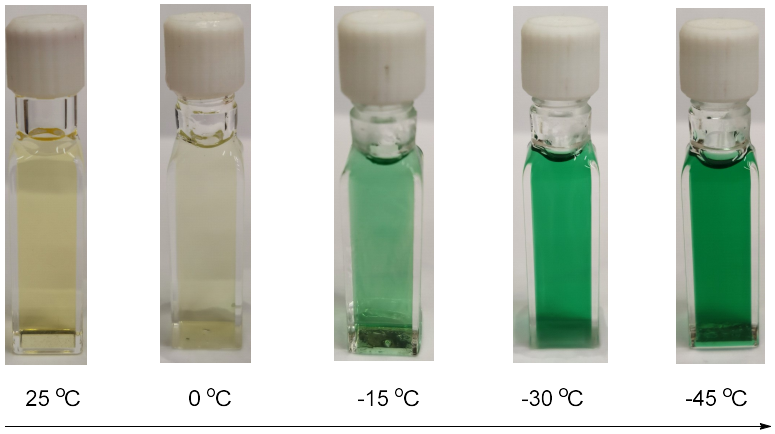


Figure *S19.* Photoswitchability of **5m** (acetonitrile, 0.01 M) at different temperatures.

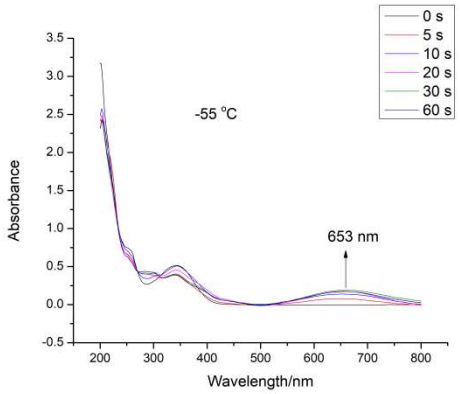


Figure *S20.* Time-dependent ultraviolet-visible absorption spectra of **5m** in ethanol

(4×10^{-5} M) under photoirradiation at 395 nm.

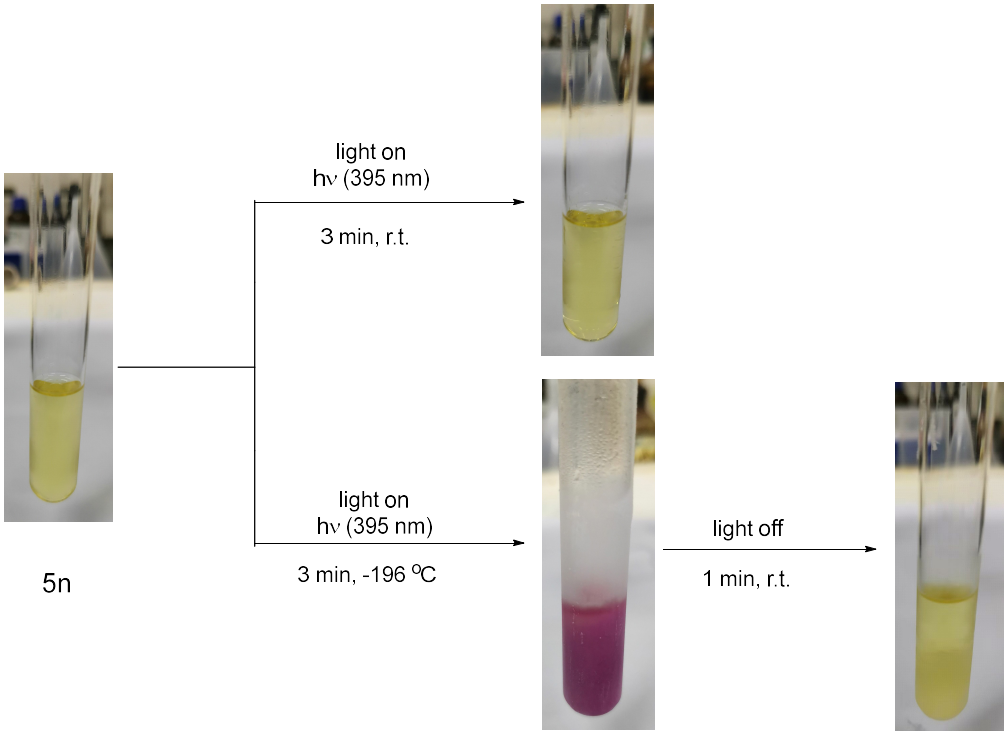


Figure *S21.* Photoswitchability of **5n** in ethyl acetate (0.01 M).

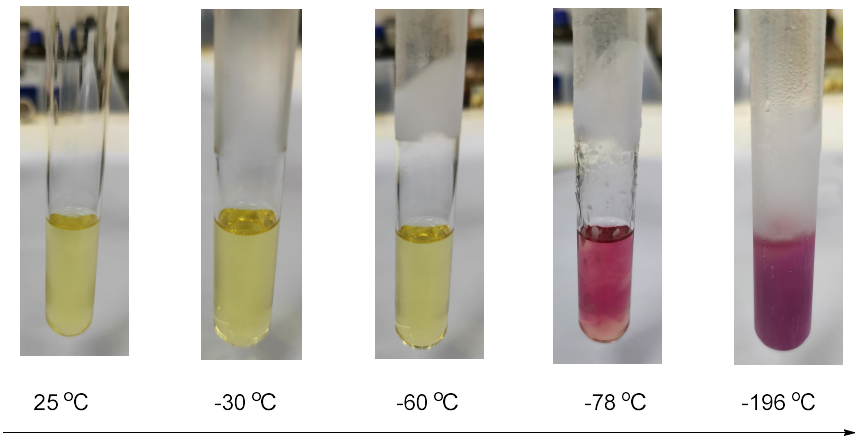


Figure *S22.* Photoswitchability of **5n** in ethyl acetate (0.01 M) at different temperatures.

5. Density Functional Theory (DFT) Calculations

All calculations are performed at the M062X/6-311+G(d)[13,14] level of theory using the Gaussian 09 package (version D01)[15] with tight SCF convergence and ultrafine integration grids. The solvent effect was taken into account by using the implicit solvent model CPCM (the conductor polarizable continuum model)[16] in the acetonitrile solvent. Theoretical analysis of corresponding absorption spectra for metastable 1,8-dioxatetraene species are conducted with time-dependent DFT.

The optimized Cartesian coordinates for **5a** and the excited state of **5a** in gas：

5a: (with the bond length of C_{spiro}-O is 1.39508 Å)
The total energy of **5a** is -1624.04460417 a.u.

C	-4.397278	0.329847	0.391055
C	-4.774773	-0.283224	-0.799557
C	-5.924623	0.097846	-1.479444
C	-6.675723	1.123722	-0.919217
C	-6.305424	1.753292	0.278743
C	-5.157873	1.356278	0.946182
C	-3.162418	-0.318676	0.832253
C	-2.819384	-1.343237	-0.297072
H	-6.212202	-0.390069	-2.402159
H	-7.578624	1.446937	-1.425642
H	-6.922041	2.549135	0.677939
H	-4.845796	1.820409	1.874962
C	-1.754360	-3.556241	-0.564278
C	-2.604534	-2.742796	0.133222
C	-0.965700	-1.650214	-1.792616
C	-0.968141	-2.993563	-1.659224
O	-2.498843	-0.161694	1.816608
O	-3.942009	-1.274312	-1.207892
O	-1.692983	-0.840421	-0.948720
C	-0.231559	-3.898883	-2.577343
C	-0.536737	-3.934881	-3.939075
C	0.780340	-4.729491	-2.088471
C	0.165834	-4.772190	-4.797886
H	-1.321716	-3.290838	-4.320982
C	1.481747	-5.569420	-2.946820
H	1.033467	-4.695056	-1.033211
C	1.177104	-5.591219	-4.304684
H	-0.078229	-4.786250	-5.854215
H	2.271750	-6.201226	-2.556248
C	-0.210200	-0.839247	-2.768134

C	-0.811552	0.300808	-3.310242
C	1.092963	-1.169952	-3.152059
C	-0.133687	1.078405	-4.240775
H	-1.814675	0.568945	-2.999581
C	1.769403	-0.386897	-4.078014
H	1.580823	-2.034472	-2.718286
C	1.157181	0.735077	-4.629742
H	-0.613517	1.955372	-4.660417
H	2.781437	-0.650062	-4.363832
C	-2.668878	-5.046625	0.955974
H	1.724825	-6.244189	-4.974777
H	1.687971	1.343890	-5.353056
S	-3.454294	-3.570341	1.376100
C	-1.802183	-4.904326	-0.083041
H	-1.222155	-5.719602	-0.493558
H	-2.888045	-5.941192	1.519266

The HOMO and LUMO of **5a** on the ground state

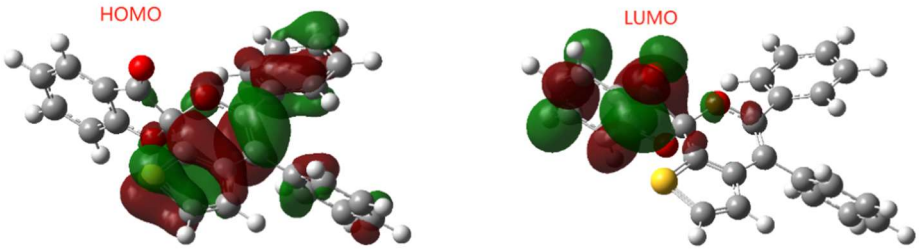


Figure *S23.* The HOMO and LUMO of **5a** on the ground state.

Excited State 1: Singlet-?Sym 1.8783 eV 660.08 nm f=0.0080
<S**2>=0.000

97 ->107	-0.10693
99 ->107	0.12183
106 ->107	0.65177

This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1623.94800548 a. u.
Delta energy between the Ground state and the excited state of **5a** is:
(-1623.94800548+-1624.04460417) a. u. * 627.4626 = 60 kcal/mol

the excited state of **5a:** (with the bond length of C_{spiro}-O is 1.46679 Å).

C	-2.961497	0.264678	1.012238
C	-4.279863	0.274908	0.531282

C	-5.250179	1.123762	0.991858
C	-4.880265	2.022031	2.007516
C	-3.574136	2.044500	2.499541
C	-2.599434	1.179928	2.011442
C	-2.215639	-0.696567	0.258669
C	-3.286030	-1.325994	-0.686839
H	-6.252540	1.099615	0.582357
H	-5.619482	2.705521	2.406905
H	-3.313122	2.753269	3.277395
H	-1.582721	1.204338	2.383695
C	-2.325986	-3.559861	-1.049684
C	-3.355795	-2.781505	-0.532340
C	-1.670625	-1.649830	-2.382329
C	-1.375341	-2.942431	-1.910140
O	-1.013248	-0.979422	0.140390
O	-4.478681	-0.675632	-0.462407
O	-2.791434	-1.034306	-2.036572
C	-0.178655	-3.697781	-2.328615
C	0.113838	-3.923562	-3.677517
C	0.666021	-4.225367	-1.346448
C	1.234525	-4.660976	-4.035758
H	-0.540668	-3.519881	-4.442421
C	1.793461	-4.952593	-1.709337
H	0.445045	-4.030250	-0.302108
C	2.078914	-5.172700	-3.053691
H	1.449971	-4.836021	-5.083564
H	2.452100	-5.342570	-0.941769
C	-0.858596	-0.889522	-3.344135
C	-1.501272	-0.156042	-4.346988
C	0.535486	-0.845121	-3.235841
C	-0.754161	0.578203	-5.257686
H	-2.583272	-0.171469	-4.407401
C	1.274229	-0.093770	-4.138910
H	1.029380	-1.367712	-2.425766
C	0.633980	0.607955	-5.157127
H	-1.255729	1.133964	-6.041389
H	2.352552	-0.047815	-4.040946
C	-3.534034	-5.130145	0.141125
H	2.957243	-5.741899	-3.336187
H	1.216022	1.188531	-5.863923
S	-4.449902	-3.676210	0.425835
C	-2.447086	-4.932427	-0.643500
H	-1.766624	-5.717104	-0.945730
H	-3.884600	-6.059908	0.563845

The optimized Cartesian coordinates for the metastable 1,8-dioxatetraene species **5-B** in the acetonitrile:

5a-B

C	-2.706574	0.528639	0.977253
C	-3.818271	-0.024224	1.599025
C	-4.613455	0.686203	2.482326
C	-4.236954	2.003640	2.725118
C	-3.117431	2.584547	2.108623
C	-2.340716	1.851014	1.224162
C	-2.148393	-0.508415	0.101579
C	-3.034276	-1.675580	0.336581
H	-5.477316	0.236982	2.955601
H	-4.828217	2.598295	3.411807
H	-2.864232	3.614330	2.328362
H	-1.475412	2.283493	0.735065
C	-1.927837	-3.660134	-0.858010
C	-2.909519	-2.979594	0.006739
C	-1.771268	-1.930017	-2.687966
C	-1.296620	-3.169527	-1.961622
O	-1.168896	-0.453023	-0.618340
O	-4.024076	-1.327800	1.235850
O	-2.957954	-1.691722	-2.772352
C	-0.246756	-3.959819	-2.647589
C	-0.312172	-4.174341	-4.029380
C	0.843358	-4.472058	-1.934795
C	0.680327	-4.899071	-4.679037
H	-1.148787	-3.780782	-4.598487
C	1.841006	-5.187374	-2.586600
H	0.915539	-4.286511	-0.867935
C	1.761030	-5.404430	-3.960168
H	0.611285	-5.066446	-5.747715
H	2.684154	-5.569744	-2.022813
C	-0.769328	-1.093703	-3.421010
C	-1.200581	-0.380152	-4.539460
C	0.562890	-1.001681	-3.011683
C	-0.305606	0.409676	-5.253624
H	-2.236753	-0.458022	-4.848365
C	1.452653	-0.200761	-3.715271
H	0.895037	-1.536399	-2.129345
C	1.021122	0.499923	-4.841423
H	-0.641910	0.952778	-6.129254
H	2.482892	-0.121355	-3.388091
C	-1.861882	-5.072485	-0.467559

C	-2.836876	-5.450860	0.366238
H	-1.173706	-5.770977	-0.920815
H	-3.052376	-6.455631	0.701159
H	2.539461	-5.961380	-4.468902
H	1.720111	1.116462	-5.395384
S	-3.887246	-4.150612	0.896918

5b-B:

C	-2.700136	0.519352	0.974576
C	-3.811914	-0.029722	1.599354
C	-4.597027	0.680059	2.491702
C	-4.209983	1.993425	2.740346
C	-3.090306	2.570727	2.120813
C	-2.323817	1.837778	1.227101
C	-2.155126	-0.515005	0.088571
C	-3.046548	-1.680108	0.324610
H	-5.461031	0.233684	2.967328
H	-4.792990	2.587658	3.434392
H	-2.828880	3.597345	2.345549
H	-1.458572	2.267420	0.735478
C	-1.945306	-3.663605	-0.871829
C	-2.928650	-2.983628	-0.008746
C	-1.786657	-1.934567	-2.699378
C	-1.308460	-3.168488	-1.970360
O	-1.182326	-0.460965	-0.640036
O	-4.028549	-1.330304	1.229396
O	-2.971967	-1.694340	-2.786663
C	-0.243507	-3.949448	-2.642149
C	-0.282676	-4.164739	-4.024215
C	0.840040	-4.452742	-1.914504
C	0.722323	-4.877904	-4.665427
H	-1.111941	-3.783622	-4.611510
C	1.857520	-5.159713	-2.542208
H	0.899077	-4.270267	-0.846710
C	1.785204	-5.365833	-3.914623
H	0.677355	-5.049202	-5.733558
H	2.696434	-5.537056	-1.971137
C	-0.785527	-1.097156	-3.434098
C	-1.215170	-0.392801	-4.557452
C	0.543158	-0.991321	-3.019777
C	-0.329711	0.401177	-5.277195
H	-2.248321	-0.475683	-4.874103
C	1.436007	-0.190401	-3.717393
H	0.879632	-1.514001	-2.132210

C	0.987309	0.491171	-4.844860
H	-0.659497	0.938780	-6.157177
H	2.463773	-0.096006	-3.390691
C	-1.876963	-5.074311	-0.479869
C	-2.853360	-5.452420	0.353135
H	-1.189058	-5.773931	-0.931989
H	-3.067789	-6.457519	0.687883
S	-3.906296	-4.154624	0.881604
Br	2.210097	1.575659	-5.815697
Br	3.172332	-6.332393	-4.783228

5c-B:

C	-2.760190	0.528898	0.995420
C	-3.852629	-0.045407	1.631329
C	-4.649480	0.648248	2.525570
C	-4.294851	1.972694	2.764176
C	-3.195199	2.575569	2.133342
C	-2.416347	1.858081	1.237886
C	-2.195682	-0.494939	0.110499
C	-3.055371	-1.683236	0.359890
H	-5.498193	0.182284	3.009797
H	-4.888094	2.555439	3.459266
H	-2.959048	3.609843	2.350701
H	-1.566197	2.307227	0.737524
C	-1.911313	-3.643530	-0.834182
C	-2.907777	-2.984449	0.031157
C	-1.794322	-1.914479	-2.665455
C	-1.292111	-3.136572	-1.936493
O	-1.231716	-0.419656	-0.627223
O	-4.038177	-1.353729	1.269570
O	-2.981036	-1.687489	-2.750472
C	-0.216201	-3.897463	-2.617083
C	-0.275739	-4.124055	-3.996611
C	0.892059	-4.361214	-1.899884
C	0.741965	-4.809750	-4.644906
H	-1.126646	-3.770900	-4.569653
C	1.916565	-5.040933	-2.542738
H	0.960262	-4.165109	-0.835419
C	1.837369	-5.260489	-3.914897
H	0.684098	-4.985201	-5.712381
H	2.776653	-5.385035	-1.980723
C	-0.803696	-1.065024	-3.409544
C	-1.239605	-0.400121	-4.552116
C	0.517341	-0.922156	-2.978540

C	-0.360298	0.395925	-5.278698
H	-2.267380	-0.515357	-4.874956
C	1.394323	-0.118288	-3.687657
H	0.850027	-1.416779	-2.073933
C	0.949947	0.532227	-4.839089
H	-0.696042	0.905419	-6.173200
H	2.416180	0.007559	-3.348417
C	-1.803341	-5.048998	-0.434665
C	-2.765845	-5.447155	0.405465
H	-1.099150	-5.733222	-0.885388
H	-2.950661	-6.455518	0.748076
S	-3.850874	-4.176010	0.931871
C	1.932592	1.359703	-5.614267
C	2.919529	-6.037846	-4.602444
F	1.345554	2.128367	-6.540060
F	2.640840	2.175470	-4.814978
F	2.830882	0.591616	-6.259472
F	3.048790	-5.699535	-5.893732
F	4.117631	-5.861392	-4.025092
F	2.676959	-7.363297	-4.577870

5d-B:

C	-2.521776	0.502332	0.999709
C	-3.673700	0.000150	1.579005
C	-4.430213	0.740791	2.471052
C	-3.966756	2.018251	2.756609
C	-2.796268	2.571125	2.188278
C	-2.071970	1.791017	1.294459
C	-2.014478	-0.533383	0.095920
C	-2.976380	-1.655882	0.277644
H	-5.331781	0.344914	2.921214
H	-4.543190	2.614722	3.455226
H	-1.168790	2.152964	0.818687
C	-1.955376	-3.661345	-0.951092
C	-2.923239	-2.952985	-0.092378
C	-1.646371	-1.888397	-2.715912
C	-1.264480	-3.169892	-2.017226
O	-1.024795	-0.514495	-0.611428
O	-3.957633	-1.276959	1.168716
O	-2.807994	-1.562591	-2.823329
C	-0.231897	-3.991990	-2.693663
C	-0.267222	-4.168745	-4.080875
C	0.814326	-4.565894	-1.962350
C	0.711982	-4.913202	-4.724640

H	-1.069477	-3.729526	-4.664488
C	1.800519	-5.303861	-2.599869
H	0.865453	-4.410248	-0.890258
C	1.745541	-5.472776	-3.980889
H	0.672287	-5.049173	-5.798515
H	2.613792	-5.733405	-2.026675
C	-0.570571	-1.098860	-3.405939
C	-0.921164	-0.364651	-4.536463
C	0.744946	-1.077932	-2.939665
C	0.038605	0.377440	-5.214681
H	-1.946442	-0.384005	-4.886134
C	1.704451	-0.328137	-3.601842
H	1.012388	-1.625370	-2.043854
C	1.345202	0.391240	-4.740561
H	-0.231138	0.941685	-6.099049
H	2.723171	-0.297589	-3.234105
C	-1.970015	-5.082831	-0.596502
C	-2.986655	-5.429914	0.201584
H	-1.306953	-5.805810	-1.049110
H	-3.260175	-6.430964	0.504100
S	-3.985683	-4.094486	0.738971
C	2.403997	1.145851	-5.489480
C	2.788302	-6.310560	-4.658041
F	2.922859	-6.009489	-5.957336
F	2.492484	-7.623988	-4.597767
F	3.997216	-6.169923	-4.091816
F	3.328343	1.669780	-4.669706
F	1.899422	2.155250	-6.212725
F	3.067335	0.350469	-6.351097
C	-2.379362	3.990993	2.576522
C	-2.137627	4.053774	4.093579
H	-1.835340	5.063933	4.382430
H	-3.036185	3.801156	4.660787
H	-1.344211	3.362588	4.389357
C	-3.498323	4.973996	2.195119
H	-3.207691	5.993166	2.463470
H	-3.689839	4.946070	1.119373
H	-4.433682	4.748816	2.712065
C	-1.094860	4.422958	1.864678
H	-0.251844	3.775443	2.119381
H	-1.213927	4.424480	0.778091
H	-0.835072	5.439010	2.169978

5e-B:

C	-2.616558	0.466213	1.096920
C	-3.716787	-0.095654	1.729176
C	-4.474821	0.608058	2.642072
C	-4.086613	1.919997	2.911008
C	-2.974422	2.503372	2.278617
C	-2.227806	1.772883	1.356721
C	-2.088433	-0.552042	0.179916
C	-2.976175	-1.723402	0.411522
H	-5.333511	0.166592	3.131675
H	-4.666925	2.487870	3.626019
H	-1.373043	2.222372	0.864689
C	-1.889197	-3.680266	-0.842766
C	-2.860208	-3.019434	0.049211
C	-1.753265	-1.912255	-2.634192
C	-1.270275	-3.161808	-1.940177
O	-1.131718	-0.481150	-0.566641
O	-3.941165	-1.394249	1.336970
O	-2.935378	-1.655764	-2.697420
C	-0.219366	-3.930629	-2.650125
C	-0.298016	-4.122730	-4.033841
C	0.885389	-4.436448	-1.956096
C	0.696999	-4.815618	-4.709367
H	-1.146224	-3.736274	-4.589023
C	1.887449	-5.123281	-2.625989
H	0.968891	-4.267571	-0.888056
C	1.789294	-5.308050	-4.002194
H	0.624213	-4.964022	-5.780000
H	2.745372	-5.499875	-2.081720
C	-0.753780	-1.067191	-3.371518
C	-1.192883	-0.359401	-4.488198
C	0.576123	-0.967149	-2.959906
C	-0.307225	0.435270	-5.205793
H	-2.228653	-0.440341	-4.795434
C	1.462307	-0.165003	-3.662276
H	0.912027	-1.493704	-2.074722
C	1.014868	0.527959	-4.785689
H	-0.645650	0.979884	-6.078865
H	2.491573	-0.073354	-3.336729
C	-1.809400	-5.096974	-0.477881
C	-2.771295	-5.492915	0.364115
H	-1.126350	-5.786196	-0.952885
H	-2.975556	-6.504751	0.684782
S	-3.820255	-4.210144	0.933076
O	-2.558348	3.775609	2.507794

C	-3.288541	4.560132	3.437425
H	-2.792330	5.526309	3.467579
H	-4.323386	4.692245	3.112128
H	-3.268546	4.109322	4.432656
C	1.992305	1.342048	-5.581636
C	2.847698	-6.092144	-4.718414
F	2.959433	-5.740048	-6.007525
F	2.586776	-7.414306	-4.705098
F	4.058177	-5.939778	-4.160008
F	2.944485	1.888537	-4.810545
F	1.400220	2.343470	-6.247915
F	2.630656	0.593764	-6.502341

5f-B:

C	-2.762519	0.527079	0.993208
C	-3.856447	-0.045507	1.624595
C	-4.655600	0.652722	2.515608
C	-4.306094	1.975121	2.757043
C	-3.203381	2.544020	2.117177
C	-2.408960	1.854546	1.227296
C	-2.195629	-0.499162	0.108854
C	-3.056854	-1.683148	0.356987
H	-5.507436	0.192580	2.999102
H	-4.882710	2.583506	3.443253
H	-1.561490	2.323189	0.741813
C	-1.907360	-3.644552	-0.830665
C	-2.906712	-2.985655	0.031186
C	-1.788023	-1.915978	-2.662741
C	-1.285740	-3.137733	-1.931800
O	-1.229705	-0.420064	-0.624910
O	-4.042976	-1.353080	1.263373
O	-2.975085	-1.691886	-2.748493
C	-0.208798	-3.899171	-2.609700
C	-0.264826	-4.125392	-3.989390
C	0.897021	-4.363510	-1.889101
C	0.754195	-4.811950	-4.634673
H	-1.113801	-3.771574	-4.564879
C	1.923043	-5.043448	-2.529200
H	0.962333	-4.167401	-0.824467
C	1.847332	-5.263077	-3.901532
H	0.699242	-4.987431	-5.702278
H	2.781485	-5.387812	-1.964848
C	-0.798523	-1.064592	-3.405508
C	-1.239426	-0.390172	-4.542131

C	0.523483	-0.926256	-2.980157
C	-0.362651	0.408905	-5.265390
H	-2.269202	-0.500647	-4.860081
C	1.400612	-0.119444	-3.688723
H	0.860136	-1.426199	-2.079935
C	0.951912	0.539746	-4.831579
H	-0.702034	0.927850	-6.153651
H	2.423353	0.001817	-3.352722
C	-1.801478	-5.050503	-0.432092
C	-2.766074	-5.448245	0.405531
H	-1.097097	-5.734941	-0.882120
H	-2.953412	-6.456360	0.747375
S	-3.850238	-4.175320	0.930407
C	1.919243	1.358965	-5.634691
C	2.931358	-6.040882	-4.585885
F	3.062732	-5.704561	-5.877398
F	2.689508	-7.366340	-4.559372
F	4.128154	-5.862538	-4.006493
F	2.865856	1.922514	-4.869509
F	1.314177	2.348167	-6.307821
F	2.564471	0.611132	-6.550884
F	-2.912643	3.830918	2.390286

5g-B:

C	-2.639617	0.524602	1.023327
C	-3.746572	-0.029014	1.651361
C	-4.529349	0.675270	2.554863
C	-4.145873	1.982144	2.809489
C	-3.027083	2.555451	2.180129
C	-2.260500	1.838917	1.276624
C	-2.098551	-0.504725	0.125225
C	-2.987974	-1.667863	0.361300
H	-5.389152	0.226186	3.034281
H	-4.721498	2.574807	3.511803
H	-1.399621	2.274980	0.784367
C	-1.895042	-3.646565	-0.847027
C	-2.875585	-2.971041	0.023917
C	-1.738168	-1.901344	-2.660611
C	-1.264090	-3.143806	-1.944439
O	-1.132426	-0.440032	-0.609180
O	-3.964133	-1.320055	1.277514
O	-2.919687	-1.647971	-2.738351
C	-0.209133	-3.925035	-2.633979

C	-0.274875	-4.134290	-4.015772
C	0.886103	-4.425545	-1.921341
C	0.724120	-4.840323	-4.671465
H	-1.115681	-3.751904	-4.584841
C	1.892441	-5.124427	-2.571978
H	0.959125	-4.242905	-0.854822
C	1.807152	-5.327154	-3.946444
H	0.661753	-5.002851	-5.740657
H	2.743375	-5.496939	-2.014119
C	-0.730958	-1.067256	-3.398552
C	-1.160229	-0.370043	-4.525744
C	0.596374	-0.967331	-2.978631
C	-0.266898	0.413824	-5.245574
H	-2.194082	-0.450972	-4.839310
C	1.490053	-0.175864	-3.683537
H	0.924854	-1.485087	-2.085493
C	1.052599	0.506362	-4.817351
H	-0.597424	0.950207	-6.126715
H	2.517367	-0.084206	-3.351972
C	-1.825359	-5.059122	-0.464152
C	-2.798494	-5.440285	0.370972
H	-1.140046	-5.756690	-0.923315
H	-3.012762	-6.446523	0.702277
S	-3.847442	-4.144222	0.912144
C	2.038285	1.308659	-5.615296
C	2.870173	-6.124816	-4.640986
F	2.993211	-5.793965	-5.934516
F	2.606354	-7.445864	-4.607815
F	4.075994	-5.965186	-4.074790
F	2.988412	1.857986	-4.843848
F	1.454394	2.306308	-6.294182
F	2.678209	0.548735	-6.525166
C	-2.697504	3.982098	2.498708
F	-1.541051	4.376647	1.953012
F	-3.647749	4.826927	2.056112
F	-2.601463	4.190161	3.823832

5h-B:

C	-2.758239	0.521194	0.997680
C	-3.853847	-0.054989	1.626196
C	-4.656774	0.635441	2.516693
C	-4.304804	1.960003	2.759559
C	-3.202190	2.565156	2.136451

C	-2.417018	1.850227	1.244508
C	-2.186682	-0.499785	0.114427
C	-3.050345	-1.690591	0.356459
H	-5.507859	0.167643	2.994845
H	-4.902920	2.540897	3.451975
H	-2.968572	3.599299	2.356942
H	-1.564402	2.301035	0.749988
C	-1.908424	-3.649841	-0.842744
C	-2.904784	-2.988300	0.020901
C	-1.787534	-1.918146	-2.666663
C	-1.283967	-3.142454	-1.941481
O	-1.218734	-0.426328	-0.615969
O	-4.037330	-1.363847	1.259768
O	-2.974431	-1.690354	-2.744799
C	-0.203492	-3.900932	-2.616538
C	-0.256344	-4.127634	-3.996294
C	0.902045	-4.362003	-1.893456
C	0.766062	-4.811153	-4.639228
H	-1.105202	-3.776228	-4.573380
C	1.931118	-5.039639	-2.531309
H	0.965812	-4.164374	-0.828940
C	1.858842	-5.259439	-3.903663
H	0.713943	-4.986783	-5.706948
H	2.789316	-5.381449	-1.965074
C	-0.799812	-1.066424	-3.410802
C	-1.243446	-0.390899	-4.545795
C	0.522606	-0.927151	-2.987159
C	-0.368717	0.410063	-5.269278
H	-2.273649	-0.501978	-4.862148
C	1.397674	-0.118237	-3.696007
H	0.861171	-1.427663	-2.087985
C	0.946404	0.541863	-4.837240
H	-0.710026	0.929872	-6.156299
H	2.420708	0.003960	-3.361284
C	-1.792671	-5.052692	-0.443524
C	-2.760784	-5.438659	0.395749
H	-1.087998	-5.740855	-0.887063
S	-3.864481	-4.175428	0.917390
C	1.911125	1.363570	-5.641045
C	2.946456	-6.034185	-4.585976
F	1.303784	2.355570	-6.308043
F	2.860998	1.923784	-4.877556
F	2.552152	0.618837	-6.562640
F	3.081143	-5.695209	-5.876433

F	4.141038	-5.854676	-4.002530
F	2.706717	-7.360003	-4.562564
Br	-3.065454	-7.183862	0.992299

5i-B:

C	-2.761604	0.299919	1.007668
C	-3.932577	-0.229407	1.530938
C	-4.781837	0.497644	2.350258
C	-4.396259	1.804331	2.630498
C	-3.215858	2.361490	2.111631
C	-2.386789	1.613200	1.290117
C	-2.163286	-0.743018	0.169560
C	-3.087034	-1.901526	0.331103
H	-5.692560	0.067792	2.747780
H	-5.028349	2.410693	3.269025
H	-2.958129	3.384273	2.357358
H	-1.474300	2.026584	0.875864
C	-1.868840	-3.750599	-0.862045
C	-2.945930	-3.207235	-0.008245
C	-1.793902	-2.002905	-2.663646
C	-1.272404	-3.240314	-1.961965
O	-1.136861	-0.687641	-0.482867
O	-4.138280	-1.522633	1.146735
O	-2.987104	-1.807612	-2.753266
C	-0.208340	-3.989632	-2.674231
C	-0.315917	-4.218483	-4.050566
C	0.919324	-4.459099	-1.993683
C	0.674664	-4.920298	-4.727166
H	-1.182896	-3.853336	-4.592710
C	1.914471	-5.153401	-2.673315
H	1.029339	-4.253641	-0.933722
C	1.792941	-5.387936	-4.040215
H	0.575163	-5.099603	-5.791465
H	2.788207	-5.503711	-2.135999
C	-0.815966	-1.112112	-3.363353
C	-1.266656	-0.376011	-4.459844
C	0.512452	-0.994565	-2.948109
C	-0.394492	0.462303	-5.145857
H	-2.299504	-0.474788	-4.773708
C	1.379157	-0.145719	-3.624059
H	0.858087	-1.545511	-2.081518
C	0.928555	0.578045	-4.727670
H	-0.745331	1.023231	-6.004344
H	2.406143	-0.046642	-3.292126

C	-3.094077	-5.475314	0.473953
H	-3.431335	-6.416691	0.887971
H	2.569030	-5.928220	-4.570048
H	1.609750	1.232643	-5.259700
C	-3.731180	-4.297248	0.588814
S	-1.581833	-5.455197	-0.401663
C	-5.041113	-4.146699	1.308595
H	-4.922554	-3.613409	2.252130
H	-5.759322	-3.587419	0.707620
H	-5.456584	-5.132900	1.517086

5j-B:

C	-2.733117	0.537950	1.000510
C	-3.845621	-0.020180	1.616083
C	-4.651678	0.687748	2.490764
C	-4.284819	2.008438	2.731635
C	-3.164912	2.594815	2.121179
C	-2.377349	1.863706	1.244643
C	-2.163940	-0.496280	0.131244
C	-3.042139	-1.677008	0.369188
H	-5.516177	0.234864	2.959213
H	-4.884735	2.601592	3.412048
H	-1.511595	2.299902	0.759807
C	-1.906832	-3.650260	-0.803215
C	-2.906855	-2.977646	0.046750
C	-1.805441	-1.924950	-2.641442
C	-1.298145	-3.146574	-1.912529
O	-1.188365	-0.435276	-0.591334
O	-4.041343	-1.327066	1.255301
O	-2.992371	-1.698177	-2.721382
C	-0.222356	-3.900145	-2.604007
C	-0.307159	-4.144960	-3.978823
C	0.909573	-4.332879	-1.905360
C	0.709307	-4.819600	-4.640571
H	-1.176455	-3.813901	-4.537320
C	1.932810	-5.001937	-2.561640
H	0.996534	-4.121871	-0.845067
C	1.828335	-5.240649	-3.928781
H	0.632244	-5.009212	-5.704461
H	2.810918	-5.322877	-2.014092
C	-0.819292	-1.076434	-3.393152
C	-1.262726	-0.417446	-4.536377
C	0.504255	-0.929826	-2.970944
C	-0.388789	0.375937	-5.272247

H	-2.292213	-0.535473	-4.852654
C	1.376014	-0.128709	-3.689562
H	0.842873	-1.418867	-2.065667
C	0.924008	0.515610	-4.841469
H	-0.730622	0.880597	-6.167192
H	2.399766	-0.000138	-3.357162
C	-1.763702	-5.056949	-0.404906
C	-2.703310	-5.534534	0.417164
H	-1.020996	-5.700645	-0.855810
H	-2.815795	-6.564407	0.725485
C	1.901049	1.339712	-5.627254
C	2.908373	-6.007104	-4.631812
F	3.020465	-5.661357	-5.922937
F	2.674690	-7.334228	-4.611807
F	4.111586	-5.825437	-4.067375
F	2.616926	2.157002	-4.836401
F	1.306992	2.106311	-6.550305
F	2.792946	0.568732	-6.277856
H	-2.920103	3.626908	2.339289
Se	-3.959896	-4.248127	1.008508

5k-B:

C	-2.759026	-0.339851	1.147565
C	-3.833748	-1.065814	1.639285
C	-4.737330	-0.543780	2.549248
C	-4.510283	0.767342	2.956457
C	-3.430148	1.522306	2.472364
C	-2.543021	0.974996	1.557572
C	-2.060508	-1.208798	0.195307
C	-2.828836	-2.492179	0.257880
H	-5.570660	-1.126602	2.920478
H	-5.190652	1.218205	3.669610
H	-3.294916	2.539475	2.818465
H	-1.705652	1.542804	1.168481
C	-1.409998	-4.055120	-1.109780
C	-2.547635	-3.721417	-0.226290
C	-1.614533	-2.195755	-2.768352
C	-0.906815	-3.393403	-2.172582
O	-1.076417	-0.962855	-0.472037
O	-3.889802	-2.333191	1.124316
O	-2.826090	-2.152904	-2.806550
C	0.251655	-3.923390	-2.932567
C	0.165925	-4.073303	-4.321263
C	1.443414	-4.263582	-2.285616

C	1.243563	-4.571164	-5.043878
H	-0.751436	-3.806483	-4.837244
C	2.524435	-4.754464	-3.010365
H	1.533349	-4.114586	-1.214221
C	2.426015	-4.911640	-4.390021
H	1.161452	-4.691267	-6.117970
H	3.445591	-5.006357	-2.497626
C	-0.791941	-1.129736	-3.421670
C	-1.372590	-0.396255	-4.457297
C	0.515497	-0.846456	-3.019801
C	-0.648701	0.603042	-5.098410
H	-2.388253	-0.623643	-4.760349
C	1.232337	0.162984	-3.649522
H	0.959842	-1.396982	-2.199099
C	0.653963	0.883202	-4.694097
H	-1.098743	1.161270	-5.911184
H	2.242166	0.389552	-3.327559
H	3.268658	-5.293007	-4.955224
H	1.219529	1.663309	-5.191214
S	-0.838616	-5.704064	-0.710222
C	-2.365037	-6.069655	0.096236
C	-3.198259	-4.952231	0.248977
C	-2.740065	-7.329209	0.543361
C	-4.454346	-5.118295	0.839817
C	-3.992317	-7.475734	1.133122
H	-2.079637	-8.180117	0.424311
C	-4.845960	-6.381221	1.270474
H	-5.122494	-4.276367	0.951115
H	-4.307326	-8.453754	1.478115
H	-5.823954	-6.513260	1.717476

5l-B:

C	-2.938092	-0.387583	1.074599
C	-3.925570	-1.166084	1.659945
C	-4.789795	-0.680974	2.625939
C	-4.615333	0.650585	2.991960
C	-3.623528	1.458567	2.414425
C	-2.773779	0.946199	1.445142
C	-2.257959	-1.233377	0.088392
C	-2.950152	-2.553513	0.219639
H	-5.555098	-1.305205	3.069304
H	-5.267446	1.074722	3.746649
H	-3.526552	2.489547	2.731267

H	-2.004392	1.555240	0.984668
C	-1.597229	-4.173545	-1.222455
C	-2.649650	-3.785945	-0.247926
C	-1.675975	-2.277835	-2.844951
C	-1.046916	-3.503348	-2.273853
O	-1.323709	-0.951273	-0.634113
O	-3.938339	-2.446564	1.171879
O	-2.878972	-2.110694	-2.856308
C	0.070449	-4.110618	-3.037029
C	0.012448	-4.193304	-4.433456
C	1.215712	-4.581745	-2.382018
C	1.067554	-4.729118	-5.158943
H	-0.867227	-3.838123	-4.959700
C	2.273833	-5.119531	-3.100274
H	1.285428	-4.502839	-1.302458
C	2.197286	-5.187251	-4.488723
H	1.009722	-4.786103	-6.239268
H	3.159739	-5.468377	-2.582710
C	-0.777687	-1.276630	-3.518007
C	-1.284591	-0.545111	-4.588687
C	0.528237	-1.054793	-3.076677
C	-0.487838	0.392082	-5.237158
H	-2.302283	-0.719906	-4.917199
C	1.322537	-0.109296	-3.705729
H	0.912682	-1.605898	-2.226502
C	0.810366	0.604153	-4.789055
H	-0.877216	0.952953	-6.077796
H	2.331544	0.076490	-3.356176
C	-2.245198	-6.042846	-0.078781
C	-3.129289	-5.037555	0.343715
C	-2.369784	-7.359801	0.340148
C	-4.168285	-5.352428	1.219794
C	-3.420826	-7.659164	1.203260
H	-1.678365	-8.123883	0.005712
C	-4.309674	-6.672289	1.638918
H	-4.860036	-4.592373	1.555089
H	-3.549713	-8.680659	1.542523
H	-5.118589	-6.937224	2.308892
C	1.705625	1.578592	-5.495808
C	3.322403	-5.809475	-5.258696
F	2.433938	2.309009	-4.635290
F	2.587454	0.953008	-6.299696
F	1.026584	2.438747	-6.266187
F	4.515779	-5.581469	-4.688064

F	3.193440	-7.148747	-5.343870
F	3.393267	-5.354395	-6.518226
N	-1.286289	-5.492623	-0.923046
H	-0.760308	-6.062533	-1.570993

5m-B:

C	-2.718529	-0.385285	1.084021
C	-3.728662	-1.115531	1.689179
C	-4.491294	-0.622219	2.733086
C	-4.186175	0.668147	3.157312
C	-3.168409	1.428019	2.560144
C	-2.423484	0.908008	1.511759
C	-2.174484	-1.219909	0.008025
C	-2.958537	-2.495163	0.115800
H	-5.277143	-1.209275	3.191017
H	-4.754258	1.097672	3.974315
H	-2.968529	2.428118	2.924230
H	-1.636672	1.480652	1.034401
C	-1.828816	-4.183225	-1.449709
C	-2.803227	-3.729854	-0.420719
C	-1.768438	-2.227905	-2.968249
C	-1.154329	-3.454732	-2.407973
O	-1.273107	-0.957592	-0.759899
O	-3.873511	-2.359953	1.133794
O	-2.972151	-2.035664	-2.952733
C	0.132022	-3.929218	-2.967299
C	0.385067	-3.929749	-4.346372
C	1.149004	-4.350358	-2.102175
C	1.613445	-4.334346	-4.844494
H	-0.393652	-3.626141	-5.037357
C	2.383005	-4.756313	-2.592365
H	0.971494	-4.348017	-1.031738
C	2.611819	-4.747339	-3.964261
H	1.790388	-4.339530	-5.913786
H	3.160124	-5.076006	-1.908393
C	-0.888355	-1.225865	-3.671121
C	-1.398589	-0.593213	-4.802038
C	0.389471	-0.900154	-3.210902
C	-0.634303	0.341930	-5.491649
H	-2.394744	-0.844290	-5.146742
C	1.149919	0.045560	-3.880445
H	0.777870	-1.372346	-2.317115
C	0.635749	0.655969	-5.024124

H	-1.028259	0.822976	-6.378490
H	2.135602	0.310699	-3.515815
C	-2.611003	-6.012227	-0.326701
C	-3.360840	-4.941577	0.180685
C	-2.811528	-7.317892	0.101781
C	-4.360213	-5.180371	1.123722
C	-3.813646	-7.539022	1.044259
H	-2.210940	-8.139642	-0.267341
C	-4.584793	-6.488726	1.544078
H	-4.959397	-4.370890	1.514583
H	-3.993243	-8.549188	1.393889
H	-5.362268	-6.691024	2.270759
C	1.497629	1.627793	-5.773587
C	3.954190	-5.132684	-4.504230
F	2.193299	2.427224	-4.948246
F	2.406980	0.998777	-6.544040
F	0.790497	2.422777	-6.588388
F	4.749354	-4.060063	-4.695601
F	4.621405	-5.956179	-3.681871
F	3.865850	-5.749988	-5.693863
N	-1.703982	-5.549763	-1.285034
C	-1.147706	-6.461723	-2.275642
H	-1.250549	-6.028439	-3.268868
H	-0.095273	-6.676376	-2.087049
H	-1.714956	-7.389450	-2.246406

5n-B:

C	-2.024756	0.409606	0.643175
C	-3.401742	0.332604	0.797303
C	-4.169729	1.407736	1.213213
C	-3.482901	2.588893	1.477802
C	-2.090570	2.690330	1.329905
C	-1.346123	1.597292	0.910565
C	-1.566520	-0.906589	0.177637
C	-2.835875	-1.688255	0.061796
H	-5.243555	1.328390	1.326443
H	-4.042569	3.456477	1.807932
H	-1.599882	3.631215	1.546484
H	-0.270354	1.655276	0.788901
C	-2.049654	-3.838865	-0.823943
C	-3.043503	-3.024777	-0.122990
C	-2.034200	-2.221340	-2.738267
C	-1.414357	-3.354061	-1.937125
O	-0.419604	-1.283049	0.023105

O	-3.890773	-0.906597	0.490834
O	-3.201070	-2.313078	-3.068117
C	-0.258175	-4.022515	-2.561014
C	-0.192410	-4.176667	-3.951969
C	0.815352	-4.467146	-1.777128
C	0.909468	-4.783966	-4.541983
H	-1.012894	-3.832628	-4.574119
C	1.919645	-5.065602	-2.369786
H	0.788146	-4.312046	-0.703607
C	1.967890	-5.228416	-3.753058
H	0.943317	-4.907818	-5.618156
H	2.747444	-5.397238	-1.753698
C	-1.195522	-1.074973	-3.204043
C	-1.796784	-0.122460	-4.034254
C	0.137985	-0.909169	-2.818765
C	-1.076047	0.978818	-4.474982
H	-2.831324	-0.258182	-4.326182
C	0.858408	0.194931	-3.261199
H	0.610028	-1.627861	-2.162388
C	0.254282	1.137740	-4.088840
H	-1.547171	1.712517	-5.118665
H	1.891422	0.319778	-2.958192
C	-1.954191	-5.230742	-0.416258
C	-2.968265	-5.796055	0.278433
H	-1.142034	-5.841265	-0.788686
C	-4.188175	-3.692697	0.449475
C	-4.130782	-5.028907	0.660358
H	-2.942865	-6.855681	0.503895
H	-5.024982	-3.101379	0.799223
H	-4.952532	-5.534388	1.154473
H	2.830879	-5.694099	-4.214904
H	0.819095	1.996894	-4.432971

The optimized Cartesian coordinates for the transition states between the benzofuranone-based spiropyrans **5** and the 1,8-dioxatatraene species **5-B** in the acetonitrile:

TS-5a:

C	-4.077013	0.316506	0.523383
C	-5.193304	-0.039686	-0.216323
C	-6.317866	0.750649	-0.317408
C	-6.278017	1.959323	0.379038
C	-5.163706	2.345160	1.133418
C	-4.046366	1.522367	1.215487
C	-3.111092	-0.783656	0.390914
C	-3.797036	-1.721639	-0.612541
H	-7.177874	0.448142	-0.900710
H	-7.138117	2.616841	0.332771
H	-3.175358	1.803617	1.795660
C	-2.218818	-3.565094	-1.103778
C	-3.508582	-3.059461	-0.821122
C	-1.462052	-1.542332	-2.232549
C	-1.164477	-2.806039	-1.670620
O	-2.071192	-0.981491	0.956218
O	-5.047230	-1.276562	-0.834694
O	-2.445090	-0.810154	-1.913090
C	0.076522	-3.551236	-2.038700
C	0.277918	-4.049142	-3.329327
C	1.042860	-3.801099	-1.062696
C	1.432151	-4.759146	-3.642781
H	-0.473431	-3.869177	-4.091971
C	2.198559	-4.514693	-1.372537
H	0.889023	-3.424615	-0.056250
C	2.397904	-4.990997	-2.665073
H	1.576866	-5.135339	-4.649469
H	2.942881	-4.694961	-0.604932
C	-0.642215	-1.023673	-3.379570
C	-1.286247	-0.673771	-4.567205
C	0.734362	-0.831683	-3.257766
C	-0.553884	-0.171128	-5.637162
H	-2.359510	-0.805660	-4.650846
C	1.461527	-0.308524	-4.323002
H	1.237625	-1.088484	-2.332105
C	0.822157	0.012840	-5.517485
H	-1.058087	0.081864	-6.563005
H	2.529511	-0.153920	-4.218582
C	-3.495271	-5.514311	-0.932013

C	-2.247939	-5.010187	-1.082564
H	-1.371796	-5.625776	-1.233003
S	-4.730497	-4.315013	-0.779174
H	-3.779803	-6.556890	-0.915262
H	-5.177443	3.292775	1.657113
H	1.392120	0.410949	-6.349266
H	3.297938	-5.543897	-2.909402

TS-5f:

C	-3.997181	0.239777	0.673279
C	-5.151609	-0.013360	-0.046551
C	-6.238067	0.836295	-0.056214
C	-6.121583	1.992667	0.710923
C	-4.959000	2.244468	1.434676
C	-3.873225	1.389667	1.443561
C	-3.091966	-0.898062	0.436665
C	-3.857850	-1.728531	-0.603674
H	-7.131543	0.618067	-0.626083
H	-6.931790	2.710183	0.755268
H	-2.982233	1.611136	2.018250
C	-2.376969	-3.592977	-1.286583
C	-3.633846	-3.056133	-0.925814
C	-1.554907	-1.517801	-2.272157
C	-1.305321	-2.833961	-1.825000
O	-2.050913	-1.185469	0.955302
O	-5.088007	-1.212188	-0.749806
O	-2.493550	-0.767565	-1.875767
C	-0.114260	-3.600109	-2.296100
C	0.035848	-3.966371	-3.637512
C	0.850205	-4.006163	-1.372489
C	1.139079	-4.697874	-4.053186
H	-0.717882	-3.672614	-4.360114
C	1.958431	-4.741795	-1.778092
H	0.734585	-3.736702	-0.328264
C	2.098641	-5.081728	-3.118926
H	1.246668	-4.977040	-5.094987
H	2.703636	-5.047903	-1.053628
C	-0.725997	-0.941412	-3.384880
C	-1.367897	-0.474798	-4.532881
C	0.656676	-0.812102	-3.260432
C	-0.629235	0.080280	-5.567499
H	-2.445522	-0.555155	-4.615106
C	1.398904	-0.240322	-4.286802

H	1.157495	-1.152869	-2.361591
C	0.753206	0.195519	-5.438725
H	-1.126601	0.429271	-6.464967
H	2.471977	-0.132498	-4.184972
C	3.314119	-5.826605	-3.579736
C	1.549340	0.754314	-6.578544
F	2.729264	1.254963	-6.184553
F	0.897540	1.738256	-7.219366
F	1.823447	-0.183254	-7.507918
F	3.043349	-6.663890	-4.594332
F	4.277013	-4.994166	-4.025346
F	3.869193	-6.559006	-2.602651
C	-3.734799	-5.490984	-1.226594
C	-2.470252	-5.030351	-1.380390
H	-1.629593	-5.670885	-1.608932
S	-4.908016	-4.257633	-0.938980
H	-4.064746	-6.518738	-1.281160
F	-4.898598	3.375349	2.159195

TS-5i:

C	-3.723722	0.435867	0.750131
C	-4.912286	0.032424	0.164117
C	-6.039282	0.823943	0.114383
C	-5.923381	2.086416	0.698326
C	-4.735303	2.520549	1.297348
C	-3.617502	1.694192	1.331653
C	-2.782113	-0.684498	0.608746
C	-3.575231	-1.696765	-0.230640
H	-6.956372	0.483638	-0.348846
H	-6.781721	2.747774	0.686463
H	-4.691509	3.508580	1.738195
H	-2.690012	2.013085	1.792620
C	-1.993278	-3.464081	-0.787092
C	-3.290067	-3.049535	-0.386975
C	-1.445786	-1.518296	-2.135731
C	-1.044141	-2.738250	-1.531623
O	-1.689855	-0.847933	1.079604
O	-4.835080	-1.253413	-0.359912
O	-2.418952	-0.808506	-1.759850
C	0.168655	-3.481639	-1.982697
C	0.263053	-4.018498	-3.270470
C	1.215153	-3.697154	-1.083441
C	1.391657	-4.731937	-3.658097

H	-0.551989	-3.867370	-3.971262
C	2.345745	-4.413804	-1.468646
H	1.143359	-3.290774	-0.079331
C	2.438297	-4.927862	-2.758588
H	1.453762	-5.138476	-4.661369
H	3.154073	-4.566034	-0.762273
C	-0.752872	-1.041693	-3.379495
C	-1.516017	-0.763117	-4.514199
C	0.623693	-0.814474	-3.398511
C	-0.901501	-0.297131	-5.671259
H	-2.588475	-0.922240	-4.488023
C	1.232414	-0.326196	-4.550803
H	1.219006	-1.015462	-2.514584
C	0.474294	-0.077147	-5.691898
H	-1.497267	-0.100322	-6.555377
H	2.300906	-0.142977	-4.556443
C	-3.549563	-5.335135	-0.182869
C	-4.199771	-4.153005	-0.129016
S	-1.872269	-5.203420	-0.647369
H	0.952175	0.293103	-6.591751
H	3.318996	-5.482965	-3.061373
C	-5.634854	-3.996794	0.279213
H	-5.727349	-3.345089	1.151056
H	-6.228535	-3.552795	-0.521539
H	-6.061264	-4.968425	0.528338
H	-3.949518	-6.307799	0.066541

TS-5j:

C	-3.930471	0.237986	0.715740
C	-5.094172	0.044452	-0.011079
C	-6.151856	0.927259	0.002963
C	-5.991143	2.057554	0.805796
C	-4.827087	2.279416	1.550633
C	-3.779648	1.366116	1.514948
C	-3.064518	-0.918781	0.446222
C	-3.857855	-1.699782	-0.615860
H	-7.050704	0.750981	-0.573574
H	-6.794539	2.783317	0.852070
H	-2.871853	1.520707	2.086195
C	-2.442387	-3.592722	-1.332471
C	-3.681897	-3.025412	-0.967873
C	-1.576716	-1.517222	-2.287133
C	-1.354472	-2.844421	-1.854671

O	-2.028869	-1.255246	0.949185
O	-5.070599	-1.136439	-0.746780
O	-2.500028	-0.752757	-1.883851
C	-0.162763	-3.613781	-2.319782
C	-0.004676	-3.977866	-3.660794
C	0.797715	-4.018758	-1.391590
C	1.102239	-4.706610	-4.071563
H	-0.754807	-3.683723	-4.387002
C	1.909644	-4.751608	-1.792143
H	0.676110	-3.750154	-0.347797
C	2.057714	-5.089472	-3.132665
H	1.216239	-4.983878	-5.113193
H	2.651787	-5.056819	-1.064164
C	-0.736430	-0.945815	-3.394021
C	-1.368245	-0.468853	-4.543322
C	0.646898	-0.830419	-3.262663
C	-0.619384	0.082889	-5.572471
H	-2.446189	-0.538671	-4.631203
C	1.399365	-0.262054	-4.283391
H	1.140271	-1.179625	-2.362962
C	0.763393	0.184465	-5.436705
H	-1.109199	0.439994	-6.470865
H	2.472968	-0.165053	-4.176139
C	-3.770553	-5.551311	-1.316205
C	-2.528641	-5.034647	-1.443814
H	-1.667034	-5.650757	-1.666608
H	-4.041429	-6.594656	-1.395952
H	-4.746671	3.171138	2.159551
C	3.277499	-5.830580	-3.588159
C	1.571276	0.739406	-6.570096
F	4.239547	-4.995138	-4.029996
F	3.013735	-6.668994	-4.603690
F	3.830888	-6.560942	-2.608603
F	0.927289	1.722517	-7.219827
F	2.747947	1.239553	-6.165487
F	1.853823	-0.200839	-7.494266
Se	-5.102013	-4.277010	-1.008521

TS-5l:

C	-3.573845	0.624433	0.857163
C	-4.810026	0.201043	0.396328
C	-5.936139	0.994019	0.408231
C	-5.768360	2.282149	0.919885

C	-4.532401	2.737105	1.392522
C	-3.416544	1.907399	1.368691
C	-2.653671	-0.510929	0.694023
C	-3.516656	-1.550479	-0.041121
H	-6.890500	0.636734	0.043584
H	-6.623701	2.946692	0.951300
H	-4.449012	3.744333	1.781083
H	-2.452528	2.242694	1.732854
C	-2.030128	-3.400738	-0.661136
C	-3.262084	-2.908769	-0.160638
C	-1.519943	-1.500475	-2.067253
C	-1.108717	-2.716738	-1.499840
O	-1.532649	-0.675260	1.089187
O	-4.781296	-1.111527	-0.071615
O	-2.482195	-0.772413	-1.663864
C	0.025387	-3.519473	-2.036449
C	0.054739	-3.965769	-3.362719
C	1.065346	-3.892050	-1.179069
C	1.113121	-4.731396	-3.831704
H	-0.758087	-3.707718	-4.032429
C	2.125703	-4.665016	-1.637230
H	1.046939	-3.561734	-0.145936
C	2.147091	-5.077000	-2.965407
H	1.125412	-5.068876	-4.861395
H	2.928254	-4.941675	-0.963780
C	-0.834917	-0.984940	-3.298999
C	-1.602320	-0.648152	-4.414559
C	0.544688	-0.780331	-3.317444
C	-0.991887	-0.149020	-5.556455
H	-2.676907	-0.785691	-4.387070
C	1.158264	-0.262499	-4.450999
H	1.141668	-1.020452	-2.444949
C	0.387535	0.043679	-5.568070
H	-1.586777	0.098316	-6.427781
H	2.228532	-0.094340	-4.459952
C	3.316727	-5.858394	-3.481429
C	1.051940	0.542583	-6.815133
F	2.189196	1.206503	-6.558718
F	0.262177	1.369962	-7.517576
F	1.380201	-0.465459	-7.648455
F	2.979028	-6.678170	-4.488957
F	4.289297	-5.054303	-3.957052
F	3.885126	-6.615846	-2.530562
C	-3.271957	-5.182883	-0.012477

C	-3.708436	-6.469589	0.281981
C	-4.088573	-4.049996	0.175649
C	-5.003954	-6.608164	0.766696
H	-3.065842	-7.329281	0.132431
C	-5.381778	-4.207945	0.678544
C	-5.829450	-5.492131	0.963396
H	-5.381248	-7.598000	0.995607
H	-6.024621	-3.349362	0.832589
H	-6.834779	-5.634900	1.342179
N	-2.042552	-4.756500	-0.504439
H	-1.331500	-5.370258	-0.876979

TS-5m:

C	-3.179226	0.546170	0.737878
C	-4.505884	0.187998	0.565772
C	-5.556588	1.061810	0.731897
C	-5.211274	2.366555	1.091316
C	-3.880617	2.757088	1.273587
C	-2.844451	1.844749	1.101768
C	-2.382260	-0.668034	0.503650
C	-3.439336	-1.685433	0.033354
H	-6.584676	0.753196	0.593265
H	-6.000699	3.095025	1.233906
H	-3.659309	3.779548	1.552993
H	-1.808469	2.129896	1.242176
C	-2.196654	-3.640735	-0.763647
C	-3.303506	-3.055143	-0.093823
C	-1.762065	-1.751696	-2.232705
C	-1.313560	-2.954618	-1.660303
O	-1.222788	-0.894775	0.712509
O	-4.650585	-1.154269	0.212634
O	-2.737620	-1.031264	-1.847071
C	-0.012902	-3.565747	-2.041618
C	0.328539	-3.900043	-3.359416
C	0.911881	-3.831823	-1.027306
C	1.556222	-4.470905	-3.652758
H	-0.383187	-3.727412	-4.158801
C	2.144804	-4.410004	-1.310206
H	0.660153	-3.579840	-0.002285
C	2.463589	-4.726727	-2.624611
H	1.802567	-4.732593	-4.675856
H	2.848016	-4.609383	-0.510660
C	-1.061270	-1.202008	-3.444094
C	-1.746881	-1.101420	-4.654124

C	0.246472	-0.730682	-3.342148
C	-1.115757	-0.567521	-5.769182
H	-2.768627	-1.456626	-4.725652
C	0.877984	-0.181987	-4.451336
H	0.776629	-0.803258	-2.398659
C	0.197139	-0.114464	-5.662834
H	-1.640209	-0.508277	-6.715726
H	1.895761	0.181289	-4.373227
C	3.799073	-5.308907	-2.967591
C	0.857999	0.510876	-6.853270
F	0.588033	1.828887	-6.946083
F	0.451024	-0.038326	-8.008701
F	2.194538	0.400919	-6.813649
F	3.701811	-6.305483	-3.865591
F	4.624028	-4.393416	-3.516302
F	4.438128	-5.805399	-1.898738
C	-3.498807	-5.309734	0.043109
C	-4.003341	-6.552451	0.414955
C	-4.175208	-4.115481	0.353249
C	-5.218606	-6.576902	1.091375
H	-3.480411	-7.475742	0.199335
C	-5.387640	-4.156335	1.042807
C	-5.904176	-5.395582	1.400429
H	-5.638861	-7.531603	1.385275
H	-5.915871	-3.242368	1.286799
H	-6.849669	-5.449929	1.927272
N	-2.320259	-4.998044	-0.648241
C	-1.554905	-6.003877	-1.374893
H	-1.507271	-5.742373	-2.430932
H	-0.544594	-6.096788	-0.979269
H	-2.063404	-6.958605	-1.279099

TS-5n:

C	-2.293573	0.229097	1.663910
C	-3.601358	0.387266	1.235330
C	-4.386149	1.466411	1.582824
C	-3.785278	2.416699	2.409239
C	-2.466067	2.281767	2.858127
C	-1.703157	1.179604	2.489483
C	-1.810138	-1.037048	1.092236
C	-2.984333	-1.489539	0.220659
H	-5.406303	1.565867	1.235098
H	-4.360480	3.283890	2.711767

H	-2.040994	3.044442	3.498585
H	-0.680857	1.058276	2.828206
C	-2.114643	-3.489148	-0.919880
C	-3.198934	-2.754152	-0.309423
C	-1.160425	-1.468175	-1.985620
C	-1.086968	-2.863671	-1.655107
O	-0.790725	-1.638596	1.301701
O	-4.022167	-0.658227	0.426329
O	-1.705971	-0.581973	-1.286037
C	-0.025283	-3.662600	-2.334429
C	-0.302252	-4.693478	-3.239825
C	1.312402	-3.332963	-2.093383
C	0.726307	-5.374477	-3.881273
H	-1.333477	-4.945576	-3.464951
C	2.345316	-4.012868	-2.732685
H	1.541268	-2.530255	-1.398866
C	2.054592	-5.037057	-3.629057
H	0.490348	-6.163382	-4.586705
H	3.375396	-3.741339	-2.530582
C	-0.614487	-0.992223	-3.303061
C	-0.875292	-1.655660	-4.504193
C	0.125153	0.192131	-3.319278
C	-0.392474	-1.144837	-5.703860
H	-1.468771	-2.562469	-4.502385
C	0.628213	0.690103	-4.516918
H	0.314338	0.712047	-2.386677
C	0.369077	0.022295	-5.710887
H	-0.610393	-1.657472	-6.633857
H	1.217401	1.600049	-4.518697
C	-2.271312	-4.918720	-0.905506
C	-3.475324	-5.495115	-0.625065
H	-1.426322	-5.543258	-1.163424
C	-4.484804	-3.364113	-0.159242
C	-4.624980	-4.709043	-0.321087
H	-3.564003	-6.575763	-0.645221
H	-5.311112	-2.753418	0.184526
H	-5.580425	-5.188557	-0.147752
H	2.855984	-5.566985	-4.131367
H	0.754909	0.412207	-6.646052

The optimized Cartesian coordinates for the benzofuranone-based spiropyrans **5** in the acetonitrile:

5a:

C	0	-4.404830	0.324248	0.387753
C	0	-4.771522	-0.286444	-0.809167
C	0	-5.921912	0.081786	-1.493312
C	0	-6.688221	1.094890	-0.929419
C	0	-6.331114	1.723769	0.275017
C	0	-5.182120	1.340858	0.945818
C	0	-3.164760	-0.302056	0.821114
C	0	-2.812587	-1.331967	-0.297201
H	0	-6.201314	-0.400983	-2.421117
H	0	-7.592490	1.409326	-1.437961
H	0	-6.960745	2.508690	0.674672
H	0	-4.884662	1.808601	1.877310
C	0	-1.740820	-3.544706	-0.546713
C	0	-2.597690	-2.729932	0.143500
C	0	-0.950461	-1.644416	-1.782586
C	0	-0.957669	-2.987005	-1.647915
O	0	-2.479858	-0.124679	1.794228
O	0	-3.920867	-1.266365	-1.219609
O	0	-1.672749	-0.831265	-0.932135
C	0	-0.239268	-3.893858	-2.580309
C	0	-0.570801	-3.921328	-3.937051
C	0	0.774842	-4.733780	-2.112083
C	0	0.109567	-4.760954	-4.812993
H	0	-1.360224	-3.273367	-4.303721
C	0	1.454461	-5.575201	-2.987524
H	0	1.048251	-4.709986	-1.061876
C	0	1.124791	-5.589169	-4.340600
H	0	-0.155309	-4.770525	-5.864294
H	0	2.245781	-6.214968	-2.613593
C	0	-0.191088	-0.835966	-2.756878
C	0	-0.797697	0.288244	-3.327182
C	0	1.124160	-1.156259	-3.109679
C	0	-0.110979	1.061457	-4.256634
H	0	-1.812212	0.547206	-3.045582
C	0	1.809821	-0.377266	-4.033810
H	0	1.613503	-2.008380	-2.652728
C	0	1.192961	0.729115	-4.614432
H	0	-0.594333	1.924080	-4.700804
H	0	2.830912	-0.629969	-4.295568
C	0	-2.648462	-5.030354	0.984383

H	0	1.655128	-6.243634	-5.022963
H	0	1.729698	1.333626	-5.336690
S	0	-3.449737	-3.556975	1.388188
C	0	-1.779847	-4.889638	-0.053684
H	0	-1.189020	-5.704902	-0.448586
H	0	-2.863819	-5.920441	1.556448

5b:

C	-4.406790	0.324531	0.383378
C	-4.774350	-0.289049	-0.811658
C	-5.925928	0.075491	-1.495232
C	-6.693105	1.088660	-0.932428
C	-6.335346	1.720663	0.270124
C	-5.184877	1.341159	0.940331
C	-3.165393	-0.299110	0.816476
C	-2.814648	-1.331438	-0.300601
H	-6.205760	-0.409828	-2.421554
H	-7.598565	1.400525	-1.440396
H	-6.965720	2.505407	0.668926
H	-4.886961	1.811372	1.870406
C	-1.738618	-3.544560	-0.544230
C	-2.596670	-2.728335	0.143000
C	-0.950711	-1.644536	-1.782317
C	-0.954852	-2.986724	-1.644523
O	-2.478534	-0.119605	1.787557
O	-3.922239	-1.269194	-1.221153
O	-1.674959	-0.830100	-0.938543
C	-0.231195	-3.890490	-2.573960
C	-0.548595	-3.911130	-3.933573
C	0.776805	-4.734720	-2.102633
C	0.133283	-4.743726	-4.813563
H	-1.333380	-3.263695	-4.309682
C	1.466948	-5.575551	-2.968944
H	1.045551	-4.720589	-1.051574
C	1.136386	-5.567372	-4.318199
H	-0.116778	-4.752325	-5.867084
H	2.253873	-6.220201	-2.598057
C	-0.190721	-0.839876	-2.758182
C	-0.794924	0.283145	-3.331173
C	1.124151	-1.159114	-3.109990
C	-0.115315	1.058567	-4.262536
H	-1.808781	0.547609	-3.053754
C	1.816572	-0.388420	-4.034527
H	1.620325	-2.006051	-2.651564
C	1.184496	0.709533	-4.606736

H	-0.592314	1.920381	-4.712099
H	2.837283	-0.635155	-4.297943
C	-2.647748	-5.027215	0.987576
S	-3.449573	-3.553489	1.387515
C	-1.777827	-4.888594	-0.049685
Br	2.075712	-6.712821	-5.513254
Br	2.126370	1.765170	-5.877232
H	-1.187878	-5.705757	-0.441936
H	-2.863840	-5.916359	1.560778

5c:

C	-4.417822	0.315377	0.350360
C	-4.770356	-0.312779	-0.841549
C	-5.918483	0.035653	-1.538704
C	-6.698339	1.048480	-0.992644
C	-6.355883	1.695191	0.206467
C	-5.208427	1.331372	0.890451
C	-3.175319	-0.293786	0.800265
C	-2.806326	-1.332522	-0.305330
H	-6.186485	-0.461086	-2.462453
H	-7.601701	1.348141	-1.511569
H	-6.995673	2.479016	0.591838
H	-4.922270	1.813190	1.818250
C	-1.696800	-3.534408	-0.516110
C	-2.574548	-2.723145	0.151998
C	-0.924455	-1.635302	-1.765320
C	-0.908585	-2.975390	-1.612268
O	-2.498187	-0.100359	1.775284
O	-3.906539	-1.290780	-1.233606
O	-1.667034	-0.822342	-0.939295
C	-0.157666	-3.876394	-2.522163
C	-0.459176	-3.914656	-3.884784
C	0.859992	-4.695242	-2.023448
C	0.253600	-4.742397	-4.742907
H	-1.251431	-3.285306	-4.274569
C	1.576245	-5.524984	-2.874583
H	1.111223	-4.661110	-0.968927
C	1.272423	-5.540284	-4.233522
H	0.018069	-4.761880	-5.800067
H	2.374456	-6.146005	-2.484649
C	-0.167992	-0.832915	-2.747381
C	-0.790604	0.266582	-3.345466
C	1.157964	-1.134686	-3.074098

C	-0.112247	1.034443	-4.282245
H	-1.811761	0.513991	-3.080859
C	1.841230	-0.365916	-4.004414
H	1.663372	-1.960728	-2.589202
C	1.201186	0.713238	-4.608396
H	-0.602631	1.879888	-4.749437
H	2.871704	-0.597381	-4.246358
C	-2.604378	-5.014656	1.017723
S	-3.431477	-3.548500	1.392915
C	-1.723271	-4.874048	-0.009723
C	2.022797	-6.471323	-5.137042
C	1.926204	1.506591	-5.653873
F	1.536671	-7.727413	-5.080501
F	3.322478	-6.556801	-4.809224
F	3.243756	1.583452	-5.410643
F	1.468531	2.763198	-5.751573
F	1.797786	0.957128	-6.877831
F	1.964333	-6.097659	-6.423128
H	-1.117388	-5.686779	-0.386627
H	-2.815895	-5.901196	1.596597

5d:

C	-4.229342	0.327571	0.610683
C	-4.652573	-0.305124	-0.550131
C	-5.854965	0.037160	-1.153613
C	-6.597038	1.038674	-0.545561
C	-6.195447	1.709272	0.633841
C	-4.990127	1.336079	1.210702
C	-2.951726	-0.263998	0.973385
C	-2.650848	-1.306318	-0.149943
H	-6.193303	-0.455221	-2.056580
H	-7.537490	1.315365	-1.009964
H	-4.618168	1.802234	2.114933
C	-1.558771	-3.511185	-0.418587
C	-2.390621	-2.694582	0.299765
C	-0.862111	-1.618428	-1.721009
C	-0.839036	-2.958147	-1.563885
O	-2.207431	-0.058895	1.896658
O	-3.807025	-1.271632	-1.007319
O	-1.553197	-0.800358	-0.856686
C	-0.147581	-3.864014	-2.515156
C	-0.527130	-3.899314	-3.858441
C	0.890648	-4.691039	-2.076280

C	0.128279	-4.732272	-4.755983
H	-1.335425	-3.263531	-4.202083
C	1.549337	-5.527237	-2.967074
H	1.203365	-4.659117	-1.038315
C	1.167547	-5.539792	-4.305995
H	-0.167669	-4.749076	-5.797957
H	2.363049	-6.155307	-2.623445
C	-0.160654	-0.821526	-2.747503
C	-0.811501	0.279060	-3.311992
C	1.143936	-1.129104	-3.147600
C	-0.183800	1.042777	-4.287047
H	-1.815125	0.531169	-2.990854
C	1.776881	-0.364543	-4.115801
H	1.672436	-1.956282	-2.690003
C	1.107967	0.716209	-4.685279
H	-0.696657	1.888983	-4.727781
H	2.791458	-0.600373	-4.414616
C	-2.372504	-4.982360	1.175744
S	-3.169695	-3.511880	1.595900
C	-1.557255	-4.848717	0.094408
C	1.851870	-6.478790	-5.252687
C	1.780370	1.504235	-5.769266
F	1.330683	-7.720697	-5.193563
F	3.160825	-6.607408	-4.981902
F	3.103392	1.613798	-5.570494
F	1.292803	2.748448	-5.876274
F	1.625621	0.927214	-6.977353
F	1.750243	-6.084102	-6.530014
C	-7.094532	2.801430	1.214820
C	-6.497874	3.413401	2.484607
H	-6.372944	2.668012	3.274304
H	-5.528308	3.880498	2.293133
H	-7.168418	4.187587	2.864065
C	-8.466153	2.200742	1.563382
H	-9.116430	2.972902	1.982928
H	-8.966220	1.787554	0.684667
H	-8.363963	1.402154	2.302615
C	-7.274083	3.919755	0.175134
H	-7.741891	3.554196	-0.741679
H	-7.912384	4.708705	0.581662
H	-6.310442	4.362820	-0.088933
H	-0.978874	-5.665101	-0.316216
H	-2.549531	-5.865796	1.770713

5e:

C	-4.376733	0.146541	0.580179
C	-4.757065	-0.465338	-0.610190
C	-5.930939	-0.111663	-1.250558
C	-6.711297	0.881601	-0.663928
C	-6.332354	1.508592	0.537118
C	-5.151081	1.138159	1.170846
C	-3.110087	-0.455274	0.978548
C	-2.761504	-1.463252	-0.162032
H	-6.234734	-0.587035	-2.174515
H	-7.630548	1.166739	-1.158494
H	-4.852616	1.614765	2.097428
C	-1.609656	-3.633565	-0.458686
C	-2.480385	-2.856888	0.257968
C	-0.923804	-1.690585	-1.691050
C	-0.873379	-3.033176	-1.569136
O	-2.407654	-0.271426	1.936437
O	-3.890651	-1.429372	-1.048580
O	-1.653409	-0.913118	-0.821071
C	-0.136952	-3.897681	-2.525120
C	-0.485570	-3.912506	-3.877028
C	0.913569	-4.706247	-2.080890
C	0.211997	-4.707303	-4.777632
H	-1.302995	-3.290822	-4.224848
C	1.614829	-5.503444	-2.974721
H	1.201495	-4.689755	-1.035372
C	1.263089	-5.495988	-4.321995
H	-0.060339	-4.708601	-5.826148
H	2.438040	-6.116708	-2.626943
C	-0.220856	-0.850125	-2.681024
C	-0.886899	0.250333	-3.227587
C	1.097644	-1.116743	-3.064951
C	-0.259949	1.054831	-4.169902
H	-1.901913	0.470140	-2.918738
C	1.729670	-0.311360	-3.999996
H	1.637005	-1.944092	-2.620510
C	1.045976	0.769104	-4.552487
H	-0.784594	1.900628	-4.597219
H	2.754749	-0.515407	-4.286261
C	-2.431397	-5.167158	1.071427
S	-3.275236	-3.727928	1.508527
C	-1.590182	-4.984545	0.017540
C	1.995656	-6.394140	-5.272130

C	1.721074	1.600451	-5.601798
F	1.519384	-7.654952	-5.240572
F	3.304075	-6.479611	-4.981799
F	3.032474	1.755195	-5.359522
F	1.191121	2.827375	-5.704294
F	1.626052	1.038633	-6.823142
F	1.900036	-5.982956	-6.544625
O	-7.059974	2.481038	1.144019
C	-8.272731	2.888981	0.530564
H	-8.685621	3.663035	1.171607
H	-8.090177	3.300152	-0.465312
H	-8.978212	2.057164	0.463709
H	-0.981248	-5.775534	-0.398618
H	-2.603275	-6.070636	1.637104

5f:

C	-4.412500	0.313482	0.358276
C	-4.769172	-0.312076	-0.831273
C	-5.920789	0.041764	-1.523824
C	-6.698893	1.052994	-0.979471
C	-6.325631	1.674317	0.214830
C	-5.190527	1.331136	0.911747
C	-3.168378	-0.300888	0.804714
C	-2.805895	-1.337854	-0.304345
H	-6.196573	-0.450552	-2.447191
H	-7.608139	1.376322	-1.472226
H	-4.920333	1.825030	1.837233
C	-1.697854	-3.539189	-0.520348
C	-2.574907	-2.729166	0.150278
C	-0.926616	-1.638728	-1.768104
C	-0.910176	-2.978783	-1.616045
O	-2.492110	-0.107960	1.778582
O	-3.910709	-1.292413	-1.228332
O	-1.669604	-0.826695	-0.940794
C	-0.158320	-3.878642	-2.526355
C	-0.459933	-3.916881	-3.888904
C	0.860397	-4.696190	-2.027740
C	0.253902	-4.743542	-4.747212
H	-1.252995	-3.288448	-4.278517
C	1.577689	-5.524795	-2.879092
H	1.111549	-4.661981	-0.973202
C	1.273778	-5.540177	-4.238007
H	0.018377	-4.763112	-5.804365

H	2.376732	-6.144849	-2.489337
C	-0.171251	-0.834587	-2.749431
C	-0.794908	0.264974	-3.346249
C	1.154809	-1.135212	-3.076769
C	-0.117344	1.034183	-4.282506
H	-1.816191	0.511440	-3.081263
C	1.837227	-0.365052	-4.006522
H	1.660926	-1.961358	-2.592805
C	1.196204	0.714203	-4.609292
H	-0.608472	1.879689	-4.748780
H	2.867794	-0.595564	-4.248990
C	-2.604508	-5.021943	1.011470
S	-3.431227	-3.556663	1.390232
C	-1.724239	-4.879669	-0.016456
C	2.025477	-6.469995	-5.141739
C	1.920578	1.509004	-5.654175
F	1.541479	-7.726866	-5.084950
F	3.325372	-6.553196	-4.814246
F	3.237710	1.588582	-5.409585
F	1.460398	2.764604	-5.752438
F	1.794514	0.959046	-6.878120
F	1.965996	-6.096455	-6.427791
F	-7.121190	2.649531	0.693889
H	-1.118768	-5.691753	-0.395365
H	-2.815752	-5.909485	1.588912

5g:

C	-4.339024	0.317460	0.468240
C	-4.716764	-0.302750	-0.719410
C	-5.885122	0.047773	-1.389357
C	-6.653758	1.048615	-0.821944
C	-6.275343	1.681689	0.376187
C	-5.115023	1.324332	1.037236
C	-3.082575	-0.292977	0.887064
C	-2.739454	-1.325557	-0.231713
H	-6.173250	-0.441427	-2.310421
H	-7.570934	1.353317	-1.314312
H	-4.812036	1.801811	1.961294
C	-1.656171	-3.533146	-0.484943
C	-2.512198	-2.720627	0.209786
C	-0.895755	-1.630724	-1.736411
C	-0.887079	-2.971679	-1.593074
O	-2.387801	-0.100971	1.847119

O	-3.866027	-1.268360	-1.139143
O	-1.617257	-0.818126	-0.889257
C	-0.161937	-3.871512	-2.524973
C	-0.492390	-3.896965	-3.881150
C	0.858759	-4.702275	-2.053379
C	0.194550	-4.725035	-4.759626
H	-1.286900	-3.257810	-4.249782
C	1.549033	-5.532820	-2.925117
H	1.132646	-4.677694	-1.004264
C	1.216039	-5.536250	-4.277176
H	-0.063358	-4.734959	-5.811699
H	2.349389	-6.163876	-2.556409
C	-0.153201	-0.825403	-2.726214
C	-0.779081	0.282858	-3.304015
C	1.164095	-1.134609	-3.080244
C	-0.112856	1.052956	-4.247829
H	-1.793267	0.535786	-3.018682
C	1.835180	-0.363623	-4.017285
H	1.672354	-1.967974	-2.611170
C	1.191641	0.724739	-4.601013
H	-0.605935	1.905185	-4.699472
H	2.859232	-0.600641	-4.280446
C	-2.541742	-5.017844	1.056912
S	-3.348254	-3.548997	1.462941
C	-1.682600	-4.876315	0.011053
C	1.935780	-6.469421	-5.203302
C	1.904998	1.520000	-5.653228
F	1.427017	-7.716823	-5.155051
F	3.238261	-6.582879	-4.896490
F	3.223324	1.606816	-5.416922
F	1.438150	2.772806	-5.752790
F	1.774484	0.964839	-6.874277
F	1.864743	-6.078381	-6.483618
C	-7.174904	2.747071	0.923659
F	-8.386656	2.260188	1.249253
F	-6.676603	3.324142	2.023072
F	-7.394639	3.725620	0.027401
H	-1.091965	-5.690798	-0.385609
H	-2.747613	-5.907283	1.633388

5h:

C	-4.413733	0.323883	0.349361
C	-4.771393	-0.315823	-0.834743

C	-5.919835	0.027699	-1.532948
C	-6.695539	1.048611	-0.995737
C	-6.348286	1.707145	0.195449
C	-5.200271	1.347629	0.880745
C	-3.172601	-0.284540	0.803256
C	-2.806733	-1.330435	-0.297754
H	-6.191465	-0.478402	-2.450498
H	-7.599354	1.345167	-1.515613
H	-6.984924	2.496883	0.573865
H	-4.910578	1.838533	1.802618
C	-1.684862	-3.526874	-0.499709
C	-2.563369	-2.717572	0.167044
C	-0.929048	-1.633868	-1.764311
C	-0.904409	-2.972784	-1.603599
O	-2.494204	-0.089053	1.776614
O	-3.910690	-1.301619	-1.218216
O	-1.671932	-0.820653	-0.940098
C	-0.151904	-3.877059	-2.508932
C	-0.463014	-3.932247	-3.868692
C	0.876599	-4.680913	-2.008343
C	0.251481	-4.762582	-4.722807
H	-1.263649	-3.314226	-4.259424
C	1.594009	-5.513706	-2.855588
H	1.136045	-4.632391	-0.956288
C	1.280631	-5.546164	-4.211947
H	0.009014	-4.795339	-5.778047
H	2.400369	-6.123366	-2.464571
C	-0.182341	-0.834556	-2.756164
C	-0.816367	0.254288	-3.361498
C	1.143841	-1.130704	-3.086132
C	-0.148184	1.017273	-4.309382
H	-1.838014	0.496874	-3.094299
C	1.816976	-0.366223	-4.027409
H	1.657249	-1.948559	-2.595798
C	1.165888	0.701882	-4.638887
H	-0.646905	1.854362	-4.782754
H	2.847766	-0.592754	-4.272389
C	-2.574687	-4.998224	1.034309
S	-3.416719	-3.536535	1.419040
C	-1.695663	-4.866699	0.005900
C	2.033263	-6.479884	-5.111148
C	1.878633	1.490050	-5.696937
F	1.557679	-7.739042	-5.039429
F	3.335429	-6.551244	-4.790361

F	3.198996	1.566875	-5.470745
F	1.420415	2.746514	-5.794069
F	1.733740	0.935327	-6.916552
F	1.963806	-6.118903	-6.400223
H	-1.089641	-5.680335	-0.367640
Br	-2.904729	-6.556739	2.020019

5i:

C	-4.397029	0.296724	0.415778
C	-4.836428	-0.283934	-0.771668
C	-6.017775	0.112769	-1.383120
C	-6.738411	1.123353	-0.756726
C	-6.307763	1.721245	0.439010
C	-5.128558	1.309590	1.037193
C	-3.148105	-0.361714	0.771583
C	-2.873479	-1.378832	-0.379416
H	-6.355123	-0.346872	-2.303458
H	-7.665005	1.459657	-1.208008
H	-6.904183	2.504570	0.889593
H	-4.774832	1.751969	1.961449
C	-1.759045	-3.540890	-0.640633
C	-2.684745	-2.793813	0.035560
C	-0.978611	-1.654774	-1.860361
C	-0.934748	-2.995246	-1.703237
O	-2.406801	-0.208468	1.707177
O	-4.026442	-1.272211	-1.242549
O	-1.758603	-0.861186	-1.051677
C	-0.152784	-3.902024	-2.582245
C	-0.420853	-3.966345	-3.951737
C	0.850224	-4.713460	-2.045358
C	0.312252	-4.815629	-4.773376
H	-1.202687	-3.340879	-4.369924
C	1.581312	-5.566012	-2.867491
H	1.076369	-4.658762	-0.985214
C	1.315688	-5.617001	-4.233195
H	0.097437	-4.854860	-5.835292
H	2.363492	-6.184038	-2.441547
C	-0.217846	-0.836988	-2.824666
C	-0.841720	0.260237	-3.428121
C	1.116170	-1.121988	-3.135372
C	-0.152265	1.040788	-4.349169
H	-1.870938	0.492273	-3.178753

C	1.803963	-0.335310	-4.051295
H	1.618443	-1.951451	-2.651539
C	1.170802	0.743412	-4.665305
H	-0.648480	1.882052	-4.819299
H	2.839331	-0.560186	-4.280207
C	-3.054298	-4.836176	1.016953
H	1.886948	-6.279208	-4.873727
H	1.709473	1.353988	-5.380967
H	-3.443025	-5.629732	1.638819
C	-3.450135	-3.531668	0.994062
C	-4.555125	-2.958942	1.834061
H	-4.178867	-2.209279	2.534403
H	-5.314723	-2.478848	1.210554
H	-5.043253	-3.743375	2.411887
S	-1.788306	-5.185093	-0.108980

5j:

C	-4.419701	0.324851	0.348371
C	-4.765442	-0.306078	-0.844107
C	-5.914185	0.035552	-1.544043
C	-6.700843	1.044419	-1.000616
C	-6.365002	1.693800	0.199050
C	-5.217289	1.336771	0.886003
C	-3.174520	-0.276365	0.801509
C	-2.799182	-1.318471	-0.298208
H	-6.177143	-0.463045	-2.468245
H	-7.604544	1.338795	-1.521994
H	-7.010145	2.474254	0.582344
H	-4.936039	1.820657	1.814234
C	-1.706662	-3.524616	-0.500246
C	-2.576031	-2.708027	0.167634
C	-0.921541	-1.626656	-1.753513
C	-0.917417	-2.966686	-1.599430
O	-2.500837	-0.075963	1.777762
O	-3.894851	-1.278195	-1.233763
O	-1.657942	-0.808732	-0.928719
C	-0.171010	-3.868211	-2.513942
C	-0.497136	-3.921741	-3.870190
C	0.868539	-4.667378	-2.028482
C	0.211816	-4.745756	-4.735361
H	-1.305127	-3.306438	-4.249952
C	1.580917	-5.493423	-2.886314
H	1.139146	-4.620592	-0.979207

C	1.251701	-5.524331	-4.239164
H	-0.042703	-4.776639	-5.787858
H	2.395597	-6.099197	-2.506654
C	-0.161461	-0.831097	-2.738625
C	-0.778851	0.271631	-3.336378
C	1.161570	-1.141483	-3.069197
C	-0.098685	1.033963	-4.276353
H	-1.797628	0.525811	-3.069066
C	1.846740	-0.378190	-4.002668
H	1.663800	-1.969583	-2.584751
C	1.211673	0.704097	-4.606197
H	-0.585298	1.881766	-4.743223
H	2.875005	-0.616442	-4.247405
C	-2.550768	-5.112162	1.010883
C	-1.703550	-4.880879	-0.022556
C	1.998243	-6.451411	-5.149945
C	1.938309	1.491127	-5.655313
F	1.525606	-7.712040	-5.081462
F	3.303363	-6.522400	-4.841148
F	3.257203	1.559452	-5.416822
F	1.488742	2.750653	-5.753162
F	1.801891	0.940848	-6.878044
F	1.916877	-6.083508	-6.436492
H	-1.080125	-5.659307	-0.443566
H	-2.702483	-6.043060	1.536747
Se	-3.501244	-3.590051	1.521608

5k:

C	-4.414732	0.233367	0.395961
C	-4.833419	-0.325538	-0.809410
C	-6.005722	0.079557	-1.432396
C	-6.739484	1.075441	-0.798160
C	-6.330281	1.651297	0.416007
C	-5.160019	1.231783	1.025468
C	-3.169492	-0.428136	0.759525
C	-2.873670	-1.419928	-0.408854
H	-6.326192	-0.362624	-2.367171
H	-7.659610	1.417944	-1.257869
H	-6.936610	2.423916	0.871765
H	-4.822555	1.657369	1.963540
C	-1.767360	-3.575989	-0.704436
C	-2.685170	-2.840558	-0.018914
C	-0.967599	-1.665804	-1.872507

C	-0.936396	-3.011636	-1.750742
O	-2.447273	-0.298109	1.712855
O	-4.010115	-1.298932	-1.288712
O	-1.748400	-0.889390	-1.053699
C	-0.154894	-3.900535	-2.648946
C	-0.430046	-3.939131	-4.017856
C	0.854327	-4.717381	-2.132390
C	0.301792	-4.770004	-4.859240
H	-1.216267	-3.308618	-4.419890
C	1.583465	-5.552004	-2.974335
H	1.087175	-4.680707	-1.072908
C	1.310370	-5.578171	-4.339269
H	0.081873	-4.789619	-5.920615
H	2.370245	-6.174941	-2.564425
C	-0.189137	-0.830585	-2.806848
C	-0.796861	0.289552	-3.384075
C	1.144532	-1.121732	-3.113202
C	-0.090797	1.088369	-4.276253
H	-1.826063	0.524791	-3.137905
C	1.849069	-0.315707	-3.998832
H	1.633910	-1.969685	-2.648864
C	1.232350	0.786470	-4.587500
H	-0.573886	1.947515	-4.727189
H	2.884336	-0.544241	-4.224266
C	-3.037518	-4.952907	0.935194
C	-3.623133	-5.897797	1.778286
C	-3.447822	-3.603546	0.932781
C	-4.641939	-5.483670	2.621100
H	-3.292230	-6.929793	1.770246
C	-4.489063	-3.210465	1.789996
C	-5.073734	-4.148162	2.622619
H	-5.112398	-6.201048	3.283118
H	-4.841293	-2.184392	1.803887
H	-5.876677	-3.847501	3.285307
S	-1.761231	-5.252623	-0.223748
H	1.880418	-6.226232	-4.995145
H	1.784109	1.411671	-5.280169

5l:

C	-4.459124	0.337939	0.413679
C	-4.916903	-0.211790	-0.782104
C	-6.128307	0.172367	-1.342318
C	-6.858530	1.135925	-0.656679

C	-6.409152	1.702183	0.548122
C	-5.200630	1.305341	1.094262
C	-3.177042	-0.287171	0.702034
C	-2.928271	-1.289315	-0.467363
H	-6.479821	-0.261387	-2.269906
H	-7.808023	1.460527	-1.067197
H	-7.014681	2.449037	1.045996
H	-4.831132	1.724635	2.023098
C	-1.839875	-3.477020	-0.707440
C	-2.753716	-2.692499	-0.052096
C	-1.017078	-1.623493	-1.927829
C	-0.979731	-2.963573	-1.751186
O	-2.403328	-0.132552	1.611062
O	-4.089947	-1.148210	-1.319192
O	-1.810949	-0.804154	-1.168643
C	-0.161885	-3.889802	-2.571204
C	-0.342082	-3.966076	-3.954655
C	0.790921	-4.708084	-1.958027
C	0.429579	-4.831216	-4.717322
H	-1.085221	-3.338035	-4.432908
C	1.562838	-5.580275	-2.715427
H	0.954274	-4.639704	-0.887516
C	1.382069	-5.632403	-4.093419
H	0.290840	-4.880218	-5.790814
H	2.309306	-6.201948	-2.235605
C	-0.217458	-0.834491	-2.885957
C	-0.816405	0.247642	-3.537834
C	1.125967	-1.131703	-3.135953
C	-0.095213	1.002102	-4.452668
H	-1.851526	0.491517	-3.331884
C	1.851614	-0.375506	-4.044625
H	1.612542	-1.942287	-2.607620
C	1.236177	0.685655	-4.702810
H	-0.566405	1.834243	-4.961715
H	2.895065	-0.602656	-4.227116
C	2.182244	-6.603174	-4.908829
C	2.006152	1.466291	-5.725671
F	3.315656	1.526272	-5.440171
F	1.568189	2.728727	-5.840155
F	1.908967	0.916288	-6.952126
F	2.381216	-6.171597	-6.163276
F	3.390187	-6.841349	-4.376069
F	1.568744	-7.798989	-5.010528
C	-2.910390	-4.819525	0.728927

C	-3.355915	-5.903128	1.488022
C	-3.462663	-3.521782	0.874074
C	-4.375607	-5.669354	2.395524
H	-2.921152	-6.888668	1.367833
C	-4.497702	-3.314428	1.799568
C	-4.942149	-4.388856	2.549505
H	-4.746488	-6.489439	2.999364
H	-4.942830	-2.332474	1.926132
H	-5.740003	-4.246487	3.269084
N	-1.930669	-4.762033	-0.242651
H	-1.379267	-5.543869	-0.564390

5m:

C	-4.395690	0.330306	0.465769
C	-4.871253	-0.172595	-0.743787
C	-6.061153	0.278321	-1.300668
C	-6.750530	1.259507	-0.597982
C	-6.282417	1.779180	0.620602
C	-5.096339	1.315686	1.163649
C	-3.145583	-0.359242	0.747302
C	-2.928848	-1.339827	-0.446897
H	-6.427082	-0.119229	-2.238859
H	-7.681955	1.635716	-1.005841
H	-6.855751	2.542519	1.131437
H	-4.713231	1.697876	2.102950
C	-1.932316	-3.584701	-0.736976
C	-2.808497	-2.758019	-0.071823
C	-1.023962	-1.712693	-1.892280
C	-1.023561	-3.057102	-1.742476
O	-2.373732	-0.261535	1.665956
O	-4.084994	-1.133470	-1.297150
O	-1.798193	-0.876110	-1.133360
C	-0.150629	-3.923783	-2.581481
C	-0.456931	-4.141439	-3.923490
C	0.990217	-4.514354	-2.030999
C	0.364578	-4.939486	-4.712945
H	-1.339540	-3.681052	-4.352970
C	1.814096	-5.311598	-2.810696
H	1.238998	-4.334549	-0.990409
C	1.496124	-5.518919	-4.151796
H	0.124402	-5.102154	-5.756523
H	2.703001	-5.760100	-2.382259
C	-0.221851	-0.927211	-2.856155

C	-0.848279	0.119136	-3.541331
C	1.132437	-1.184397	-3.086368
C	-0.144402	0.873408	-4.468947
H	-1.892803	0.334458	-3.350638
C	1.842235	-0.426591	-4.007628
H	1.642704	-1.962217	-2.533532
C	1.199509	0.595392	-4.699174
H	-0.638354	1.675860	-5.003622
H	2.894481	-0.623696	-4.173673
C	2.371222	-6.417603	-4.973441
C	1.950631	1.375674	-5.735977
F	3.260320	1.462735	-5.459223
F	1.489551	2.628907	-5.863851
F	1.855858	0.809164	-6.955172
F	2.214269	-6.224924	-6.290180
F	3.674267	-6.240049	-4.700373
F	2.111262	-7.719329	-4.741370
C	-3.096788	-4.875371	0.671198
C	-3.613836	-5.933546	1.426389
C	-3.570514	-3.550717	0.834817
C	-4.620982	-5.644198	2.332139
H	-3.244365	-6.946452	1.323212
C	-4.595909	-3.285425	1.756306
C	-5.111451	-4.334377	2.495315
H	-5.038502	-6.445723	2.930504
H	-4.978002	-2.278032	1.889693
H	-5.901872	-4.149114	3.213298
N	-2.112894	-4.880445	-0.302435
C	-1.451834	-6.093492	-0.764619
H	-1.365565	-6.090134	-1.848508
H	-0.462094	-6.202676	-0.320330
H	-2.064825	-6.944531	-0.478142

5n:

C	-4.480381	0.350362	0.240206
C	-4.766786	-0.219654	-0.997690
C	-5.848576	0.199038	-1.760665
C	-6.629159	1.220331	-1.232192
C	-6.351956	1.808846	0.013084
C	-5.270818	1.376067	0.761850
C	-3.297346	-0.324825	0.754371
C	-2.890742	-1.340138	-0.354956
H	-6.066015	-0.252018	-2.720486

H	-7.480907	1.573738	-1.802150
H	-6.989860	2.601787	0.382712
H	-5.035888	1.811787	1.726192
C	-0.994687	-1.658220	-1.751237
C	-1.096772	-3.000968	-1.700964
O	-2.686215	-0.181427	1.781404
O	-3.912033	-1.212319	-1.365830
O	-1.691999	-0.853647	-0.876431
C	-0.390945	-3.867849	-2.684416
C	-0.781441	-3.866853	-4.024690
C	0.674659	-4.681156	-2.289046
C	-0.109749	-4.652185	-4.957326
H	-1.608226	-3.236692	-4.336063
C	1.345495	-5.468123	-3.219474
H	0.993024	-4.678557	-1.251193
C	0.955931	-5.453477	-4.557003
H	-0.419353	-4.637527	-5.996275
H	2.176753	-6.087120	-2.901389
C	-0.170157	-0.841713	-2.666096
C	-0.711693	0.339672	-3.184662
C	1.134561	-1.205557	-3.014974
C	0.027261	1.126989	-4.060399
H	-1.717663	0.632404	-2.905511
C	1.873632	-0.411435	-3.883911
H	1.576371	-2.101887	-2.597031
C	1.320820	0.752224	-4.414084
H	-0.406918	2.033914	-4.465349
H	2.886601	-0.698495	-4.141824
H	1.480655	-6.064155	-5.282932
H	1.899046	1.367943	-5.093588
C	-2.734026	-5.477069	0.658518
C	-1.930656	-4.972030	-0.355968
C	-1.939153	-3.603507	-0.655975
C	-2.799728	-2.771694	0.074276
C	-3.601644	-3.276953	1.092099
C	-3.566402	-4.633711	1.391612
H	-2.710250	-6.538109	0.879055
H	-1.293378	-5.644376	-0.916896
H	-4.262066	-2.617969	1.646591
H	-4.190036	-5.031298	2.183198

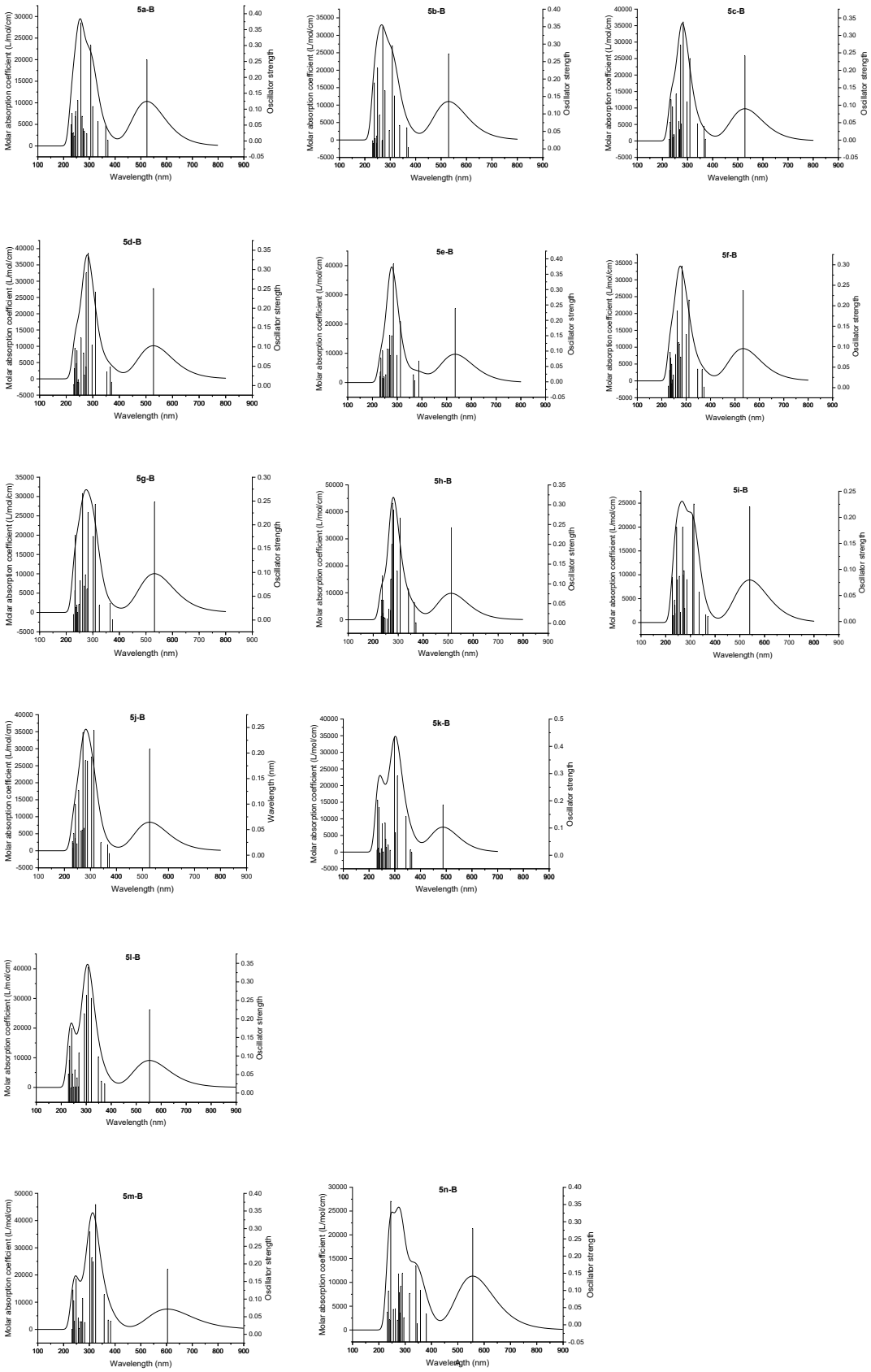


Figure *S24.* Calculated UV-vis spectra of **5a-B**–**5n-B** at the M062X/6-311+G(d) level of theory

6. X-Ray Diffraction Data for the Benzofuranone-Based Spiropyran 5b

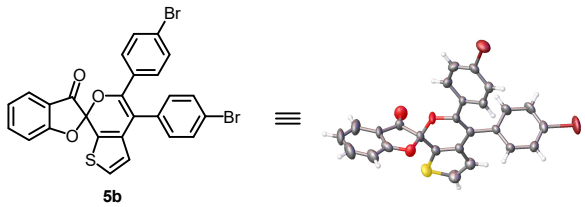


Figure S25. X-ray structure of 4',5'-bis(4-bromophenyl)-3*H*-spiro[benzofuran-2,7'-thieno[2,3-*c*]pyran]-3-one（**5b**） (ORTEP view at 50% ellipsoidal probability).

Table *S1*. Crystal data and structure refinement for **5b**.

Identification code	**5b**
Empirical formula	$C_{26}H_{14}Br_2O_3S$
Formula weight	566.25
Temperature/K	293(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.0340(4)
b/Å	17.0933(9)
c/Å	11.0048(3)
α/°	90
β/°	92.379(3)
γ/°	90
Volume/Å^3	2261.74(15)
Z	4
ρ_{calc}g/cm^3	1.663
μ/mm^{-1}	5.629
F(000)	1120.0
Crystal size/mm^3	0.3 × 0.3 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.352 to 133.158
Index ranges	$-14 \le h \le 9$, $-19 \le k \le 20$, $-12 \le l \le 13$
Reflections collected	7666
Independent reflections	3983 [R_{int} = 0.0303, R_{sigma} = 0.0406]
Data/restraints/parameters	3983/0/289
Goodness-of-fit on F^2	1.078
Final R indexes [I>=2σ (I)]	R_1 = 0.0733, wR_2 = 0.1797
Final R indexes [all data]	R_1 = 0.0811, wR_2 = 0.1860

Largest diff. peak/hole / e $Å^{-3}$ 1.15/-1.29

Table *S2*. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **5b**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ}tensor.

Atom	x	y	z	U(eq)
Br1	10080.0(6)	4904.6(7)	8196.1(8)	84.9(4)
Br2	7344.5(7)	3708.0(6)	671.4(7)	70.9(3)
S1	2732.0(14)	3663.6(12)	8651.7(16)	58.6(5)
O1	3908(3)	3335(3)	5326(4)	53.7(12)
O2	2747(5)	2035(3)	6545(6)	73.8(15)
O3	2285(4)	4000(2)	5640(4)	50.4(10)
C1	6564(4)	3709(4)	2134(5)	42.5(13)
C2	5743(5)	3181(4)	2313(6)	50.7(15)
C3	5204(5)	3165(4)	3413(6)	45.3(14)
C4	5511(4)	3702(3)	4332(5)	32.1(10)
C5	6326(4)	4263(3)	4094(5)	37.0(11)
C6	6850(4)	4273(3)	3011(5)	40.3(12)
C7	4936(4)	3697(3)	5493(5)	34.6(11)
C8	5313(4)	3961(3)	6579(5)	33.5(11)
C9	4543(4)	3928(3)	7583(5)	35.8(11)
C10	4749(5)	4129(4)	8818(6)	49.0(14)
C11	3853(6)	4014(5)	9500(6)	61.5(18)
C12	6473(4)	4211(3)	6885(5)	32.4(11)
C13	7340(5)	3674(4)	6855(6)	46.9(14)
C14	8401(5)	3881(4)	7226(6)	51.3(16)
C15	8610(5)	4629(4)	7642(5)	46.2(14)
C16	7784(5)	5176(4)	7663(6)	46.8(14)
C17	6714(5)	4959(3)	7295(5)	39.5(12)
C18	3485(4)	3668(3)	7368(5)	39.4(12)
C19	3050(4)	3427(3)	6148(5)	37.6(12)
C20	2408(4)	2648(3)	6107(5)	39.1(12)
C21	1342(5)	2817(4)	5514(6)	46.9(14)
C22	1352(5)	3611(4)	5249(6)	48.4(15)
C23	490(6)	3985(5)	4631(7)	65.0(19)
C24	-391(6)	3524(7)	4291(9)	87(3)
C25	-467(6)	2725(7)	4545(8)	83(3)
C26	429(7)	2358(6)	5171(8)	81(3)

Table *S3*. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 5b. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	30.9(4)	143.4(10)	78.7(6)	1.9(5)	-17.5(3)	-17.8(4)
Br2	60.9(5)	98.5(7)	54.6(4)	-6.8(4)	17.2(3)	9.1(4)
S1	42.5(8)	78.5(12)	55.8(9)	-0.7(8)	14.9(7)	-10.3(8)
O1	27(2)	81(3)	53(2)	-23(2)	7.0(17)	-23(2)
O2	65(3)	49(3)	107(4)	8(3)	-4(3)	0(2)
O3	47(2)	36(2)	68(3)	5(2)	-5(2)	-3.2(18)
C1	28(3)	51(3)	49(3)	0(3)	4(2)	9(2)
C2	51(4)	52(4)	49(3)	-18(3)	2(3)	-1(3)
C3	39(3)	39(3)	58(4)	-10(3)	5(3)	-9(2)
C4	23(2)	33(3)	40(3)	-3(2)	-0.4(19)	-2(2)
C5	31(3)	38(3)	41(3)	-2(2)	-5(2)	-4(2)
C6	31(3)	43(3)	46(3)	2(2)	-1(2)	-3(2)
C7	22(2)	33(3)	49(3)	-4(2)	1(2)	-1.8(19)
C8	25(2)	33(3)	43(3)	3(2)	2(2)	-1(2)
C9	26(2)	37(3)	44(3)	1(2)	3(2)	0(2)
C10	42(3)	58(4)	47(3)	1(3)	1(3)	-3(3)
C11	59(4)	80(5)	46(3)	-5(3)	11(3)	-10(4)
C12	22(2)	38(3)	37(3)	0(2)	0.3(19)	3(2)
C13	32(3)	39(3)	70(4)	1(3)	2(3)	7(2)
C14	29(3)	63(4)	61(4)	8(3)	-5(3)	19(3)
C15	29(3)	71(4)	39(3)	0(3)	-3(2)	-6(3)
C16	37(3)	51(3)	53(3)	-12(3)	-1(2)	-8(3)
C17	29(3)	41(3)	49(3)	-7(2)	-1(2)	4(2)
C18	30(3)	41(3)	47(3)	-1(2)	7(2)	-2(2)
C19	23(2)	38(3)	51(3)	3(2)	1(2)	-5(2)
C20	30(3)	29(3)	59(3)	5(2)	-1(2)	0(2)
C21	24(3)	60(4)	56(3)	-8(3)	4(2)	-17(3)
C22	37(3)	64(4)	45(3)	2(3)	4(2)	16(3)
C23	41(4)	84(5)	69(4)	3(4)	-6(3)	12(4)
C24	35(4)	133(9)	93(6)	-2(6)	-4(4)	-2(5)
C25	34(4)	124(8)	91(6)	-21(6)	-6(4)	-30(4)
C26	54(5)	106(7)	84(5)	-23(5)	12(4)	-43(5)

Table *S4*. Bond Lengths for **5b**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C15	1.906(6)	C9	C10	1.413(8)
Br2	C1	1.897(6)	C9	C18	1.360(8)

S1	C11	1.717(7)	C10	C11	1.353(9)
S1	C18	1.710(6)	C12	C13	1.392(8)
O1	C7	1.388(6)	C12	C17	1.381(8)
O1	C19	1.410(7)	C13	C14	1.371(9)
O2	C20	1.217(7)	C14	C15	1.378(10)
O3	C19	1.442(7)	C15	C16	1.366(9)
O3	C22	1.359(8)	C16	C17	1.384(8)
C1	C2	1.358(9)	C18	C19	1.479(8)
C1	C6	1.398(8)	C19	C20	1.538(7)
C2	C3	1.397(9)	C20	C21	1.444(8)
C3	C4	1.405(8)	C21	C22	1.388(10)
C4	C5	1.403(7)	C21	C26	1.390(9)
C4	C7	1.478(7)	C22	C23	1.374(9)
C5	C6	1.371(8)	C23	C24	1.361(12)
C7	C8	1.339(8)	C24	C25	1.397(15)
C8	C9	1.473(7)	C25	C26	1.403(14)
C8	C12	1.485(7)			

Table *S5*. Bond Angles for **5b**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C18	S1	C11	90.9(3)	C13	C14	C15	119.6(5)
C7	O1	C19	122.5(4)	C14	C15	Br1	119.3(5)
C22	O3	C19	107.2(4)	C16	C15	Br1	119.5(5)
C2	C1	Br2	120.7(5)	C16	C15	C14	121.2(5)
C2	C1	C6	121.2(5)	C15	C16	C17	118.8(6)
C6	C1	Br2	118.0(4)	C12	C17	C16	121.5(5)
C1	C2	C3	120.3(6)	C9	C18	S1	112.5(4)
C2	C3	C4	119.6(5)	C9	C18	C19	122.9(5)
C3	C4	C7	120.0(5)	C19	C18	S1	124.6(4)
C5	C4	C3	118.5(5)	O1	C19	O3	107.4(5)
C5	C4	C7	121.4(5)	O1	C19	C18	111.9(4)
C6	C5	C4	121.4(5)	O1	C19	C20	105.4(5)
C5	C6	C1	118.8(5)	O3	C19	C18	111.0(5)
O1	C7	C4	109.6(4)	O3	C19	C20	105.3(4)
C8	C7	O1	122.4(5)	C18	C19	C20	115.2(5)
C8	C7	C4	128.0(5)	O2	C20	C19	125.0(5)
C7	C8	C9	117.1(5)	O2	C20	C21	128.9(6)
C7	C8	C12	125.5(5)	C21	C20	C19	106.0(5)
C9	C8	C12	117.1(5)	C22	C21	C20	106.0(5)
C10	C9	C8	128.4(5)	C22	C21	C26	120.6(7)

C18	C9	C8	119.7(5)	C26	C21	C20	133.4(8)
C18	C9	C10	111.8(5)	O3	C22	C21	115.2(5)
C11	C10	C9	112.7(6)	O3	C22	C23	121.7(7)
C10	C11	S1	112.0(5)	C23	C22	C21	123.1(7)
C13	C12	C8	120.2(5)	C24	C23	C22	115.5(9)
C17	C12	C8	121.5(5)	C23	C24	C25	124.6(8)
C17	C12	C13	118.2(5)	C24	C25	C26	118.7(7)
C14	C13	C12	120.8(6)	C21	C26	C25	117.6(9)

Table *S6*. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **5b**.

Atom	x	y	z	U(eq)
H2	5539.7	2827.61	1700.18	61
H3	4645.93	2800.7	3535.49	54
H5	6513.64	4635.71	4682.34	44
H6	7386.87	4648.85	2863.41	48
H10	5426.77	4319.13	9127.6	59
H11	3846.4	4113.42	10330.47	74
H13	7197.54	3167.8	6578.88	56
H14	8976.25	3518.76	7197.33	62
H16	7936.76	5684.08	7919.21	56
H17	6143.6	5324.76	7324.5	47
H23	507.24	4517.13	4457.88	78
H24	-983.21	3756.64	3858.24	105
H25	-1098.82	2442.92	4305.12	100
H26	412.8	1826.41	5348.69	97

Experimental

Single crystals of $C_{26}H_{14}Br_2O_3S$ **5b** were obtained by recrystallization from dichloromethane and petroleum ether (1:10). A suitable crystal was selected and analyzed on a diffractometer. The crystal was kept at 293(10) K during data collection. Using Olex2, the structure was solved with the Unknown structure solution program using Unknown and refined with the Unknown refinement package using Unknown minimisation.

7. References

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8. NMR Spectra

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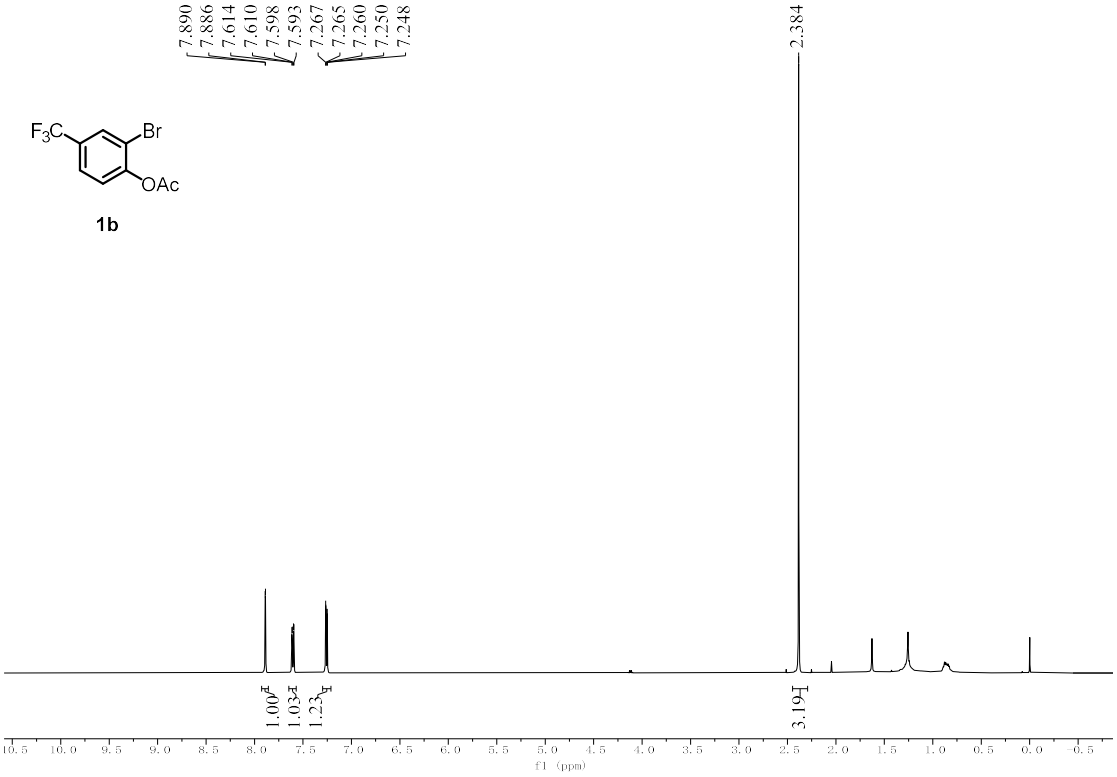
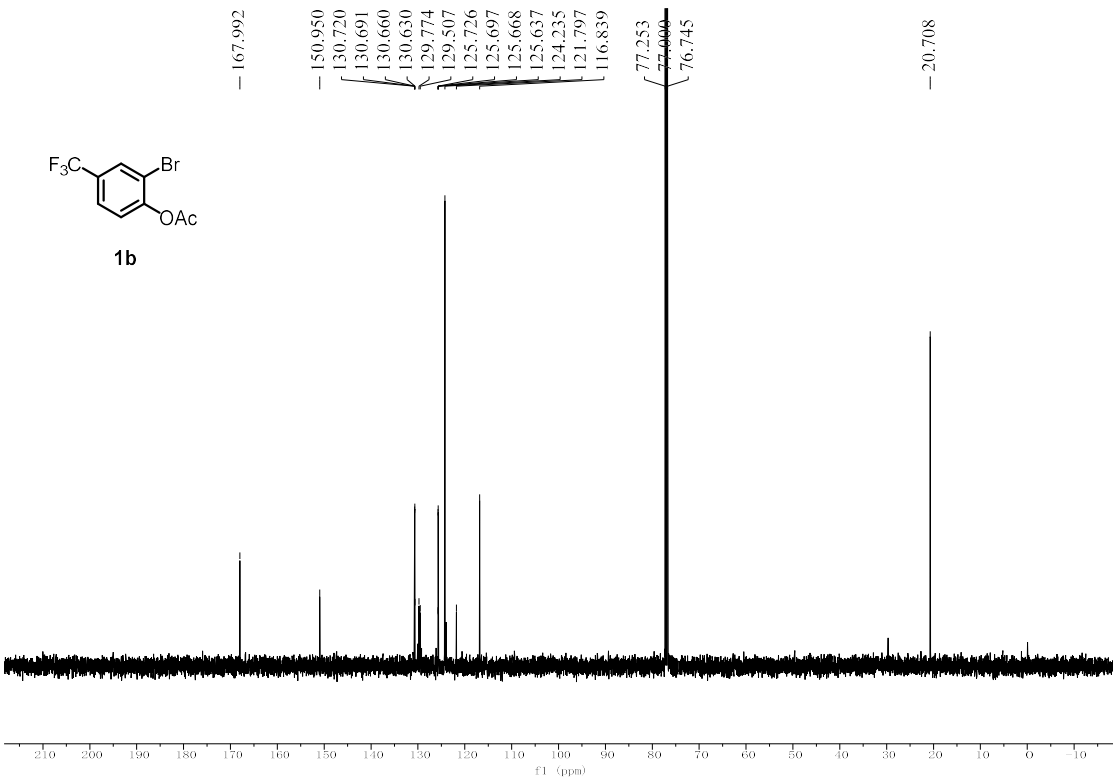


^{13}C NMR (126 MHz, $CDCl_3$)



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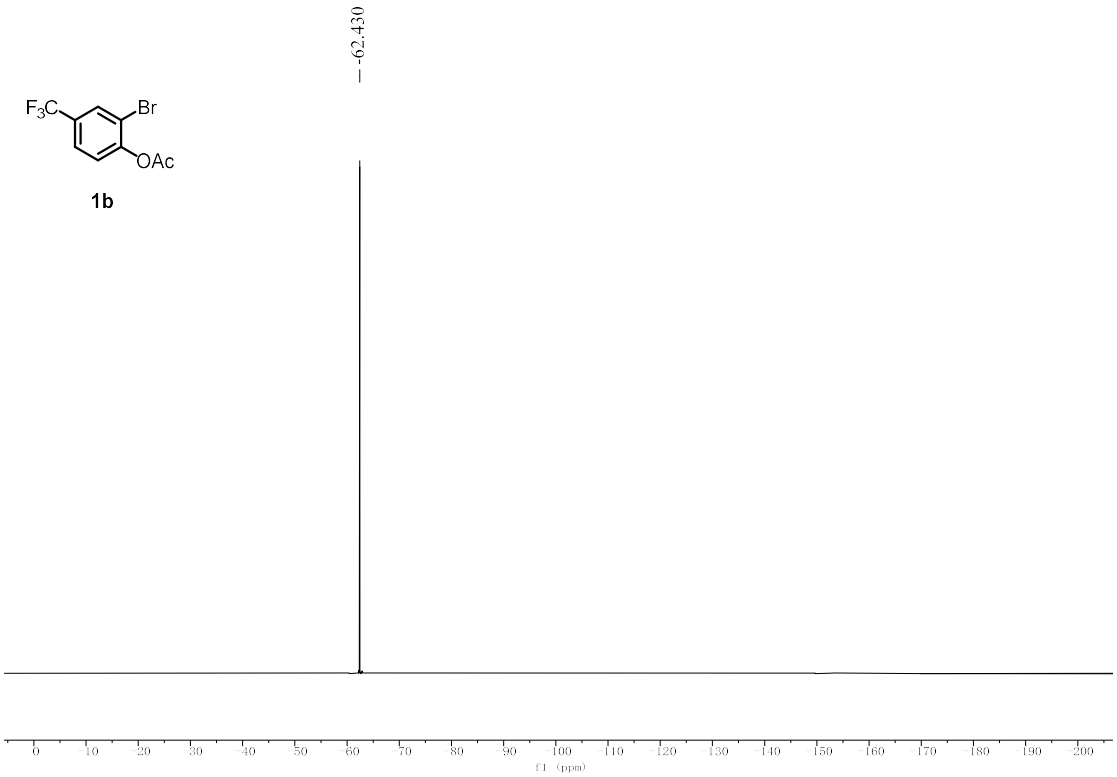

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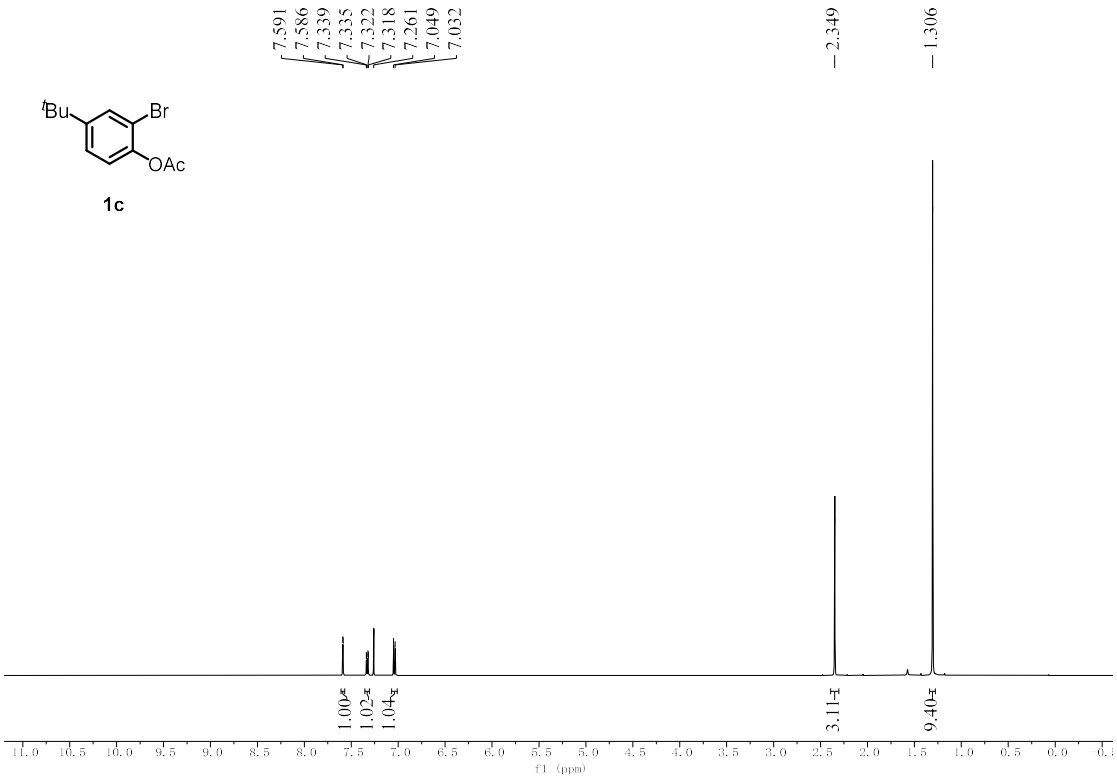

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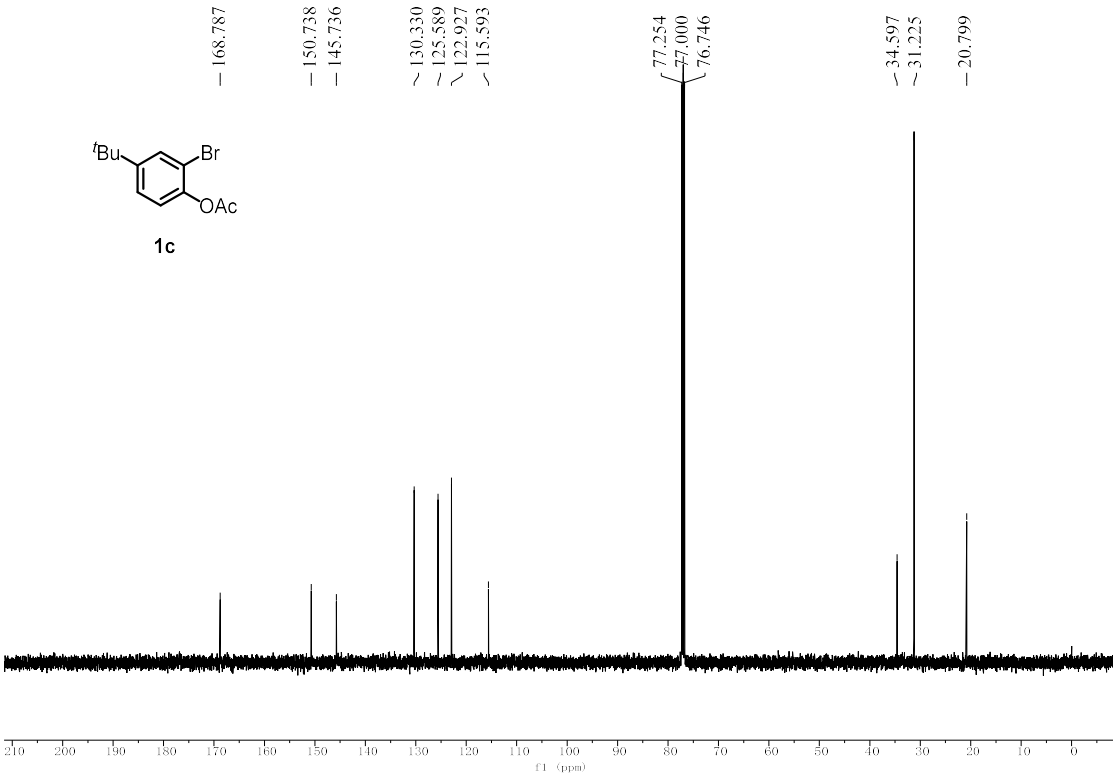

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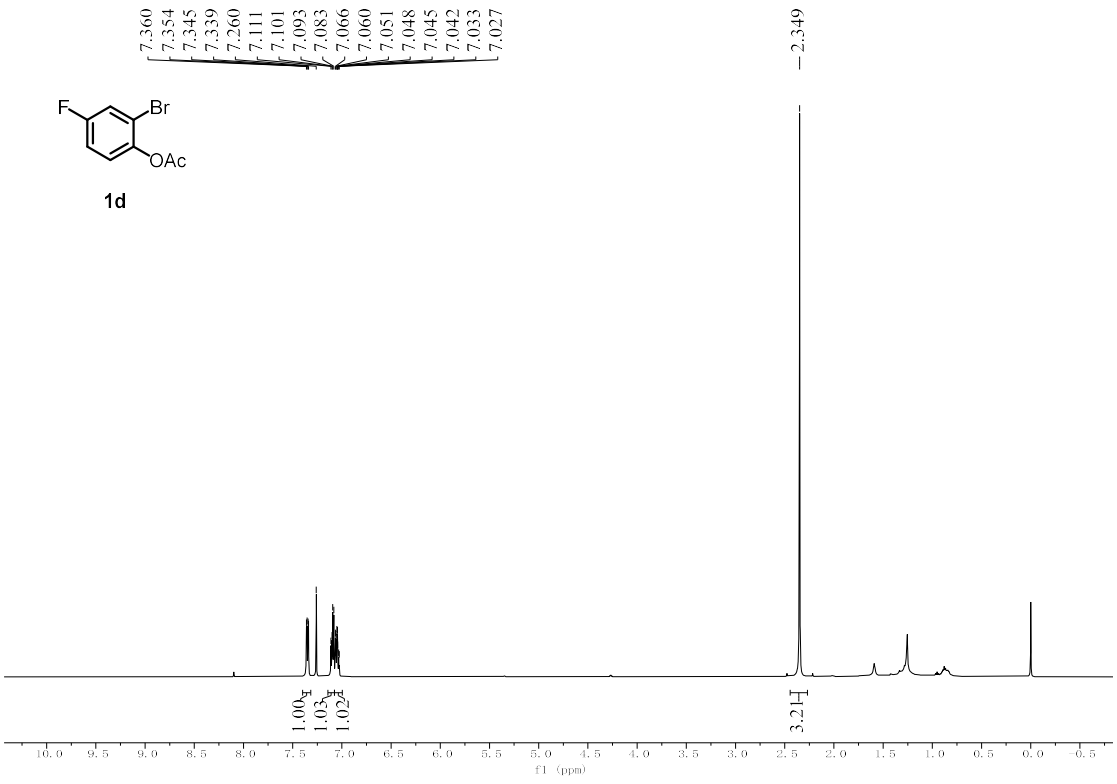

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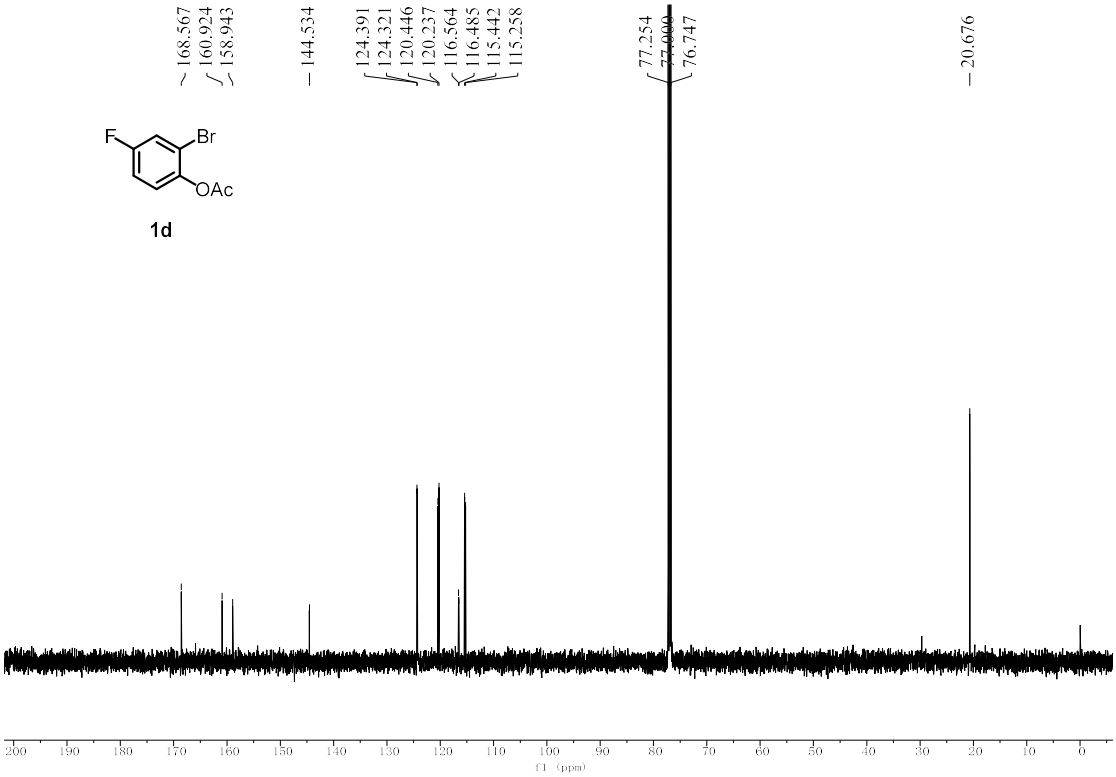

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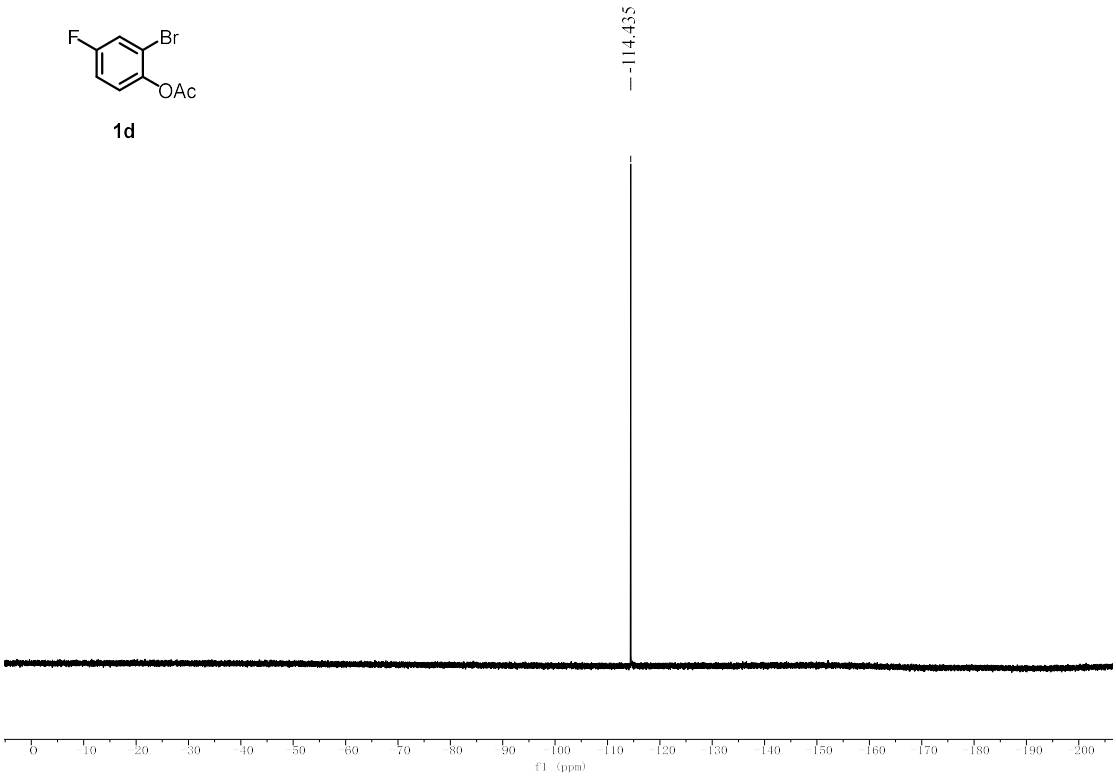

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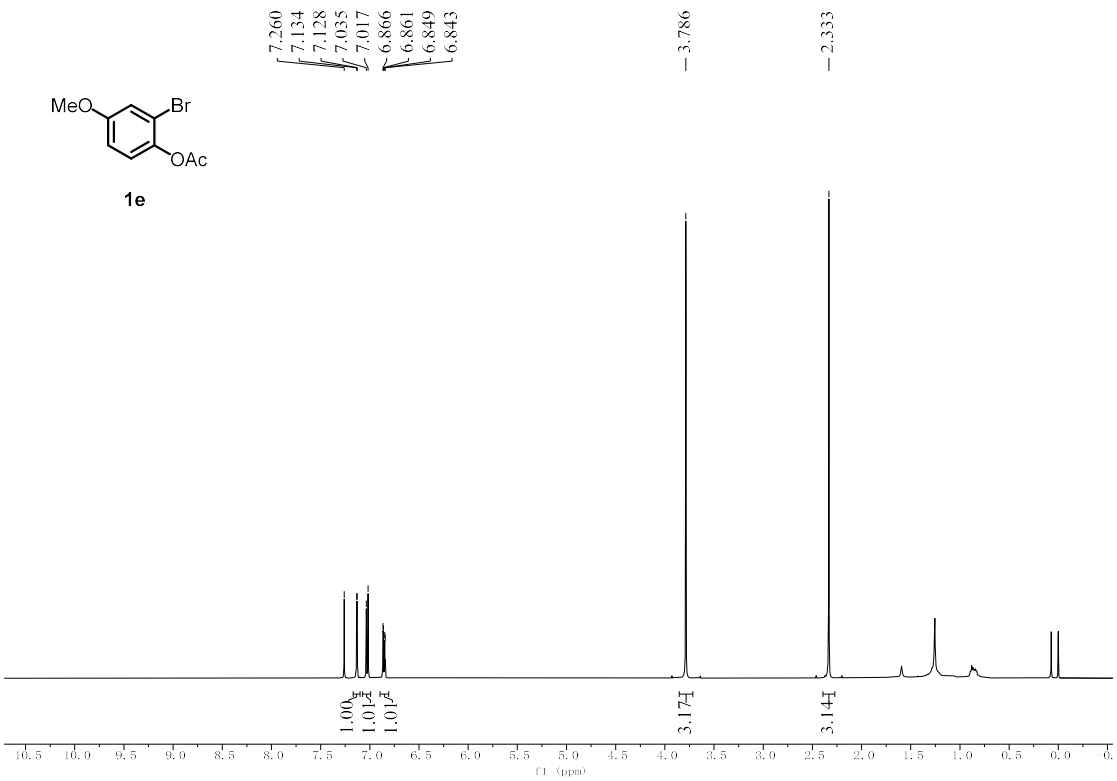

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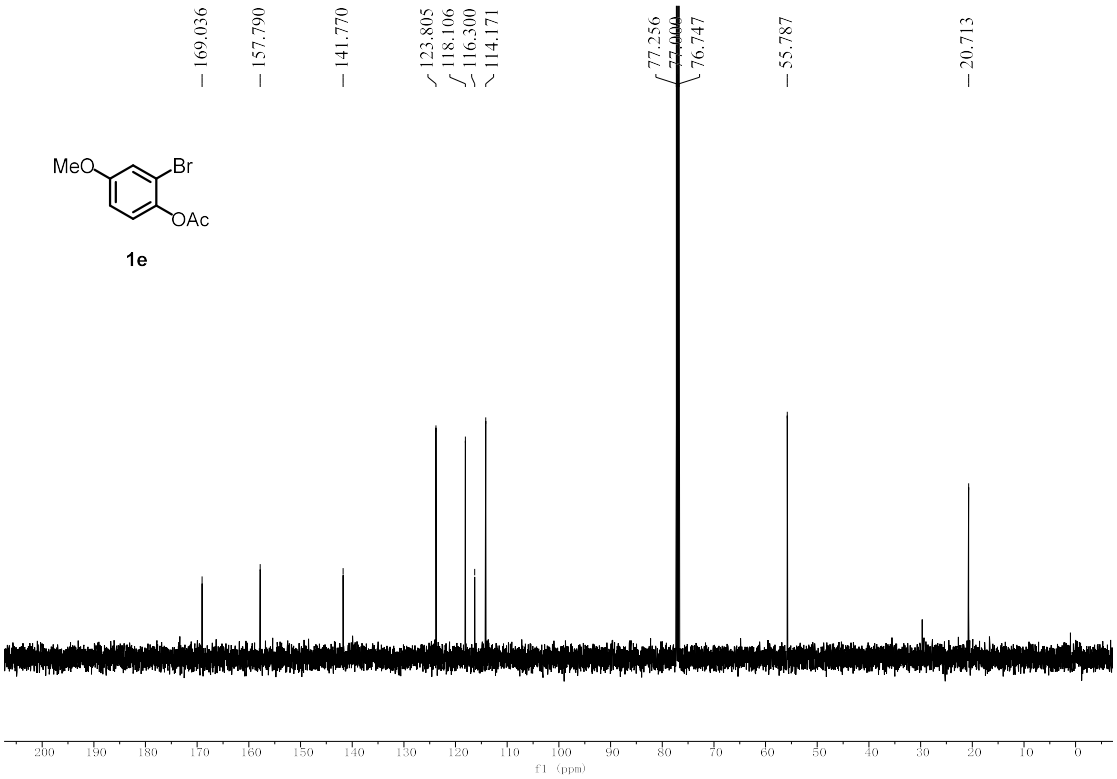

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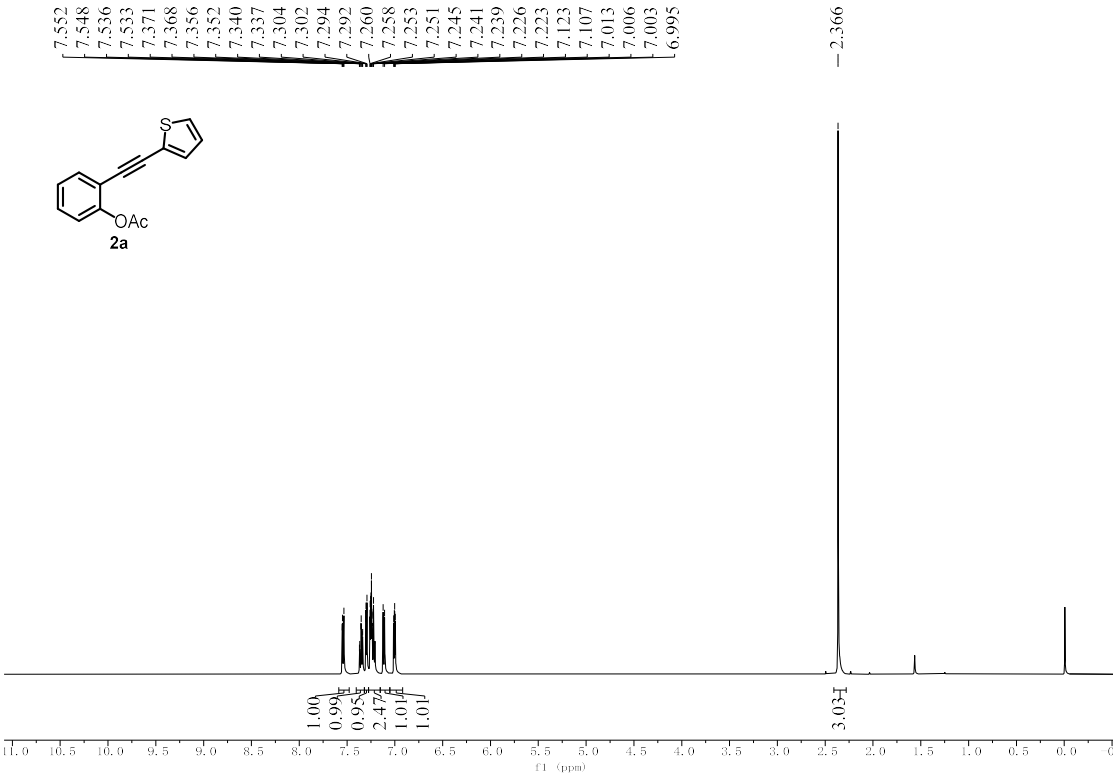

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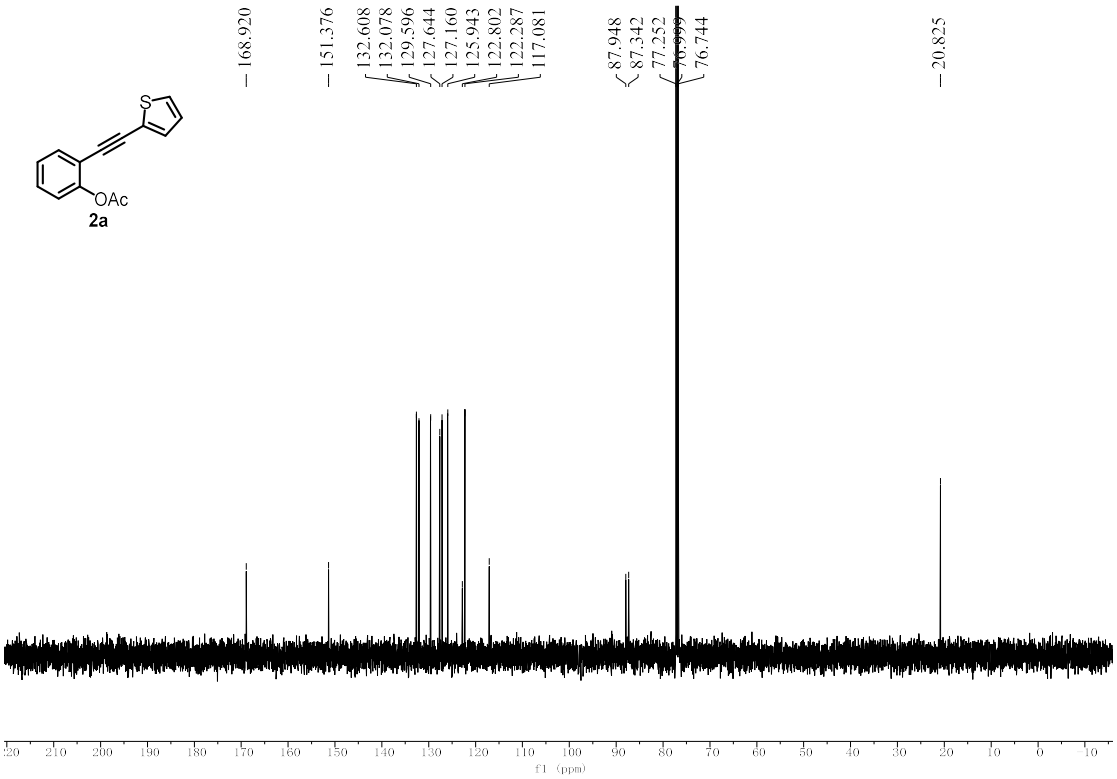

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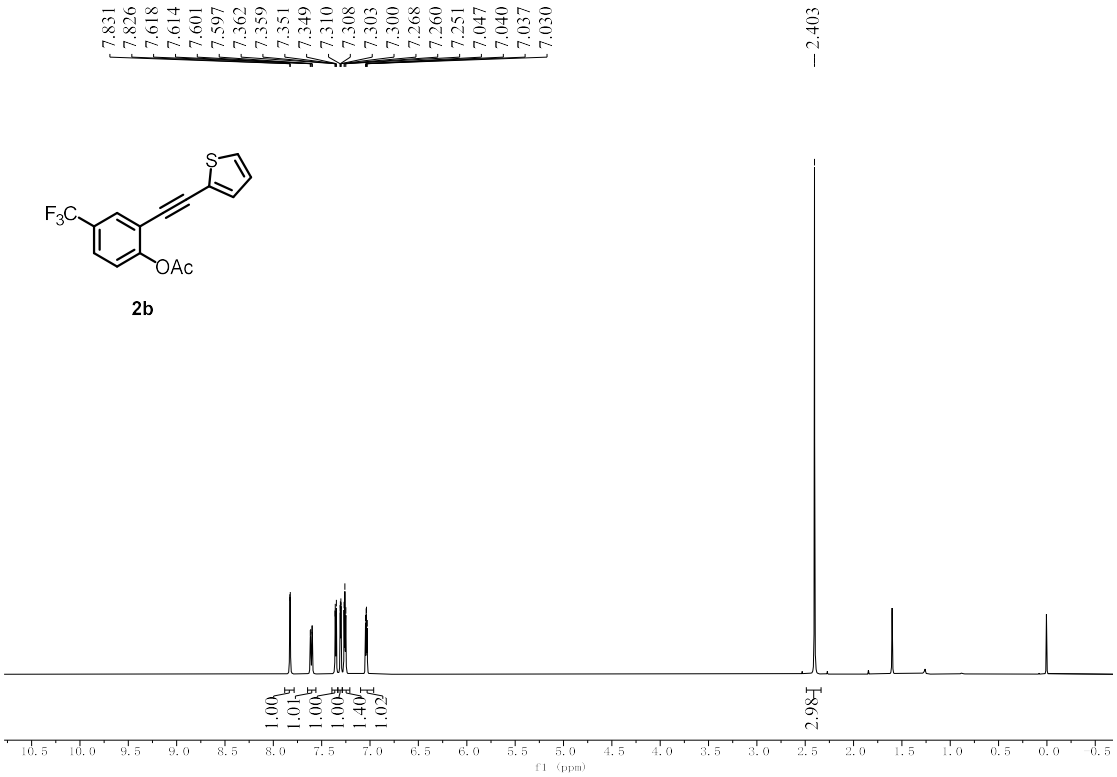

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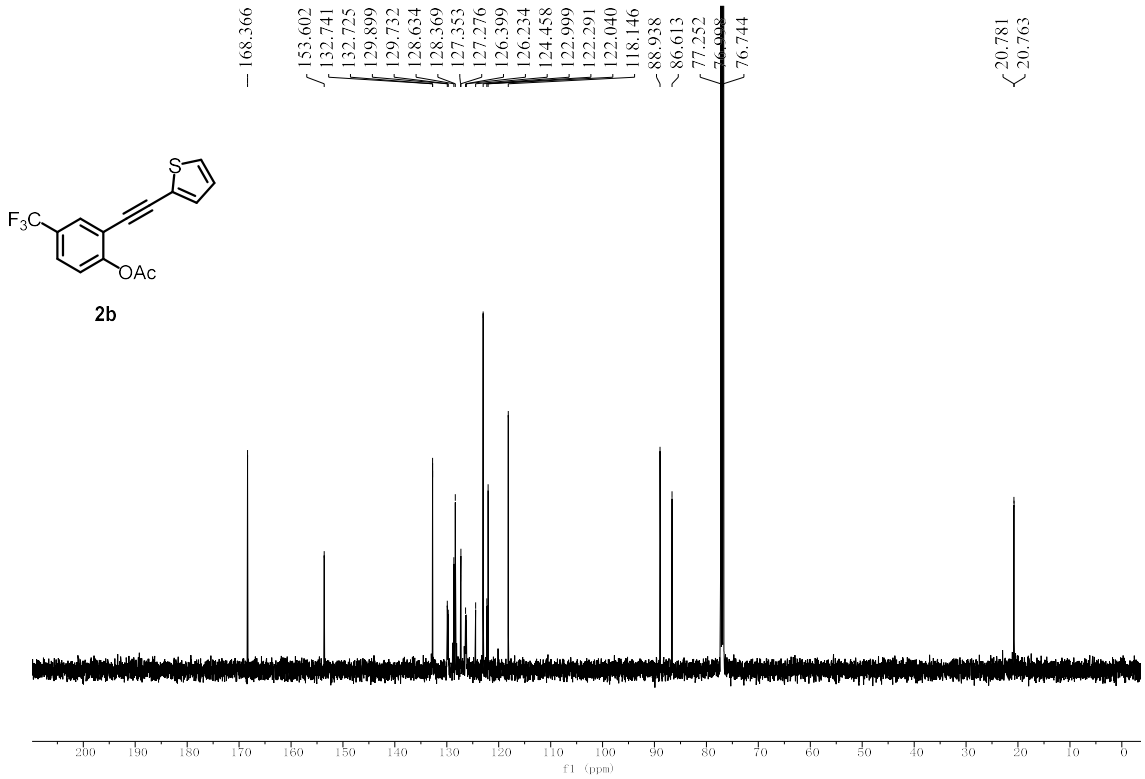

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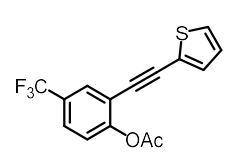

2b

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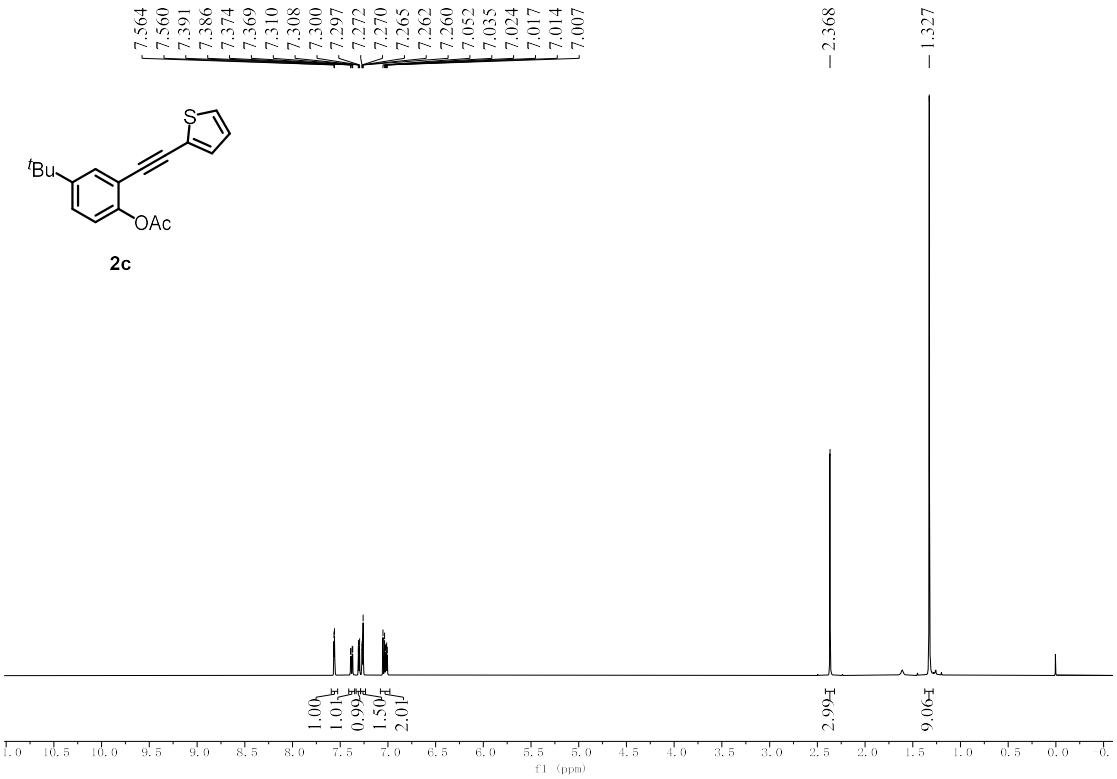

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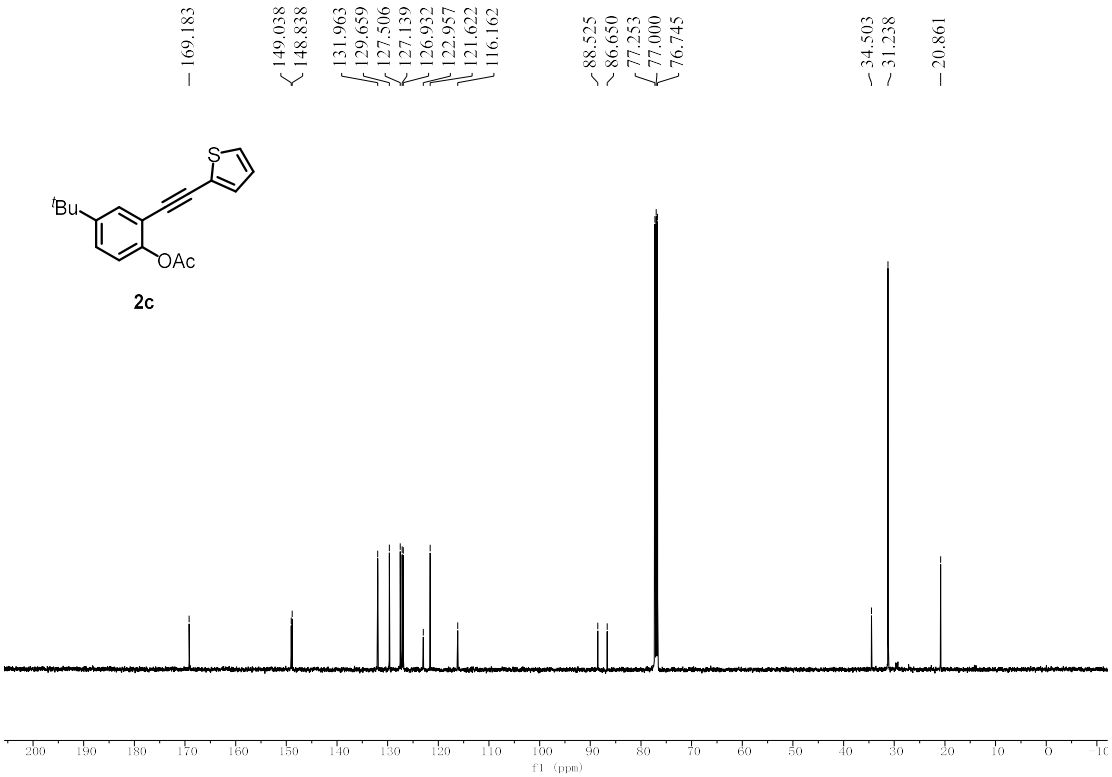

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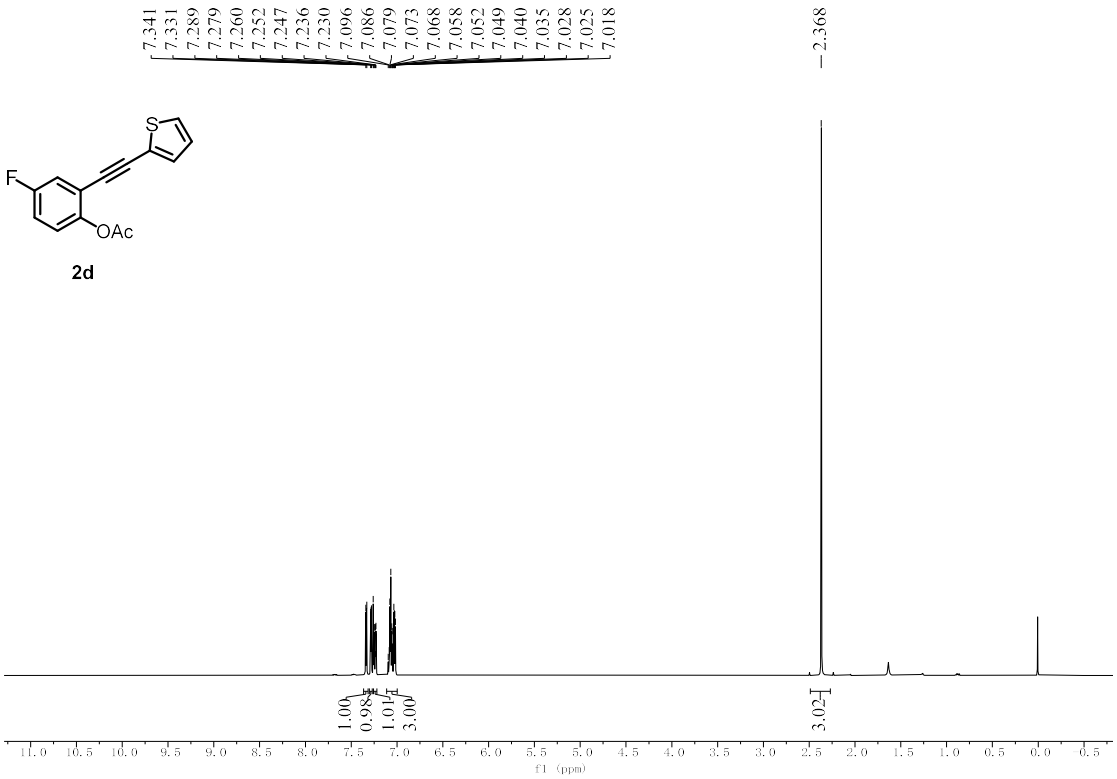

2d

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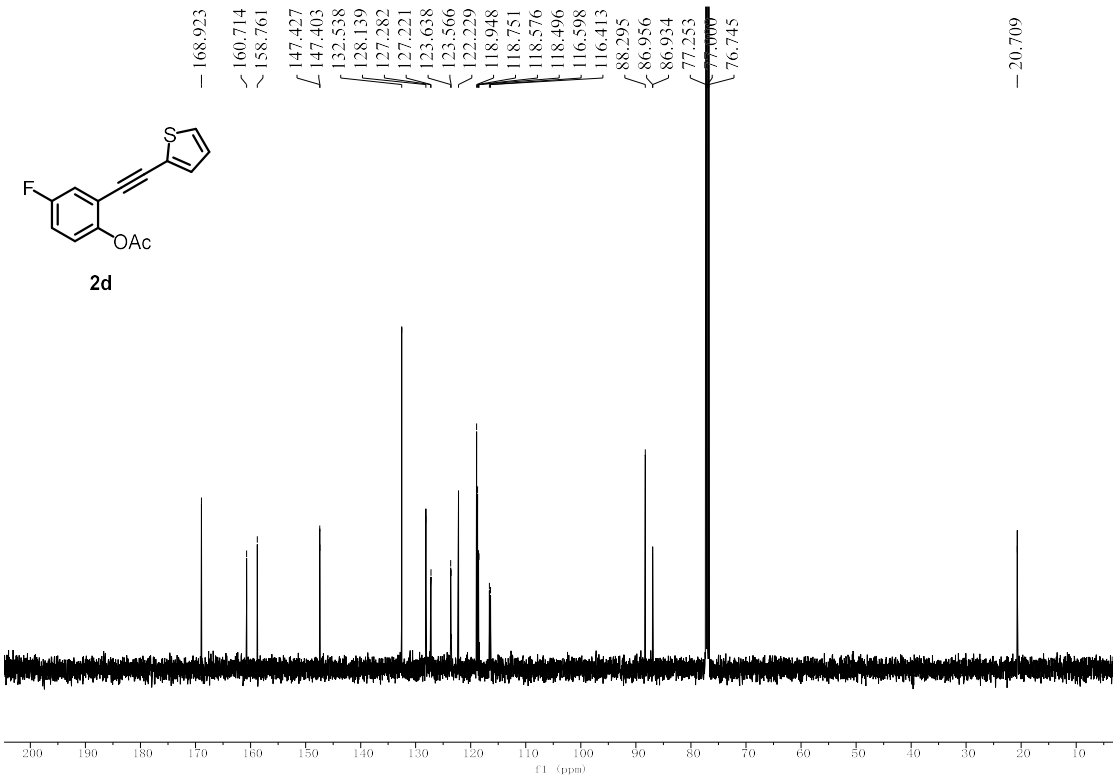

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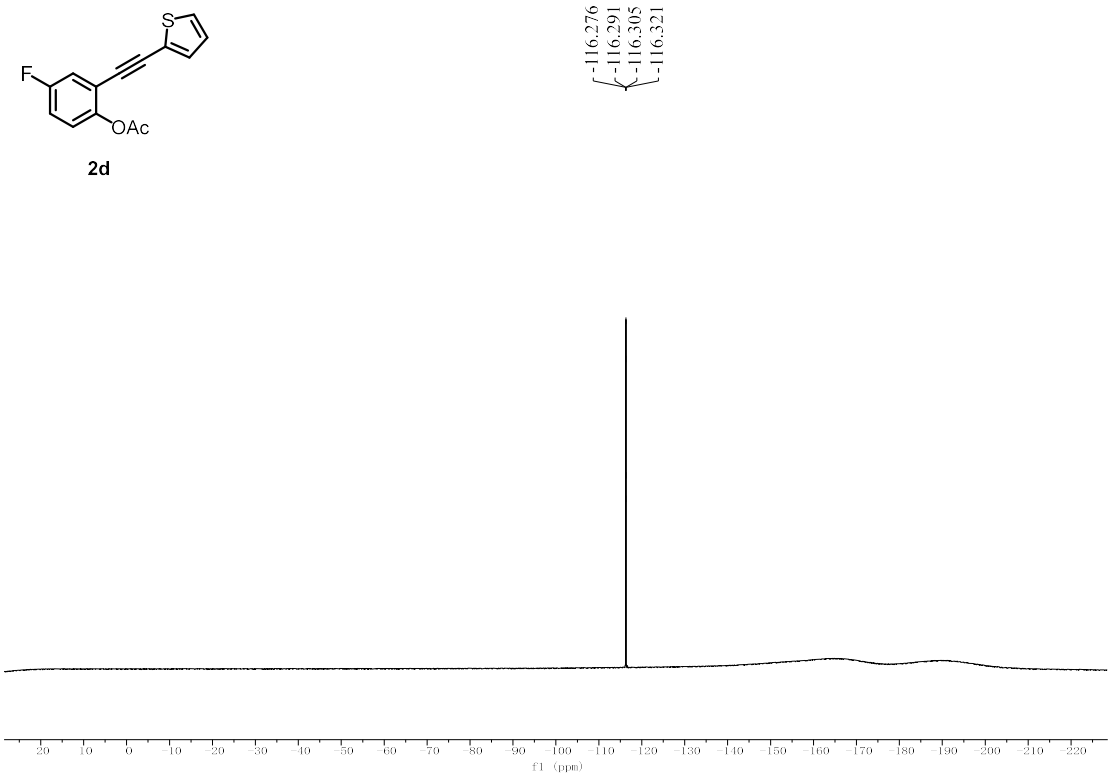

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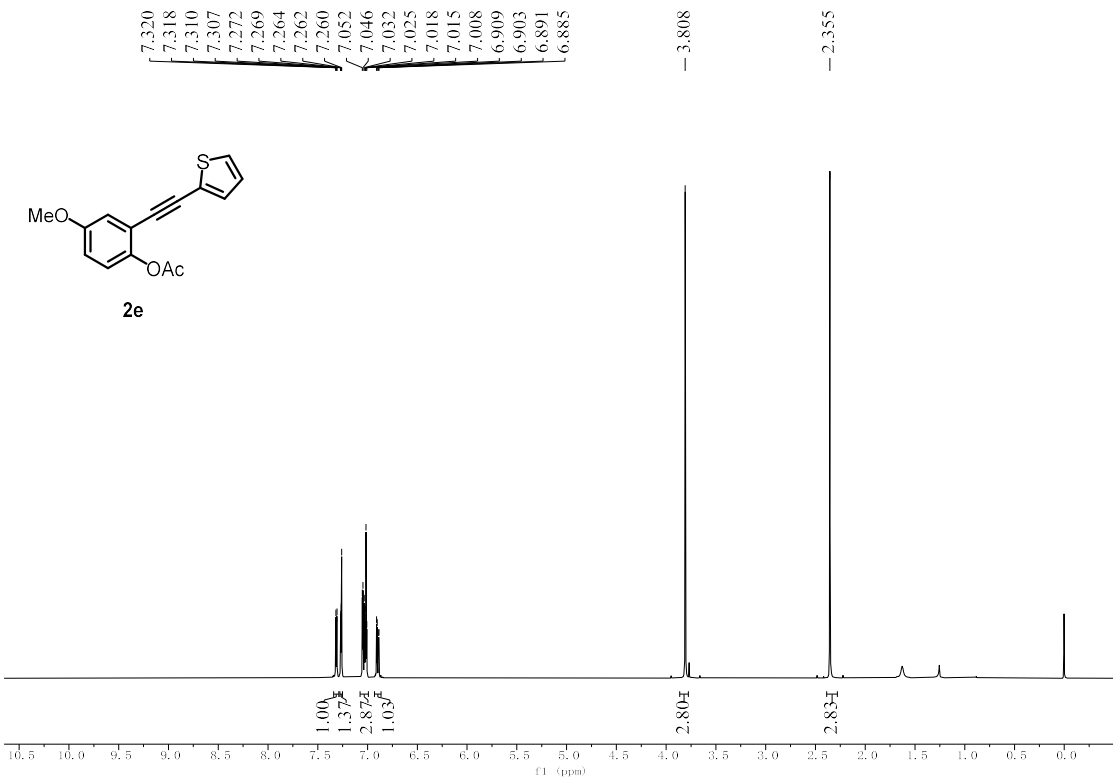

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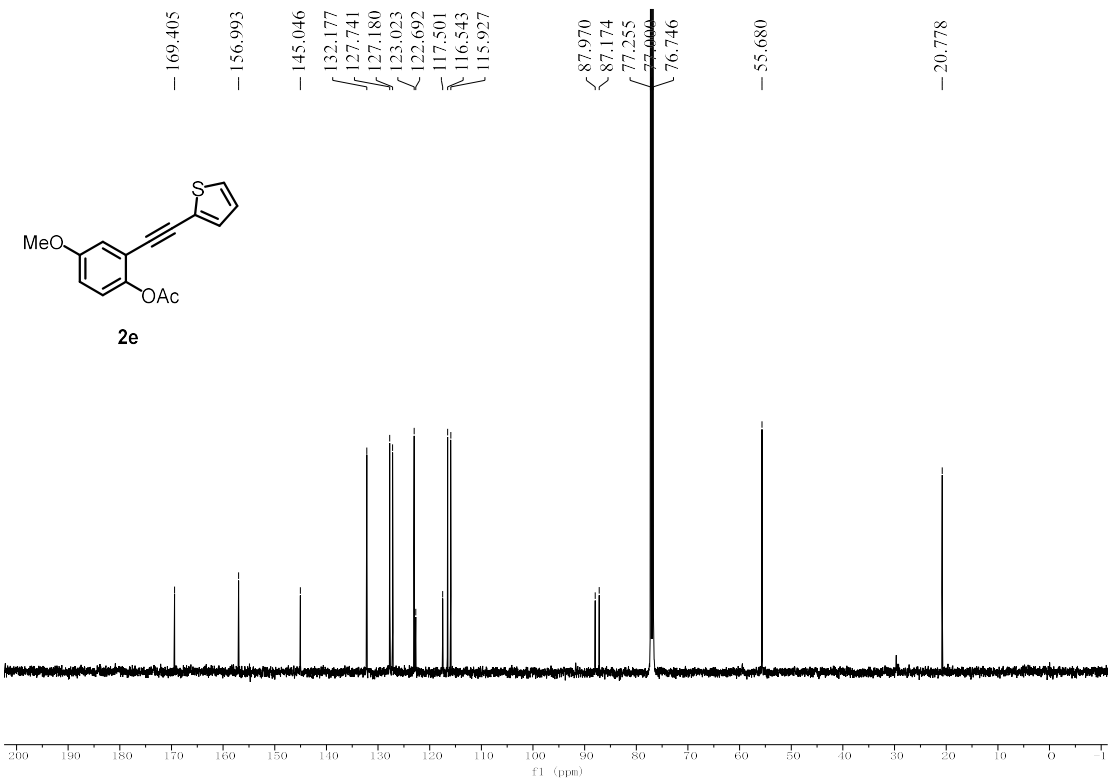

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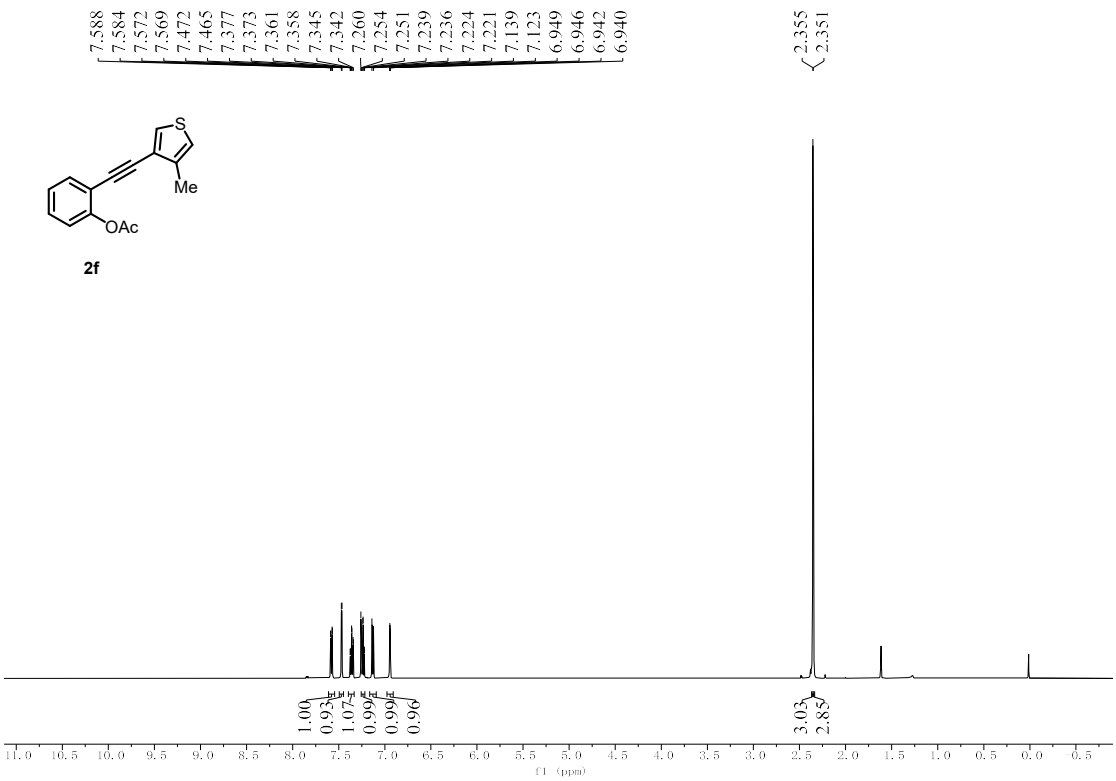

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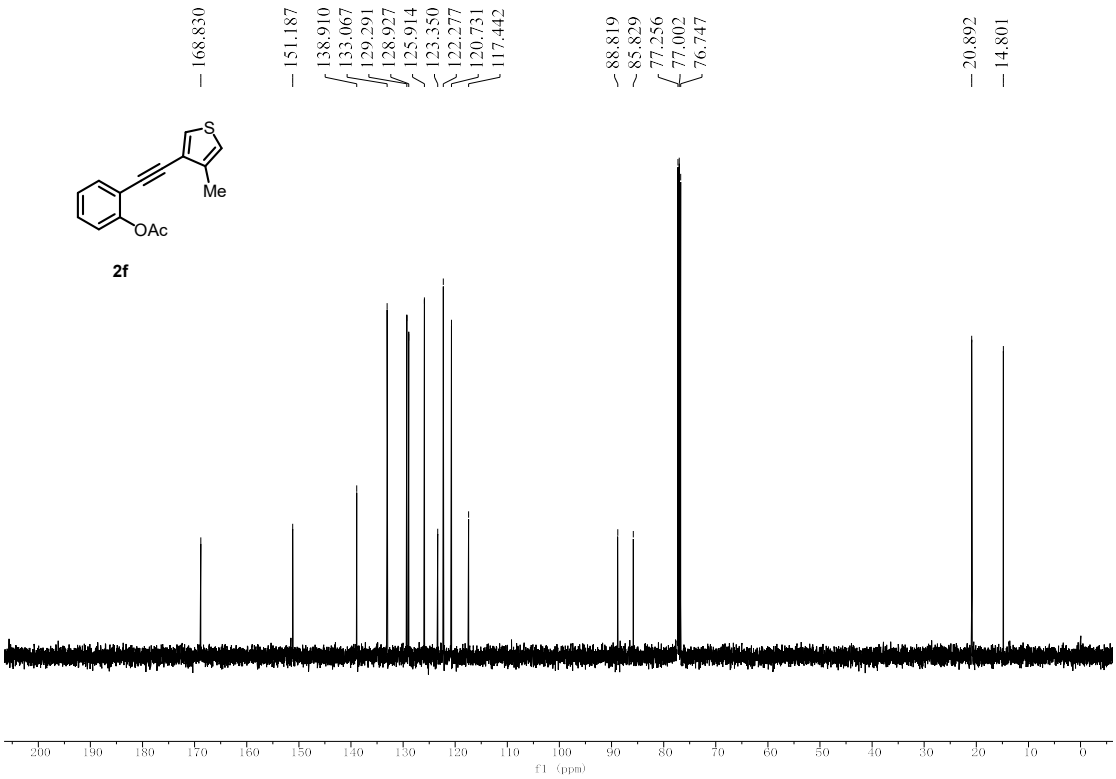

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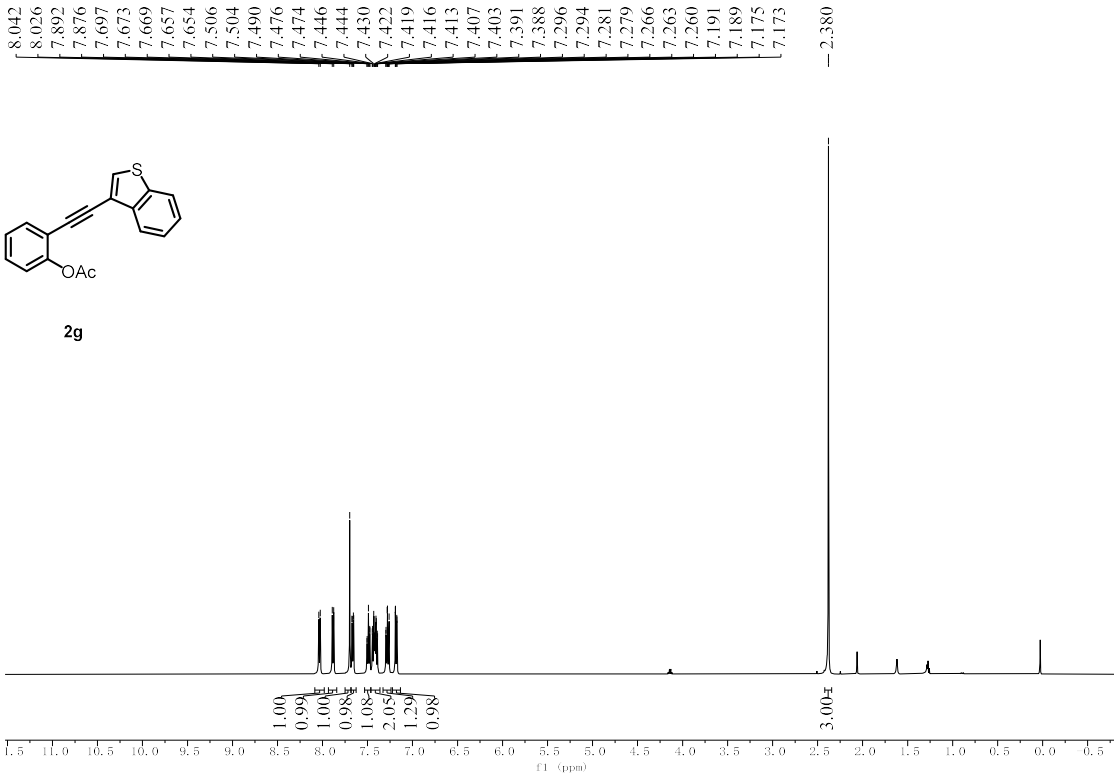

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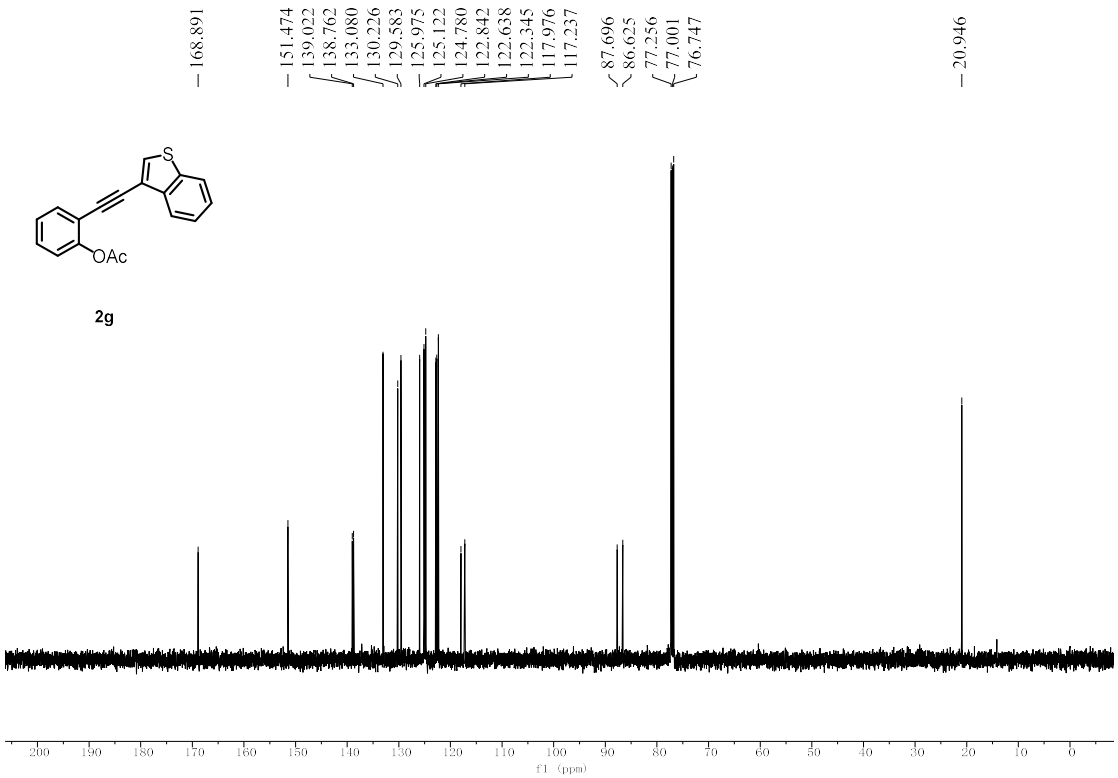

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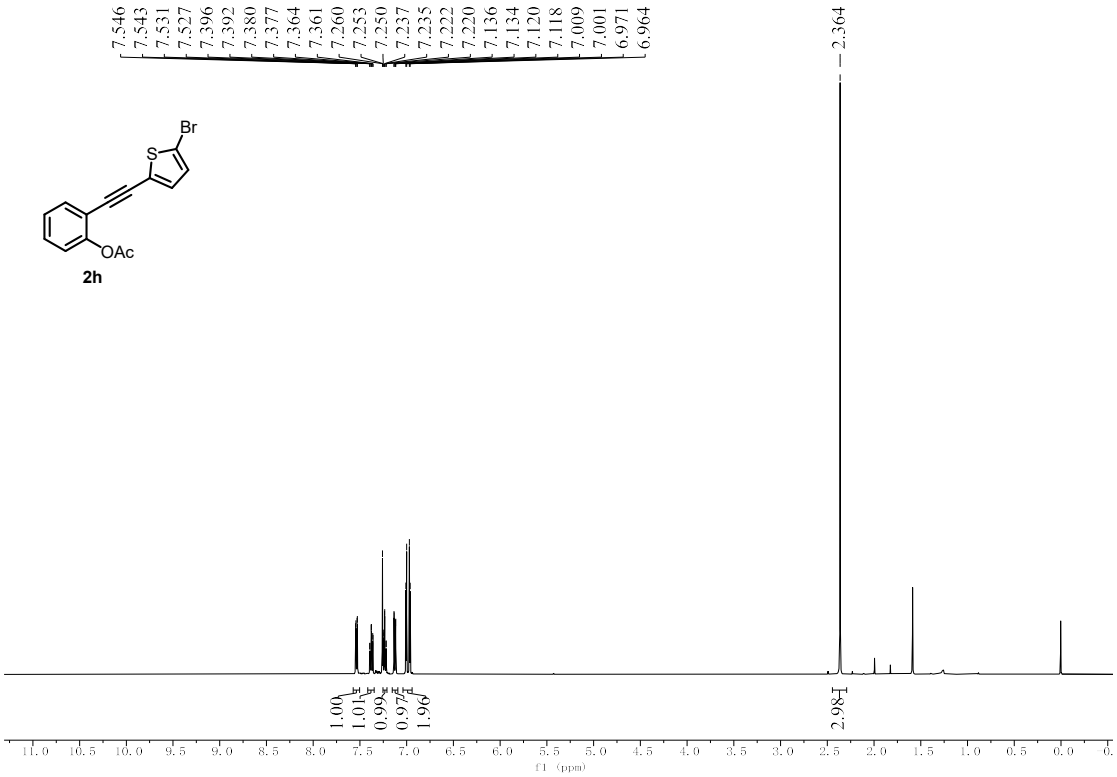

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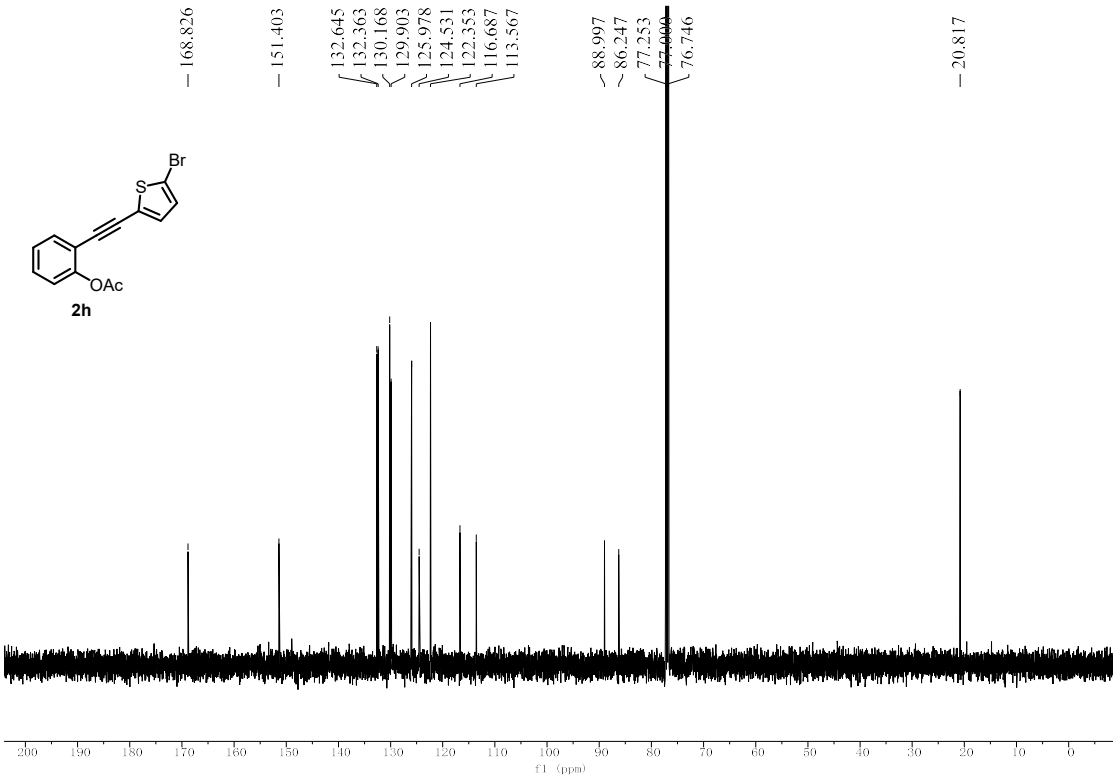

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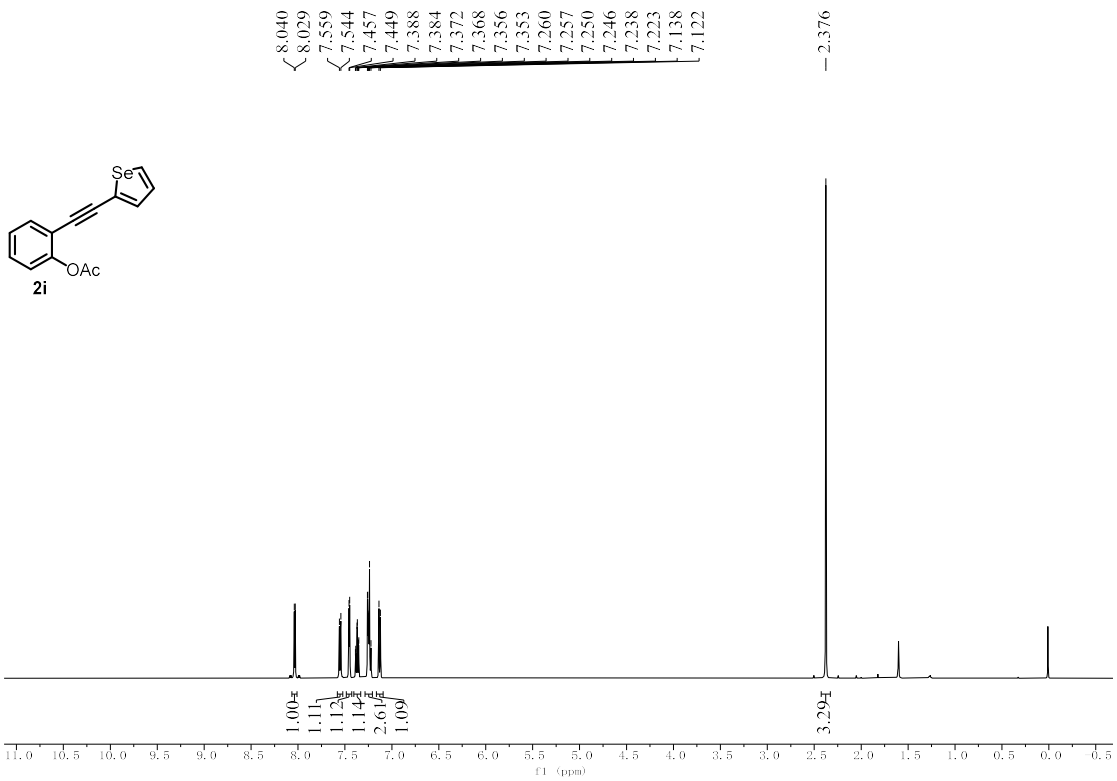

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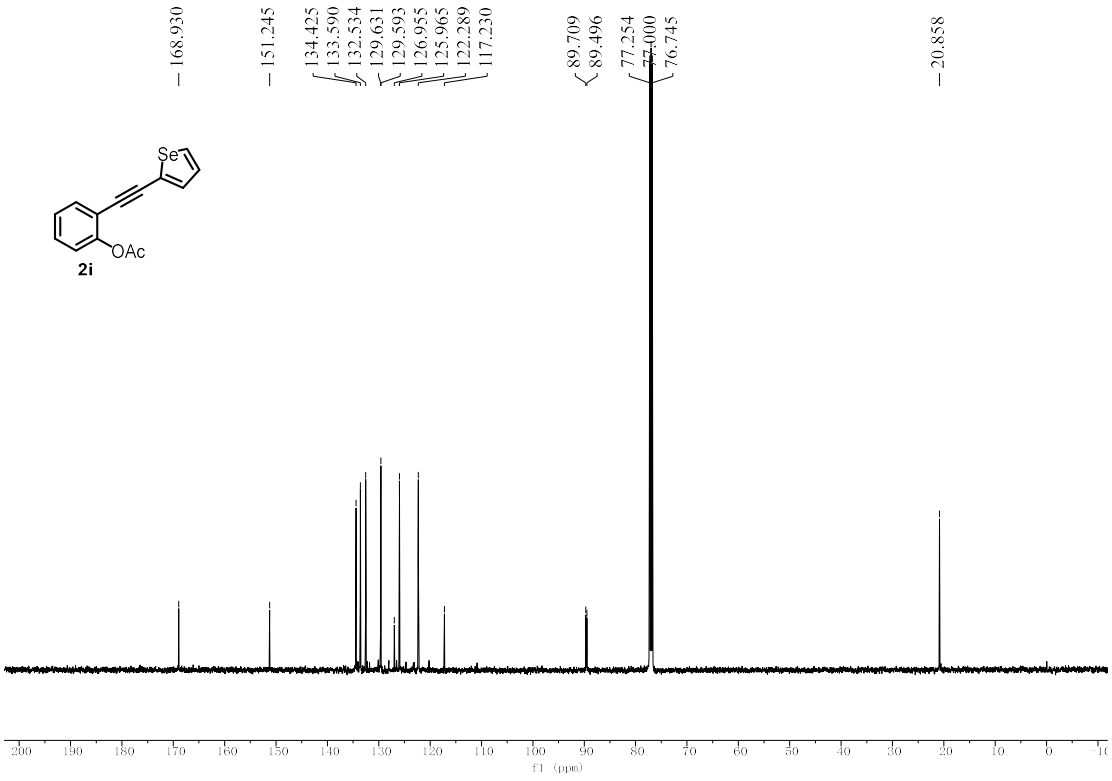

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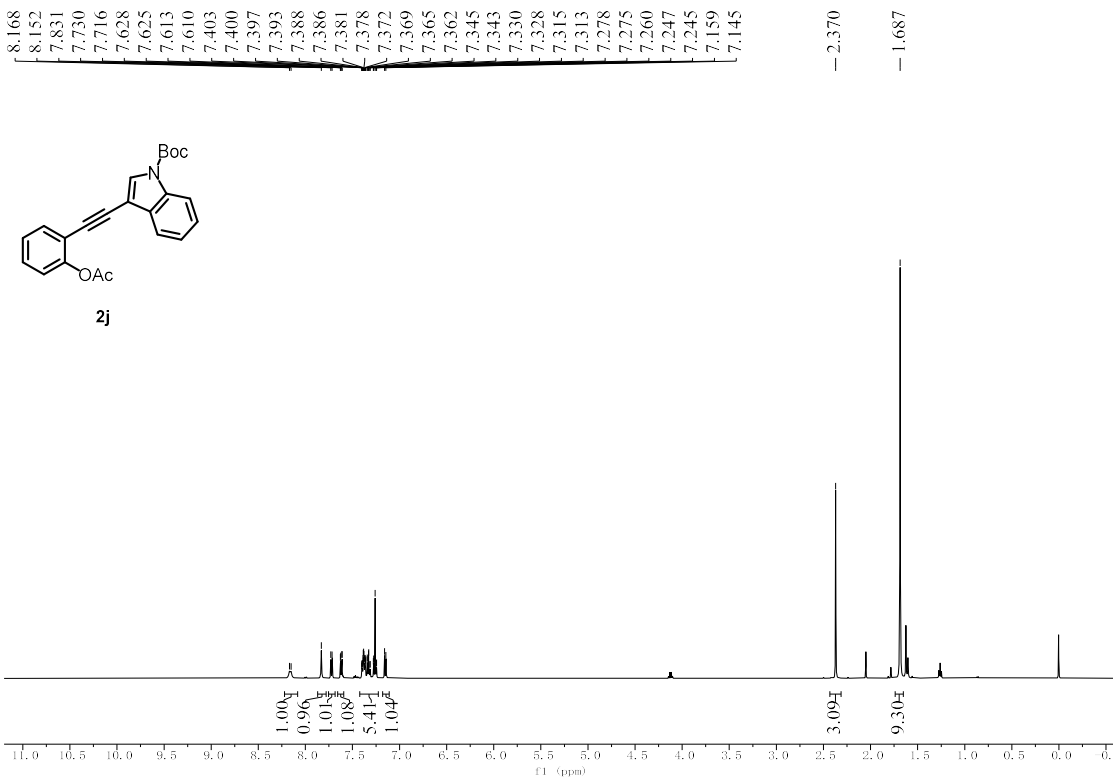

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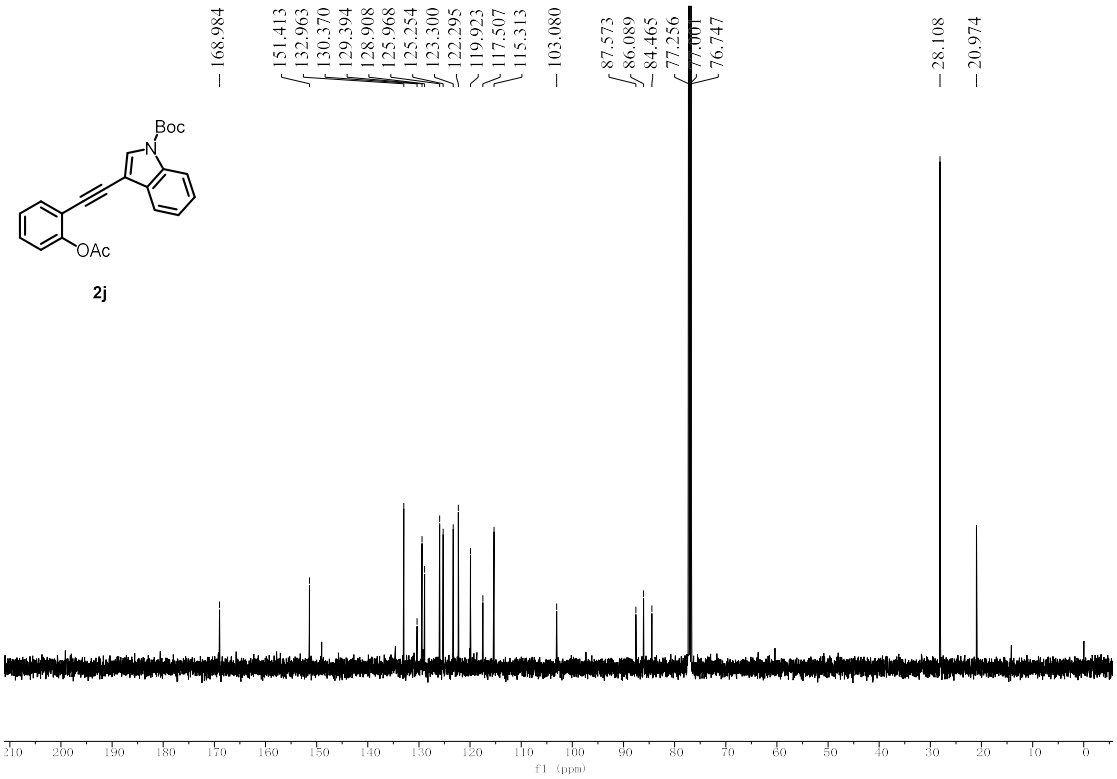

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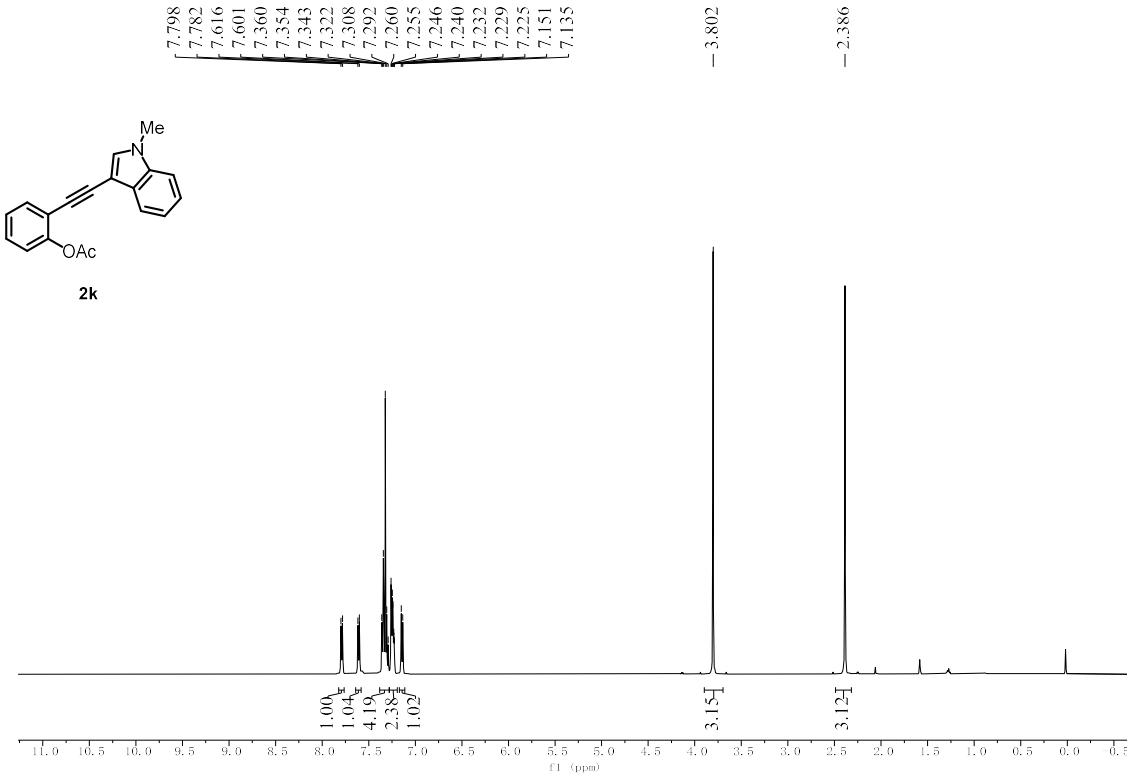

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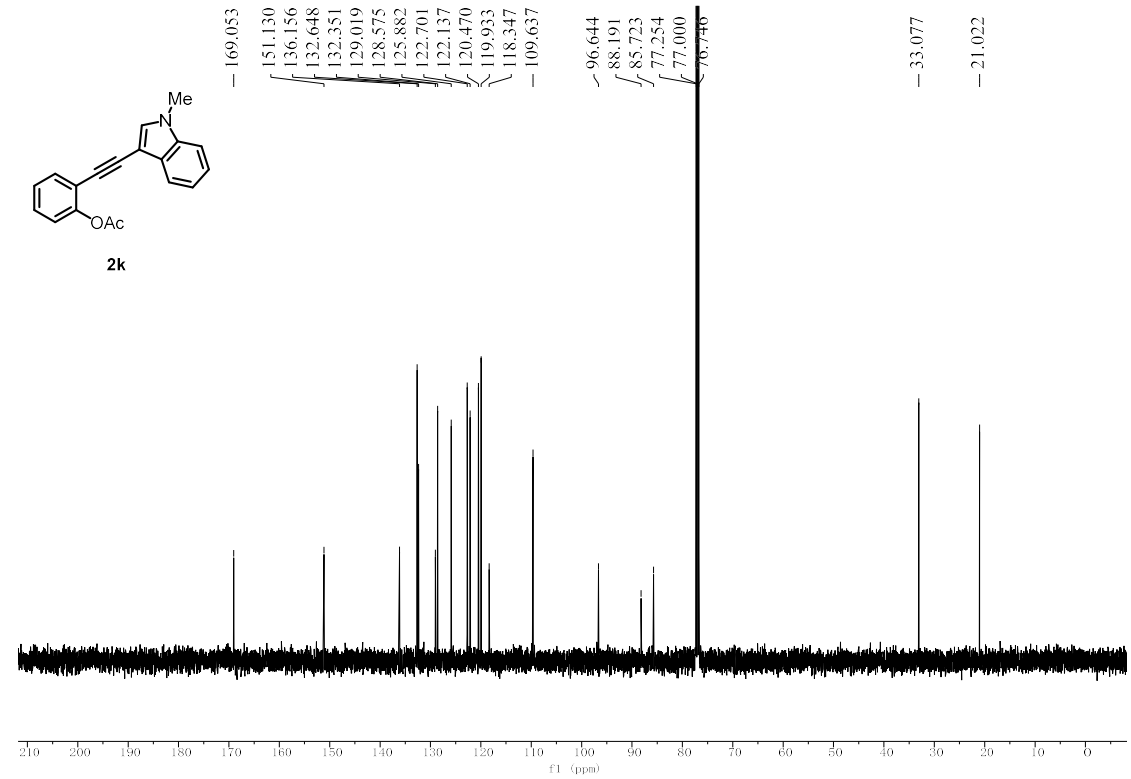

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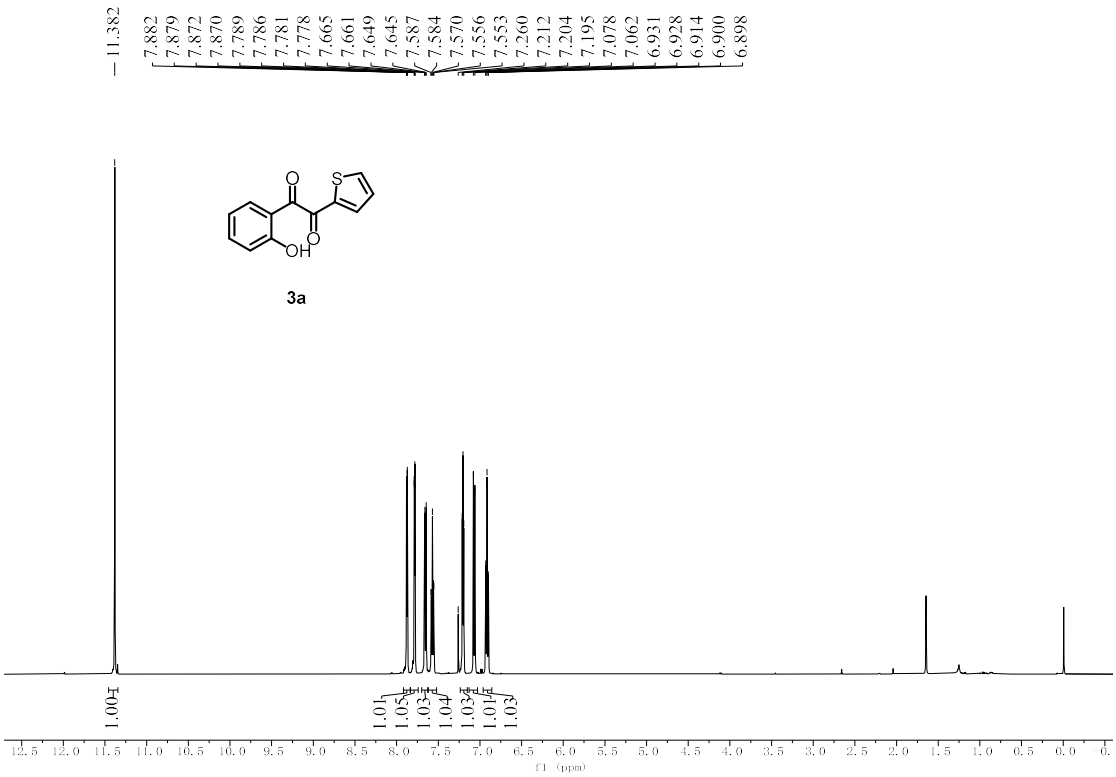
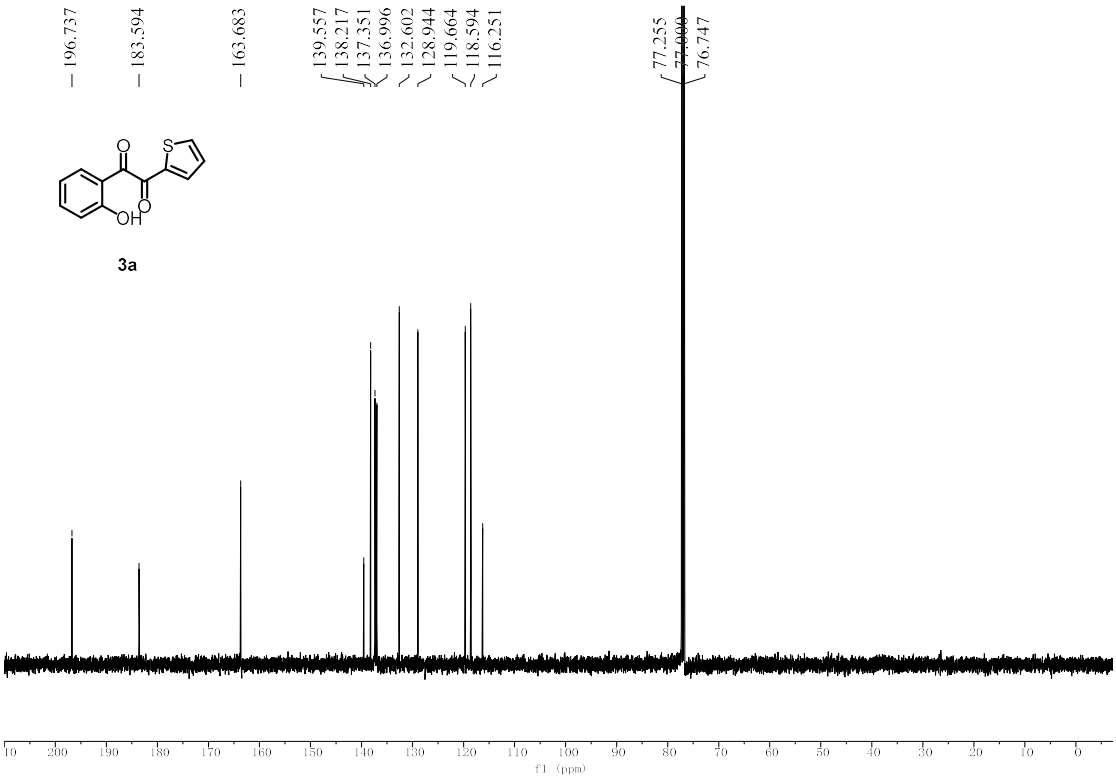
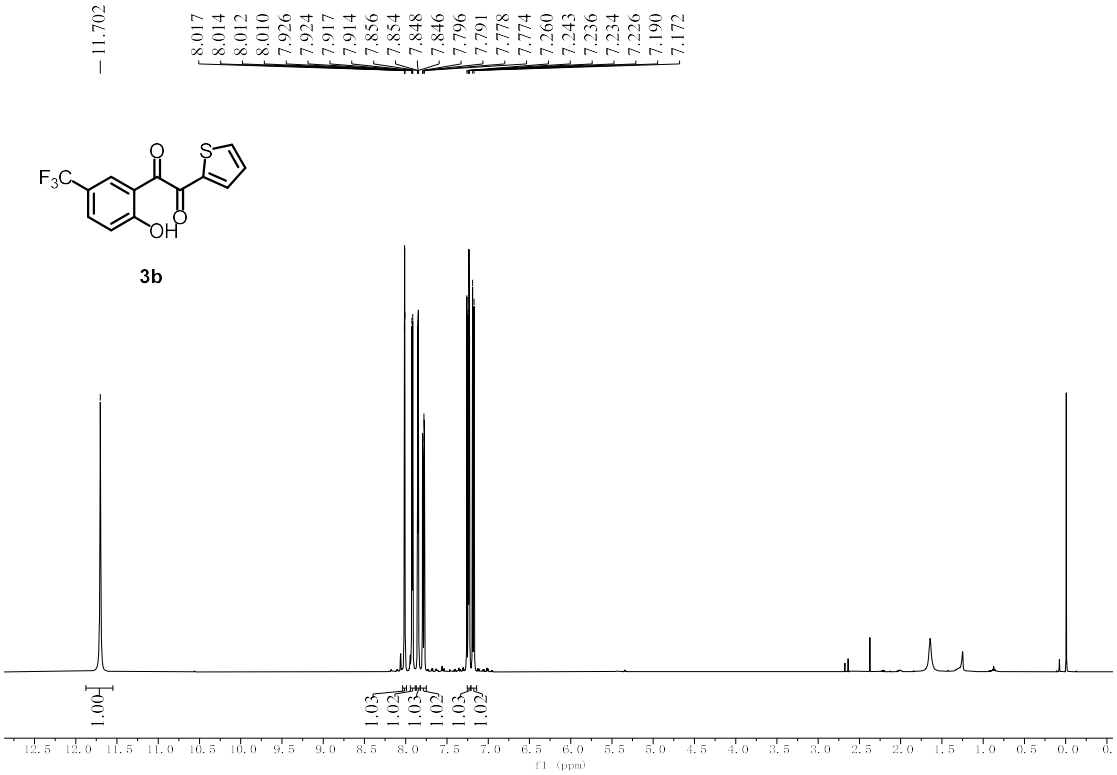


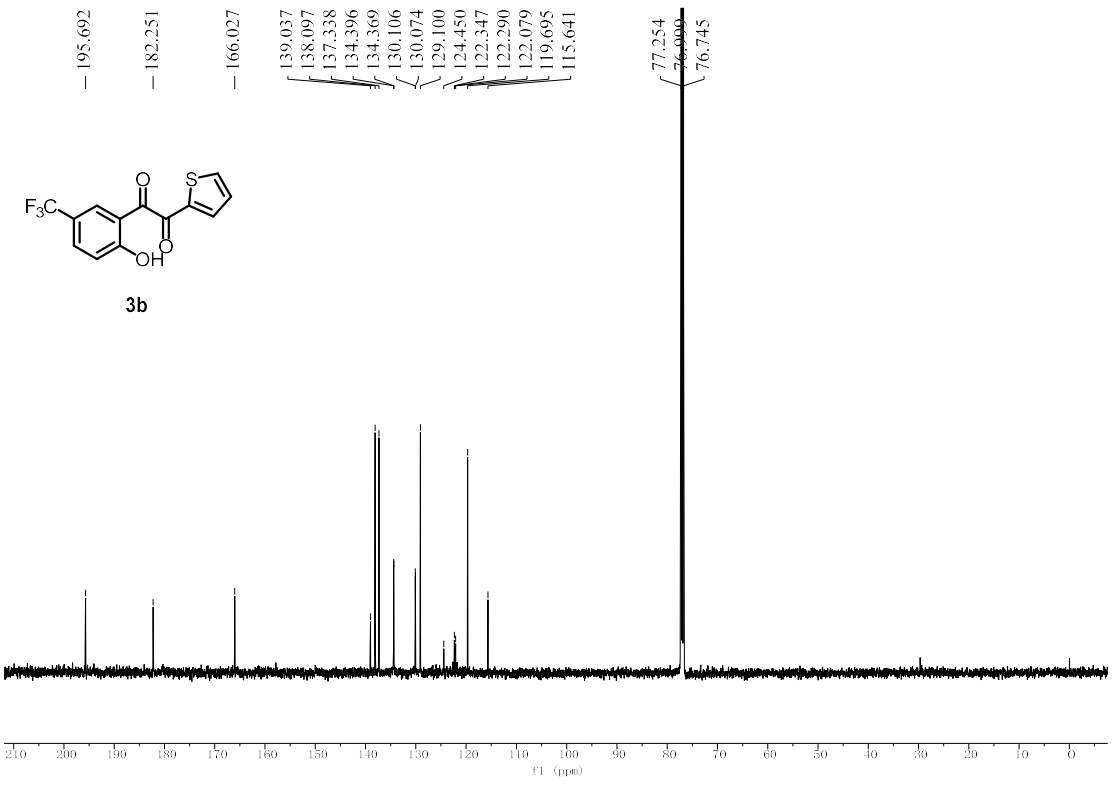
^{13}C NMR (126 MHz, $CDCl_3$)



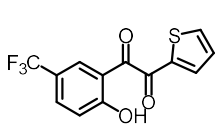
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)

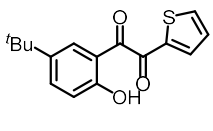


^{19}F NMR (471 MHz, $CDCl_3$)



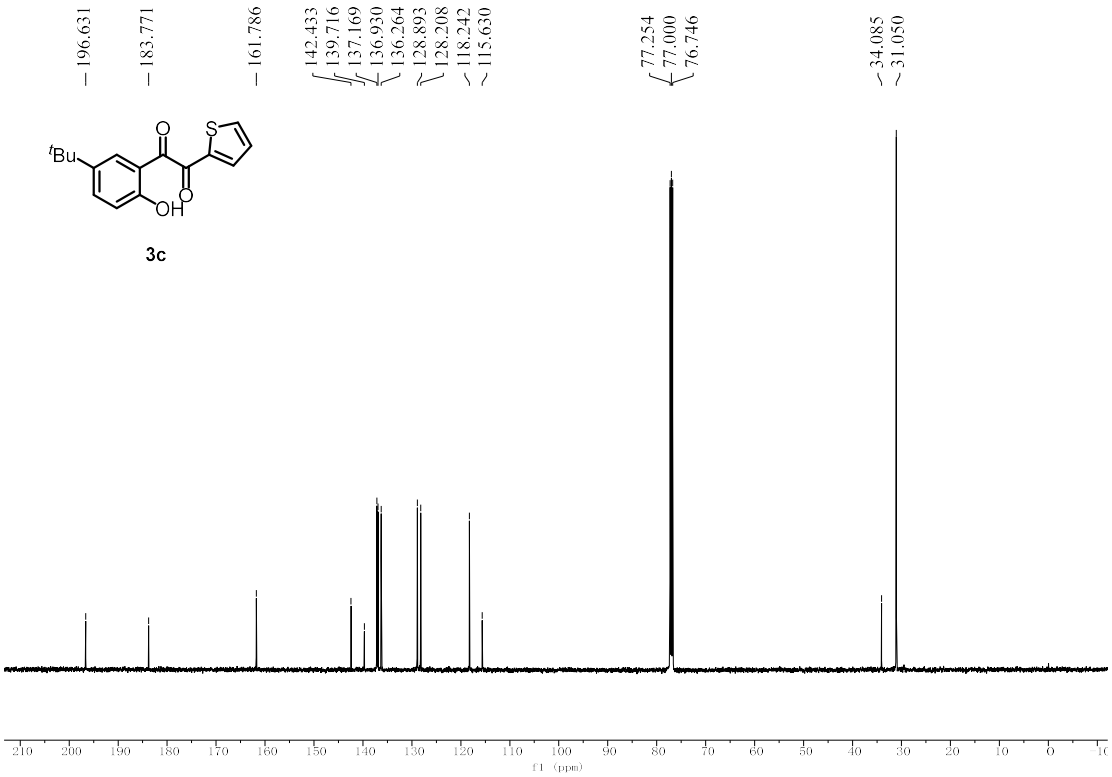
3b

^{1}H NMR (500 MHz, $CDCl_3$)



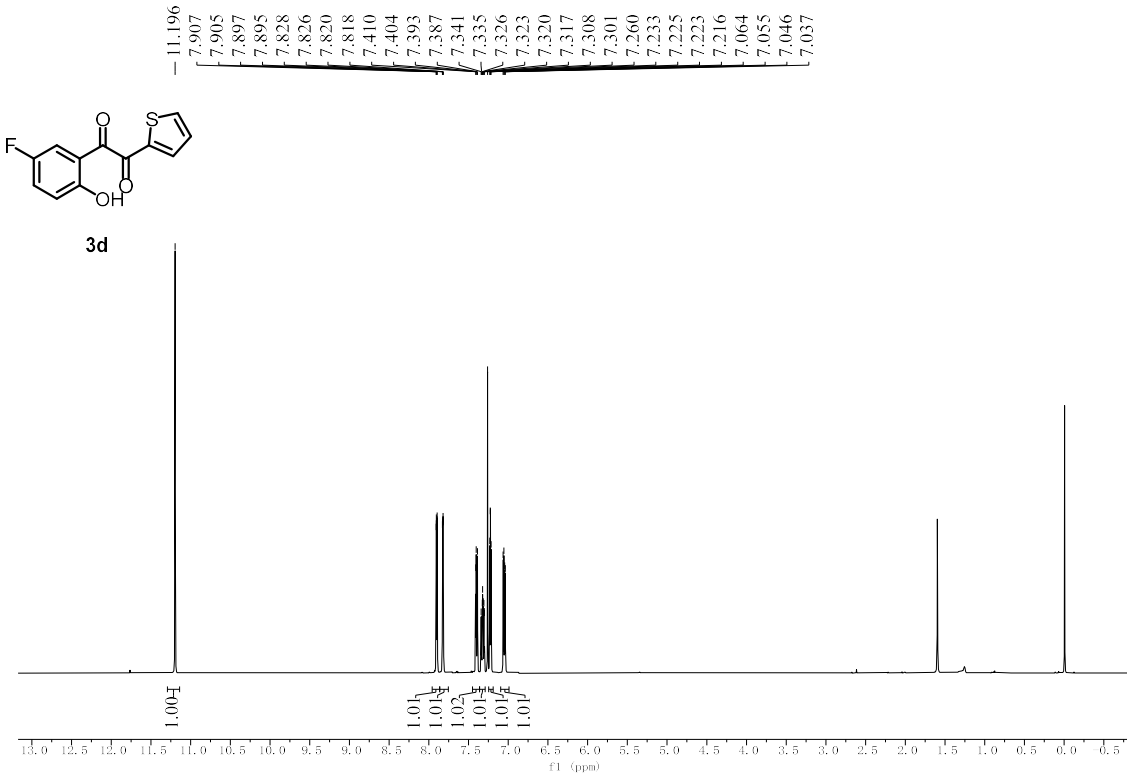
3c

^{13}C NMR (126 MHz, $CDCl_3$)



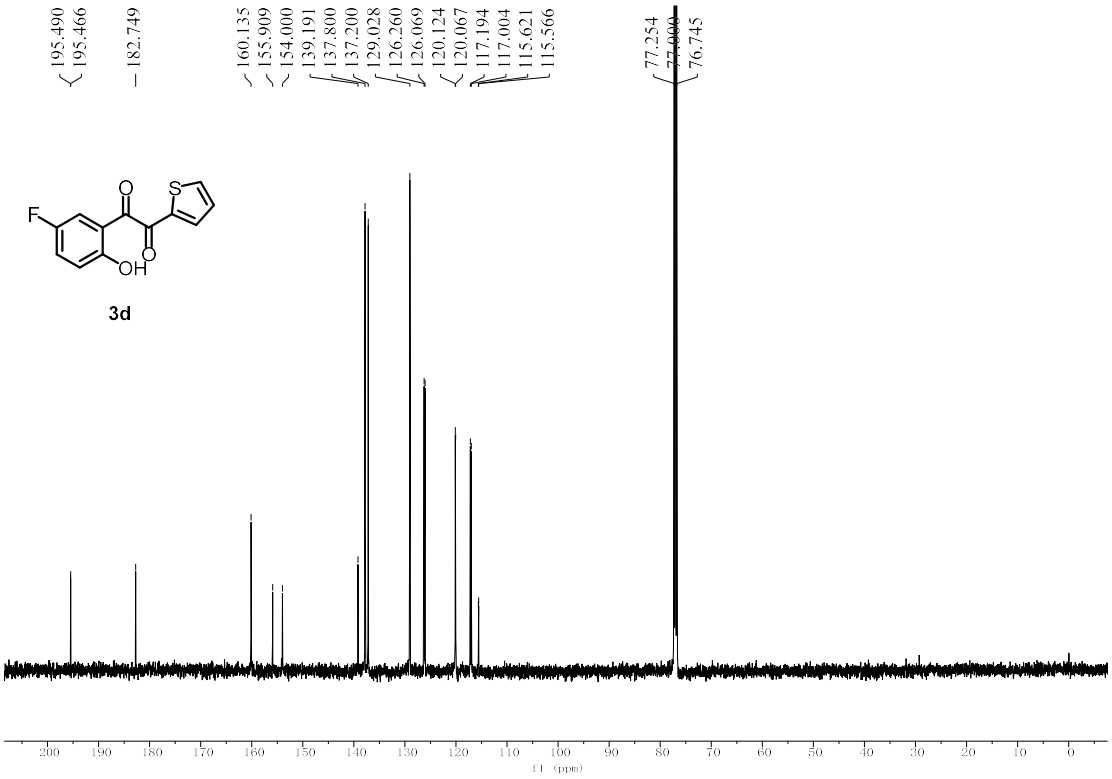
3c

^{1}H NMR (500 MHz, $CDCl_3$)

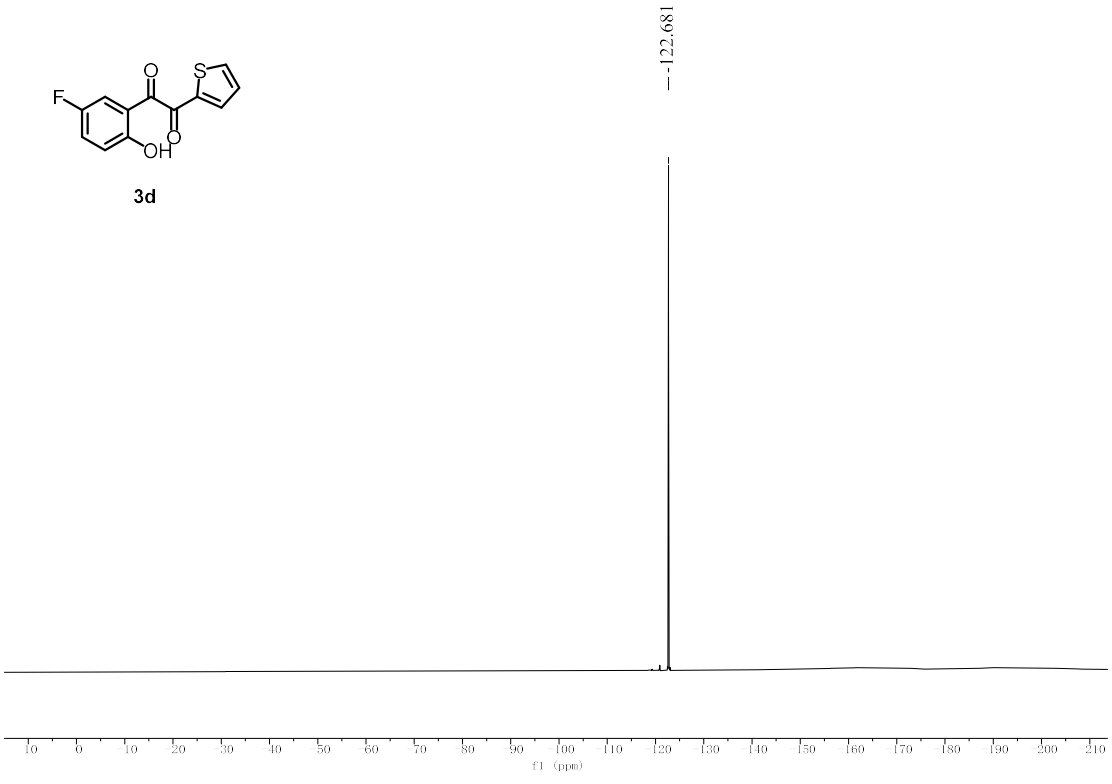


3d

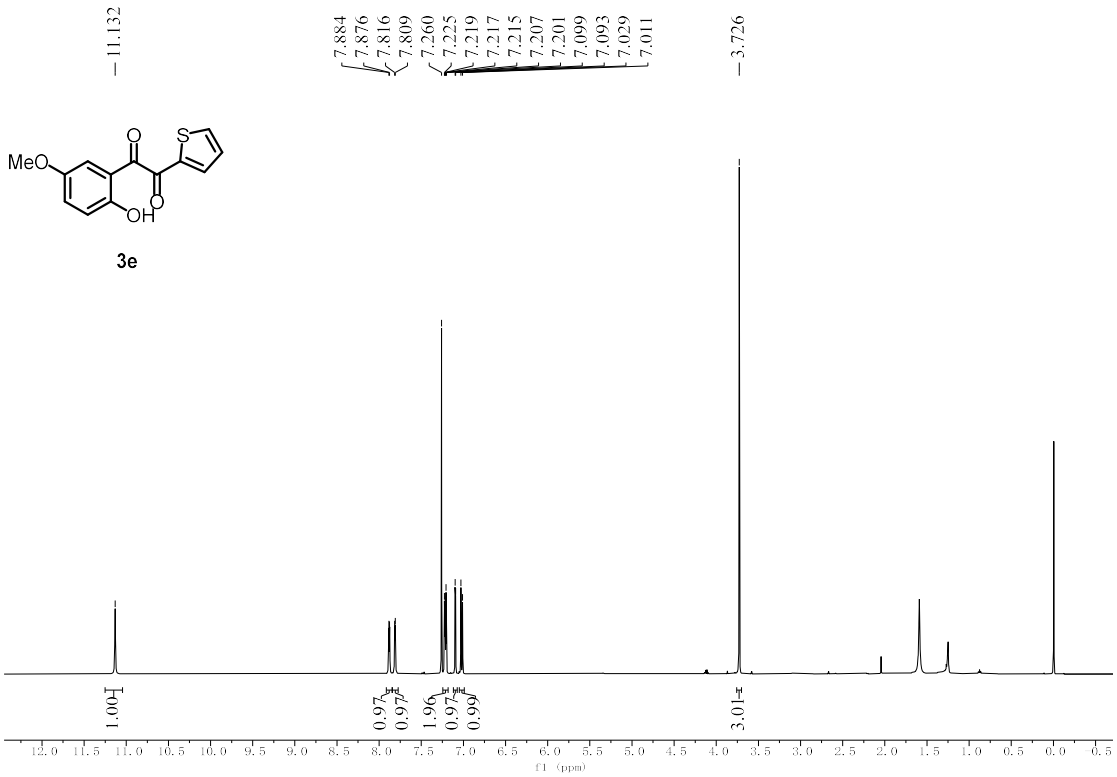
^{13}C NMR (126 MHz, $CDCl_3$)



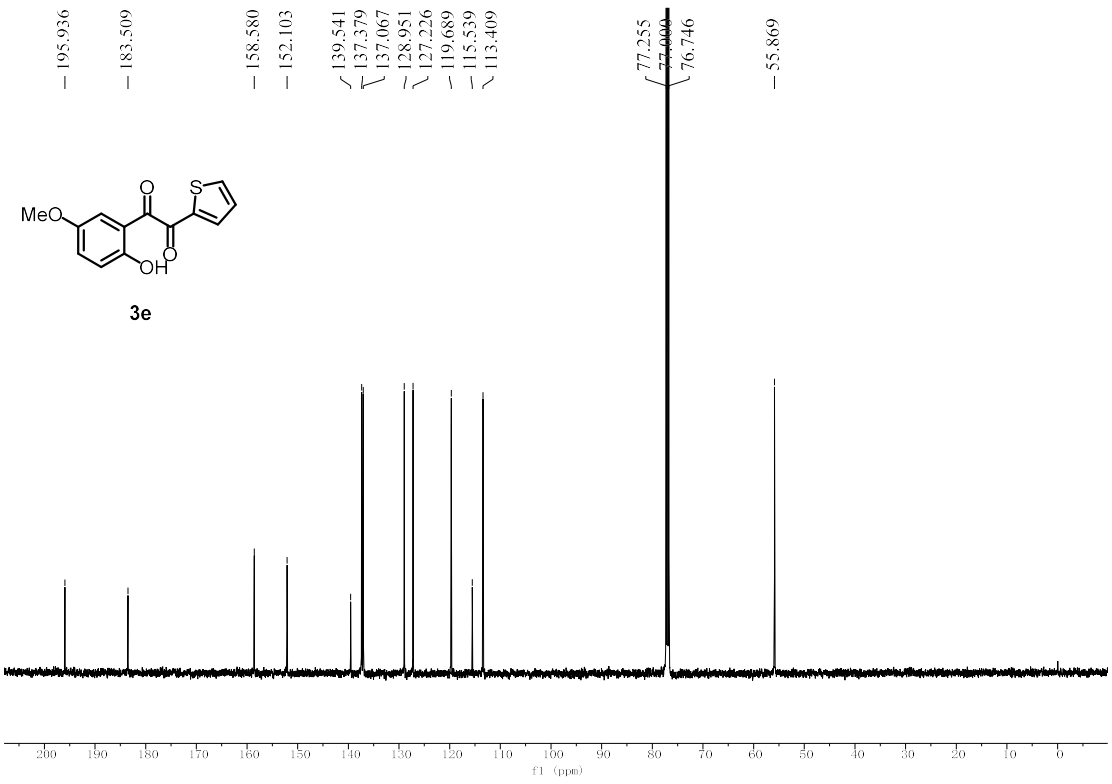
^{19}F NMR (471 MHz, $CDCl_3$)



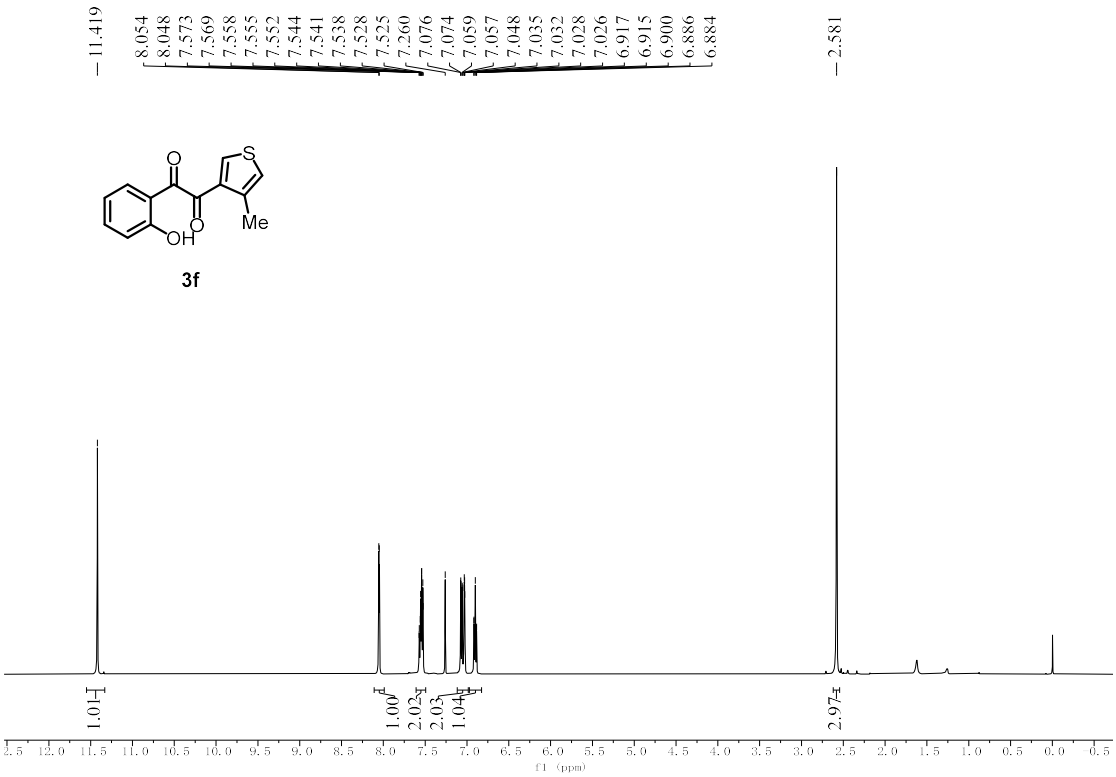
^{1}H NMR (500 MHz, $CDCl_3$)



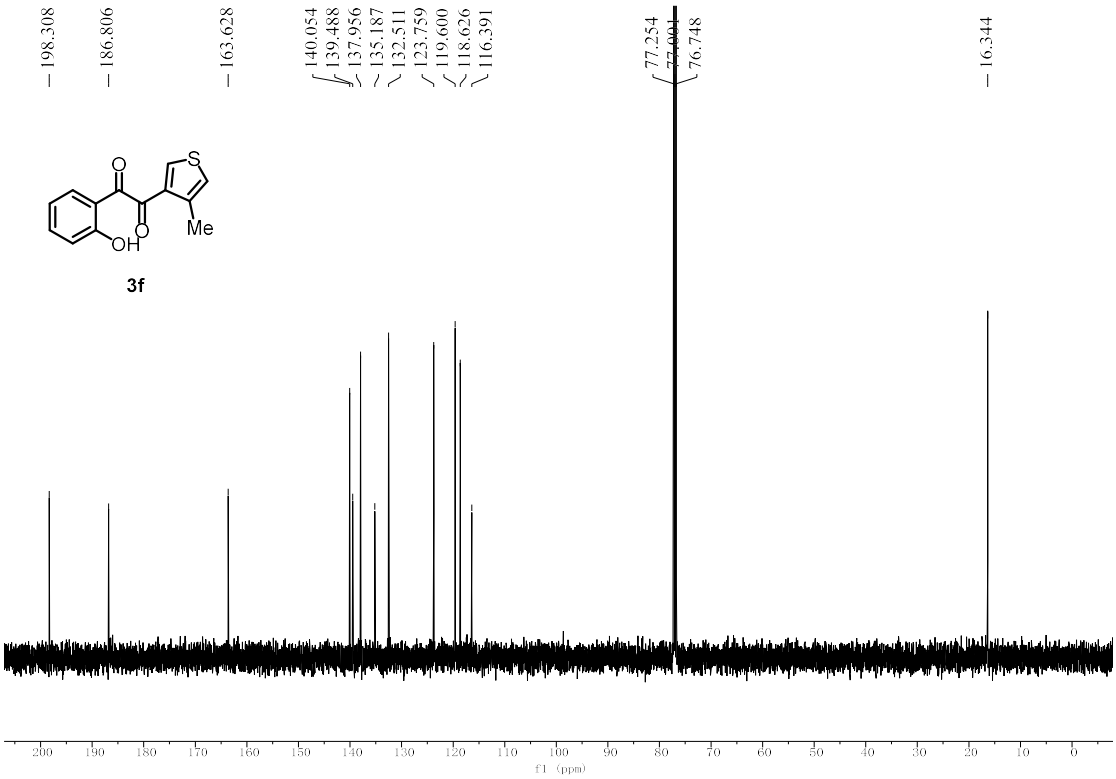
^{13}C NMR (126 MHz, $CDCl_3$)



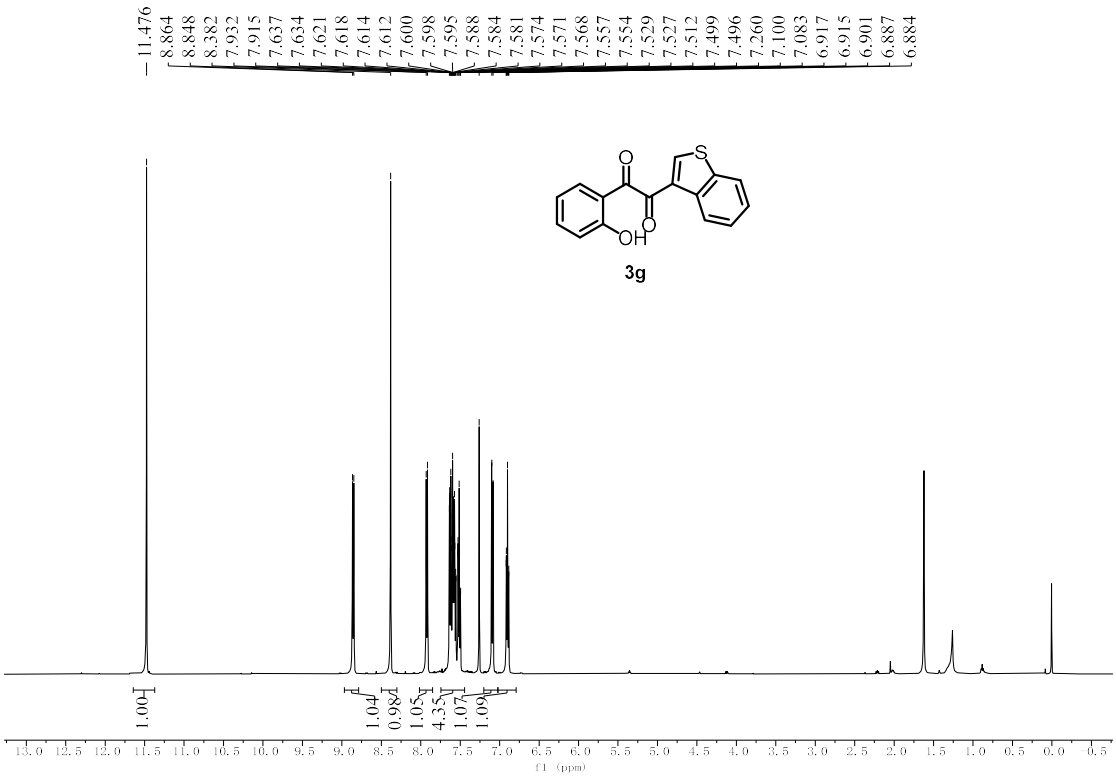
^{1}H NMR (500 MHz, $CDCl_3$)



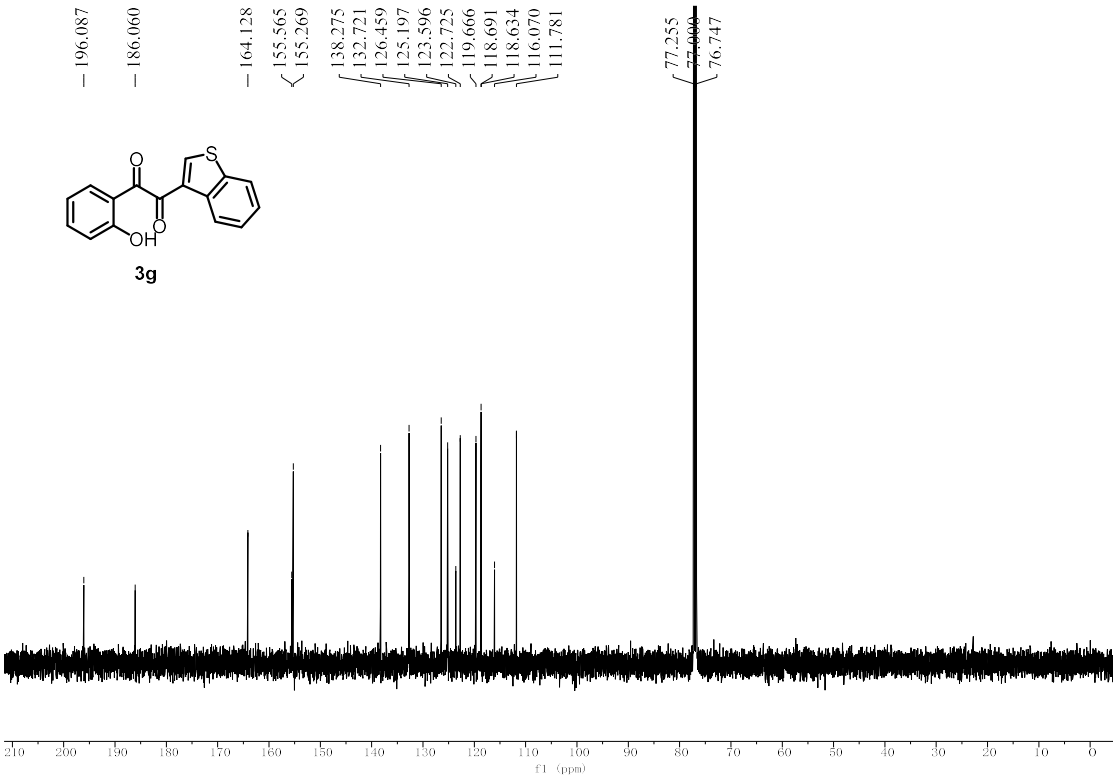
^{13}C NMR (126 MHz, $CDCl_3$)



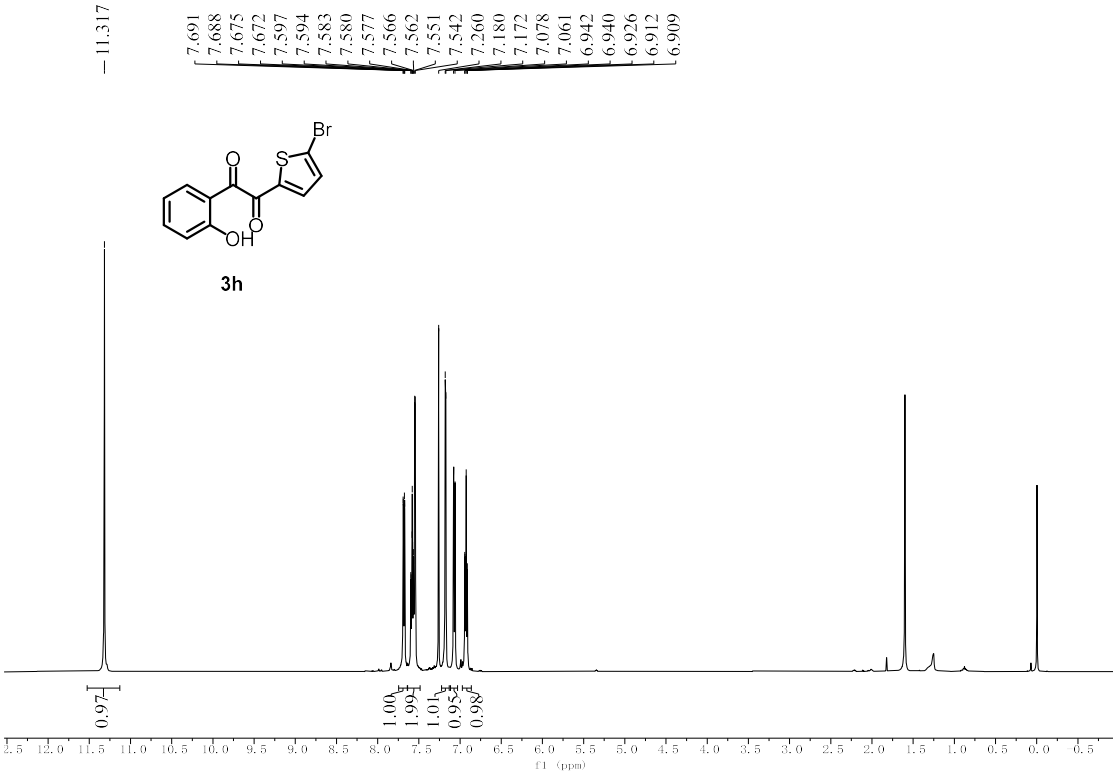
^{1}H NMR (500 MHz, $CDCl_3$)



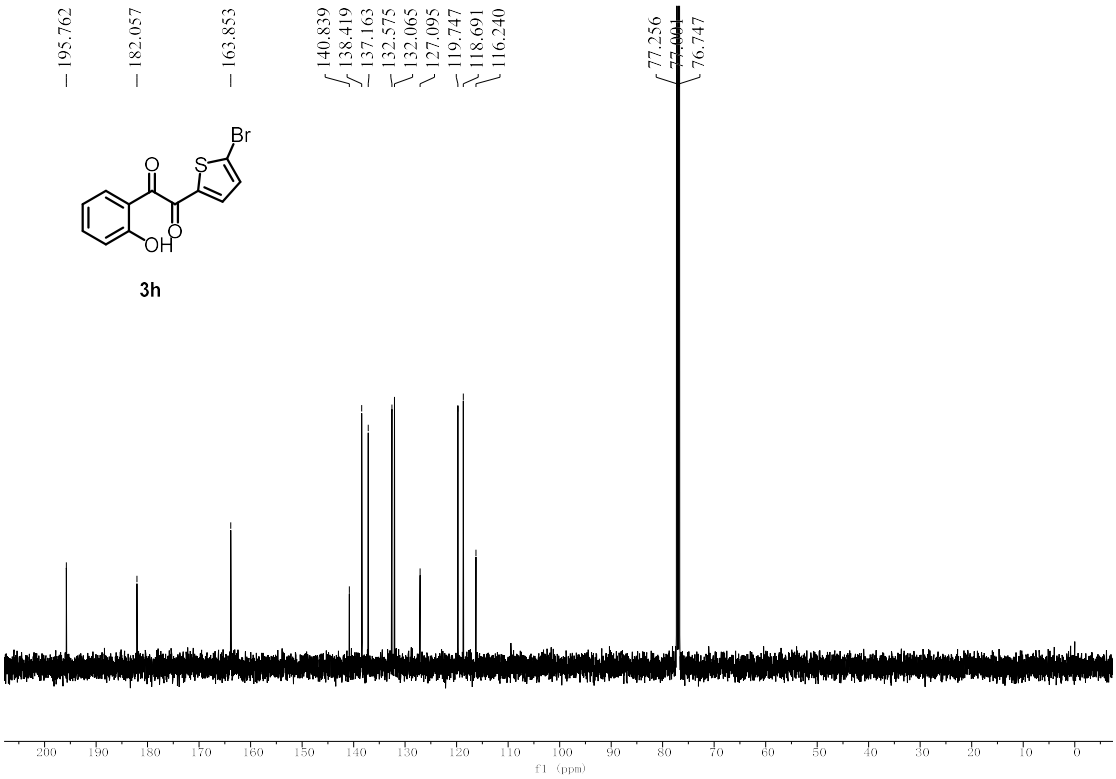
^{13}C NMR (126 MHz, $CDCl_3$)



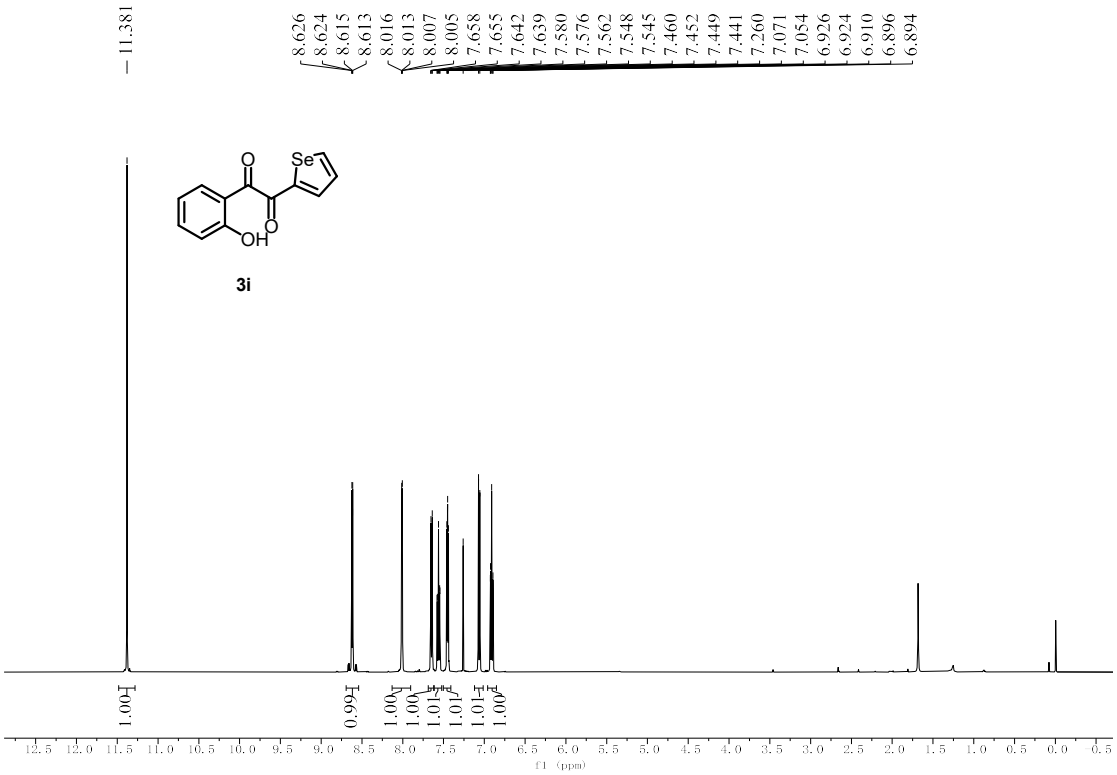
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)

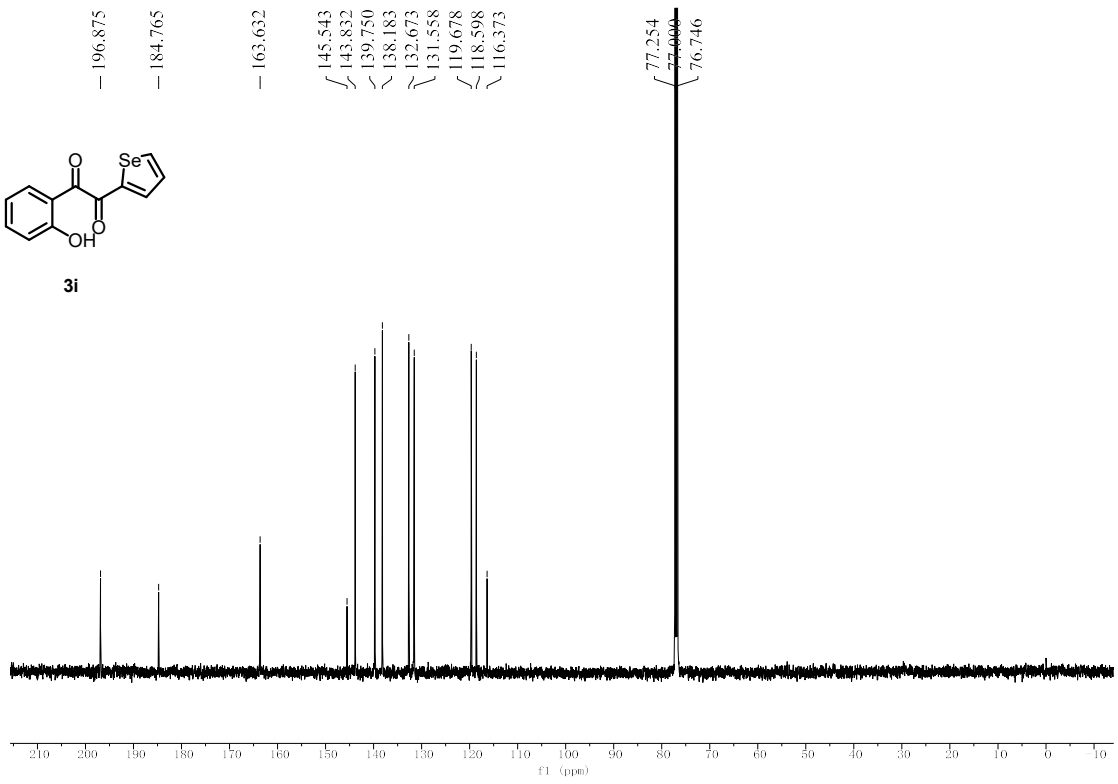


^{1}H NMR (500 MHz, $CDCl_3$)



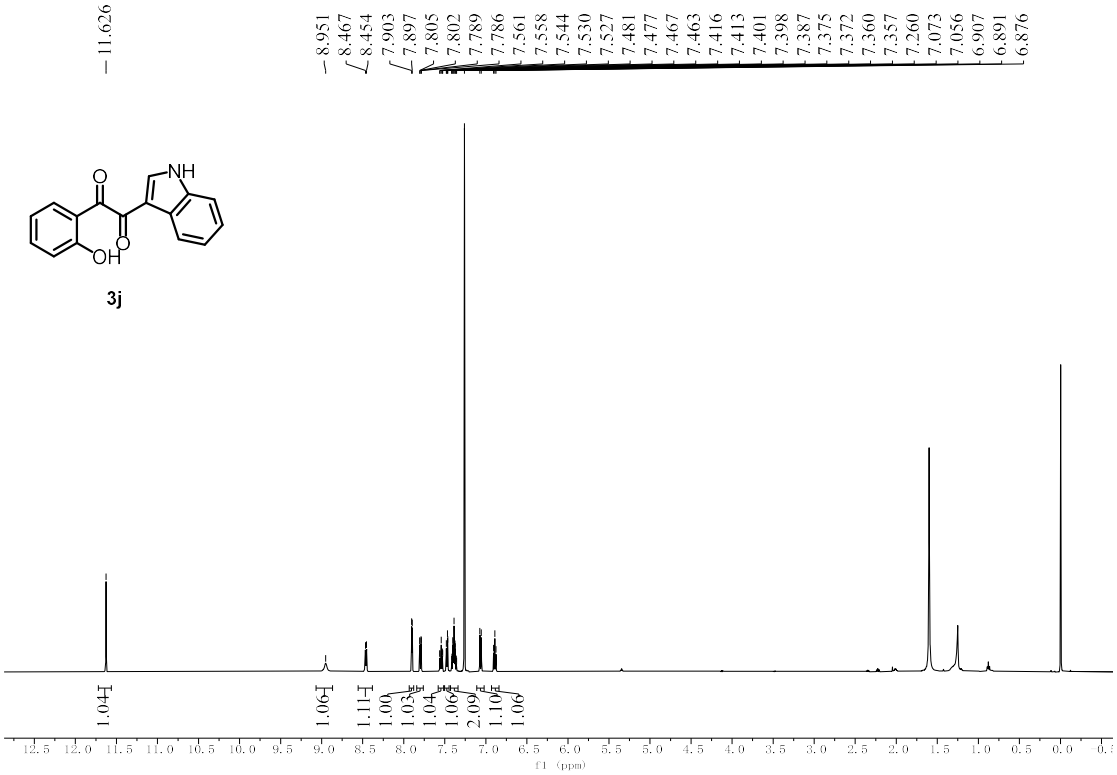
3i

^{13}C NMR (126 MHz, $CDCl_3$)

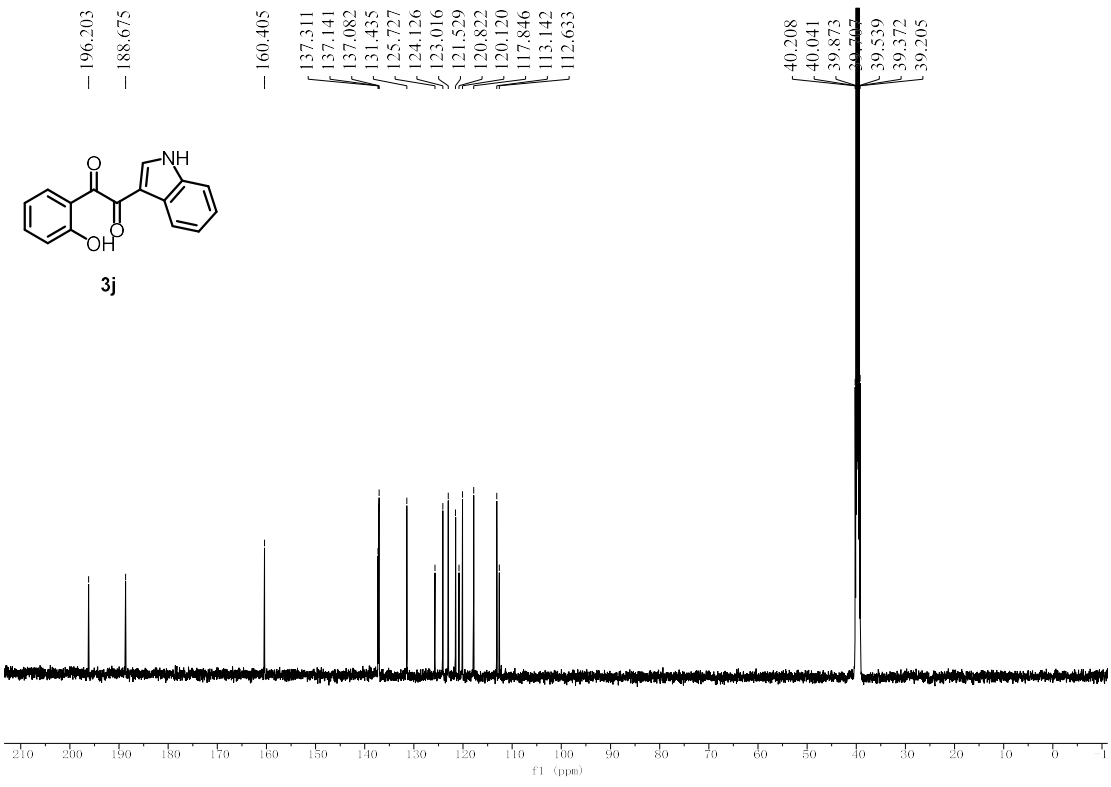


3i

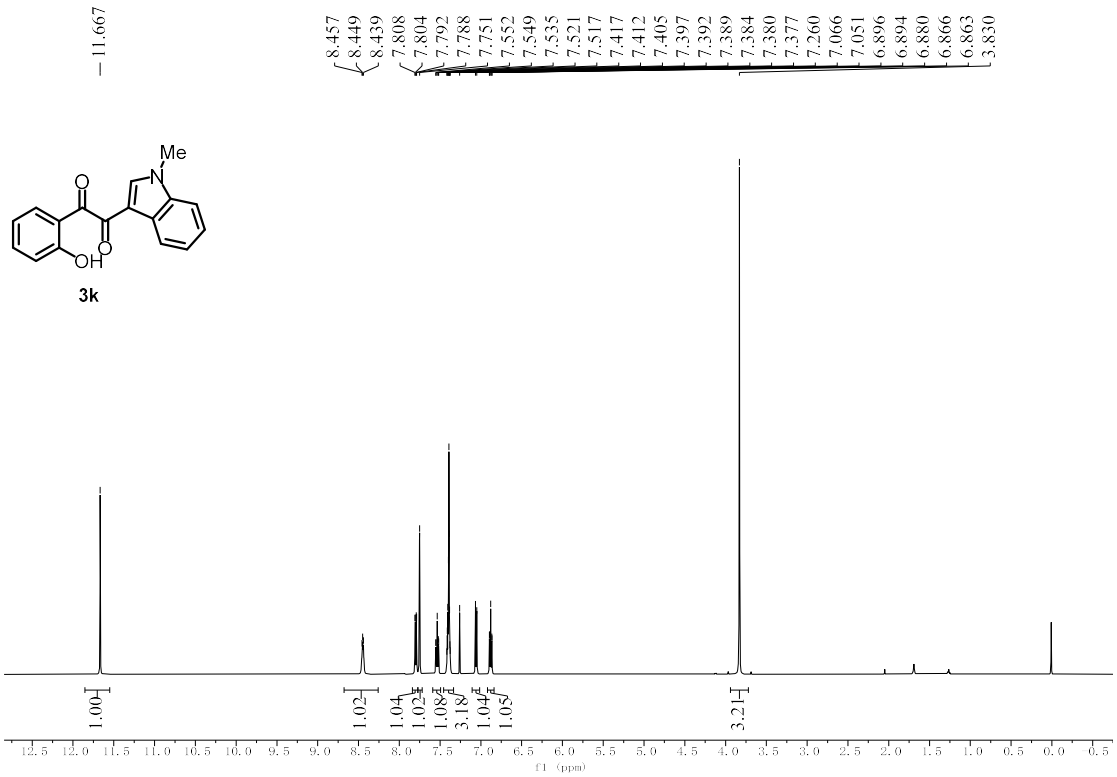
^{1}H NMR (500 MHz, $CDCl_3$)



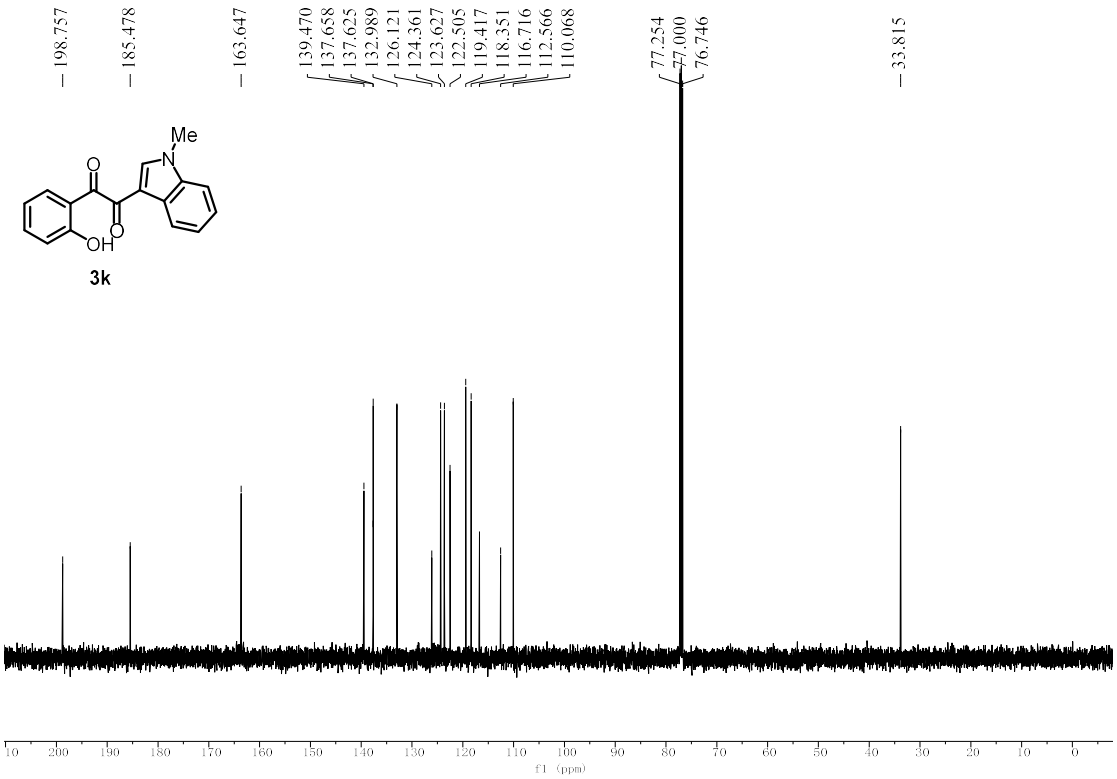
^{13}C NMR (126 MHz, DMSO-d_6)



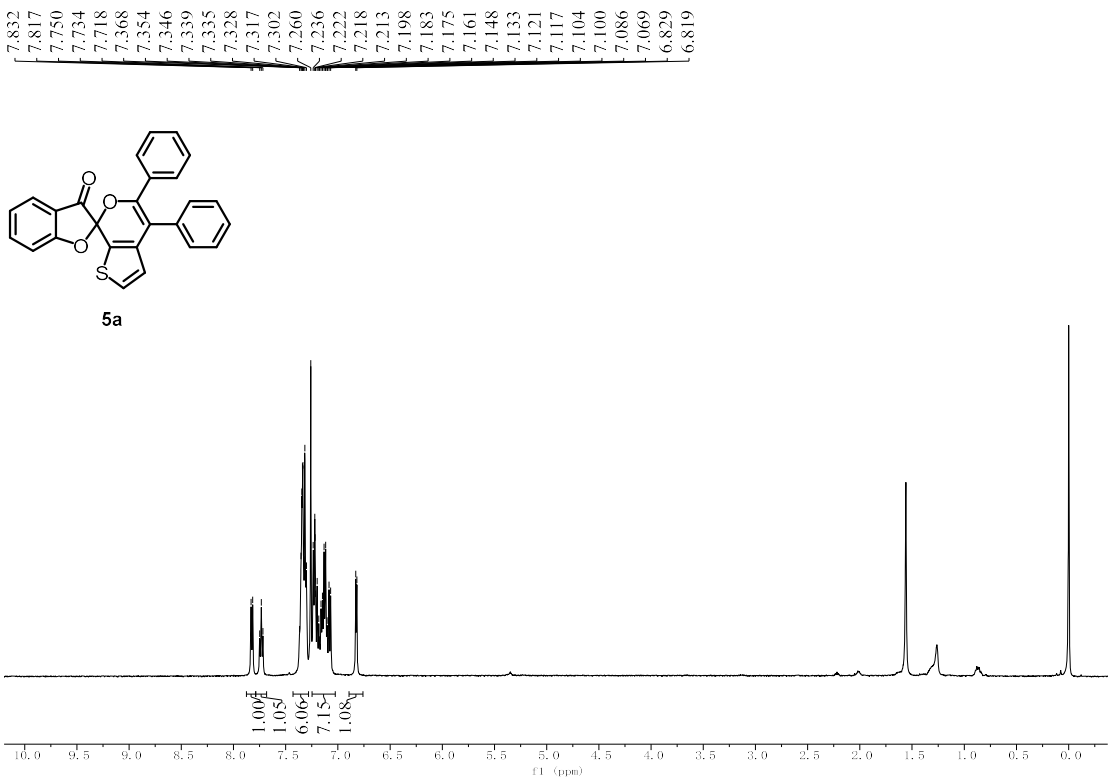
^{1}H NMR (500 MHz, $CDCl_3$)



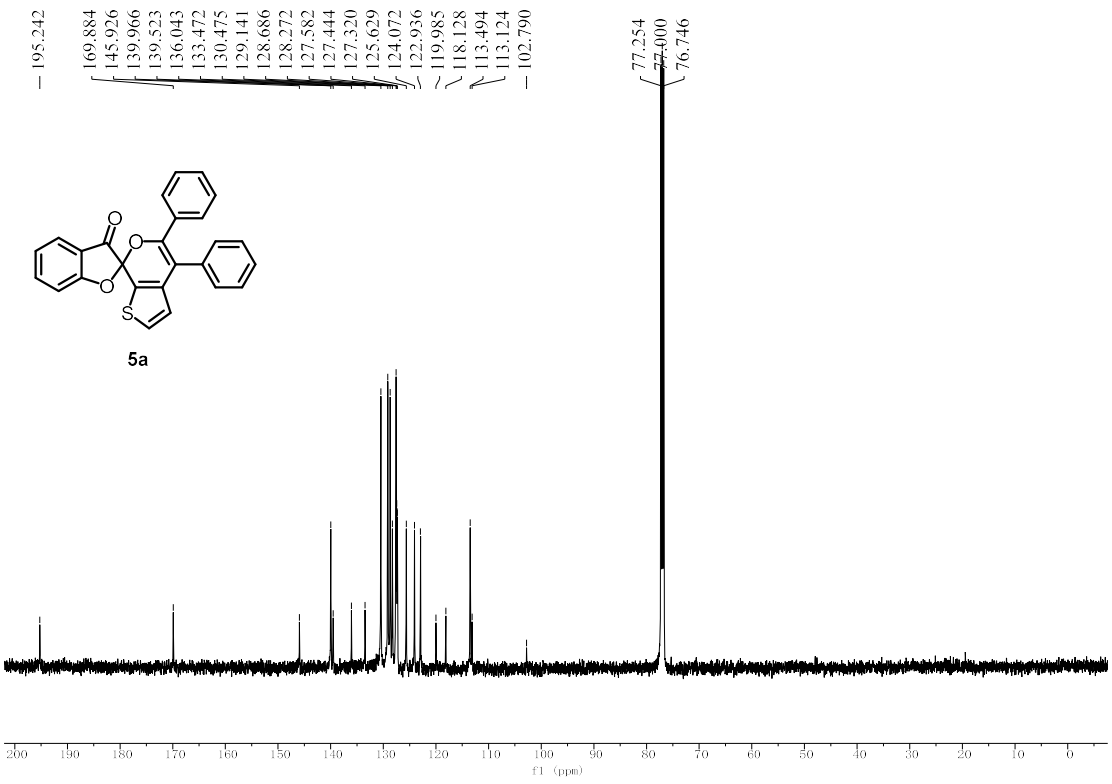
^{13}C NMR (126 MHz, $CDCl_3$)



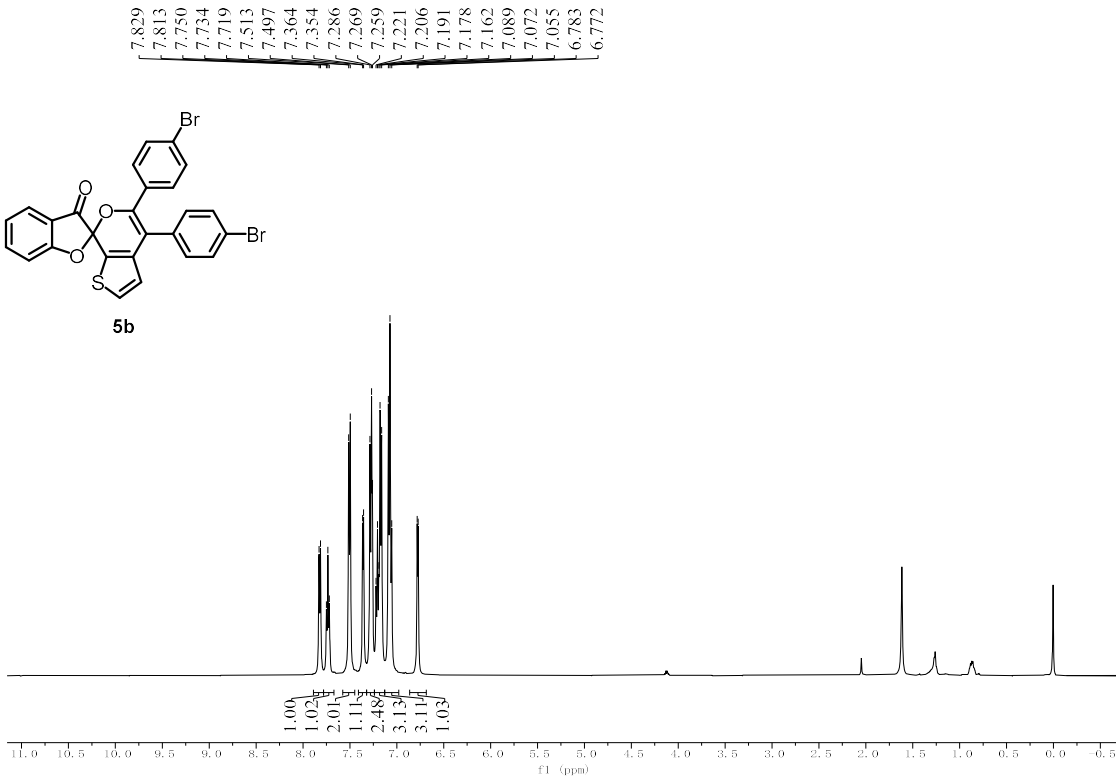
^{1}H NMR (500 MHz, $CDCl_3$)



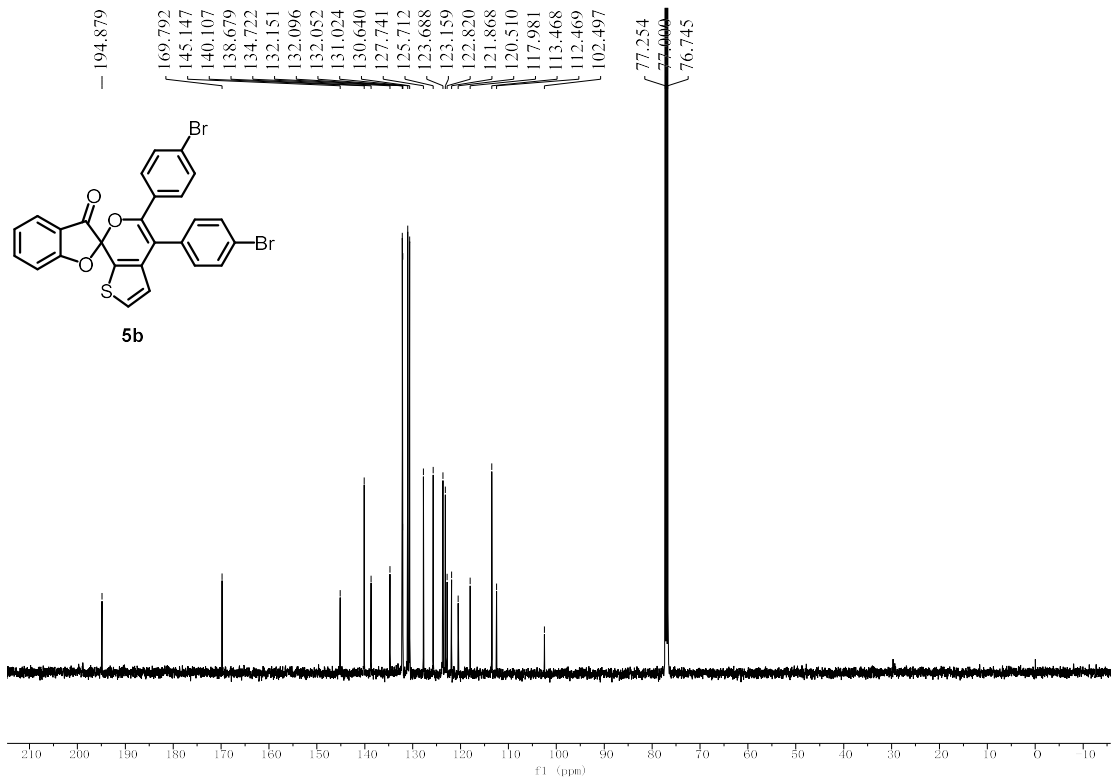
^{13}C NMR (126 MHz, $CDCl_3$)



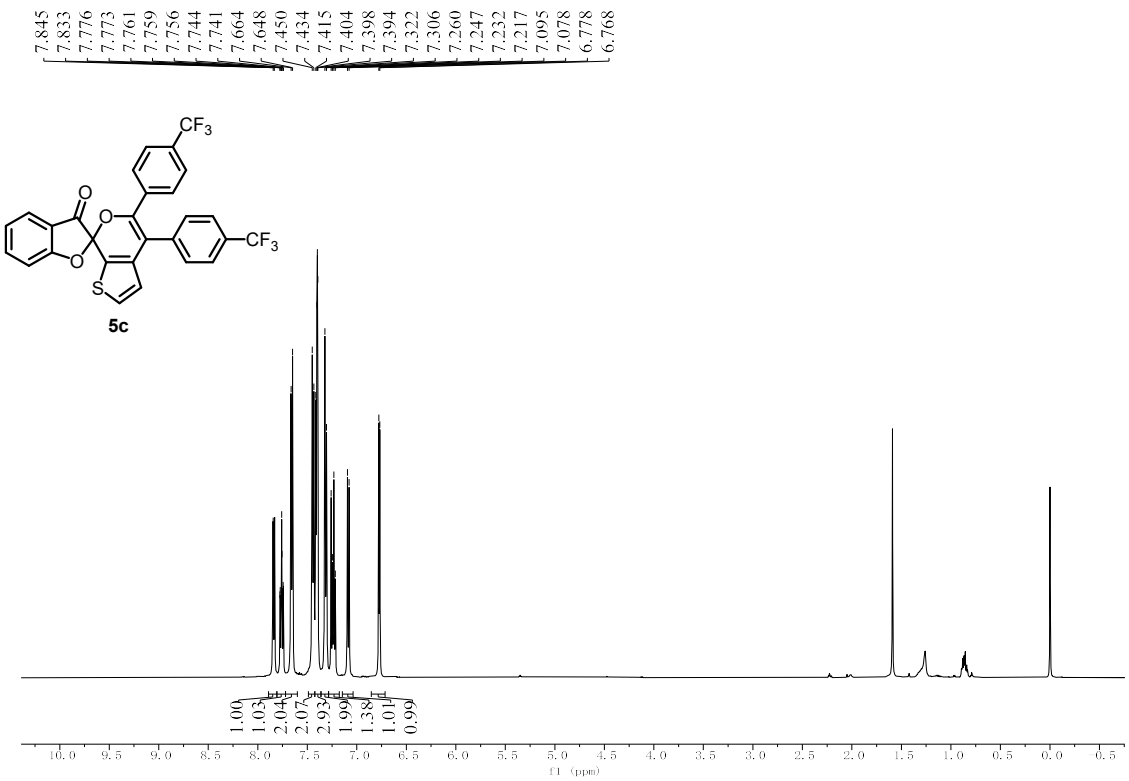
^{1}H NMR (500 MHz, $CDCl_3$)



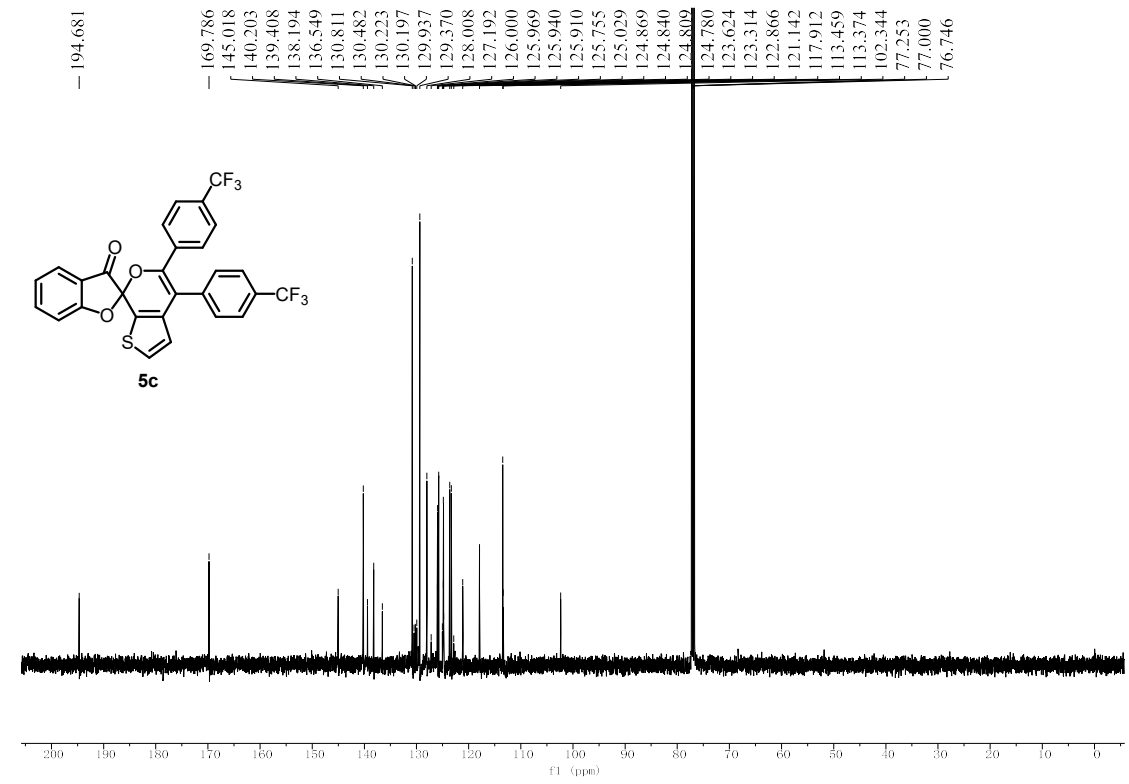
^{13}C NMR (126 MHz, $CDCl_3$)



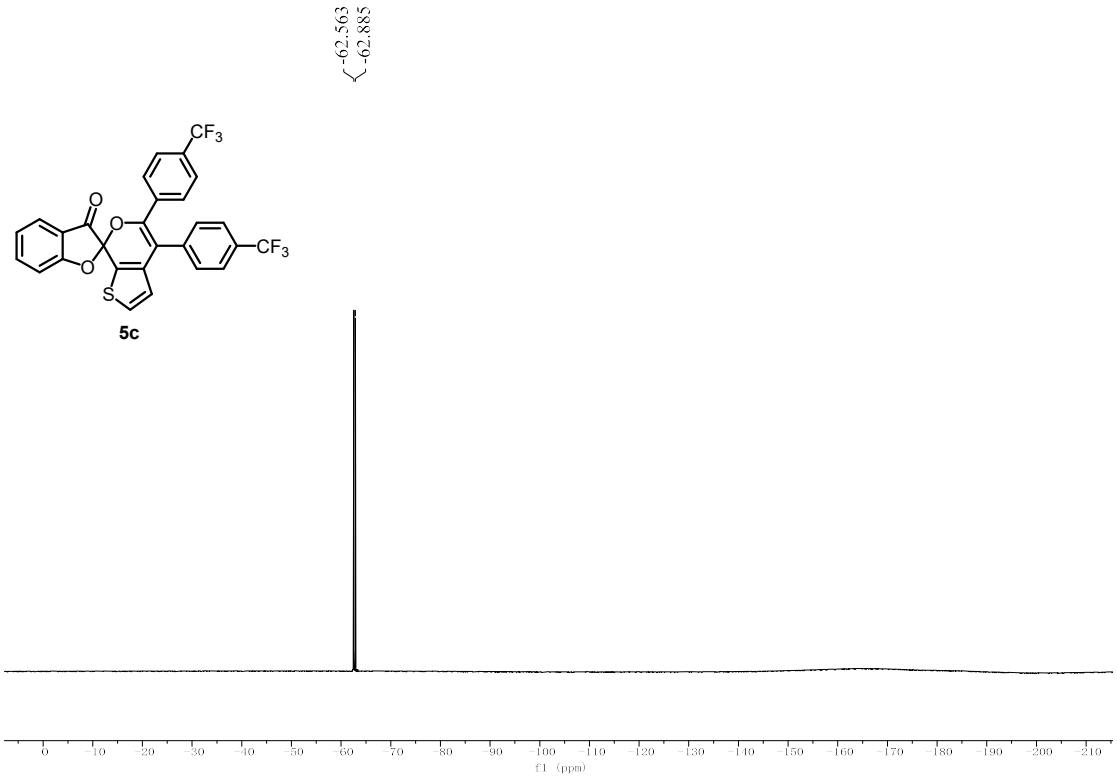
^{1}H NMR (500 MHz, $CDCl_3$)



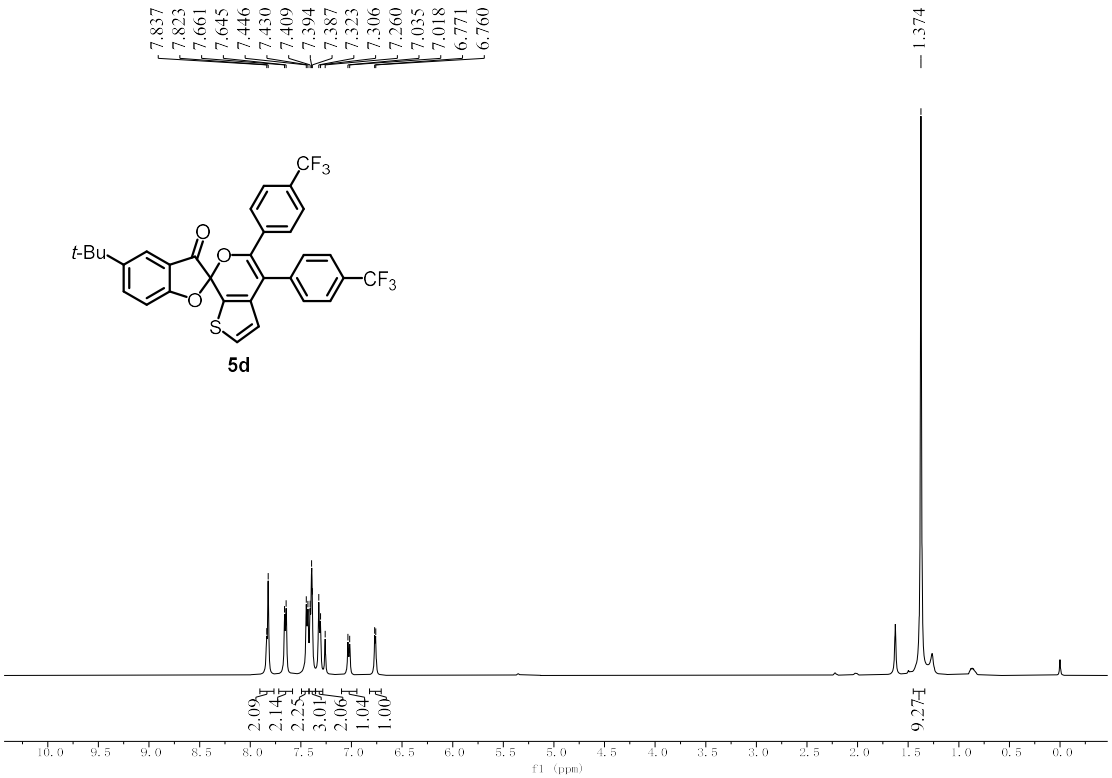
^{13}C NMR (126 MHz, $CDCl_3$)



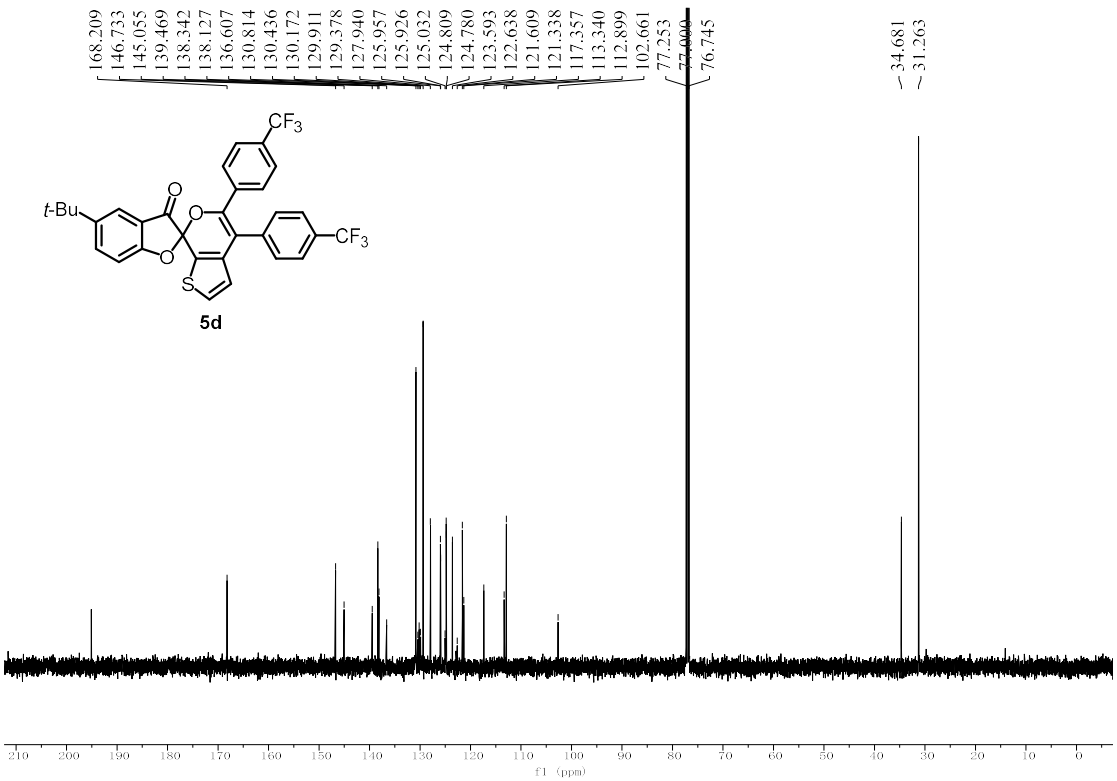
^{19}F NMR (471 MHz, $CDCl_3$)



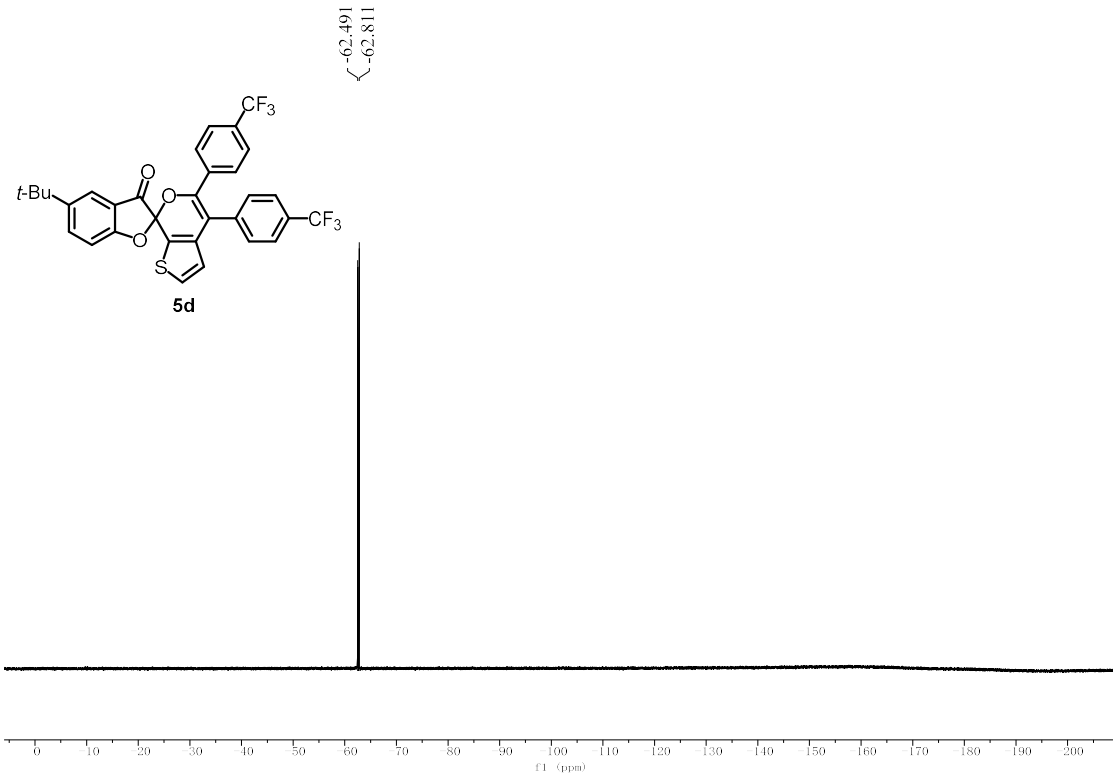
^{1}H NMR (500 MHz, $CDCl_3$)



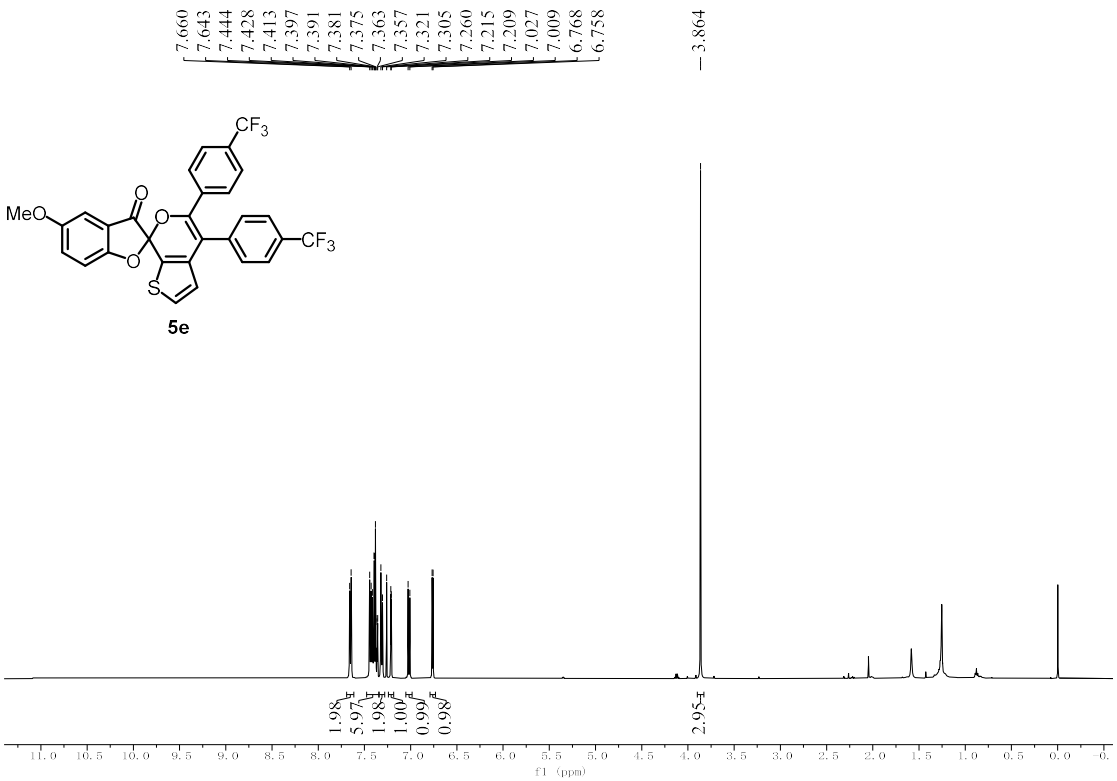
^{13}C NMR (126 MHz, $CDCl_3$)



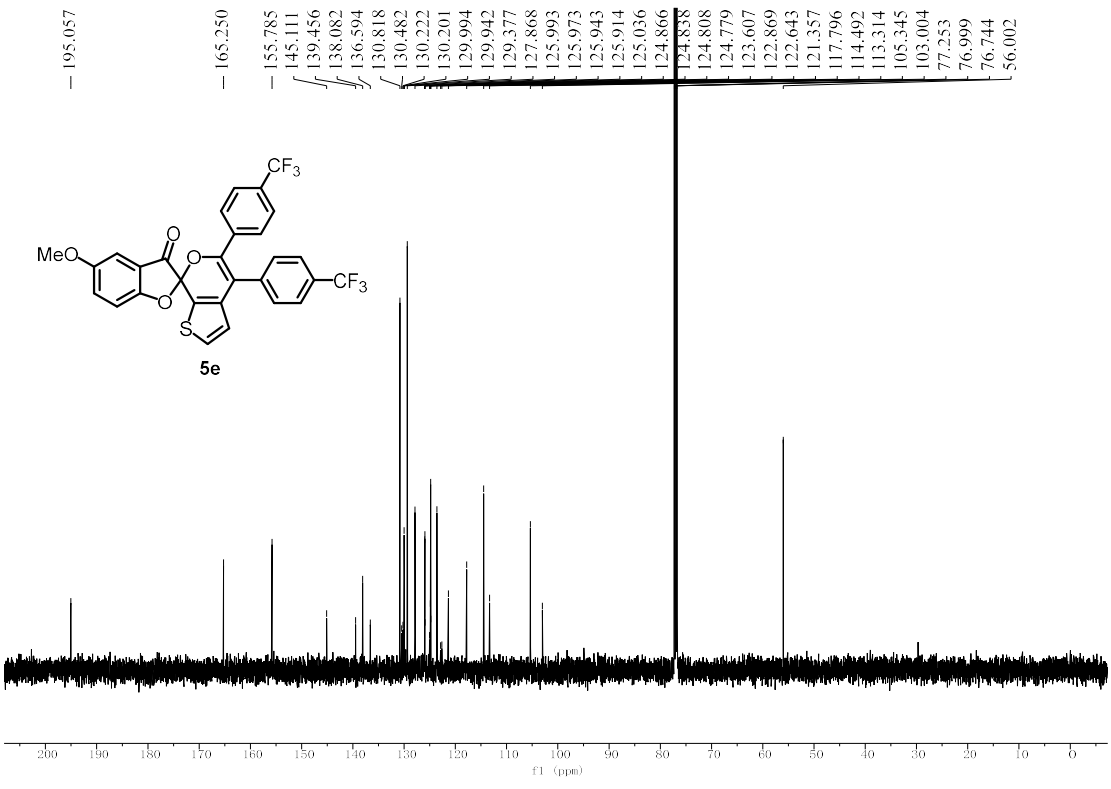
^{19}F NMR (471 MHz, $CDCl_3$)



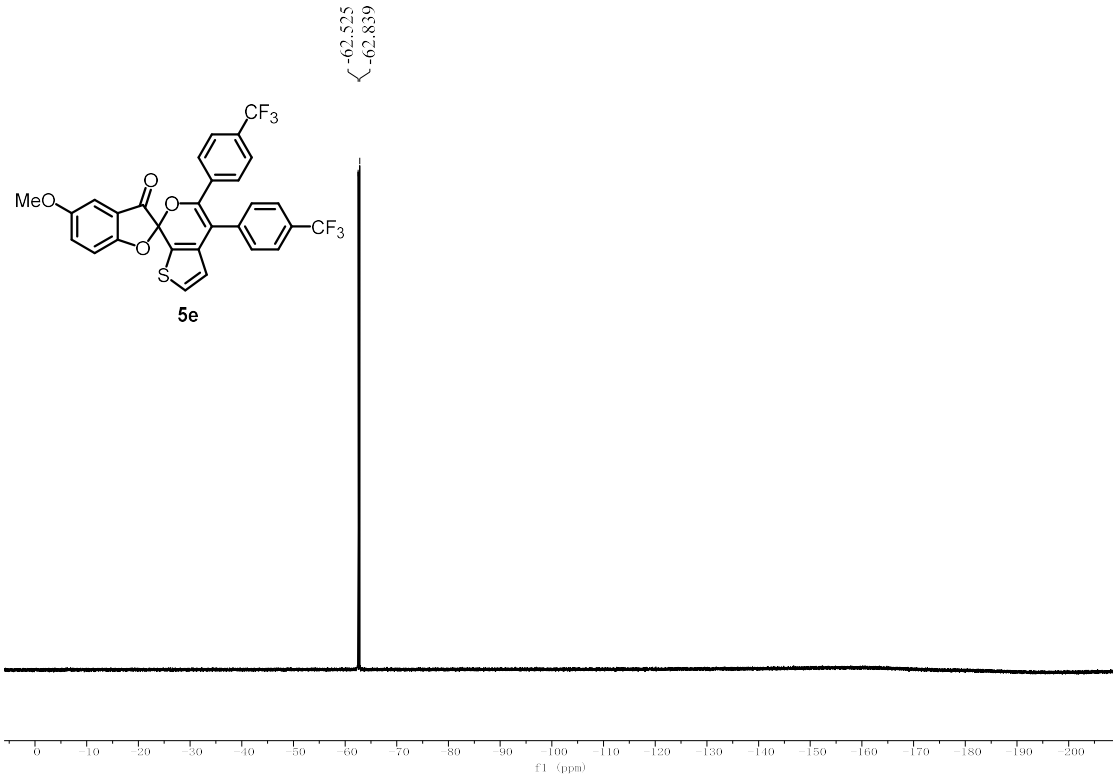
^{1}H NMR (500 MHz, $CDCl_3$)



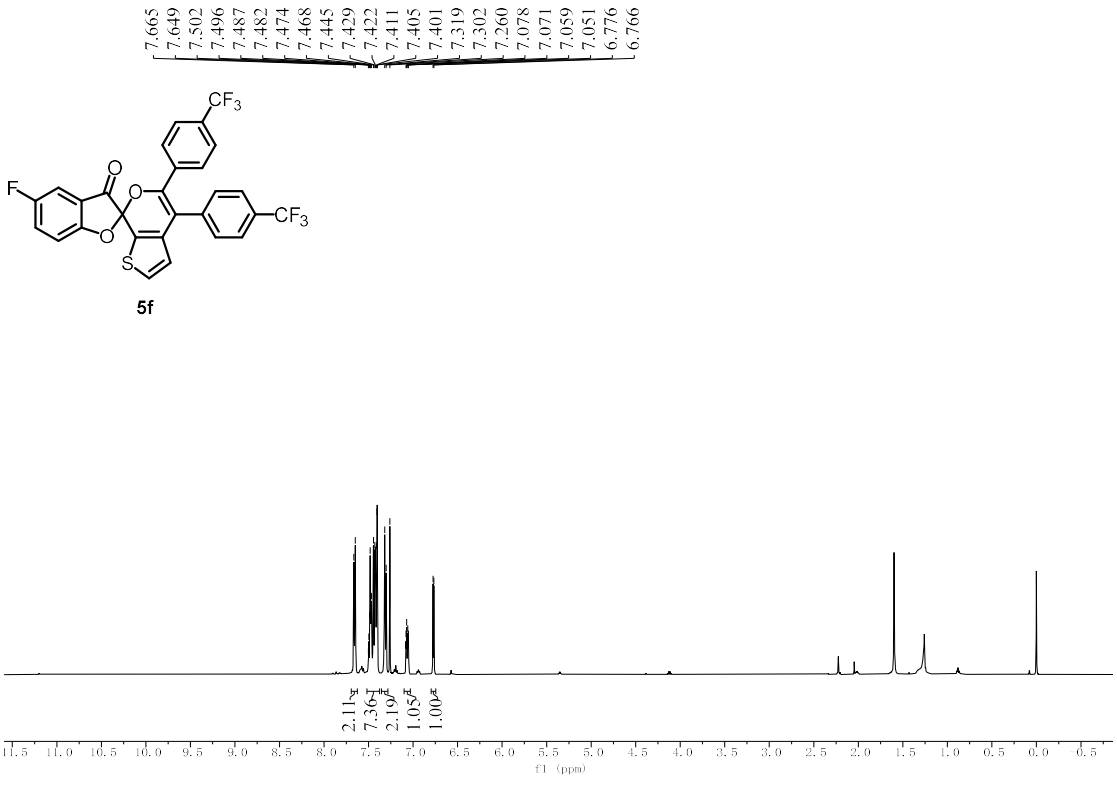
^{13}C NMR (126 MHz, $CDCl_3$)



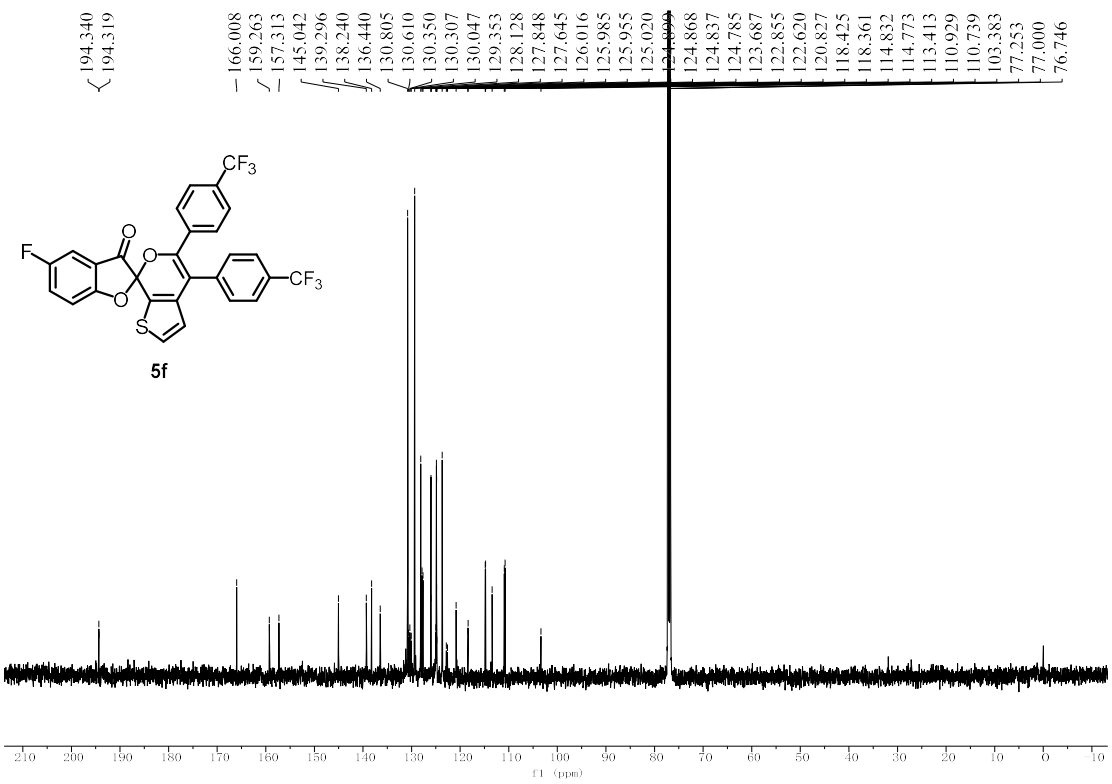
^{19}F NMR (471 MHz, $CDCl_3$)



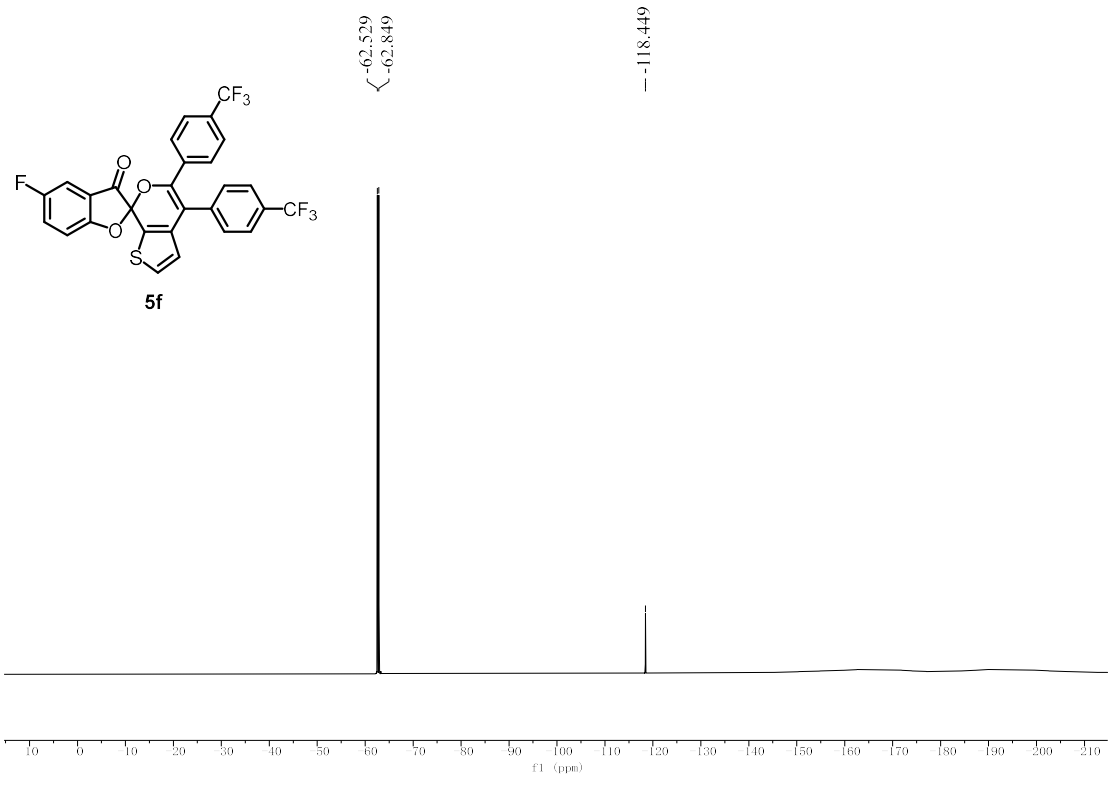
^{1}H NMR (500 MHz, $CDCl_3$)



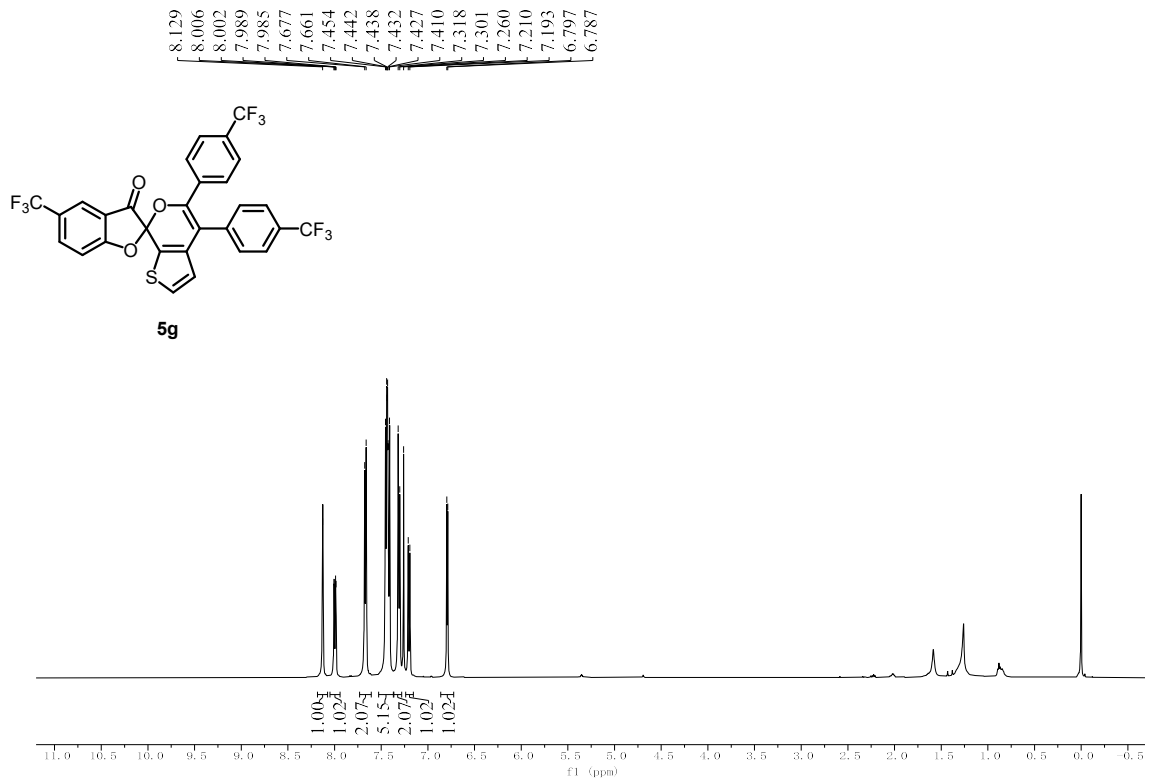
^{13}C NMR (126 MHz, $CDCl_3$)



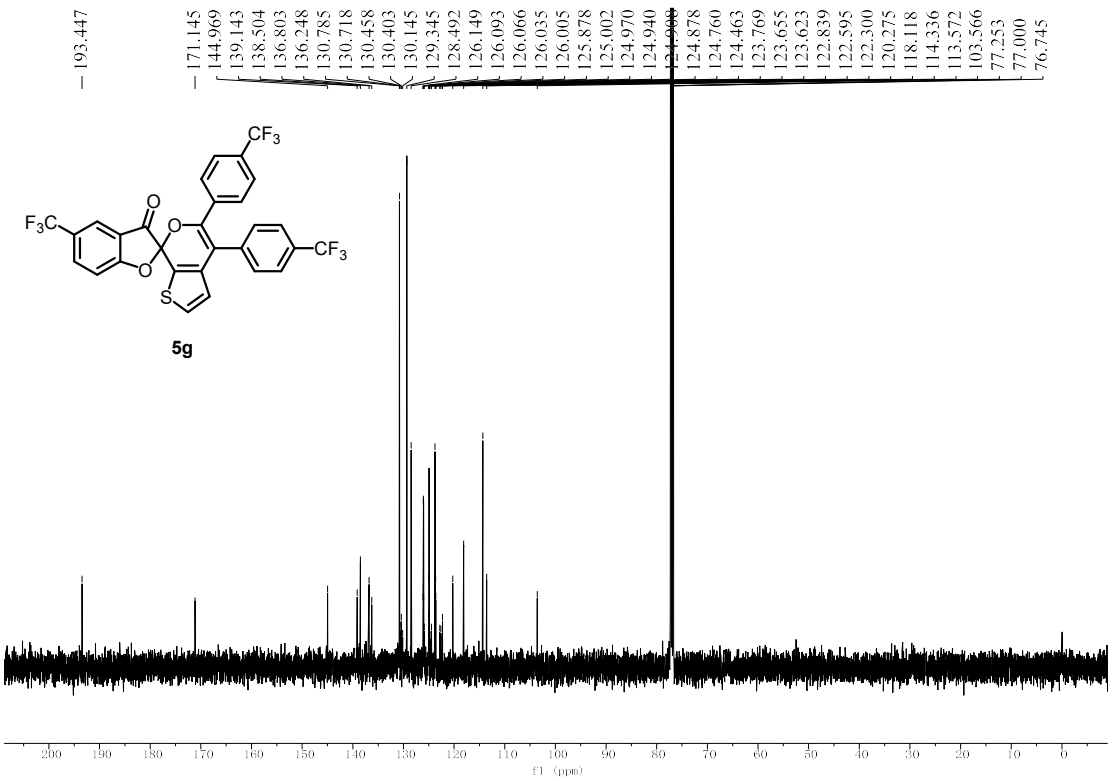
^{19}F NMR (471 MHz, $CDCl_3$)



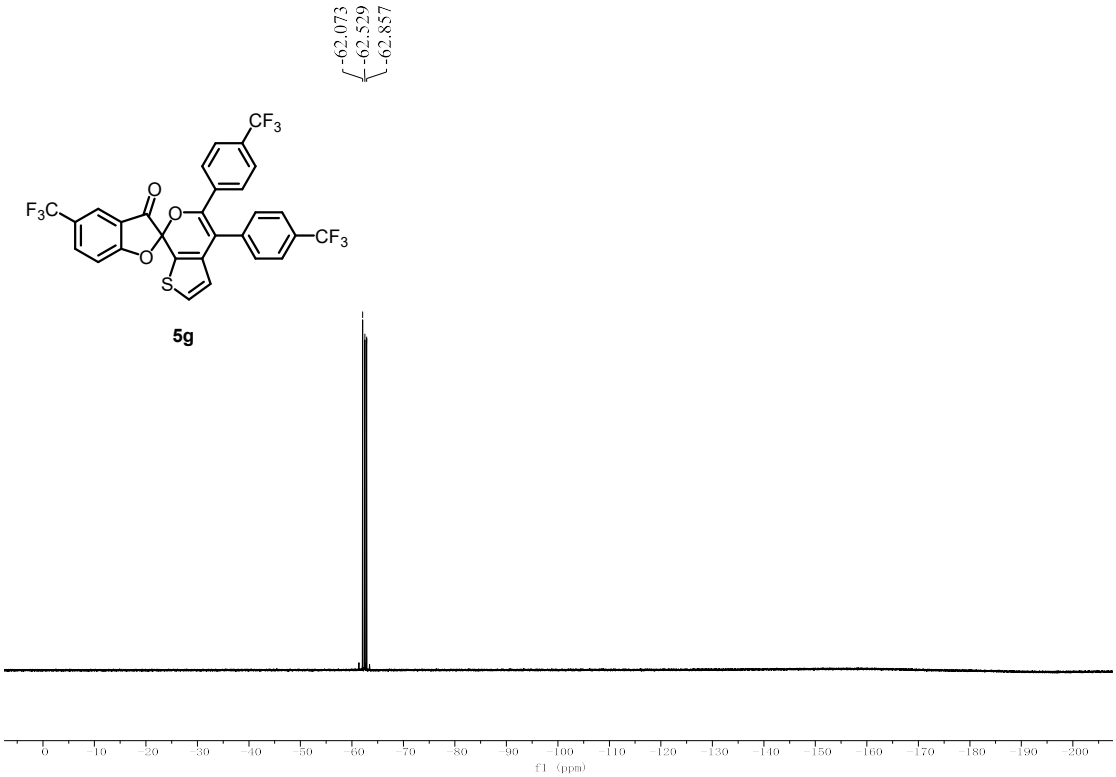
^{1}H NMR (500 MHz, $CDCl_3$)



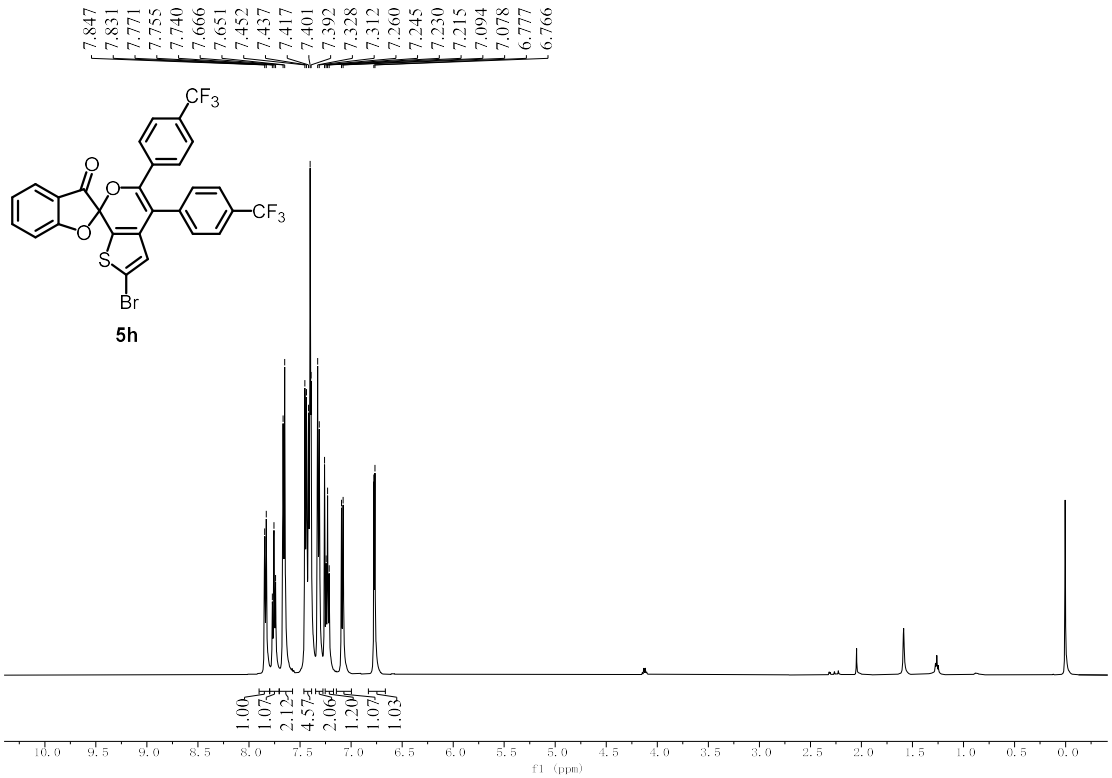
^{13}C NMR (126 MHz, $CDCl_3$)



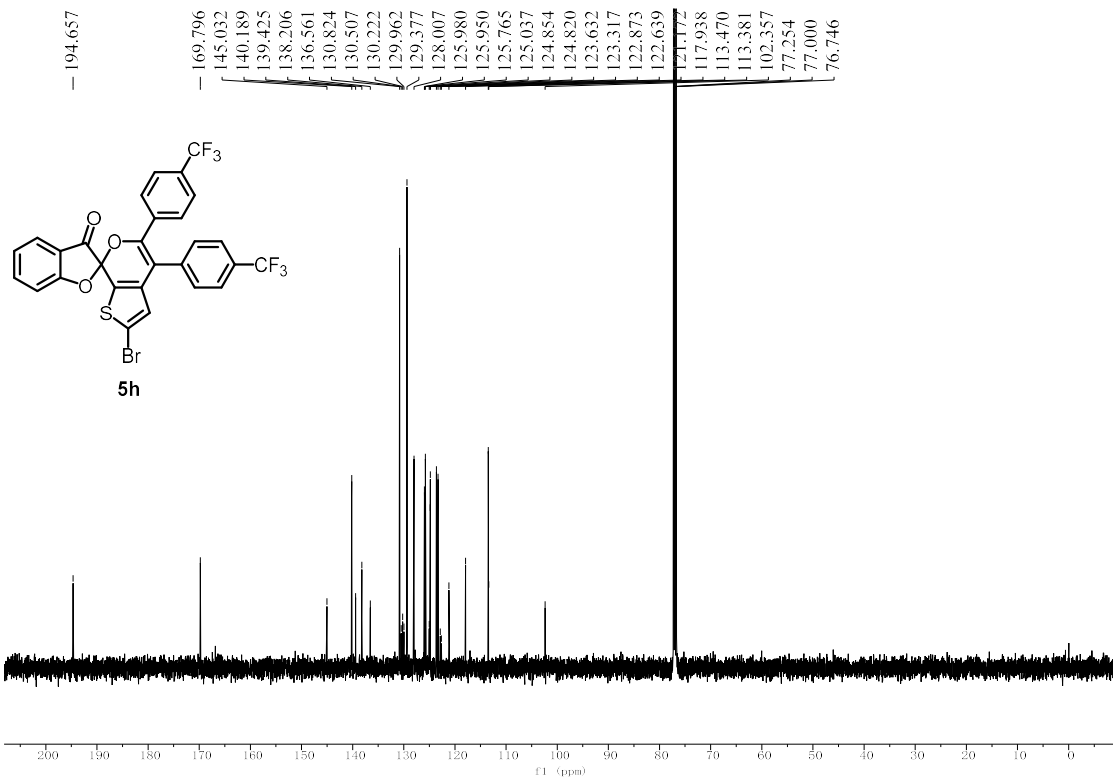
^{19}F NMR (471 MHz, $CDCl_3$)



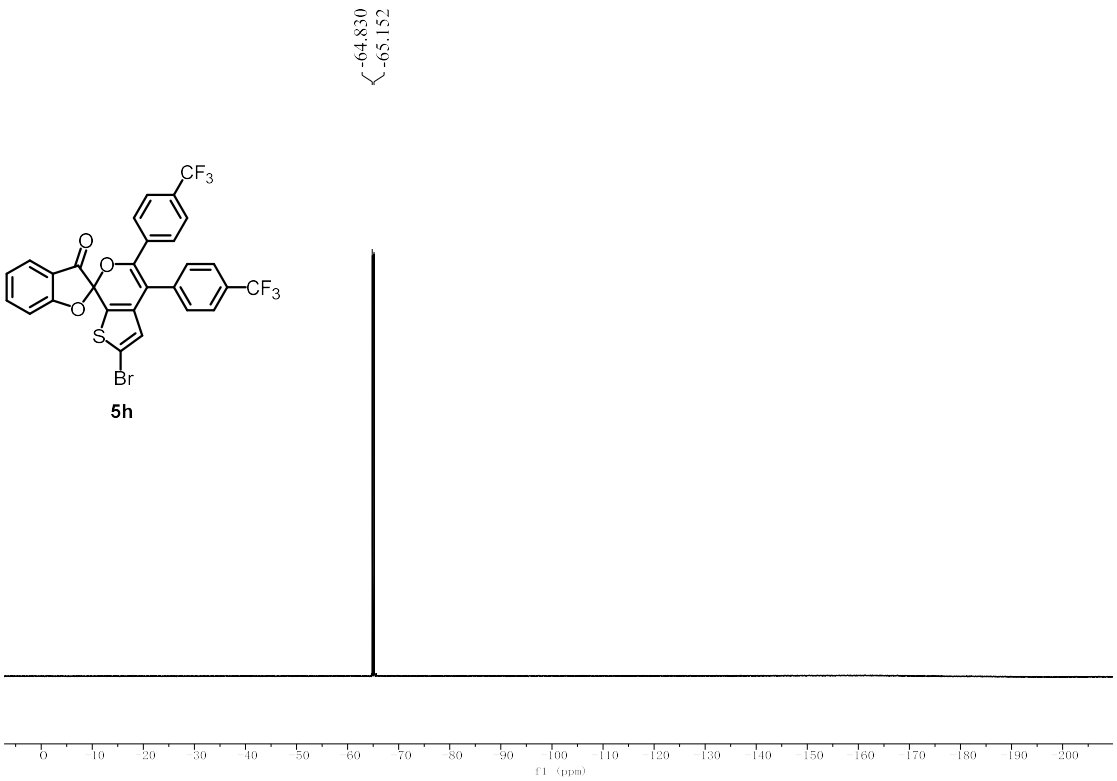
^{1}H NMR (500 MHz, $CDCl_3$)



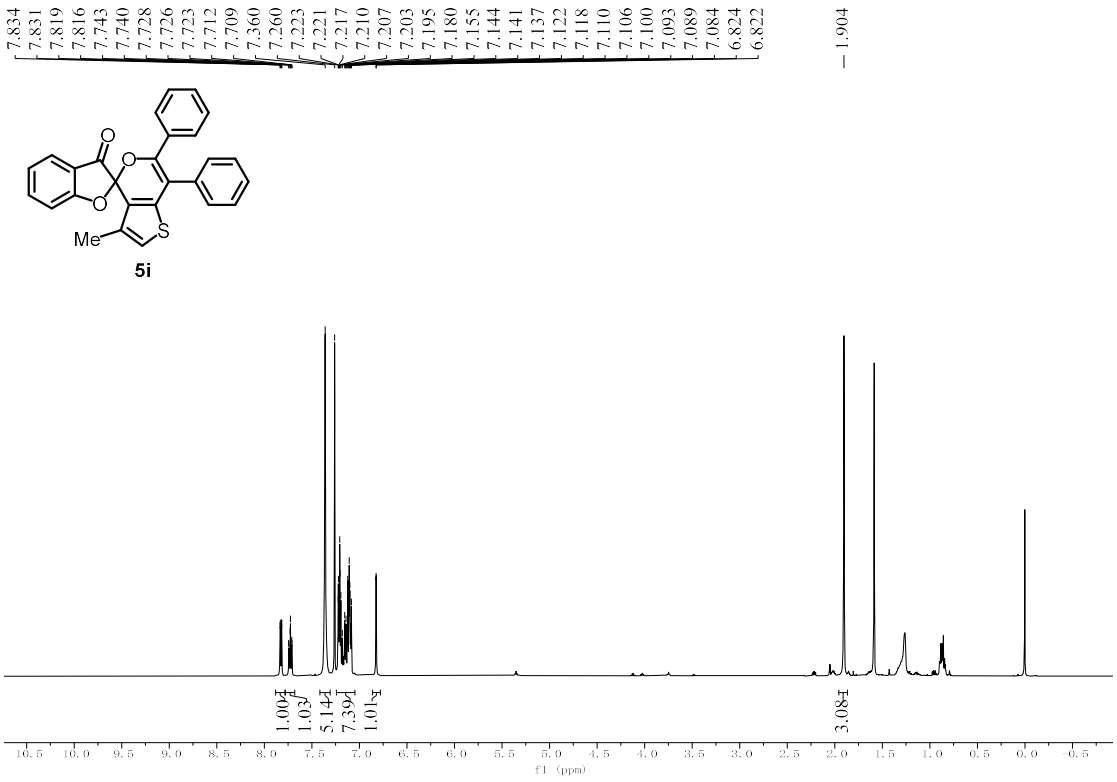
^{13}C NMR (126 MHz, $CDCl_3$)



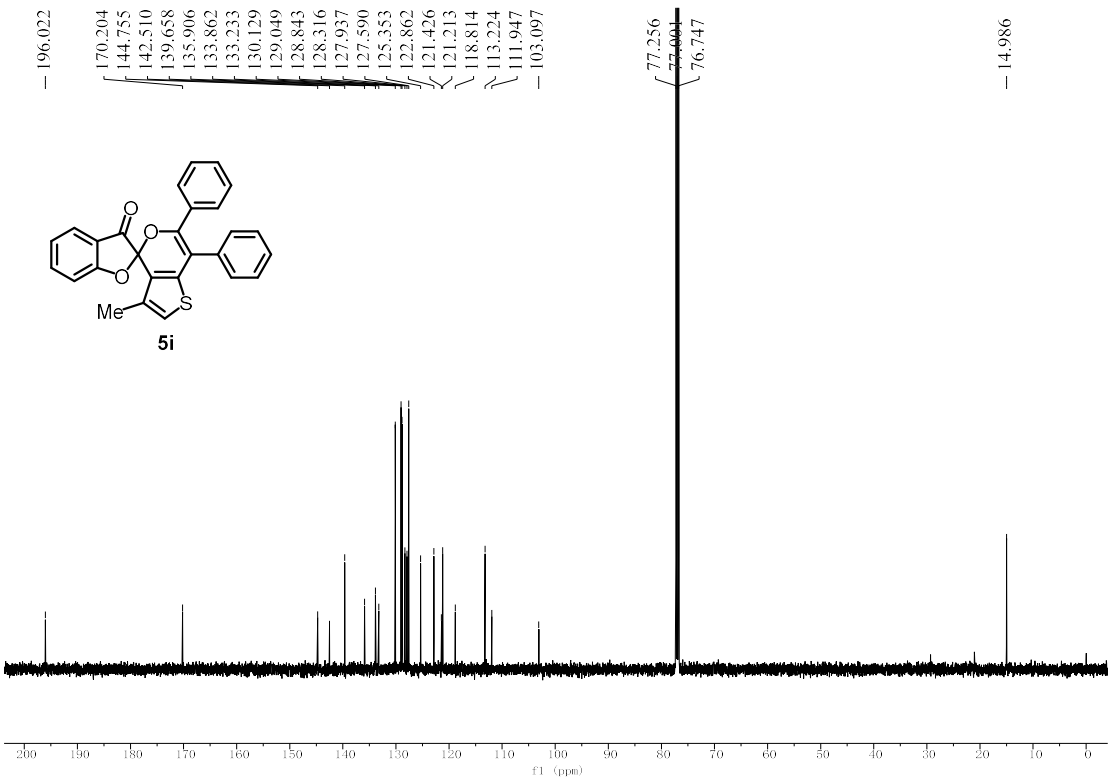
^{19}F NMR (471 MHz, $CDCl_3$)



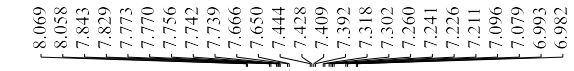
^{1}H NMR (500 MHz, $CDCl_3$)

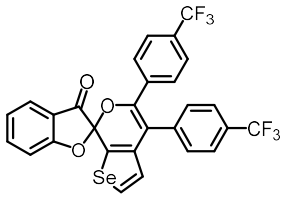


^{13}C NMR (126 MHz, $CDCl_3$)

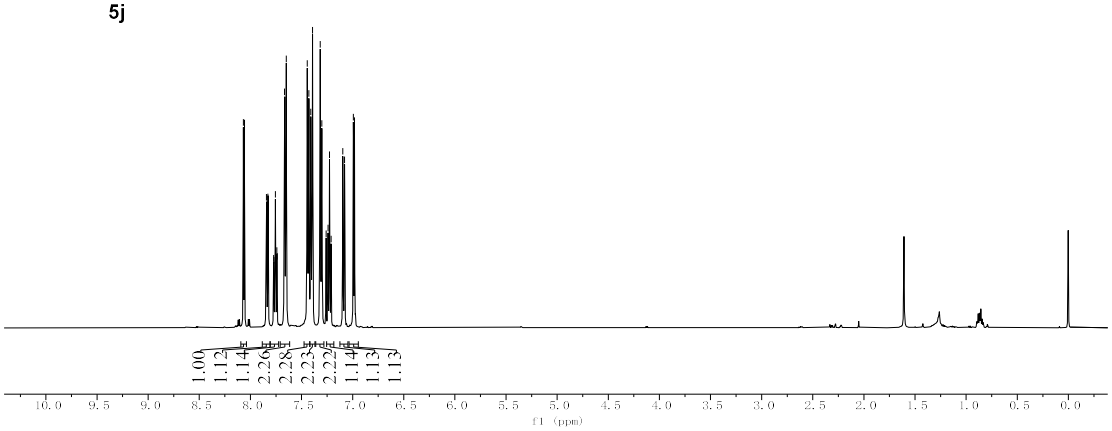


^{1}H NMR (500 MHz, $CDCl_3$)

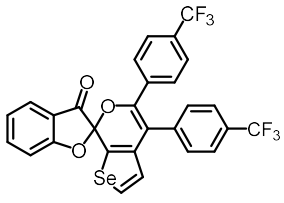




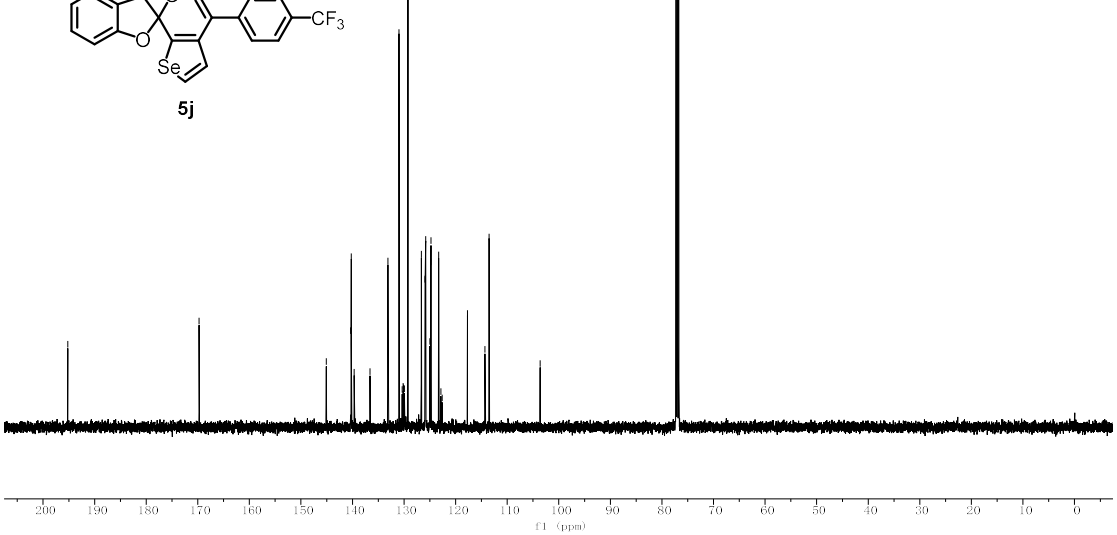
5j



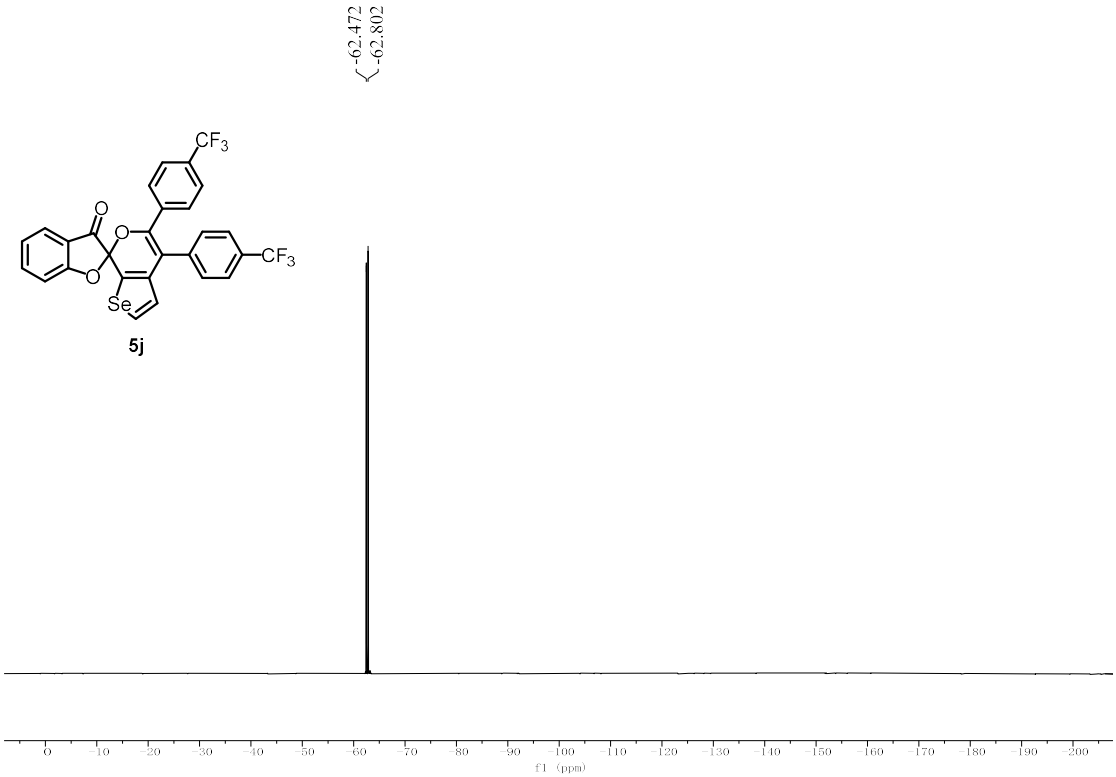
^{13}C NMR (126 MHz, $CDCl_3$)



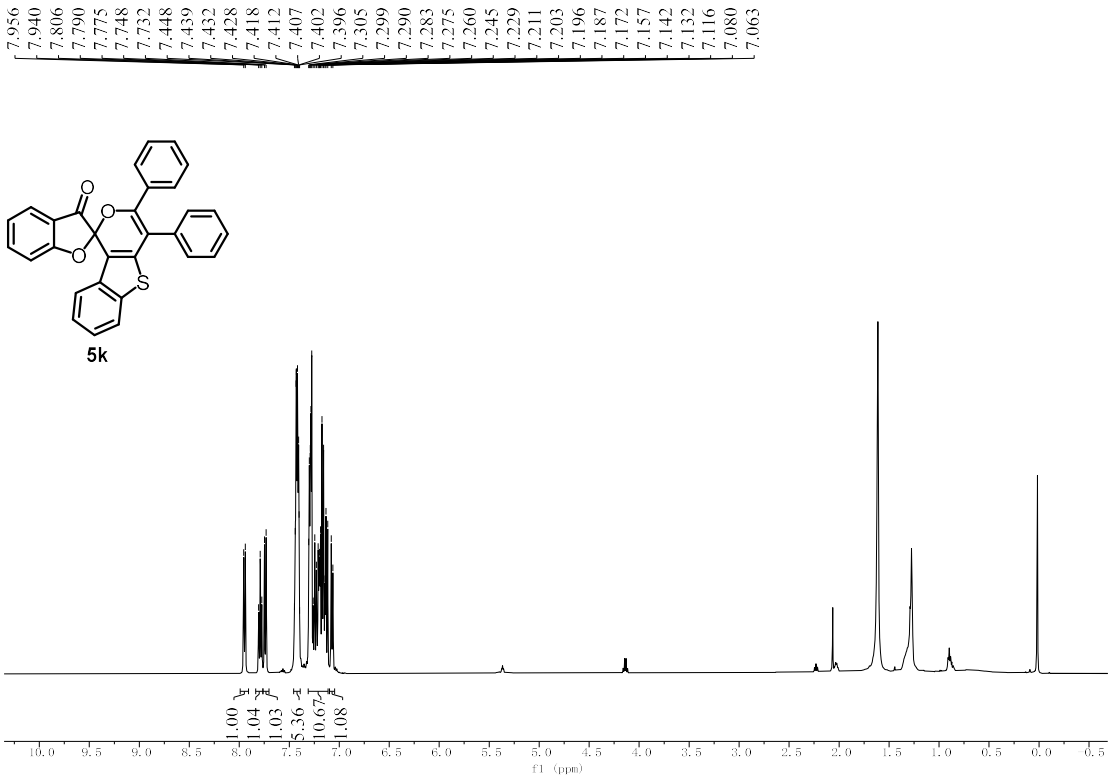
5j



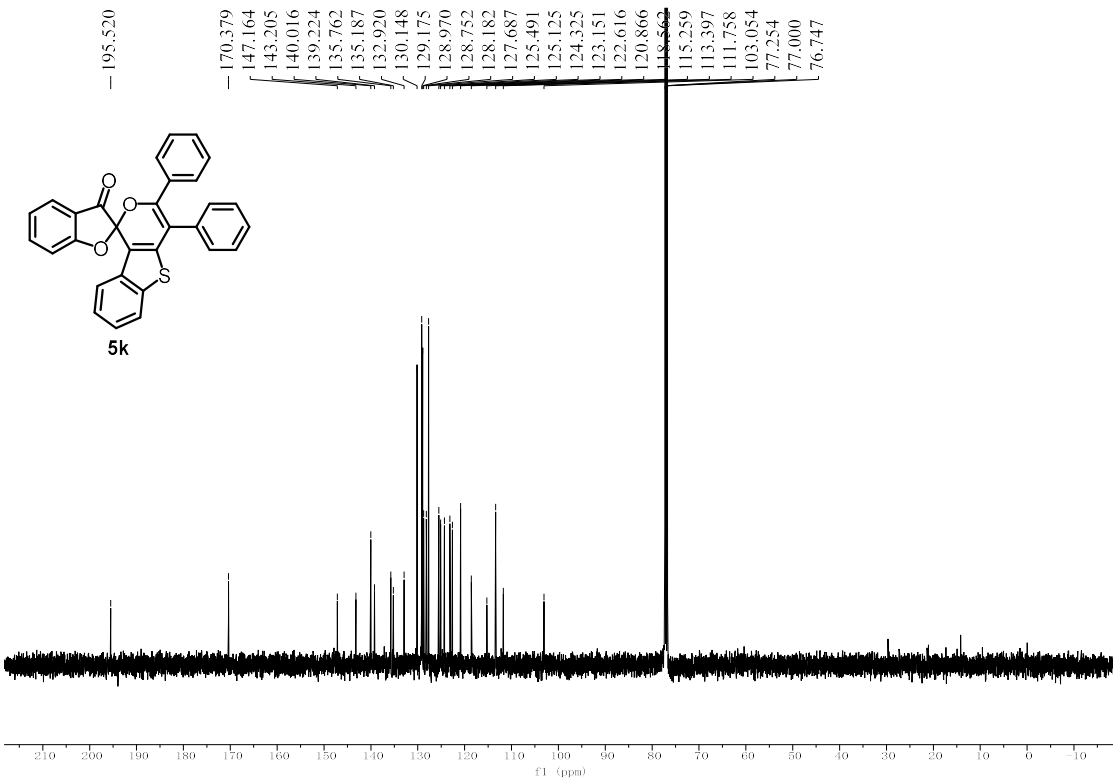
^{19}F NMR (471 MHz, $CDCl_3$)



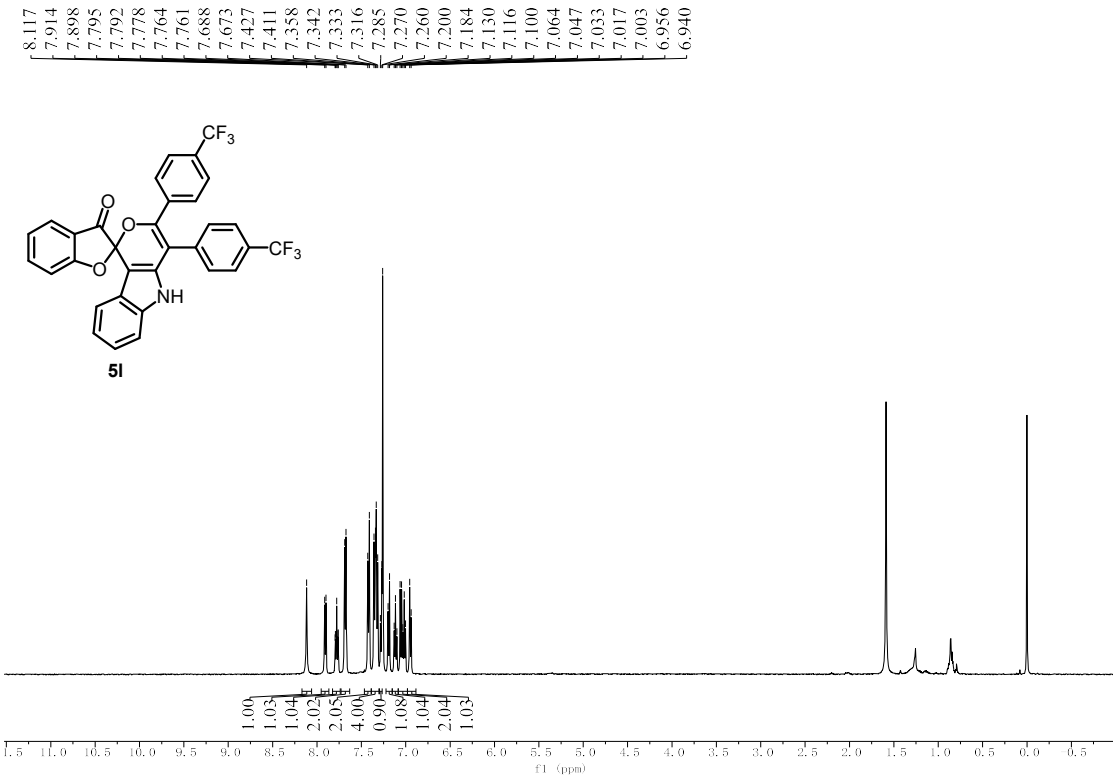
^{1}H NMR (500 MHz, $CDCl_3$)



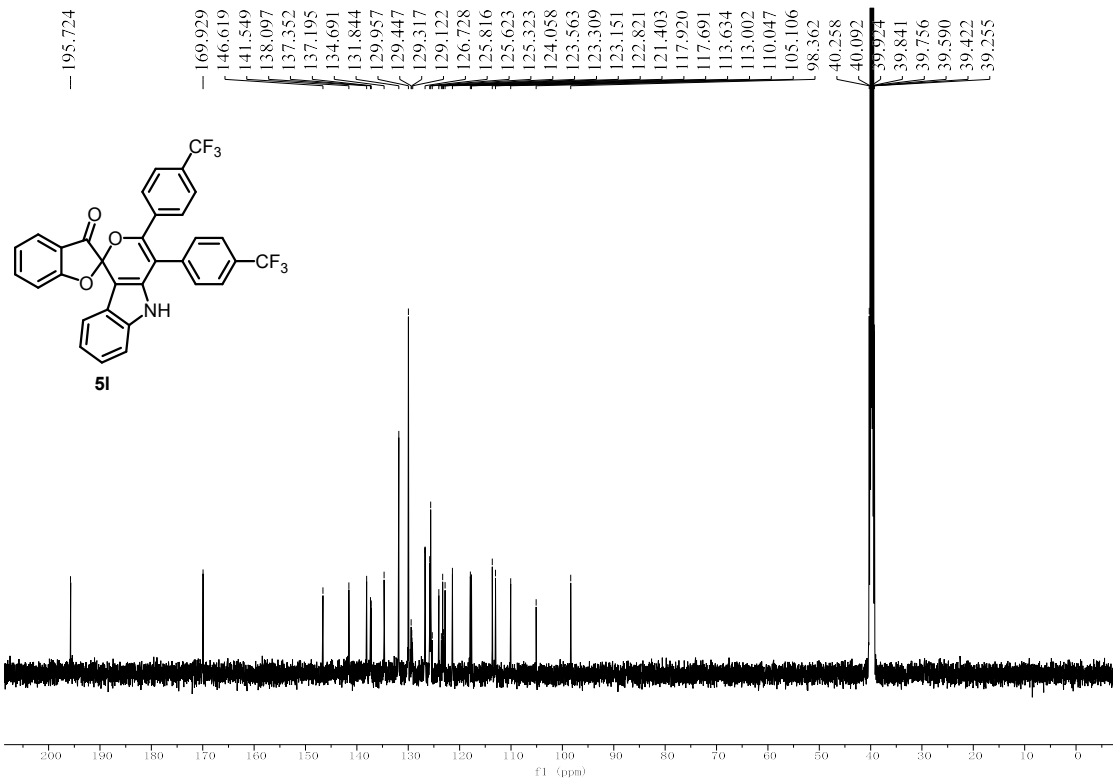
^{13}C NMR (126 MHz, $CDCl_3$)



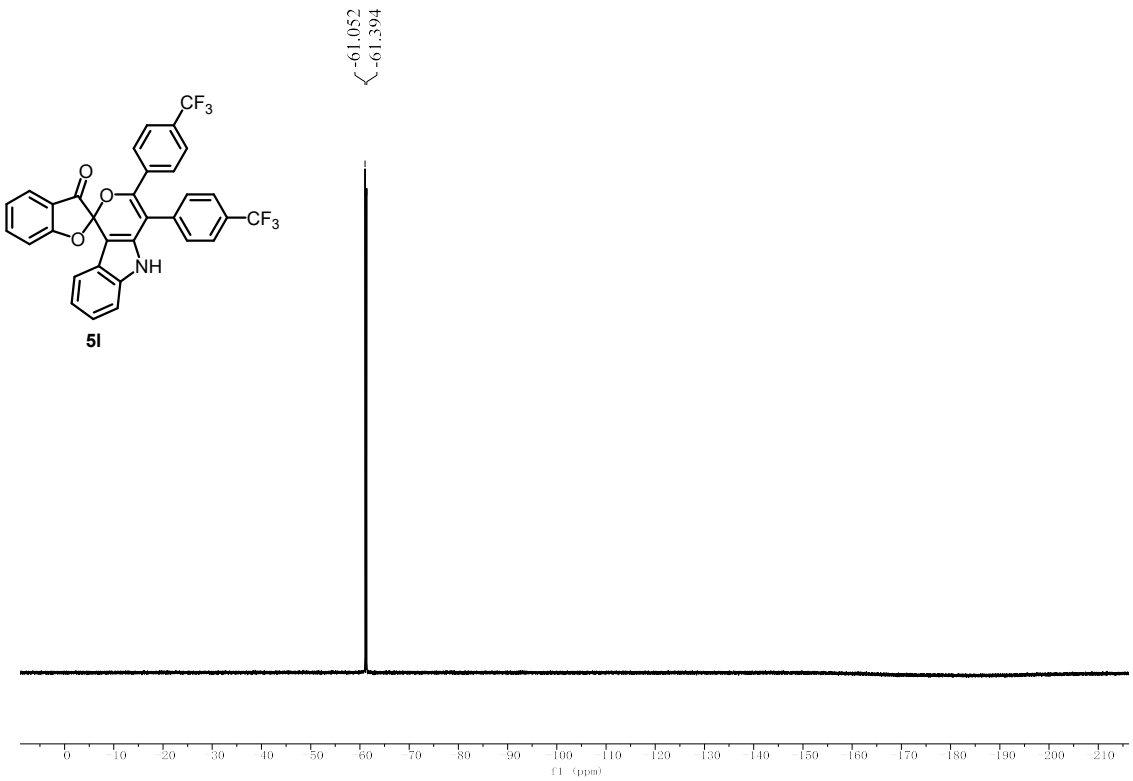
^{1}H NMR (500 MHz, $CDCl_3$)



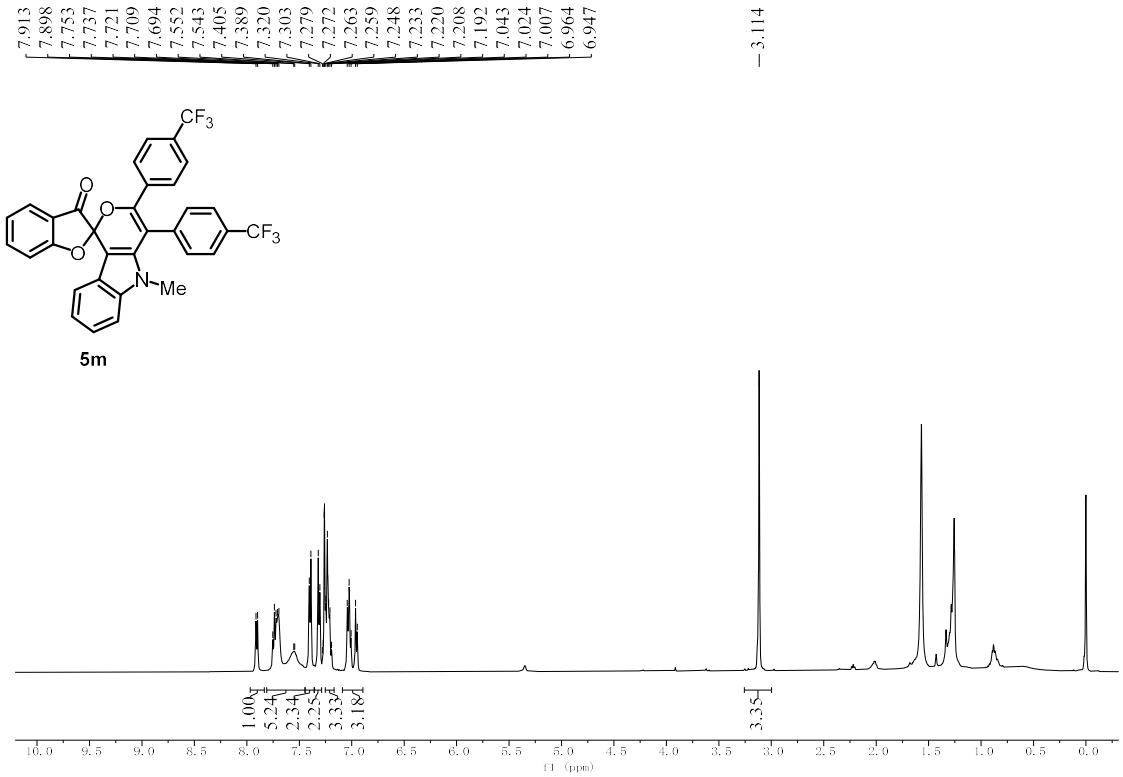
^{13}C NMR (126 MHz, DMSO-d_6)



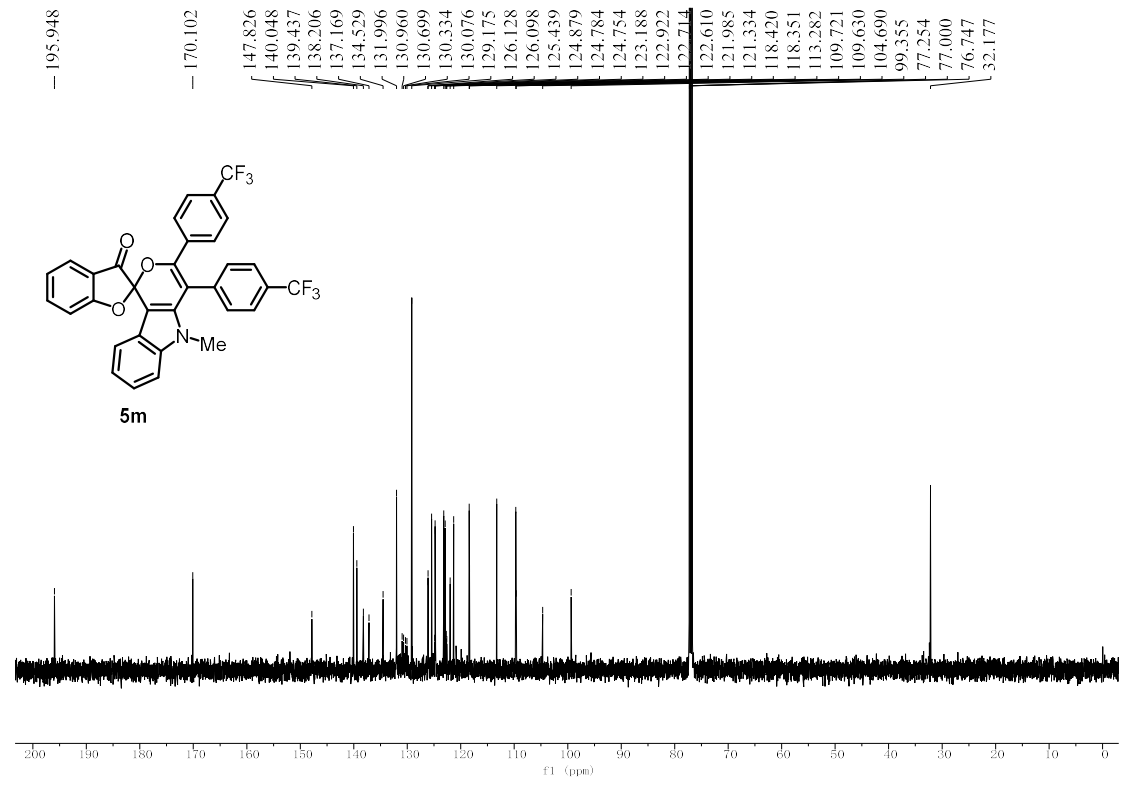
^{19}F NMR (471 MHz, DMSO-d_6)



^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)



^{19}F NMR (471 MHz, $CDCl_3$)