Supporting Information

Brønsted Acid-Catalyzed Solvent-Controlled Regioselective Hydrothiolation and Diastereoselective Cascade Cyclization of Dienes

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1. General considerations

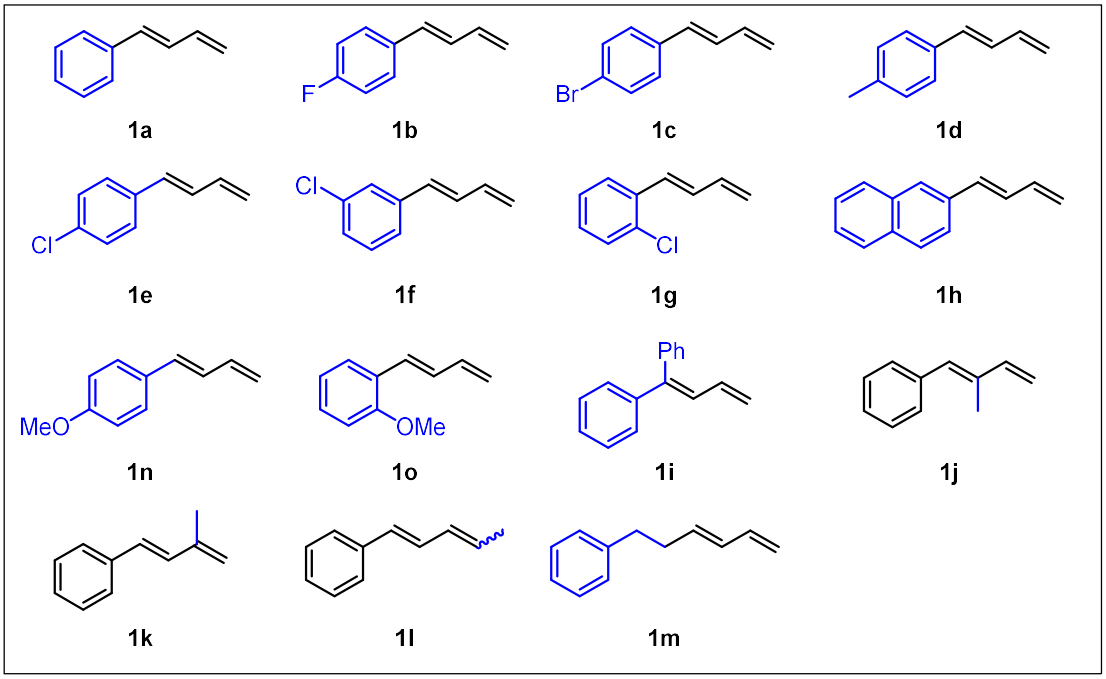
Unless otherwise noted, all reactions were carried out under an atmosphere of argon, using over-dried or flame-dried glassware equipped with a magnetic stir bar. All chemicals were purchased from commercial suppliers and used without further purification. In addition to commercially available extra dry solvents, all solvents were purified by standard operating method. Thin-layer chromatography was performed with EMD silica gel 60 F_{254} plates eluting with solvents indicated, visualized by a 254 nm UV lamp and stained with phosphomolybdic acid (PMA). **^{1}H NMR**, **^{13}C NMR** and **^{19}F NMR** spectra were obtained on Bruker AM-400 and Bruker AM-500. Chemical shifts (δ) were quoted in ppm relative to tetramethylsiane or deuterated solvent as internal standard (Chloroform-*d*: 7.26 ppm for **^{1}H NMR**; Chloroform-*d*: 77.16 ppm for **^{13}C NMR**), multiplicities are as indicated: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution mass spectral analysis (HRMS) data were measured on a MALDI-Fourier Transform Ion Cyclotron (SolariX 7.0T) mass spectrometer. Crystallographic data was obtained from a Bruker D8 VENTURE diffractometer. Melting points were measured on a melting point apparatus and were uncorrected.

2. The preparation of substrates

2.1 All of the used 1,3-dienes are known compounds. Compounds **1a-1m** were prepared according to reported literatures[1-2].

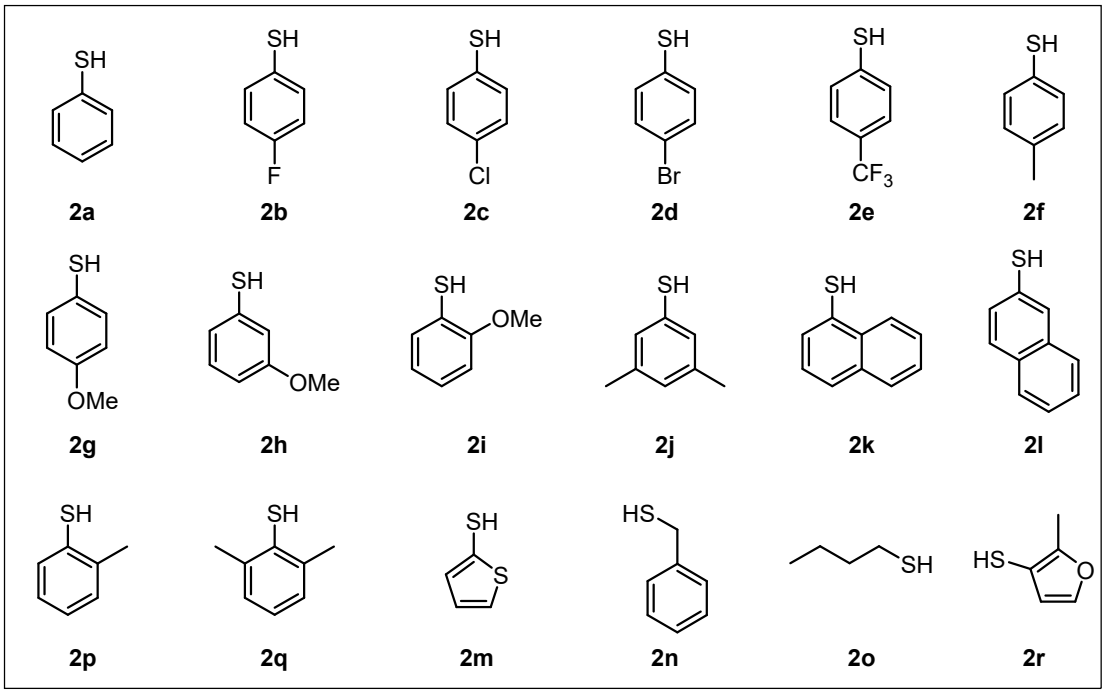
Our analytical data (**^{1}H NMR**, **^{13}C NMR** and **^{19}F NMR**) match with the literatures[1-2]. (**Figure S1** and **Figure S2)**.

Figure S1. Substrate scope of known linear 1,3-dienes



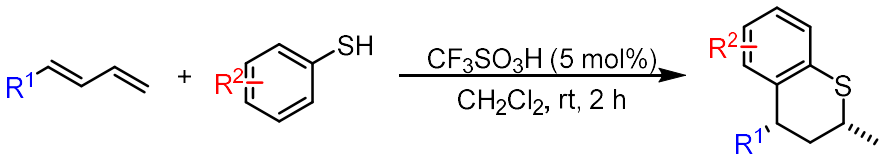
2.2 All of thiols were purchased from commercial suppliers (*Energy Chemical* and *TCI company*) and used without further purification, TfOH were purchased from commercial suppliers (*Energy Chemical*) and used without further purification.

Figure S2. Substrate scope of thiols



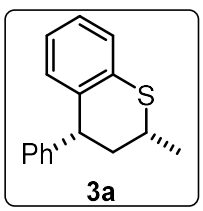
3. General procedure for the synthesis of products 3 and 4.

3.1 General procedure **A**: reactions for the synthesis of **3** using 1-substituted 1,3-dienes as substrates



1 **2** **3**

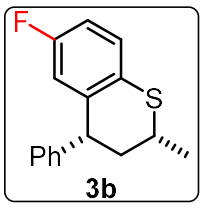
At room temperature, **1** (0.1 mmol), **2** (0.2 mmol), anhydrous DCM (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then TfOH (0.005 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The product **3** is obtained by column chromatography.



3a

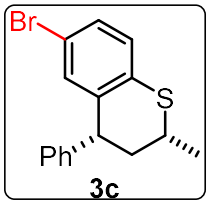
According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2a** (20.6 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column

chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3a** (16.1 mg, 67%) as a white solid, Rf =0.25 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.34 (t, *J* = 7.4 Hz, 2H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.20 (d, *J* = 7.4 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 4.10 (dd, *J* = 12.3, 4.5 Hz, 1H), 3.58 (dtd, *J* = 16.3, 9.4, 8.1, 5.3 Hz, 1H), 2.38 (dt, *J* = 13.5, 3.7 Hz, 1H), 2.04 (q, *J* = 12.4 Hz, 1H), 1.36 (d, *J* = 6.6 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 145.51, 136.93, 134.37, 130.08, 128.85, 128.83, 126.79, 126.59, 126.31, 124.08, 47.49, 42.71, 36.62, 21.89; **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{16}H_{16}AgS$ 347.0019, found 347.0019.



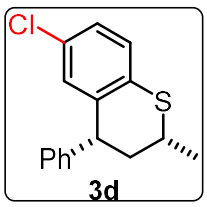
3b

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3b** (17.6 mg, 68%) as a colorless oil, Rf =0.25 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 (t, *J* = 7.3 Hz, 2H), 7.32 – 7.26 (m, 1H), 7.22 – 7.14 (m, 2H), 7.07 (dd, *J* = 8.7, 5.6 Hz, 1H), 6.78 (td, *J* = 8.3, 7.9, 2.8 Hz, 1H), 6.41 (ddd, *J* = 10.4, 2.8, 1.1 Hz, 1H), 4.05 (dd, *J* = 12.3, 4.5 Hz, 1H), 3.56 (dtd, *J* = 13.4, 6.7, 2.9 Hz, 1H), 2.39 (ddd, *J* = 13.5, 4.5, 2.9 Hz, 1H), 2.08 – 1.94 (m, 1H), 1.36 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.12 (d, J = 243.0 Hz), 144.63, 139.09 (d, *J* = 6.3 Hz), 129.22 (d, *J* = 6.1 Hz), 129.00, 128.75, 127.47 (d, *J* = 7.5 Hz), 127.09, 116.76 (d, *J* = 22.0 Hz), 114.05 (d, *J* = 22.0 Hz), 47.58 (d, *J* = 1.3 Hz), 42.23, 36.59, 21.86; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.62 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{16}H_{15}FS$ 258.0873, found 258.0880.



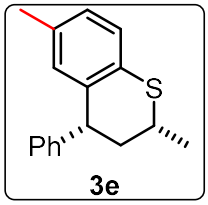
3c

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2d** (37.8 mg, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3c** (22.8 mg, 71%) as a colorless oil, Rf =0.26 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.40 – 7.32 (m, 2H), 7.32 – 7.25 (m, 1H), 7.21 – 7.11 (m, 3H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.79 (s, 1H), 4.04 (dd, *J* = 12.3, 4.5 Hz, 1H), 3.62 – 3.49 (m, 1H), 2.37 (dt, *J* = 13.6, 3.5 Hz, 1H), 2.00 (q, *J* = 12.4 Hz, 1H), 1.35 (d, *J* = 6.6 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 144.49, 139.10, 133.70, 132.61, 129.64, 129.06, 128.71, 127.79, 127.14, 117.41, 47.37, 42.27, 36.62, 21.77; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{16}H_{15}BrS$ 318.0073, found 318.0073.



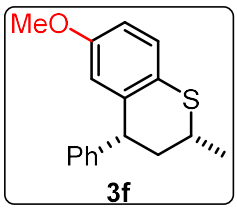
3d

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2c** (28.9 mg, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3d** (19.9 mg, 73%) as a colorless oil, Rf =0.26 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 (t, *J* = 7.4 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 7.5 Hz, 2H), 7.08 – 6.98 (m, 2H), 6.66 (s, 1H), 4.04 (dd, *J* = 12.3, 4.5 Hz, 1H), 3.62 – 3.49 (m, 1H), 2.37 (dt, *J* = 13.6, 3.7 Hz, 1H), 2.01 (q, *J* = 12.4 Hz, 1H), 1.36 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 144.53, 138.77, 133.00, 129.78, 129.65, 129.06, 128.74, 127.48, 127.13, 126.80, 47.43, 42.27, 36.65, 21.80; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{16}H_{15}ClS$ 274.0578, found 274.0582.



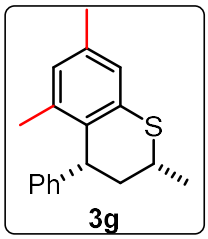
3e

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2f** (23.7 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3e** (19.8 mg, 78%) as a colorless oil, Rf =0.22 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.35 (t, *J* = 7.3 Hz, 2H), 7.28 (d, *J* = 7.3 Hz, 1H), 7.20 (d, *J* = 6.6 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.50 (s, 1H), 4.07 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.54 (dtd, *J* = 13.4, 6.7, 2.8 Hz, 1H), 2.36 (ddd, *J* = 13.5, 4.6, 2.8 Hz, 1H), 2.10 (s, 3H), 2.09 – 1.95 (m, 1H), 1.35 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 145.67, 136.72, 133.69, 130.71, 130.68, 128.85, 128.80, 127.54, 126.70, 126.29, 47.46, 43.11, 36.53, 21.89, 21.02; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}S$ 254.1124, found 254.1124.



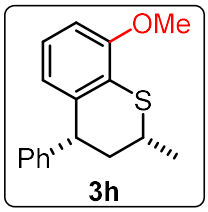
3f

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2g** (24.6 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=10:1, v/v) to afford **3f** (13.5 mg, 50%) as a colorless oil, Rf =0.35 (silica gel, PE:DCM = 4:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.33 (t, *J* = 7.3 Hz, 2H), 7.28 – 7.23 (m, 1H), 7.23 – 7.17 (m, 2H), 7.04 (d, *J* = 8.6 Hz, 1H), 6.66 (ddd, *J* = 8.7, 2.8, 0.8 Hz, 1H), 6.26 (dd, *J* = 2.9, 1.1 Hz, 1H), 4.06 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.58 (s, 3H), 3.59 – 3.48 (m, 1H), 2.38 (ddd, *J* = 13.5, 4.6, 3.0 Hz, 1H), 2.00 (dt, *J* = 13.3, 11.8 Hz, 1H), 1.35 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 156.74, 145.23, 138.45, 128.83, 127.25, 126.83, 125.19, 116.14, 112.61, 55.34, 55.29, 47.67, 42.82, 36.57, 21.96; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}OS$ 270.1073, found 270.1074.



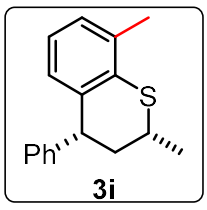
3g

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2j** (27.2 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3g** (22.3 mg, 83%) as a white solid, Rf =0.20 (silica gel, PE), **M.P.** 61 – 62 ºC; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.30 – 7.13 (m, 3H), 7.06 (d, *J* = 7.6 Hz, 2H), 6.93 (s, 1H), 6.67 (s, 1H), 4.32 (t, *J* = 8.4 Hz, 1H), 3.28 (td, *J* = 6.9, 3.3 Hz, 1H), 2.60 (ddd, *J* = 14.0, 7.7, 2.8 Hz, 1H), 2.25 (s, 3H), 2.07 (dt, *J* = 13.6, 9.8 Hz, 1H), 1.82 (s, 3H), 1.22 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 146.98, 138.78, 135.95, 135.19, 131.68, 128.96, 128.69, 127.63, 126.11, 125.91, 46.48, 44.12, 36.22, 21.31, 21.17, 20.79; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{18}H_{20}S$ 268.1281, found 268.1280.



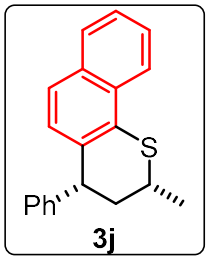
3h

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2i** (24.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=10:1, v/v) to afford **3h** (13.6 mg, 50%) as a colorless oil, Rf =0.33 (silica gel, PE:DCM = 4:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.33 (t, *J* = 7.3 Hz, 2H), 7.28 – 7.22 (m, 1H), 7.21 – 7.16 (m, 2H), 6.84 (t, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.33 (d, *J* = 7.9 Hz, 1H), 4.13 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.90 (s, 3H), 3.47 (ddd, *J* = 11.6, 6.8, 2.5 Hz, 1H), 2.34 (ddd, *J* = 13.4, 4.7, 2.5 Hz, 1H), 2.10 – 1.96 (m, 1H), 1.39 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 154.56, 145.83, 137.94, 128.81, 128.77, 126.71, 123.71, 123.51, 122.83, 107.74, 56.07, 47.57, 42.39, 35.48, 21.81; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}OS$ 270.1073, found 270.1073.



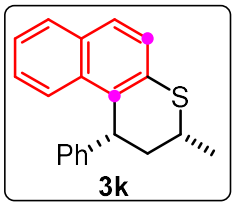
3i

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2p** (23.6 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3i** (9.7 mg, 38%) as a colorless oil, Rf =0.20 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.33 (t, *J* = 7.4 Hz, 2H), 7.29 – 7.23 (m, 1H), 7.19 (d, *J* = 7.1 Hz, 2H), 6.95 (d, *J* = 7.3 Hz, 1H), 6.78 (t, *J* = 7.6 Hz, 1H), 6.54 (d, *J* = 7.8 Hz, 1H), 4.13 (dd, *J* = 12.4, 4.5 Hz, 1H), 3.54 (ddd, *J* = 11.6, 6.7, 2.8 Hz, 1H), 2.36 (ddd, *J* = 13.5, 4.5, 2.9 Hz, 1H), 2.30 (s, 3H), 2.11 – 1.97 (m, 1H), 1.39 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 145.97, 136.84, 134.08, 133.88, 128.83, 128.79, 127.94, 127.73, 126.68, 123.18, 47.90, 42.36, 36.43, 22.05, 20.39; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}S$ 254.1124, found 254.1128.



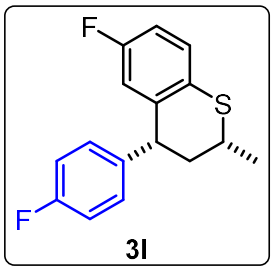
3j

According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2k** (27.9 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **3j** (15.0 mg, 52%) as a white solid, Rf =0.37 (silica gel, PE:DCM = 5:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 7.9 Hz, 1H), 7.72 (d, *J* = 9.5 Hz, 1H), 7.56 – 7.42 (m, 2H), 7.39 – 7.29 (m, 3H), 7.28 – 7.23 (m, 1H), 7.23 – 7.15 (m, 2H), 6.87 (d, *J* = 8.6 Hz, 1H), 4.37 (dd, *J* = 12.1, 5.5 Hz, 1H), 3.58 (ddd, *J* = 11.7, 6.8, 2.4 Hz, 1H), 2.50 (ddd, *J* = 13.6, 5.5, 2.4 Hz, 1H), 2.20 – 2.05 (m, 1H), 1.47 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 146.30, 133.41, 132.21, 130.79, 130.54, 128.86, 128.85, 128.38, 128.30, 126.72, 126.12, 125.94, 123.85, 123.79, 48.16, 43.62, 36.28, 21.61; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{20}H_{18}S$ 290.1124, found 290.1124.



3k

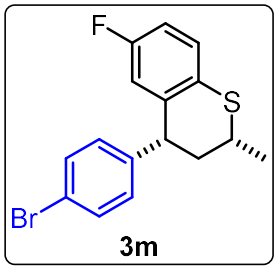
According to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2l** (32.0 mg, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **3k** and its isomer (24.3 mg, 84%, 6:1 rr) as a colorless oil, Rf =0.37 (silica gel, PE:DCM = 5:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.55 (d, *J* = 8.5 Hz, 1H), 7.32 – 7.22 (m, 2H), 7.23 – 7.16 (m, 3H), 7.13 (d, *J* = 7.3 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 2H), 4.90 (dd, *J* = 9.4, 7.4 Hz, 1H), 3.43 – 3.29 (m, 1H), 2.73 (ddd, *J* = 14.1, 7.4, 2.6 Hz, 1H), 2.17 (dt, *J* = 14.0, 9.8 Hz, 1H), 1.29 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 147.42, 133.84, 132.89, 132.23, 129.57, 128.81, 128.61, 127.60, 127.35, 126.56, 124.51, 124.35, 46.11, 43.32, 36.11, 36.08, 21.18; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{20}H_{18}S$ 290.1124, found 290.1126.



3l

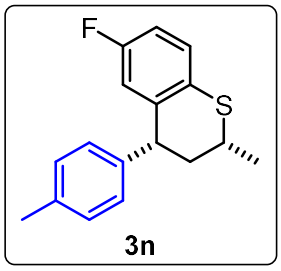
According to the general procedure **A**, the reaction of **1b** (14.8 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3l** (19.8 mg, 72%) as a colorless oil, Rf =0.33 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.20 – 7.11 (m, 2H), 7.10 – 6.99 (m, 3H), 6.78 (td, *J* = 8.3, 2.7 Hz, 1H), 6.37 (d, *J* = 9.0 Hz, 1H), 4.05 (dd, *J* = 12.4, 4.5 Hz, 1H), 3.62 – 3.45 (m,

1H), 2.36 (dt, *J* = 13.7, 3.7 Hz, 1H), 1.96 (q, *J* = 12.4 Hz, 1H), 1.35 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 161.93 (d, *J* = 245.2 Hz), 160.15 (d, *J* = 242.6 Hz), 140.38 (d, *J* = 3.3 Hz), 138.82 (d, *J* = 6.4 Hz), 130.19 (d, *J* = 7.8 Hz), 129.27 (d, *J* = 3.0 Hz), 127.61 (d, *J* = 7.6 Hz), 116.64 (d, *J* = 22.3 Hz), 115.87 (d, *J* = 21.3 Hz), 114.20 (d, *J* = 22.3 Hz), 46.83, 42.39, 36.54, 21.83; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -115.76 (s, 1F), -118.46 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{16}H_{14}F_2S$ 276.0779, found 276.0782.



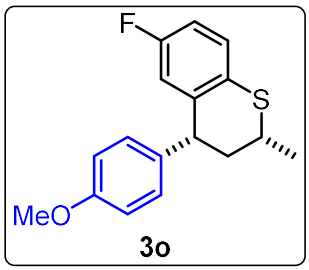
3m

According to the general procedure **A**, the reaction of **1c** (20.9 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (1.3 ul, 0.015 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3m** (23.5 mg, 70%) as a white solid, Rf =0.30 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.11 – 7.02 (m, 3H), 6.79 (td, *J* = 8.3, 2.8 Hz, 1H), 6.37 (ddd, *J* = 10.3, 2.8, 1.1 Hz, 1H), 4.03 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.53 (dqd, *J* = 11.3, 6.7, 2.8 Hz, 1H), 2.35 (ddd, *J* = 13.5, 4.6, 2.9 Hz, 1H), 2.02 – 1.88 (m, 1H), 1.35 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.11 (d, *J* = 242.6 Hz), 143.73, 138.26 (d, *J* = 6.4 Hz), 132.14, 130.46, 129.30, 129.27, 127.65 (d, *J* = 7.6 Hz), 120.90, 116.66 (d, *J* = 22.4 Hz), 114.29 (d, *J* = 22.4 Hz), 47.02 (d, *J* = 1.4 Hz), 42.20, 36.45, 21.76; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.32 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{16}H_{14}BrFS$ 335.9979, found 335.9977.



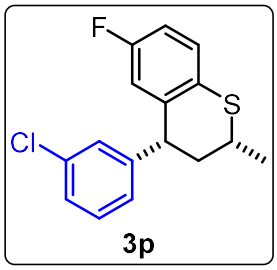
3n

According to the general procedure **A**, the reaction of **1d** (14.4 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3n** (13.0 mg, 50%) as a colorless oil, Rf =0.22 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.16 (d, *J* = 7.9 Hz, 2H), 7.10 – 7.02 (m, 3H), 6.80 – 6.72 (m, 1H), 6.45 – 6.38 (m, 1H), 4.01 (dd, *J* = 12.3, 4.5 Hz, 1H), 3.62 – 3.47 (m, 1H), 2.41 – 2.30 (m, 4H), 2.05 – 1.92 (m, 1H), 1.35 (d, *J* = 6.6 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.13 (d, *J* = 242.0 Hz), 141.58, 139.33 (d, *J* = 6.3 Hz), 136.67, 129.67, 129.15 (d, *J* = 3.0 Hz), 128.60, 127.40 (d, *J* = 7.4 Hz), 116.73 (d, *J* = 22.3 Hz), 113.98 (d, *J* = 22.3 Hz), 47.15 (d, *J* = 1.3 Hz), 42.26, 36.60, 21.88, 21.22; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.72; **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{17}H_{16}FS$ 271.0952, found 271.0946.



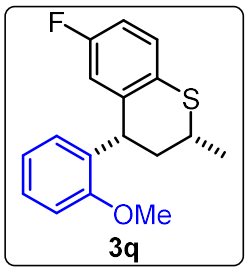
3o

According to the general procedure **A**, the reaction of **1n** (16.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=10:1, v/v) to afford **3o** (19.2 mg, 66%) as a colorless oil, Rf =0.35 (silica gel, PE:DCM = 5:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.14 – 7.02 (m, 3H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.77 (td, *J* = 8.3, 2.7 Hz, 1H), 6.42 (ddd, *J* = 10.4, 2.9, 1.2 Hz, 1H), 3.99 (dd, *J* = 12.5, 4.4 Hz, 1H), 3.82 (s, 3H), 3.55 (dqd, *J* = 13.3, 6.6, 2.9 Hz, 1H), 2.40 – 2.31 (m, 1H), 2.04 – 1.90 (m, 1H), 1.35 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.16 (d, J = 242.1 Hz), 158.66, 139.56 (d, *J* = 6.2 Hz), 136.65, 129.68, 129.17 (d, *J* = 2.8 Hz), 127.42 (d, *J* = 7.6 Hz), 116.67 (d, *J* = 22.7 Hz), 114.39, 113.98 (d, *J* = 22.2 Hz), 55.44, 46.74, 42.29, 36.64, 21.93; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.68 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{17}OS$ 288.0978, found 288.0978.



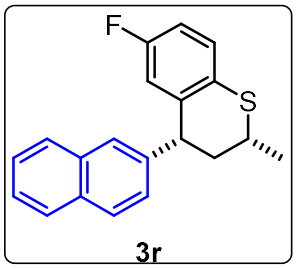
3p

According to the general procedure **A**, the reaction of **1f** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (1.3 ul, 0.015 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3p** (21.1 mg, 72%) as a colorless oil, Rf =0.35 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.32 – 7.24 (m, 2H), 7.18 (s, 1H), 7.11 – 7.03 (m, 2H), 6.84 – 6.75 (m, 1H), 6.39 (ddd, *J* = 10.3, 2.8, 1.1 Hz, 1H), 4.04 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.60 – 3.47 (m, 1H), 2.37 (ddd, *J* = 13.5, 4.7, 2.9 Hz, 1H), 1.97 (dt, *J* = 13.5, 11.9 Hz, 1H), 1.36 (d, *J* = 6.6 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.13 (d, *J* = 242.9 Hz), 146.75, 138.09 (d, *J* = 6.3 Hz), 134.79, 130.29, 129.29 (d, *J* = 3.1 Hz), 128.86, 127.69 (d, *J* = 7.6 Hz), 127.36, 126.98, 116.71 (d, *J* = 22.7 Hz), 114.34 (d, *J* = 22.7 Hz), 47.28 (d, *J* = 1.3 Hz), 42.17, 36.45, 21.74; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.29 (s, 1F) ; **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{16}H_{14}AgClFS$ 398.9535, found 398.9528.



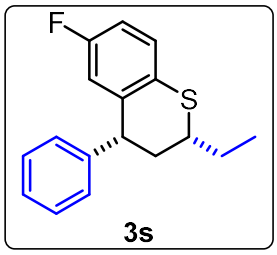
3q

According to the general procedure **A**, the reaction of **1o** (16.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=10:1, v/v) to afford **3q** (19.3 mg, 67%) as a white solid, Rf =0.35 (silica gel, PE:DCM = 4:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.31 – 7.23 (m, 1H), 7.10 – 7.02 (m, 2H), 6.98 – 6.89 (m, 2H), 6.80 – 6.71 (m, 1H), 6.40 (ddd, *J* = 10.5, 2.8, 1.2 Hz, 1H), 4.54 (dd, *J* = 12.2, 4.5 Hz, 1H), 3.80 (s, 3H), 3.63 – 3.49 (m, 1H), 2.32 (ddd, *J* = 13.4, 4.5, 3.0 Hz, 1H), 2.09 – 1.96 (m, 1H), 1.35 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.22 (d, *J* = 241.8 Hz), 157.27, 139.35 (d, *J* = 6.5 Hz), 132.77, 129.51, 129.19 (d, *J* = 2.9 Hz), 128.11, 127.37 (d, J = 7.8 Hz), 121.23, 116.05 (d, *J* = 22.4 Hz), 113.59 (d, *J* = 22.4 Hz), 111.02, 55.62, 40.40, 36.88, 21.88; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -114.43 (s, 1F). **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{17}OS$ 288.0979, found 288.0978.



3r

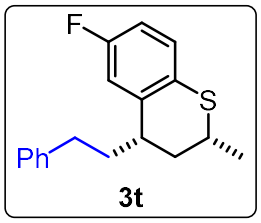
According to the general procedure **A**, the reaction of **1h** (1.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **3r** (17.6 mg, 57%) as a white solid, Rf =0.40 (silica gel, PE:DCM = 10:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 – 7.78 (m, 3H), 7.71 (s, 2H), 7.52 – 7.47 (m, 2H), 7.28 – 7.22 (m, 1H), 7.09 (dd, *J* = 8.7, 5.6 Hz, 1H), 6.79 (td, *J* = 8.7, 3.5 Hz, 1H), 6.46 – 6.38 (m, 1H), 4.24 (dd, *J* = 12.3, 4.6 Hz, 1H), 3.66 – 3.55 (m, 1H), 2.44 (ddd, *J* = 13.6, 4.6, 2.9 Hz, 1H), 2.12 (dt, *J* = 13.5, 11.9 Hz, 1H), 1.38 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.16 (d, *J* = 242.8 Hz), 141.98, 138.78 (d, *J* = 6.3 Hz), 133.71, 132.66, 129.24 (d, *J* = 3.0 Hz), 128.89, 127.87, 127.76, 127.58, 127.52 (d, *J* = 7.6 Hz), 126.57, 126.42, 125.96, 116.95 (d, *J* = 22.5 Hz), 114.17 (d, *J* = 22.5 Hz), 47.69 (d, *J* = 1.3 Hz), 42.15, 36.57, 21.83; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.56 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{20}H_{17}FS$ 308.1030, found 308.1032.



3s

According to the general procedure **A**, the reaction of **1l** (14.4 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (1.3 ul, 0.015 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **3s** (13.9 mg, 51%) as a colorless oil, Rf =0.35 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.41 – 7.25 (m, 3H), 7.23 – 7.17 (m, 2H), 7.09 (dd, *J* = 8.7, 5.6 Hz, 1H), 6.81 – 6.74 (m, 1H), 6.39 (ddd, *J* = 10.4, 2.8, 1.4 Hz, 1H), 4.02 (dd, *J* = 12.4, 4.3 Hz, 1H), 3.42 (dtd, *J* = 10.3, 6.7, 3.1 Hz, 1H), 2.43 (dt, *J* = 13.4, 3.7 Hz, 1H), 2.04 – 1.91 (m, 1H), 1.78 – 1.60 (m, 2H), 1.05 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 160.14 (d, *J* =

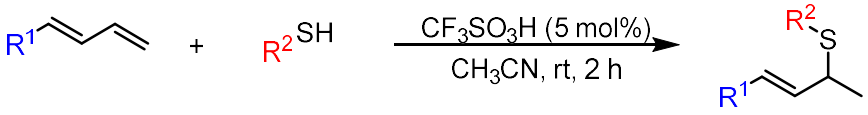
242.4 Hz), 144.51, 139.91 (d, J = 6.5 Hz), 129.12 (d, J = 3.0 Hz), 129.01, 128.77, 127.72 (d, J = 7.6 Hz), 127.12, 116.52 (d, J = 22.5 Hz), 114.03 (d, J = 22.5 Hz), 47.48 (d, J = 1.3 Hz), 43.75, 39.81, 29.64, 11.40; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -118.64 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{17}FS$ 272.1030, found 272.1030.



3t

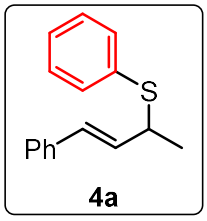
According to the general procedure **A**, the reaction of **1m** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford the mixture of **3t** (11.7 mg, 41%) as a colorless oil, Rf =0.29 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.45 – 7.40 (m, 2H), 7.16 – 7.07 (m, 4H), 7.01 (t, J = 8.7 Hz, 1H), 3.56 (dt, J = 5.5, 3.5 Hz, 1H), 3.01 (ddd, J = 16.5, 10.1, 6.0 Hz, 1H), 2.82 – 2.67 (m, 3H), 2.20 – 2.08 (m, 1H), 1.90 – 1.63 (m, 3H), 0.92 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.45 (d, J = 247.5 Hz), 138.49, 135.59, 135.08 (d, J = 8.0 Hz), 130.31 (d, J = 3.3 Hz), 129.69, 128.98, 126.00 (d, J = 19.3), 116.12 (d, J = 22.5 Hz), 47.43, 44.88, 30.24, 25.84, 24.04, 11.84; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -114.50 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{18}H_{19}FS$ 286.1186, found 286.1186.

3.2 General procedure B: hydrothiolation reactions for the synthesis of **4** using 1-substituted 1,3-dienes as substrates



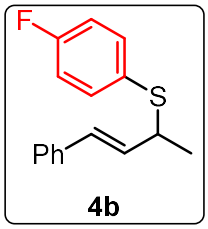
1 **2** **4**

At room temperature, **1** (0.1 mmol), **2** (0.2 mmol), anhydrous MeCN (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then TfOH (0.005 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), quenched with saturated $NaHCO_3$ aqueous solution. The organic phase was separated, extracted with MeCN, dried over Na_2SO_4, removed the solvent under reduce pressure. The product **4** is obtained by column chromatography.



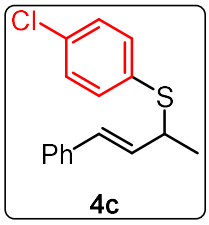
4a

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2a** (20.6 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4a** (17.2 mg, 72%) as a colorless oil, Rf =0.23 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.43 (d, *J* = 7.8 Hz, 2H), 7.35 – 7.16 (m, 8H), 6.27 – 6.11 (m, 2H), 3.97 - 3.85 (m, 1H), 1.50 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 137.01, 134.66, 133.49, 131.78, 130.08, 128.83, 128.63, 127.54, 127.49, 126.43, 46.65, 20.75; **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{16}H_{16}AgS$ 347.0019, found 347.0020.



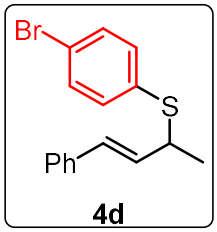
4b

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4b** (19.4 mg, 75%) as a colorless oil, Rf =0.23 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.43 – 7.36 (m, 2H), 7.31 – 7.16 (m, 5H), 6.99 – 6.90 (m, 2H), 6.18 – 6.05 (m, 2H), 3.77 (qdd, *J* = 6.8, 5.0, 2.3 Hz, 1H), 1.45 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.76 (d, J = 247.3 Hz), 136.86, 136.54 (d, *J* = 8.3 Hz), 131.58, 130.18, 129.44 (d, *J* = 3.4 Hz), 128.66, 127.62, 126.39, 115.88 (d, *J* = 21.8 Hz), 47.60, 20.54; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.73 (s, 1F); **HRMS** (MALDI) m/z: $[M+H]^+$ calcd for $C_{16}H_{16}FS$ 259.0952, found 259.0956.



4c

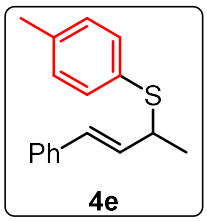
According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2c** (28.9 mg, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4c** (22.0 mg, 80%) as a colorless oil, Rf =0.23 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.34 – 7.17 (m, 9H), 6.22 – 6.05 (m, 2H), 3.90 – 3.78 (m, 1H), 1.45 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 136.78, 134.86, 133.72, 133.13, 131.45, 130.35, 128.98, 128.68, 127.69, 126.44, 46.97, 20.65; **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{16}H_{14}ClS$ 273.0500, found 273.0498.



4d

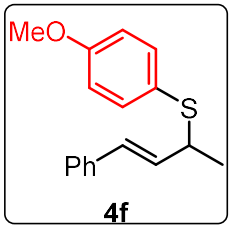
According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2d** (37.8 mg, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4d** (20.8 mg, 65%) as a colorless oil, Rf

=0.23 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.39 – 7.33 (m, 2H), 7.30 – 7.17 (m, 7H), 6.27 – 6.06 (m, 2H), 3.90 – 3.79 (m, 1H), 1.45 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 136.76, 134.94, 133.85, 131.92, 131.41, 130.38, 128.69, 127.71, 126.45, 121.74, 46.80, 20.67; **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{16}H_{15}AgBrS$ 424.9124, found 424.9124.



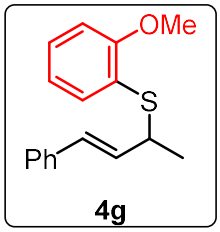
4e

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2f** (23.7 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4e** (16.6 mg, 61%) as a colorless oil, Rf =0.18 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 8.1 Hz, 2H), 7.31 – 7.27 (m, 4H), 7.25 – 7.17 (m, 1H), 7.15 – 7.05 (m, 2H), 6.26 – 6.11 (m, 2H), 3.84 (pd, *J* = 6.8, 0.8 Hz, 1H), 2.32 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 137.71, 137.10, 134.09, 131.97, 130.77, 129.89, 129.61, 128.61, 127.48, 126.43, 46.94, 21.26, 20.70; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}S$ 254.1124, found 254.1127.



4f

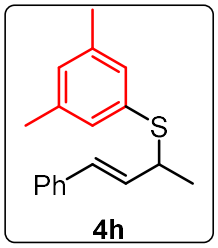
According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2g** (24.6 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=10:1, v/v) to afford **4f** (20.7 mg, 77%) as a colorless oil, Rf =0.33 (silica gel, PE:DCM = 4:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.43 – 7.34 (m, 2H), 7.32 – 7.27 (m, 4H), 7.27 – 7.17 (m, 1H), 6.88 – 6.75 (m, 2H), 6.21 – 6.05 (m, 2H), 3.78 (s, 3H), 3.74 (t, *J* = 6.9 Hz, 1H), 1.45 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 159.82, 137.12, 136.77, 131.99, 129.83, 128.61, 127.45, 126.39, 124.70, 114.35, 55.41, 47.72, 20.52; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}OS$ 270.1073, found 270.1076.



4g

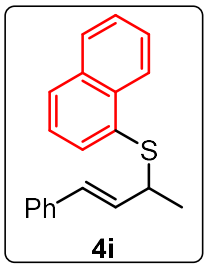
According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2i** (24.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=10:1, v/v) to afford **4g** (19.4 mg, 72%) as a colorless oil, Rf =0.31 (silica gel, PE:DCM = 4:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.41 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.31 – 7.14 (m, 6H), 6.92 – 6.82 (m, 2H), 6.25 – 6.10 (m, 2H), 4.05 (p, *J* = 6.9 Hz, 1H), 3.87 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 159.15, 137.13, 134.79, 132.02,

129.78, 129.06, 128.55, 127.41, 126.38, 122.73, 120.91, 110.82, 55.90, 44.72, 20.61; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}OS$ 270.1073, found 270.1075.



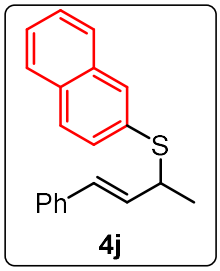
4h

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2j** (27.2 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4h** (21.6 mg, 81%) as a colorless oil, Rf =0.20 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.30 – 7.16 (m, 5H), 7.03 (s, 2H), 6.84 (s, 1H), 6.25 – 6.10 (m, 2H), 3.87 (p, *J* = 7.0 Hz, 1H), 2.23 (s, 6H), 1.46 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 138.32, 137.08, 134.09, 131.88, 131.00, 130.02, 129.24, 128.59, 127.48, 126.42, 46.39, 21.27, 20.76; **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{18}H_{19}S$ 267.1202, found 267.1202.



4i

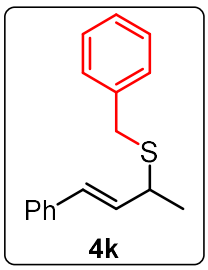
According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2k** (27.9 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **4i** (20.4 mg, 70%) as a colorless oil, Rf =0.35 (silica gel, PE:DCM = 5:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.60 (d, *J* = 8.5 Hz, 1H), 7.83 (dd, *J* = 21.0, 8.2 Hz, 2H), 7.71 (d, *J* = 7.3 Hz, 1H), 7.63 – 7.48 (m, 2H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.31 – 7.16 (m, 5H), 6.27 – 6.01 (m, 2H), 3.94 (p, *J* = 6.9 Hz, 1H), 1.53 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 136.96, 134.22, 133.92, 131.76, 130.05, 129.00, 128.67, 128.54, 127.47, 126.69, 126.38, 126.21, 126.10, 125.53, 46.93, 20.89. **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{20}H_{18}S$ 290.1124, found 290.1125.



4j

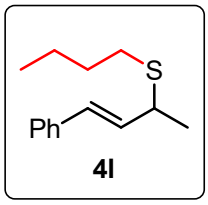
According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2l** (32.0 mg, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **4j** (17.3 mg, 60%) as a colorless oil, Rf =0.35 (silica gel, PE:DCM = 5:1); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 (s, 1H), 7.82 – 7.68 (m, 3H), 7.53 – 7.40 (m, 3H), 7.29 – 7.15 (m, 5H), 4.02 (p, *J* = 6.9 Hz, 1H), 1.52 (d, *J* = 6.9 Hz, 3H); **^{13}C**

NMR (101 MHz, Chloroform-*d*) δ 136.95, 133.73, 132.53, 132.18, 132.08, 131.74, 130.59, 130.25, 128.62, 128.29, 127.78, 127.60, 126.49, 126.25, 46.51, 20.82; **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{20}H_{17}S$ 289.1046, found 289.1043.



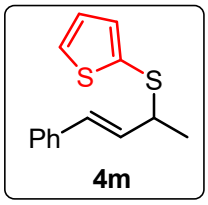
4k

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2n** (23.4 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4k** (21.5 mg, 85%) as a colorless oil, Rf =0.16 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 7.6 Hz, 2H), 7.37 – 7.19 (m, 8H), 6.33 (d, *J* = 15.7 Hz, 1H), 6.08 (dd, *J* = 15.7, 9.0 Hz, 1H), 3.68 (s, 2H), 3.46 – 3.33 (m, 1H), 1.38 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 138.78, 136.86, 132.38, 130.02, 129.06, 128.73, 128.60, 127.65, 126.98, 126.47, 42.31, 35.50, 20.60; **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{18}S$ 254.1124, found 254.1130.



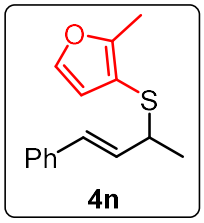
4l

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2o** (21.4 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4l** (18.8 mg, 85%) as a colorless oil, Rf =0.20 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.20 (m, 1H), 6.36 (d, *J* = 15.7 Hz, 1H), 6.07 (dd, *J* = 15.7, 9.0 Hz, 1H), 3.56 – 3.45 (m, 1H), 2.58 – 2.32 (m, 2H), 1.63 – 1.49 (m, 2H), 1.47 – 1.33 (m, 5H), 0.90 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 136.98, 132.80, 129.35, 128.70, 127.54, 126.43, 42.67, 31.94, 30.62, 22.23, 20.85, 13.85; **HRMS** (MALDI) m/z: $[M+K]^+$ calcd for $C_{14}H_{20}KS$ 259.0918, found 259.0917.



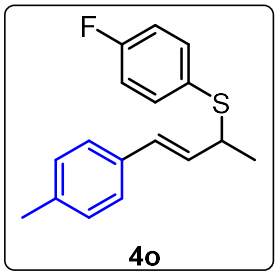
4m

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2m** (18.4 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4m** (14.8 mg, 52%) as a colorless oil, Rf =0.22 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.33 – 7.15 (m, 6H), 7.06 (dd, *J* = 3.5, 1.2 Hz, 1H), 6.92 (dd, *J* = 5.4, 3.6 Hz, 1H), 6.16 – 6.05 (m, 1H), 3.76 – 3.60 (m, 1H), 1.42 (d, *J* = 6.8 Hz, 1H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 137.00, 135.96, 132.54, 131.23, 130.58, 130.46, 128.65, 127.62, 127.58, 126.48, 49.53, 20.19; **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{14}H_{14}AgS_2$ 352.9582, found 352.9588.



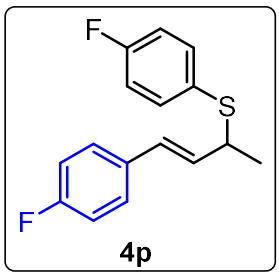
4n

According to the general procedure **B**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2r** (19.9 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4n** (2.5 mg, 11%) as a colorless oil, Rf =0.20 (silica gel, PE); the reaction could also be carried out according to the general procedure **A**, the reaction of **1a** (13.0 mg, 0.10 mmol), **2r** (19.9 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4n** (5.5 mg, 23%) as a colorless oil, Rf =0.20 (silica gel, PE); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 - 7.26 (m, 3H), 7.24 – 7.13 (m, 3H), 6.29 (d, *J* = 1.9 Hz, 1H), 6.14 – 6.01 (m, 2H), 3.61 – 3.49 (m, 1H), 2.24 (s, 3H), 1.40 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.94, 140.34, 137.15, 131.73, 129.66, 128.70, 127.50, 126.35, 116.38, 109.05, 47.05, 20.29, 12.06; **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{15}H_{16}AgOS$ 350.9967, found 350.9972.



4o

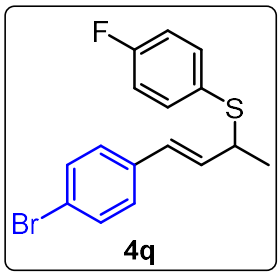
According to the general procedure **B**, the reaction of **1d** (14.4 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4o** (13.2 mg, 51%) as a colorless oil, Rf =0.20 (silica gel, PE) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.44 – 7.35 (m, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.96 (t, *J* = 8.7 Hz, 2H), 6.11 – 6.02 (m, 2H), 3.77 (qdd, *J* = 6.9, 4.7, 2.5 Hz, 1H), 2.33 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.76 (d, *J* = 247.4 Hz), 137.47, 136.55 (d, *J* = 8.2 Hz), 134.08, 130.58, 130.10, 129.37, 126.31, 115.86 (d, *J* = 21.7 Hz), 47.71, 21.32, 20.60; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.87 (s ,1F); **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{17}H_{16}FS$ 271.0952, found 271.0954.



4p

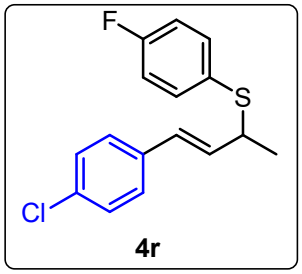
According to the general procedure **B**, the reaction of **1b** (14.8 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4p** (15.6 mg, 56%) as a colorless oil, Rf =0.27 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.40 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.25 –

7.18 (m, 2H), 6.97 (td, *J* = 8.7, 2.6 Hz, 4H), 6.12 – 5.94 (m, 2H), 3.77 (p, *J* = 6.8 Hz, 1H), 1.45 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.80 (d, *J* = 245.6 Hz) 162.40 (d, *J* = 246.6 Hz), 136.59 (d, *J* = 8.2 Hz), 133.00 (d, *J* = 3.2 Hz), 131.31 (d, *J* = 2.2 Hz), 129.41 (d, *J* = 3.5 Hz), 129.01, 127.86 (d, *J* = 8.0 Hz), 115.90 (d, *J* = 22.0 Hz), 115.59 (d, J = 22.0 Hz), 47.57, 20.52. **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.65 (s, 1F), -114.56 (s, 1F); **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{16}H_{13}F_2S$ 275.0701, found 275.0705.



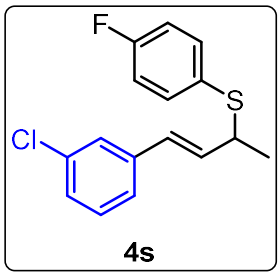
4q

According to the general procedure **B**, the reaction of **1c** (20.9 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4q** (19.0 mg, 60%) as a colorless oil, Rf =0.30 (silica gel, PE) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.46 – 7.34 (m, 4H), 7.12 (d, *J* = 8.4 Hz, 2H), 6.96 (t, *J* = 8.5 Hz, 2H), 6.17 – 5.96 (m, 2H), 3.76 (p, *J* = 7.1 Hz, 1H), 1.45 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.84 (d, *J* = 248.2 Hz), 136.67 (d, *J* = 8.1 Hz), 135.79, 132.36, 131.78, 129.28 (d, *J* = 3.5 Hz), 128.97, 127.89, 121.38, 115.92 (d, *J* = 22.0 Hz), 47.57, 20.39; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.47 (s ,1F); **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{16}H_{13}BrFS$ 334.9900, found 334.9898.



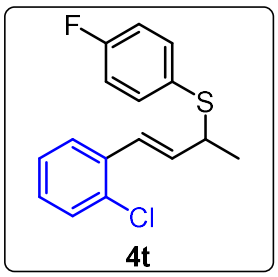
4r

According to the general procedure **B**, the reaction of **1e** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4r** (17.2 mg, 59%) as a colorless oil, Rf =0.27 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.44 – 7.34 (m, 2H), 7.28 – 7.14 (m, 4H), 7.03 – 6.91 (m, 2H), 6.18 – 5.94 (m, 2H), 3.76 (p, *J* = 7.0 Hz, 1H), 1.45 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.83 (d, *J* = 248.0 Hz), 136.66 (d, *J* = 8.3 Hz), 135.35, 133.25, 132.22, 129.30 (d, *J* = 3.4 Hz), 128.93, 128.84, 127.57, 115.93 (d, *J* = 21.7 Hz), 47.58, 20.42; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.52 (s, 1F); **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{16}H_{13}ClFS$ 291.0406, found 291.0406.



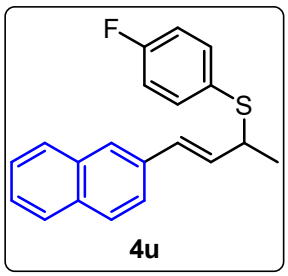
4s

According to the general procedure **B**, the reaction of **1f** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4s** (22.9 mg, 78%) as a colorless oil, Rf =0.27 (silica gel, PE) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.44 – 7.35 (m, 2H), 7.26 – 7.07 (m, 4H), 7.02 – 6.91 (m, 2H), 6.19 – 5.98 (m, 2H), 3.76 (p, *J* = 7.2 Hz, 1H), 1.45 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.82 (d, *J* = 248.2 Hz), 138.73, 136.62 (d, *J* = 8.3 Hz), 134.62, 133.09, 129.89, 129.23 (*d*, J = 3.3 Hz), 128.76, 127.56, 126.25, 124.62, 115.95 (d, *J* = 21.6 Hz), 47.47, 20.38; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.45 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{20}H_{18}S$ 290.1124, found 290.1122.



4t

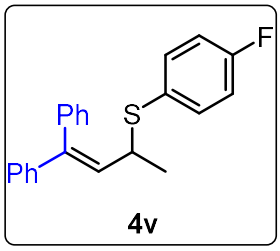
According to the general procedure **B**, the reaction of **1g** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4t** (10.5 mg, 36%) as a colorless oil, Rf =0.27 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.47 – 7.37 (m, 3H), 7.30 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.24 – 7.10 (m, 2H), 7.04 – 6.89 (m, 2H), 6.49 (d, *J* = 15.7 Hz, 1H), 6.08 (dd, *J* = 15.7, 8.6 Hz, 1H), 3.84 (dtd, *J* = 8.6, 6.9, 5.9 Hz, 1H), 1.48 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.81 (d, *J* = 247.7 Hz), 136.41 (d, *J* = 8.4 Hz), 135.01, 134.39, 133.09, 129.77, 129.24 (d, *J* = 3.3 Hz), 128.62, 126.93, 126.44, 116.01 (d, *J* = 21.8 Hz), 47.58, 20.40; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.70 (s, 1F); **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{16}H_{13}ClFS$ 291.0406, found 291.0398.



4u

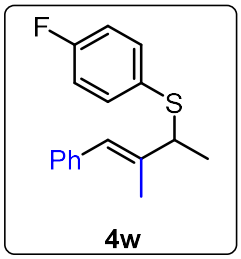
According to the general procedure **B**, the reaction of **1h** (1.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **4u** (13.1 mg, 42%) as a colorless oil, Rf =0.55 (silica gel, PE:DCM = 4:1) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.83 – 7.73 (m, 3H), 7.60 (s,

1H), 7.55 – 7.38 (m, 6H), 6.96 (t, J = 8.7 Hz, 2H), 6.30 – 6.19 (m, 2H), 3.84 (qt, J = 6.9, 3.6 Hz, 1H), 1.50 (d, J = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.81 (d, J = 248.1 Hz), 136.66 (d, J = 8.2 Hz), 134.29, 133.68, 133.06, 131.93, 130.28, 129.41 (d, J = 3.4 Hz), 128.31, 128.05, 127.79, 126.42, 126.22, 125.98, 123.62, 115.91 (d, J = 21.5 Hz), 47.82, 20.56; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.65 (s, 1F); **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{20}H_{16}FS$ 307.0952, found 307.0952.



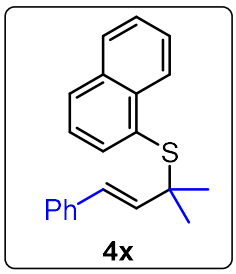
4v

According to the general procedure **B**, the reaction of **1i** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=25:1, v/v) to afford **4v** (28.8 mg, 86%) as a colorless oil, Rf =0.26 (silica gel, PE) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.33 – 7.19 (m, 8H), 7.13 (dd, J = 7.5, 2.1 Hz, 2H), 6.94 – 6.81 (m, 4H), 5.95 (d, J = 10.6 Hz, 1H), 3.87 (dq, J = 10.6, 6.8 Hz, 1H), 1.43 (d, J = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.73 (d, J = 248.2 Hz), 141.99 (d, J = 25.1 Hz), 139.26, 136.46 (d, J = 8.1 Hz), 131.32, 129.75, 129.48 (d, J = 3.4 Hz), 128.28, 128.19, 127.53, 127.44, 127.37, 115.78 (d, J = 21.7 Hz), 44.29, 21.16; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -114.00 (s, 1F); **HRMS** (MALDI) m/z: $[M+Ag]^+$ calcd for $C_{22}H_{20}FS$ 441.0237, found 441.0212.



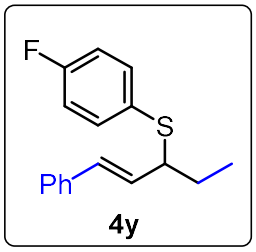
4w

According to the general procedure **B**, the reaction of **1j** (14.4 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4w** (18.7 mg, 69%) as a colorless oil, Rf =0.25 (silica gel, PE) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.41 – 7.34 (m, 2H), 7.32 – 7.26 (m, 2H), 7.23 – 7.15 (m, 1H), 7.05 (dd, J = 7.9, 1.3 Hz, 2H), 7.01 – 6.93 (m, 2H), 5.97 (s, 1H), 3.80 (q, J = 7.1 Hz, 1H), 1.92 (d, J = 1.3 Hz, 3H), 1.47 (d, J = 7.0 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.76 (d, J = 248.1 Hz), 137.99, 137.65, 136.49 (d, J = 8.3 Hz), 130.16 (d, J = 3.3 Hz), 128.91, 128.16, 127.42, 126.50, 115.78 (d, J = 21.6 Hz), 54.61, 19.17, 13.70; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.85 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{17}FS$ 272.1030, found 272.1034.



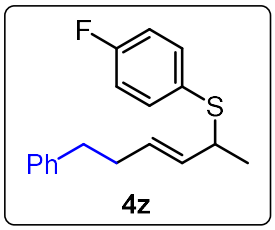
4x

According to the general procedure **B**, the reaction of **1k** (14.4 mg, 0.10 mmol), **2k** (27.9 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=20:1, v/v) to afford **4x** (23.4 mg, 77%) as a colorless oil, Rf =0.18 (silica gel, PE); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.72 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.93 – 7.66 (m, 3H), 7.55 – 7.42 (m, 2H), 7.41 – 7.33 (m, 1H), 7.28 – 7.13 (m, 5H), 6.31 (d, *J* = 16.1 Hz, 1H), 5.96 (d, *J* = 16.1 Hz, 1H), 1.50 (s, 6H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 137.78, 137.22, 136.93, 134.21, 130.07, 128.53, 128.35, 127.32, 127.30, 126.84, 126.54, 126.37, 126.07, 125.20, 51.67, 28.36; **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{21}H_{19}S$ 303.1202, found 303.1196.

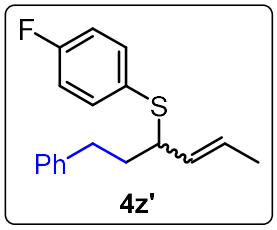


4y

According to the general procedure **B**, the reaction of **1l** (14.4 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford **4y** (19.6 mg, 72%) as a colorless oil, Rf =0.33 (silica gel, PE) **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.43 – 7.37 (m, 2H), 7.32 – 7.18 (m, 5H), 6.95 (t, *J* = 8.7 Hz, 2H), 6.18 – 5.90 (m, 2H), 3.53 (td, *J* = 8.2, 5.8 Hz, 1H), 1.91 – 1.64 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.70 (d, *J* = 248.1 Hz), 136.94, 136.54 (d, *J* = 8.1 Hz), 131.27, 130.46, 129.47 (d, *J* = 3.4 Hz), 128.66, 127.57, 126.37, 115.85 (d, *J* = 21.7 Hz), 55.20, 27.81, 12.19; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -113.95 (s, 1F); **HRMS** (MALDI) m/z: $[M]^+$ calcd for $C_{17}H_{17}FS$ 272.1030, found 272.1032.



4z

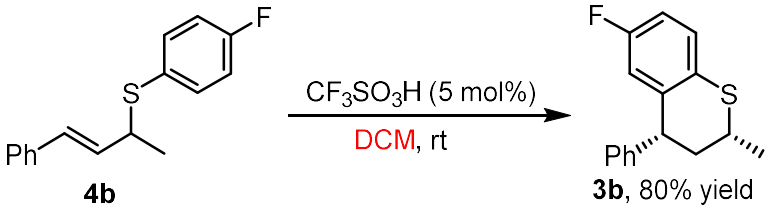


4z'

According to the general procedure **B**, the reaction of **1m** (16.5 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol) and TfOH (0.5 ul, 0.005 mmol) was stirred for 2 h, followed by flash column chromatography (SiO_2, PE:DCM=30:1, v/v) to afford the mixture of **4z** and **4z'** (23.4 mg, 82%，rr = 1.5:1), Rf =0.27 (silica gel, PE), **6x** were separated by PTLC (silica gel, PE) as a colorless oil; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 2H), 7.22 – 7.15 (m, 1H), 7.11 (d, *J* = 6.8 Hz, 2H), 6.98 (t, *J* = 8.7 Hz, 2H), 5.45 – 5.22 (m, 2H), 3.61 (p, *J* = 7.1 Hz, 1H), 2.56 (td, *J* = 7.5, 3.1 Hz, 2H), 2.31 – 2.20 (m, 2H), 1.33 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.60 (d, *J* = 247.3 Hz), 141.79, 136.11 (d, *J* = 8.1 Hz), 132.39, 130.61, 129.94 (d, *J* = 3.3 Hz), 128.51, 128.42, 125.97, 115.76 (d, *J* = 21.7 Hz), 47.00, 35.83, 34.00, 20.67; ^{19}F NMR (376 MHz, Chloroform-d) δ -114.24 (s, 1F). **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{18}H_{18}FS$ 285.1108, found 285.1114.

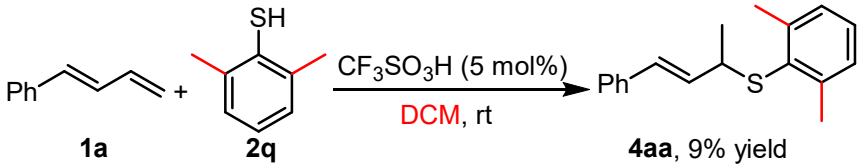
4. Control experiments and deuterium-labelling

4.1



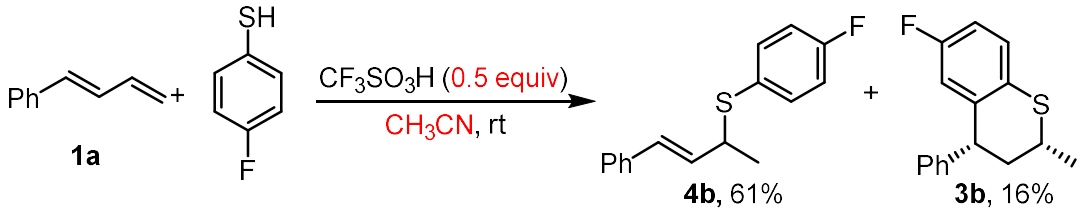
At room temperature, **4b** (25.8 mg, 0.10 mmol), anhydrous DCM (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (0.5 ul, 0.005 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The product **3b** (20.6 mg, 80%) is obtained by column chromatography.

4.2

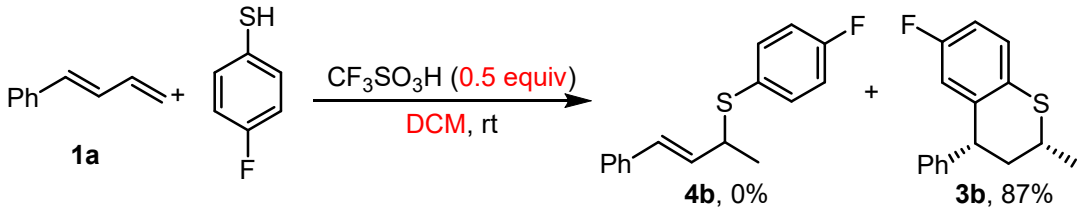


At room temperature, **1a** (13.0 mg, 0.10 mmol), **2q** (26.6 ul, 0.20 mmol), anhydrous DCM (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (0.5 ul, 0.005 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The product **4aa** (2.4 mg, 9%) is obtained by column chromatography; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.34 – 7.17 (m, 5H), 7.14 – 6.96 (m, 3H), 6.19 – 5.81 (m, 2H), 3.64 (dq, *J* = 8.7, 6.8 Hz, 1H), 2.51 (s, 6H); **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 143.75, 137.11, 132.99, 131.70, 129.11, 128.57, 128.46, 128.14, 127.38, 126.29, 46.94, 22.42, 20.67; **HRMS** (MALDI) m/z: $[M-H]^+$ calcd for $C_{18}H_{19}S$ 267.1202, found 267.1197.

4.3

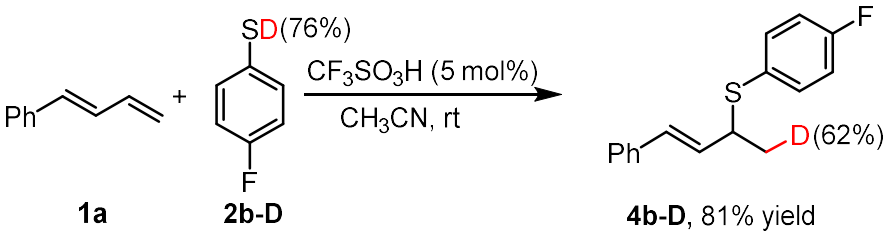


At room temperature, **1a** (13.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol), anhydrous MeCN (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (4.40 ul, 0.05 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The mixture of product **4b** (15.8 mg, 70%) and **3b** (4.1 mg, 16%) is obtained by column chromatography.



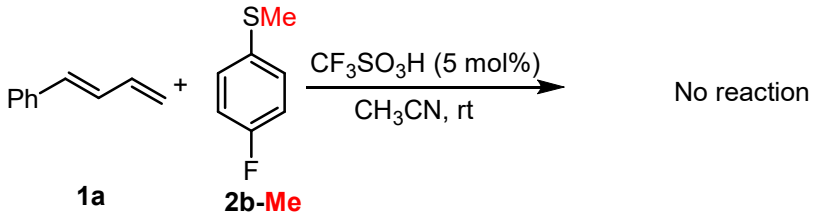
At room temperature, **1a** (13.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol), anhydrous DCM (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (4.40 ul, 0.05 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The mixture of product **3b** (22.5 mg, 87%) is obtained by column chromatography.

4.4



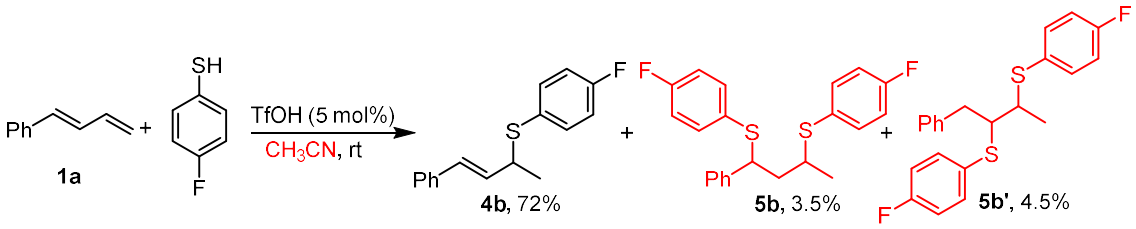
At room temperature, **1a** (13.0 mg, 0.10 mmol), **2b-D** (21.3 ul, 0.20 mmol), anhydrous MeCN (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (0.5 ul, 0.005 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The product **4b-D** (15.8 mg, 70%) is obtained by column chromatography. (NMR spectrum of **4b-D** see *Supporting information*, the beginning of capture **8**)

4.5

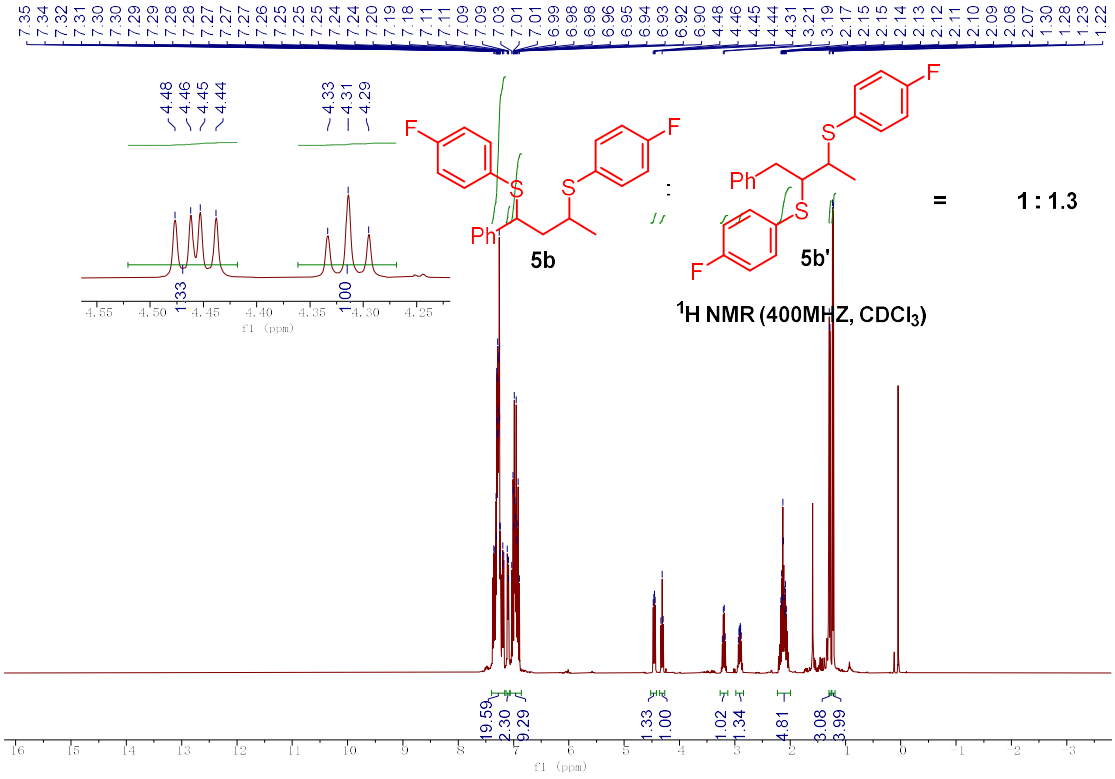


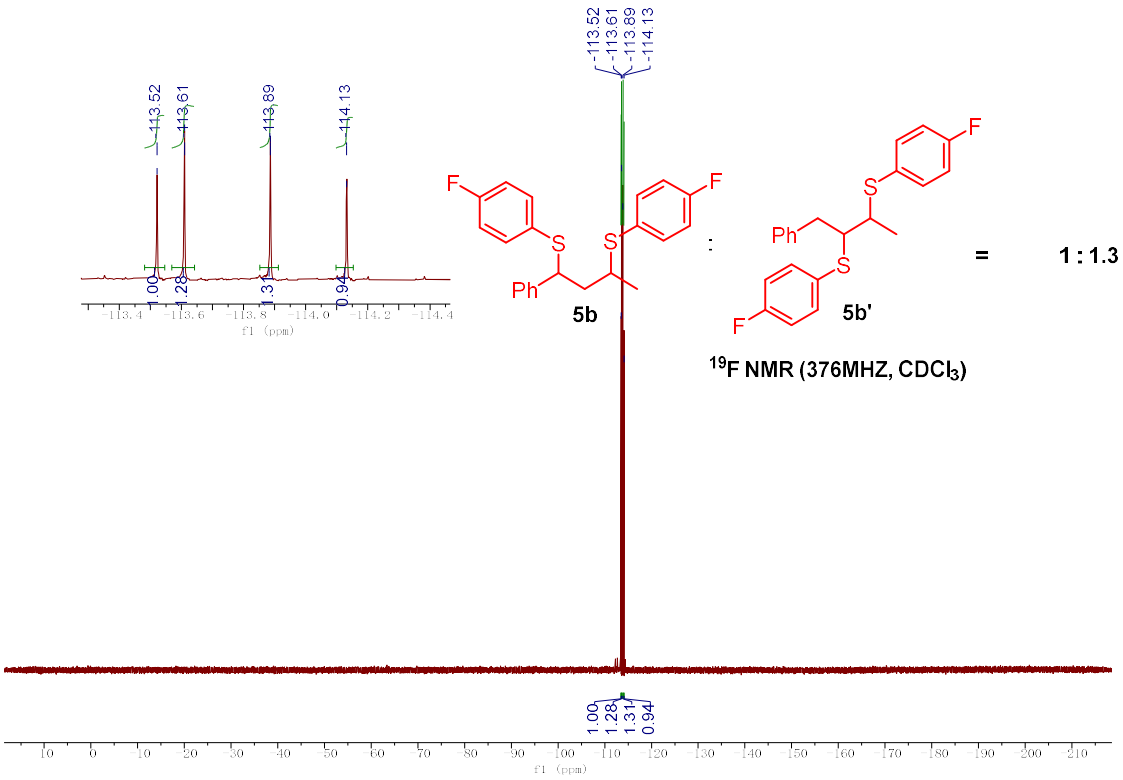
At room temperature, **1a** (13.0 mg, 0.10 mmol), **2b-Me** (24.4 ul, 0.20 mmol), anhydrous DCM (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (0.5 ul, 0.005 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. There was no product detected.

4.6

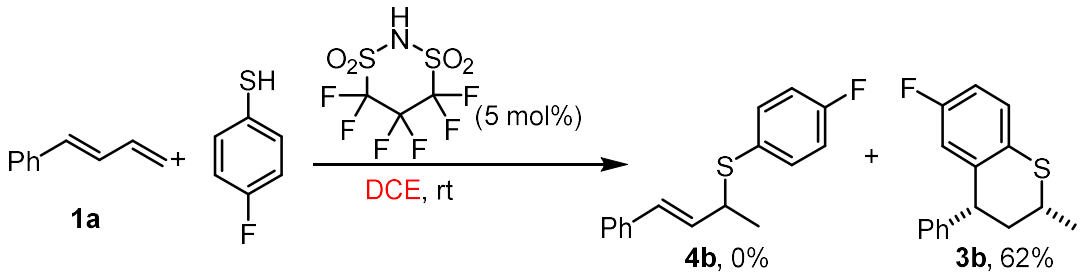


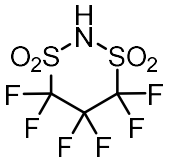
At room temperature, **1a** (26.0 mg, 0.20 mmol), **2b-D** (42.6 ul, 0.40 mmol), anhydrous MeCN (2 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **TfOH** (0.9 ul, 0.010 mmol) were added by a pipette gun and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The product **4b** (15.8 mg, 70%, Rf =0.23 (silica gel, PE)) and the mixture of **5b** and **5b'** (6.5 mg, 8%, **5b**:**5b'**=1:1.3, Rf =0.08 (silica gel, PE)) is obtained by column chromatography. The ratio of **5b** and **5b'** was measured by **NMR**.



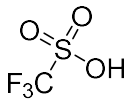


4.7





PKa = 0.6 (in DCE)

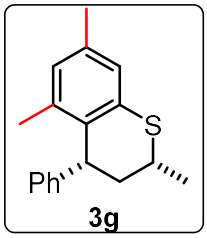


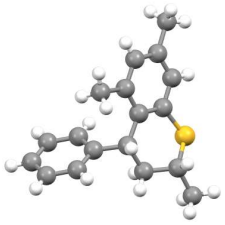
PKa = 0.7 (in CH_3CN)

At room temperature, **1a** (13.0 mg, 0.10 mmol), **2b** (21.3 ul, 0.20 mmol), anhydrous 1,2-dichloroethane (DCE) (1 mL) were added into an oven dried 10 mL tube charged with a stir bar, seal the flask with its septum, and the solution was stirred for about 3 minutes under argon atmosphere at room temperature, then **1,1,2,2,3,3-hexafluoropropane-1,3-disulfonimide** (1.5 mg, 0.005 mmol) were added and stirred for 2 hours under argon atmosphere at room temperature. After the reaction was completed (monitored by TLC), removed the solvent under reduce pressure. The product **3b** (16.1 mg, 62%) was obtained as a colorless oil by column chromatography, Rf =0.25 (silica gel, PE).

5. Crystal Data

5.1 Crystal Data of **3g**





CCDC: 2102317

Procedure for the recrystallization of **3g**: To a 5 mL vial containing **3g** (20 mg), was added acetone (3 mL) to form a clear solution. The solution was kept aside 2 days at room temperature to obtain crystals.

5.2 Crystal data and structure refinement for **3g**:

Identification code	**3g**
Empirical formula	$C_{18}H_{20}S$
Formula weight	268.40
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	29.0653(6)
b/Å	5.67134(10)
c/Å	19.4203(4)
α /°	90
β /°	108.856(2)
γ /°	90
Volume/Å^3	3029.43(11)
Z	8
ρ_{calc}g/cm^3	1.177
μ /mm^{-1}	1.743
F(000)	1152.0
Crystal size/mm^3	0.1 × 0.05 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.426 to 149.916
Index ranges	-36 ⩽ h ⩽ 32, -6 ⩽ k ⩽ 6, -24 ⩽ l ⩽ 24
Reflections collected	9077
Independent reflections	2955 [R_{int} = 0.0184, R_{sigma} = 0.0182]
Data/restraints/parameters	2955/0/175
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0392, wR_2 = 0.1119
Final R indexes [all data]	R_1 = 0.0451, wR_2 = 0.1176
Largest diff. peak/hole / e Å^{-3}	0.20/-0.27

6. DFT calculations

6.1 Computational Details

All the calculations were carried out by Gaussian 09 programs[3] using M06-2X functional[4] theory level. The optimized structures were obtained via the Pople's basis set 6-311G(d,p), while the single point energy calculations applied Ahlrichs basis sets Def2-TZVPP as TZVP provides good performance on the basis set superposition error (BSSE)[5]. And the SMD solvation model[6] was used to stimulate the solvation effect of acetonitrile. Vibrational frequency analyses were carried out to make sure that the optimized catalyst, reactants, intermediates, and products have no imaginary frequencies while the transition states have only one imaginary frequency. The Gibbs free energies ware obtained by the addition of thermal correction of free energy and single point energy of each calculated geometries. The GaussView (Version 6)[7] and CYLview (version 1.0b)[8] softwares were employed to present the optimized structures.

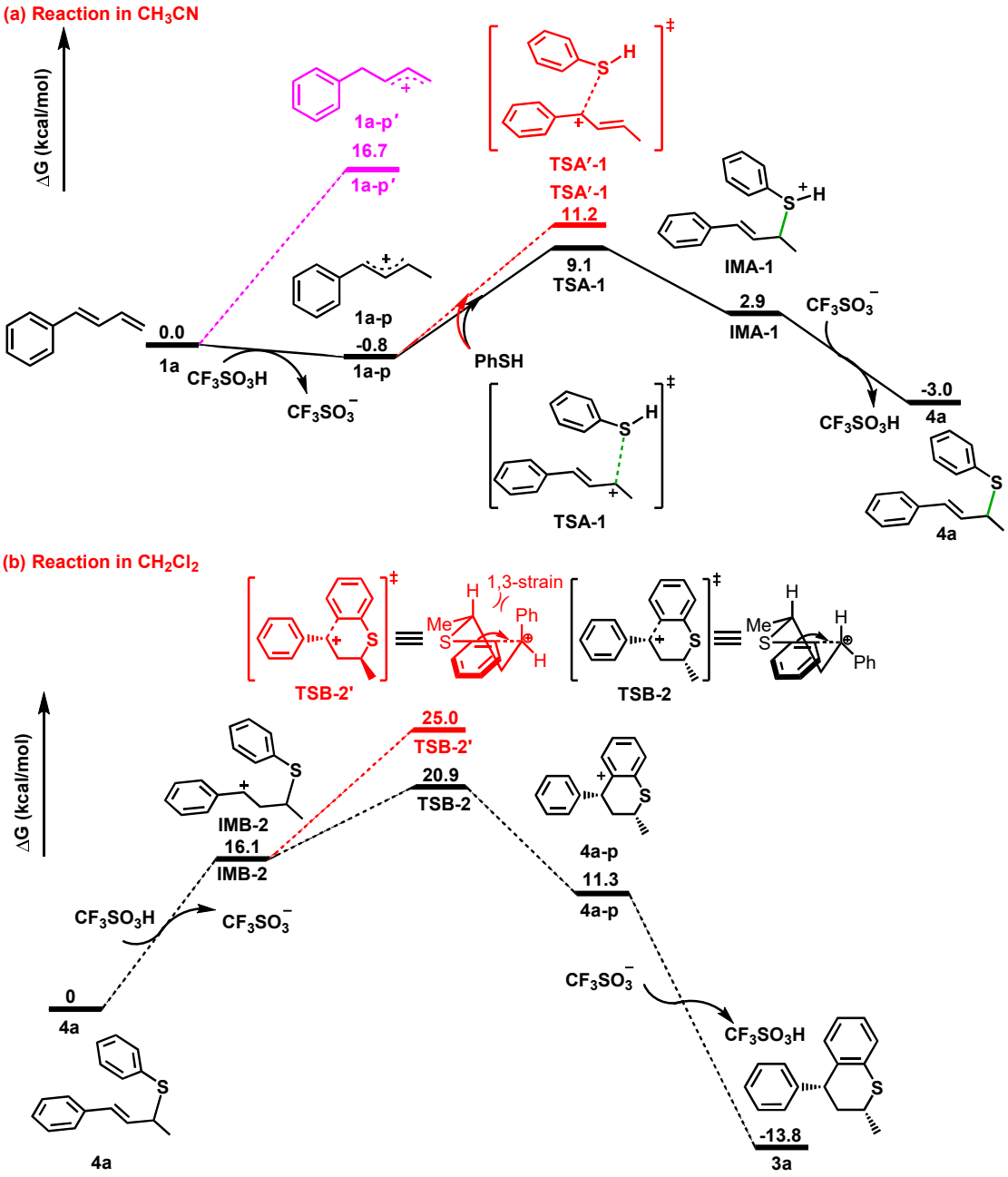
6.2 Results

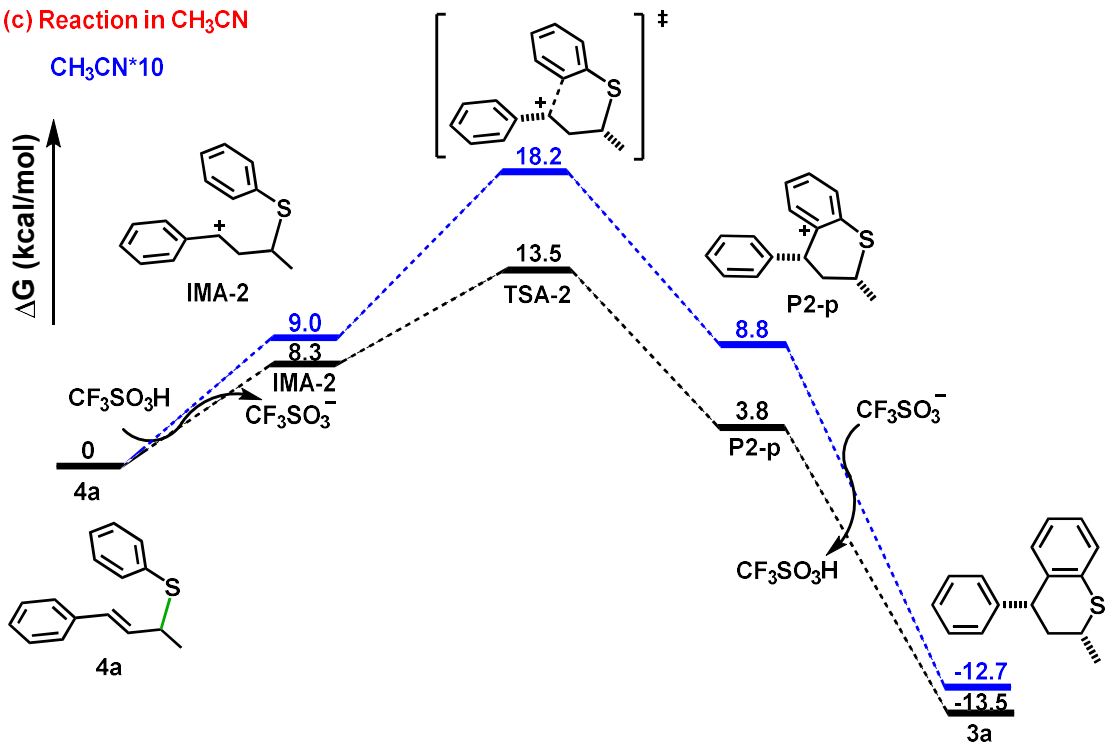
As shown in Figure (a), firstly, the reactant **1a** obtains a proton from catalyst TfOH, and DFT calculations indicated that terminal protonation of the alkenyl carbon atom has a lower energy barrier (−0.8 kcal/mol) than the carbon atom close to the phenyl group (16.7 kcal/mol). Thus, intermediate **1a-p** is more favorable. Then the Gibbs free energy barrier of the electrophilic attack at C3 is 9.9 kcal/mol, which is lower than the barrier for attack at C1 (12.0 kcal/mol). Therefore, after the electrophilic attack of PhSH and deprotonation of **IMA-1**, the cationic intermediate **1a-p** is expected to generate the 4,3-addition product **4a**. The experimental results were consistent with this theoretical calculation.

We also investigated the mechanism of further cyclization reaction of hydrothiolation product in dichloromethane (Figure b). DFT calculation showed that the energy barrier for protonation of **4a** is 16.1 kcal/mol. The next Friedel-Crafts type transformation can provide two diastereomers and DFT calculations indicated the source of diastereoselectivity in this step. Because of the exitance of 1,3-strain between phenyl at C4 and hydrogen at C2 in TSB-2', the preferred transition state is TSB-2, which may response to the excellent diastereoselectivity (Figure 5b). DFT calculation indicated that the Gibbs energy barrier from intermediate **IMB-2** to **TSB-2** is 4.8 kcal/mol, which is lower than the barrier to **TSB-2'** (8.9 kcal/mol). This result matches our theoretical explanation and experimental configuration determined by X-ray crystallography.

Interestingly, as shown in Figure (c), we found that in acetonitrile, the energy barrier of protonation was 8.3 kcal/mol (black part), which was significantly lower than the energy barrier in DCM (16.1 kcal/mol). This result indicated that the protonation of hydrothiolation product can also happen in acetonitrile. Meanwhile, we observed the di-hydrothiolation product **5b** and **5b'** in the model reaction (See *Supporting Information* Chapter 4.6). The calculation and experimental results conformably suggest the acidity of 0.05 equiv of TfOH in acetonitrile (PKa = 0.7 in CH_3CN[9]) was enough for the protonation of hydrothiolation product, but the Friedel-Crafts type cyclization process is inhibited in the polar and coordinating acetonitrile. To confirm this thought, we used 0.05 equiv of 1,1,2,2,3,3-hexafluoropropane-1,3-disulfonimide (PKa = 0.6 in DCE[10]) as the catalyst, and the model reaction was performed in low-polar and non-coordinating DCE. We found that the 4,3-hydrothiolation/Friedel-Crafts product **3b** was solely obtained in 62% yield (See *Supporting Information* Chapter 4.7). This control experimental result further confirmed that acetonitrile

influenced the Friedel-Crafts type cyclization process but not the protonation. Thus, we reconsidered the role of acetonitrile in the reaction and did a new DFT calculation (blue part). We initially assumed that ten acetonitrile molecules participate in the reaction process. The new calculation showed that the energy barrier of **4a** to IMA-2 was 9.0 kcal/mol, which was slightly higher than the foregoing result (8.3 kcal/mol). But the energy barrier from IMA-2 to TSA-2 went through a sharp increase, which from 5.2 kcal/mol increased to 9.2 kcal/mol. Thus, we can boldly assume that the energy barrier from IMA-2 to TSA-2 will be further obviously increased and the Gibbs free energy of TSA-2 will be visibly higher than 21 kcal/mol (in DCM) when a large amount of acetonitrile is involved in the reaction. Combined with experimental results and initial DFT calculation, we may conclude that the high polar and coordinating acetonitrile solvent inhibited the Friedel-Crafts type cyclization process and made the reaction in acetonitrile to produce the hydrothiolation product.





6.3 Cartesian Coordinates

CF_3SO_3H (CH_3CN)

S	0.84857900	-0.13707000	0.06091600
O	1.21528500	-1.25459200	-0.75536600
O	1.23048200	-0.01685100	1.43973500
O	1.24220600	1.16920700	-0.74435400
H	1.31407600	1.95369600	-0.16514000
C	-0.99481300	0.00564000	-0.00243600
F	-1.40074000	-0.06626800	-1.25357600
F	-1.35372200	1.16380100	0.52116700
F	-1.51512100	-0.98381200	0.69740600

CF_3SO_3H (CH_2Cl_2)

S	0.84840600	-0.13722400	0.06496700
O	1.21097000	-1.27983200	-0.71640600
O	1.23181000	0.03035600	1.43819700
O	1.24155600	1.14480100	-0.78061200
H	1.33737600	1.94025700	-0.22214500
C	-0.99418600	0.00623800	-0.00225100
F	-1.39619300	-0.04402500	-1.25582400
F	-1.35551700	1.15576500	0.53997300

F	-1.51733900	-0.99448400	0.67882300

1a (CH_3CN)

C	3.24574200	0.38888400	0.00000000
C	2.84949600	-0.94456300	0.00000000
C	1.49717700	-1.26920200	0.00000100
C	0.51436400	-0.27085200	0.00000000
C	0.92861800	1.06974900	0.00000000
C	2.27827600	1.39336900	0.00000000
H	4.29848500	0.64635000	0.00000000
H	3.59260100	-1.73380700	0.00000100
H	1.19052300	-2.31011400	0.00000100
H	0.19340100	1.86630700	0.00000000
H	2.57927800	2.43478400	0.00000000
C	-0.89888100	-0.67294300	0.00000000
C	-1.96552200	0.14054300	-0.00000200
H	-1.07423300	-1.74742200	0.00000300
C	-3.33480000	-0.35616200	-0.00000200
H	-1.84369500	1.22145500	-0.00000500
C	-4.40773400	0.43882100	0.00000300
H	-3.45970200	-1.43705900	-0.00000600
H	-5.41295500	0.03357900	0.00000300
H	-4.30412800	1.52005700	0.00000700

PhSH (CH_3CN)

C	-1.57956600	1.20730100	-0.00053100
C	-0.18837200	1.20694100	-0.00073300
C	0.50315500	-0.00485600	0.00042600
C	-0.20244800	-1.20926400	0.00121500
C	-1.59267200	-1.19681700	0.00048300
C	-2.28776000	0.00937100	-0.00020700
H	-2.10901200	2.15316400	-0.00107100
H	0.35320500	2.14621500	-0.00183400
H	0.33071900	-2.15375000	0.00294900
H	-2.13218600	-2.13689000	0.00114900
H	-3.37113900	0.01547200	-0.00032800
S	2.28247600	-0.08394000	-0.00200000
H	2.49477800	1.24276400	0.02722000

$CF_3SO_3^-$ (CH_3CN)

S	-0.90458600	0.00014300	-0.00001100
O	-1.22791000	1.41982800	-0.13625300
O	-1.22722000	-0.59170600	1.29777700
O	-1.22813000	-0.82794100	-1.16118000
C	0.93894800	0.00002300	-0.00014900
F	1.41915600	0.52447400	-1.12940300
F	1.41806500	-1.24063100	0.11035400
F	1.41897500	0.71572600	1.01886100

$CF_3SO_3^-$ (CH_2Cl_2)

S	-0.90581100	0.00022100	0.00004600
O	-1.22780500	1.42618400	0.02444900
O	-1.22840200	-0.73426000	1.22272200
O	-1.22718000	-0.69172400	-1.24709000
C	0.93817400	-0.00004000	0.00019200
F	1.41924700	0.66032100	-1.05548900
F	1.41890400	-1.24464300	-0.04441400
F	1.42085200	0.58377900	1.09962200

1a-p

C	-3.27874200	0.38272000	-0.00003200
C	-2.89719800	-0.95870200	0.00000600
C	-1.55343500	-1.28311800	0.00004100
C	-0.57585400	-0.26308000	0.00004800
C	-0.98092100	1.09194500	0.00003200
C	-2.32420100	1.40542000	-0.00000400
H	-4.33219300	0.63835700	-0.00008200
H	-3.64831600	-1.73843200	0.00001000
H	-1.23403000	-2.31914600	0.00008200
H	-0.24120100	1.88280000	0.00008100
H	-2.64112000	2.44059600	-0.00000800
C	0.78964600	-0.65202200	-0.00001800
C	1.90378900	0.18941900	-0.00008800
H	0.98447900	-1.72307700	-0.00007500
C	3.14748700	-0.37961900	-0.00007800
H	1.80088000	1.26830900	-0.00010300
C	4.40913600	0.37137300	0.00004100
H	3.21371900	-1.46590000	-0.00006200
H	5.00166900	0.07080400	-0.87239100
H	4.25656700	1.44898400	0.00013100
H	5.00129700	0.07069400	0.87272100

1a-p′

C	2.54881300	-0.70148000	-0.39594000
C	2.18829500	0.51790900	-0.96683000

C	1.02815700	1.14966100	-0.55444900
C	0.23196800	0.56059800	0.5554200
C	0.59311600	-0.68407600	1.00080400
C	1.75622800	-1.30079200	0.58792900
H	3.45549100	-1.19678600	-0.72348300
H	2.80973200	0.96873600	-1.72991900
H	0.72473600	2.09807800	-0.98439900
H	-0.04026300	-1.13644700	1.75519600
H	2.05184600	-2.24783700	1.02113900
C	-0.95612200	1.36155100	1.05973500
C	-1.55491600	0.68895000	-0.05683400
H	-1.21176700	0.99750800	2.04873700
C	-2.30453600	-0.54524300	0.02975700
H	-1.54192200	1.18766500	-1.02083400
C	-2.96359000	-0.99648500	-1.04161000
H	-2.36411100	-1.04236400	0.99220900
H	-2.89375800	-0.48742600	-1.99763300
H	-3.59634000	-1.87429800	-0.98181900
H	-0.79811500	2.42961100	0.97218100

TSA-1

Value of imaginary frequency = -134.44 cm^{-1}

C	-4.01470700	-0.70542000	0.26735500
C	-3.57298400	-0.39925900	-1.01697600
C	-2.23715400	-0.58112900	-1.34512400
C	-1.32994500	-1.07752500	-0.39401700
C	-1.78947400	-1.37828100	0.90175700
C	-3.12250800	-1.19374200	1.22492600
H	-5.05699300	-0.56183100	0.52799300
H	-4.26682200	-0.01721000	-1.75578600
H	-1.87832900	-0.33739100	-2.33957700
H	-1.10141500	-1.74897400	1.65236300
H	-3.47347700	-1.42573500	2.22316600
C	0.05293000	-1.21294400	-0.77938400
C	1.08552500	-1.67984200	-0.00623000
H	0.29113500	-0.91246000	-1.79836000
C	2.38623500	-1.66236400	-0.52033800
H	0.93222200	-2.00185400	1.01852700
C	3.51810400	-2.34757800	0.15226100
H	2.50213600	-1.42068500	-1.57340400
H	4.48491300	-1.94848600	-0.15331400
H	3.41952100	-2.33028900	1.23809900
H	3.48279400	-3.39585800	-0.17368900
C	-0.59743400	1.79043900	1.39810600
C	0.71081000	1.32404800	1.35819600

C	1.42924400	1.40407300	0.16344200
C	0.83901800	1.92957700	-0.98883000
C	-0.47250600	2.38732800	-0.93461100
C	-1.19294100	2.31809100	0.25454500
H	-1.15507700	1.73108700	2.32540700
H	1.16718100	0.90310700	2.24712800
H	1.39869400	1.98410400	-1.91631500
H	-0.93138700	2.79486300	-1.82763300
H	-2.21640000	2.67231100	0.29042800
S	3.06326100	0.75536400	0.01801600
H	3.23585600	0.43666300	1.31625300

TSA′-1

Value of imaginary frequency = -134.77 cm^{-1}

C	-1.64765500	2.73435700	0.11045000
C	-1.54662400	1.92128300	1.23801500
C	-0.5083200	1.10122600	1.39437200
C	0.57992500	1.08870600	0.42534500
C	0.45722900	1.90322400	-0.71646200
C	-0.64705700	2.72528800	-0.86308600
H	-2.51118100	3.37775900	-0.01348300
H	-2.32853000	1.92798000	1.98777800
H	-0.34556900	0.46481800	2.26797700
H	1.22394800	1.89411600	-1.48165800
H	-0.73660800	3.35809600	-1.73750800
C	1.70690500	0.21504300	0.63769800
C	2.93465100	0.27173500	-0.09604300
H	1.75599600	-0.26143100	1.61307300
C	4.04423600	-0.30878600	0.40720000
H	2.97799500	0.80543500	-1.03934300
C	5.38176000	-0.26339200	-0.22751300
H	3.96253400	-0.84597000	1.35063000
H	5.73101800	-1.28402800	-0.41647600
H	5.37483800	0.29836100	-1.16117500
H	6.10394700	0.18267800	0.46368900
C	-2.89938100	-0.38168100	-1.26772500
C	-1.56078600	-0.74897400	-1.33569000
C	-1.01136300	-1.51122600	-0.30375000
C	-1.78844600	-1.90542700	0.78826900
C	-3.12420700	-1.52789200	0.84294100
C	-3.68026400	-0.76323500	-0.17964200
H	-3.32942300	0.21037400	-2.06705200
H	-0.95392700	-0.5726600	-2.18198500
H	-1.35482000	-2.49725900	1.58700200
H	-3.72949600	-1.83142400	1.68868000

H	-4.72212100	-0.46988800	-0.13137000
S	0.70781300	-1.91820200	-0.27128400
H	1.00785000	-1.49261400	-1.51450500
IMA-1			
C	-4.51978700	-0.05180800	0.22721300
C	-3.81479000	0.77695700	-0.63942700
C	-2.49611000	0.47867800	-0.96578300
C	-1.86158500	-0.64498000	-0.42331500
C	-2.58241500	-1.47536500	0.5586800
C	-3.90014500	-1.17947200	0.76581400
H	-5.54926900	0.17420800	0.47952800
H	-4.29100000	1.65269300	-1.06468000
H	-1.94426200	1.12187000	-1.64378500
H	-2.11652900	-2.36098900	0.86327600
H	-4.44998800	-1.83169600	1.43441500
C	-0.45682500	-0.88831100	-0.77627100
C	0.38249900	-1.73292300	-0.16645000
H	-0.07298000	-0.28517700	-1.59815200
C	1.80088900	-1.84307400	-0.57350900
H	0.07866300	-2.33587800	0.68571400
C	2.43016200	-3.21284900	-0.39551100
H	1.97928000	-1.42962100	-1.56787300
H	3.48700500	-3.21316400	-0.66549900
H	2.31460200	-3.57027600	0.63018700
H	1.90650100	-3.90517200	-1.05794900
C	0.20364500	2.34074500	1.08005500
C	0.91337700	1.15929100	1.25701000
C	1.97330800	0.88953300	0.39485700
C	2.33928400	1.75641200	-0.63067500
C	1.60760900	2.92616100	-0.79992600
C	0.54509100	3.21560600	0.05179500
H	-0.62214300	2.57024100	1.74226400
H	0.64204700	0.46576500	2.04452000
H	3.17269700	1.52673900	-1.28500200
H	1.87447100	3.61143100	-1.59475300
H	-0.01835000	4.13096200	-0.08426400
S	2.86255700	-0.64661100	0.49171500
H	2.42310300	-1.06376100	1.70413900
4a			
C	-4.61749000	0.22901000	0.25274200
C	-3.85230200	1.05697200	-0.56238000
C	-2.54694100	0.70147200	-0.88666200
C	-1.97996600	-0.48180600	-0.39813000
C	-2.76404700	-1.31095700	0.41642100

C	-4.06750000	-0.95674900	0.73850900
H	-5.63611400	0.50021700	0.50470000
H	-4.27113900	1.97934700	-0.94825600
H	-1.95044500	1.34859600	-1.52206500
H	-2.35676300	-2.24326100	0.79131800
H	-4.66125800	-1.61092000	1.36687400
C	-0.58561800	-0.79556800	-0.75351700
C	0.19973700	-1.69986500	-0.16181700
H	-0.16303900	-0.18887500	-1.55352600
C	1.63196800	-1.89184400	-0.52927500
H	-0.15990900	-2.29949200	0.67262200
C	2.05859600	-3.35431900	-0.52895400
H	1.84440500	-1.42886800	-1.49462900
H	3.11518500	-3.45744400	-0.78328200
H	1.88732900	-3.80922700	0.45012100
H	1.46997800	-3.90337200	-1.26743700
C	0.72391000	2.52489700	1.04597000
C	1.20637500	1.24317200	1.29622700
C	2.13493400	0.66531300	0.42955900
C	2.58058900	1.37734900	-0.68549500
C	2.08880100	2.65442600	-0.93723800
C	1.16025600	3.22924800	-0.07253600
H	0.00075900	2.96780400	1.72105800
H	0.85406000	0.68373900	2.15516800
H	3.30472600	0.92817500	-1.35613200
H	2.43421300	3.20138300	-1.80693500
H	0.77951900	4.22472400	-0.26955000
S	2.70504300	-1.00231500	0.70996300

4a-p

C	2.42103200	-1.15424800	1.02480000
C	1.26513800	-0.87290600	0.29611600
C	1.37160100	-0.65625000	-1.08089600
C	2.61042300	-0.71009500	-1.71033900
C	3.75917700	-0.99094800	-0.97406500
C	3.66121200	-1.21708800	0.39453500
H	2.34720500	-1.32433800	2.09413700
H	0.48588000	-0.45011300	-1.67422900
H	2.67820600	-0.53663400	-2.77810500
H	4.72328400	-1.03678100	-1.46693000
H	4.54876300	-1.44209500	0.97468700
C	-0.06769700	-0.76553300	1.01208000
C	-1.14031100	-1.70613300	0.43156000
H	0.09298300	-1.01145100	2.06214400
C	-2.55342700	-1.12671600	0.38752900

H	-0.87203100	-2.01603500	-0.58107900
C	-3.58093400	-2.12915500	-0.11797500
H	-2.85500000	-0.74081600	1.36460100
H	-4.57665500	-1.68660000	-0.18129800
H	-3.29922900	-2.51612600	-1.09994000
H	-3.62292500	-2.96519500	0.58272200
S	-2.55708900	0.29601100	-0.77019900
C	-1.22244500	1.17625200	-0.19713000
C	-0.55058500	0.74597300	1.05156900
C	-0.78491900	2.30746800	-0.89739200
C	0.54862500	1.62152300	1.51044100
H	-1.31834400	0.76370500	1.84419500
C	0.26646800	3.04035000	-0.39815100
H	-1.26812400	2.60164300	-1.82125100
C	0.93579500	2.71316700	0.82017400
H	1.04341500	1.33002200	2.43138600
H	0.59929800	3.91010700	-0.95437600
H	1.74652400	3.34096100	1.16530600
H	-1.17475100	-2.61039600	1.04407800

4a (CH_2Cl_2)

C	4.24154000	1.35668300	0.03962200
C	3.36267200	0.26988400	0.11075800
C	3.89059800	-1.02242800	-0.02093800
C	5.25104500	-1.21379000	-0.21680800
C	6.11536200	-0.12173100	-0.28583000
C	5.60527500	1.16525500	-0.15665700
H	3.84581000	2.36203900	0.13951000
H	3.23712300	-1.88564300	0.02970700
H	5.64140300	-2.22007900	-0.31667900
H	7.17700500	-0.27613500	-0.43916900
H	6.26763700	2.02164400	-0.20863600
C	1.92838600	0.53624100	0.31831300
C	0.95158100	-0.36939800	0.40373600
H	1.66471700	1.58851600	0.41169900
C	-0.48480200	-0.01179100	0.63062900
H	1.15920700	-1.43353600	0.31157500
C	-1.10099100	-0.83598200	1.75357800
H	-0.57148400	1.05515700	0.84448500
H	-2.14721800	-0.57105800	1.91628600
H	-1.04332000	-1.90370600	1.52645700
H	-0.55357300	-0.64783600	2.68113000
S	-1.34245000	-0.30703000	-0.99307200
C	-3.04510300	-0.02390000	-0.53168600
C	-3.94080900	-1.09254200	-0.48869300

C	-3.48607800	1.26424300	-0.22103100
C	-5.26938300	-0.87276500	-0.13486200
H	-3.59506600	-2.09176100	-0.72673400
C	-4.80983600	1.47567400	0.14849700
H	-2.79249900	2.09628500	-0.27007100
C	-5.70388900	0.40832700	0.18964000
H	-5.96194000	-1.70604300	-0.10598900
H	-5.14516800	2.47653300	0.39467200
H	-6.73684500	0.57621900	0.47129200

IMB-2

C	2.15396600	-0.54756200	1.28006200
C	1.12462400	-1.06077800	0.5741200
C	1.45423000	-1.55507300	-0.84404000
C	2.76534100	-1.55907000	-1.25945600
C	3.76796800	-1.06925600	-0.41005800
C	3.46790600	-0.56249100	0.85328500
H	1.89118000	-0.15969600	2.25830500
H	0.67699300	-1.92578800	-1.50001100
H	3.02692100	-1.93717700	-2.23932600
H	4.79816900	-1.08141200	-0.74723300
H	4.25645300	-0.18286900	1.49003500
C	-0.18320300	-1.05095200	0.94446200
C	-1.37874400	-1.65591300	0.34908700
H	-0.31266200	-0.64938000	1.94847000
C	-2.66607200	-0.82180600	0.47915200
H	-1.23765500	-2.00359900	-0.67418900
C	-3.90535100	-1.67603700	0.25074200
H	-2.70602000	-0.36409500	1.46903100
H	-4.81158700	-1.07046600	0.30402400
H	-3.86931700	-2.16503600	-0.72553800
H	-3.96500600	-2.44694900	1.02154800
S	-2.67920900	0.52584100	-0.77203700
C	-1.11924700	1.29209700	-0.39599300
C	-0.85985600	1.79228000	0.88661600
C	-0.14532600	1.39308600	-1.39337000
C	0.38178500	2.34873900	1.17685400
H	-1.63100300	1.75421900	1.64849300
C	1.09202800	1.94709600	-1.09520500
H	-0.35014400	1.01004600	-2.38643100
C	1.36184900	2.41503200	0.19251200
H	0.57961300	2.73087100	2.17152000
H	1.85352800	2.00601700	-1.86437000
H	2.33159000	2.84229300	0.41982000
H	-1.53510700	-2.54676700	0.98606600

TSB-2

Value of imaginary frequency = -198.32 cm^{-1}

C	2.27557700	-0.88171700	1.18459600
C	1.14850200	-0.94195900	0.34328500
C	1.33516000	-1.05657500	-1.04633600
C	2.61610900	-1.14017700	-1.57095900
C	3.72013200	-1.10940700	-0.72202800
C	3.55082900	-0.97986600	0.65704000
H	2.12962100	-0.77347000	2.25440200
H	0.48073600	-1.07152400	-1.71315600
H	2.75603100	-1.22979000	-2.64109900
H	4.71899200	-1.18174800	-1.13644100
H	4.41348500	-0.95349200	1.31123500
C	-0.16212300	-0.89280800	0.94883700
C	-1.34266000	-1.56715900	0.33473000
H	-0.16090000	-0.87137900	2.03532900
C	-2.70111400	-0.86280600	0.42882400
H	-1.16011600	-1.84116600	-0.70389800
C	-3.83919200	-1.77507700	-0.00753800
H	-2.88923200	-0.50704700	1.44168200
H	-4.79214500	-1.24354300	0.00101300
H	-3.66427900	-2.16890200	-1.01119100
H	-3.91181900	-2.61381000	0.68750800
S	-2.66035100	0.56535000	-0.72595400
C	-1.13402000	1.26985200	-0.23788300
C	-0.72269000	1.22491300	1.11430300
C	-0.28381600	1.82453600	-1.20058300
C	0.49772200	1.83245000	1.49690900
H	-1.44485000	0.99574800	1.88749900
C	0.94116000	2.33248000	-0.81067000
H	-0.57258700	1.82328400	-2.24481200
C	1.33683300	2.34721800	0.54335000
H	0.77121400	1.84185700	2.54559900
H	1.61190300	2.73053400	-1.56361600
H	2.29212100	2.77589600	0.81912600
H	-1.43102200	-2.50043300	0.91083100

TSB-2′

Value of imaginary frequency = -220.36 cm^{-1}

C	-2.46094800	1.00645100	0.67882900
C	-1.69040300	-0.14932900	0.5320700
C	-2.27869300	-1.25177100	-0.20887500
C	-3.59811200	-1.18766400	-0.61852700
C	-4.34938600	-0.03627600	-0.37480000
C	-3.78402400	1.05837400	0.27926900

H	-2.00127000	1.85197300	1.18018700
H	-1.70883000	-2.15729800	-0.38135600
H	-4.05175400	-2.03389500	-1.11900700
H	-5.38476900	0.00444100	-0.69243500
H	-4.37708100	1.94342200	0.47259100
C	-0.33480900	-0.17055000	0.92101700
C	0.5340900	-1.42983500	1.10079300
H	-0.04533000	0.67527900	1.53862600
C	1.18379700	-2.01460100	-0.12992400
H	1.16859300	-1.29164700	1.90296800
C	1.60612500	-3.45740200	0.11112500
H	0.54569100	-1.95781300	-1.01269900
H	2.18607600	-3.84047600	-0.73028600
H	2.20624700	-3.54243400	1.01988900
H	0.71651300	-4.08037100	0.22281500
S	2.69976700	-1.03330800	-0.42252700
C	2.01394600	0.57919900	-0.33524500
C	0.73284600	0.84446000	-0.85908400
C	2.73530700	1.60201600	0.29338600
C	0.21438400	2.15631000	-0.79364700
H	0.25467700	0.12110200	-1.50823700
C	2.19434600	2.87263700	0.36749700
H	3.70557100	1.39131400	0.72688800
C	0.92922300	3.15621800	-0.17589200
H	-0.75926900	2.35749200	-1.22559800
H	2.75143300	3.65835900	0.86434700
H	0.52759600	4.15975900	-0.11223500
H	-0.27240400	-2.19569500	1.41918900

4a-p (CH_2Cl_2)

C	-2.43360300	-1.16082000	-1.02017100
C	-1.28004300	-0.86011500	-0.29618900
C	-1.38809800	-0.62135500	1.07680500
C	-2.62610100	-0.67152800	1.70702900
C	-3.77276500	-0.97143200	0.97533900
C	-3.67332700	-1.21997100	-0.38880400
H	-2.35987100	-1.35132100	-2.08613700
H	-0.50315700	-0.40130600	1.66630800
H	-2.69517300	-0.48164800	2.77183000
H	-4.73652700	-1.01535000	1.46873900
H	-4.55935900	-1.46062900	-0.96477100
C	0.05507900	-0.76401700	-1.00944100
C	1.11626200	-1.71453100	-0.42269400
H	-0.10462600	-1.01211000	-2.05947700
C	2.53768200	-1.15501200	-0.38515000

H	0.84439200	-2.01035800	0.59291500
C	3.55390500	-2.16757000	0.12351100
H	2.84211500	-0.77780300	-1.36503900
H	4.55383800	-1.73550200	0.19237500
H	3.26513700	-2.55285500	1.10392000
H	3.59342900	-3.00394300	-0.57670700
S	2.56349900	0.27283500	0.76595000
C	1.23990100	1.16823700	0.19303000
C	0.55490100	0.74205100	-1.05116200
C	0.82509600	2.31232100	0.88739000
C	-0.53482300	1.63241000	-1.50664600
H	1.32109700	0.75110900	-1.84588700
C	-0.21677400	3.05924000	0.39010100
H	1.31952000	2.60448300	1.80583600
C	-0.89974000	2.73442200	-0.82148600
H	-1.04281200	1.34460000	-2.42146600
H	-0.53089000	3.93819300	0.94265900
H	-1.70386600	3.37153800	-1.16469000
H	1.13545100	-2.62645200	-1.02437300

3a (CH_2Cl_2)

C	1.88737200	0.74692900	0.06046900
C	0.54897000	0.77623100	-0.35558900
C	-0.03911000	2.03085200	-0.56449700
C	0.64822000	3.21529300	-0.34716200
C	1.96923800	3.16913500	0.09209900
C	2.58165400	1.94268400	0.28774500
H	-1.07025800	2.07070200	-0.89875900
H	0.15691700	4.16596800	-0.51700100
H	2.52348200	4.08273300	0.27292300
H	3.61624600	1.90080100	0.61213500
C	-0.27620400	-0.47663900	-0.64428600
C	0.29213800	-1.75289800	-0.00991200
C	1.74021900	-2.01293500	-0.39181300
H	0.20748400	-1.70532300	1.08087400
C	2.23114900	-3.37161900	0.08841800
H	1.85615900	-1.93910800	-1.47582300
H	3.28791400	-3.52289100	-0.14334300
H	2.09392200	-3.47285600	1.16795400
H	1.65974700	-4.15996000	-0.40745400
S	2.81745500	-0.74009300	0.35824100
C	-1.72860000	-0.31639100	-0.23119500
C	-2.75656900	-0.50230600	-1.15355400
C	-2.05962000	-0.01078900	1.09263200
C	-4.09091000	-0.38712000	-0.76615000

H	-2.51087600	-0.73509200	-2.18488800
C	-3.38828200	0.10312200	1.48245800
H	-1.26742700	0.14802600	1.81815000
C	-4.40990300	-0.08465600	0.55231000
H	-4.87824200	-0.53099700	-1.49741800
H	-3.62939500	0.34210700	2.51208400
H	-5.44637400	0.00734000	0.85574900
H	-0.31455800	-2.59928300	-0.34822900
H	-0.26258700	-0.62403500	-1.73065800

IMA-2

Value of imaginary frequency = -595.26 cm^{-1}

C	-2.14768400	-0.56304300	-1.28731100
C	-1.12446600	-1.06897700	-0.44343000
C	-1.46038400	-1.54432200	0.85308600
C	-2.77326000	-1.53648600	1.26393200
C	-3.77005600	-1.05115700	0.40543800
C	-3.46297100	-0.56366200	-0.86388800
H	-1.87916000	-0.18967500	-2.26957700
H	-0.68654300	-1.90977500	1.51602500
H	-3.03975400	-1.90019900	2.24799600
H	-4.80123700	-1.05091700	0.74006900
H	-4.24689700	-0.18655900	-1.50786800
C	0.18683700	-1.06485100	-0.93186500
C	1.37856500	-1.65335400	-0.31538800
H	0.32556200	-0.67776200	-1.94054500
C	2.66689600	-0.82941600	-0.47817700
H	1.23662200	-1.96836500	0.71840600
C	3.90511700	-1.68147200	-0.23722300
H	2.69875500	-0.39530300	-1.47884900
H	4.81253300	-1.07876300	-0.30437200
H	3.86850700	-2.15173600	0.74838700
H	3.95859400	-2.46635200	-0.99433300
S	2.69690200	0.55014200	0.73995200
C	1.12337600	1.29967600	0.38277600
C	0.84415300	1.79600200	-0.89696900
C	0.15878200	1.38581100	1.39024200
C	-0.40705600	2.33777600	-1.17316900
H	1.60433300	1.75742400	-1.66969100
C	-1.08855100	1.92611600	1.10622900
H	0.37714200	1.00030600	2.37947100
C	-1.37699500	2.39281900	-0.17753900
H	-0.62226400	2.71230700	-2.16707600
H	-1.84322300	1.97275600	1.88300500
H	-2.35514000	2.80598900	-0.39496500

H	1.52790800	-2.56441300	-0.92579000

TSA-2

Value of imaginary frequency = -210.10 cm^{-1}

C	2.27417000	-0.89781300	1.17880600
C	1.15182900	-0.94678500	0.33092500
C	1.34489900	-1.03921800	-1.05871800
C	2.62938800	-1.11135000	-1.57850700
C	3.72940200	-1.09067500	-0.72437800
C	3.55254700	-0.98364900	0.65586100
H	2.12213800	-0.80421400	2.24912700
H	0.49448200	-1.04638800	-1.73053600
H	2.77415100	-1.18340700	-2.64941400
H	4.73057100	-1.15237200	-1.13508200
H	4.41175000	-0.96354100	1.31495100
C	-0.16290000	-0.90480200	0.93251800
C	-1.34089700	-1.56928100	0.30432700
H	-0.16625100	-0.90180800	2.01900100
C	-2.69925900	-0.86898000	0.42229500
H	-1.16037500	-1.81970200	-0.74080800
C	-3.84122000	-1.77580700	-0.01311700
H	-2.87282400	-0.52287000	1.44088300
H	-4.79414700	-1.24436800	0.00901700
H	-3.67351500	-2.16011500	-1.02181300
H	-3.90623300	-2.62104700	0.67472300
S	-2.66901500	0.57416700	-0.71473300
C	-1.13866600	1.27019800	-0.22740000
C	-0.71959300	1.19819200	1.12155900
C	-0.29405200	1.84147400	-1.18493400
C	0.50197500	1.80144100	1.50895400
H	-1.43804700	0.95435700	1.89380300
C	0.93209300	2.34493700	-0.79152400
H	-0.58667900	1.85734900	-2.22798200
C	1.33417900	2.33709900	0.56062100
H	0.78227400	1.78663300	2.55572100
H	1.59848000	2.75653900	-1.54112700
H	2.29036300	2.76225400	0.83909900
H	-1.42526500	-2.51387000	0.86242700

CF_3SO_3H (CH_3CN*10)

C	0.09434200	-3.49609300	1.11765400
N	0.98743500	-3.45210200	0.39434800
C	-1.02213100	-3.56446300	2.04795700
H	-0.77780700	-3.00108800	2.94980800
H	-1.90521100	-3.13657300	1.57438700

H	-1.21010700	-4.60584800	2.31161000
C	-1.68612100	-3.22483100	-1.65862900
N	-2.52416600	-3.21732100	-0.87158200
C	-0.61980900	-3.24485600	-2.64597100
H	0.33581700	-3.30632400	-2.12621000
H	-0.74499400	-4.10772900	-3.30064500
H	-0.65063100	-2.32844600	-3.23532900
C	-1.31955300	1.15893800	3.30122600
N	-0.25545700	1.56527200	3.45746900
C	-2.66976000	0.65025400	3.11036900
H	-3.33327300	1.09966000	3.85014100
H	-3.01296900	0.91083500	2.10929000
H	-2.67011700	-0.43373700	3.22650800
C	3.88879600	1.30345900	1.27590200
N	4.65041200	0.44430400	1.21023200
C	2.90883400	2.37640400	1.33969600
H	2.78311600	2.80890000	0.34400300
H	1.95200500	1.97512600	1.67987900
H	3.25282100	3.14764200	2.02984200
C	-1.45530800	3.66557700	1.18863500
N	-2.50483200	3.23394000	1.00535300
C	-0.13404500	4.22169900	1.42908900
H	-0.15013000	5.29583100	1.24296800
H	0.15514200	4.02607700	2.46223500
H	0.58011400	3.74371300	0.75922700
C	3.25128200	-2.68932700	-1.81634600
N	2.74563600	-2.86806700	-2.83315600
C	3.89156900	-2.44334500	-0.53381200
H	3.93909900	-3.37048800	0.03688000
H	4.89870000	-2.05675200	-0.69498900
H	3.30655200	-1.71079000	0.02138800
C	2.71755700	-1.93187700	2.76614800
N	3.47094800	-2.77298100	2.97968200
C	1.76646900	-0.86595300	2.48987500
H	1.84107500	-0.58545800	1.43717400
H	0.75296000	-1.20298600	2.70771400
H	1.99539800	0.00126600	3.11040900
C	-5.01167600	-1.42230200	-0.50730400
N	-5.37091200	-1.32250300	-1.59416000
C	-4.55501300	-1.53258400	0.86976800
H	-5.01941700	-0.74894800	1.46988500
H	-4.83386500	-2.50909300	1.26694000
H	-3.46989300	-1.42909600	0.89518000
C	-0.07806300	4.32920900	-1.98128000

N	-0.90056800	5.10546000	-1.77728300
C	0.96019100	3.33420800	-2.20367600
H	1.92005800	3.83140600	-2.34985300
H	1.01227600	2.67928700	-1.33236400
H	0.72002300	2.74099900	-3.08701100
C	3.47716400	0.86334600	-1.83633800
N	2.46242300	0.35522600	-1.67432000
C	4.75793200	1.51495600	-2.02241000
H	5.54765000	0.85928000	-1.65383200
H	4.90677100	1.71876300	-3.08315200
H	4.76376800	2.45020400	-1.45999200
S	-0.60992300	0.07737000	-0.12028300
O	-1.20388700	-0.78107200	0.87183200
O	0.13668700	1.24879500	0.27678900
O	0.20305200	-0.75945800	-1.14339600
C	-2.01834100	0.65023200	-1.19955100
F	-2.25908700	-0.24049900	-2.14408500
F	-1.70223300	1.80650100	-1.75634200
F	-3.09590200	0.79481000	-0.45033600
H	1.10969400	-0.32149100	-1.38459100

1a (CH_3CN*10)

C	-4.47549500	1.25849900	-0.89206600
C	-3.54820100	0.21525500	-0.77447200
C	-4.01757400	-1.10595400	-0.82672500
C	-5.37382100	-1.36935600	-0.96505900
C	-6.28826400	-0.32126800	-1.06306600
C	-5.83382200	0.99395200	-1.02963600
H	-4.12072600	2.28342300	-0.86105100
H	-3.31590400	-1.93161200	-0.77027900
H	-5.72020200	-2.39593100	-1.00422000
H	-7.34618800	-0.53046100	-1.17205500
H	-6.53745100	1.81453500	-1.11179500
C	-2.12366100	0.53938100	-0.62287100
C	-1.16500700	-0.31206700	-0.22530200
H	-1.83726700	1.56045500	-0.86907500
C	0.24571400	0.04791900	-0.19381100
C	1.22225000	-0.83143300	0.05539800
H	0.49557100	1.08149600	-0.42925300
H	0.99310700	-1.87245300	0.26719800
H	2.26785600	-0.53928600	0.04994200
C	0.37250600	4.09707100	-1.75496700
N	-0.49679200	3.66352200	-1.13972300
C	1.47084000	4.67381500	-2.51505800

H	2.41843300	4.38176500	-2.06052800
H	1.43775700	4.30443100	-3.53964300
H	1.38022800	5.76053700	-2.51138300
C	2.31273200	-2.96956700	-2.39456900
N	2.50116600	-2.01730200	-3.01088900
C	2.06352700	-4.17728700	-1.62259500
H	1.65320200	-3.90731100	-0.64761300
H	1.34643700	-4.80376800	-2.15327400
H	2.99875800	-4.72083800	-1.48611400
C	-0.74655200	-2.06158900	-2.78948900
N	-0.93604700	-3.02270200	-2.18698000
C	-0.50682200	-0.84382500	-3.54669500
H	-0.11578400	-1.10093100	-4.53182600
H	-1.44344000	-0.29522400	-3.65576800
H	0.22341400	-0.22683500	-3.01890400
C	-0.88614900	-3.31709800	1.95940900
N	-0.07978500	-2.81324700	2.60660500
C	-1.90294000	-3.94048000	1.12678300
H	-2.87211300	-3.49372100	1.35422800
H	-1.65758100	-3.77548800	0.07502500
H	-1.93513300	-5.01116600	1.33070000
C	3.37910500	0.08401900	2.65754200
N	4.43864200	-0.04840800	2.23106200
C	2.03478200	0.23364900	3.19228700
H	1.51291300	1.00637600	2.62492900
H	1.49993800	-0.71392500	3.09583200
H	2.08727400	0.51965300	4.24371000
C	-2.60633900	-0.66963100	2.88241400
N	-3.53696900	-1.22412000	2.49715100
C	-1.42398500	0.01822300	3.37806700
H	-1.72277100	0.93224600	3.89240400
H	-0.89132200	-0.63545900	4.06917600
H	-0.77381500	0.25822300	2.53414800
C	3.01031100	1.14688300	-2.22575600
N	2.05911000	1.57092600	-2.71387900
C	4.21327000	0.60675600	-1.61205300
H	4.27091100	-0.46262000	-1.81931000
H	5.08916000	1.10879300	-2.02477100
H	4.17415800	0.76988700	-0.53345700
C	4.06368700	-2.82719300	0.69080800
N	4.64020000	-2.54870400	-0.26405700
C	3.32418600	-3.19798800	1.88716300
H	2.42465400	-2.58564400	1.96740300
H	3.03895500	-4.24934300	1.82594900

H	3.95006600	-3.04088500	2.76614600
C	-2.01057800	2.90672500	1.92580600
N	-3.14895700	2.75268400	1.87821900
C	-0.56780500	3.07842800	2.00626300
H	-0.24592200	2.96124000	3.04255200
H	-0.08231000	2.32635600	1.38255200
H	-0.29605600	4.07133000	1.64639100
C	2.53901300	3.65779900	0.80611400
N	2.56108600	2.51690400	0.66409300
C	2.49339500	5.10140400	0.98132500
H	2.45678400	5.33782300	2.04522300
H	3.38341200	5.55143500	0.54070700
H	1.60353400	5.49969800	0.49102500
H	-1.41394000	-1.33392900	0.05272700

PhSH (CH_3CN*10)

S	0.06176400	0.14601800	0.07385700
C	-1.19516600	0.94229100	-0.90458900
C	-0.88541300	2.15605300	-1.52101600
C	-2.46748500	0.38745900	-1.05068800
C	-1.85124100	2.80747900	-2.28239300
H	0.10411500	2.58361600	-1.40762900
C	-3.41949900	1.04121000	-1.82605400
H	-2.71182200	-0.55035200	-0.56487200
C	-3.11849800	2.25323500	-2.44211800
H	-1.60544900	3.75035800	-2.75766500
H	-4.40371700	0.60028700	-1.94477900
H	-3.86514500	2.76129000	-3.04074800
C	-5.20968500	-1.45178100	-0.07068500
N	-4.78542800	-2.35556600	-0.64066600
C	-5.73938900	-0.29443900	0.63325400
H	-4.96747900	0.47488500	0.69727600
H	-6.60420000	0.09323100	0.09348600
H	-6.03760900	-0.58639000	1.64040000
C	1.89738700	-2.95152300	-1.92804800
N	2.20683800	-2.29004600	-2.81611800
C	1.50024700	-3.79002100	-0.80743600
H	1.05341500	-3.16620500	-0.03164100
H	0.76678900	-4.52182200	-1.14676500
H	2.37607000	-4.30315400	-0.40783500
C	-1.04299500	-1.93758900	-2.65616000
N	-1.34405300	-2.74500000	-1.89438000
C	-0.65517200	-0.91164400	-3.61134200
H	-0.27168700	-1.38451000	-4.51615700

H	-1.52276400	-0.29613500	-3.85577600
H	0.12492100	-0.28687200	-3.17232800
C	-0.46109500	-2.78471400	2.28274200
N	0.30241400	-2.10535600	2.81091000
C	-1.42344500	-3.62505600	1.58686800
H	-2.33866900	-3.69221200	2.17516400
H	-1.65170400	-3.18502500	0.61250400
H	-1.00131000	-4.62093200	1.44529100
C	3.42342200	1.00426900	2.30921800
N	4.44549200	0.96444400	1.78345700
C	2.12679300	1.03812000	2.96725400
H	1.50413200	1.79292000	2.48278300
H	1.64966100	0.05905100	2.87985000
H	2.25799200	1.28615700	4.02134500
C	-2.36921800	-0.23599200	2.75904600
N	-3.04696700	-0.91965200	2.13019100
C	-1.49690400	0.61451500	3.55285500
H	-2.07363300	1.43640800	3.97881400
H	-1.04821400	0.02569200	4.35371300
H	-0.70993500	1.00906000	2.90833200
C	2.75475900	0.89045000	-2.33235500
N	2.05827900	1.43904200	-3.06484800
C	3.63104000	0.19752400	-1.40090500
H	4.10841200	-0.64073100	-1.90676000
H	4.39431400	0.87960500	-1.02471100
H	3.03448400	-0.17299500	-0.56526200
C	4.38846600	-2.28389400	0.78304800
N	5.25465600	-2.32052900	0.02834500
C	3.27329600	-2.23528700	1.71674700
H	2.49658500	-1.58012800	1.31695800
H	2.86483800	-3.23674300	1.85279900
H	3.61170800	-1.84881800	2.67875100
C	-2.41652600	3.03333200	1.42943400
N	-3.48487900	2.61219800	1.37201600
C	-1.06461400	3.56390300	1.52470700
H	-0.88393700	3.91511200	2.54192200
H	-0.34346900	2.78500700	1.27247500
H	-0.94694800	4.39407000	0.82706200
C	3.01298100	3.31260100	-0.06505600
N	1.95211600	3.00464700	0.25396800
C	4.35846900	3.68461400	-0.47145700
H	5.07867900	3.10601500	0.10888200
H	4.48656700	3.47303400	-1.53402900
H	4.51392200	4.74851200	-0.29096700

H	-0.63951100	-0.97753000	0.30905800

$CF_3SO_3^-$ (CH_3CN*10)

C	-2.99477800	2.20760000	-1.70734400
N	-3.58505200	2.67777000	-0.83968000
C	-2.25960600	1.60927500	-2.81028900
H	-1.52354200	0.90922400	-2.41061800
H	-2.95446600	1.06685400	-3.45188500
H	-1.76661300	2.39285100	-3.38699100
C	-3.94812600	-0.67159000	-0.74509700
N	-3.92432600	-0.99448900	-1.84854700
C	-3.97504000	-0.26027800	0.64953900
H	-4.79744700	0.43799200	0.80798800
H	-4.11012300	-1.13922500	1.28201600
H	-3.02802100	0.22914400	0.87980200
C	3.35939000	0.47696700	-2.82840700
N	4.11440200	1.10397700	-2.22894700
C	2.39852400	-0.29899300	-3.59582400
H	2.90315900	-1.14813600	-4.05731500
H	1.61211500	-0.65899300	-2.92964000
H	1.96465300	0.33233600	-4.37267600
C	2.47552400	3.49024700	0.99749200
N	1.87517300	4.46987900	0.95020200
C	3.22577400	2.24414900	1.02051700
H	2.58615700	1.43781700	0.65099100
H	4.10389900	2.33835500	0.37997700
H	3.53411100	2.02397900	2.04298700
C	3.92077200	-2.09884300	-0.98055500
N	3.37049600	-2.79540800	-1.71076500
C	4.62507000	-1.21871200	-0.06121900
H	5.07892700	-1.80863300	0.73549200
H	5.39951400	-0.67326000	-0.60001200
H	3.90790600	-0.50955000	0.35390800
C	-2.37549800	2.86408700	2.08444100
N	-3.18271000	2.35371500	2.72531500
C	-1.34584500	3.49741800	1.27626200
H	-1.80179100	4.24074300	0.62289100
H	-0.61062600	3.97106400	1.92650000
H	-0.86181900	2.72241600	0.67815100
C	0.10500200	3.79983800	-1.83271300
N	-0.61676200	4.69295600	-1.88725600
C	0.99664200	2.65216200	-1.76761000
H	0.84689900	2.13394700	-0.81947500

H	0.77090100	1.97269700	-2.59230900
H	2.03218700	2.98566700	-1.84355900
C	-3.37242400	-3.98965000	-0.81001400
N	-4.18832500	-4.05461800	-0.00327000
C	-2.33516700	-3.90521500	-1.82665600
H	-1.51793900	-4.57925700	-1.56808200
H	-2.75071200	-4.19486300	-2.79231600
H	-1.96252900	-2.88099900	-1.88545100
C	2.84254700	-2.47126800	2.33569400
N	2.91451300	-3.53014900	1.89442000
C	2.75397700	-1.12195400	2.87356600
H	3.75490100	-0.75828200	3.11030900
H	2.28625800	-0.47433600	2.13009000
H	2.14859500	-1.12892500	3.78090400
C	-0.14633500	0.88588000	3.25446200
N	0.71613900	1.57423400	2.93121900
C	-1.22663800	0.01016900	3.68334600
H	-0.80755400	-0.87901400	4.15499800
H	-1.86070600	0.54006600	4.39371600
H	-1.82097900	-0.28062500	2.81702000
S	0.04576600	-0.55663200	-0.41053900
O	-0.27520500	-1.01221300	-1.76574300
O	1.47019900	-0.30944900	-0.16532500
O	-0.86388500	0.45813100	0.12819000
C	-0.31255400	-2.04065000	0.62465600
F	-1.62475900	-2.28109900	0.65293300
F	0.09586400	-1.85307100	1.88026400
F	0.30016800	-3.11645300	0.14123900

CH_3CN (CH_3CN*10)

C	-3.70941700	-0.14244800	1.71656000
N	-3.24055100	0.76960200	1.19632300
C	-4.32305200	-1.28941500	2.36917200
H	-3.95977200	-2.20705300	1.90564900
H	-4.05280400	-1.29315300	3.42509300
H	-5.40707900	-1.22722000	2.26903900
C	2.73626300	-1.14735000	2.10712800
N	2.30304500	-1.74246500	2.99041300
C	3.26763700	-0.38041300	0.99212200
H	2.54800400	-0.39713000	0.17166200
H	3.41950500	0.64832200	1.32240800
H	4.21810700	-0.80643900	0.66857600
C	1.40802100	1.33988900	3.69057400
N	2.21503800	1.97003600	3.16729400

C	0.37233800	0.54984700	4.33640400
H	0.83567800	-0.21422400	4.96098300
H	-0.25032700	1.20008400	4.95187600
H	-0.23996800	0.06441700	3.57392700
C	2.97779900	2.16453400	-1.14313300
N	2.80148000	1.45953100	-2.03453200
C	3.19881700	3.04819300	-0.00903700
H	3.15870400	4.08463800	-0.34323300
H	2.42218600	2.87707600	0.73912400
H	4.17600800	2.84063500	0.42937400
C	0.42005800	-2.44573400	-2.85774400
N	0.68272700	-3.56300900	-2.78975300
C	0.11914500	-1.02442500	-2.92669400
H	-0.89339700	-0.88347700	-3.30658100
H	0.19063400	-0.59567200	-1.92389600
H	0.83300300	-0.53501500	-3.59166600
C	0.23367900	3.60027200	-1.88272300
N	0.47072800	4.33705300	-1.03261400
C	-0.06275700	2.65694400	-2.94947200
H	-0.95426000	2.98131500	-3.48740100
H	0.78321900	2.60549400	-3.63512500
H	-0.22905900	1.67241200	-2.50894300
C	-0.54048500	-2.32928800	1.60249800
N	-1.23740100	-1.89884500	2.40964900
C	0.35440100	-2.87789200	0.59637200
H	1.15408200	-3.43214100	1.08589600
H	-0.20303300	-3.53291900	-0.07161700
H	0.78201100	-2.05515100	0.01780600
C	3.52389000	-2.87711800	-1.17029000
N	3.42615100	-3.63746000	-0.31372600
C	3.65373100	-1.89399800	-2.23458100
H	2.92733000	-1.09341200	-2.08411400
H	4.65823000	-1.46880300	-2.21466600
H	3.47989000	-2.37244200	-3.19889200
C	-2.99152700	2.42576900	-1.51990000
N	-2.97999600	3.53083500	-1.20298500
C	-2.98340900	1.03080500	-1.93176500
H	-2.82764300	0.97079000	-3.01009100
H	-2.18198300	0.50844700	-1.40790000
H	-3.93834500	0.57168600	-1.67319300
C	-3.36814700	-2.19589600	-1.01853000
N	-2.22483800	-2.07525300	-1.00426900
C	-4.81797400	-2.31643400	-1.03116800
H	-5.17168500	-2.35185000	-2.06171600

H	-5.11518800	-3.22872500	-0.51335000
H	-5.25521000	-1.45310600	-0.52645600
C	-0.71779200	2.68236200	1.52426200
H	-1.49725900	3.18993700	0.95570000
H	-1.13176000	2.33331800	2.47124800
H	0.11016200	3.36774700	1.70827500
C	-0.23752300	1.54005100	0.76018500
N	0.14502100	0.63884200	0.15430900

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C	-4.24014400	-2.65082700	1.53202500
C	-3.39384300	-2.18500700	0.51831300
C	-3.66501400	-2.56713900	-0.80410600
C	-4.75045500	-3.38347100	-1.09469600
C	-5.58923400	-3.83529400	-0.07594300
C	-5.32796400	-3.46771600	1.24027800
H	-4.04286300	-2.35829000	2.55845900
H	-3.02605500	-2.22647500	-1.61001800
H	-4.94633400	-3.66790000	-2.12246500
H	-6.43714400	-4.46907100	-0.30867100
H	-5.97188000	-3.81419400	2.04065600
C	-2.29836700	-1.27050000	0.88189100
C	-1.46156900	-0.66016500	0.03737600
H	-2.21696200	-1.04349000	1.94316200
C	-0.44456600	0.33702700	0.48044400
C	-0.57066800	1.65542700	-0.28171100
H	-0.52345800	0.52821800	1.54988800
H	0.21140200	2.35741500	0.01810900
H	-0.50375200	1.49108400	-1.36154700
H	-1.54648400	2.10075200	-0.06664400
S	1.26207500	-0.29902600	0.15831800
C	1.33706800	-1.73696200	1.20287300
C	0.87504300	-1.71978100	2.52195900
C	1.96314000	-2.87905700	0.70161300
C	1.04012500	-2.84169000	3.32697900
H	0.40956500	-0.82816500	2.92677000
C	2.14987300	-3.98819900	1.52343700
H	2.31798500	-2.88682600	-0.32409200
C	1.68599000	-3.97490200	2.83555300
H	0.67646500	-2.82348900	4.34806400
H	2.64979300	-4.86653600	1.13022700
H	1.82357200	-4.84174200	3.47123800
C	0.11180400	-4.01768800	-2.01676100
N	-0.61878800	-3.15895700	-2.24135500

C	1.02968500	-5.11388700	-1.75045900
H	0.86512900	-5.49067600	-0.74081100
H	0.85491100	-5.91437100	-2.47007500
H	2.05350900	-4.75118300	-1.84926700
C	-3.37977600	3.88267700	-1.01851200
N	-3.79663400	3.82877300	0.05185500
C	-2.85257300	3.93716400	-2.37321700
H	-1.96967700	3.29833500	-2.43831000
H	-3.60778800	3.57481100	-3.07083000
H	-2.58595600	4.96530400	-2.61936200
C	-4.17854600	0.76462700	-1.28094100
N	-3.53831100	0.78732600	-2.23628800
C	-4.98464700	0.73725800	-0.07048700
H	-5.71225900	1.54881600	-0.10173700
H	-5.50384400	-0.22018900	-0.00253100
H	-4.33474600	0.86613400	0.79792900
C	1.58379700	0.72871200	-3.14462900
N	2.43161500	1.46945500	-2.90664300
C	0.50658100	-0.20689700	-3.42865300
H	0.40811500	-0.89189500	-2.58538700
H	-0.42751100	0.33992100	-3.57164400
H	0.73962500	-0.77432200	-4.33058300
C	3.21086900	2.83062900	0.07323700
N	2.39143100	3.59411900	0.33483200
C	4.25321600	1.86413200	-0.23106900
H	3.78903800	0.94090500	-0.57862200
H	4.90517500	2.26117400	-1.01006200
H	4.83837900	1.66973500	0.67015300
C	3.78398400	-1.68255300	-2.94201300
N	2.89340500	-2.38853800	-2.76594800
C	4.90714700	-0.79030200	-3.18369200
H	5.83763800	-1.35472300	-3.11964700
H	4.81159200	-0.34932300	-4.17637900
H	4.90990400	-0.00232700	-2.43157100
C	-2.26864000	2.59800900	2.62398700
N	-2.85247000	1.61374200	2.73760400
C	-1.53583600	3.84565100	2.47923800
H	-2.21636000	4.62305900	2.13167800
H	-1.10645800	4.12735500	3.44113500
H	-0.73493600	3.71547800	1.75038500
C	0.00206600	5.04965700	-1.19347000
N	-0.63785100	5.49401400	-0.34792800
C	0.78442400	4.48443300	-2.28152100
H	0.82735500	3.40066000	-2.17149300

H	0.31671400	4.74028300	-3.23338200
H	1.79766600	4.88554600	-2.25224100
C	4.73176500	-1.21934800	1.01325600
N	5.09294000	-1.50205400	-0.04108800
C	4.27471300	-0.84320200	2.34219500
H	5.11422600	-0.45293800	2.91877900
H	3.49976200	-0.07842800	2.25365000
H	3.85975800	-1.71960600	2.84421700
C	1.92158800	2.24819700	3.29383100
N	0.86137300	1.81782800	3.18120200
C	3.26118800	2.79454800	3.44826800
H	3.96130600	2.22378200	2.83657600
H	3.26618700	3.83667300	3.12883000
H	3.55950200	2.73034900	4.49506200
H	-1.50331900	-0.84654100	-1.03362700

IMA-2 (CH_3CN*10)

C	-1.88978900	-2.10546100	-1.55351200
C	-1.92817400	-0.70975500	-1.80057500
C	-2.50118600	-0.22740500	-3.00794300
C	-3.05126100	-1.11921800	-3.90095500
C	-3.03149000	-2.49335600	-3.62006700
C	-2.44851500	-2.99075600	-2.45513000
H	-1.41407800	-2.46463600	-0.64821100
H	-2.51450000	0.83457000	-3.21904500
H	-3.49877200	-0.76421200	-4.82046800
H	-3.47159100	-3.18314800	-4.33150500
H	-2.42189300	-4.05547400	-2.26059200
C	-1.39675400	0.12816100	-0.81245800
C	-1.44374800	1.59060200	-0.75424000
H	-1.01166000	-0.36114200	0.08324400
C	-0.18061600	2.23698000	-0.16549100
H	-1.74894200	2.06582600	-1.68726700
C	-0.44224000	3.65609200	0.31576900
H	0.19011400	1.62836100	0.66031700
H	0.46282100	4.09204700	0.74347000
H	-0.78502000	4.29211800	-0.50504800
H	-1.21815000	3.64145100	1.08581900
S	1.13936000	2.31589900	-1.44644900
C	1.16939800	0.60967800	-1.94425200
C	1.41067700	-0.40269800	-1.00733400
C	0.93952400	0.28161000	-3.28371800
C	1.37451900	-1.73629400	-1.40418800
H	1.61768500	-0.15472900	0.02979300

C	0.91108500	-1.05089000	-3.67204700
H	0.75222700	1.06761400	-4.00612900
C	1.11548200	-2.06304300	-2.73019800
H	1.53225300	-2.51311600	-0.66535000
H	0.71175100	-1.30443500	-4.70694400
H	1.07472400	-3.10300600	-3.03436300
H	-2.23960100	1.76826100	-0.00369600
C	0.22034500	-1.55409900	2.87457900
N	0.53886200	-1.75745800	1.78780700
C	-0.18073200	-1.30883100	4.25143700
H	0.16012200	-0.31847700	4.55921100
H	-1.26801500	-1.35256500	4.32269700
H	0.25838000	-2.06934700	4.89838800
C	4.37296800	-2.48099700	-0.32529300
N	4.04270200	-2.14734800	0.72447800
C	4.77147100	-2.91207200	-1.65562200
H	4.74685500	-4.00109900	-1.70497300
H	4.08067200	-2.49223700	-2.38808700
H	5.78076200	-2.55795900	-1.86620500
C	0.24012800	-4.73078200	0.68709200
N	-0.64311100	-4.66134300	-0.04599900
C	1.35631000	-4.82744300	1.61389300
H	1.83975100	-5.79817800	1.49985000
H	2.07184800	-4.03081800	1.40545600
H	0.98034500	-4.72228900	2.63272600
C	-4.04041600	3.64917000	0.65978700
N	-4.14737100	3.00814600	1.60869200
C	-3.89259400	4.45079700	-0.54456100
H	-3.25082700	3.92279500	-1.25101000
H	-4.87182600	4.60926800	-0.99704900
H	-3.44643700	5.41250800	-0.28929400
C	-4.83954400	0.86139900	-0.81751500
N	-4.91852700	1.60510300	-1.69087900
C	-4.70618500	-0.08132500	0.28226300
H	-5.56298900	0.01182500	0.95074800
H	-4.66191100	-1.09702200	-0.11523900
H	-3.79247000	0.13999300	0.84026600
C	-1.69753200	1.50821900	2.99134800
N	-1.87017900	0.59824100	2.30935900
C	-1.47979300	2.65727900	3.85396600
H	-2.30582700	3.35856100	3.72783200
H	-1.43562200	2.32797100	4.89288200
H	-0.53803000	3.13542200	3.58265100
C	3.59688000	4.53524500	0.01446800

N	3.02046000	4.63038700	1.00429200
C	4.32408700	4.40523100	-1.23857700
H	5.39525600	4.36494500	-1.03899800
H	4.01177500	3.49097200	-1.74619900
H	4.10652700	5.26243200	-1.87634200
C	-2.20671800	-3.59006500	2.70749400
N	-1.61276500	-4.25285700	3.43518900
C	-2.94325200	-2.72788700	1.79543300
H	-2.29918200	-1.90250200	1.48249800
H	-3.25518800	-3.30433900	0.92301500
H	-3.82167200	-2.32731500	2.30388000
C	4.51817300	0.69225000	-1.12077900
N	4.62552500	0.28447000	-2.19070800
C	4.37273900	1.20838000	0.23163300
H	5.12229000	1.98027300	0.41325200
H	3.37416500	1.63525600	0.34920000
H	4.51139900	0.39115200	0.94074500
C	2.29315800	0.93159100	3.02732400
N	1.57155100	1.74593000	2.65395300
C	3.19768300	-0.10550300	3.49924600
H	4.14310900	0.34704500	3.80075400
H	2.75046500	-0.61196800	4.35648000
H	3.37460200	-0.82675800	2.69907400

TSA-2 (CH_3CN*10)

Value of imaginary frequency = -145.23 cm^{-1}

C	-1.38312200	-2.40559900	-1.57188100
C	-1.56457600	-1.03290400	-1.83245300
C	-2.07662300	-0.62899600	-3.08127300
C	-2.44339700	-1.58457000	-4.01937800
C	-2.29768800	-2.94231600	-3.72919200
C	-1.76119300	-3.35561800	-2.50673400
H	-0.93415700	-2.70926300	-0.62997200
H	-2.18715500	0.42546000	-3.31392000
H	-2.84336200	-1.27383300	-4.97840500
H	-2.59296100	-3.68307900	-4.46580800
H	-1.62789900	-4.41096400	-2.29260400
C	-1.22277400	-0.10446600	-0.78436500
C	-1.86889800	1.23031200	-0.65248700
H	-0.92060700	-0.55841300	0.16035900
C	-1.00649600	2.40099800	-0.16146100
H	-2.39168700	1.52775000	-1.56492300
C	-1.86708000	3.61544100	0.16263900
H	-0.41052800	2.11717300	0.71244400

H	-1.25066000	4.45890000	0.48245600
H	-2.45961100	3.91632500	-0.70698300
H	-2.55207200	3.36163200	0.97757400
S	0.11892900	2.87313700	-1.53679600
C	0.70107100	1.27862100	-1.97736800
C	0.95063800	0.30361000	-0.98256500
C	0.87189500	0.95049400	-3.32855500
C	1.47396000	-0.95819600	-1.35421500
H	0.97882000	0.58579100	0.06711000
C	1.30565100	-0.31993800	-3.67088600
H	0.63528800	1.67795700	-4.09818800
C	1.61976100	-1.27838700	-2.68420200
H	1.69980300	-1.67307500	-0.57077400
H	1.40538300	-0.58085200	-4.72015400
H	1.97418600	-2.26102800	-2.97868700
H	-2.63093900	1.05923400	0.12817300
C	0.84034300	-1.52871400	2.89090700
N	1.20006400	-1.55667800	1.79104100
C	0.39311500	-1.48503400	4.27796300
H	0.45210300	-0.45682800	4.64342500
H	-0.64270300	-1.82624700	4.33603400
H	1.02634900	-2.13304500	4.88737800
C	4.84135900	-1.39083200	-1.01833900
N	4.47124600	-1.38187300	0.07802500
C	5.30622900	-1.40620100	-2.39980000
H	5.59184300	-2.42262800	-2.67708600
H	4.50377500	-1.05547600	-3.05208200
H	6.16664700	-0.74232700	-2.50200300
C	1.63784800	-4.40808700	0.48873000
N	0.70350500	-4.50677500	-0.18701400
C	2.81403400	-4.29665000	1.34189700
H	3.48729800	-5.13278600	1.14283100
H	3.32709300	-3.35393900	1.13654100
H	2.49605000	-4.32328400	2.38660000
C	-5.02356400	2.06769800	0.85421200
N	-4.75755200	1.47117900	1.80982100
C	-5.33899400	2.82064700	-0.35363400
H	-4.61490500	2.56991900	-1.13189200
H	-6.34056900	2.55610400	-0.69784200
H	-5.29630800	3.89023100	-0.13887900
C	-4.68651200	-0.79094300	-0.62320200
N	-5.01251900	-0.17196900	-1.54493100
C	-4.25779100	-1.56337600	0.53680100
H	-5.06850400	-1.60388200	1.26766500

H	-3.99716300	-2.57655800	0.22208000
H	-3.39006000	-1.07970600	0.99763400
C	-1.77414200	1.05498700	2.92652100
N	-1.75034300	0.01298300	2.42305200
C	-1.81012300	2.36499400	3.56383000
H	-2.84003900	2.72823600	3.57965600
H	-1.43355200	2.28057100	4.58562800
H	-1.17408000	3.05541000	3.00508800
C	1.97583000	5.07404000	0.63558800
N	1.12674600	4.88472300	1.39806700
C	3.04856400	5.29974600	-0.32617400
H	4.01493700	5.18619000	0.16895700
H	2.96761200	4.57177400	-1.13752000
H	2.96804100	6.30827300	-0.73596800
C	-0.72945400	-4.26898800	2.75966000
N	0.10328800	-4.72689100	3.41941800
C	-1.77008700	-3.66140100	1.93847000
H	-1.48510400	-2.63017400	1.70644600
H	-1.88019000	-4.22947800	1.01192500
H	-2.71506500	-3.66014300	2.48616300
C	3.86719500	1.70784800	-1.18018400
N	4.12301100	1.59657200	-2.30322800
C	3.52619700	1.83479700	0.23189300
H	4.33597500	2.33421600	0.76905700
H	2.60435600	2.41420000	0.33637200
H	3.37413800	0.83314900	0.64327800
C	2.16482100	1.30464100	3.12686400
N	1.21404800	1.83166800	2.73026100
C	3.35465700	0.61312800	3.61026000
H	4.14582400	1.33702100	3.81414500
H	3.11255400	0.07146400	4.52771800
H	3.69453600	-0.09546000	2.85077900

P2-p (CH_3CN*10)

C	1.54708800	2.20420100	-2.11278300
C	1.51083300	0.80952200	-2.10118500
C	1.76839000	0.11968600	-3.28881700
C	2.06230800	0.81330100	-4.45841400
C	2.10653100	2.20539400	-4.45694500
C	1.84555000	2.90063300	-3.28065400
H	1.33559300	2.74825600	-1.19816400
H	1.75348600	-0.96580700	-3.30861000
H	2.26257300	0.26470400	-5.37161400
H	2.34199400	2.74324300	-5.36800200

H	1.87307500	3.98443300	-3.26895000
C	1.16824500	0.08551500	-0.81345600
C	2.16473300	-1.03324200	-0.45396800
H	1.15115200	0.81994000	-0.00457000
C	1.53514800	-2.31900200	0.08363900
H	2.78291500	-1.29146700	-1.31700600
C	2.57627300	-3.36299900	0.45948000
H	0.87377400	-2.11637100	0.93195500
H	2.10793200	-4.27280100	0.83893500
H	3.20722400	-3.61468600	-0.39661700
H	3.21436600	-2.95162400	1.24557300
S	0.47869400	-3.04233100	-1.22883100
C	-0.46434800	-1.69180200	-1.64458000
C	-0.32608900	-0.44212700	-0.85857700
C	-1.36614300	-1.77627800	-2.71086800
C	-1.23663200	0.65301400	-1.25189100
H	-0.55365400	-0.68662200	0.19602500
C	-2.16336500	-0.69173500	-3.00490900
H	-1.44491100	-2.68807400	-3.29087500
C	-2.11146700	0.53224900	-2.27288700
H	-1.15477200	1.57268900	-0.68345000
H	-2.86268700	-0.77460800	-3.83055300
H	-2.76222400	1.35093400	-2.55371600
H	2.83968900	-0.65796500	0.31982400
C	-1.13136800	1.86485200	2.81364700
N	-1.56836500	1.72464800	1.75895300
C	-0.59221400	2.03012100	4.15419200
H	-0.57764200	1.06065500	4.65591600
H	0.42549200	2.41687800	4.09097300
H	-1.21804400	2.72648600	4.71350700
C	-5.23810300	0.95995700	-0.90368900
N	-4.79836000	1.04959000	0.15505700
C	-5.79302000	0.84790400	-2.24353900
H	-6.17237300	1.81955800	-2.56094800
H	-5.01522700	0.51468700	-2.93196700
H	-6.60424900	0.11969700	-2.23858600
C	-2.09284600	4.18635200	-0.10726800
N	-1.17180000	4.10708900	-0.79164700
C	-3.25651600	4.28832700	0.75836600
H	-3.97066000	4.99003400	0.32617300
H	-3.71827900	3.30524700	0.85665400
H	-2.93896600	4.64621200	1.73867900
C	5.40434100	-1.16715100	1.11966100
N	5.03813000	-0.53450100	2.00760900

C	5.84852800	-1.97588900	-0.00480200
H	5.07398400	-1.97504100	-0.77271200
H	6.76438800	-1.55346900	-0.41862400
H	6.03413800	-2.99637000	0.33181000
C	4.59257300	1.33857700	-0.79699000
N	5.03507900	0.68512400	-1.63331000
C	4.02853500	2.16047100	0.26278000
H	4.78230100	2.32709600	1.03344900
H	3.71149500	3.11809800	-0.15245300
H	3.17283500	1.64711900	0.70785900
C	1.88653100	-0.44253600	2.99470700
N	1.69948000	0.56171700	2.46600700
C	2.12660400	-1.70759100	3.67023100
H	3.19831100	-1.91140800	3.67864100
H	1.75816000	-1.64349900	4.69511400
H	1.59543400	-2.50490300	3.14777300
C	-1.32857600	-5.04669900	1.02984700
N	-0.42003000	-4.80656000	1.69197700
C	-2.47308900	-5.34758800	0.18274600
H	-3.39124600	-5.03785800	0.68300700
H	-2.37781900	-4.81393500	-0.76473500
H	-2.50956400	-6.41989900	-0.01088000
C	0.23715700	4.63927800	2.17501700
N	-0.59400800	5.15961800	2.77497300
C	1.28231200	3.95209500	1.43227400
H	0.90300800	2.98384200	1.09783100
H	1.56763300	4.55167100	0.56685100
H	2.14936100	3.80145100	2.07719400
C	-4.15766800	-2.07404800	-0.82932100
N	-4.81445800	-2.19370100	-1.76548900
C	-3.31469000	-1.91274300	0.34485100
H	-3.84704700	-2.27165100	1.22762000
H	-2.39531400	-2.48763700	0.22171300
H	-3.07184400	-0.85520100	0.47120700
C	-1.88468100	-1.20815000	3.09288000
N	-0.92937000	-1.62893300	2.61044800
C	-3.10445000	-0.66409900	3.66984400
H	-3.72221000	-1.47658000	4.05348000
H	-2.85210000	0.01578800	4.48494100
H	-3.65116600	-0.11920200	2.89788500

3a (CH3CN*10)

C	2.04907000	2.07592000	-0.56098500
C	1.59991500	1.10449300	-1.45398000

C	1.90521900	1.24766100	-2.81176500
C	2.64142400	2.33621200	-3.26353600
C	3.08811400	3.30260200	-2.36240900
C	2.79133700	3.16866400	-1.01128000
H	1.82233100	1.96774800	0.49564000
H	1.55895100	0.49981600	-3.51897900
H	2.86950300	2.43213900	-4.31916300
H	3.66130600	4.15251000	-2.71462300
H	3.13125300	3.91712800	-0.30314400
C	0.84848700	-0.11627200	-0.95326400
C	1.79720200	-1.32138000	-0.93576300
H	0.56348200	0.08043300	0.08660500
C	1.11189200	-2.59164800	-0.45484600
H	2.22500300	-1.48860200	-1.93110200
C	2.08753500	-3.73744200	-0.23069200
H	0.55341500	-2.38942200	0.46579100
H	1.57112700	-4.64546800	0.08772500
H	2.64727300	-3.95290000	-1.14473500
H	2.79631900	-3.45824600	0.55340400
S	-0.10175000	-3.14372400	-1.70803700
C	-0.91999900	-1.61508200	-2.10190200
C	-0.44521400	-0.35114800	-1.72636400
C	-2.12353400	-1.73720200	-2.80867500
C	-1.24117900	0.75900400	-2.03729600
C	-2.88158500	-0.61990400	-3.11990700
H	-2.47627400	-2.72427700	-3.09107800
C	-2.44640900	0.64107900	-2.71543900
H	-0.88956500	1.74026600	-1.73709700
H	-3.81507400	-0.73712900	-3.65887200
H	-3.03469200	1.52551600	-2.93546000
H	2.62597300	-1.08987700	-0.25581900
C	-0.59417500	1.99358800	2.24557300
N	-1.10084800	1.73698300	1.24514800
C	0.03238300	2.31233500	3.51977500
H	0.19179100	1.39199600	4.08348200
H	0.99558900	2.79390500	3.34248500
H	-0.61482200	2.98551900	4.08328900
C	-5.36055300	0.87652600	-0.30374300
N	-4.70088100	1.04543600	0.62280400
C	-6.19107600	0.66788600	-1.47920800
H	-6.67366500	1.60626900	-1.75388500
H	-5.56778500	0.31940500	-2.30342700
H	-6.94872100	-0.08383500	-1.25778900
C	-1.62909100	4.16703300	-0.91044800

N	-0.59594600	4.53338700	-1.25866900
C	-2.93221000	3.68577900	-0.48106500
H	-3.70267700	4.05709000	-1.15796800
H	-2.92368800	2.59632200	-0.48485600
H	-3.12865200	4.03682000	0.53326200
C	5.23474000	-2.29237700	0.47436200
N	5.06928900	-1.87086600	1.53149300
C	5.43349000	-2.83168000	-0.86184000
H	4.63695800	-2.47431800	-1.51531100
H	6.39511800	-2.49478900	-1.24945600
H	5.41677500	-3.92128100	-0.81949600
C	5.12345900	0.73651700	-0.52230900
N	5.17869400	0.29051000	-1.58103400
C	5.06421300	1.28569100	0.82370200
H	5.93520100	0.95091100	1.38794900
H	5.05538100	2.37489900	0.77223700
H	4.15551300	0.93286800	1.31515000
C	2.04868600	-1.09583400	2.65828400
N	2.04380800	-0.01325900	2.26879100
C	2.06468800	-2.46023900	3.16087600
H	3.06964400	-2.86917300	3.04808300
H	1.78570800	-2.45530900	4.21523000
H	1.34567400	-3.06498200	2.60594200
C	-1.49825600	-4.84149100	1.25072300
N	-0.52123700	-4.57949000	1.79670100
C	-2.73561400	-5.16735300	0.55799400
H	-3.57892900	-4.72172700	1.08742300
H	-2.69376700	-4.77512000	-0.45984400
H	-2.86147900	-6.24977800	0.52482000
C	-0.45113400	5.23162400	1.93913000
N	-1.53994400	5.25582700	2.30716600
C	0.92746900	5.16734000	1.47953800
H	1.11879700	4.16590800	1.09133800
H	1.08221100	5.89430700	0.68224300
H	1.60103800	5.37989600	2.31029600
C	-4.14835300	-2.09019300	-0.32773000
N	-5.06798800	-2.37385800	-0.95728800
C	-2.99768800	-1.74009500	0.49152200
H	-3.26253000	-1.87969900	1.54022000
H	-2.15196800	-2.38343400	0.24042300
H	-2.72221600	-0.69738600	0.31651200
C	-1.82499600	-0.71202500	3.42646800
N	-0.93042300	-1.40696100	3.22867600
C	-2.96596000	0.16045300	3.65675800

H	-3.72132500	-0.37418900	4.23386600
H	-2.64438100	1.04292700	4.21236800
H	-3.38656100	0.46770200	2.69685500

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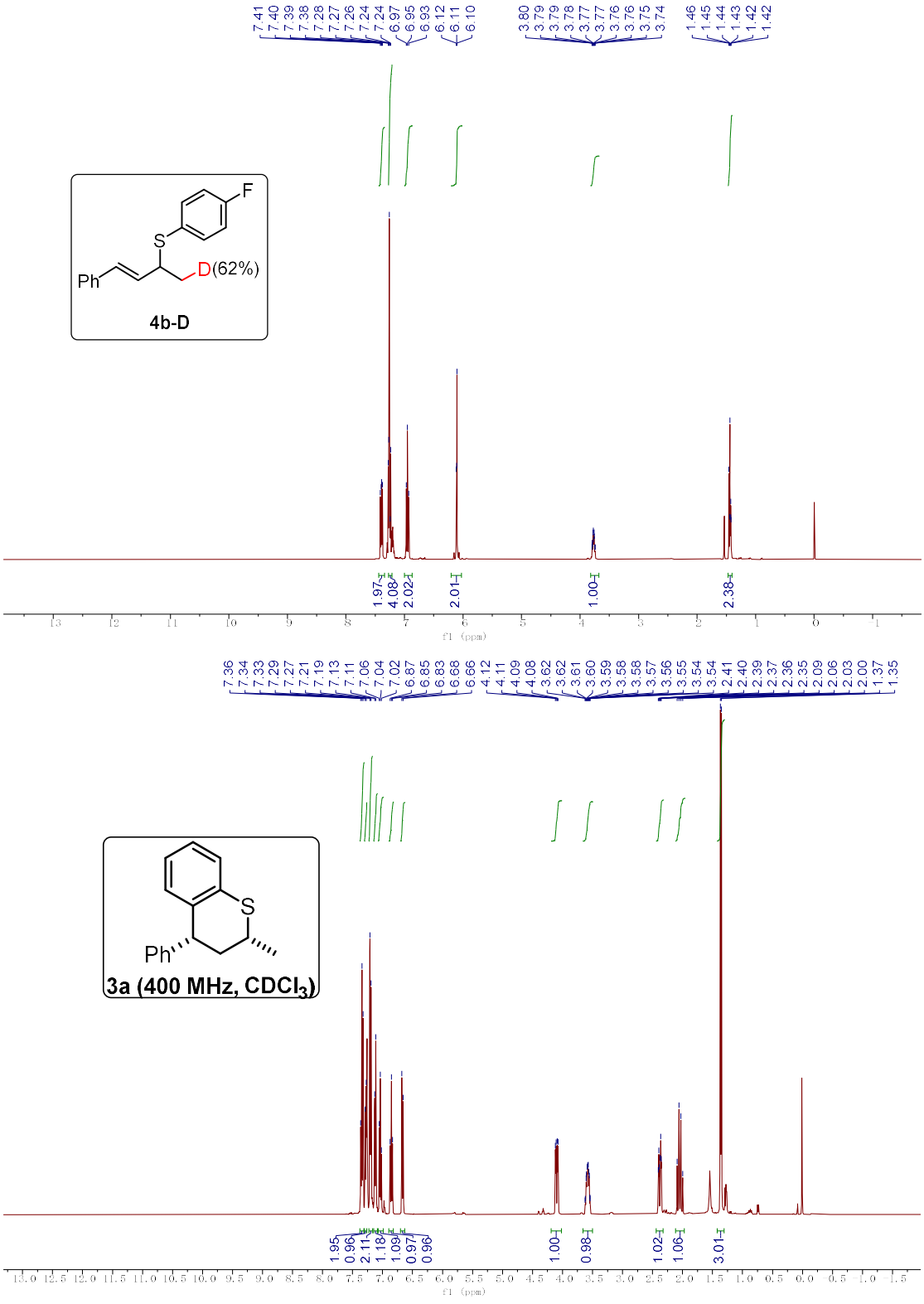
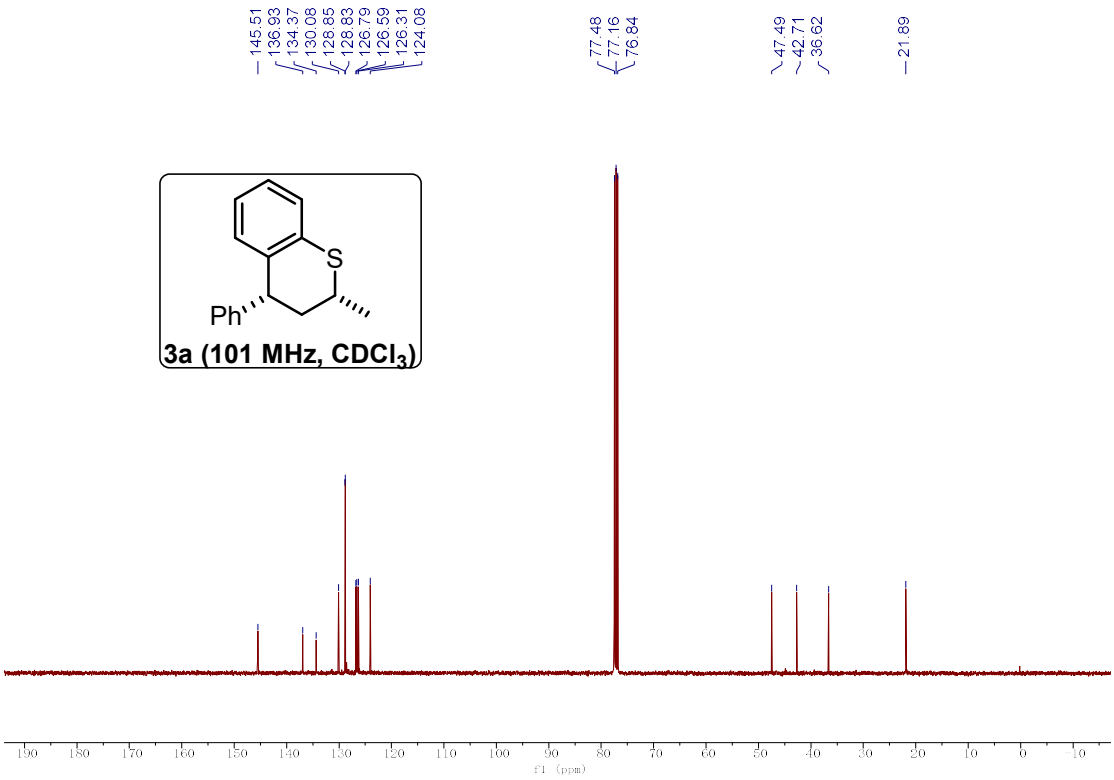
8. NMR Spectra

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134.37
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128.85
128.83
126.79
126.59
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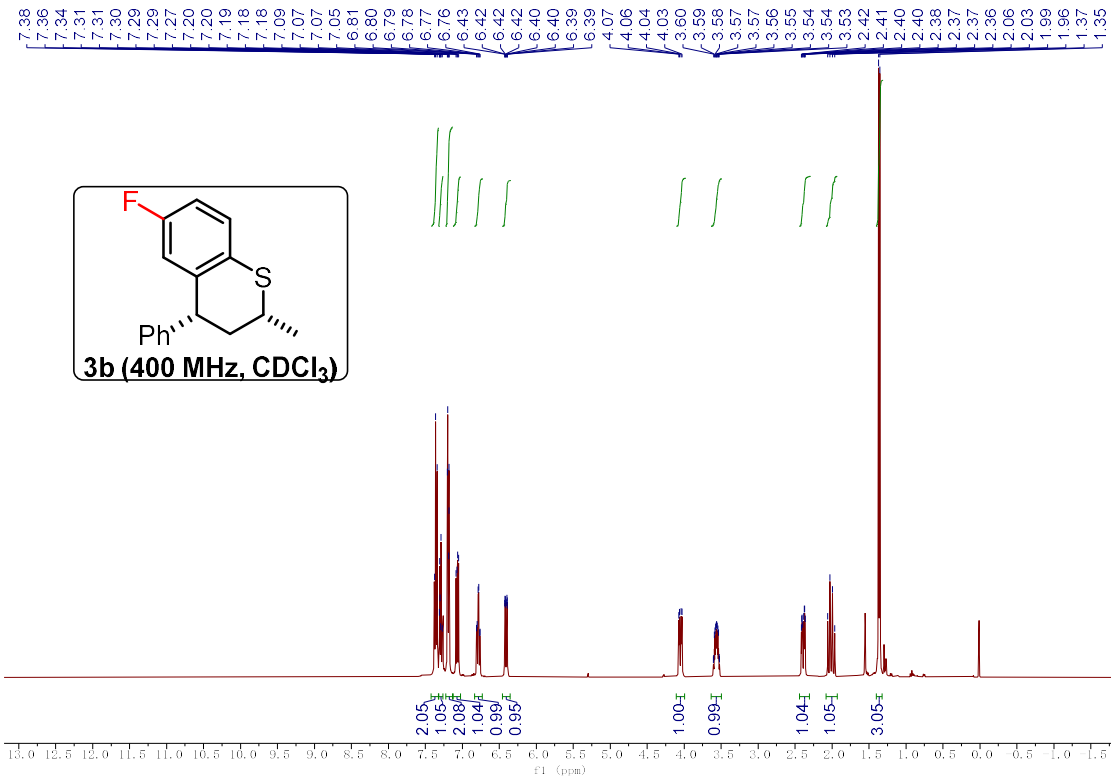
124.08
77.48
77.16
76.84
47.49
42.71
36.62
21.89
S
Ph
3a (101 MHz, CDCl3)
f1 (ppm)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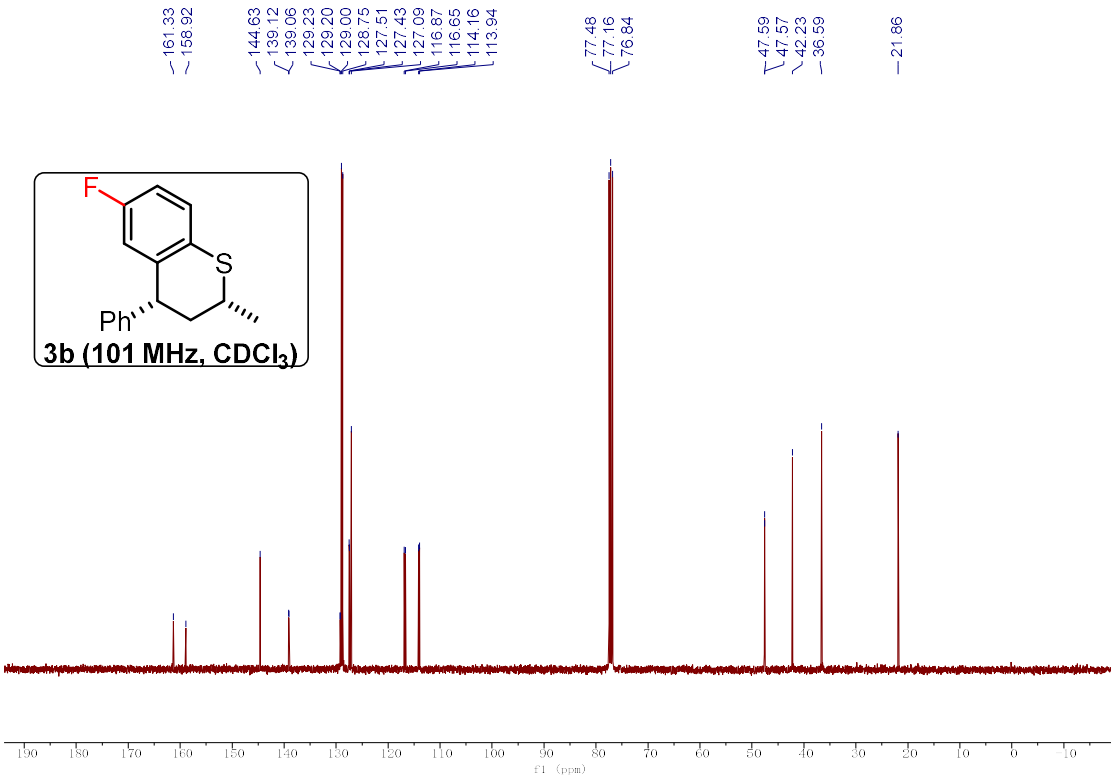
7.36
7.34
7.31
7.31
7.30
7.29
7.29
7.27
7.20
7.20
7.19
7.18
7.18
7.09
7.07
7.07
7.05
6.81
6.80
6.79
6.78
6.77
6.76
6.43
6.42
6.42
6.42
6.40
6.40
6.39
6.39
4.07
4.06
4.04
4.03
3.60
3.59
3.58
3.57
3.57
3.56
3.55
3.54
3.54
3.53
2.42
2.41
2.40
2.40
2.38
2.37
2.37
2.36
2.06
2.03
1.99
1.96
1.37
1.35
F
S
Ph
3b (400 MHz, CDCl3)
2.05
1.05
2.08
1.04
0.99
0.95
1.00
0.99
1.04
1.05
3.05
f1 (ppm)


161.33
158.92
144.63
139.12
139.06
129.23
129.20
129.00
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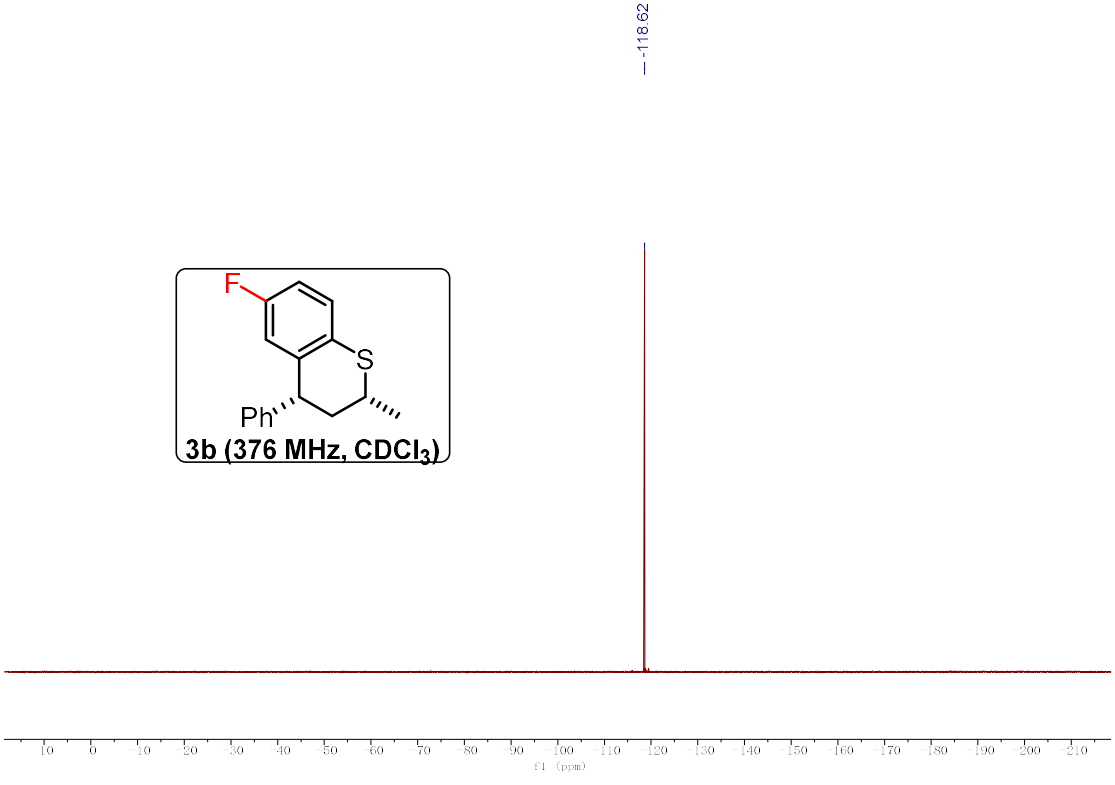
127.51
127.43
127.09
116.87
116.65
114.16
113.94
77.48
77.16
76.84
47.59
47.57
42.23
36.59
21.86
F
S
Ph
3b (101 MHz, CDCl3)
f1 (ppm)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F
S
Ph
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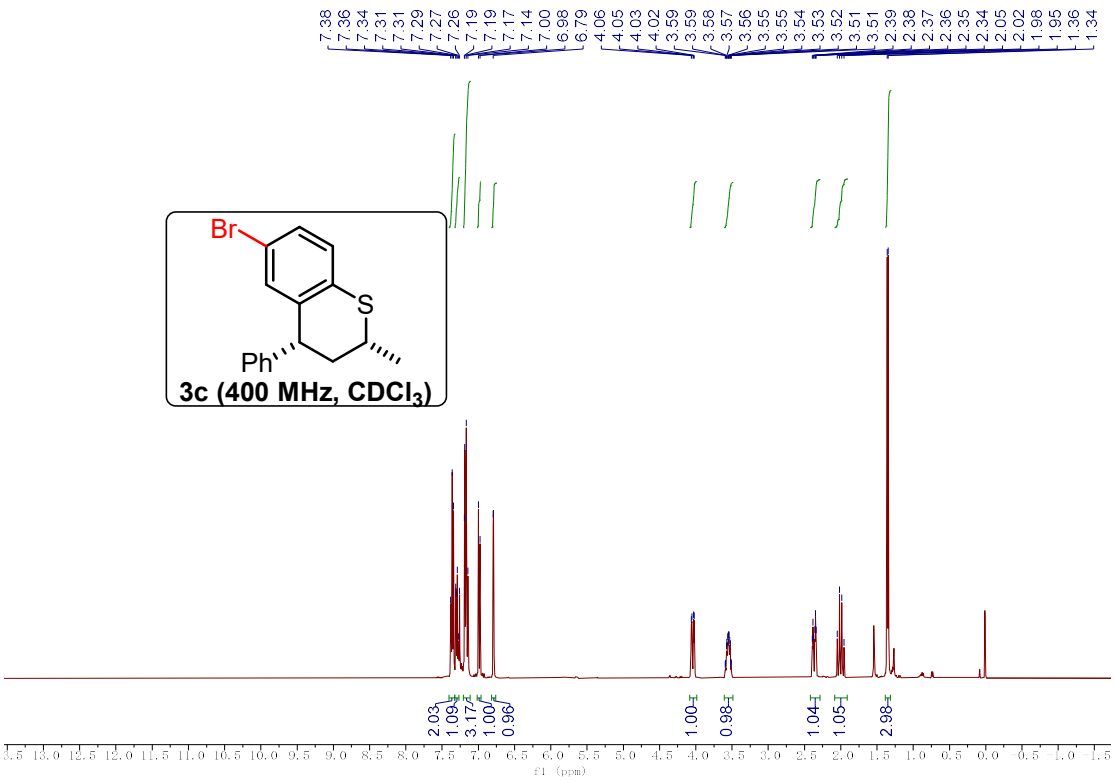
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7.31
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7.26
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7.19
7.17
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6.98
6.79
4.06
4.05
4.03
4.02
3.59
3.59
3.58
3.57
3.56
3.55
3.55
3.54
3.53
3.52
3.51
3.51
2.39
2.38
2.37
2.36
2.35
2.34
2.05
2.02
1.98
1.95
1.36
1.34
Br
S
Ph
3c (400 MHz, CDCl3)
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1.09
3.17
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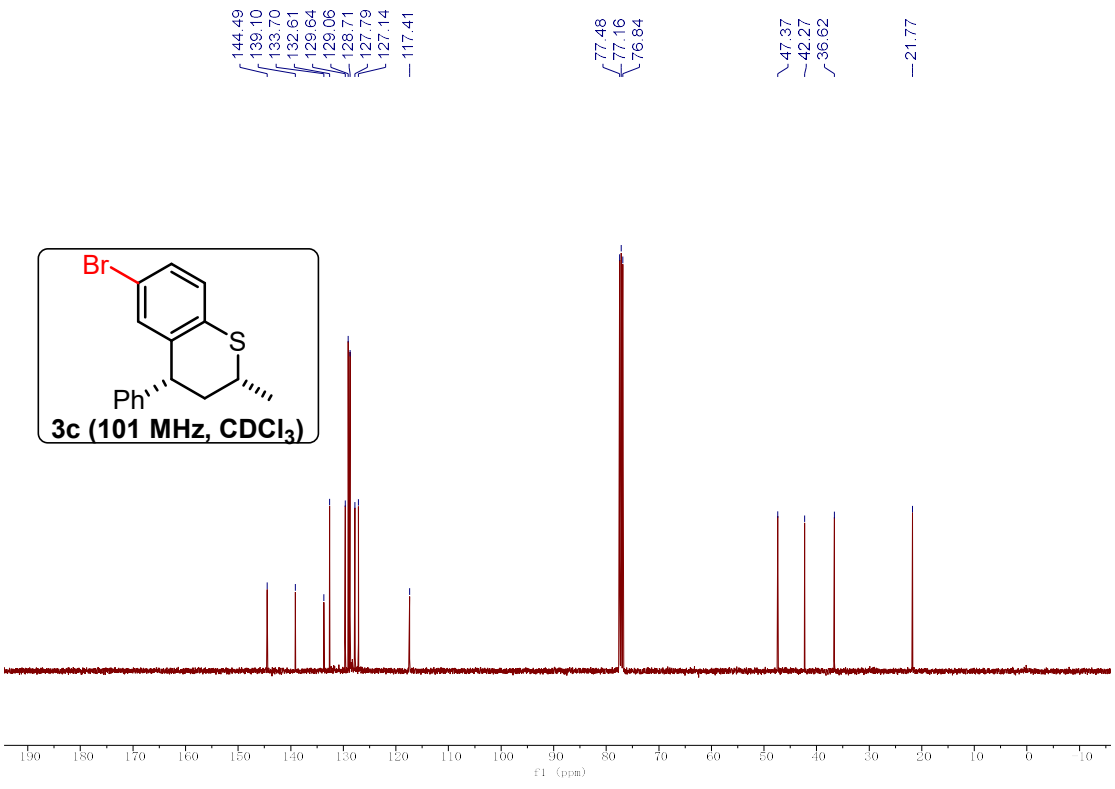
1.04
1.05
2.98
f1 (ppm)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127.79
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117.41
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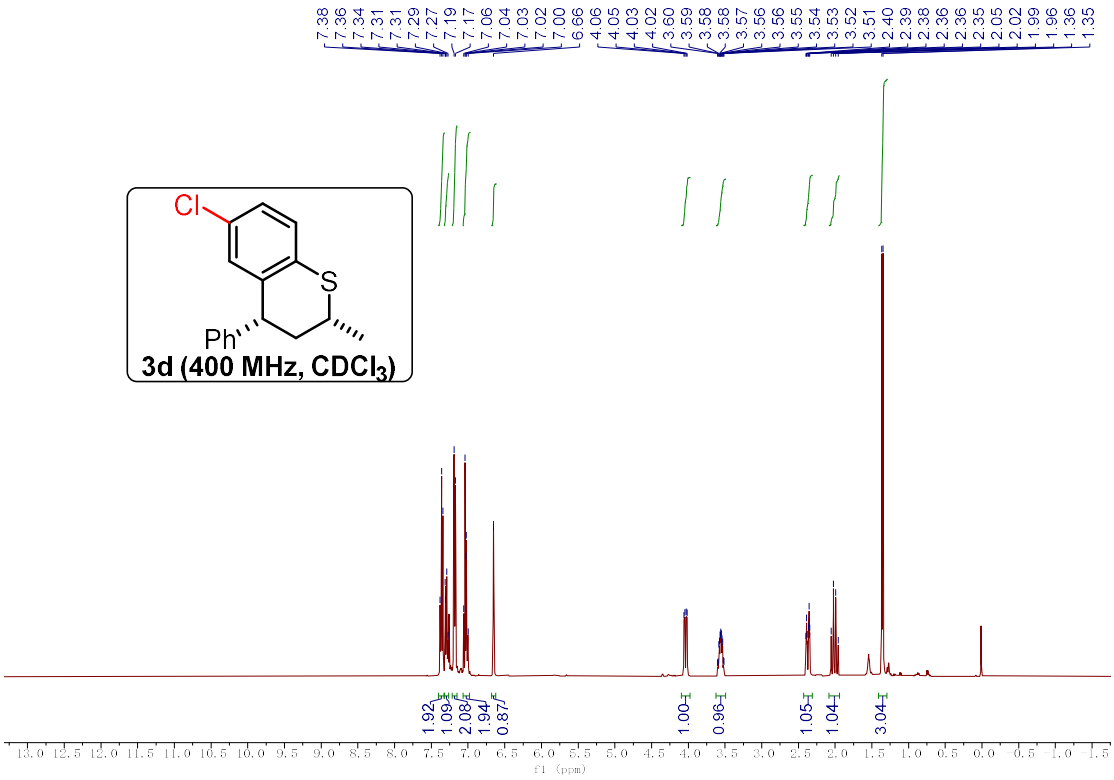
47.37
42.27
36.62
21.77
Br
S
Ph
3c (101 MHz, CDCl3)
f1 (ppm)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7.27
7.19
7.17
7.06
7.04
7.03
7.02
7.00
6.66
4.06
4.05
4.03
4.02
3.60
3.59
3.58
3.58
3.57
3.56
3.56
3.55
3.54
3.53
3.52
3.51
2.40
2.39
2.38
2.36
2.36
2.35
2.05
2.02
1.99
1.96
1.36
1.35
Cl
S
Ph
3d (400 MHz, CDCl3)
1.92
1.09
2.08
1.94
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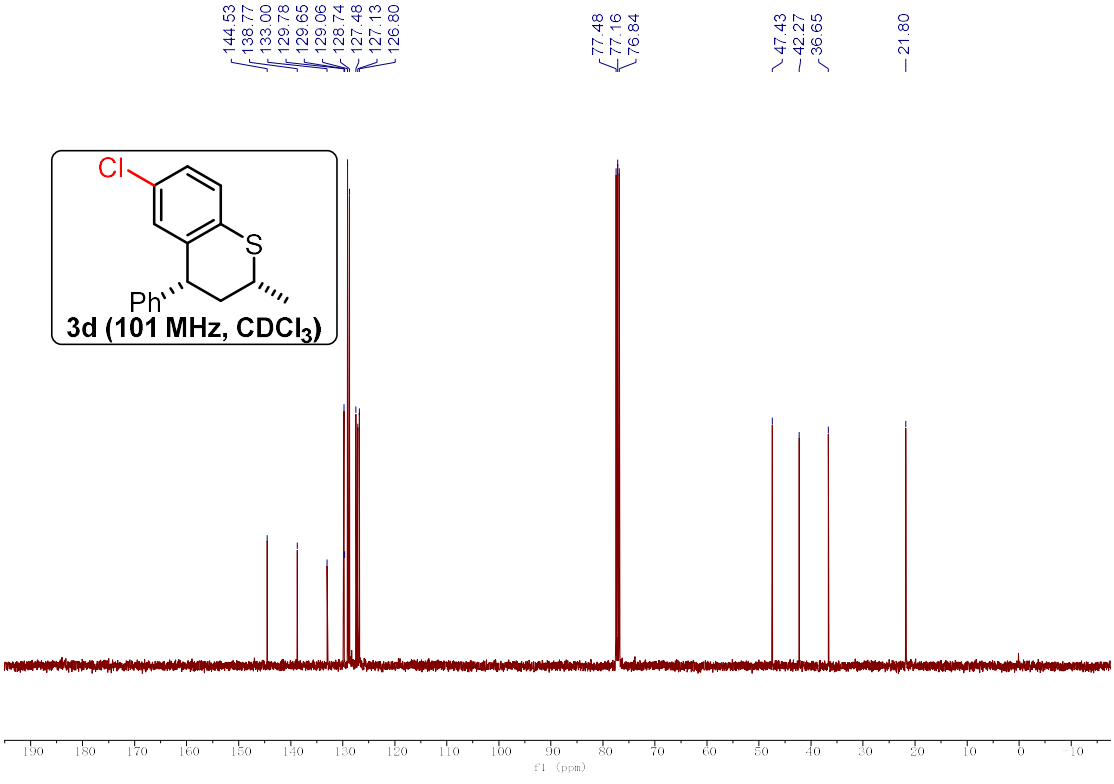
1.00
0.96
1.05
1.04
3.04
f1 (ppm)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77.16
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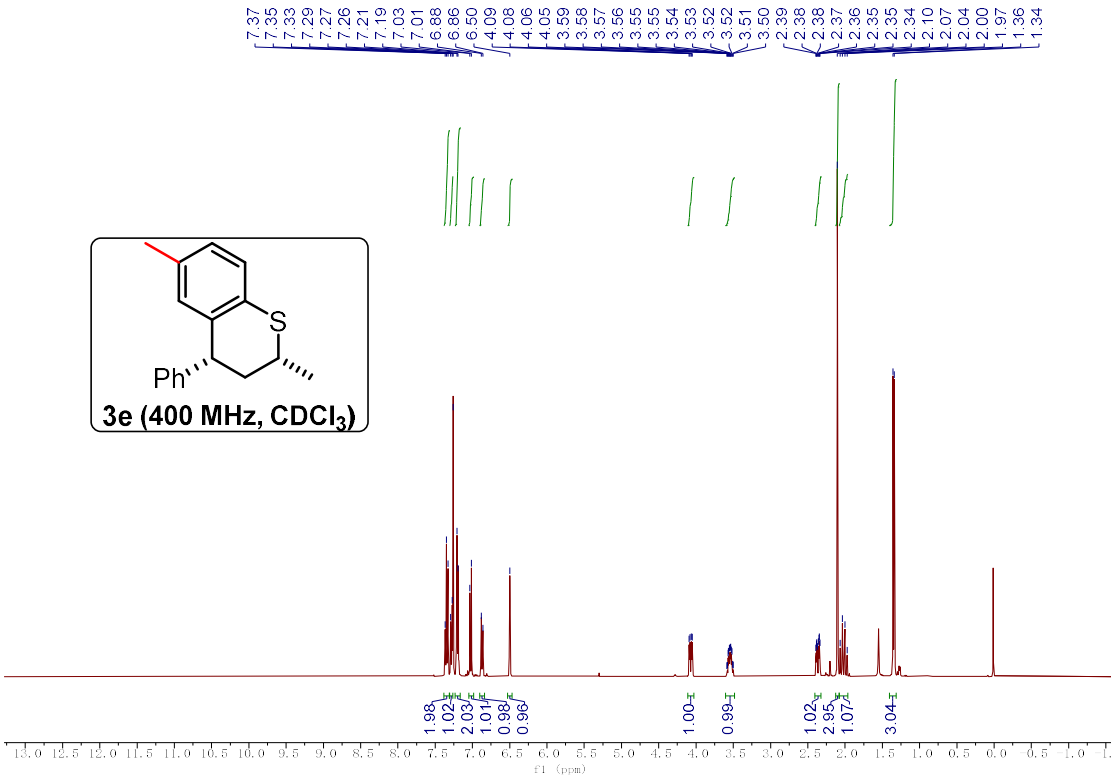
47.43
42.27
36.65
21.80
Cl
S
Ph
3d (101 MHz, CDCl3)
f1 (ppm)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7.19
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2.36
2.35
2.35
2.34
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2.00
1.97
1.36
1.34
S
Ph
3e (400 MHz, CDCl3)
1.98
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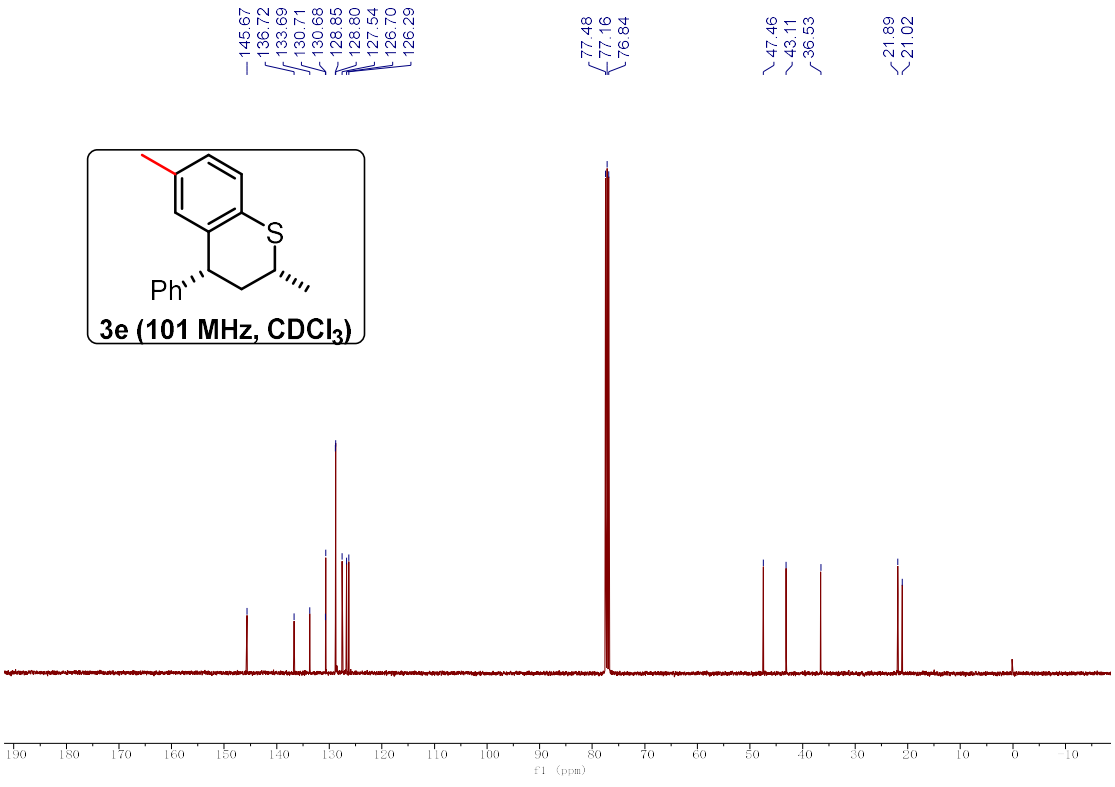
3.04
f1 (ppm)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126.29
77.48
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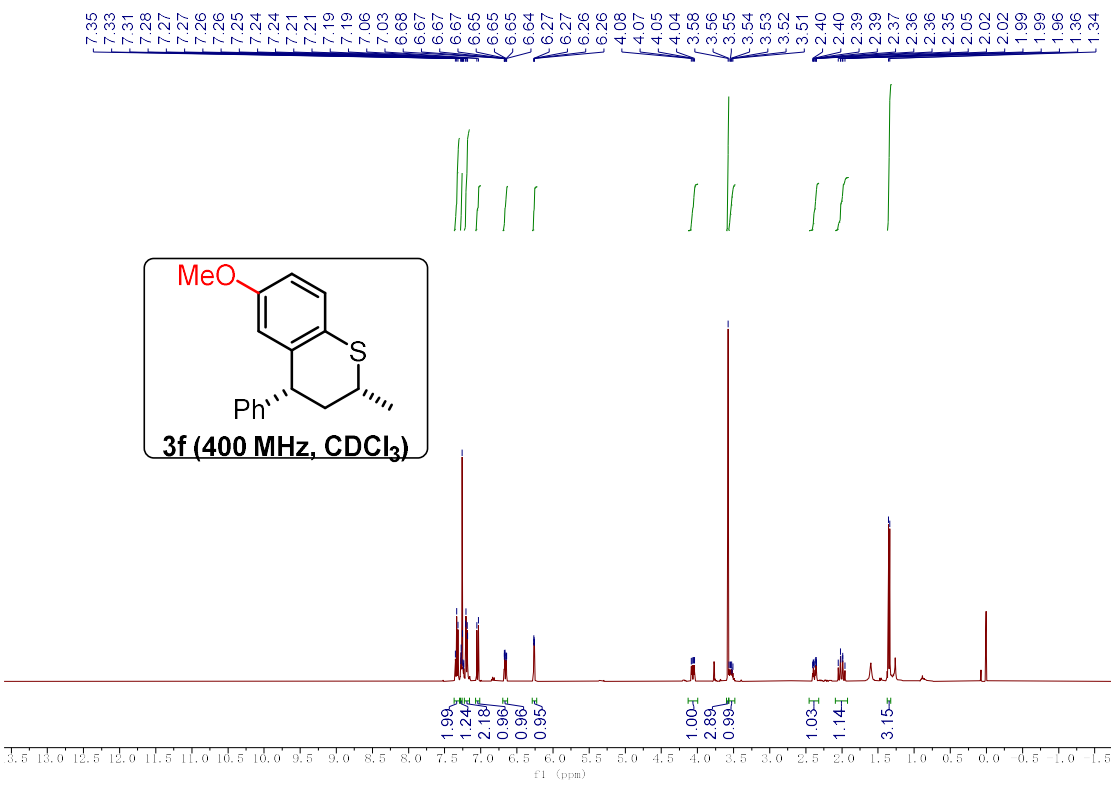
76.84
47.46
43.11
36.53
21.89
21.02
S
Ph
3e (101 MHz, CDCl3)
f1 (ppm)


MeO
S
Ph
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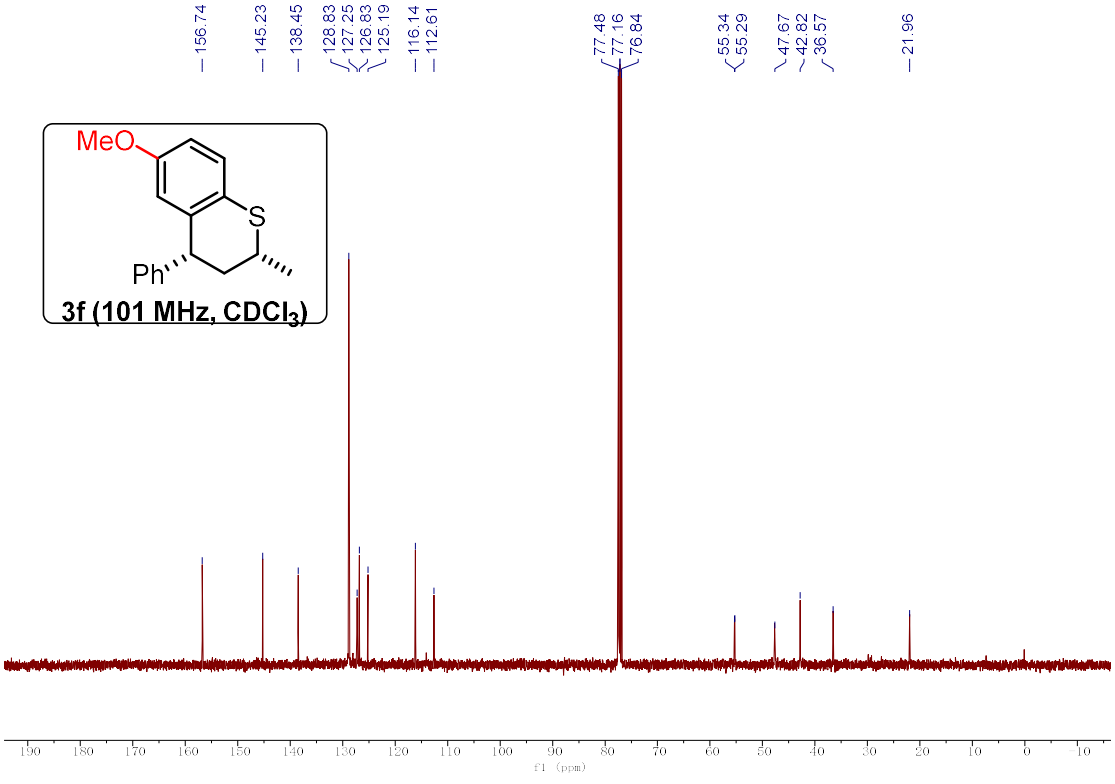
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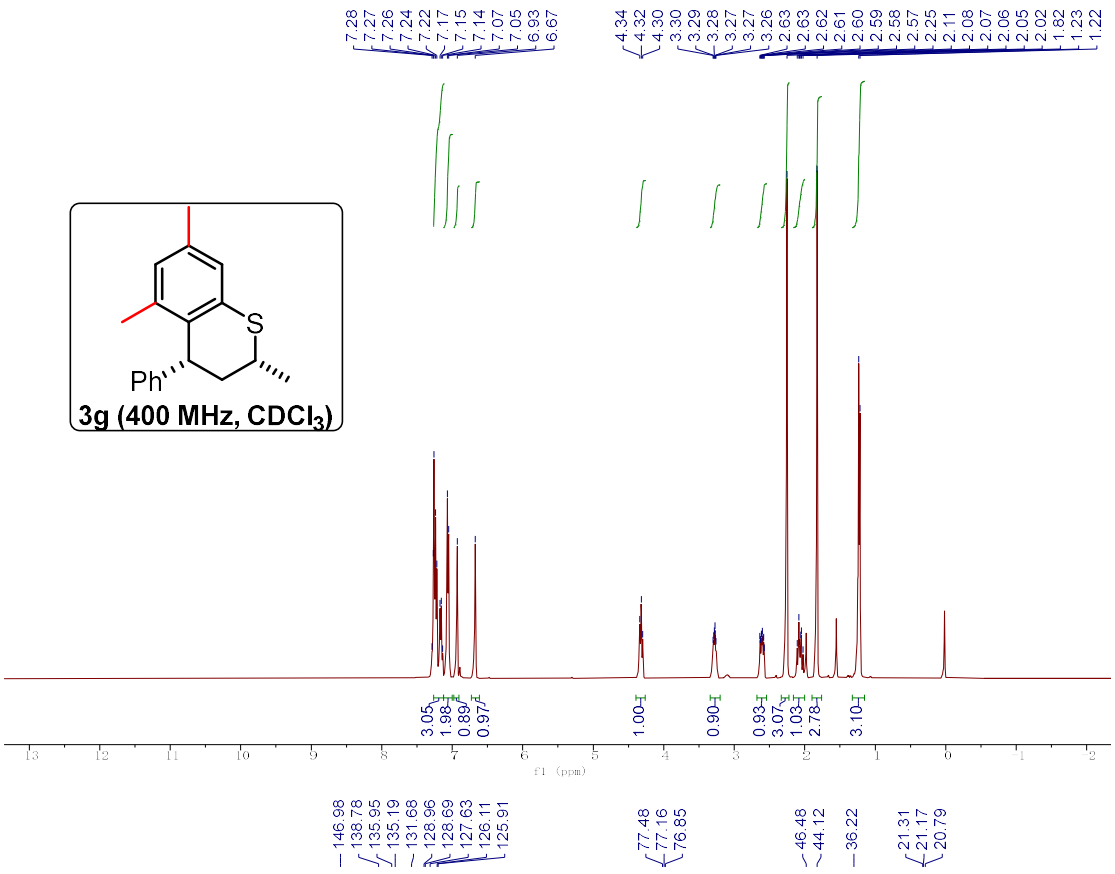
S
Ph
3f (101 MHz, CDCl3)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7.05
6.93
6.67
4.34
4.32
4.30
3.30
3.29
3.28
3.27
3.27
3.26
2.63
2.63
2.62
2.61
2.60
2.59
2.58
2.57
2.25
2.11
2.08
2.07
2.06
2.05
2.02
1.82
1.23
1.22
S
Ph
3g (400 MHz, CDCl3)
3.05
1.98
0.89
0.97
1.00
0.90
0.93
3.07
1.03
2.78
3.10
f1 (ppm)

146.98
138.78
135.95
135.19
131.68
128.96
128.69
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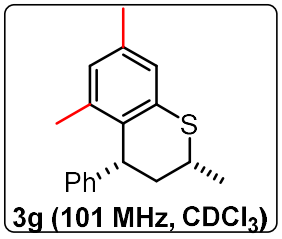
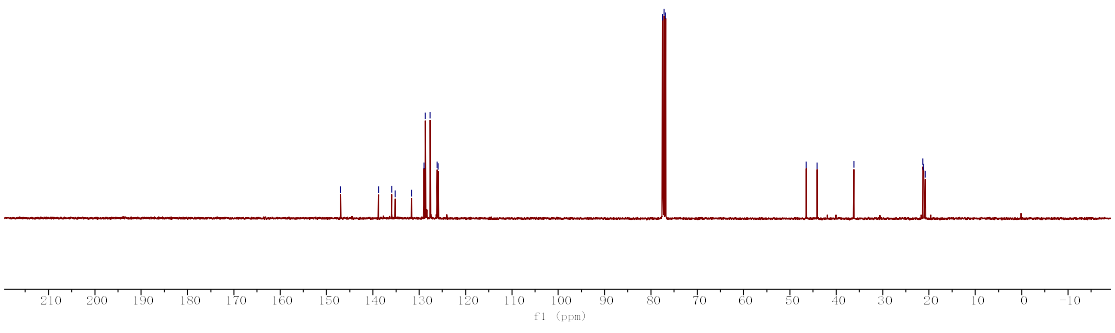
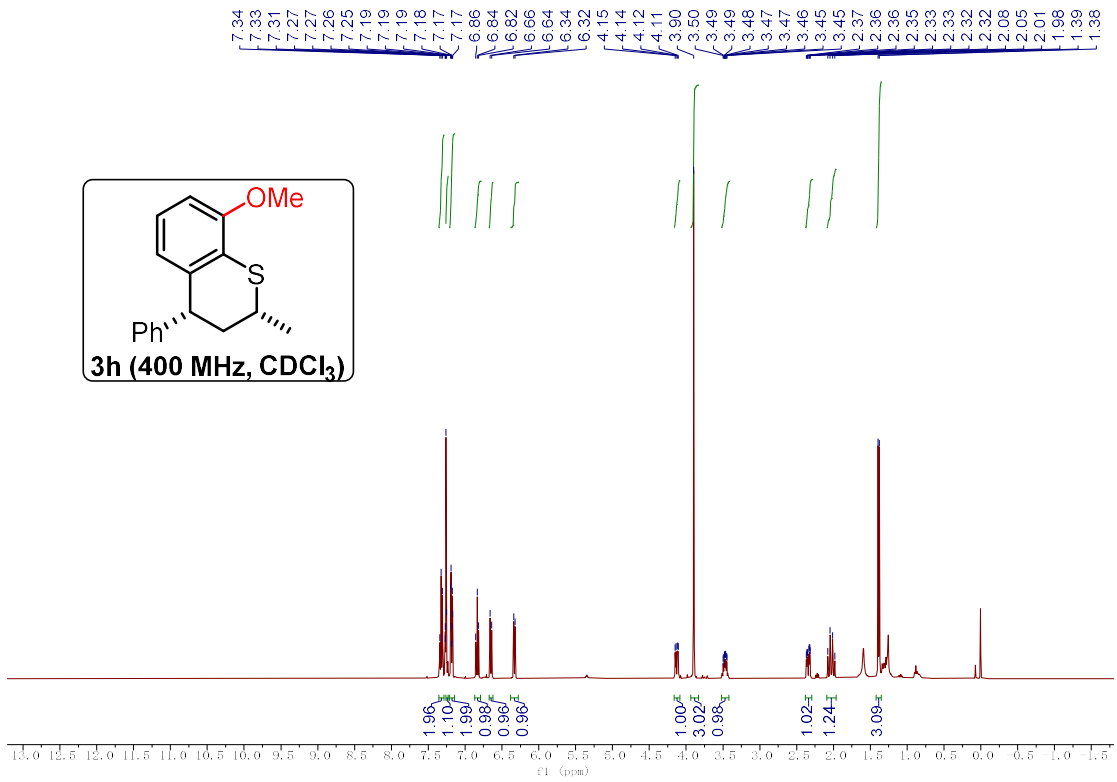

S
Ph
3g (101 MHz, CDCl3)


f1 (ppm)


OMe
S
Ph
3h (400 MHz, CDCl3)
7.34 7.33 7.31 7.27 7.27 7.26 7.25 7.19 7.19 7.19 7.18 7.17 7.17 6.86 6.84 6.82 6.66 6.64 6.34 6.32 4.15 4.14 4.12 4.11 3.90 3.50 3.49 3.49 3.48 3.47 3.47 3.46 3.45 3.45 2.37 2.36 2.36 2.35 2.33 2.33 2.32 2.32 2.08 2.05 2.01 1.98 1.39 1.38
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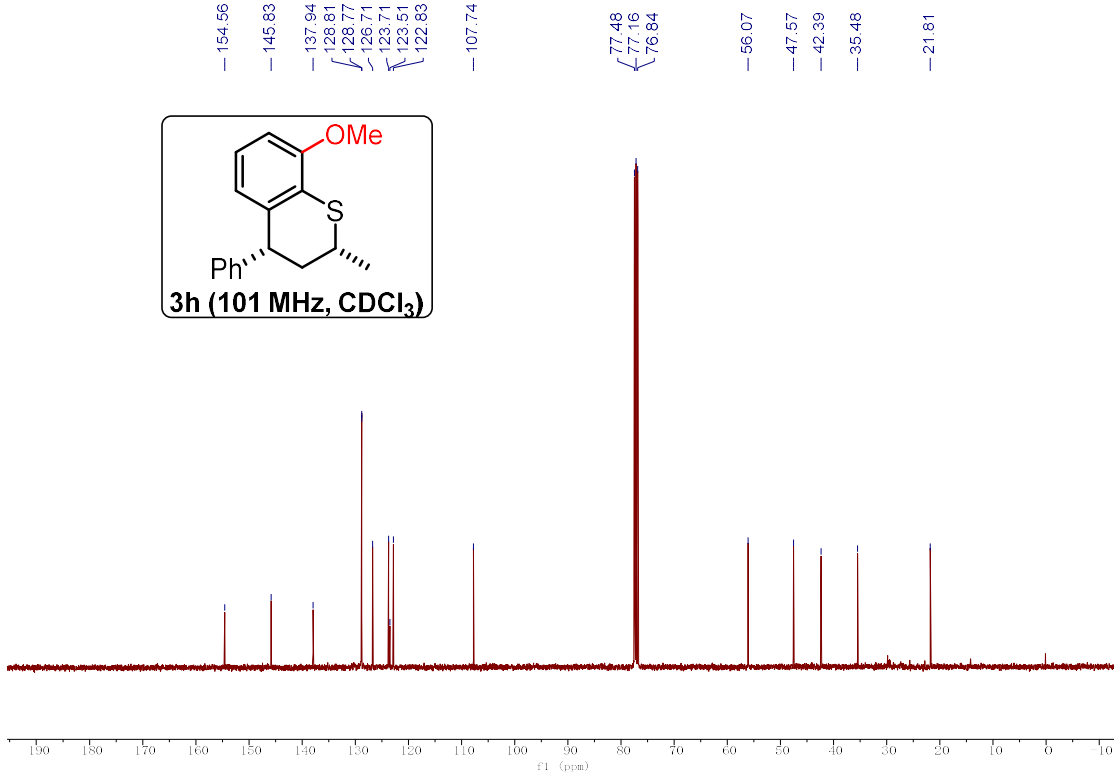
f1 (ppm)


OMe
S
Ph
3h (101 MHz, CDCl3)
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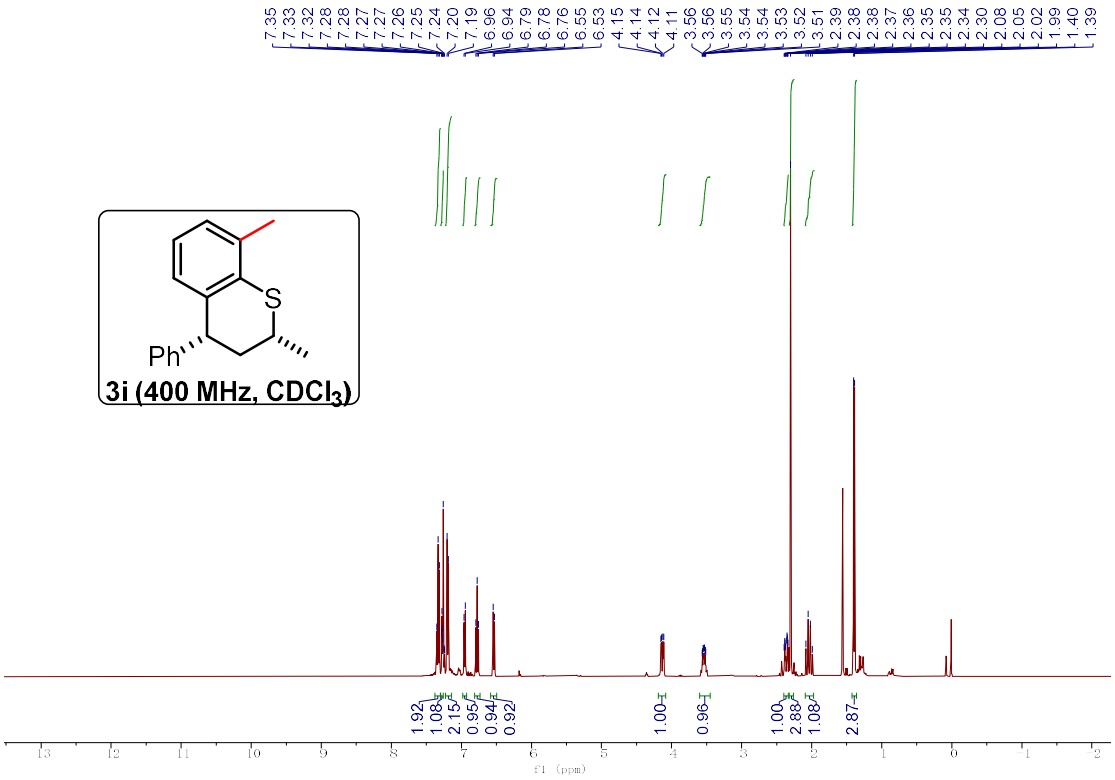
f1 (ppm)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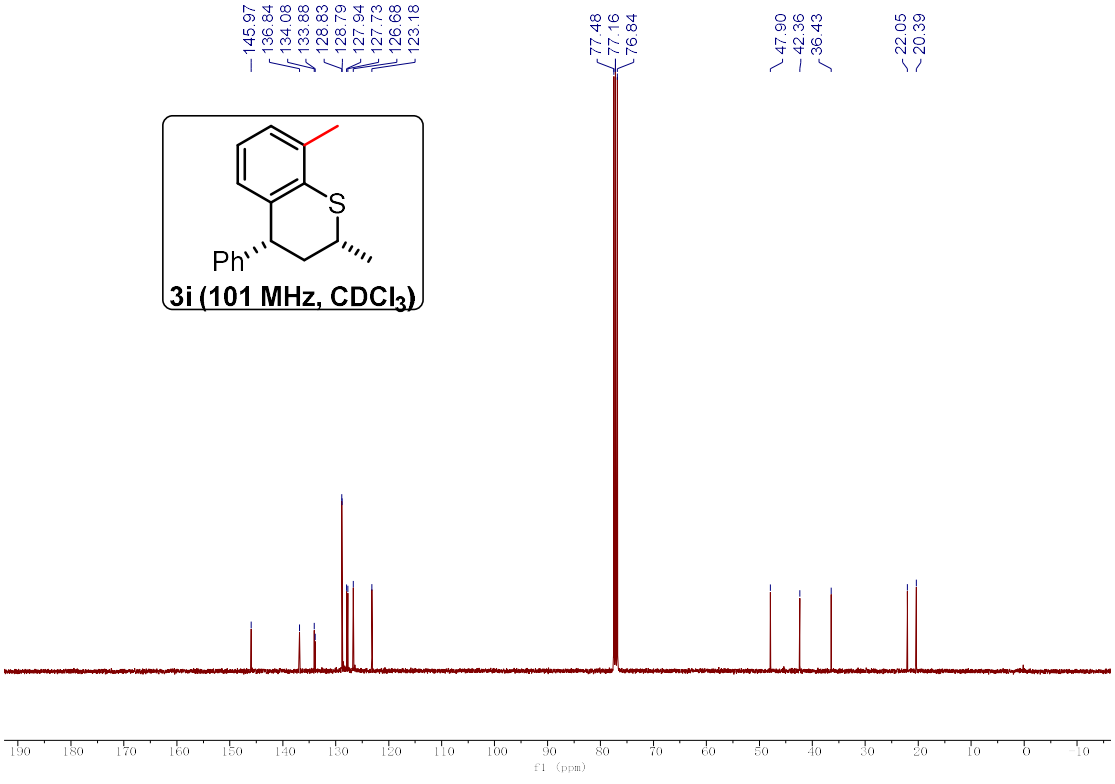
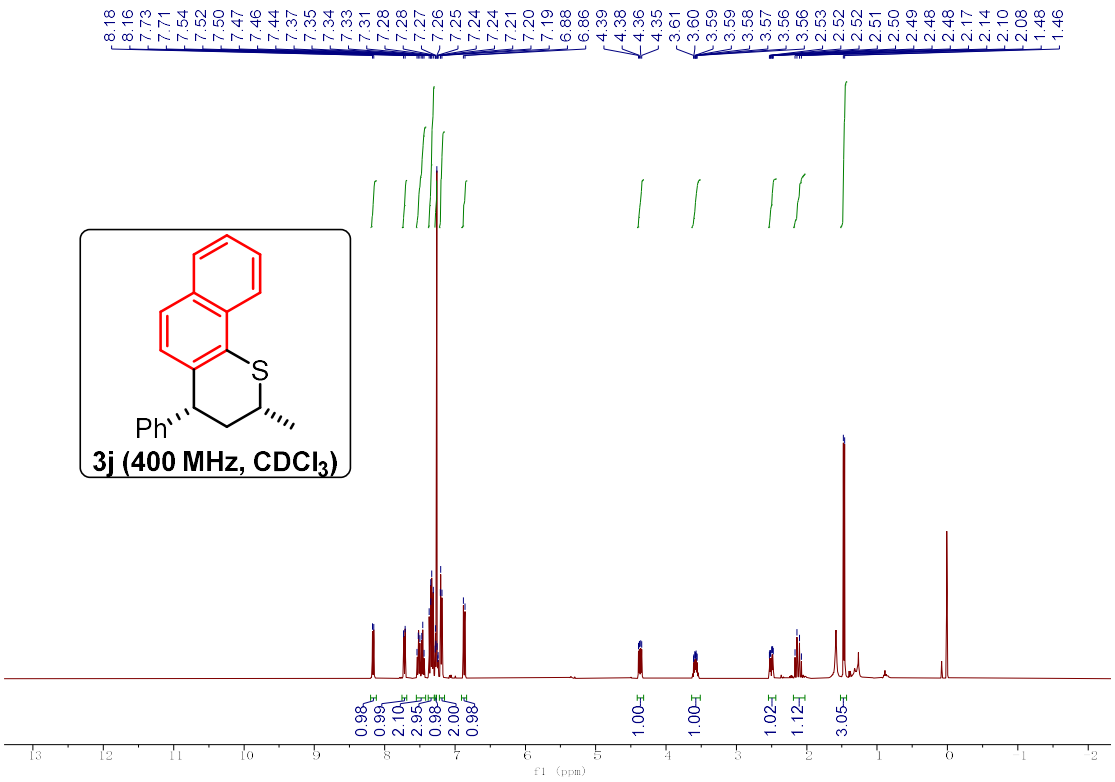
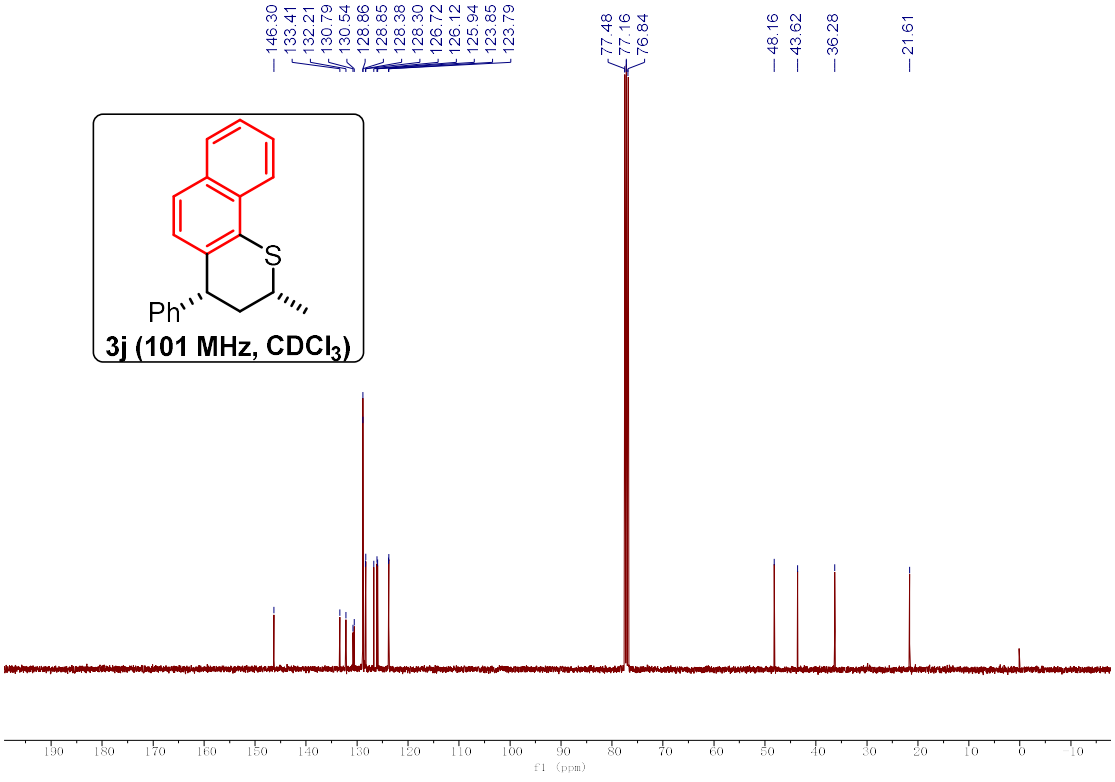
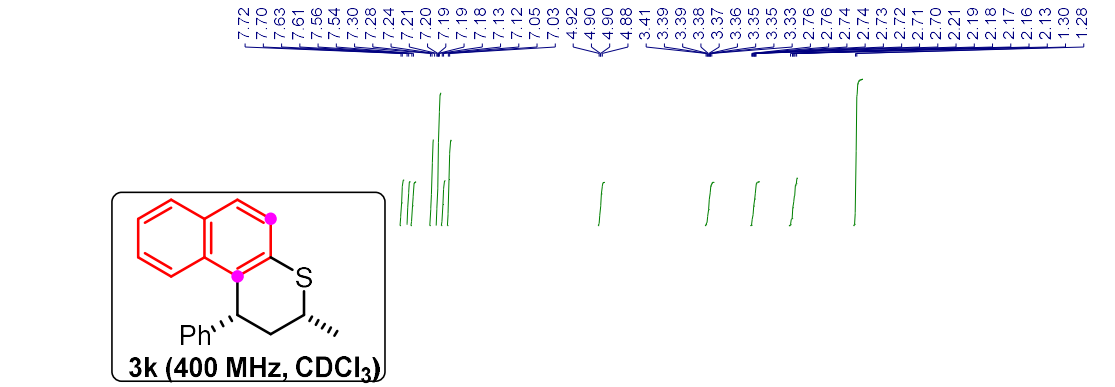
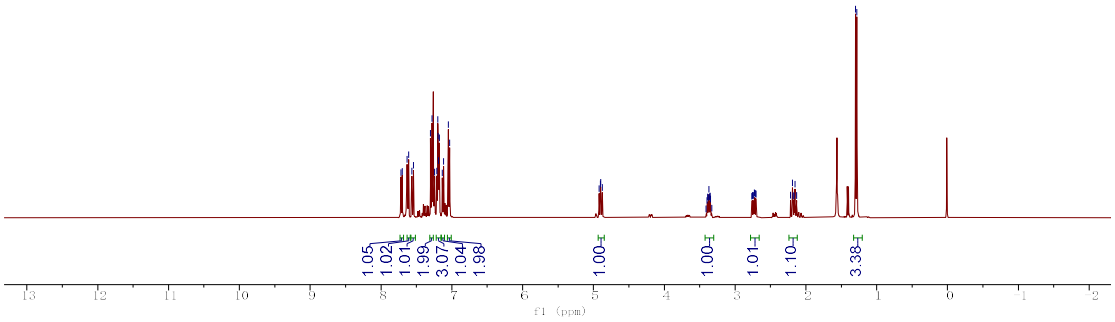
7.32
7.28
7.28
7.27
7.27
7.26
7.25
7.24
7.20
7.19
6.96
6.94
6.79
6.78
6.76
6.55
6.53
4.15
4.14
4.12
4.11
3.56
3.56
3.55
3.54
3.54
3.53
3.52
3.51
2.39
2.38
2.38
2.37
2.36
2.35
2.35
2.34
2.30
2.08
2.05
2.02
1.99
1.40
1.39
S
Ph
3i (400 MHz, CDCl3)
1.92
1.08
2.15
0.95
0.94
0.92
1.00
0.96
1.00
2.88
1.08
2.87
f1 (ppm)

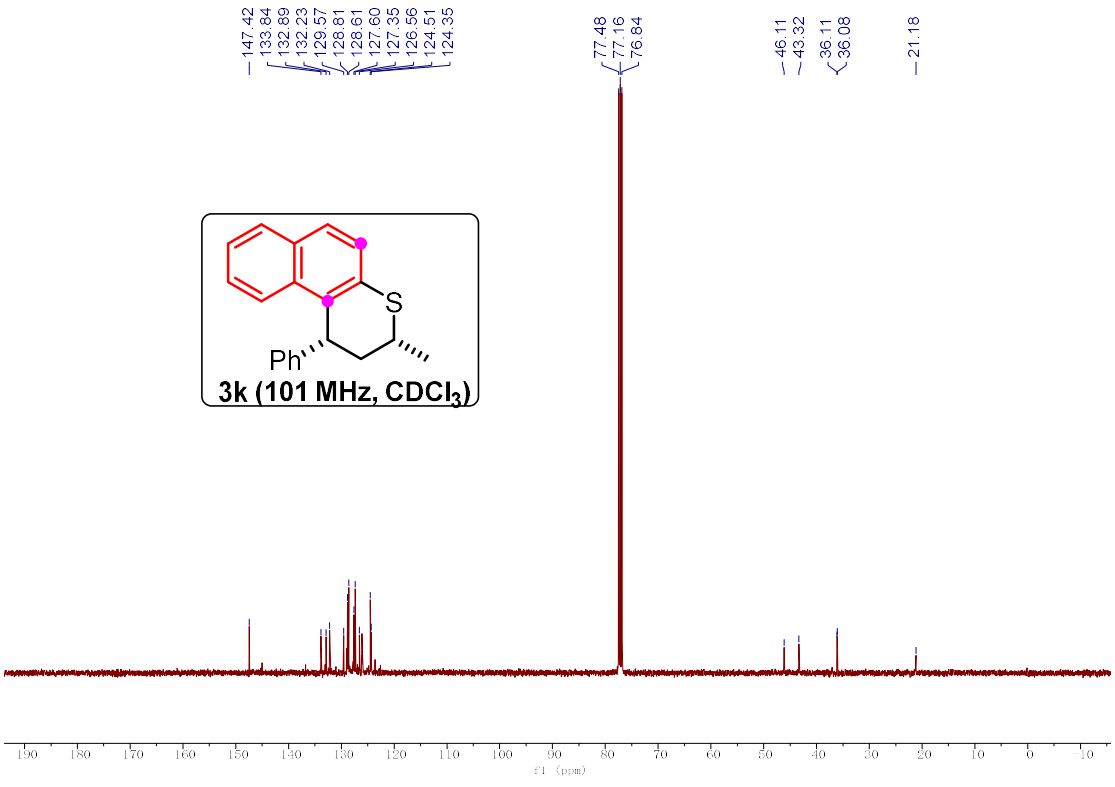

145.97
136.84
134.08
133.88
128.83
128.79
127.94
127.73
126.68
123.18
77.48
77.16
76.84
47.90
42.36
36.43
22.05
20.39
S
Ph
3i (101 MHz, CDCl3)
f1 (ppm)

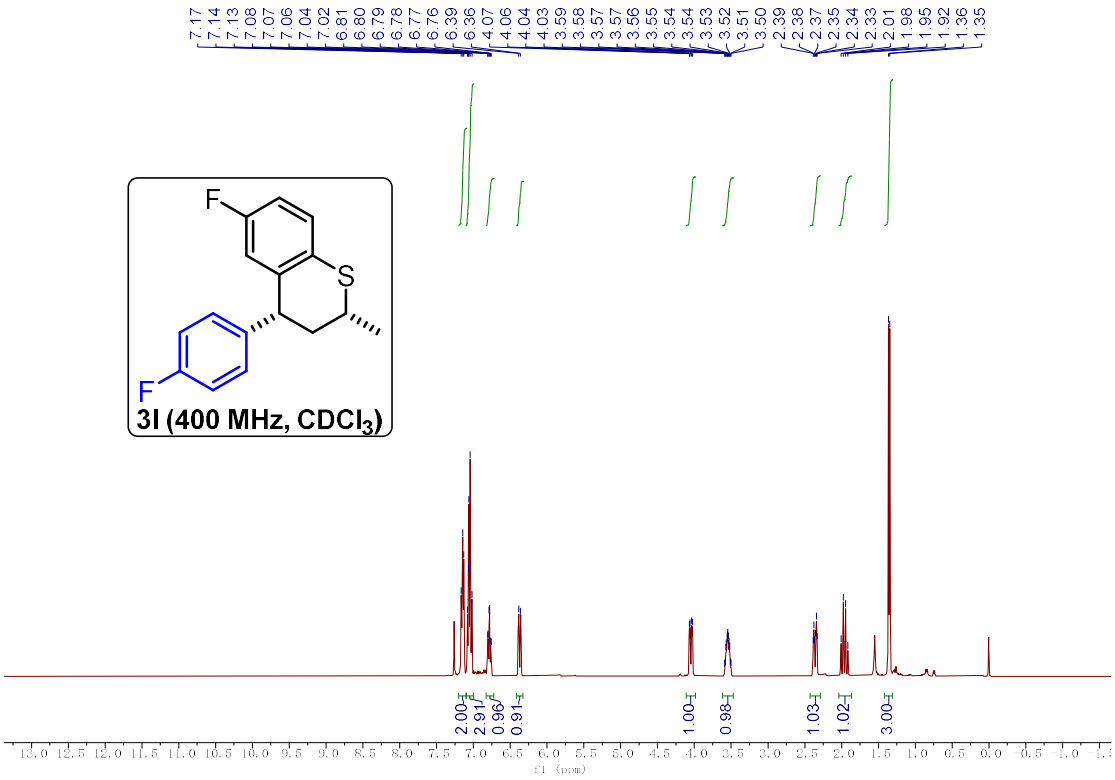

8.18 8.16 7.73 7.71 7.54 7.52 7.50 7.47 7.46 7.44 7.37 7.35 7.34 7.33 7.31 7.28 7.28 7.27 7.26 7.25 7.24 7.24 7.21 7.20 7.19 6.88 6.86 4.39 4.38 4.36 4.35 3.61 3.60 3.59 3.59 3.58 3.57 3.56 3.56 2.53 2.52 2.52 2.51 2.50 2.49 2.48 2.48 2.17 2.14 2.10 2.08 1.48 1.46
S
Ph
3j (400 MHz, CDCl3)
0.98 0.99 2.10 2.95 0.98 2.00 0.98 1.00 1.00 1.02 1.12 3.05
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

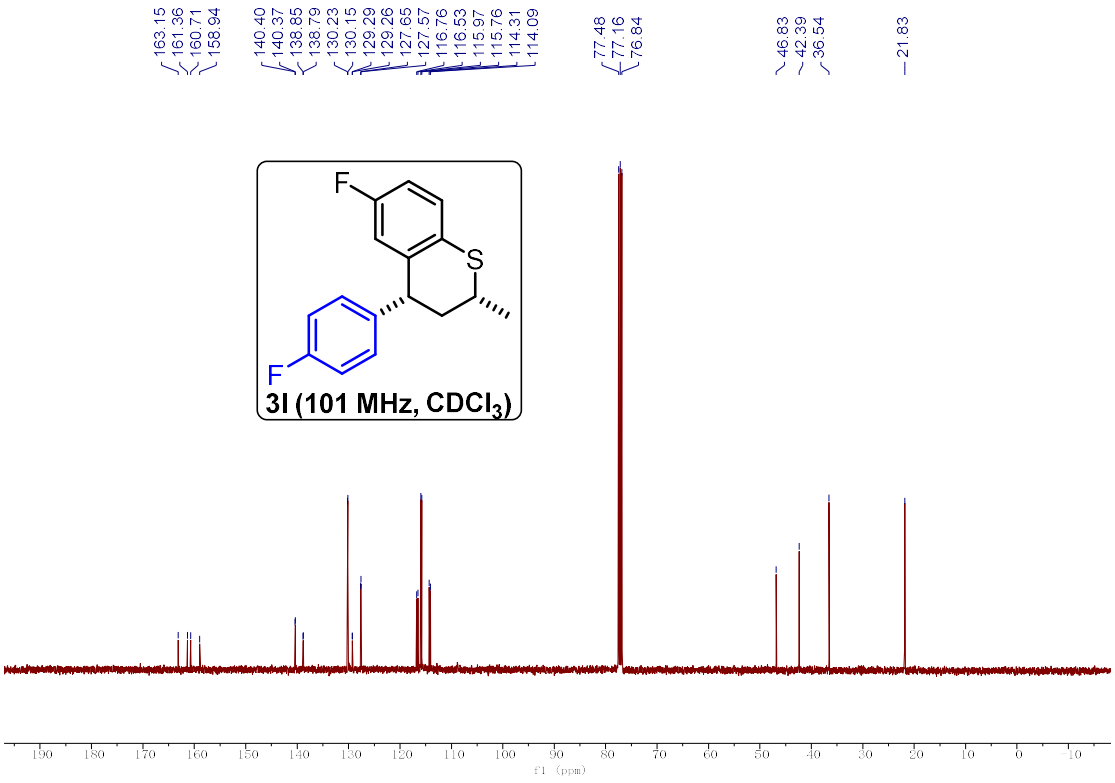

146.30 133.41 132.21 130.79 130.54 128.86 128.85 128.38 128.30 126.72 126.12 125.94 123.85 123.79
77.48 77.16 76.84
48.16 43.62 36.28 21.61
S
Ph
3j (101 MHz, CDCl3)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

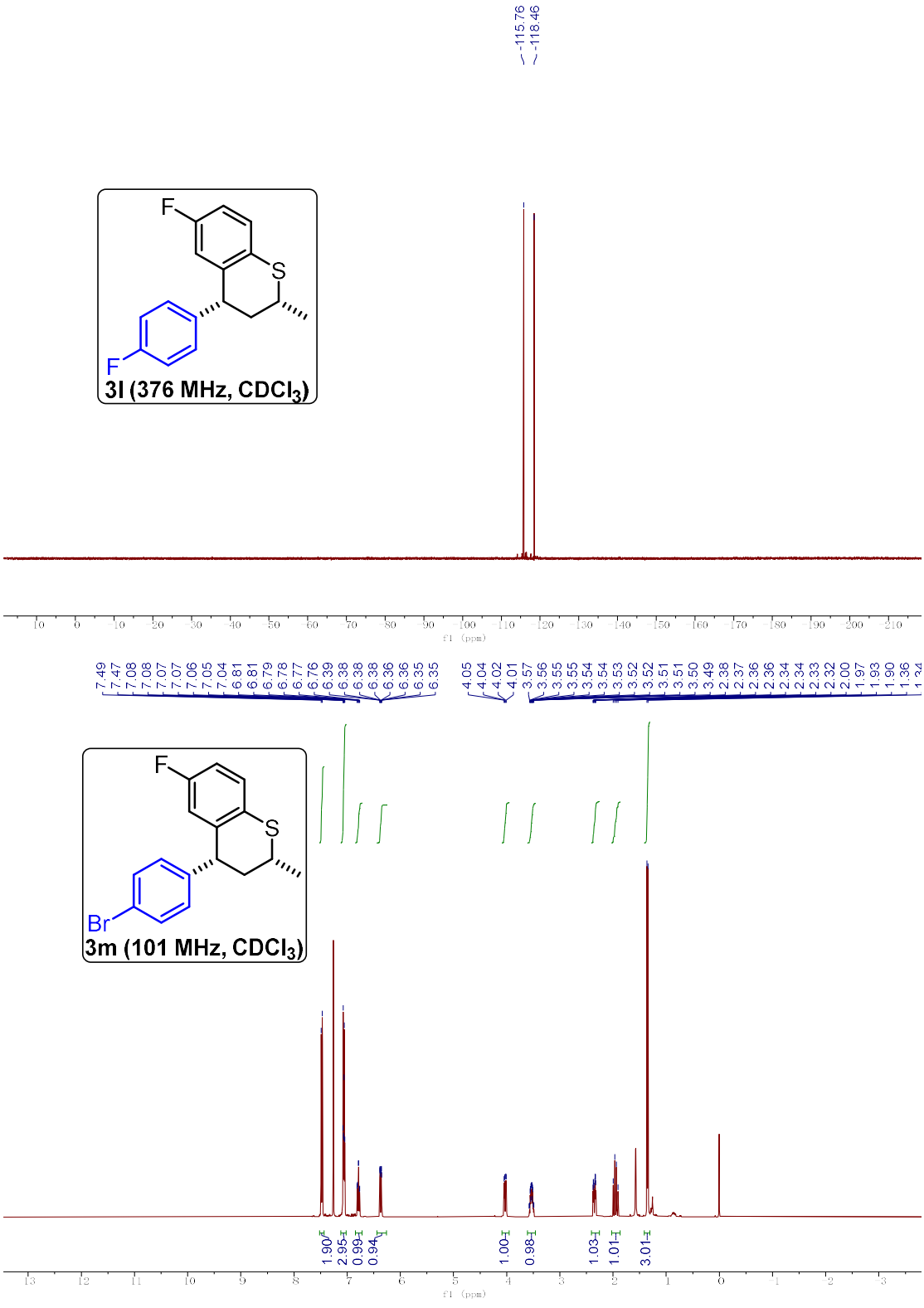

7.72
7.70
7.63
7.61
7.56
7.54
7.30
7.28
7.24
7.21
7.20
7.19
7.19
7.18
7.13
7.12
7.05
7.03
4.92
4.90
4.90
4.88
3.41
3.39
3.39
3.38
3.37
3.36
3.35
3.35
3.33
2.76
2.76
2.74
2.74
2.73
2.72
2.71
2.70
2.21
2.19
2.18
2.17
2.16
2.13
1.30
1.28
S
Ph
3k (400 MHz, CDCl3)

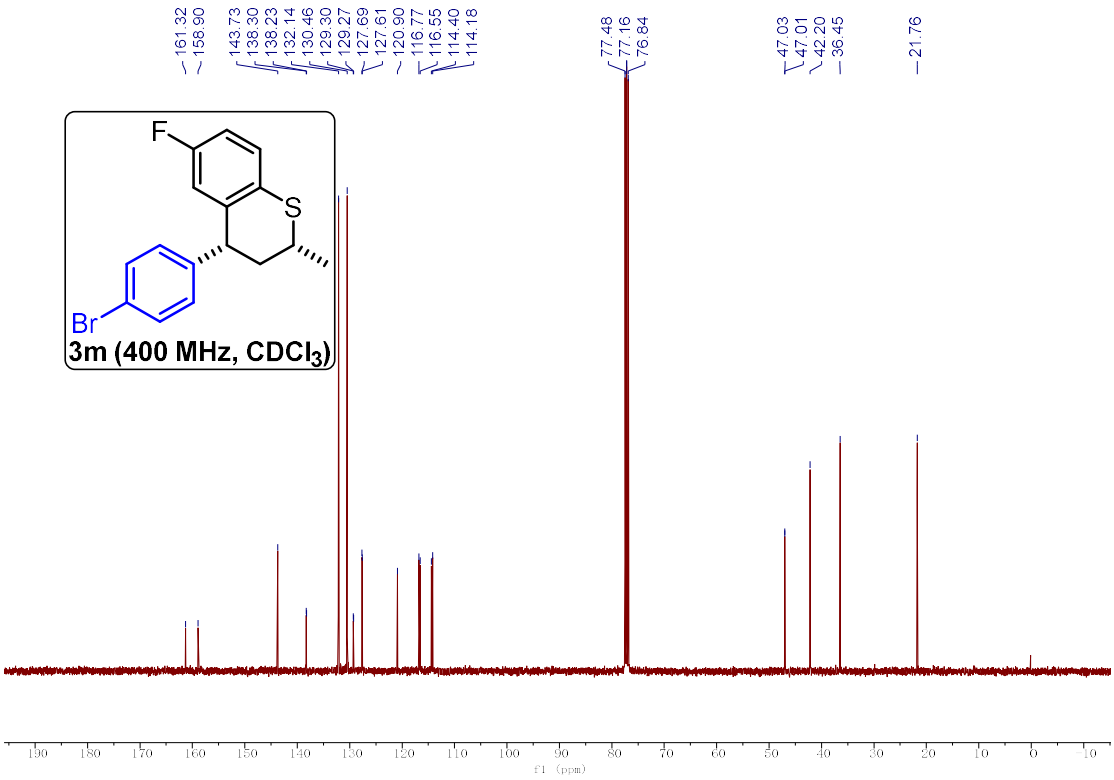

1.05
1.02
1.01
1.99
3.07
1.04
1.98
1.00
1.00
1.01
1.10
3.38
f1 (ppm)

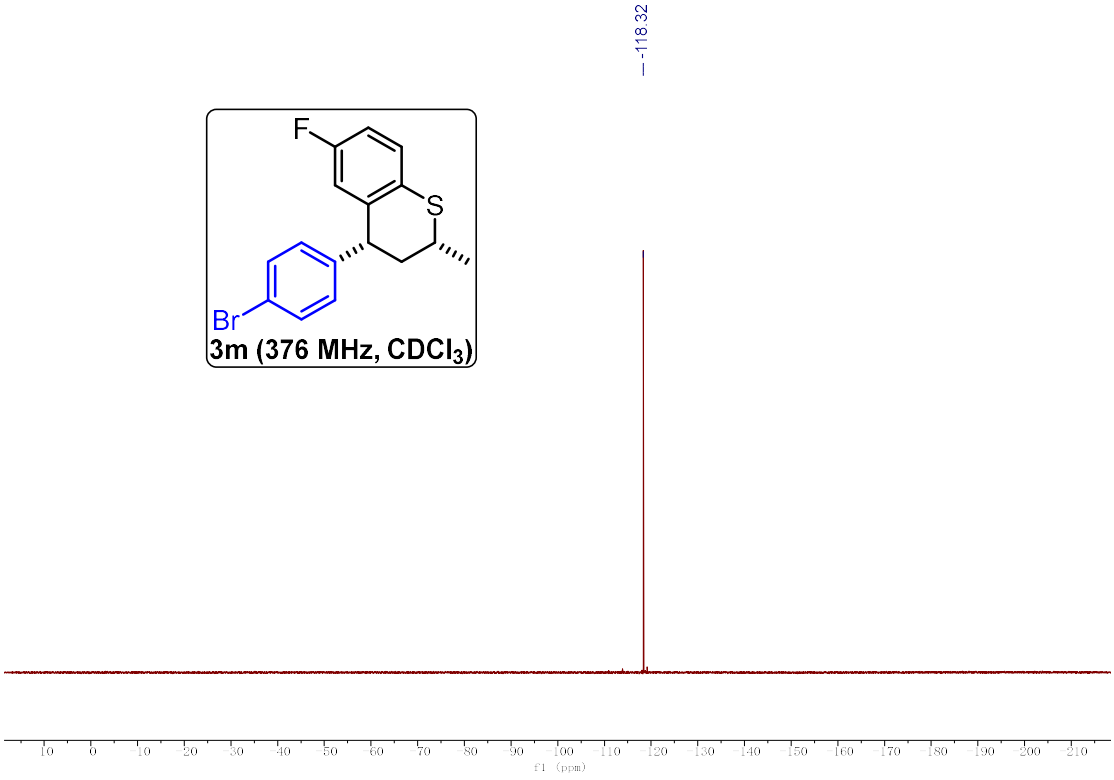

147.42
133.84
132.89
132.23
129.57
128.81
128.61
127.60
127.35
126.56
124.51
124.35
77.48
77.16
76.84
46.11
43.32
36.11
36.08
21.18
S
Ph
3k (101 MHz, CDCl3)
f1 (ppm)

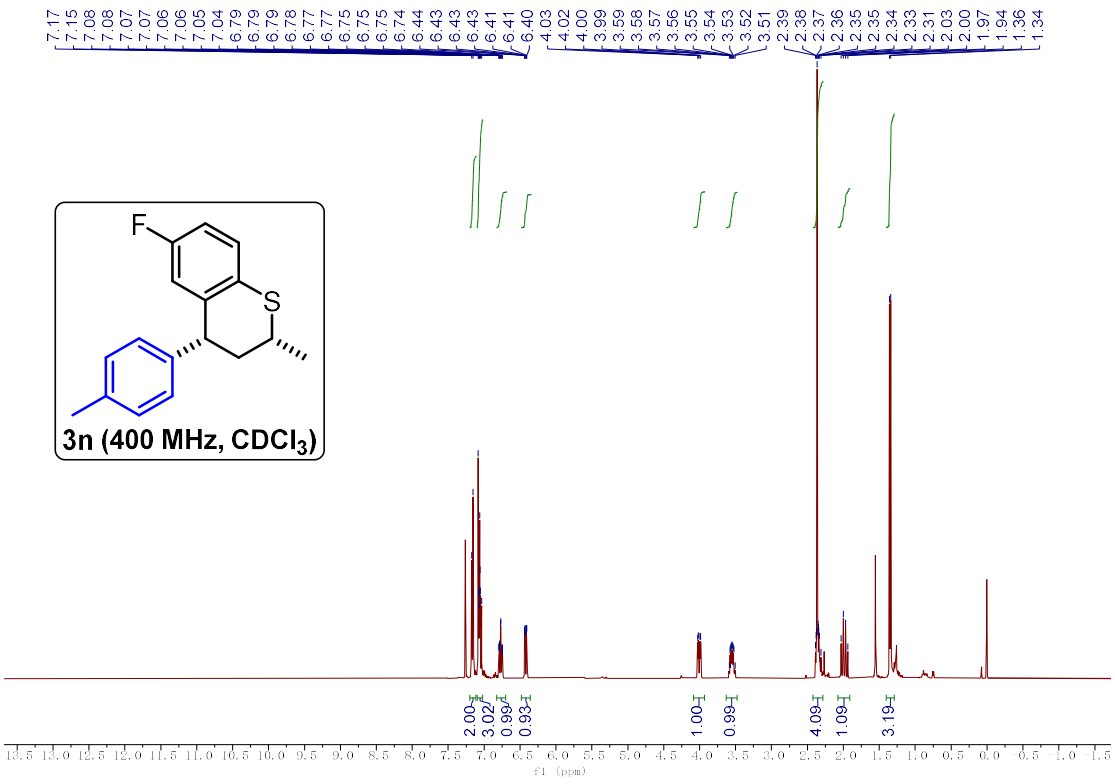

7.17
7.14
7.13
7.08
7.07
7.06
7.04
7.02
6.81
6.80
6.79
6.78
6.77
6.76
6.39
6.36
4.07
4.06
4.04
4.03
3.59
3.58
3.57
3.57
3.56
3.55
3.54
3.54
3.53
3.52
3.51
3.50
2.39
2.38
2.37
2.35
2.34
2.33
2.01
1.98
1.95
1.92
1.36
1.35
F
S
F
3l (400 MHz, CDCl3)
2.00
2.91
0.96
0.91
1.00
0.98
1.03
1.02
3.00
f1 (ppm)

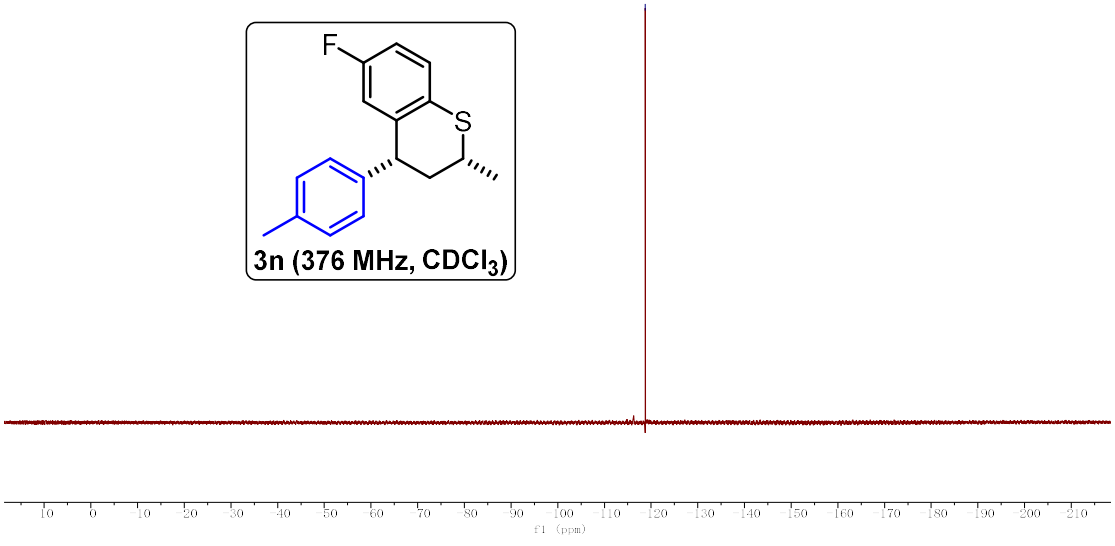

163.15
161.36
160.71
158.94
140.40
140.37
138.85
138.79
130.23
130.15
129.29
129.26
127.65
127.57
116.76
116.53
115.97
115.76
114.31
114.09
77.48
77.16
76.84
46.83
42.39
36.54
21.83
F
S
F
3l (101 MHz, CDCl3)
f1 (ppm)

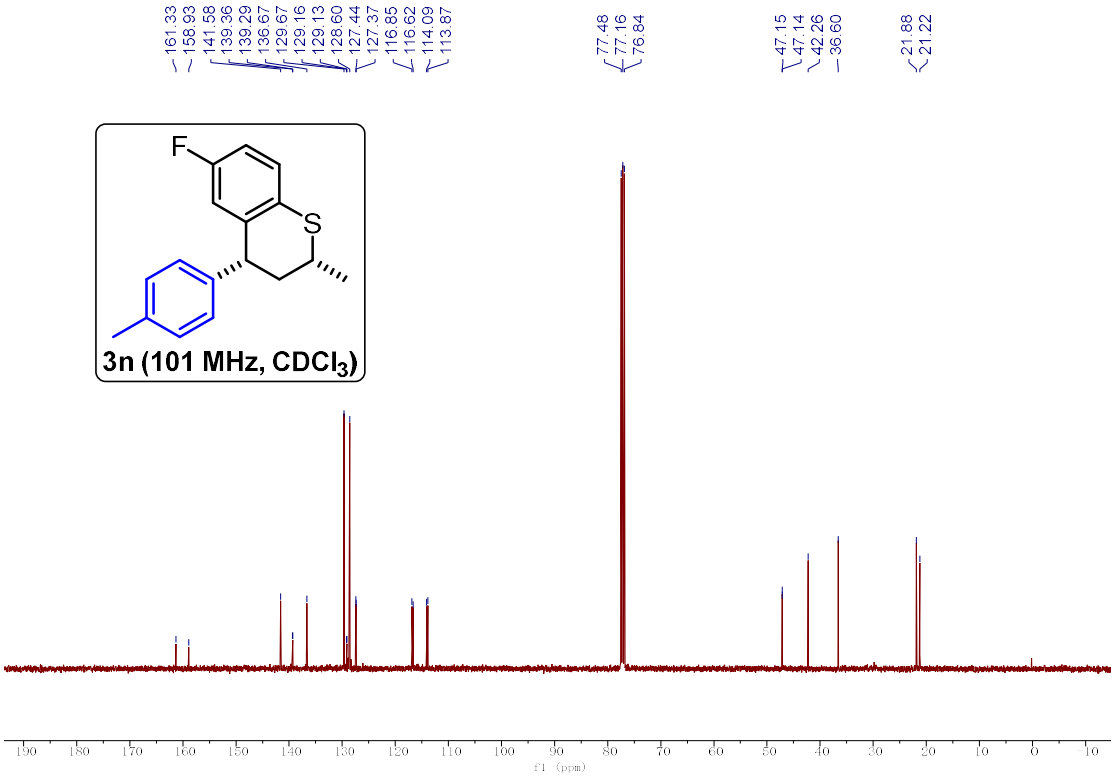

-115.76
-118.46
F
S
F
3l (376 MHz, CDCl3)
f1 (ppm)
7.49
7.47
7.08
7.08
7.07
7.07
7.06
7.05
7.04
6.81
6.81
6.79
6.78
6.77
6.76
6.39
6.38
6.38
6.38
6.36
6.36
6.35
6.35
4.05
4.04
4.02
4.01
3.57
3.56
3.55
3.55
3.54
3.54
3.53
3.52
3.52
3.51
3.51
3.50
3.49
2.38
2.37
2.36
2.36
2.34
2.34
2.33
2.32
2.00
1.97
1.93
1.90
1.36
1.24
F
S
Br
3m (101 MHz, CDCl3)
1.90
2.95
0.99
0.94
1.00
0.98
1.03
1.01
3.01
f1 (ppm)

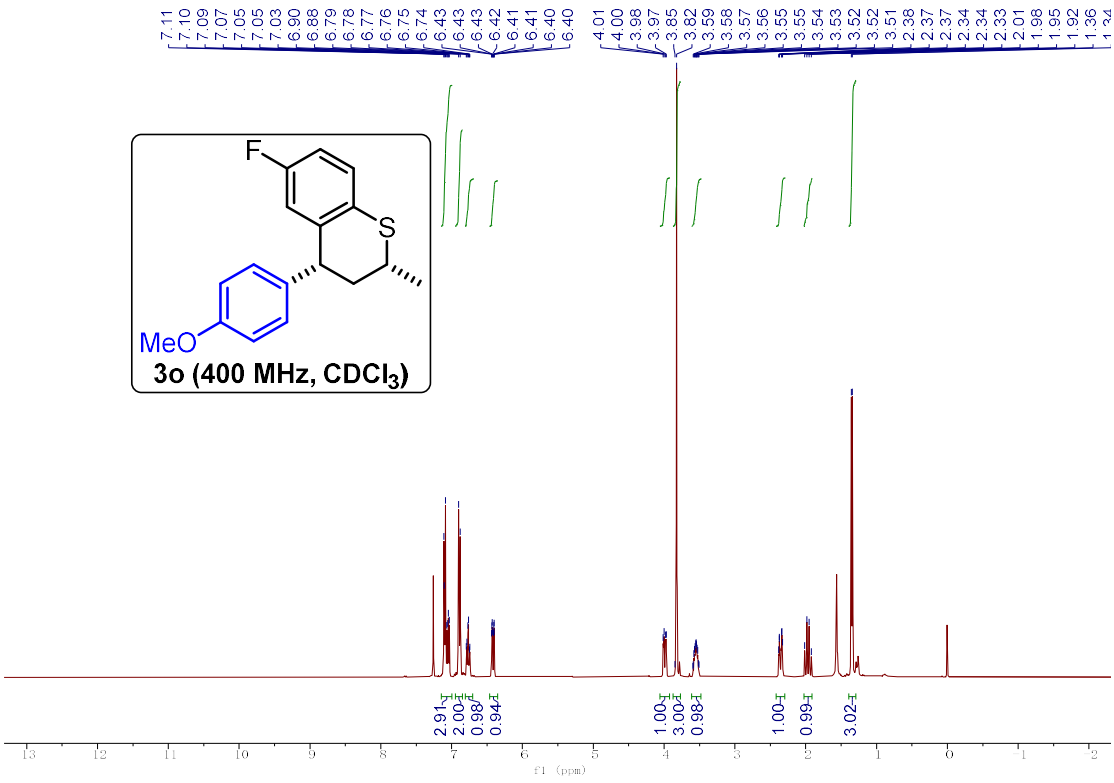

161.32
158.90
143.73
138.30
138.23
132.14
130.46
129.30
129.27
127.69
127.61
120.90
116.77
116.55
114.40
114.18
77.48
77.16
76.84
47.03
47.01
42.20
36.45
21.76
F
S
Br
3m (400 MHz, CDCl3)
f1 (ppm)

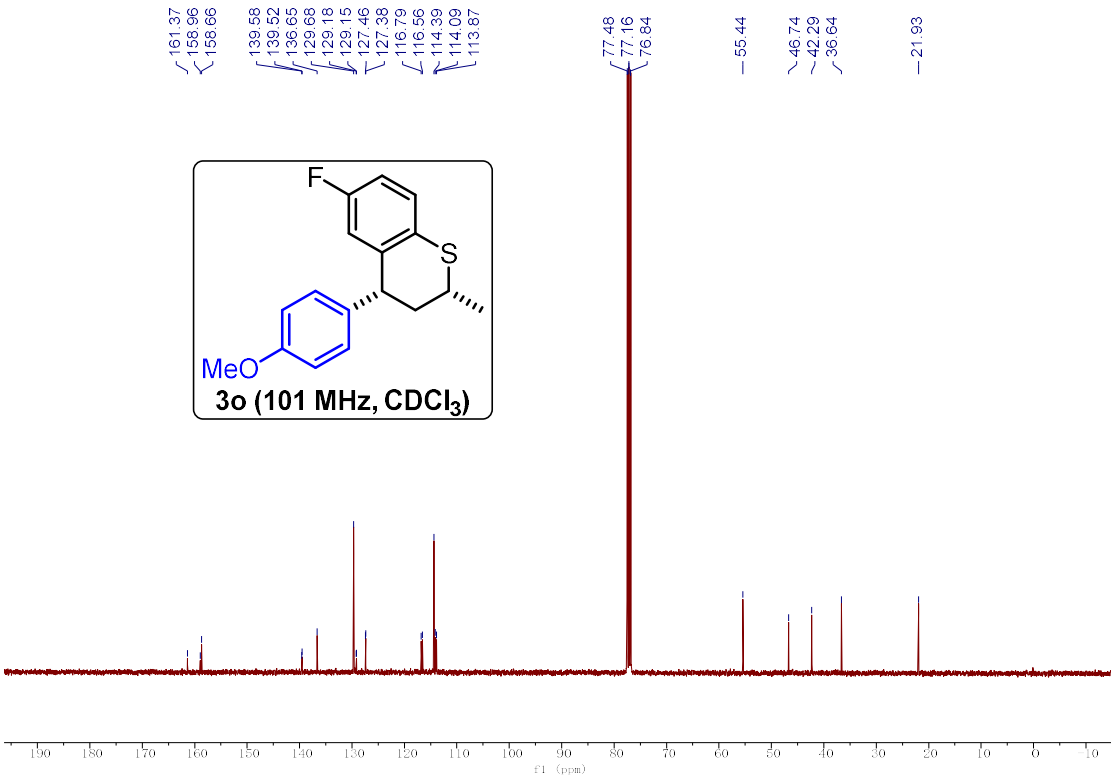

-118.32
F
S
Br
3m (376 MHz, CDCl3)
f1 (ppm)

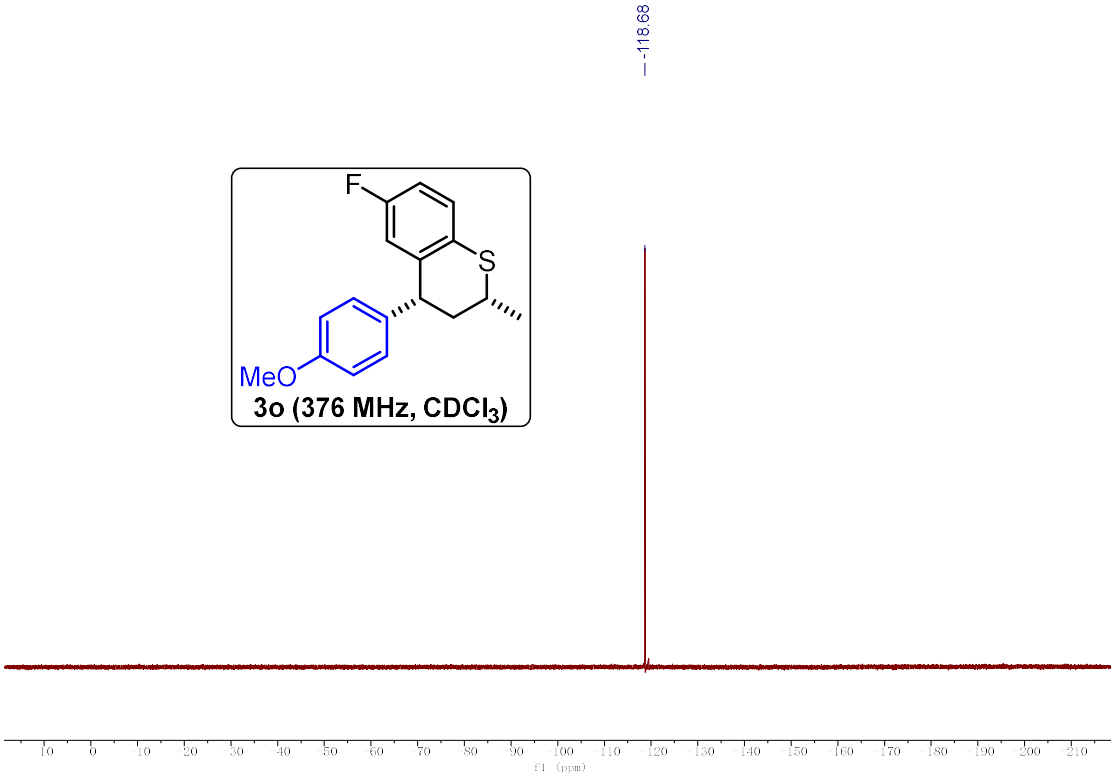

7.17
7.15
7.08
7.08
7.07
7.07
7.06
7.06
7.05
7.04
6.79
6.79
6.79
6.78
6.77
6.77
6.75
6.75
6.75
6.74
6.44
6.43
6.43
6.43
6.41
6.41
6.40
4.03
4.02
4.00
3.99
3.59
3.58
3.57
3.56
3.55
3.54
3.53
3.52
3.51
2.39
2.38
2.37
2.36
2.35
2.35
2.34
2.33
2.31
2.03
2.00
1.97
1.94
1.36
1.34
F
S
3n (400 MHz, CDCl3)
2.00
3.02
0.99
0.93
1.00
0.99
4.09
1.09
3.19
f1 (ppm)

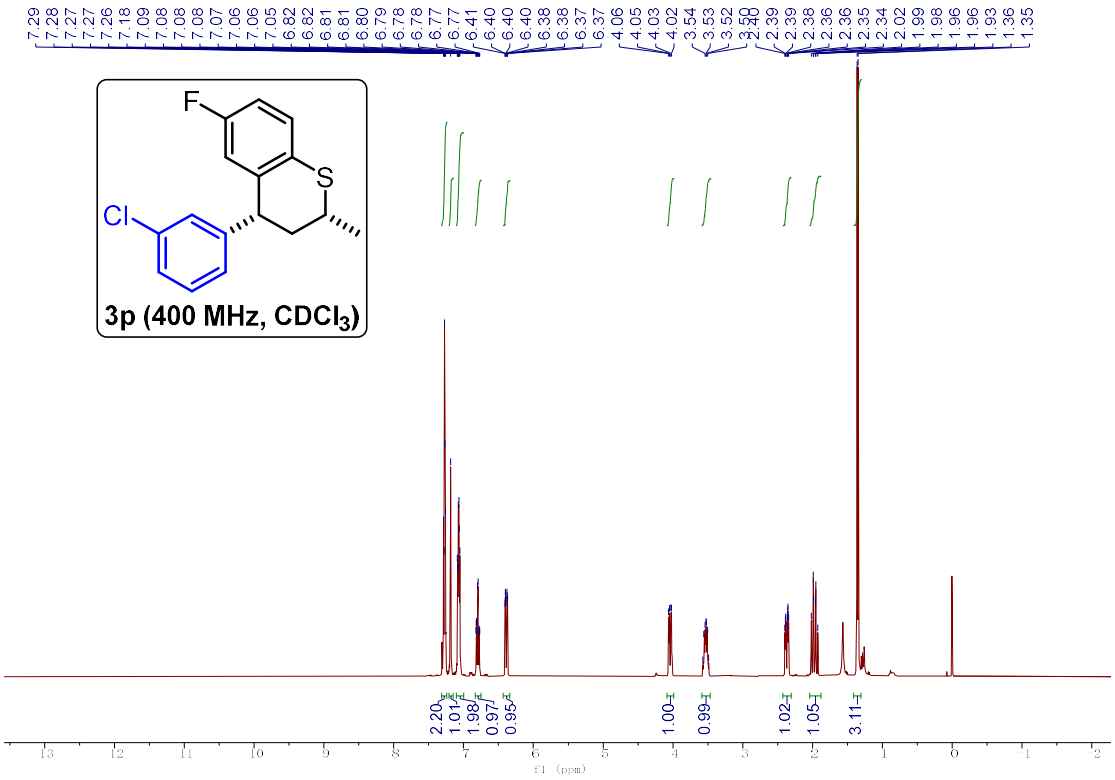

-118.72
F
S
3n (376 MHz, CDCl3)
f1 (ppm)

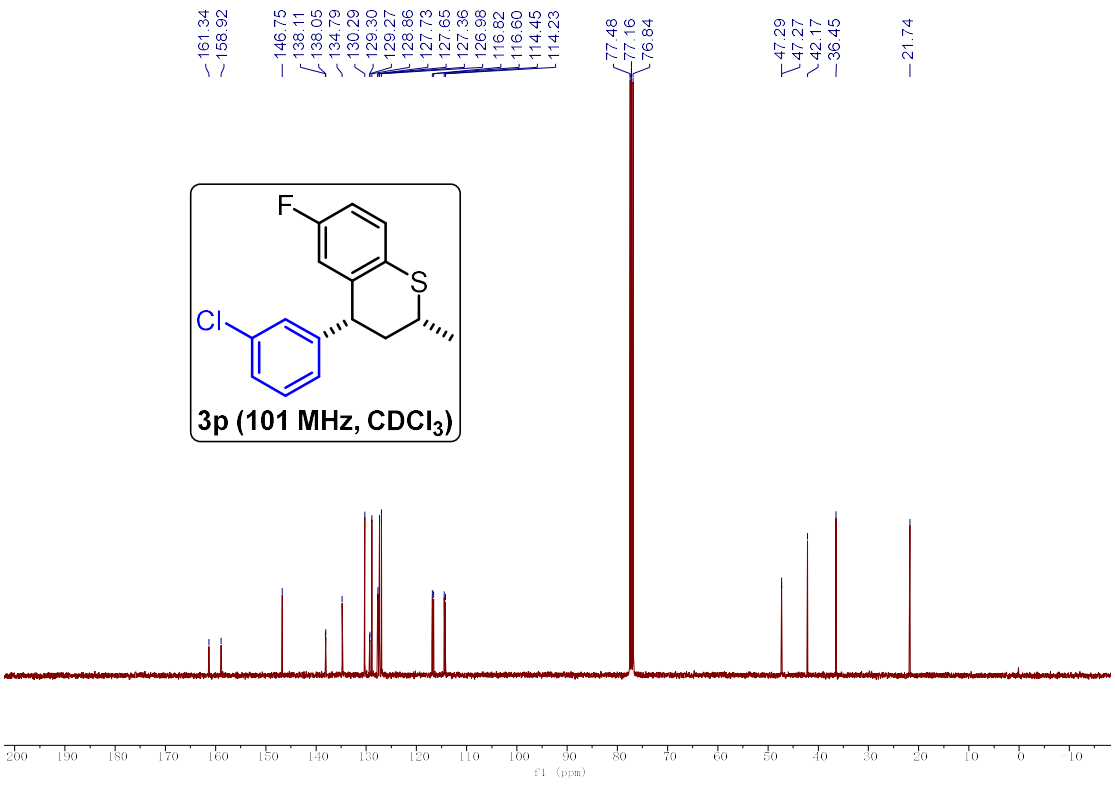

161.33
158.93
141.58
139.36
139.29
136.67
129.67
129.16
129.13
128.60
127.44
127.37
116.85
116.62
114.09
113.87
77.48
77.16
76.84
47.15
47.14
42.26
36.60
21.88
21.22
F
S
3n (101 MHz, CDCl3)
f1 (ppm)

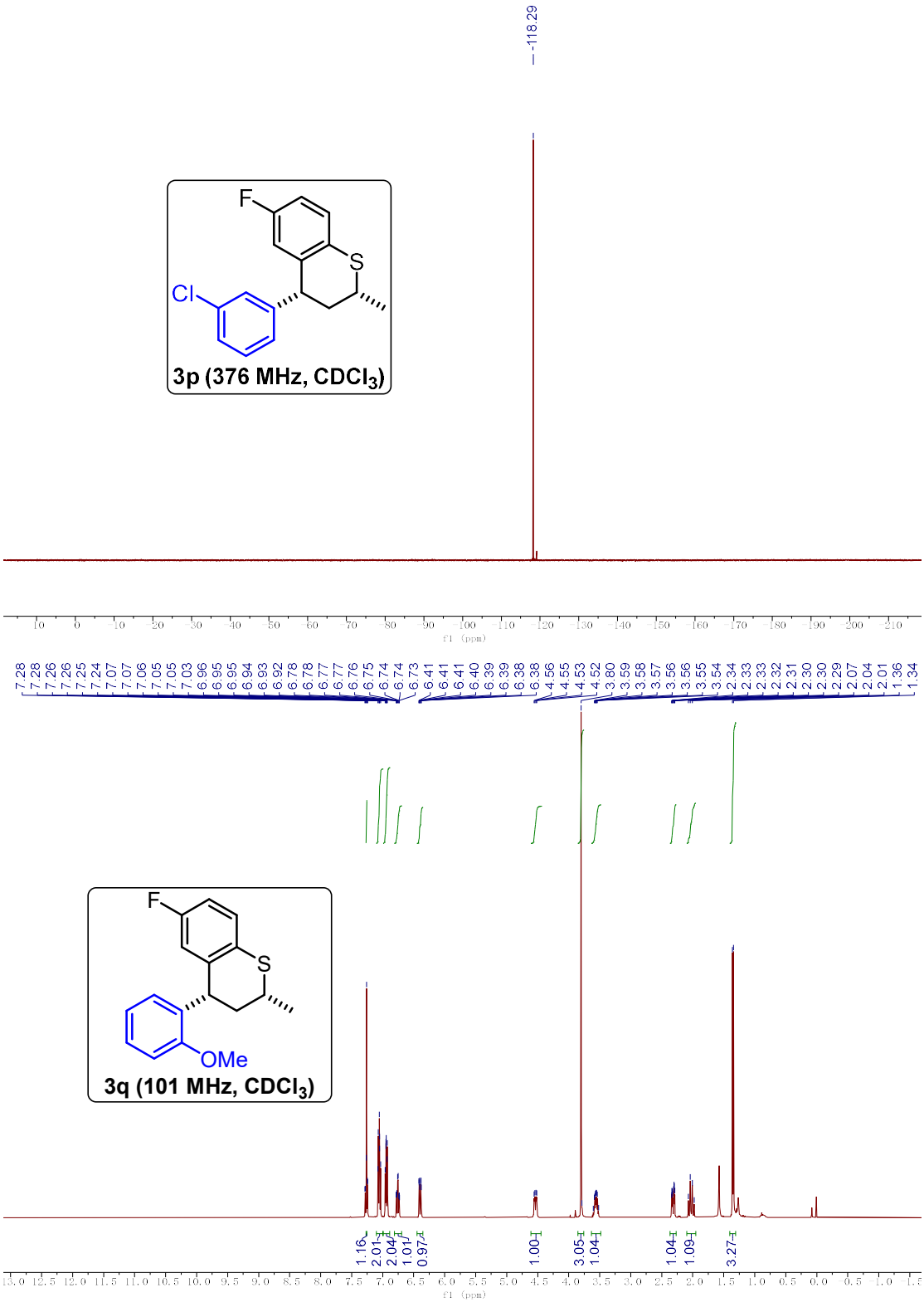

7.11
7.10
7.09
7.07
7.05
7.05
7.03
6.90
6.88
6.79
6.78
6.77
6.76
6.75
6.74
6.43
6.43
6.42
6.41
6.41
6.40
6.40
4.01
4.00
3.98
3.97
3.85
3.82
3.59
3.58
3.57
3.56
3.55
3.55
3.54
3.53
3.52
3.52
3.51
2.38
2.37
2.37
2.34
2.34
2.33
2.01
1.98
1.95
1.92
1.36
1.24
F
S
MeO
3o (400 MHz, CDCl3)
2.91
2.00
0.98
0.94
1.00
3.00
0.98
1.00
0.99
3.02
f1 (ppm)

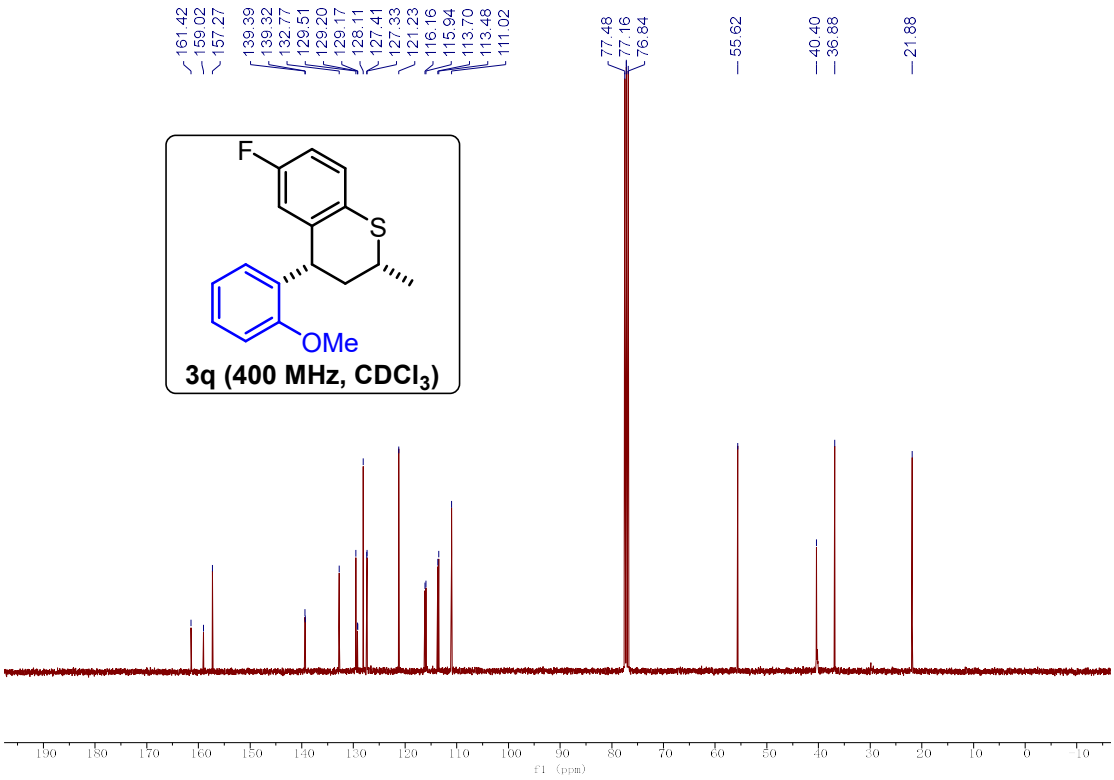

161.37
158.96
158.66
139.58
139.52
136.65
129.68
129.18
129.15
127.46
127.38
116.79
116.56
114.39
114.09
113.87
77.48
77.16
76.84
55.44
46.74
42.29
36.64
21.93
F
S
MeO
3o (101 MHz, CDCl3)
f1 (ppm)

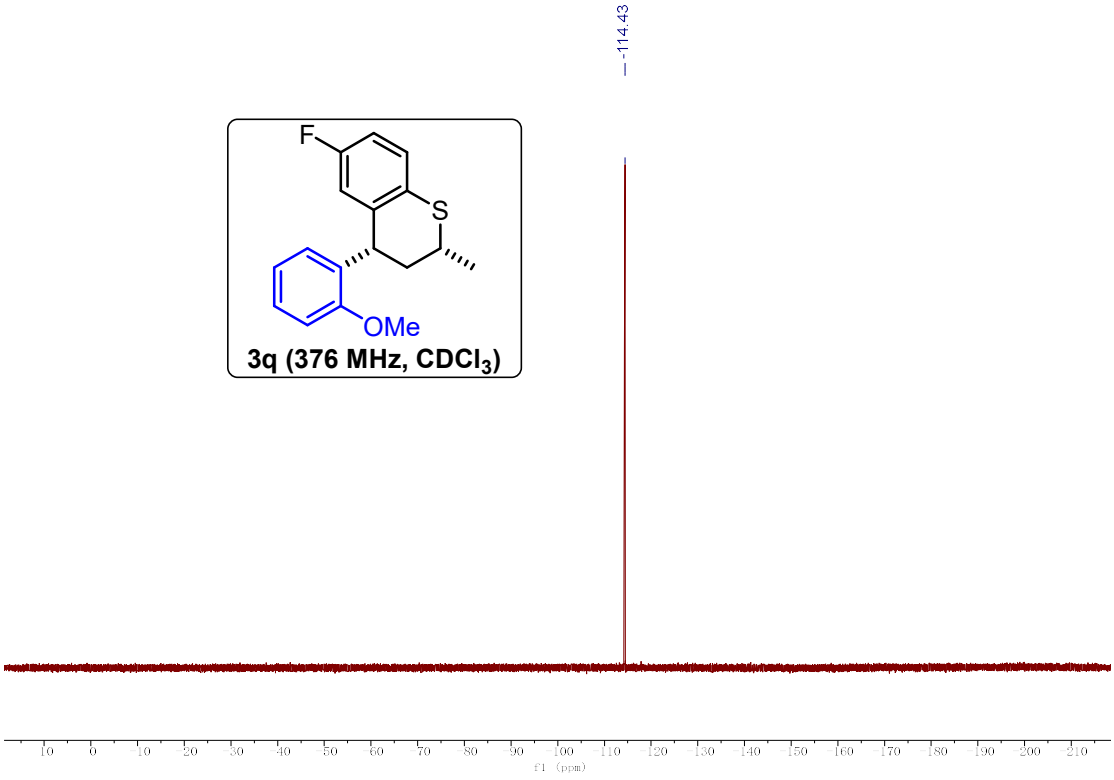

-118.68
F
S
MeO
3o (376 MHz, CDCl3)
f1 (ppm)

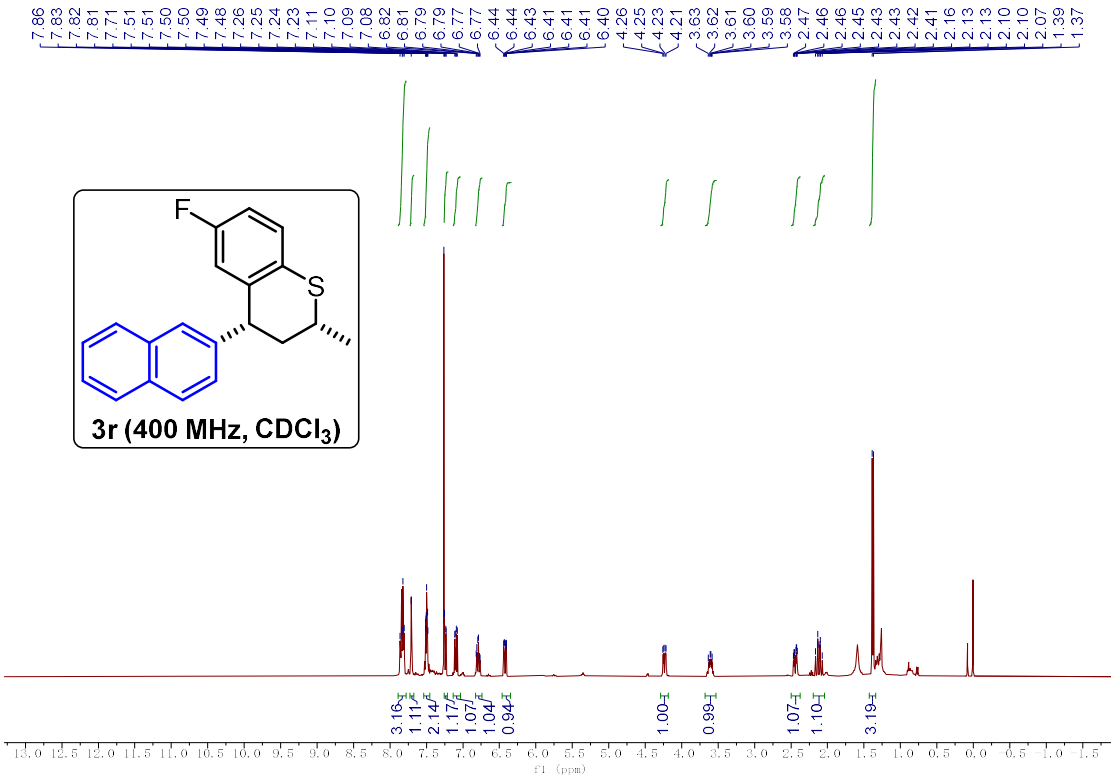

7.29
7.28
7.27
7.27
7.26
7.18
7.09
7.08
7.08
7.08
7.07
7.06
7.06
7.05
6.82
6.81
6.81
6.80
6.79
6.78
6.78
6.77
6.77
6.41
6.40
6.40
6.38
6.38
6.37
6.37
4.06
4.05
4.03
4.02
3.54
3.53
3.52
3.50
2.40
2.39
2.39
2.38
2.36
2.36
2.35
2.34
2.02
1.99
1.98
1.96
1.96
1.93
1.36
1.35
F
S
Cl
3p (400 MHz, CDCl3)
2.20
1.01
1.98
0.97
0.95
1.00
0.99
1.02
1.05
3.11
f1 (ppm)

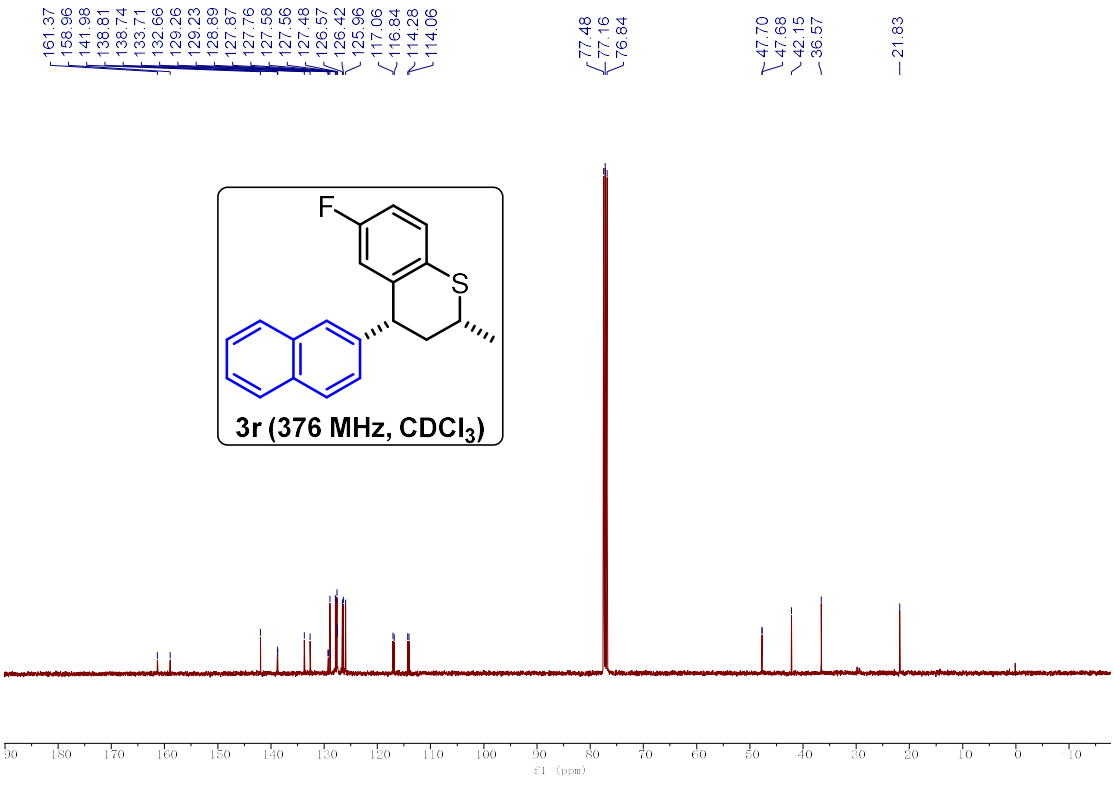

161.34
158.92
146.75
138.11
138.05
134.79
130.29
129.30
129.27
128.86
127.73
127.65
127.36
126.98
116.82
116.60
114.45
114.23
77.48
77.16
76.84
47.29
47.27
42.17
36.45
21.74
F
S
Cl
3p (101 MHz, CDCl3)
f1 (ppm)

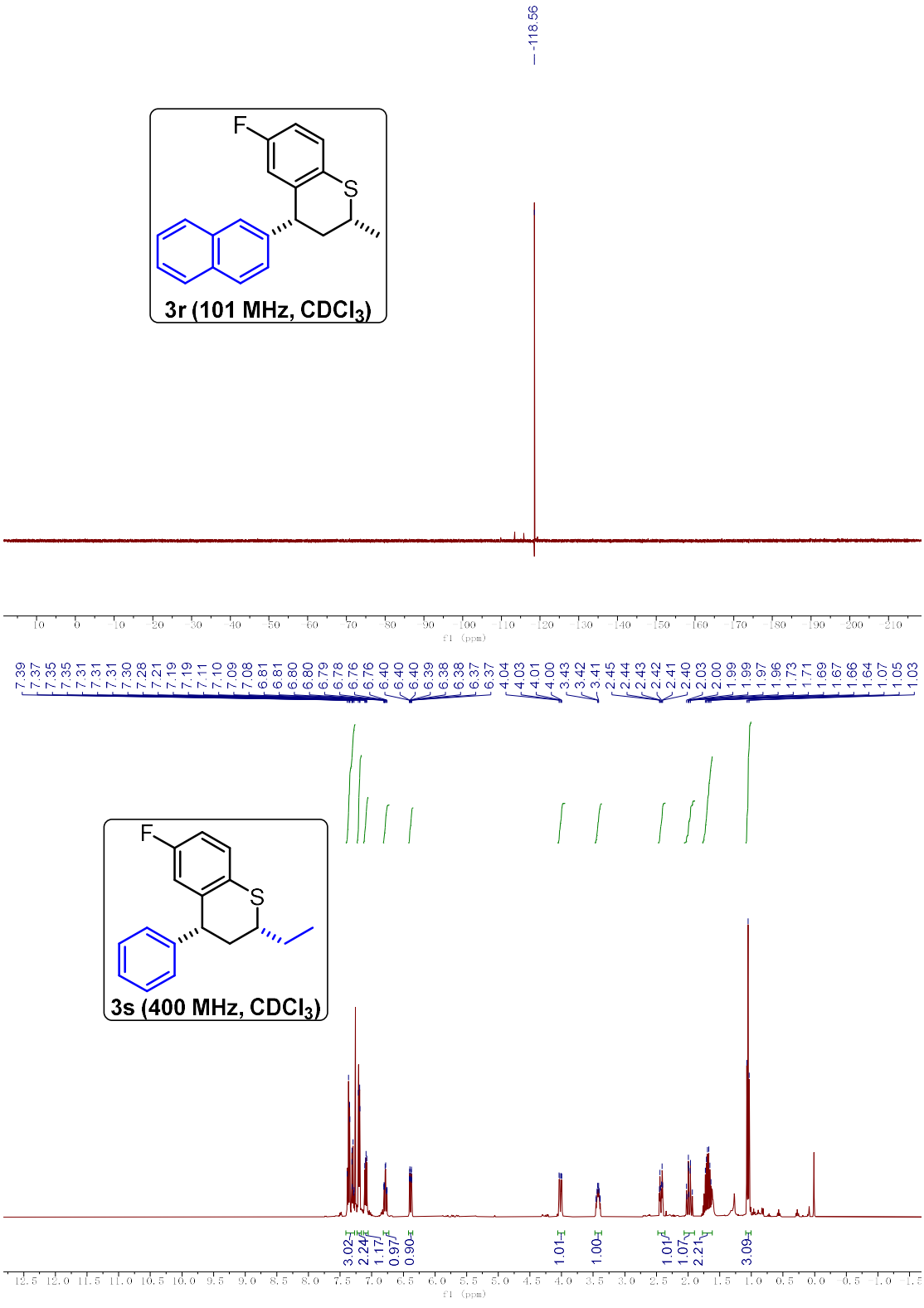

118.29
F
S
Cl
3p (376 MHz, CDCl3)
7.28
7.26
7.25
7.24
7.07
7.06
7.05
7.03
6.96
6.95
6.94
6.93
6.92
6.78
6.77
6.76
6.75
6.74
6.73
6.41
6.40
6.39
6.38
4.56
4.55
4.53
4.52
3.80
3.59
3.58
3.57
3.56
3.55
3.54
2.34
2.33
2.32
2.31
2.30
2.29
2.07
2.04
2.01
1.36
1.34
F
S
OMe
3q (101 MHz, CDCl3)
1.16
2.01
2.04
1.01
0.97
1.00
3.05
1.04
1.04
1.09
3.27
f1 (ppm)

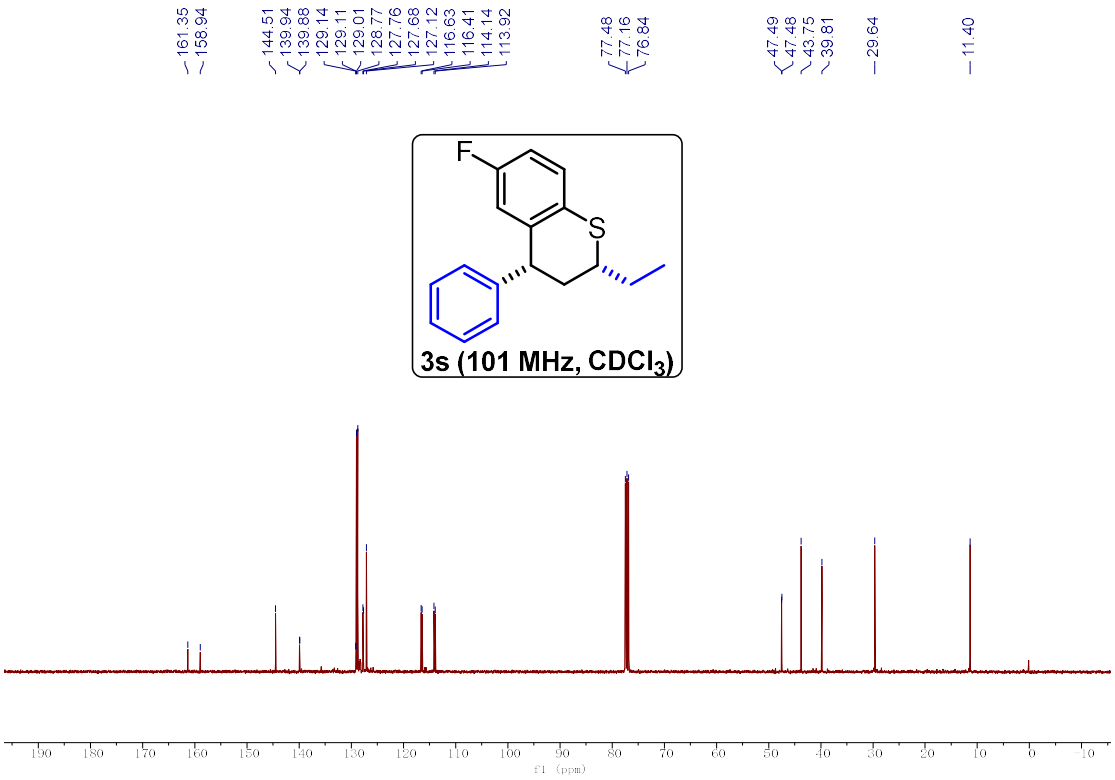

161.42
159.02
157.27
139.39
139.32
132.77
129.51
129.20
129.17
128.11
127.41
127.33
121.23
116.16
115.94
113.70
113.48
111.02
77.48
77.16
76.84
55.62
40.40
36.88
21.88
F
S
OMe
3q (400 MHz, CDCl3)
f1 (ppm)

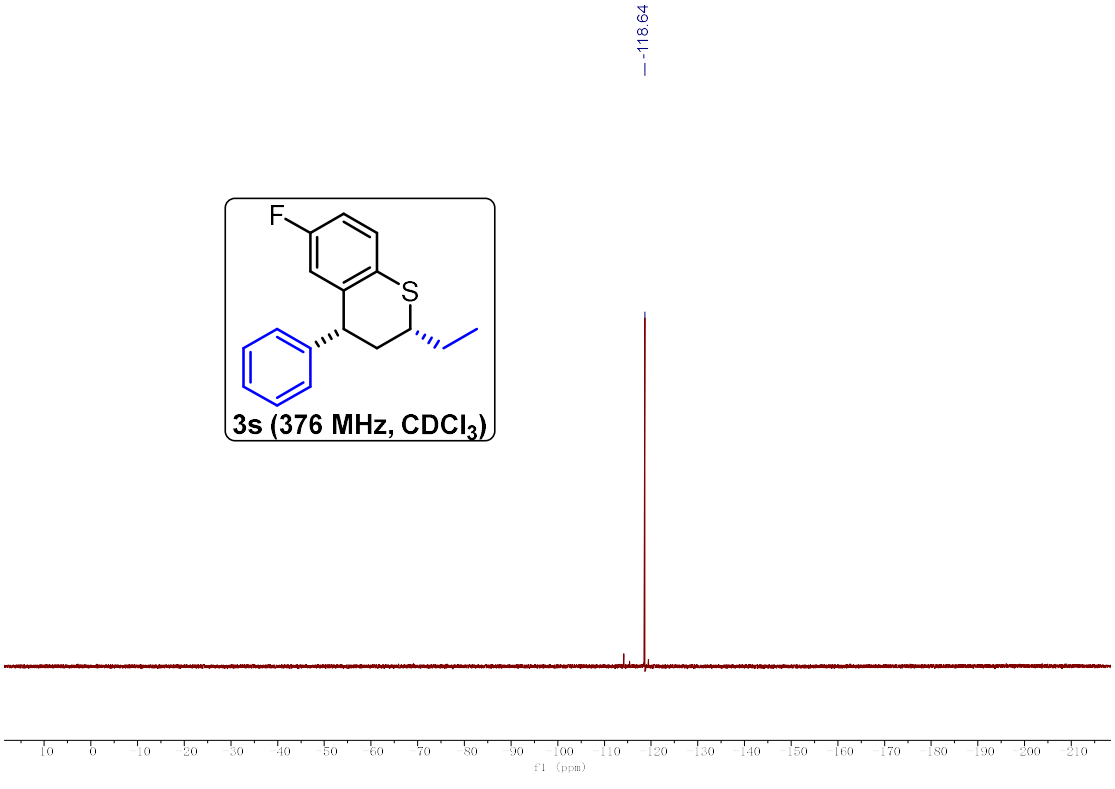

-114.43
F
S
OMe
3q (376 MHz, CDCl3)
f1 (ppm)

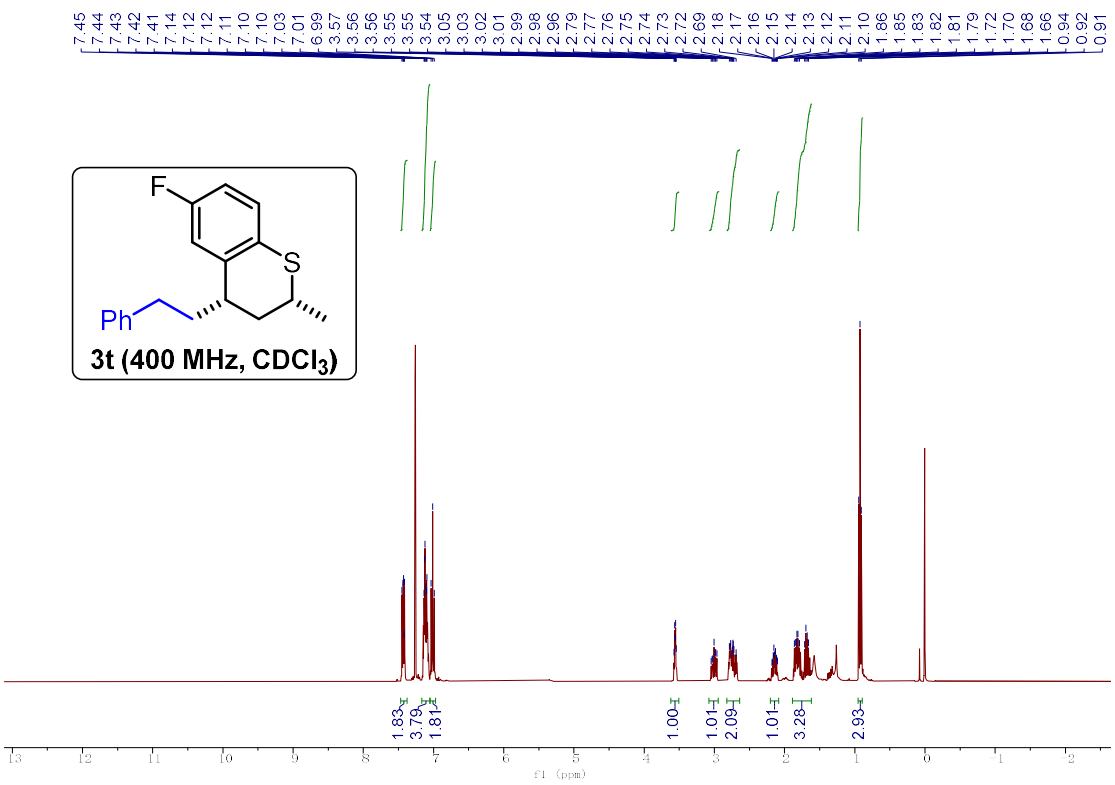

7.86
7.83
7.82
7.81
7.71
7.51
7.51
7.50
7.50
7.49
7.48
7.26
7.25
7.24
7.23
7.11
7.10
7.09
7.08
6.82
6.81
6.79
6.79
6.77
6.77
6.44
6.44
6.43
6.41
6.41
6.41
6.40
4.26
4.25
4.23
4.21
3.63
3.62
3.61
3.60
3.59
3.58
2.47
2.46
2.46
2.45
2.43
2.43
2.42
2.41
2.16
2.13
2.13
2.10
2.10
2.07
1.39
1.37
F
S
3r (400 MHz, CDCl3)
3.16
1.11
2.14
1.17
1.07
1.04
0.94
1.00
0.99
1.07
1.10
3.19
f1 (ppm)

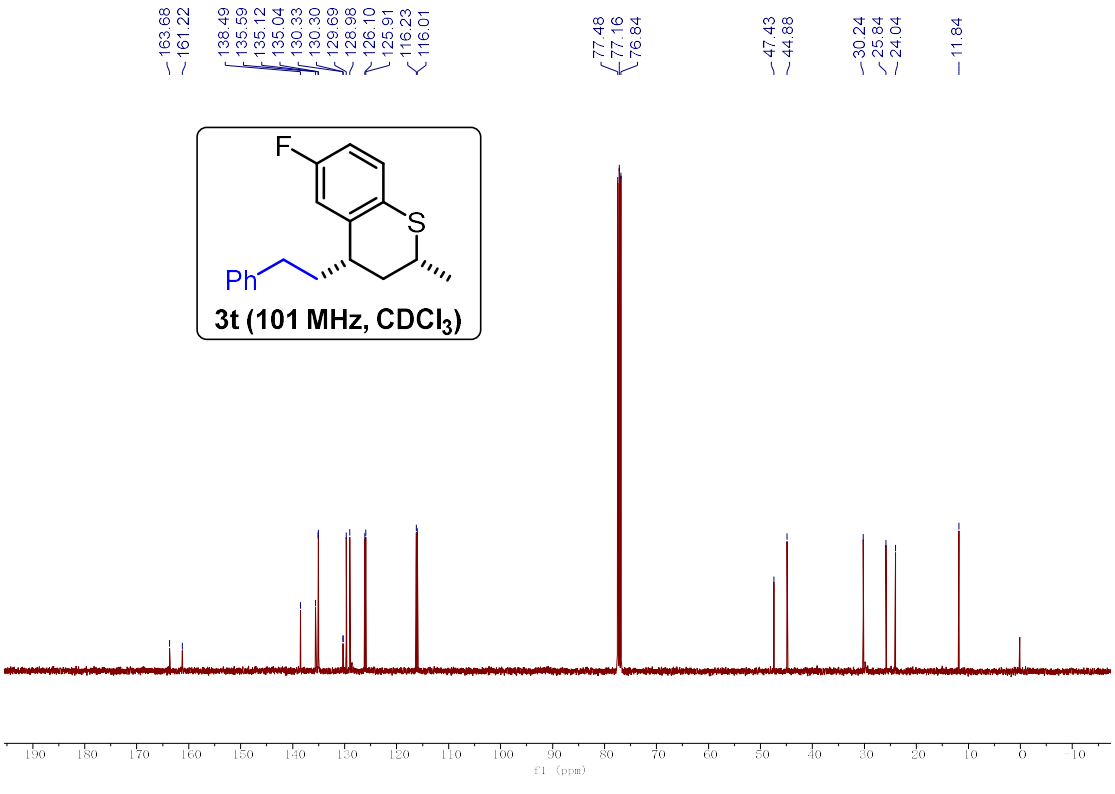

161.37
158.96
141.98
138.81
138.74
133.71
132.66
129.26
129.23
128.89
127.87
127.76
127.58
127.56
127.48
126.57
126.42
125.96
117.06
116.84
114.28
114.06
77.48
77.16
76.84
47.70
47.68
42.15
36.57
21.83
F
S
3r (376 MHz, CDCl3)
f1 (ppm)

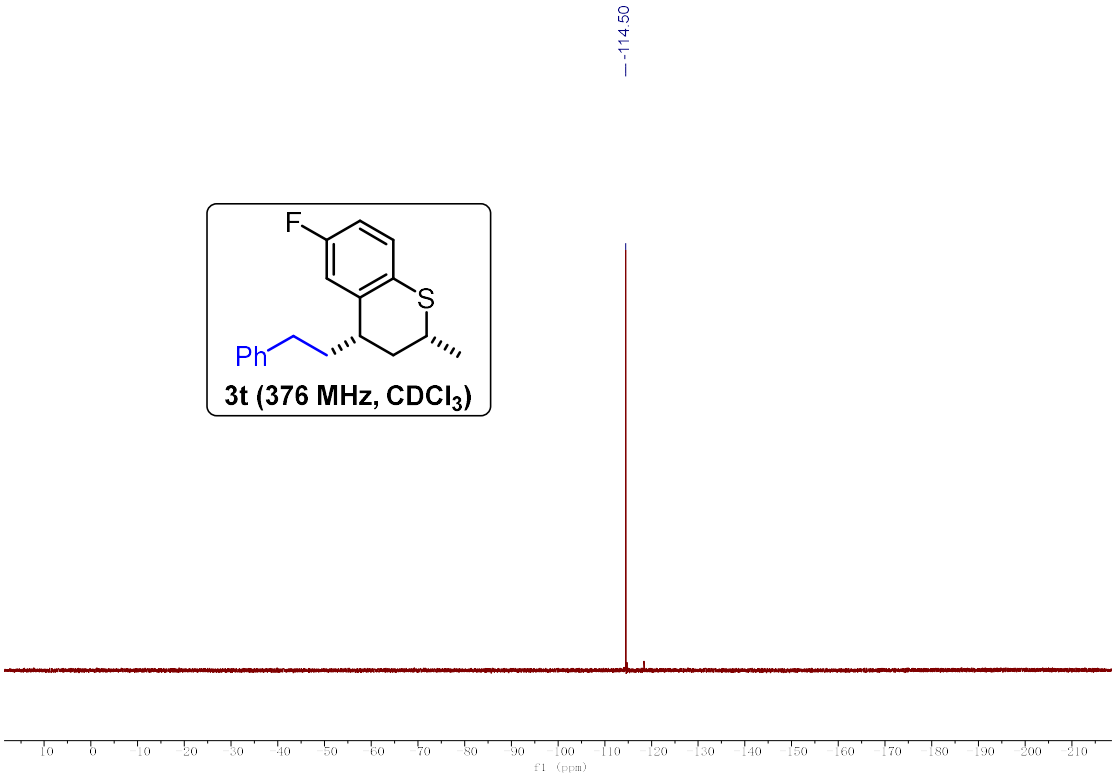

-118.56
F
S
3r (101 MHz, CDCl3)
F
S
3s (400 MHz, CDCl3)

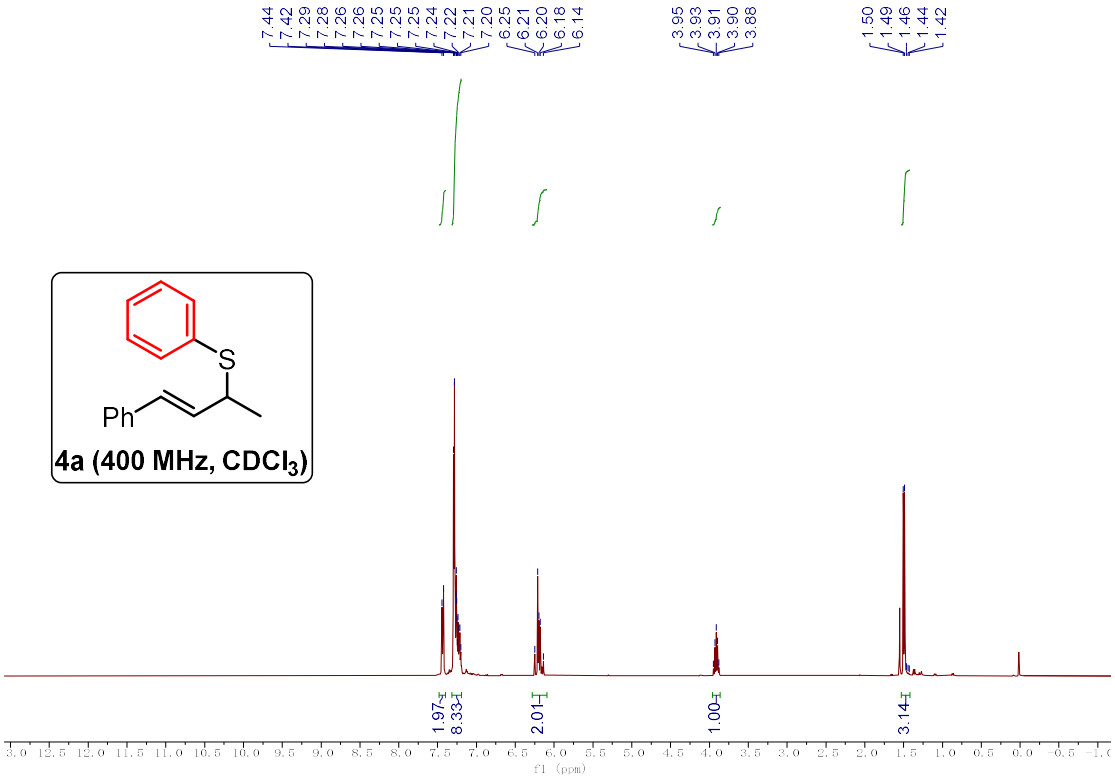

161.35
158.94
144.51
139.94
139.88
129.14
129.11
129.01
128.77
127.76
127.68
127.12
116.63
116.41
114.14
113.92
77.48
77.16
76.84
47.49
47.48
43.75
39.81
29.64
11.40
F
S
3s (101 MHz, CDCl3)
f1 (ppm)

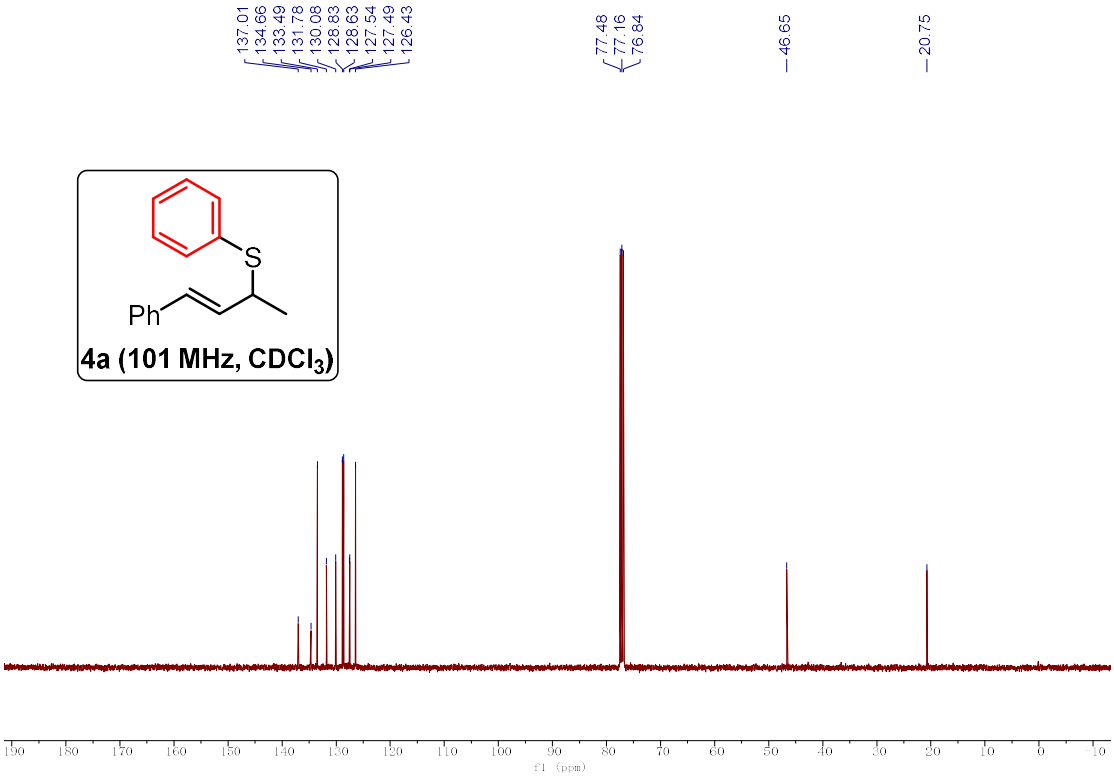

-118.64
F
S
3s (376 MHz, CDCl3)
f1 (ppm)

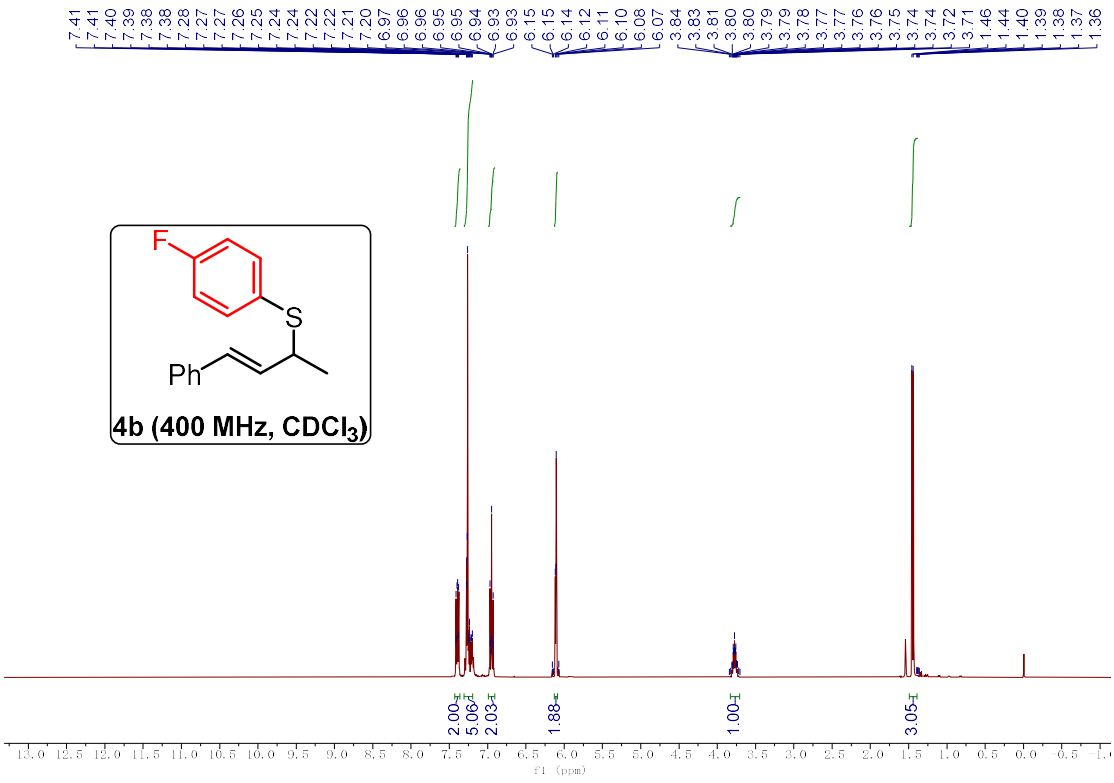

7.45 7.44 7.43 7.42 7.41 7.14 7.12 7.12 7.11 7.10 7.10 7.03 7.01 6.99 3.57 3.56 3.56 3.55 3.55 3.54 3.05 3.03 3.02 3.01 2.99 2.98 2.96 2.79 2.77 2.76 2.75 2.74 2.73 2.72 2.69 2.18 2.17 2.16 2.15 2.14 2.13 2.12 2.11 2.10 1.86 1.85 1.83 1.82 1.81 1.79 1.72 1.70 1.68 1.66 0.94 0.92 0.91
F
S
Ph
3t (400 MHz, CDCl3)
1.83 3.79 1.81 1.00 1.01 2.09 1.01 3.28 2.93
f1 (ppm)

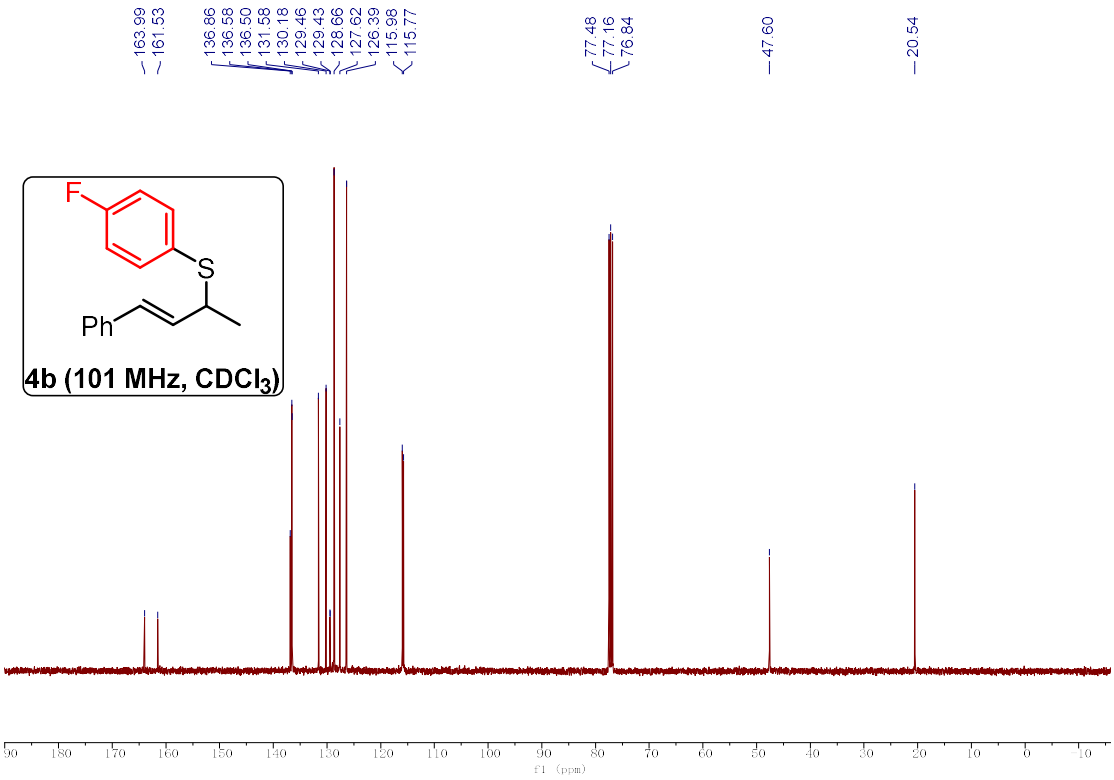

163.68 161.22 138.49 135.59 135.12 135.04 130.33 130.30 129.69 128.98 126.10 125.91 116.23 116.01 77.48 77.16 76.84 47.43 44.88 30.24 25.84 24.04 11.84
F
S
Ph
3t (101 MHz, CDCl3)
f1 (ppm)

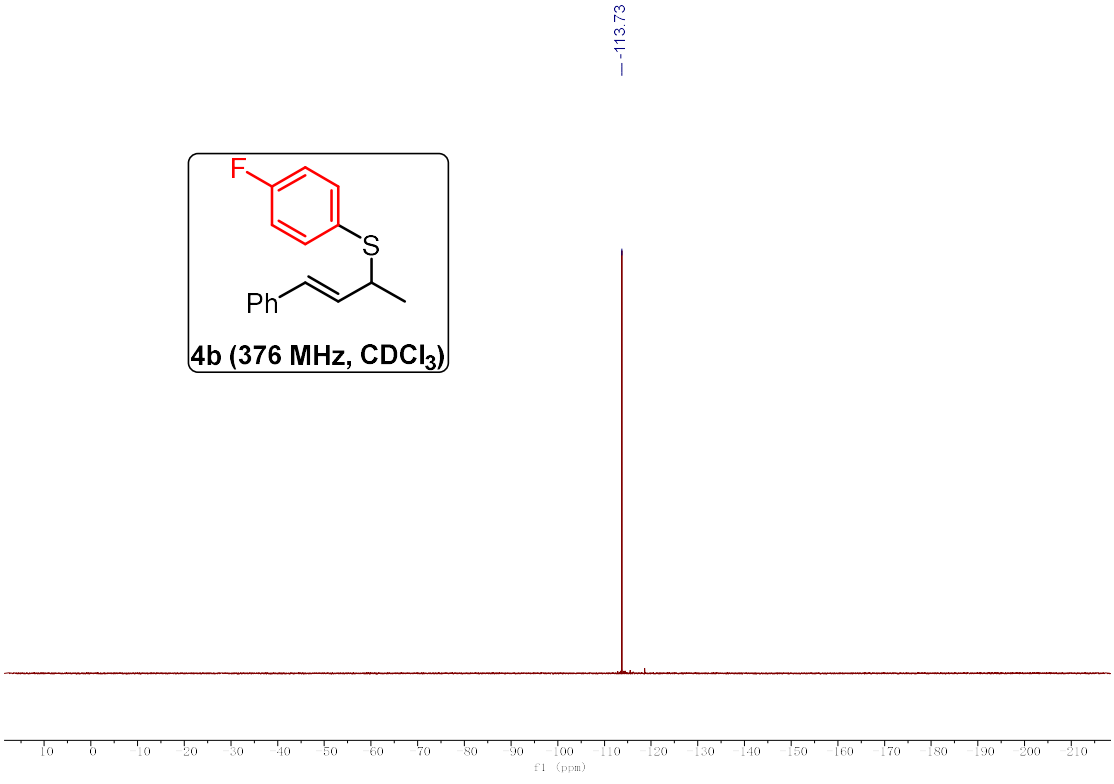

-114.50
F
S
Ph
3t (376 MHz, CDCl3)
f1 (ppm)

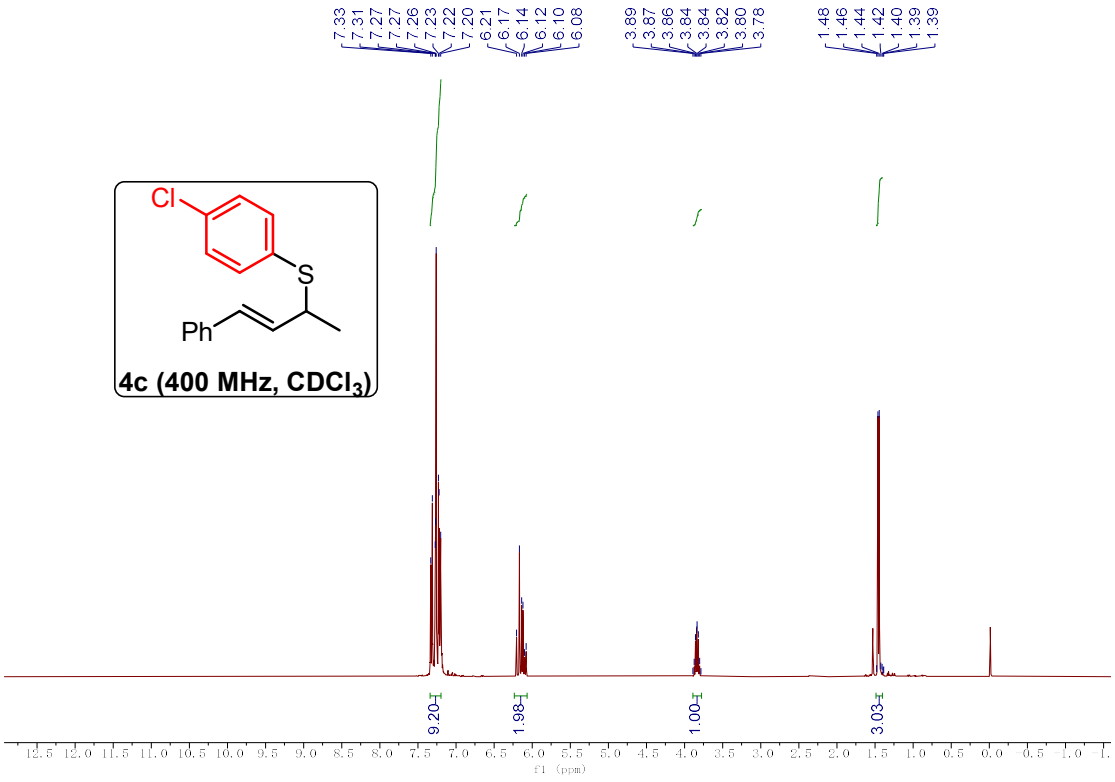

7.44
7.42
7.29
7.28
7.26
7.26
7.25
7.25
7.25
7.24
7.22
7.21
7.20
6.25
6.21
6.20
6.18
6.14
3.95
3.93
3.91
3.90
3.88
1.50
1.49
1.46
1.44
1.42
S
Ph
4a (400 MHz, CDCl3)
1.97
8.33
2.01
1.00
3.14
f1 (ppm)

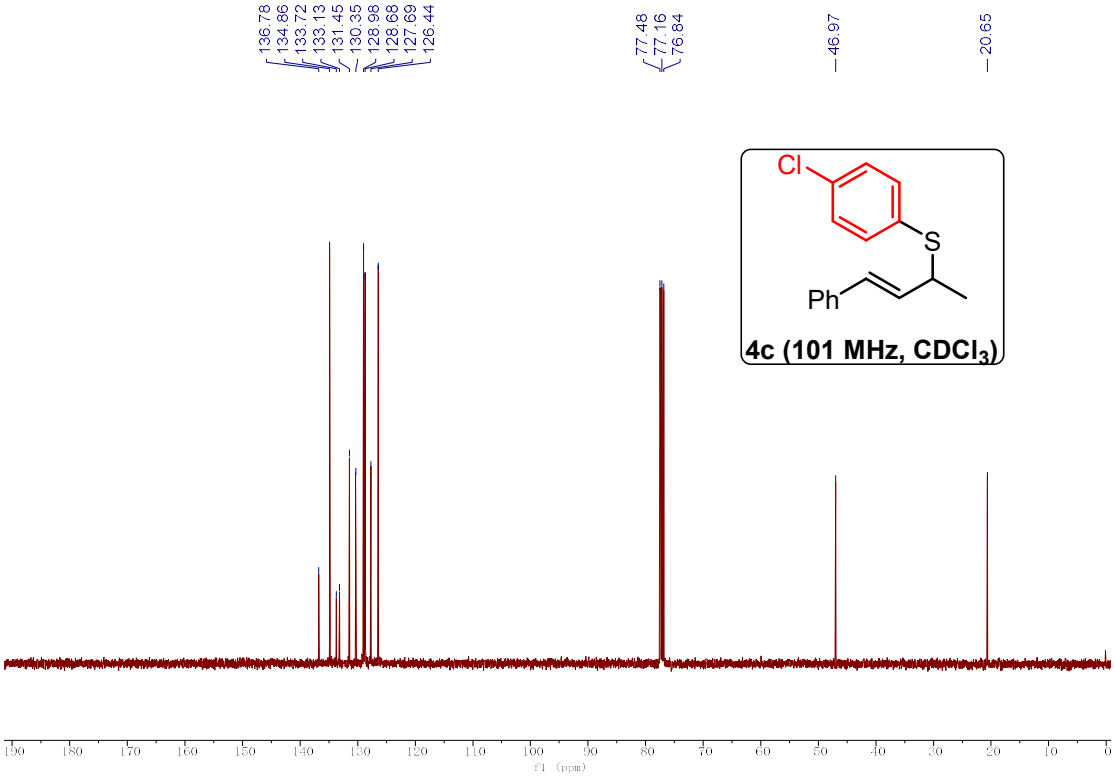

137.01
134.66
133.49
131.78
130.08
128.83
128.63
127.54
127.49
126.43
77.48
77.16
76.84
46.65
20.75
S
Ph
4a (101 MHz, CDCl3)

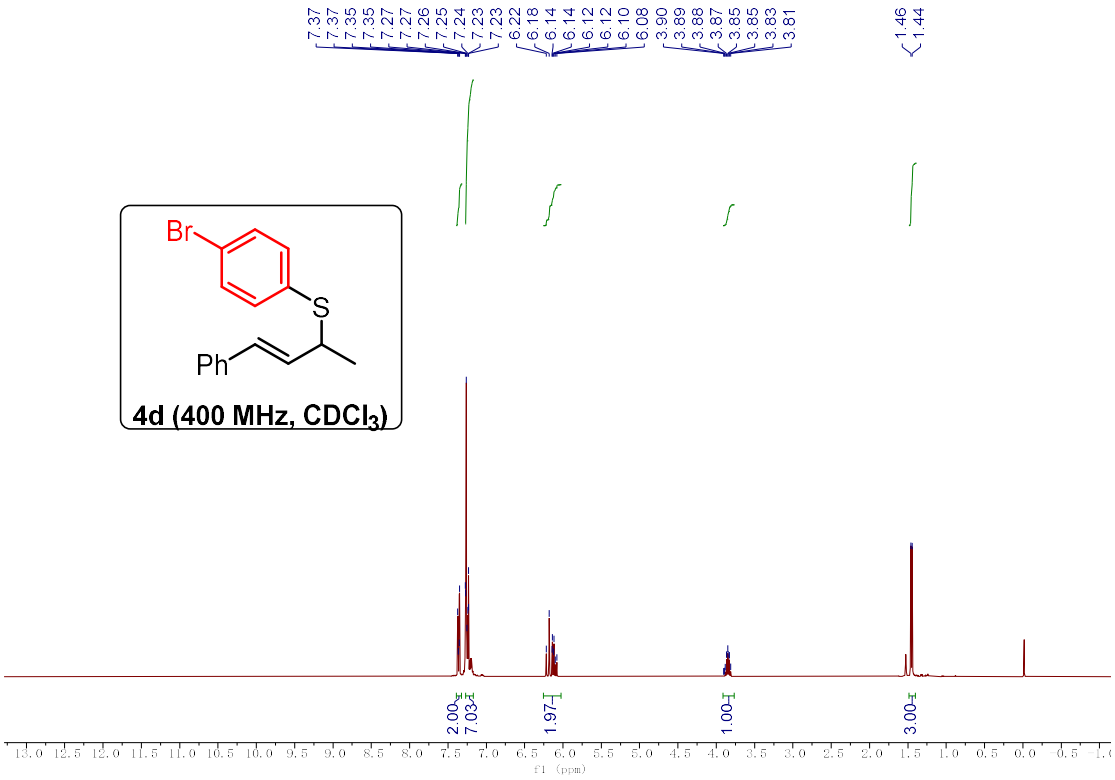

7.41
7.41
7.40
7.39
7.38
7.38
7.28
7.27
7.27
7.26
7.25
7.24
7.24
7.22
7.22
7.21
7.20
6.97
6.96
6.96
6.95
6.95
6.94
6.93
6.93
6.15
6.14
6.12
6.11
6.10
6.08
6.07
3.84
3.83
3.81
3.80
3.80
3.79
3.79
3.78
3.77
3.77
3.76
3.76
3.75
3.74
3.74
3.72
3.71
1.46
1.44
1.40
1.39
1.38
1.37
1.36
F
S
Ph
4b (400 MHz, CDCl3)
2.00
5.06
2.03
1.88
1.00
3.05

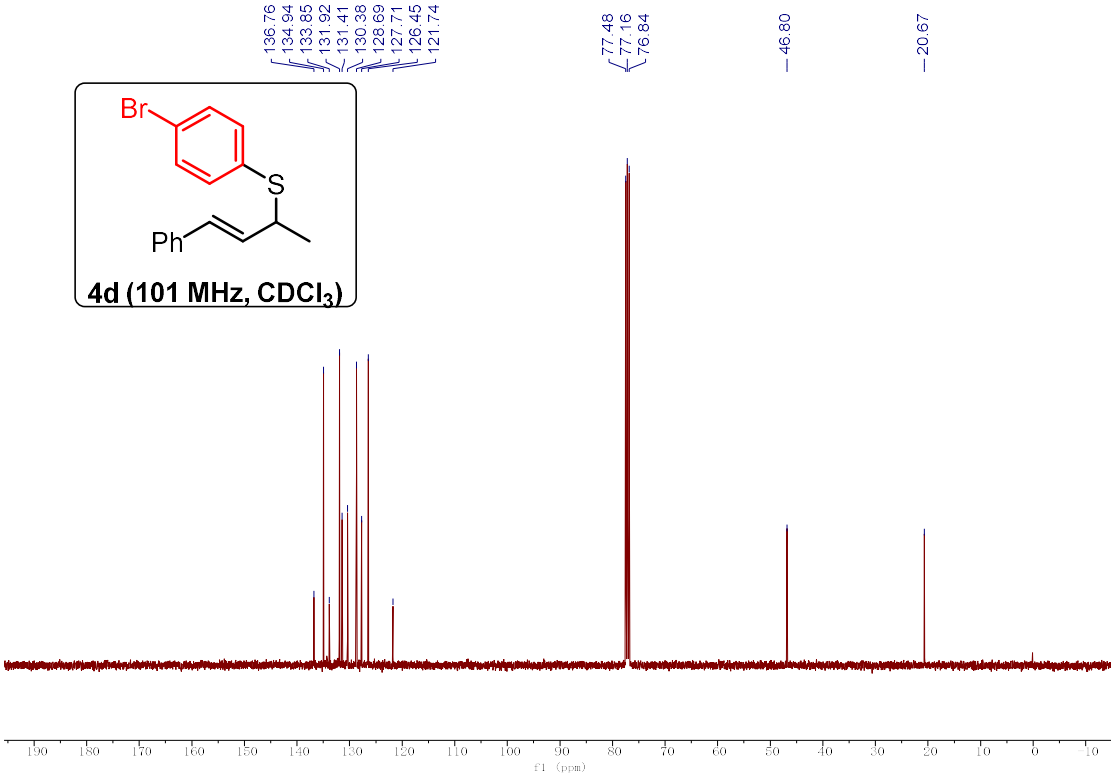

163.99
161.53
136.86
136.58
136.50
131.58
130.18
129.46
129.43
128.66
127.62
126.39
115.98
115.77
77.48
77.16
76.84
47.60
20.54
F
S
Ph
4b (101 MHz, CDCl3)
f1 (ppm)

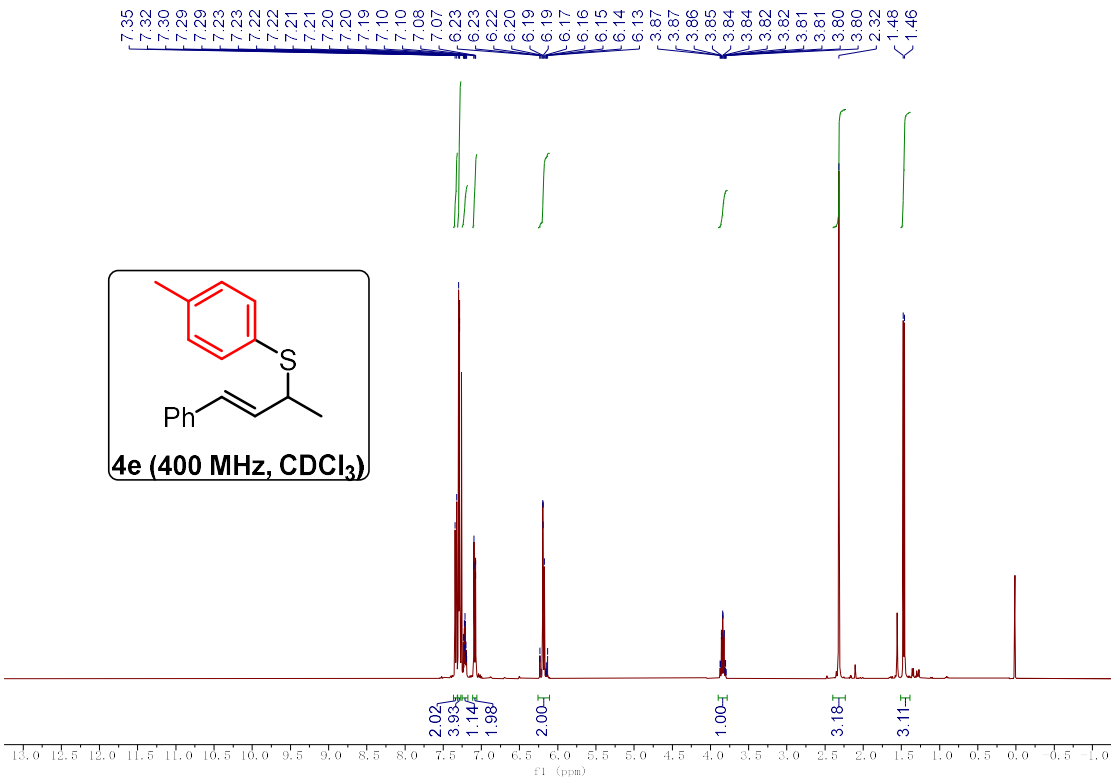

-113.73
F
S
Ph
4b (376 MHz, CDCl3)
f1 (ppm)

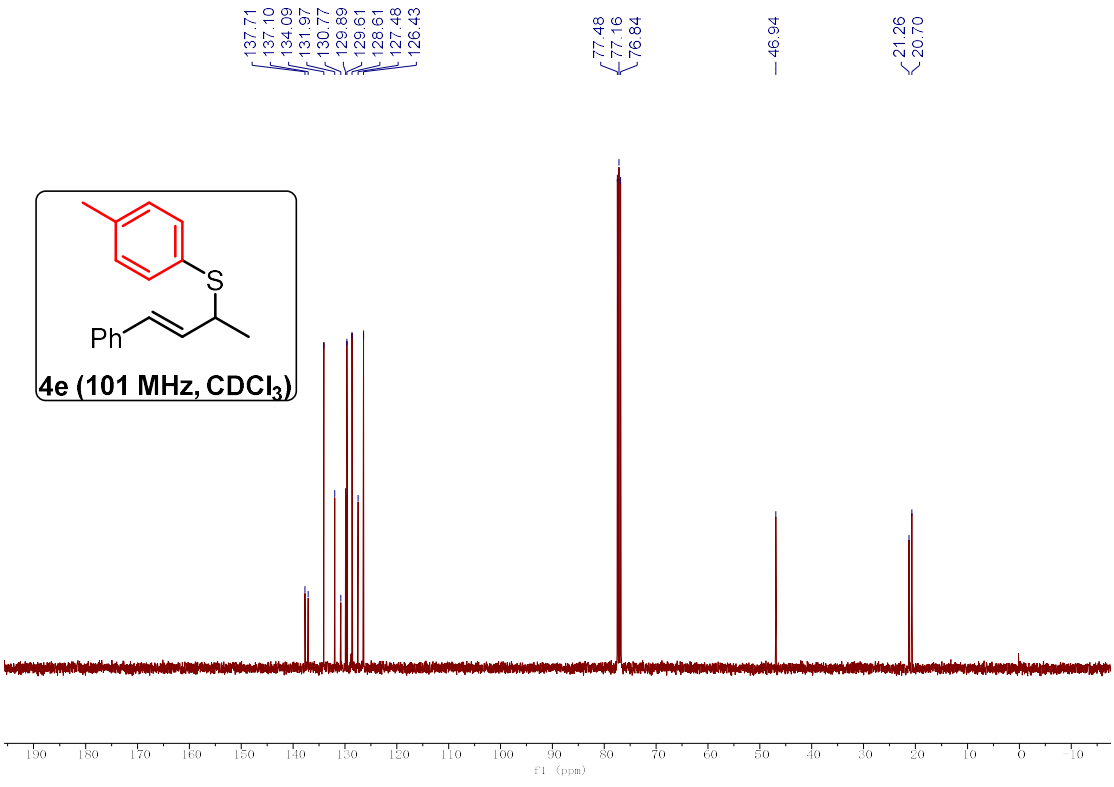

7.33
7.31
7.27
7.27
7.26
7.23
7.22
7.20
6.21
6.17
6.14
6.12
6.10
6.08
3.89
3.87
3.86
3.84
3.84
3.82
3.80
3.78
1.48
1.46
1.44
1.42
1.40
1.39
1.39
Cl
S
Ph
4c (400 MHz, CDCl3)
9.20
1.98
1.00
3.03
f1 (ppm)

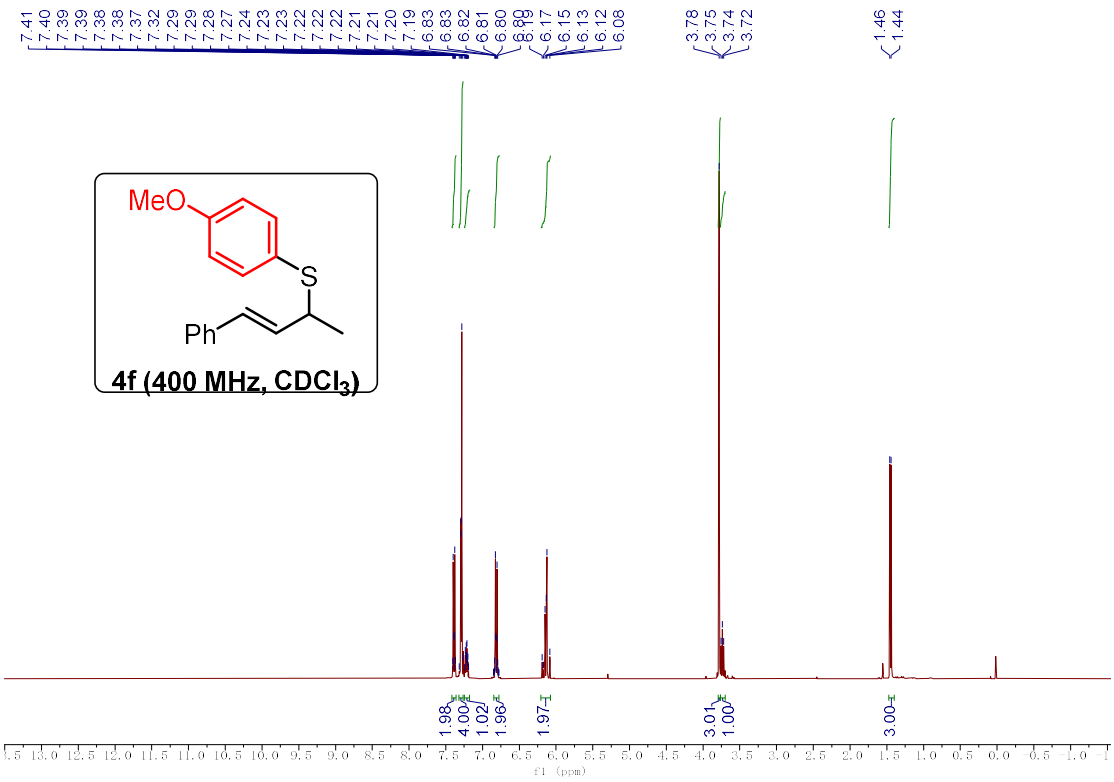

136.78
134.86
133.72
133.13
131.45
130.35
128.98
128.68
127.69
126.44
77.48
77.16
76.84
46.97
20.65
Cl
S
Ph
4c (101 MHz, CDCl3)
f1 (ppm)

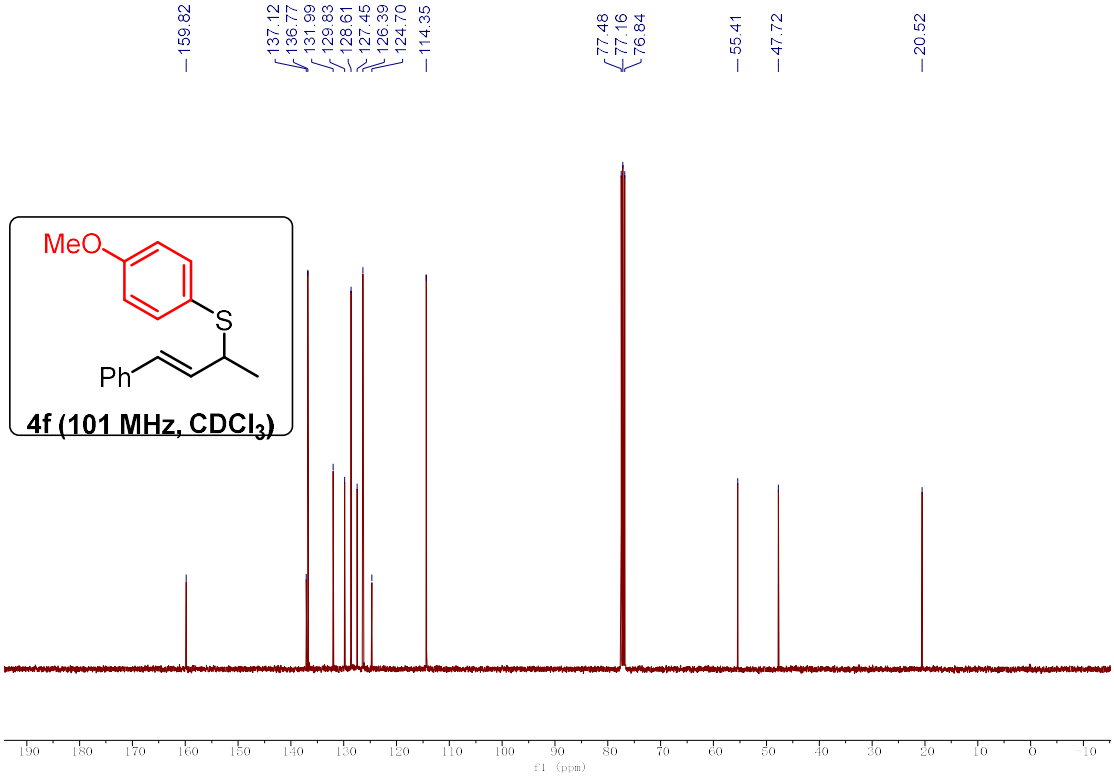

7.37
7.37
7.35
7.35
7.27
7.27
7.26
7.25
7.24
7.23
7.23
6.22
6.18
6.14
6.14
6.12
6.12
6.10
6.08
3.90
3.89
3.88
3.87
3.85
3.85
3.83
3.81
1.46
1.44
Br
S
Ph
4d (400 MHz, CDCl3)
2.00
7.03
1.97
1.00
3.00
f1 (ppm)

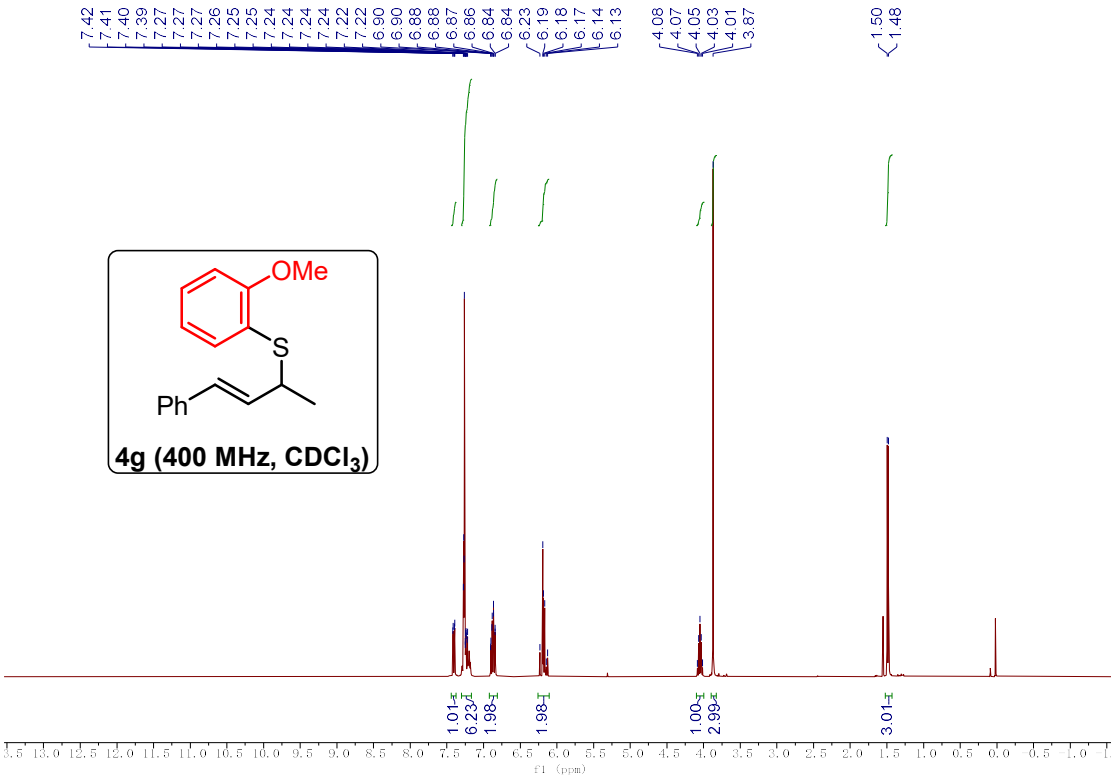

136.76
134.94
133.85
131.92
131.41
130.38
128.69
127.71
126.45
121.74
77.48
77.16
76.84
46.80
20.67
Br
S
Ph
4d (101 MHz, CDCl3)
f1 (ppm)

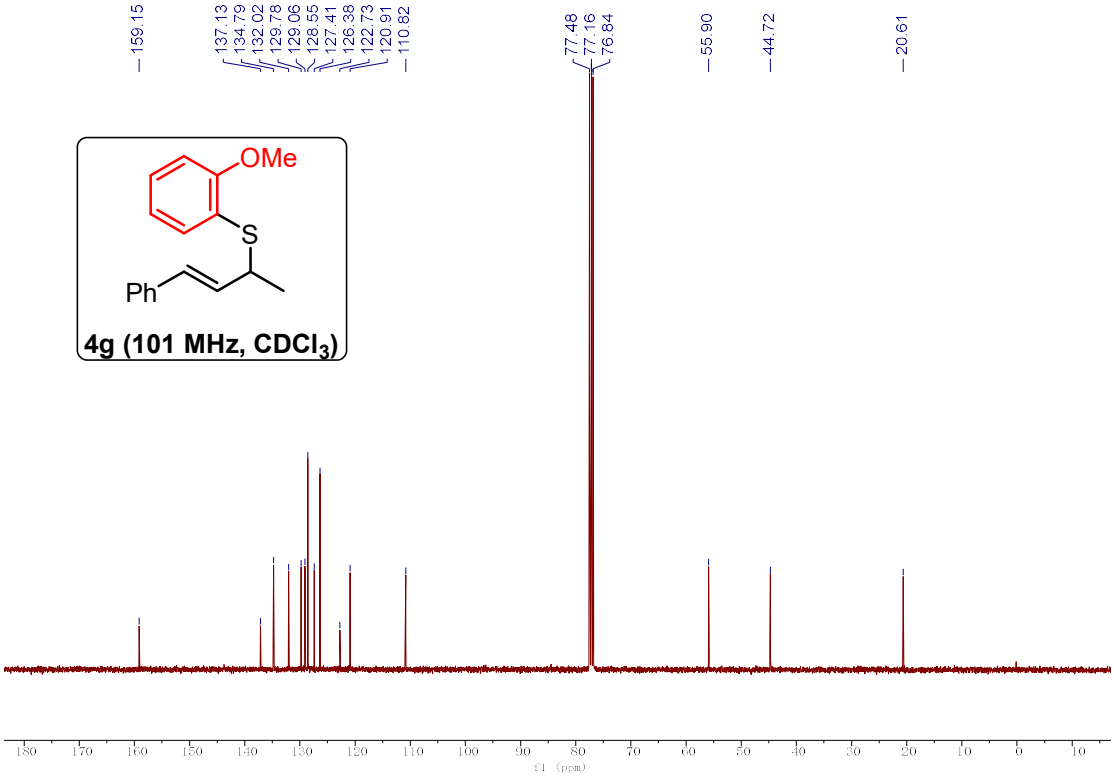

7.35
7.32
7.30
7.29
7.29
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.10
7.10
7.08
7.07
6.23
6.23
6.22
6.20
6.19
6.19
6.17
6.16
6.15
6.14
6.13
3.87
3.87
3.86
3.85
3.84
3.84
3.82
3.82
3.81
3.81
3.80
3.80
2.32
1.48
1.46
S
Ph
4e (400 MHz, CDCl3)
2.02
3.93
1.14
1.98
2.00
1.00
3.18
3.11
f1 (ppm)

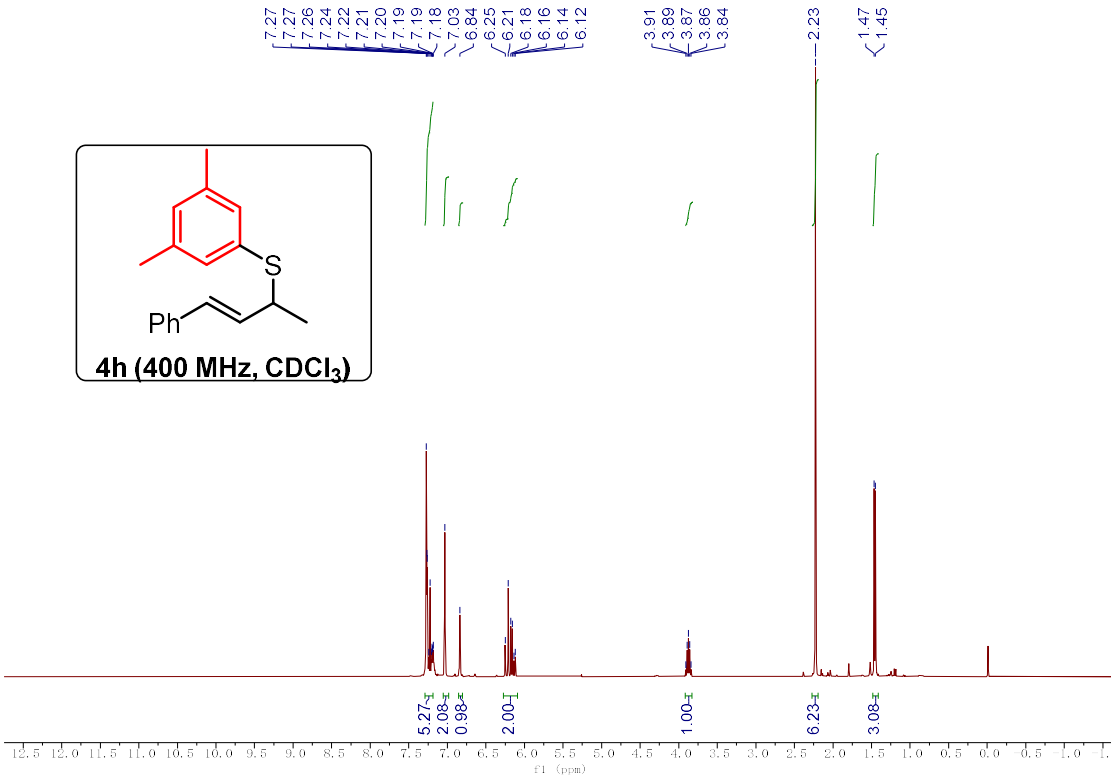

137.71
137.10
134.09
131.97
130.77
129.89
129.61
128.61
127.48
126.43
77.48
77.16
76.84
46.94
21.26
20.70
S
Ph
4e (101 MHz, CDCl3)
f1 (ppm)

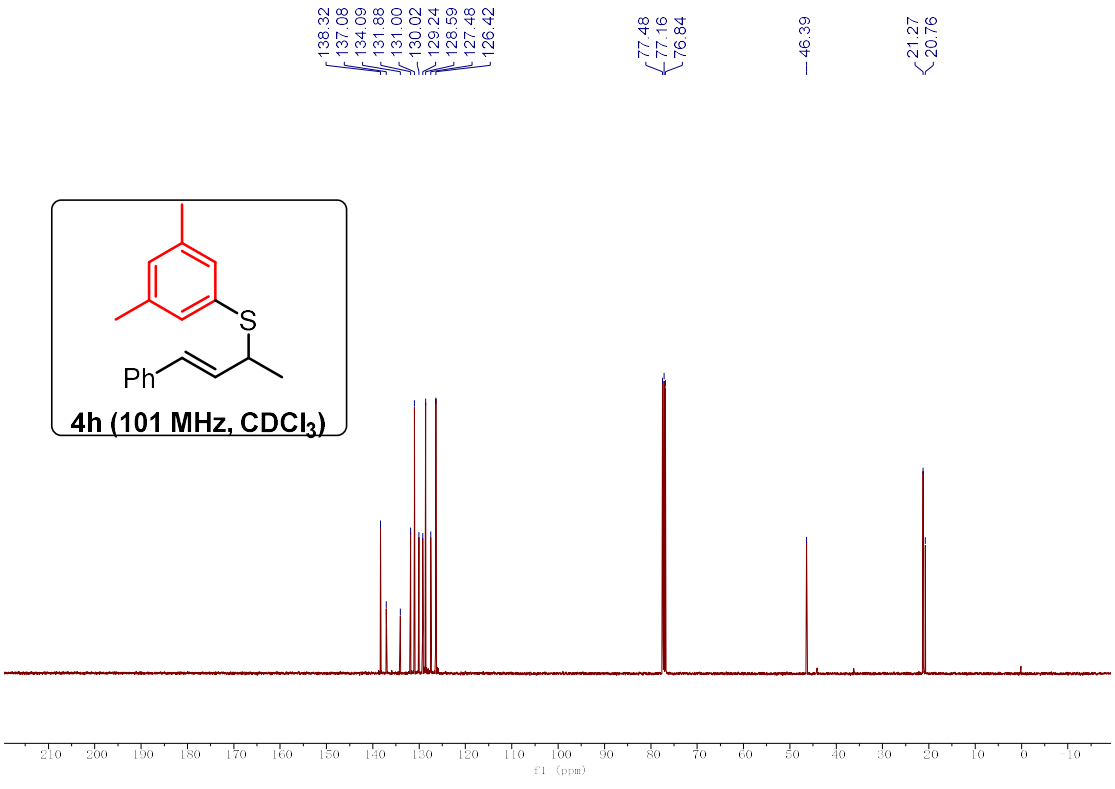

7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.32
7.29
7.29
7.28
7.27
7.24
7.23
7.23
7.22
7.22
7.22
7.21
7.21
7.20
7.19
6.83
6.83
6.82
6.81
6.80
6.80
6.17
6.15
6.13
6.12
6.08
3.78
3.75
3.74
3.72
1.46
1.44
MeO
S
Ph
4f (400 MHz, CDCl3)
1.98
4.00
1.02
1.96
1.97
3.01
1.00
3.00
f1 (ppm)

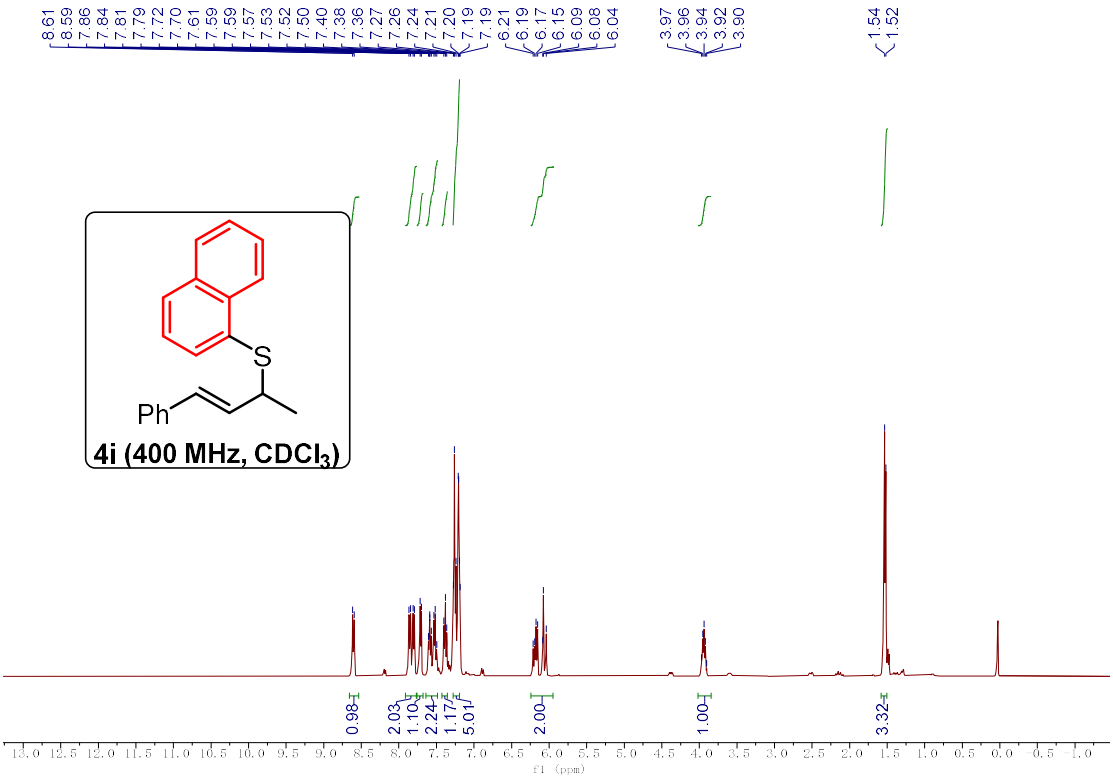

159.82
137.12
136.77
131.99
129.83
128.61
127.45
126.39
124.70
114.35
77.48
77.16
76.84
55.41
47.72
20.52
MeO
S
Ph
4f (101 MHz, CDCl3)
f1 (ppm)

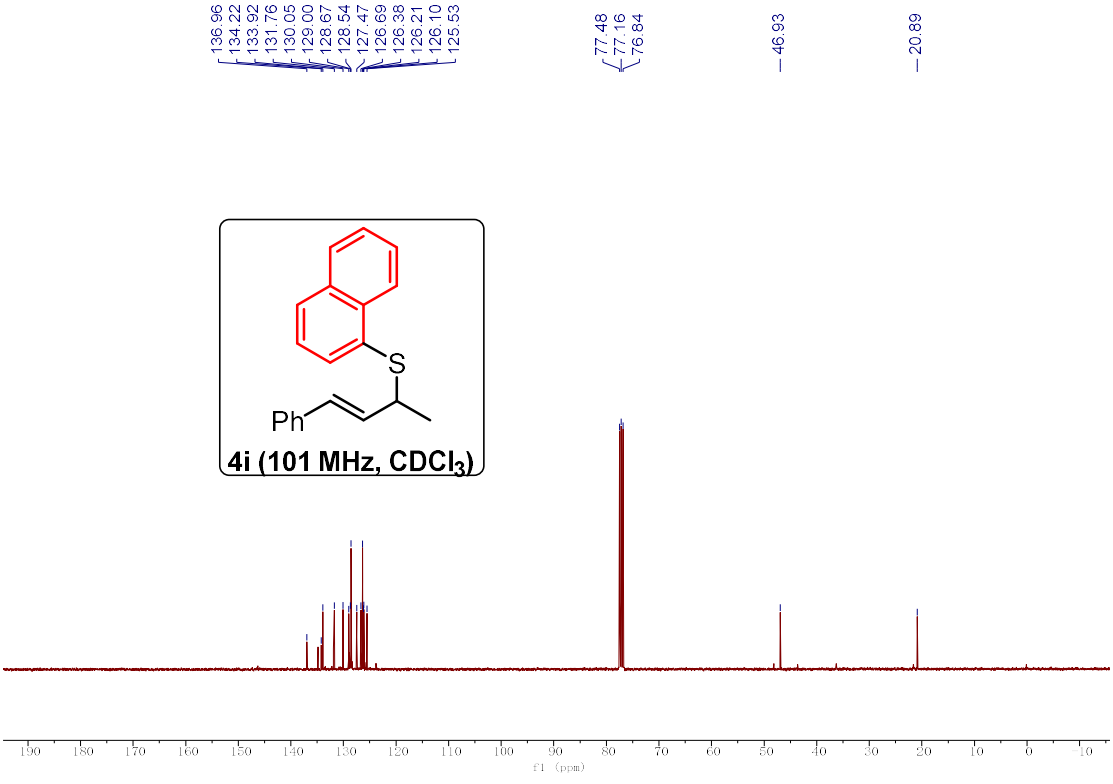

7.42
7.41
7.40
7.39
7.27
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.24
7.24
7.22
7.22
6.90
6.90
6.88
6.88
6.87
6.86
6.84
6.84
6.23
6.19
6.18
6.17
6.14
6.13
4.08
4.07
4.05
4.03
4.01
3.87
1.50
1.48
OMe
S
Ph
4g (400 MHz, CDCl3)
1.01
6.23
1.98
1.98
1.00
2.99
3.01
f1 (ppm)

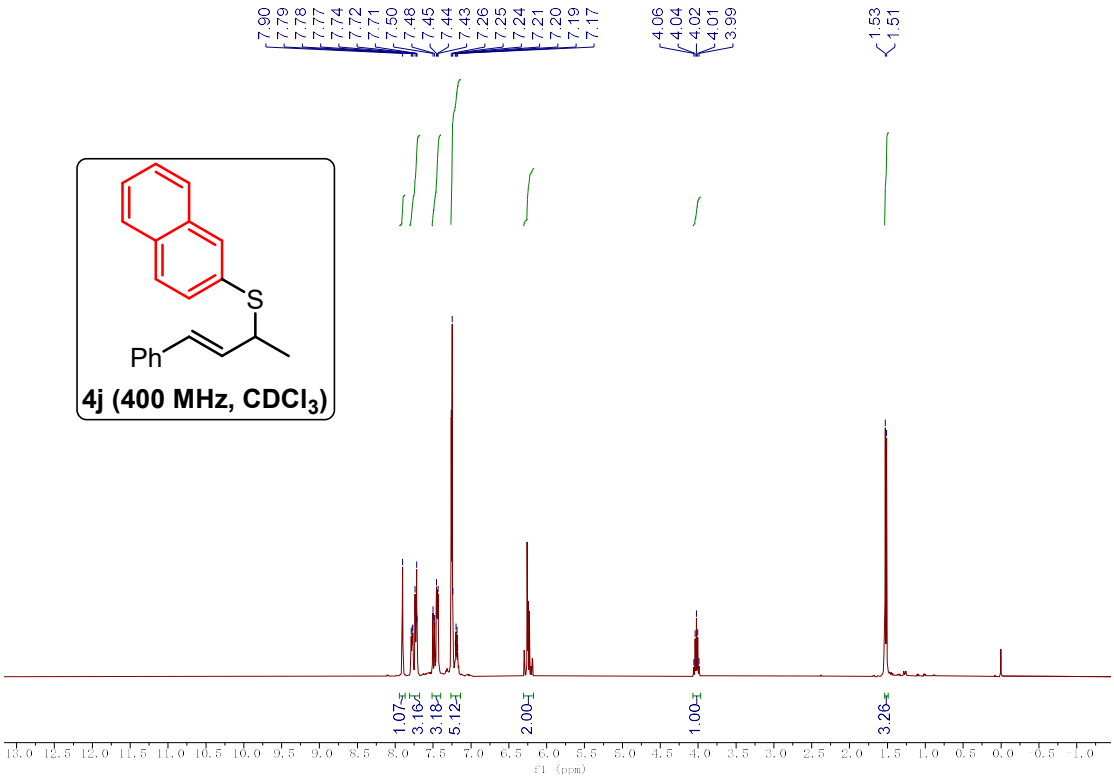

159.15
137.13
134.79
132.02
129.78
129.06
128.55
127.41
126.38
122.73
120.91
110.82
77.48
77.16
76.84
55.90
44.72
20.61
OMe
S
Ph
4g (101 MHz, CDCl3)
f1 (ppm)

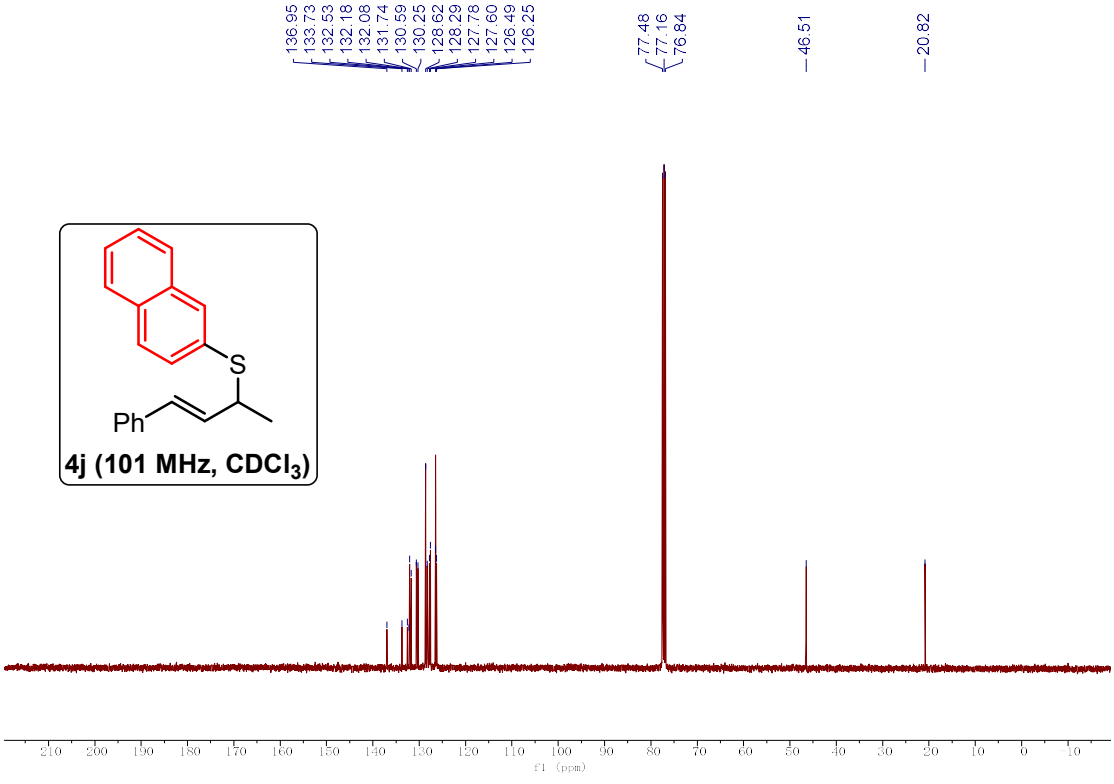

7.27
7.27
7.26
7.24
7.22
7.21
7.20
7.19
7.19
7.18
7.03
6.84
6.25
6.21
6.18
6.16
6.14
6.12
3.91
3.89
3.87
3.86
3.84
2.23
1.47
1.45
S
Ph
4h (400 MHz, CDCl3)
5.27
2.08
0.98
2.00
1.00
6.23
3.08
f1 (ppm)

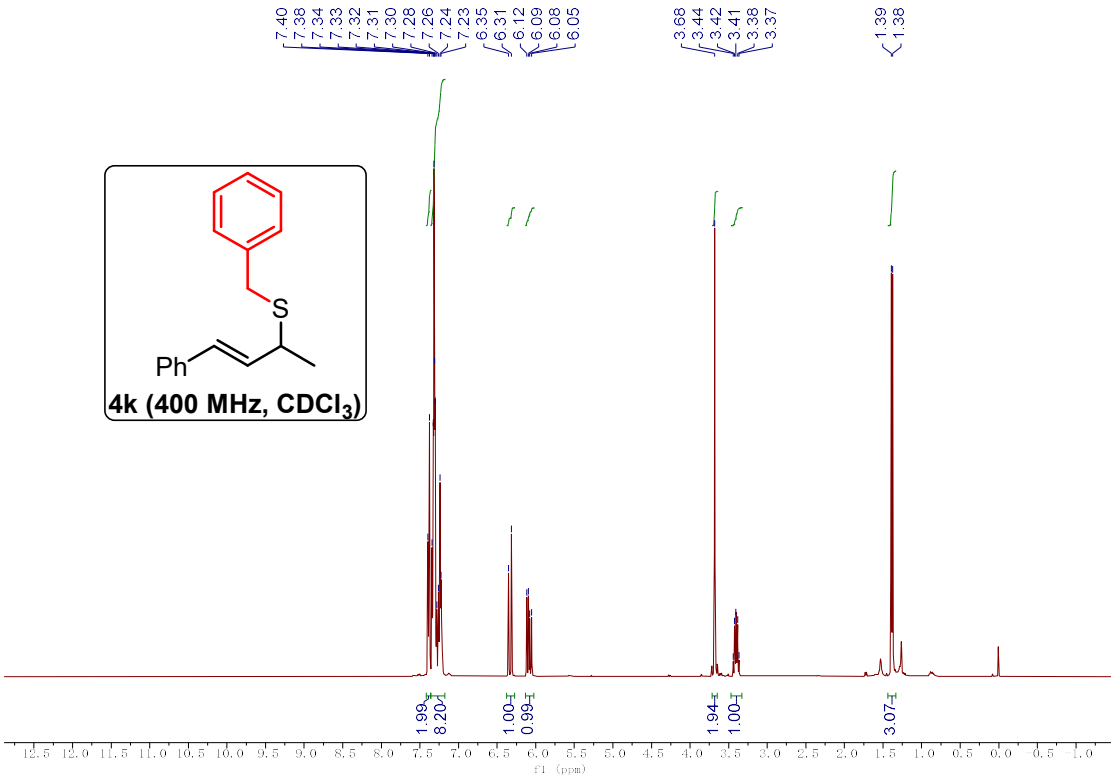

138.32
137.08
134.09
131.88
131.00
130.02
129.24
128.59
127.48
126.42
77.48
77.16
76.84
46.39
21.27
20.76
S
Ph
4h (101 MHz, CDCl3)
f1 (ppm)

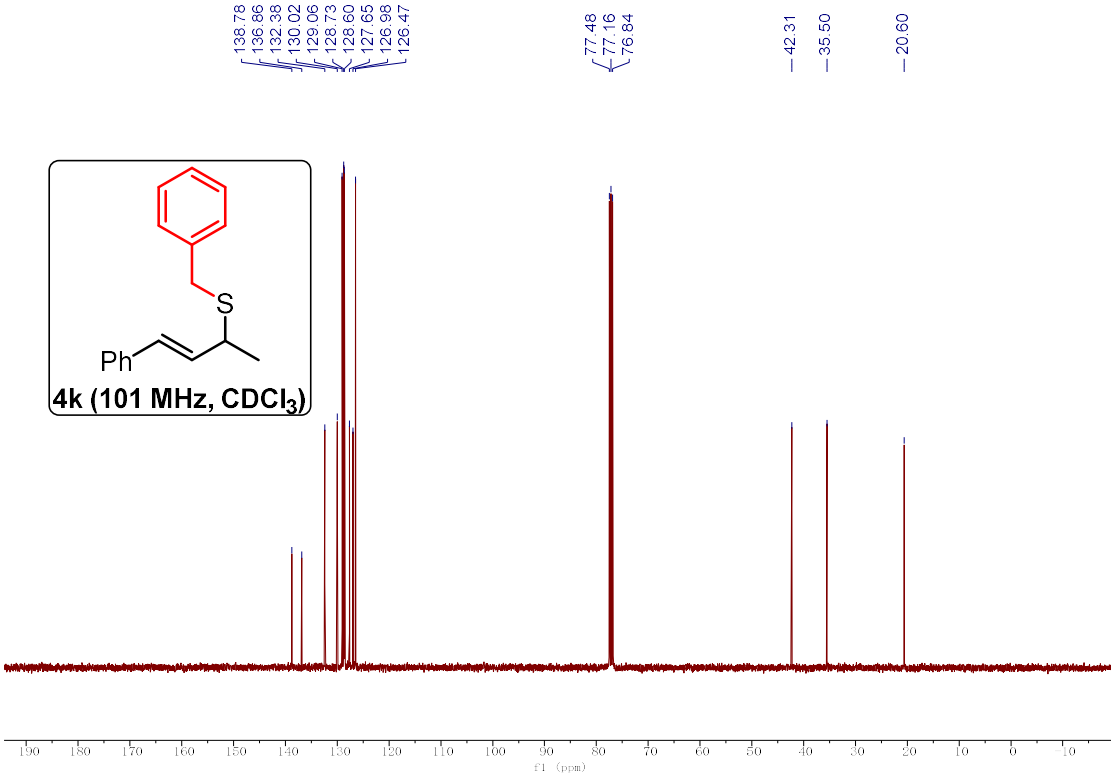

8.61
8.59
7.86
7.84
7.81
7.79
7.72
7.70
7.61
7.59
7.59
7.57
7.53
7.52
7.50
7.40
7.38
7.36
7.27
7.26
7.24
7.21
7.20
7.19
7.19
6.21
6.19
6.17
6.15
6.09
6.08
6.04
3.97
3.96
3.94
3.92
3.90
1.54
1.52
S
Ph
4i (400 MHz, CDCl3)
0.98
2.03
1.10
2.24
1.17
5.01
2.00
1.00
3.32
f1 (ppm)

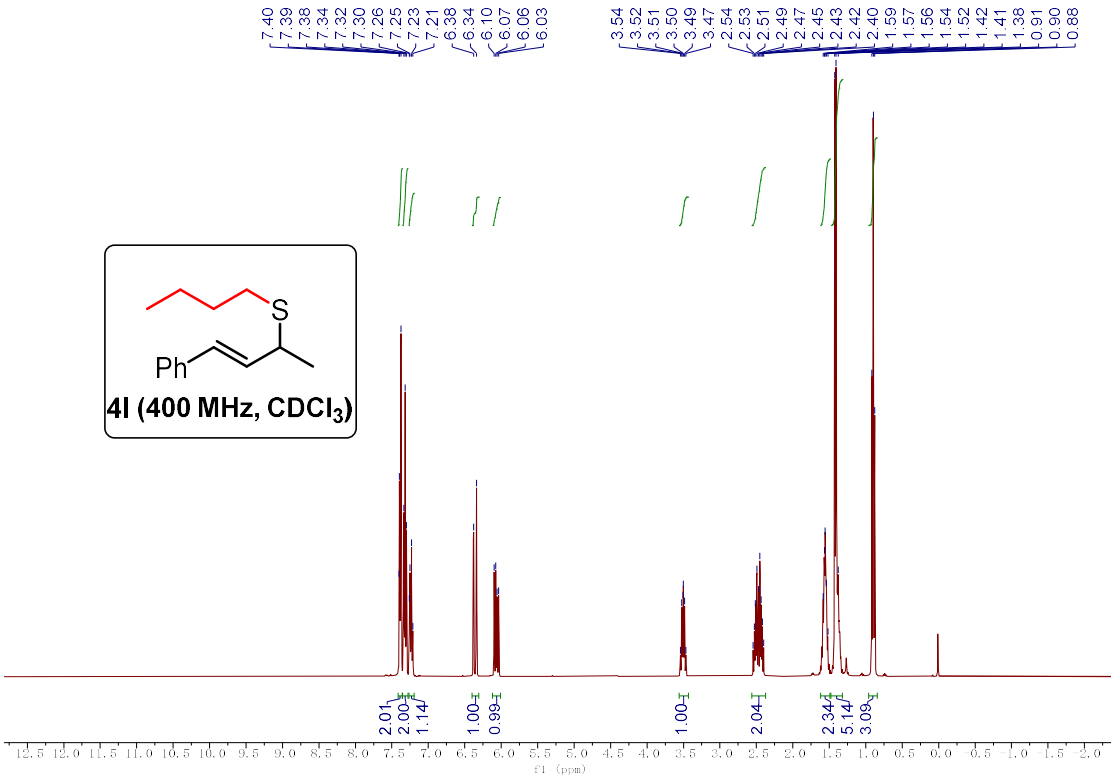

136.96
134.22
133.92
131.76
130.05
129.00
128.67
128.54
127.47
126.69
126.38
126.21
126.10
125.53
77.48
77.16
76.84
46.93
20.89
S
Ph
4i (101 MHz, CDCl3)
f1 (ppm)

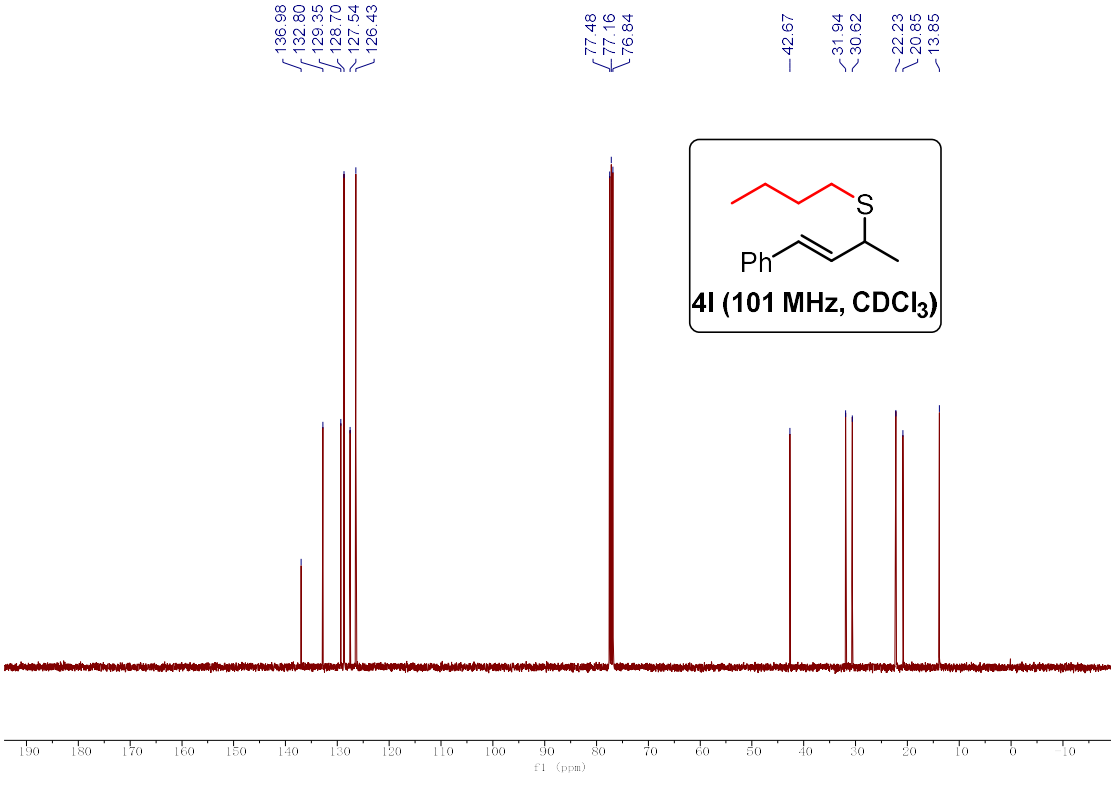

7.90
7.79
7.78
7.77
7.74
7.72
7.71
7.50
7.48
7.45
7.44
7.43
7.26
7.25
7.24
7.21
7.20
7.19
7.17
4.06
4.04
4.02
4.01
3.99
1.53
1.51
S
Ph
4j (400 MHz, CDCl3)
1.07
3.16
3.18
5.12
2.00
1.00
3.26
f1 (ppm)


136.95
133.73
132.53
132.18
132.08
131.74
130.59
130.25
128.62
128.29
127.78
127.60
126.49
126.25
77.48
77.16
76.84
46.51
20.82
S
Ph
4j (101 MHz, CDCl3)
f1 (ppm)


7.40
7.38
7.34
7.33
7.32
7.31
7.30
7.28
7.26
7.24
7.23
6.35
6.31
6.12
6.09
6.08
6.05
3.68
3.44
3.42
3.41
3.38
3.37
1.39
1.38
S
Ph
4k (400 MHz, CDCl3)
1.99
8.20
1.00
0.99
1.94
1.00
3.07
f1 (ppm)


138.78
136.86
132.38
130.02
129.06
128.73
128.60
127.65
126.98
126.47
77.48
77.16
76.84
42.31
35.50
20.60
S
Ph
4k (101 MHz, CDCl3)
f1 (ppm)


7.40
7.39
7.38
7.34
7.32
7.30
7.26
7.25
7.23
7.21
6.38
6.34
6.10
6.07
6.06
6.03
3.54
3.52
3.51
3.50
3.49
3.47
2.54
2.53
2.51
2.49
2.47
2.45
2.43
2.42
2.40
1.59
1.57
1.56
1.54
1.52
1.42
1.41
1.38
0.91
0.90
0.88
S
Ph
4l (400 MHz, CDCl3)
2.01
2.00
1.14
1.00
0.99
1.00
2.04
2.34
5.14
3.09
f1 (ppm)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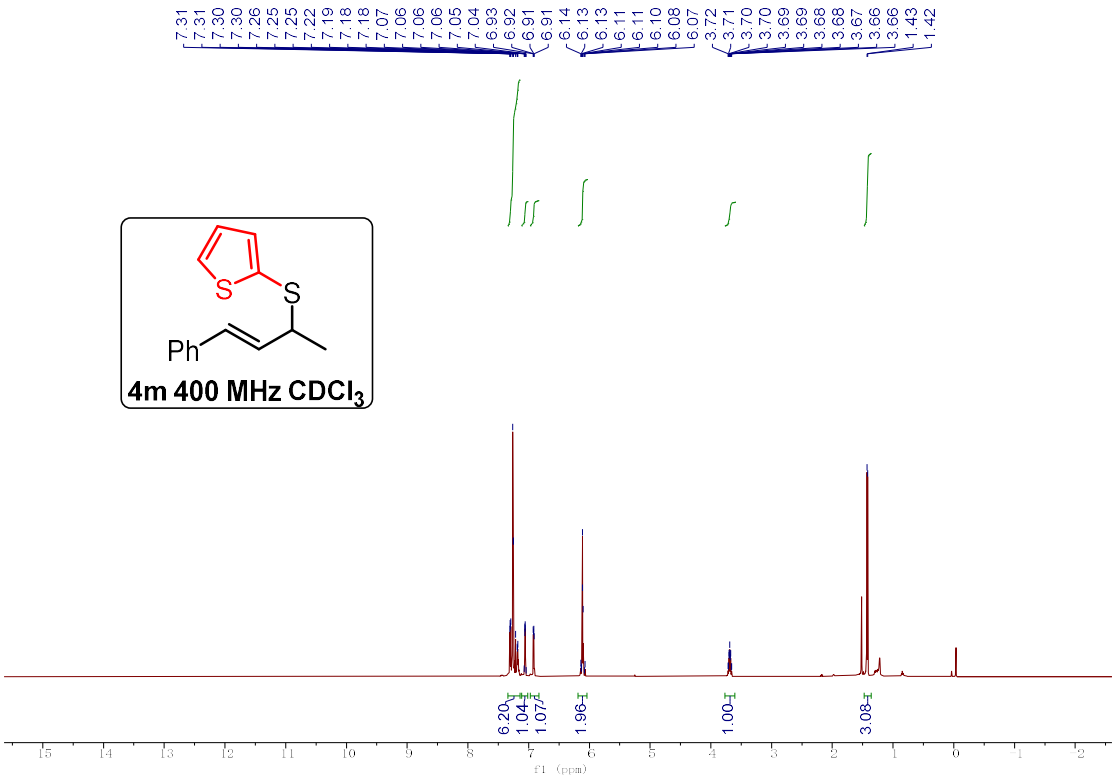
132.80
129.35
128.70
127.54
126.43
77.48
77.16
76.84
42.67
31.94
30.62
22.23
20.85
13.85
S
Ph
4l (101 MHz, CDCl3)
f1 (ppm)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7.22
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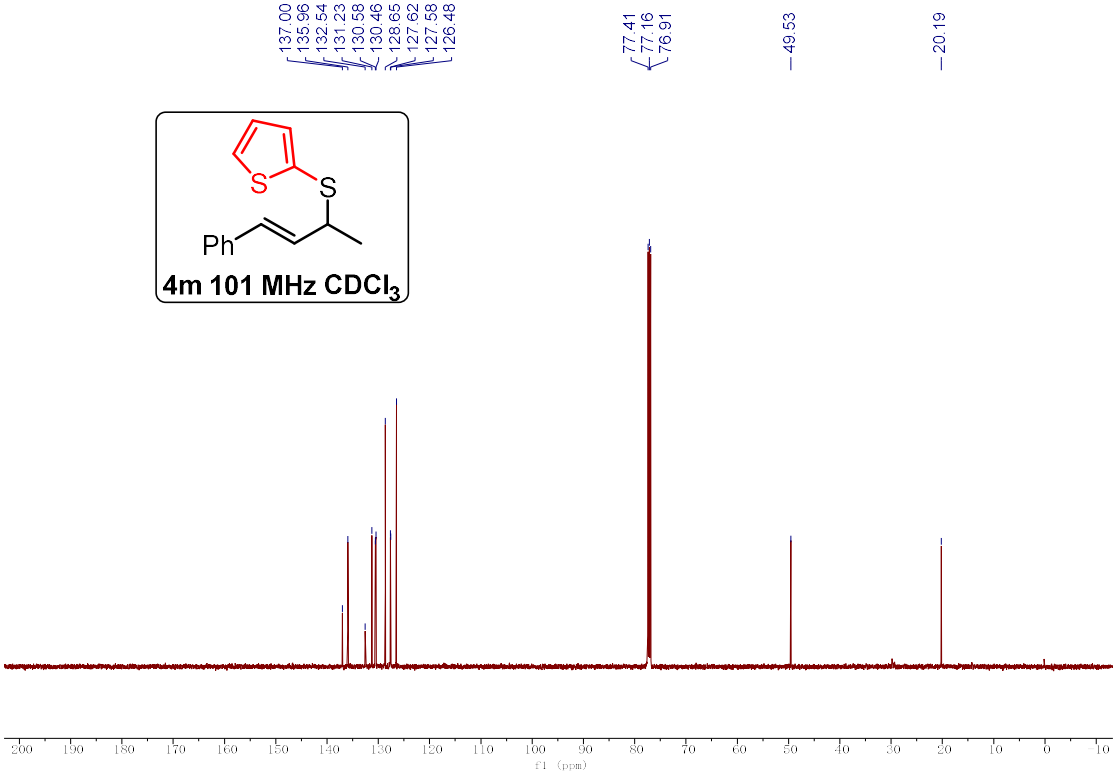
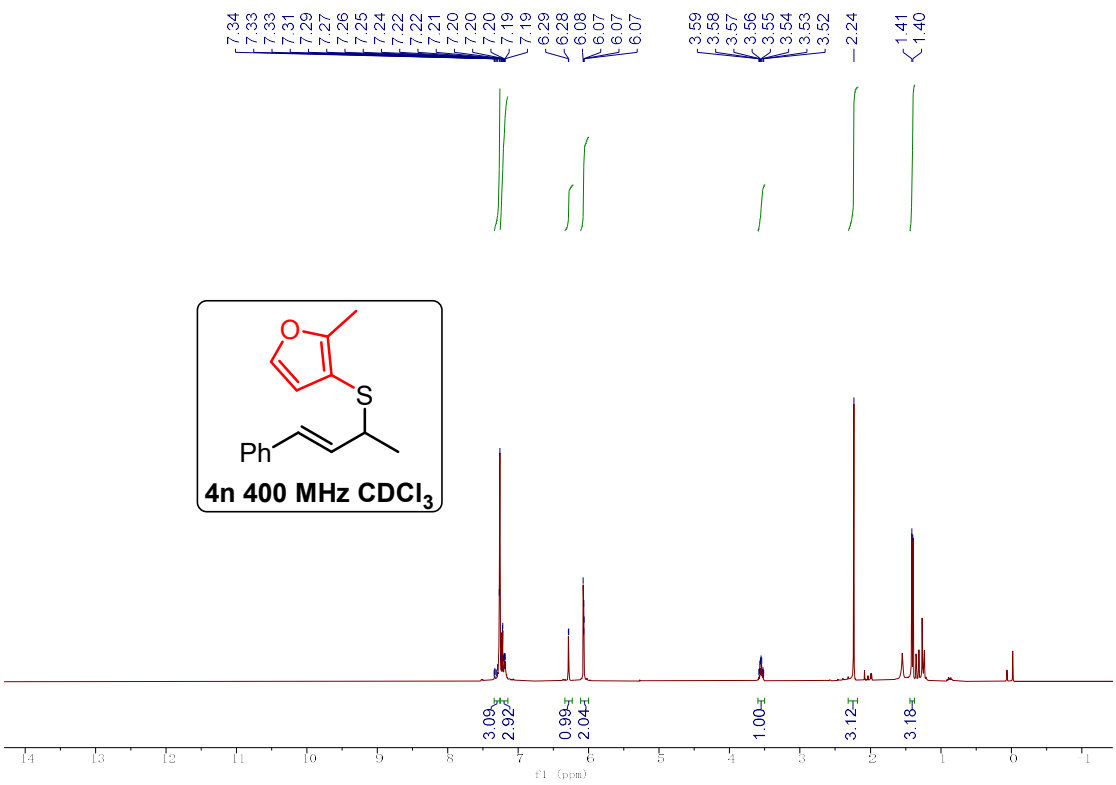
7.18
7.18
7.07
7.06
7.06
7.06
7.05
7.04
6.93
6.92
6.91
6.91
6.14
6.13
6.13
6.11
6.11
6.10
6.08
6.07
3.72
3.71
3.70
3.70
3.69
3.69
3.68
3.68
3.67
3.66
3.66
1.43
1.42
S
S
Ph
4m 400 MHz CDCl3
6.20
1.04
1.07
1.96
1.00
3.08
f1 (ppm)


137.00
135.96
132.54
131.23
130.58
130.46
128.65
127.62
127.58
126.48
77.41
77.16
76.91
49.53
20.19
S
S
Ph
4m 101 MHz CDCl3
f1 (ppm)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7.33
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7.31
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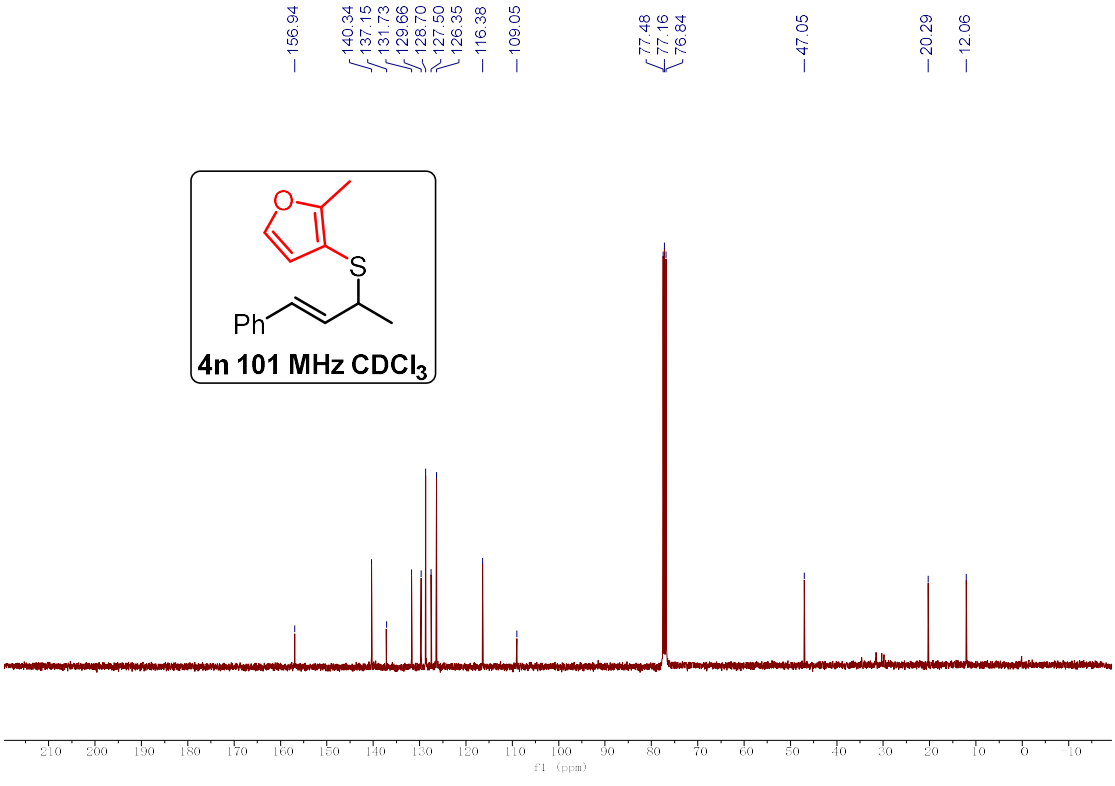
7.27
7.26
7.25
7.24
7.22
7.22
7.21
7.20
7.20
7.20
7.19
6.29
6.28
6.08
6.07
6.07
6.07
3.59
3.58
3.57
3.56
3.55
3.54
3.53
3.52
2.24
1.41
1.40
O
S
Ph
4n 400 MHz CDCl3
3.09
2.92
0.99
2.04
1.00
3.12
3.18
f1 (ppm)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140.34
137.15
131.73
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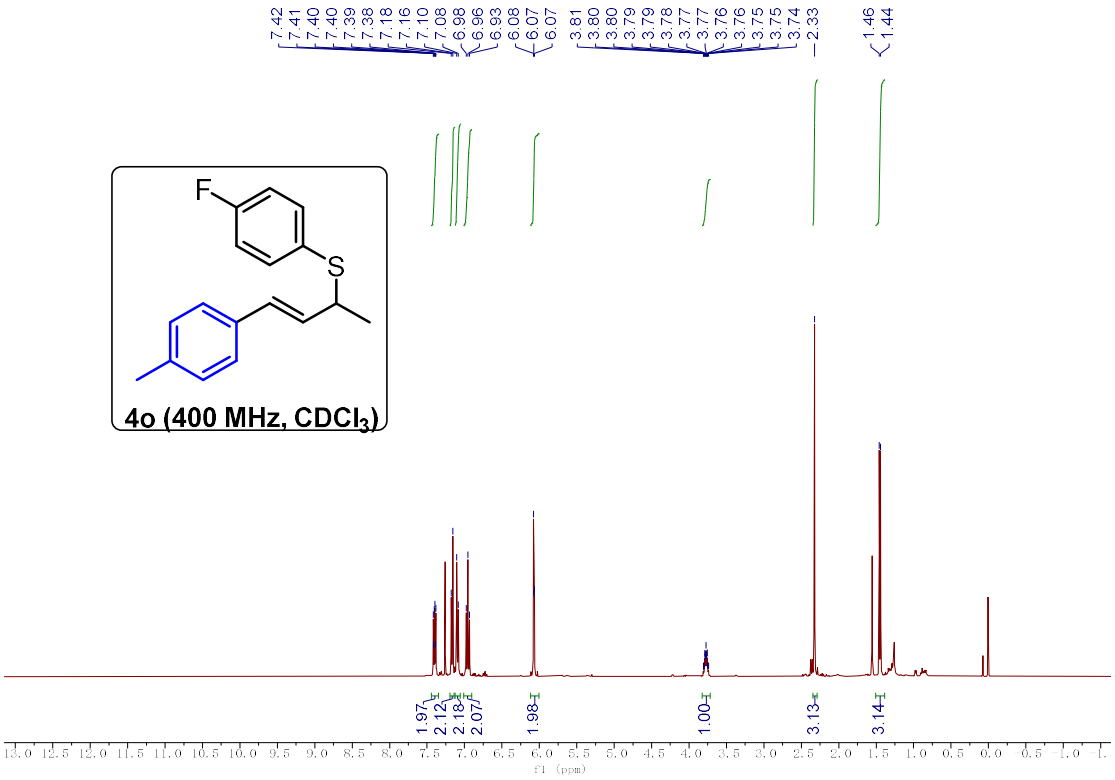
128.70
127.50
126.35
116.38
109.05
77.48
77.16
76.84
47.05
20.29
12.06
O
S
Ph
4n 101 MHz CDCl3
f1 (ppm)


7.42
7.41
7.40
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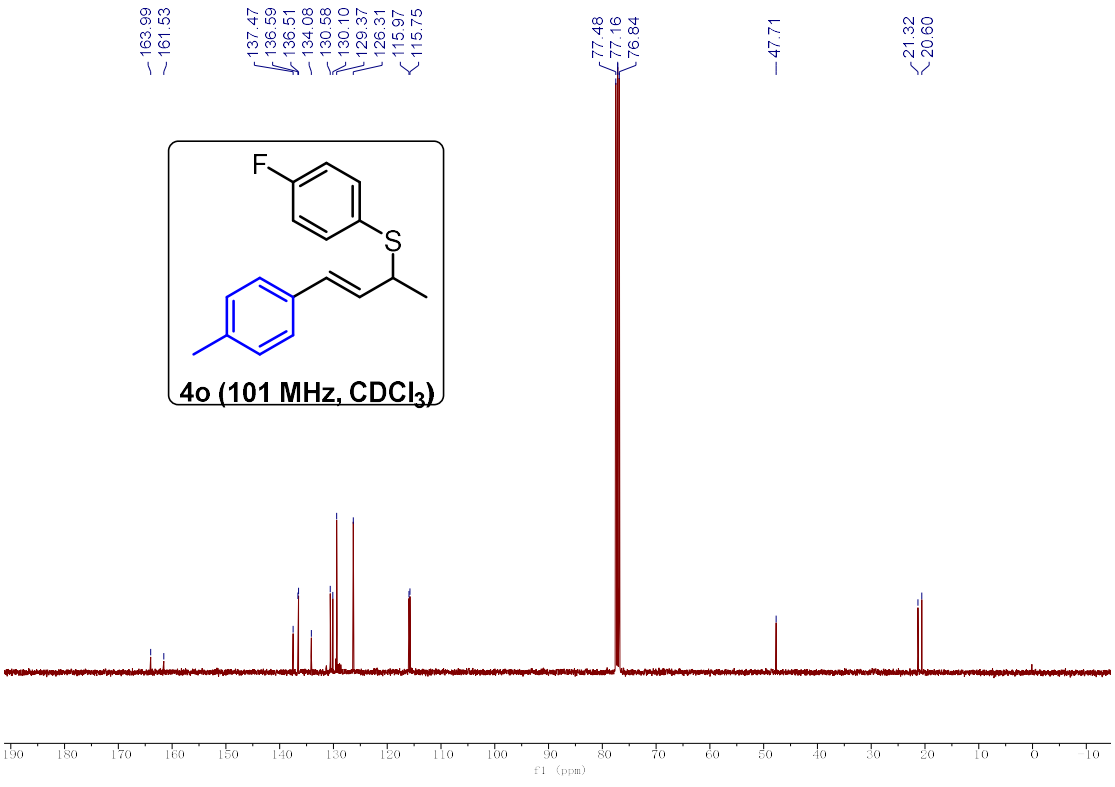
7.38
7.18
7.16
7.10
7.08
6.98
6.96
6.93
6.08
6.07
6.07
3.81
3.80
3.80
3.79
3.79
3.78
3.77
3.77
3.76
3.76
3.75
3.75
3.74
2.33
1.46
1.44
F
S
4o (400 MHz, CDCl3)
1.97
2.12
2.18
2.07
1.98
1.00
3.13
3.14
f1 (ppm)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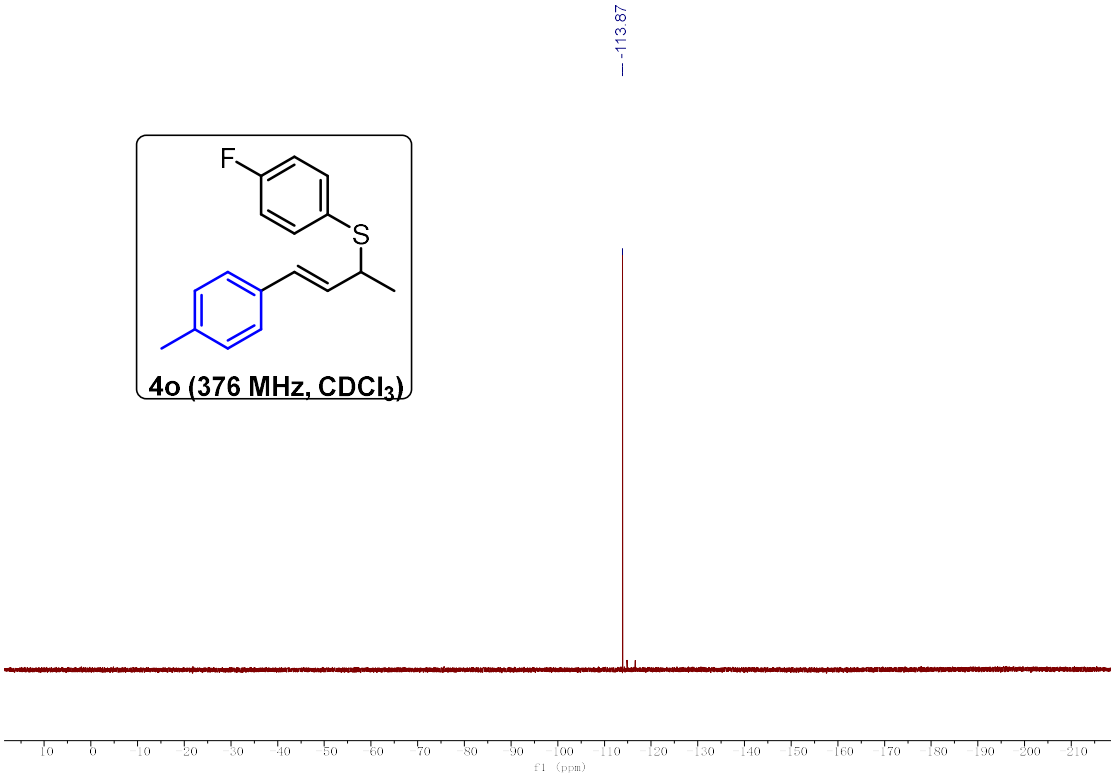
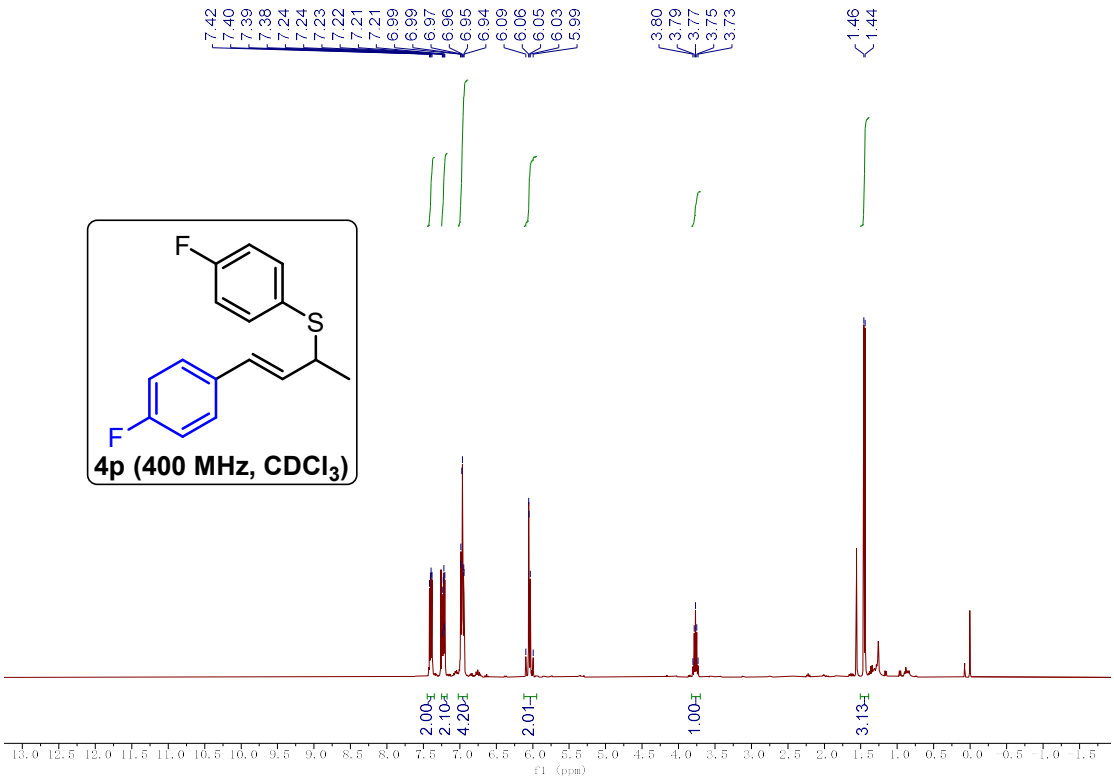
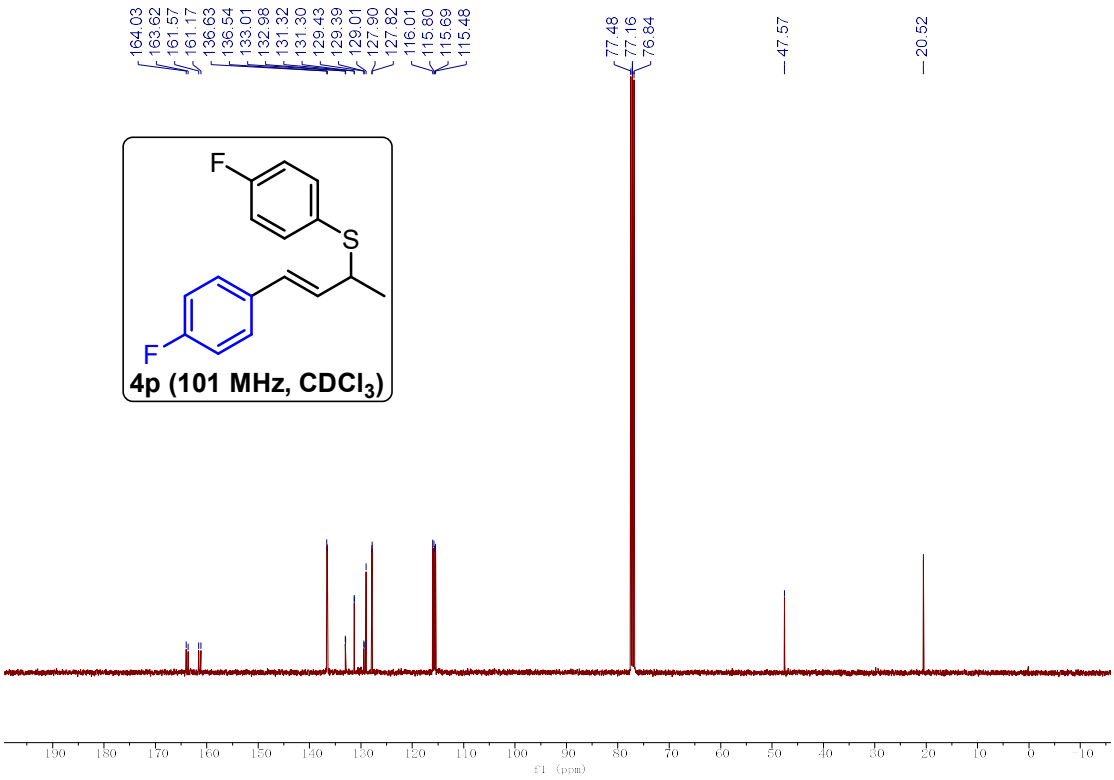
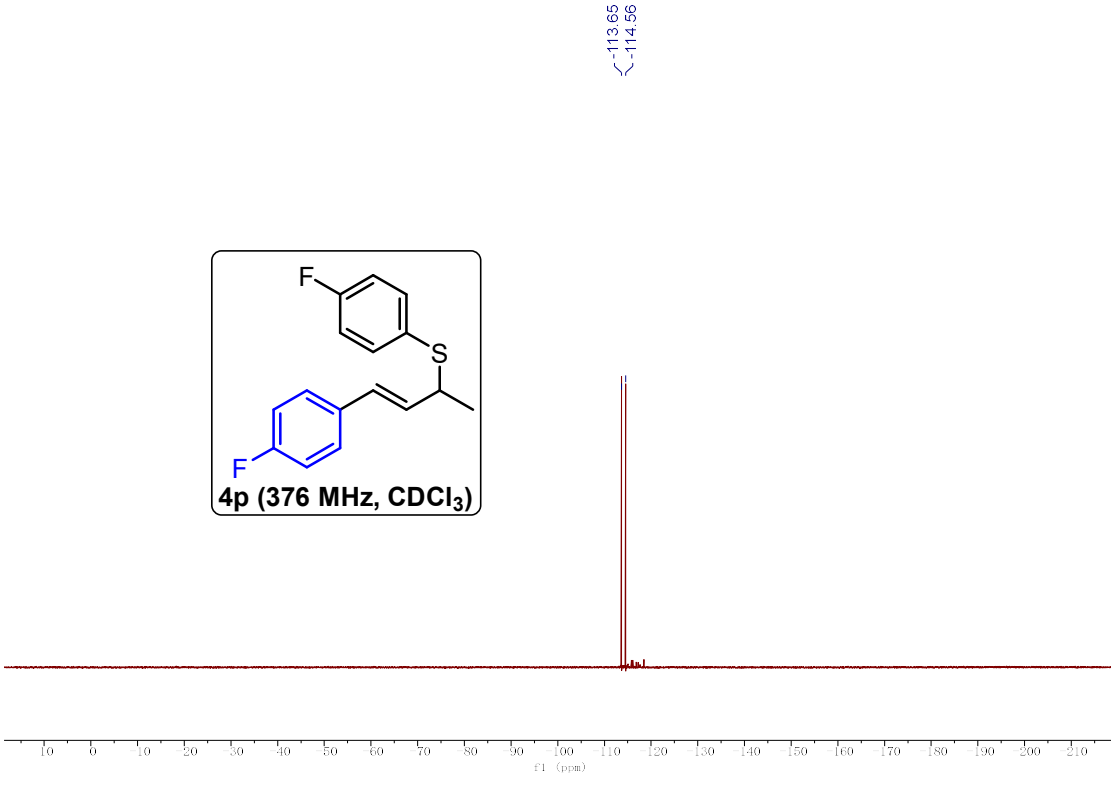
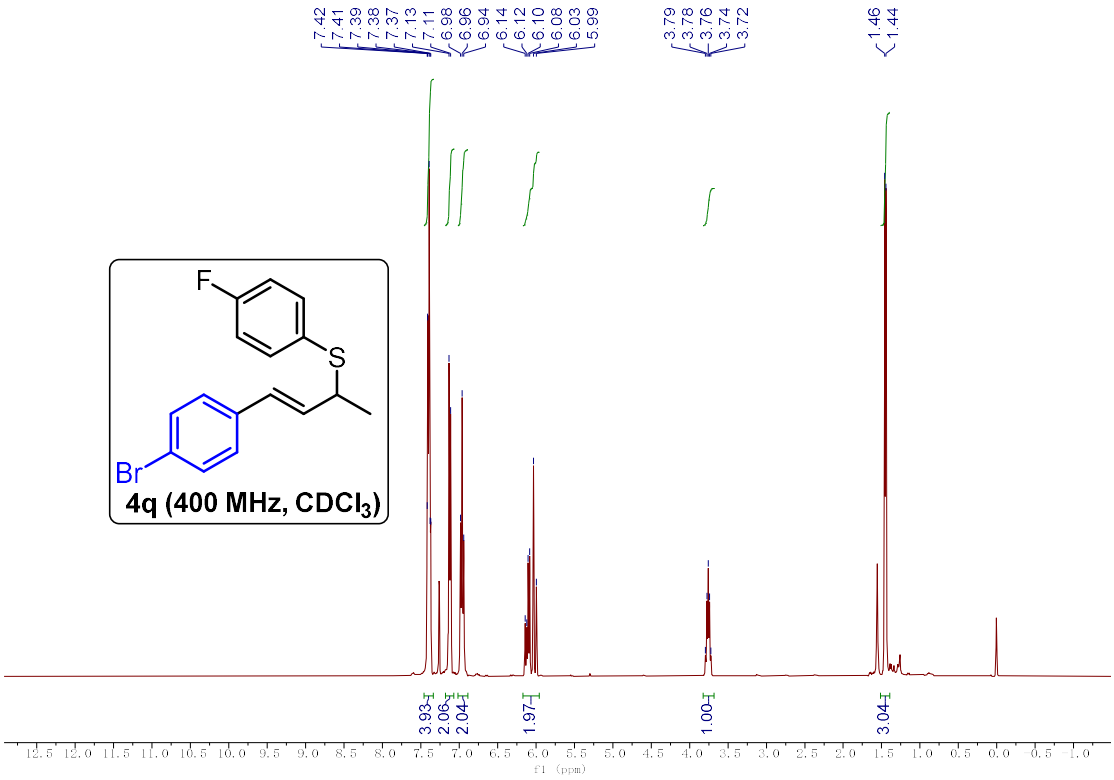
137.47
136.59
136.51
134.08
130.58
130.10
129.37
126.31
115.97
115.75
77.48
77.16
76.84
47.71
21.32
20.60
F
S
4o (101 MHz, CDCl3)
f1 (ppm)

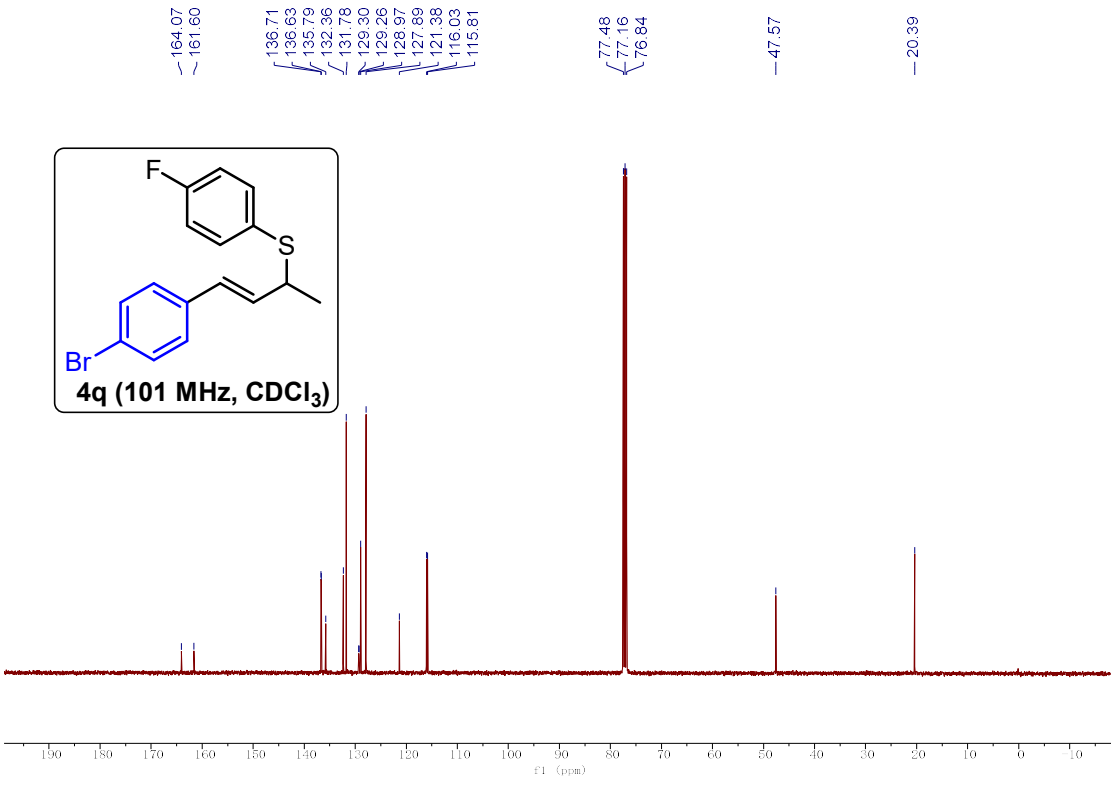

-113.87
F
S
4o (376 MHz, CDCl3)
f1 (ppm)


7.42
7.40
7.39
7.38
7.24
7.24
7.23
7.22
7.21
7.21
6.99
6.99
6.97
6.96
6.95
6.94
6.09
6.06
6.05
6.03
5.99
3.80
3.79
3.77
3.75
3.73
1.46
1.44
F
S
F
4p (400 MHz, CDCl3)
2.00
2.10
4.20
2.01
1.00
3.13
f1 (ppm)


164.03
163.62
161.57
161.17
136.63
136.54
133.01
132.98
131.32
131.30
129.43
129.39
129.01
127.90
127.82
116.01
115.80
115.69
115.48
77.48
77.16
76.84
47.57
20.52
F
S
F
4p (101 MHz, CDCl3)
f1 (ppm)


-113.65
-114.56
F
S
F
4p (376 MHz, CDCl3)
f1 (ppm)


7.42
7.41
7.39
7.38
7.37
7.13
7.11
6.98
6.96
6.94
6.14
6.12
6.10
6.08
6.03
5.99
3.79
3.78
3.76
3.74
3.72
1.46
1.44
F
S
Br
4q (400 MHz, CDCl3)
3.93
2.06
2.04
1.97
1.00
3.04
f1 (ppm)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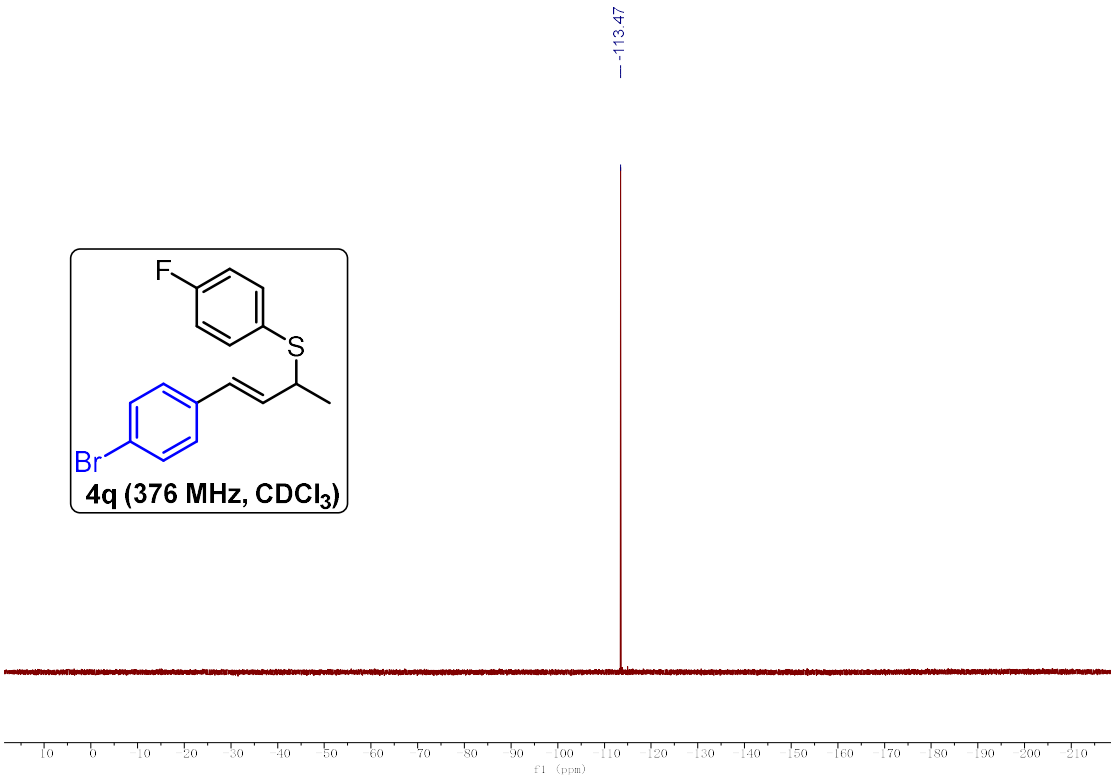
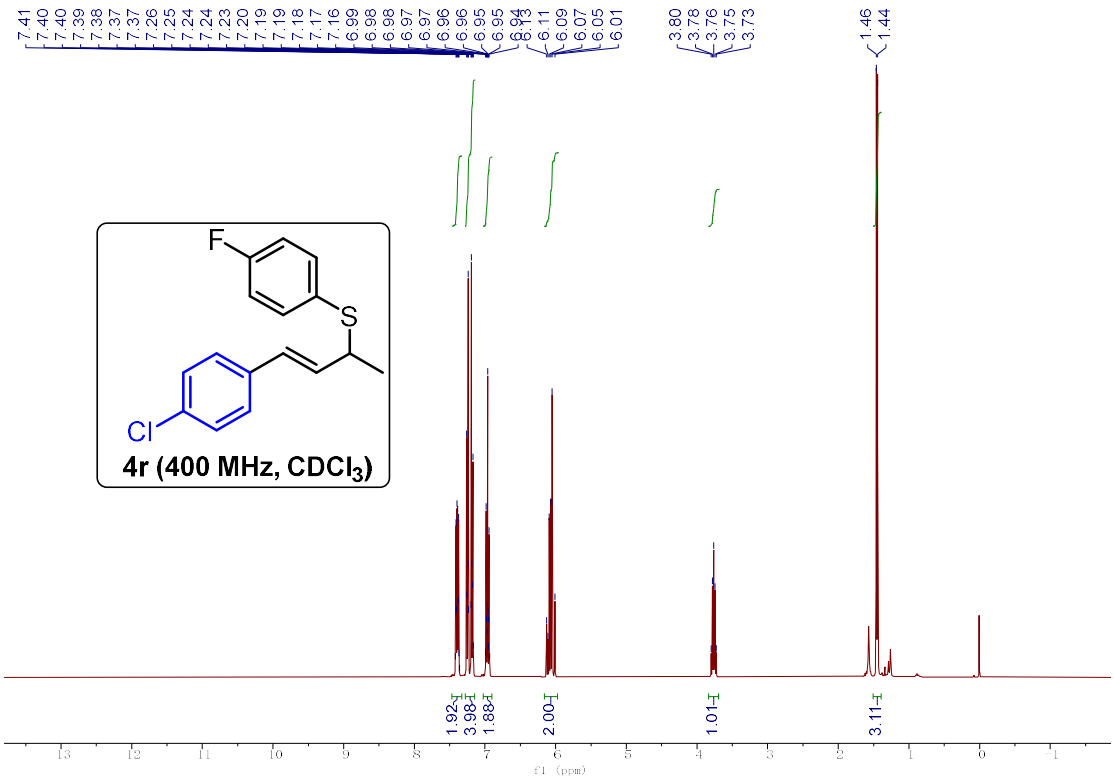
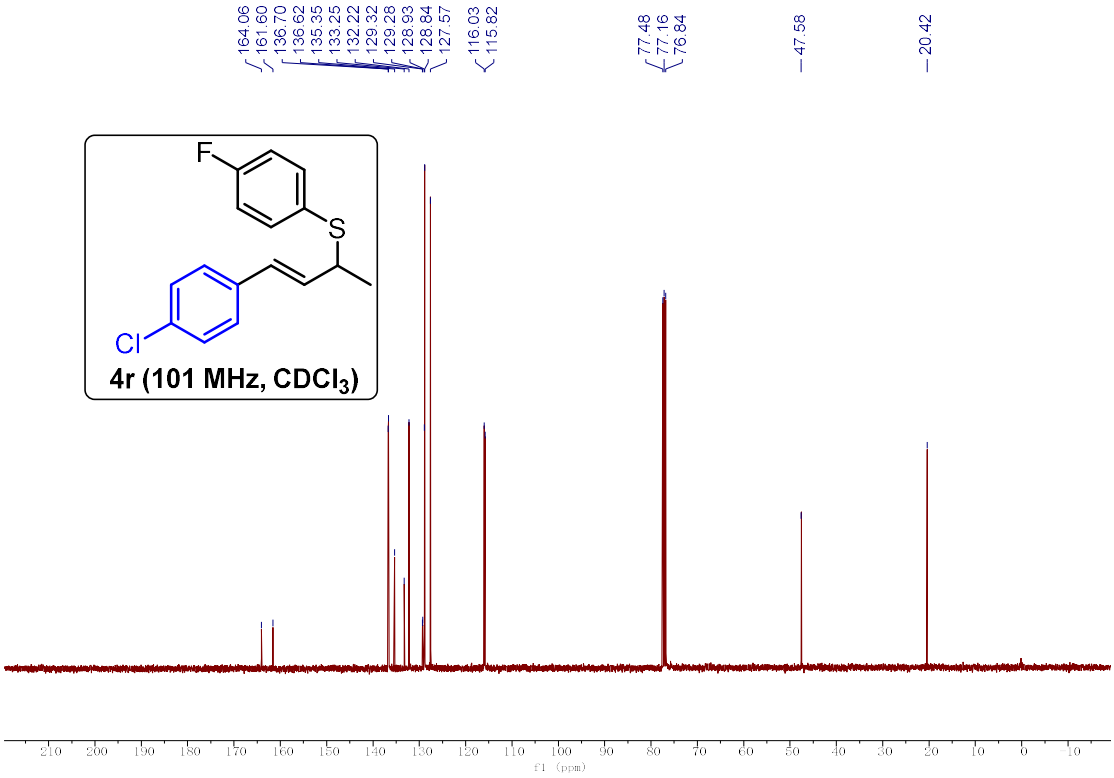
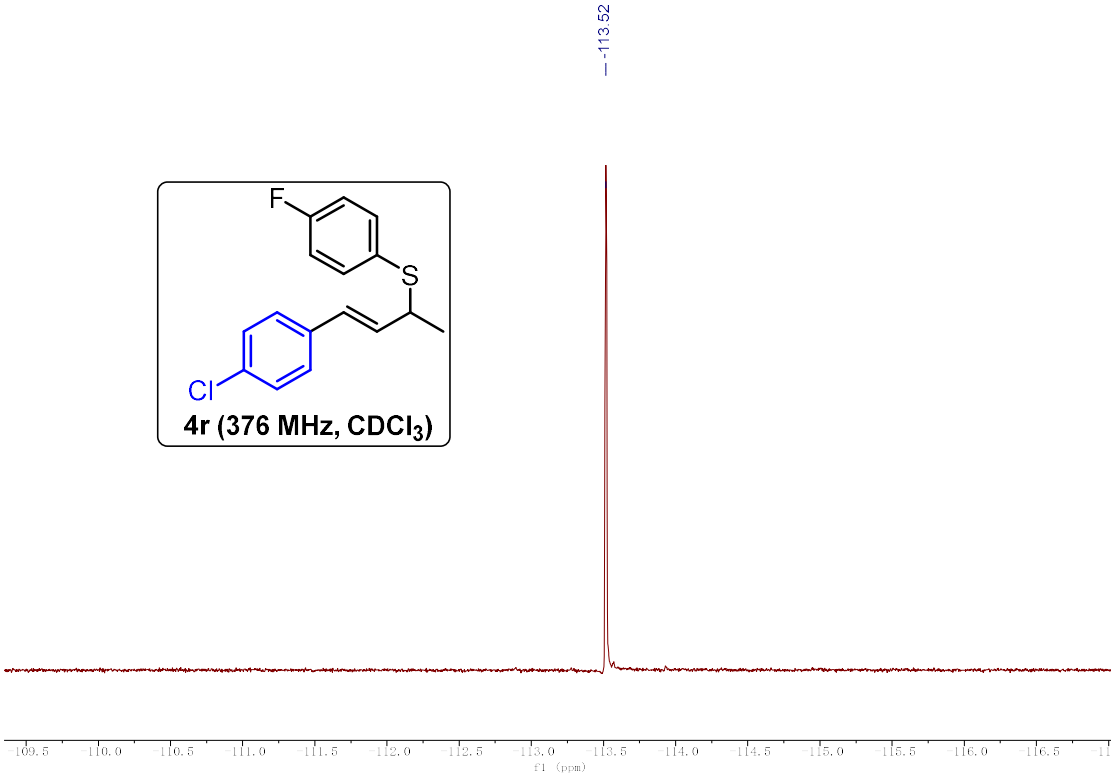
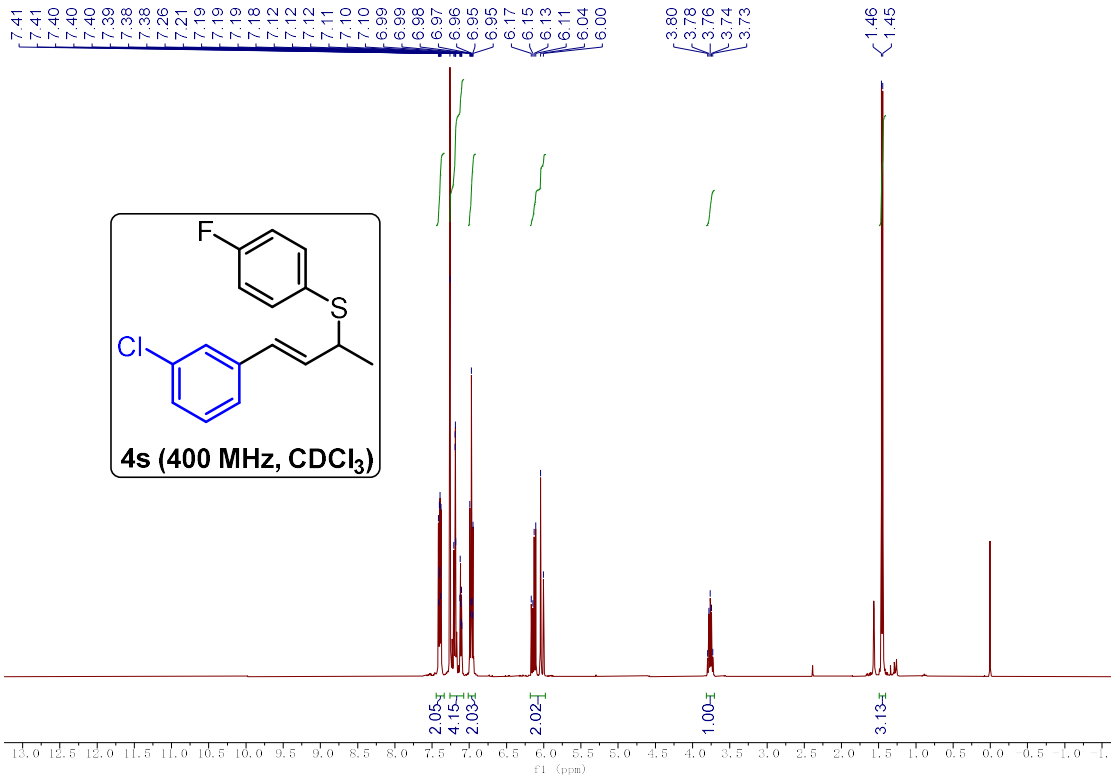
161.60
136.71
136.63
135.79
132.36
131.78
129.30
129.26
128.97
127.89
121.38
116.03
115.81
77.48
77.16
76.84
47.57
20.39
F
S
Br
4q (101 MHz, CDCl3)
f1 (ppm)

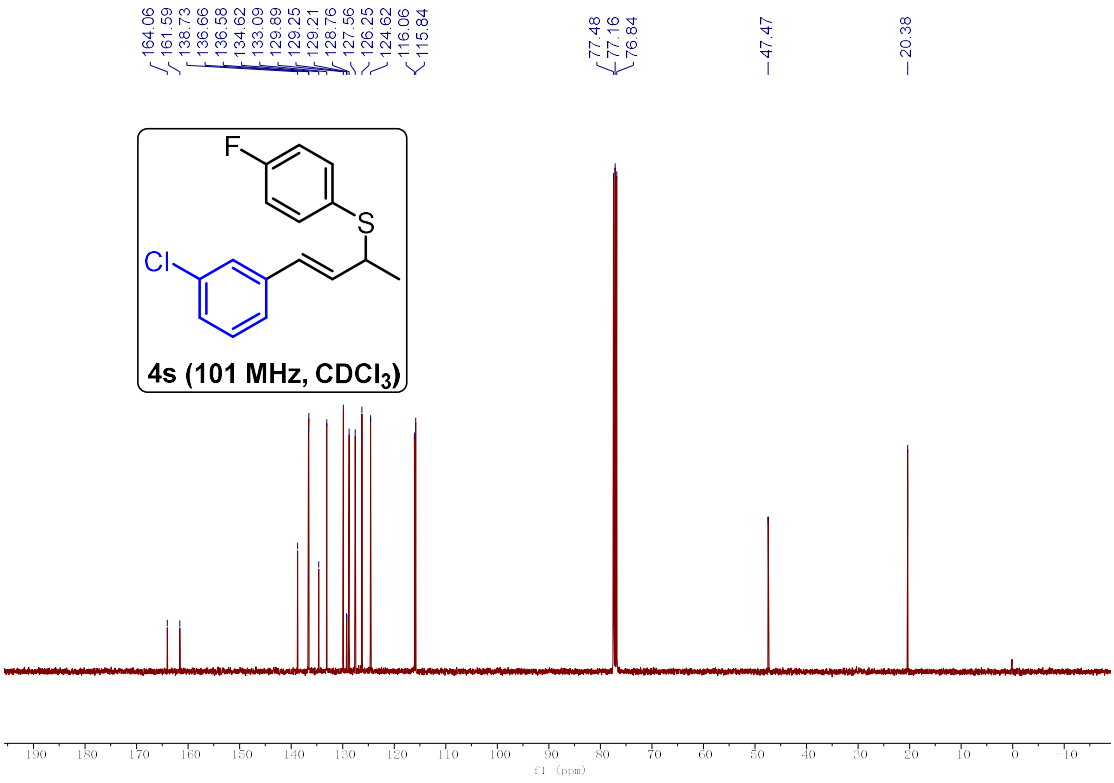

-113.47
F
S
Br
4q (376 MHz, CDCl3)


7.41
7.40
7.40
7.39
7.38
7.37
7.37
7.26
7.25
7.24
7.24
7.23
7.20
7.19
7.19
7.18
7.17
7.16
6.99
6.98
6.98
6.97
6.97
6.96
6.96
6.95
6.94
6.13
6.11
6.09
6.07
6.05
6.01
3.80
3.78
3.76
3.75
3.73
1.46
1.44
F
S
Cl
4r (400 MHz, CDCl3)
1.92
3.98
1.88
2.00
1.01
3.11


164.06
161.60
136.70
136.62
135.35
133.25
132.22
129.32
129.28
128.93
128.84
127.57
116.03
115.82
77.48
77.16
76.84
47.58
20.42
F
S
Cl
4r (101 MHz, CDCl3)
f1 (ppm)


-113.52
F
S
Cl
4r (376 MHz, CDCl3)
f1 (ppm)


7.41
7.41
7.40
7.40
7.40
7.39
7.38
7.38
7.26
7.21
7.19
7.19
7.19
7.18
7.12
7.12
7.12
7.11
7.10
7.10
6.99
6.99
6.98
6.97
6.96
6.95
6.95
6.17
6.15
6.13
6.11
6.04
6.00
3.80
3.78
3.76
3.74
3.73
1.46
1.45
F
S
Cl
4s (400 MHz, CDCl3)
2.05
4.15
2.03
2.02
1.00
3.13
f1 (ppm)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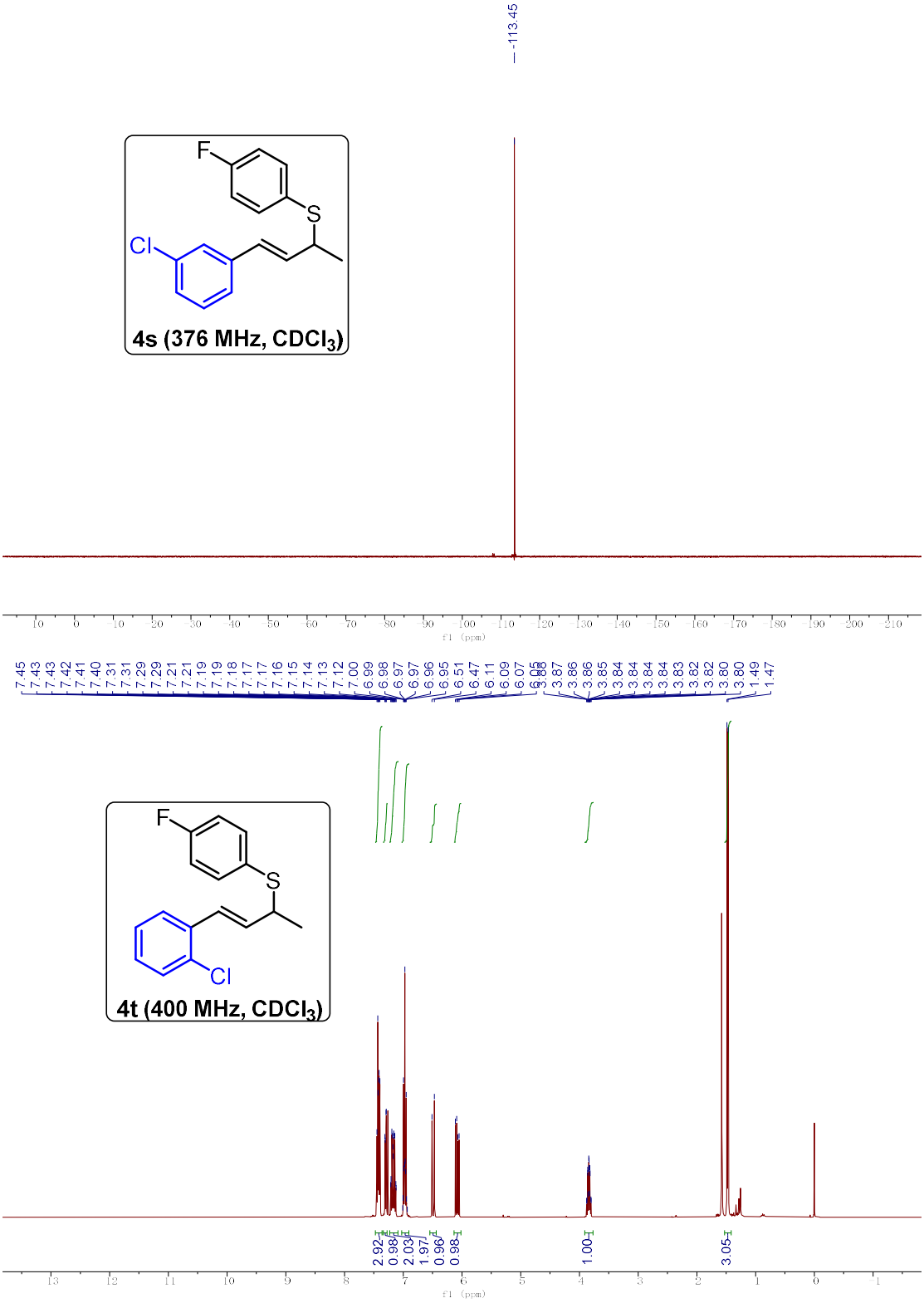
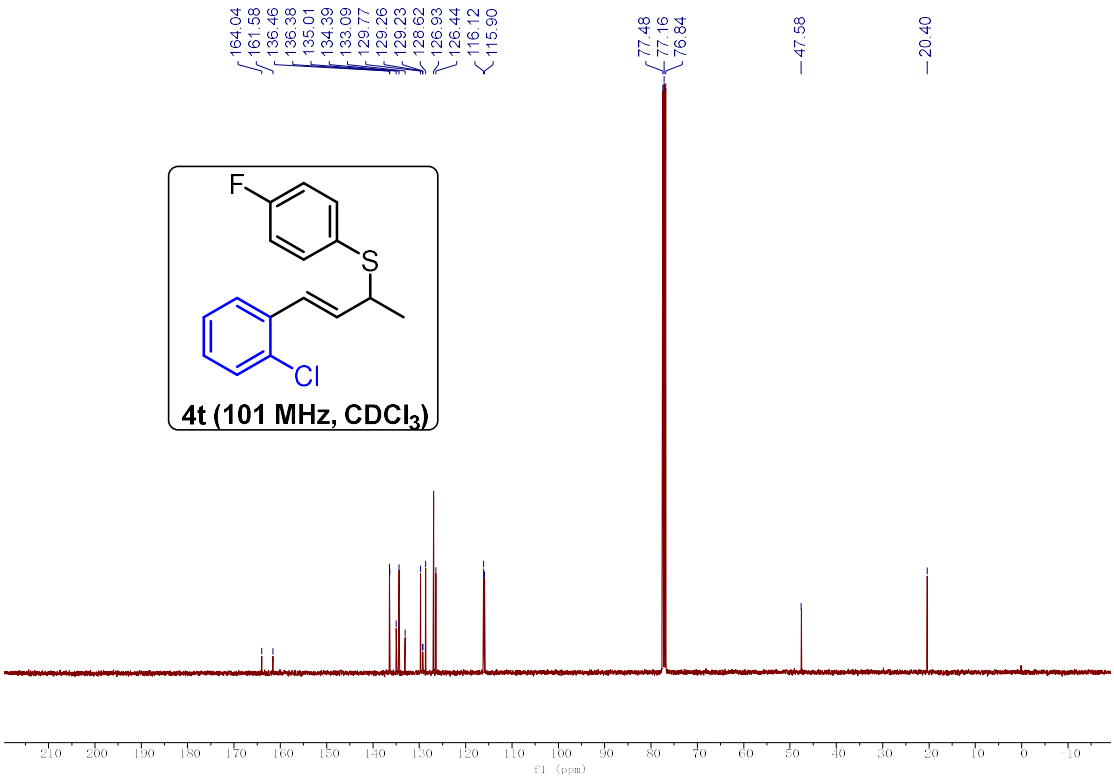
161.59
138.73
136.66
136.58
134.62
133.09
129.89
129.25
129.21
128.76
127.56
126.25
124.62
116.06
115.84
77.48
77.16
76.84
47.47
20.38
F
S
Cl
4s (101 MHz, CDCl3)
f1 (ppm)


-113.45
F
S
Cl
4s (376 MHz, CDCl3)
7.45 7.43 7.43 7.42 7.41 7.40 7.31 7.31 7.29 7.29 7.21 7.21 7.19 7.19 7.18 7.17 7.17 7.16 7.15 7.14 7.13 7.12 7.00 6.99 6.98 6.97 6.97 6.96 6.95 6.51 6.47 6.11 6.09 6.07 3.87 3.86 3.86 3.85 3.84 3.84 3.84 3.84 3.83 3.82 3.82 3.80 3.80 1.49 1.47
F
S
Cl
4t (400 MHz, CDCl3)
2.92 0.98 2.03 1.97 0.96 0.98 1.00 3.05
f1 (ppm)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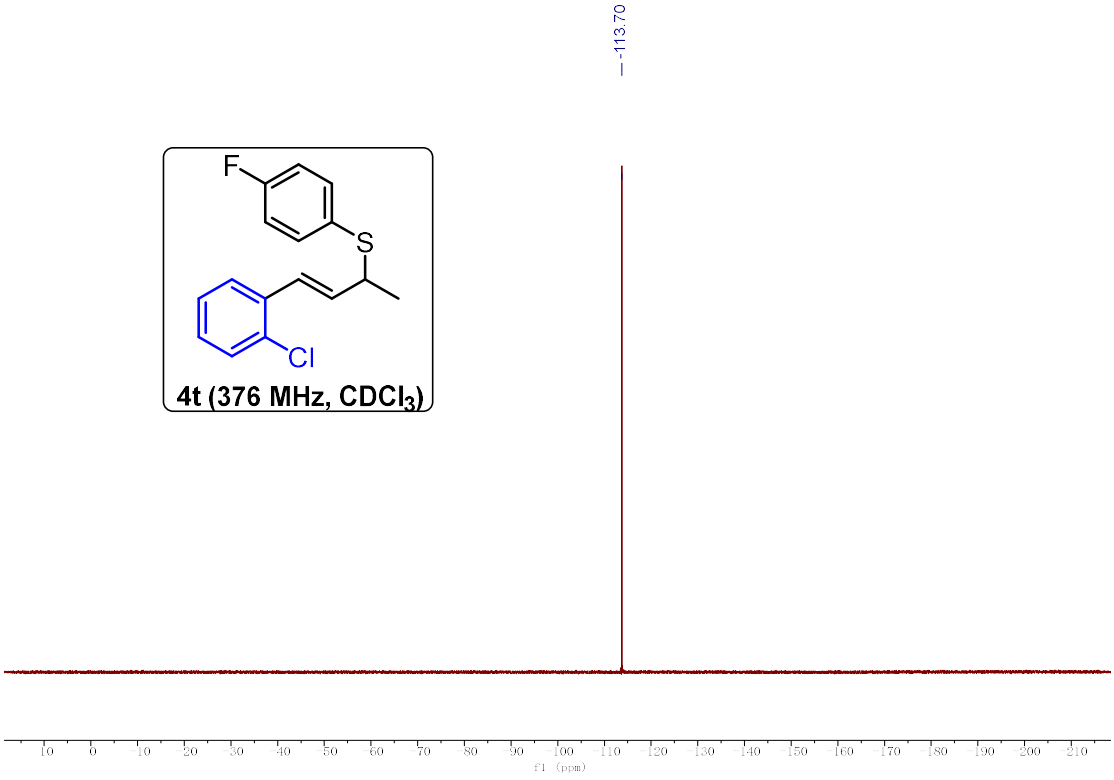
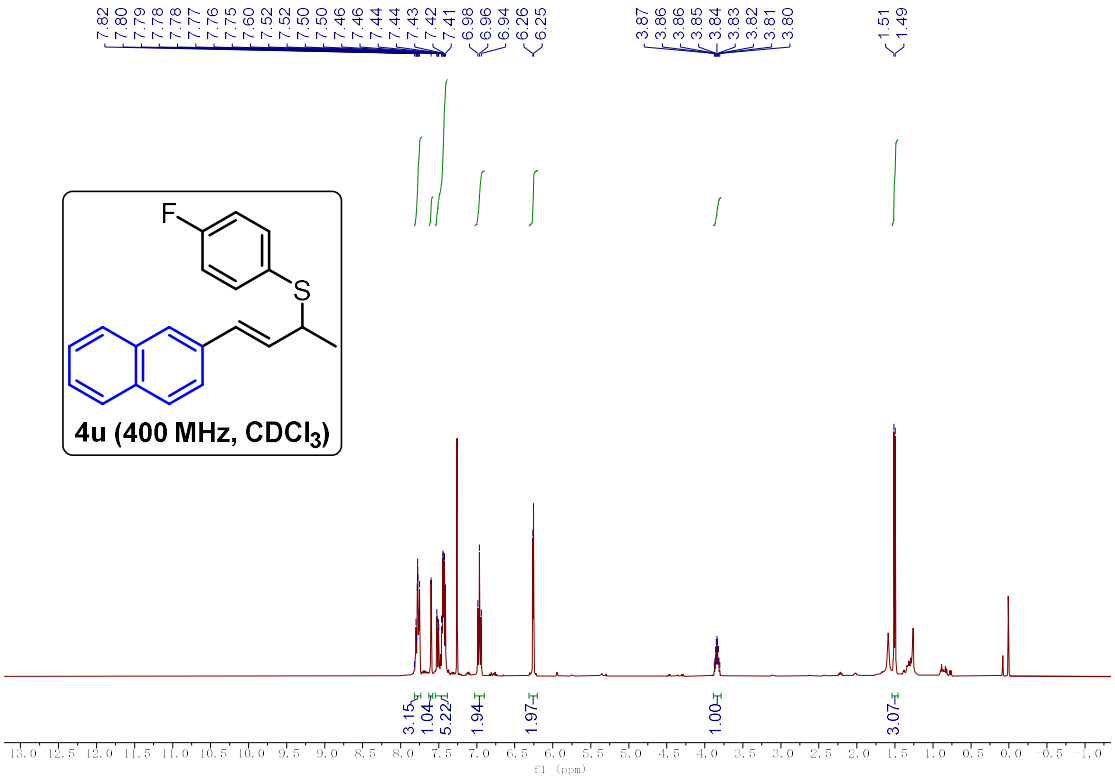
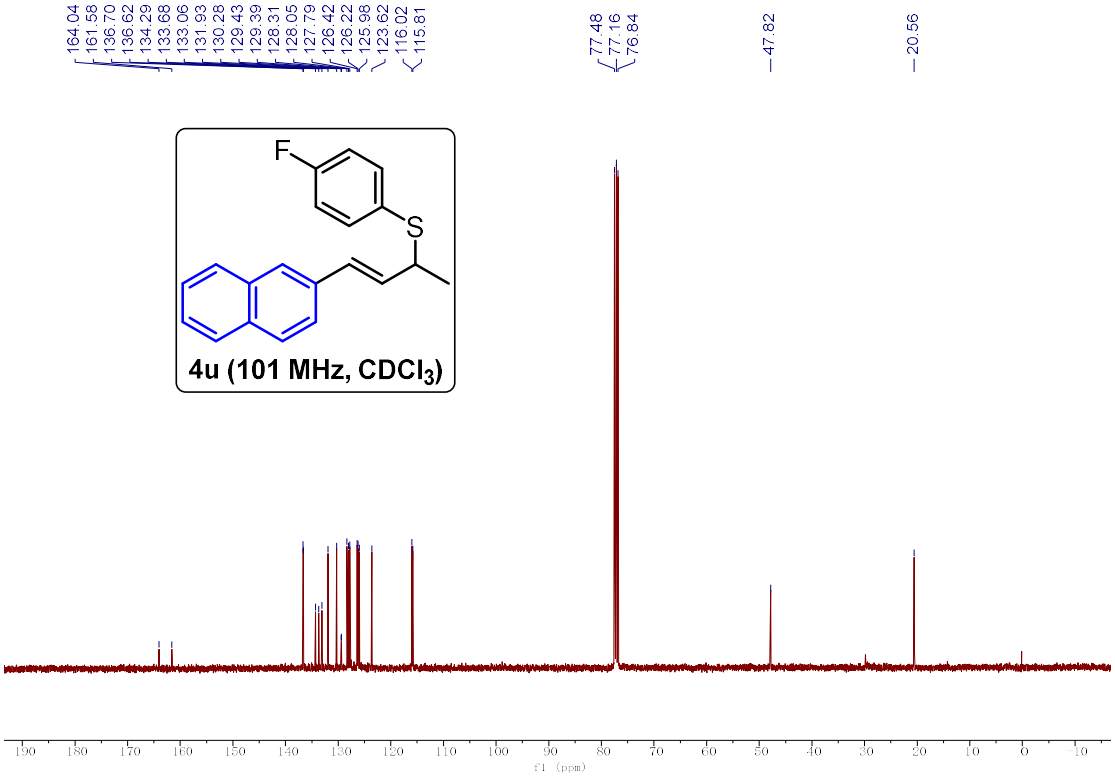
161.58
136.46
136.38
135.01
134.39
133.09
129.77
129.26
129.23
128.62
126.93
126.44
116.12
115.90
77.48
77.16
76.84
47.58
20.40
F
S
Cl
4t (101 MHz, CDCl3)
f1 (ppm)


-113.70
F
S
Cl
4t (376 MHz, CDCl3)
f1 (ppm)


7.82
7.80
7.79
7.78
7.78
7.77
7.76
7.75
7.60
7.52
7.52
7.50
7.50
7.46
7.46
7.44
7.44
7.43
7.42
7.41
6.98
6.96
6.94
6.26
6.25
3.87
3.86
3.86
3.85
3.84
3.83
3.82
3.81
3.80
1.51
1.49
F
S
4u (400 MHz, CDCl3)
3.15
1.04
5.22
1.94
1.97
1.00
3.07
f1 (ppm)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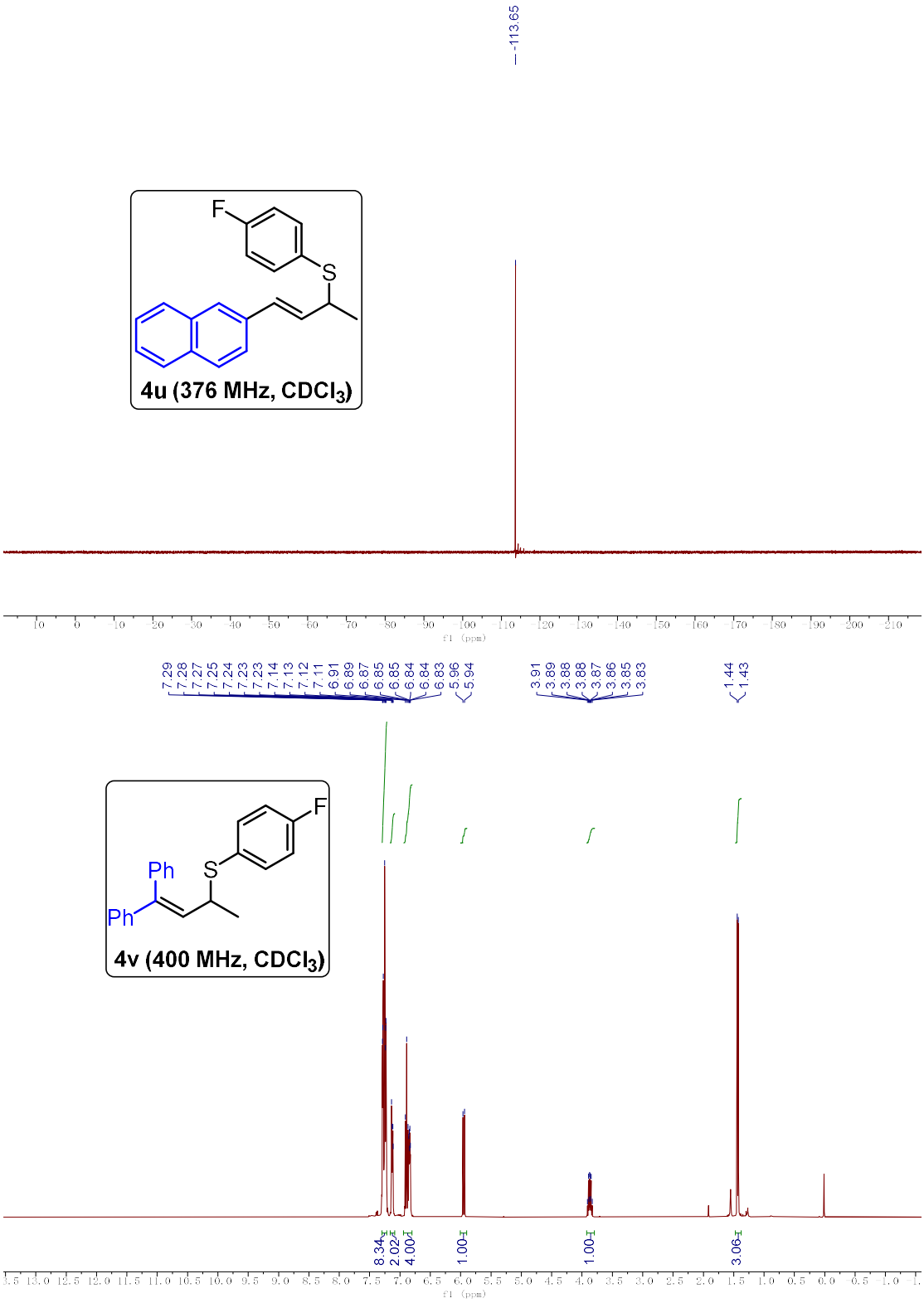
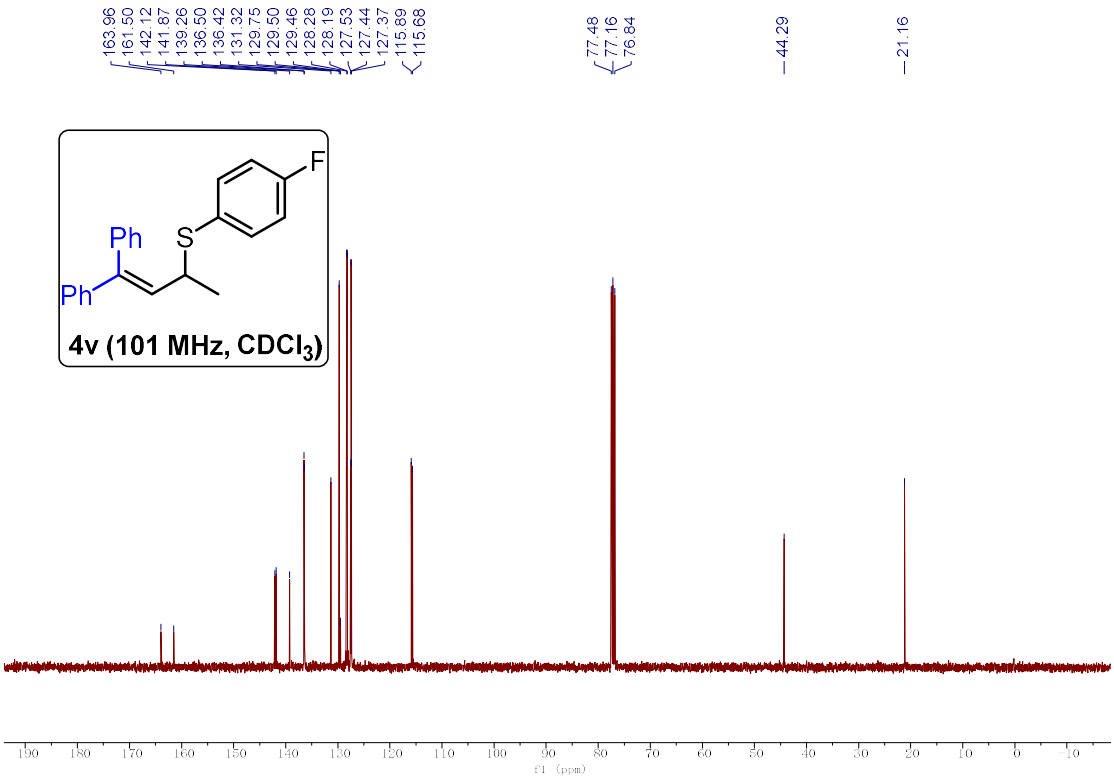
161.58
136.70
136.62
134.29
133.68
133.06
131.93
130.28
129.43
129.39
128.31
128.05
127.79
126.42
126.22
125.98
123.62
116.02
115.81
77.48
77.16
76.84
47.82
20.56
F
S
4u (101 MHz, CDCl3)
f1 (ppm)


-113.65
F
S
4u (376 MHz, CDCl3)
f1 (ppm)
7.29
7.28
7.27
7.25
7.24
7.23
7.23
7.14
7.13
7.12
7.11
6.91
6.89
6.87
6.85
6.85
6.84
6.84
6.83
5.96
5.94
3.91
3.89
3.88
3.88
3.87
3.86
3.85
3.83
1.44
1.43
F
Ph
S
Ph
4v (400 MHz, CDCl3)
8.34
2.02
4.00
1.00
1.00
3.06
f1 (ppm)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161.50
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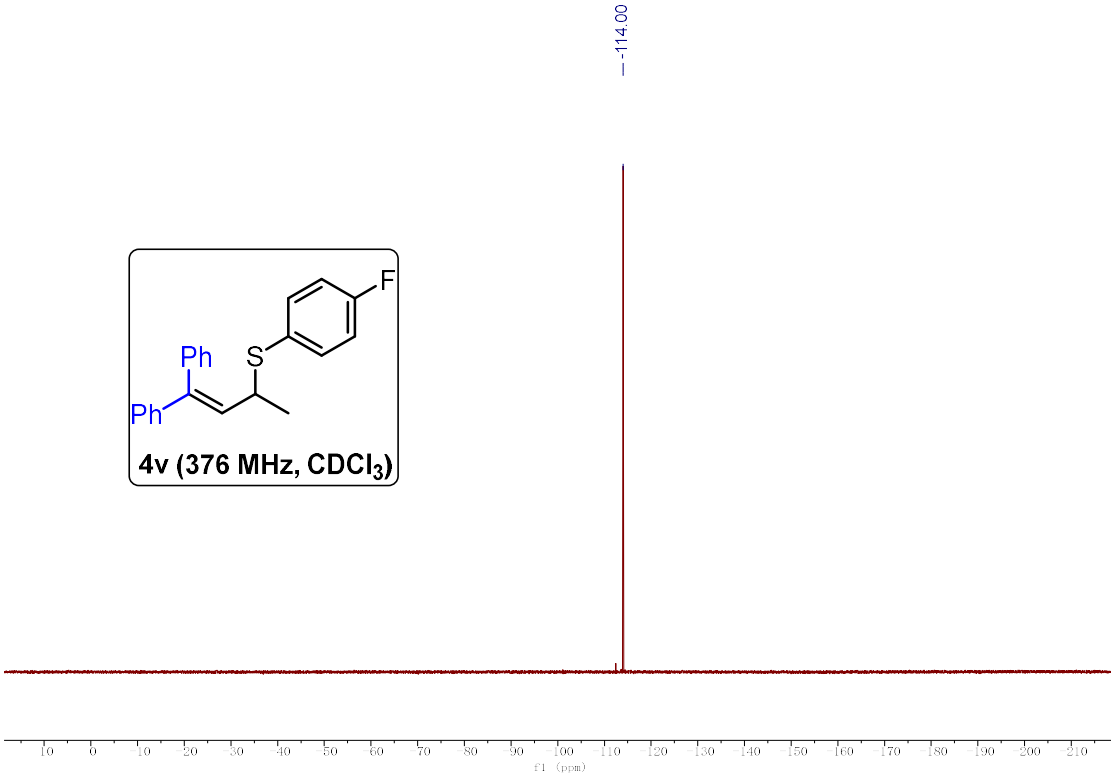
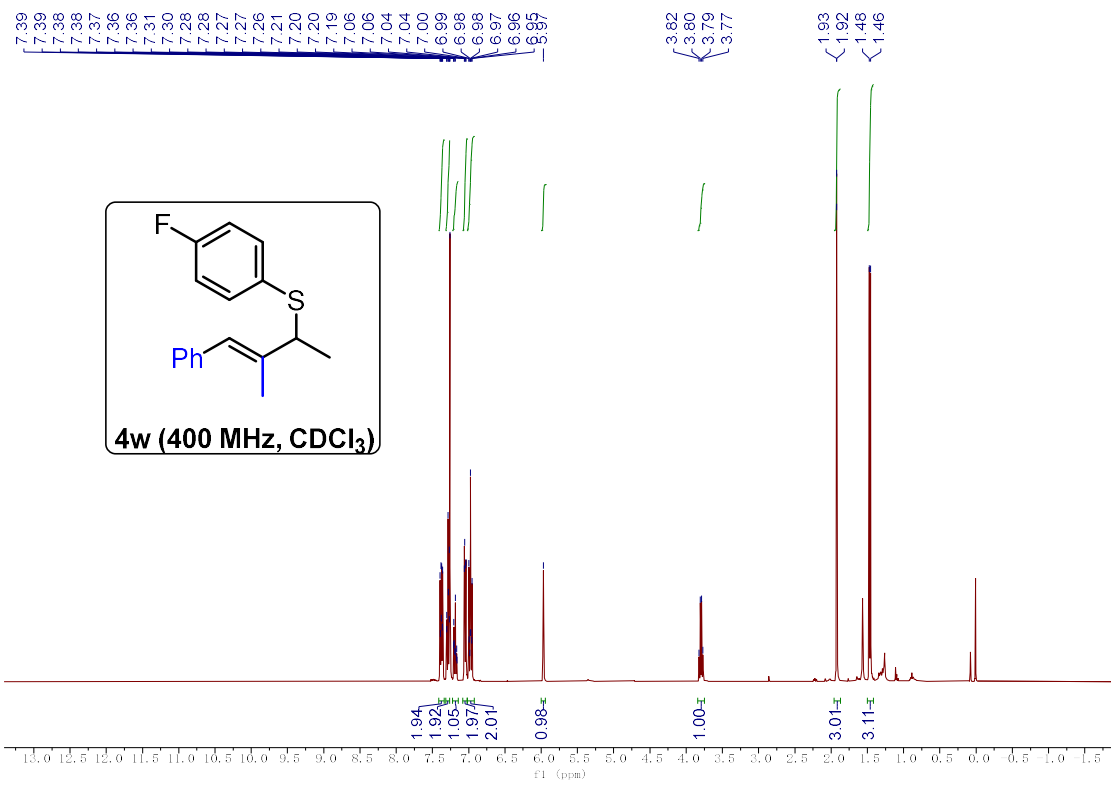
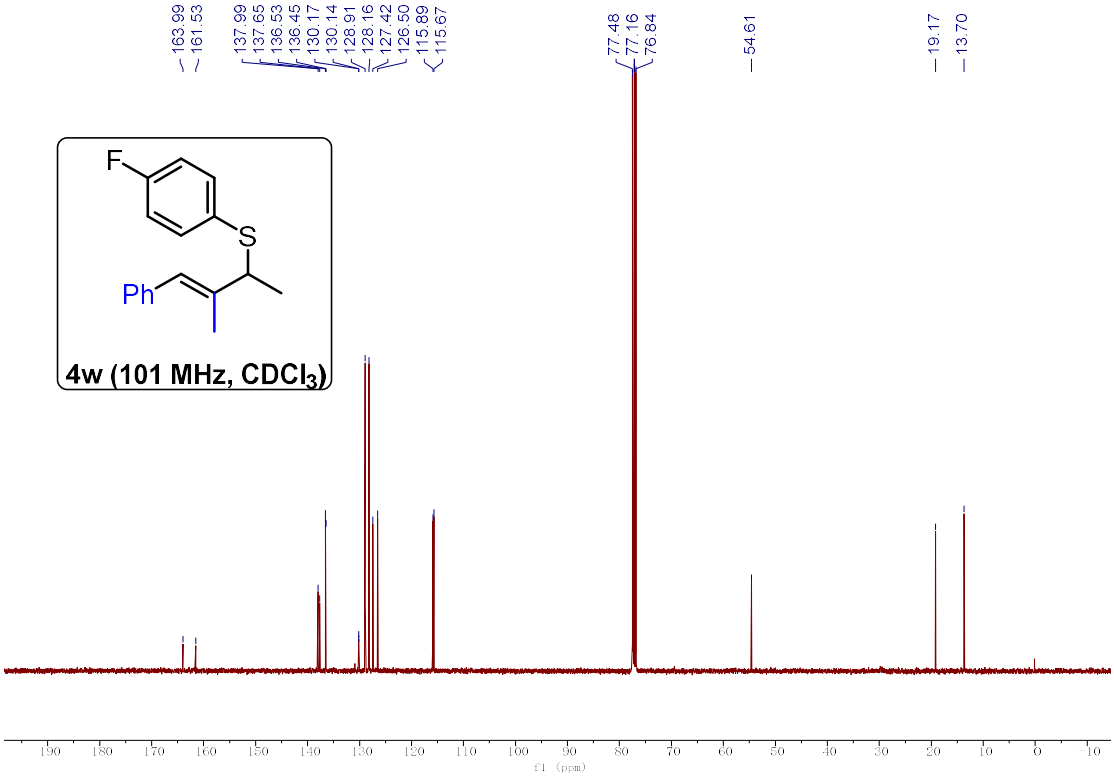
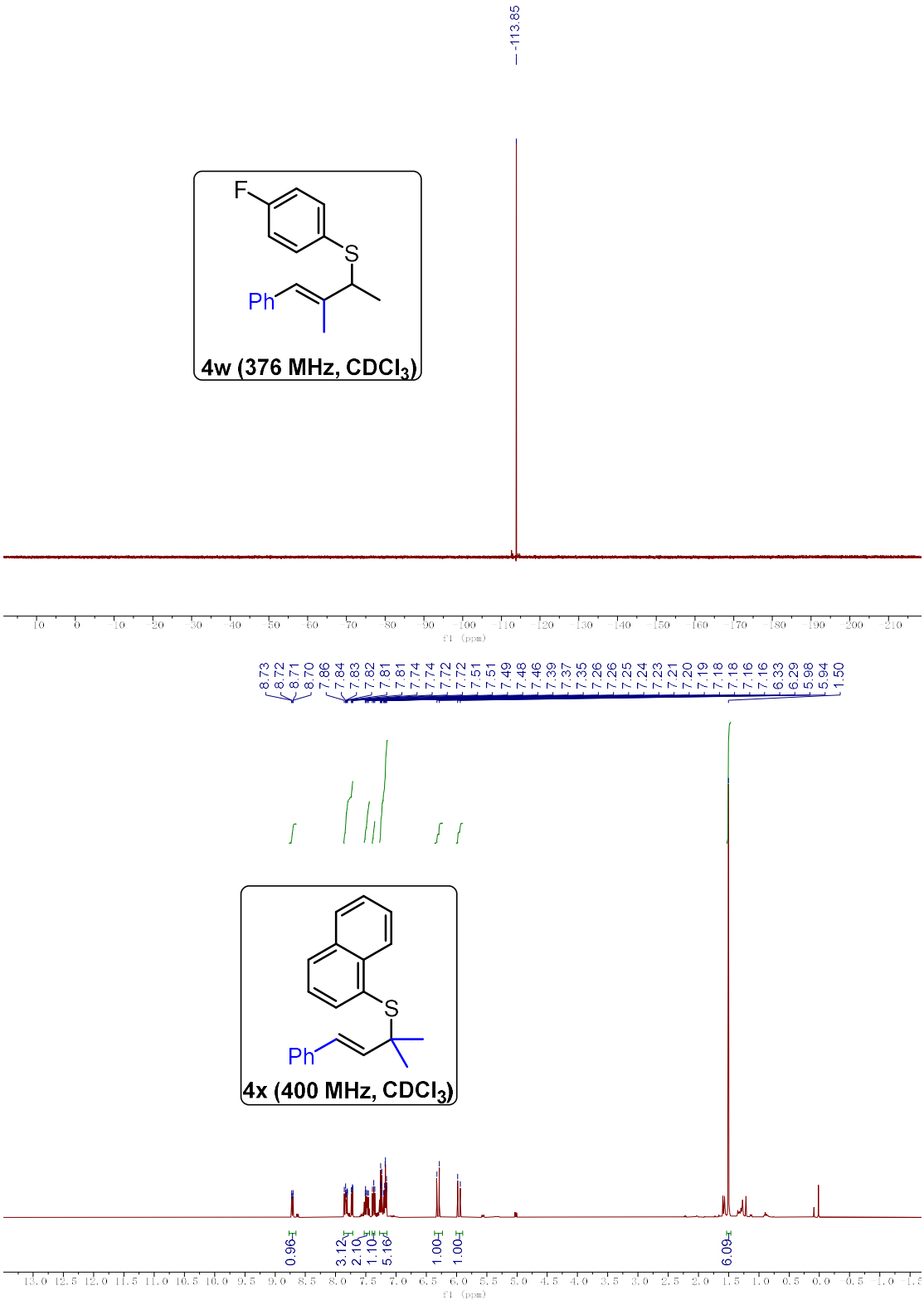
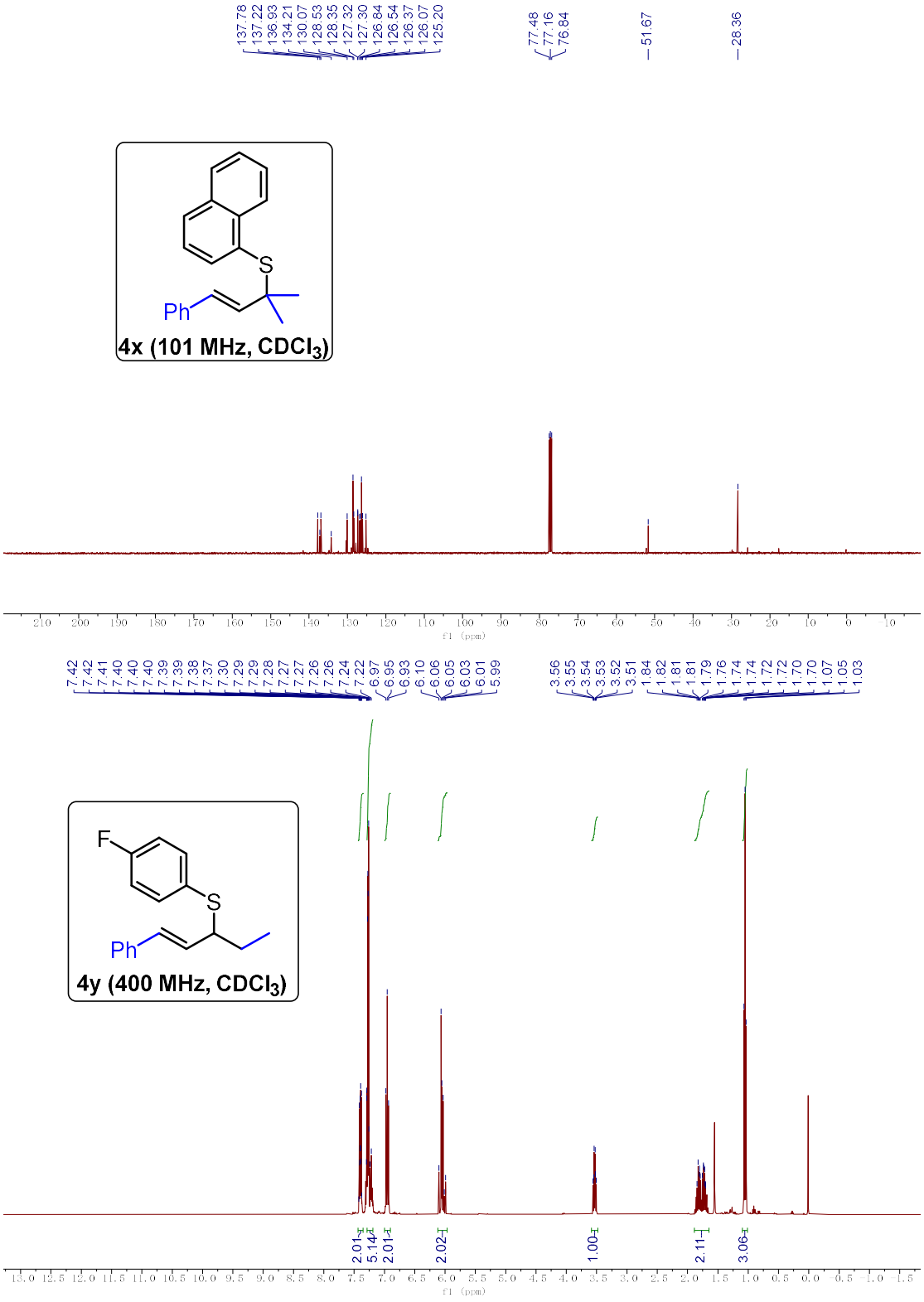
141.87
139.26
136.50
136.42
131.32
129.75
129.50
129.46
128.28
128.19
127.53
127.44
127.37
115.89
115.68
77.48
77.16
76.84
44.29
21.16
F
Ph
S
Ph
4v (101 MHz, CDCl3)
f1 (ppm)

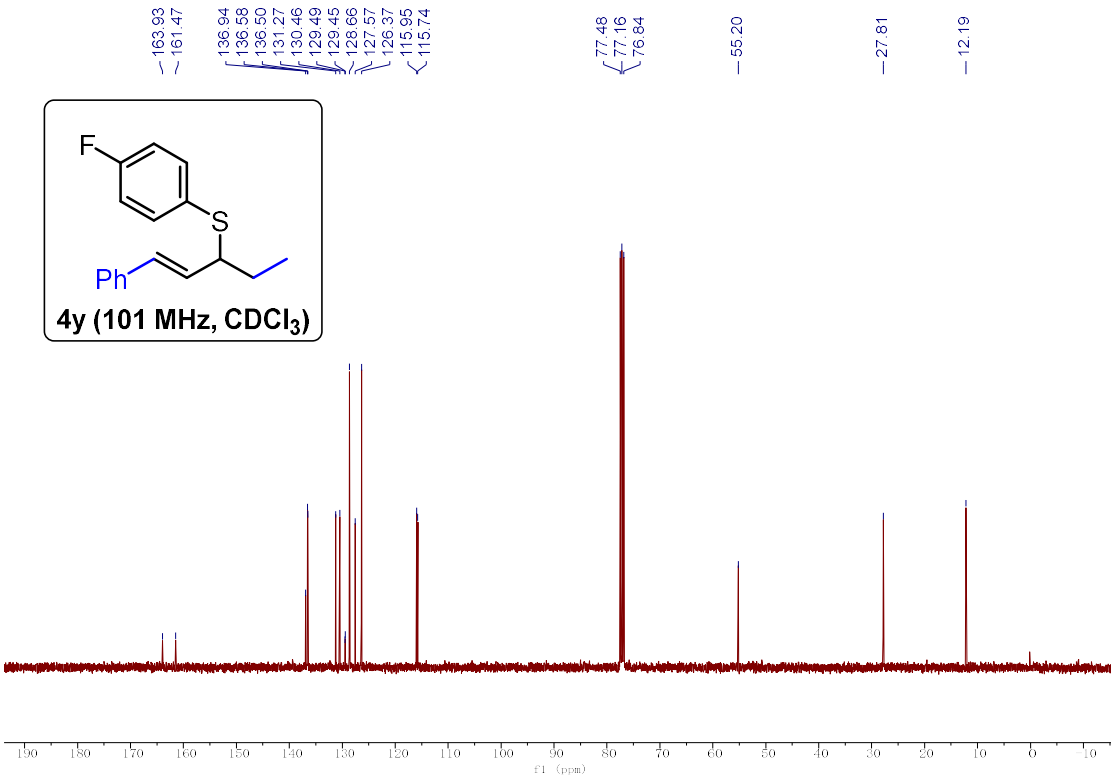

-114.00
F
Ph
S
Ph
4v (376 MHz, CDCl3)
f1 (ppm)

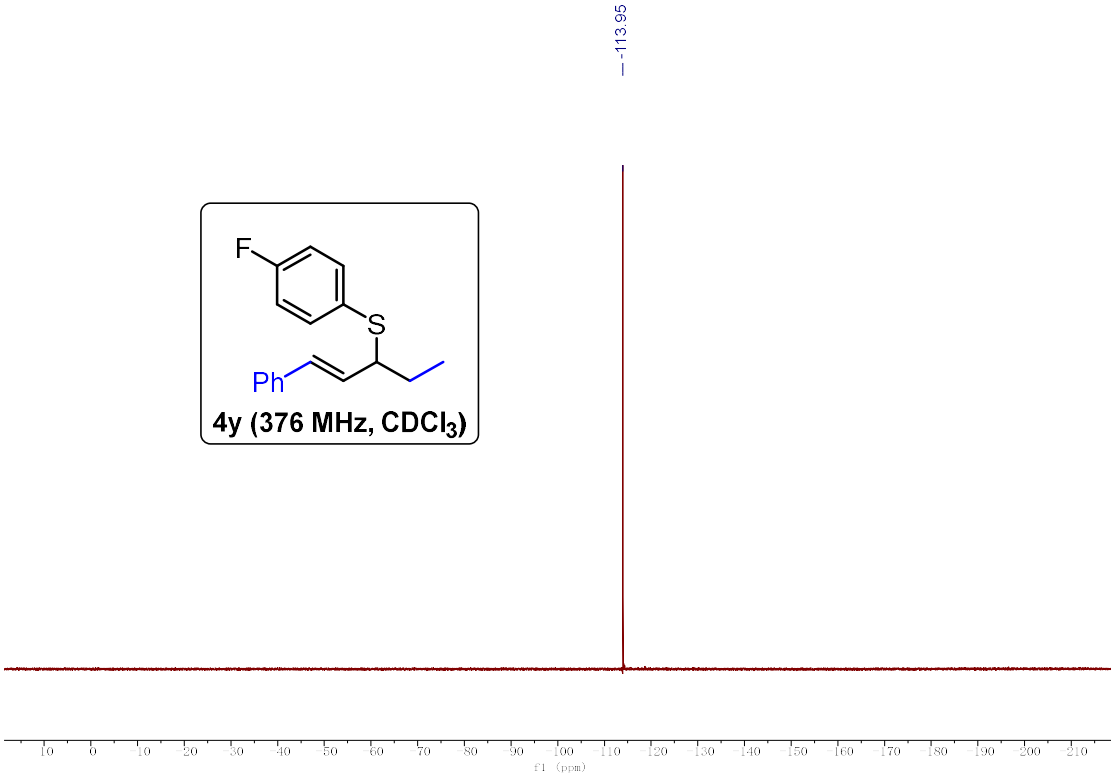

F
S
Ph
4w (400 MHz, CDCl3)

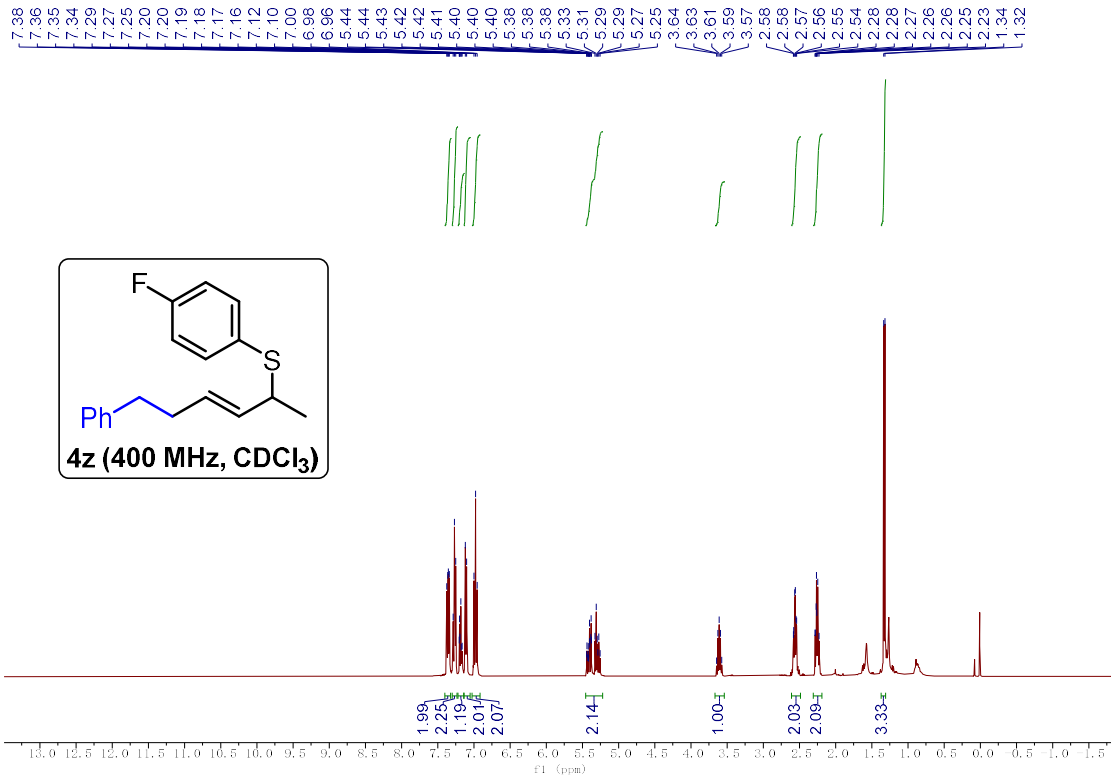

F
S
Ph
4w (101 MHz, CDCl3)

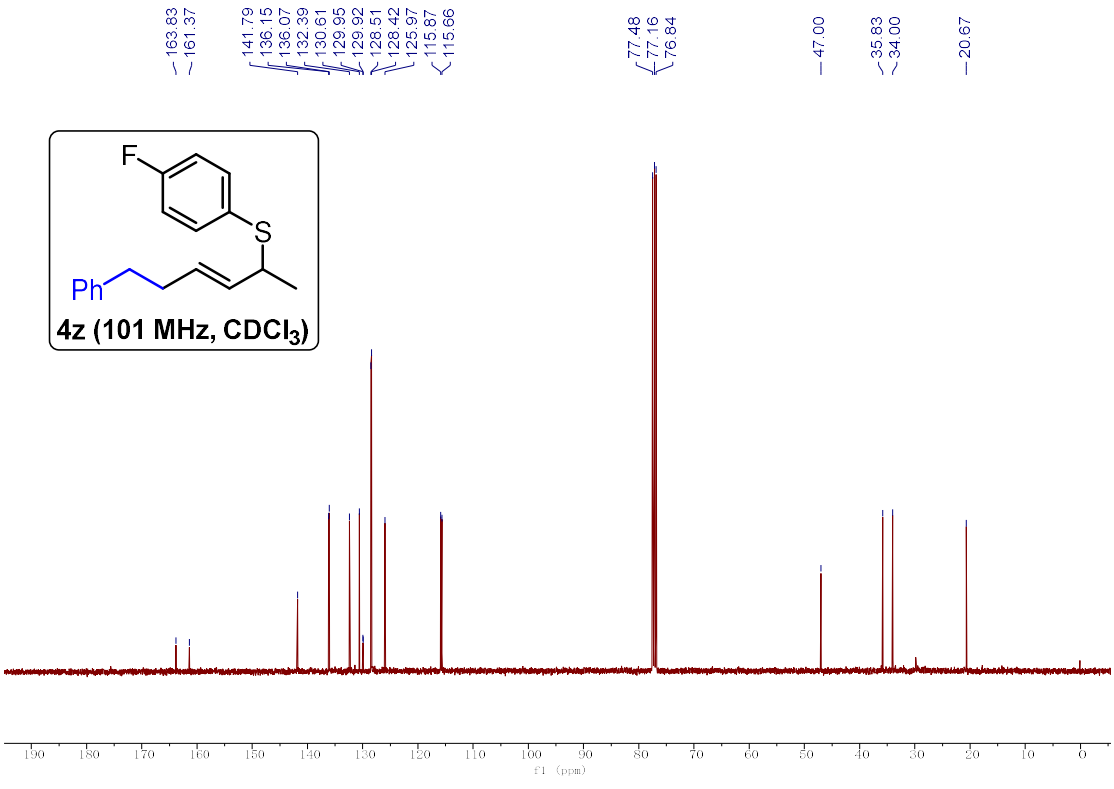

-113.85
F
S
Ph
4w (376 MHz, CDCl3)
8.73
8.72
8.71
8.70
7.86
7.84
7.83
7.82
7.81
7.81
7.74
7.74
7.72
7.72
7.51
7.51
7.49
7.48
7.46
7.39
7.37
7.35
7.26
7.26
7.25
7.24
7.23
7.21
7.20
7.19
7.18
7.18
7.16
7.16
6.33
6.29
5.98
5.94
1.50
S
Ph
4x (400 MHz, CDCl3)
0.96
3.12
2.10
1.10
5.16
1.00
1.00
6.09
f1 (ppm)

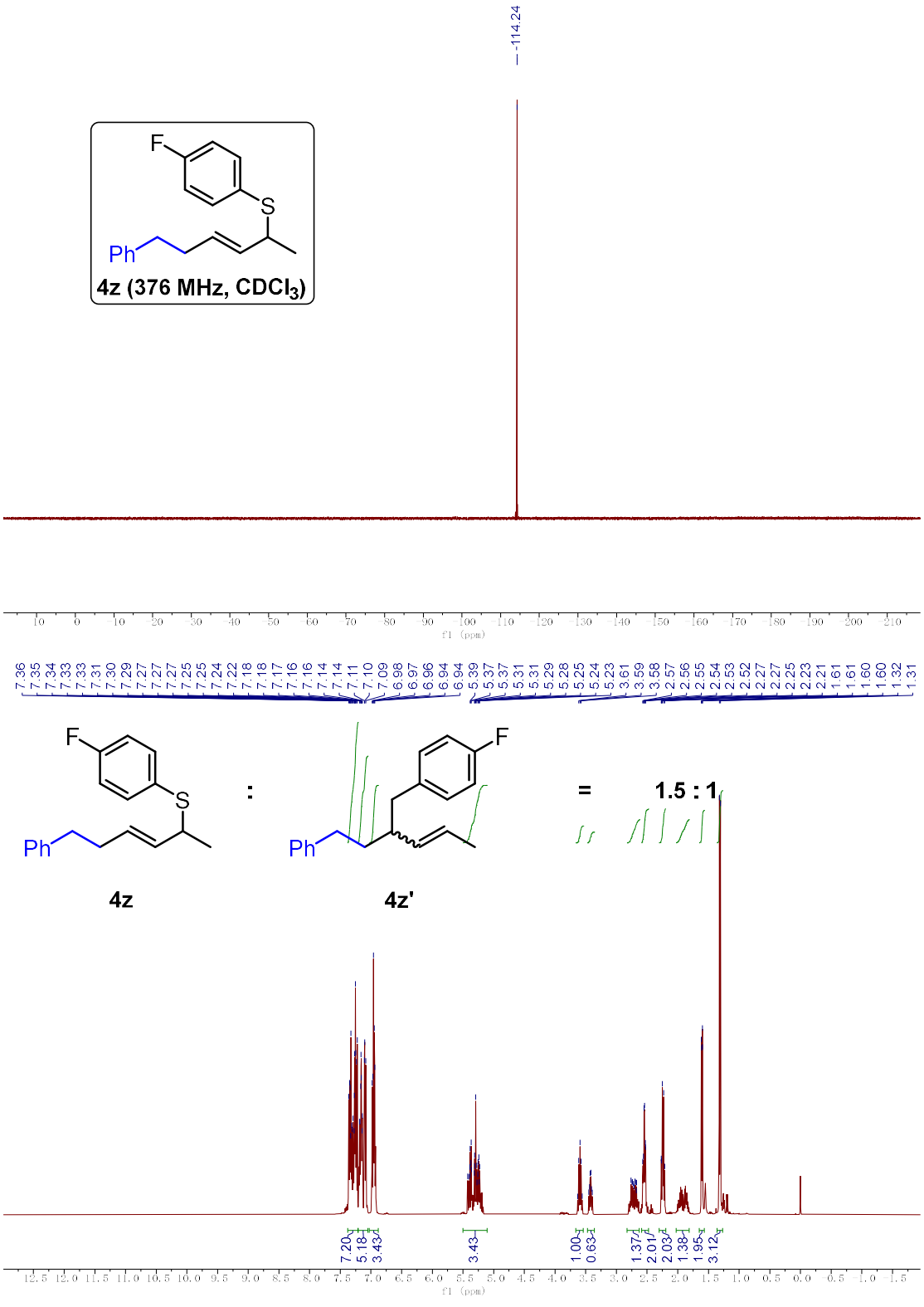

137.78
137.22
136.93
134.21
130.07
128.53
128.35
127.32
127.30
126.84
126.54
126.37
126.07
125.20
77.48
77.16
76.84
51.67
28.36
S
Ph
4x (101 MHz, CDCl3)
7.42
7.42
7.41
7.40
7.40
7.40
7.39
7.39
7.38
7.37
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.24
7.22
6.97
6.95
6.93
6.10
6.06
6.05
6.03
6.01
5.99
3.56
3.55
3.54
3.53
3.52
3.51
1.84
1.82
1.81
1.81
1.79
1.76
1.74
1.74
1.72
1.72
1.70
1.70
1.07
1.05
1.03
F
S
Ph
4y (400 MHz, CDCl3)
2.01
5.14
2.01
2.02
1.00
2.11
3.06
f1 (ppm)

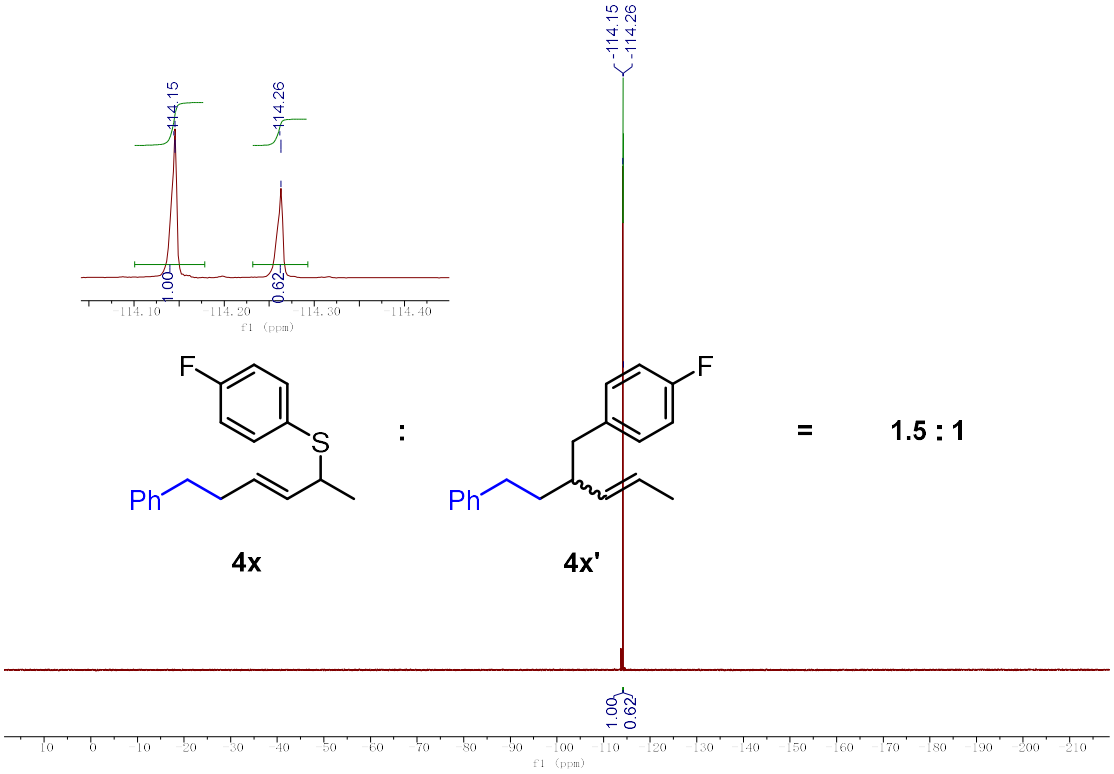

163.93
161.47
136.94
136.58
136.50
131.27
130.46
129.49
129.45
128.66
127.57
126.37
115.95
115.74
77.48
77.16
76.84
55.20
27.81
12.19
F
S
Ph
4y (101 MHz, CDCl3)
f1 (ppm)

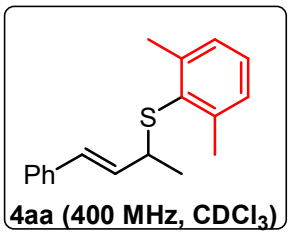

-113.95
F
S
Ph
4y (376 MHz, CDCl3)
f1 (ppm)


7.38
7.36
7.35
7.34
7.29
7.27
7.25
7.20
7.20
7.19
7.18
7.17
7.16
7.12
7.10
7.00
6.98
6.96
5.44
5.44
5.43
5.42
5.42
5.41
5.40
5.40
5.40
5.38
5.38
5.38
5.33
5.31
5.29
5.29
5.27
5.25
3.64
3.63
3.61
3.59
3.57
2.58
2.58
2.57
2.56
2.55
2.54
2.28
2.28
2.27
2.26
2.26
2.25
2.23
1.34
1.32
F
S
Ph
4z (400 MHz, CDCl3)
1.99
2.25
1.19
2.01
2.07
2.14
1.00
2.03
2.09
3.33
f1 (ppm)

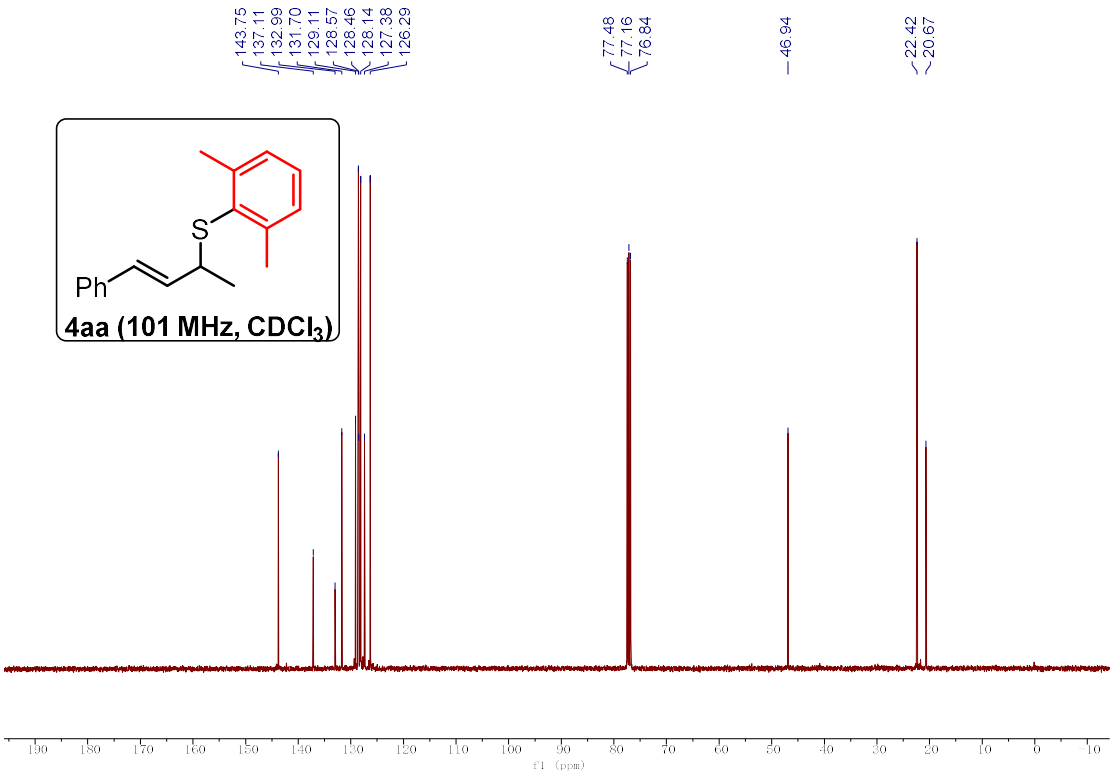

163.83
161.37
141.79
136.15
136.07
132.39
130.61
129.95
129.92
128.51
128.42
125.97
115.87
115.66
77.48
77.16
76.84
47.00
35.83
34.00
20.67
F
S
Ph
4z (101 MHz, CDCl3)
f1 (ppm)


F
S
Ph
4z (376 MHz, CDCl3)
-114.24
f1 (ppm)
7.36
7.35
7.34
7.33
7.33
7.31
7.30
7.29
7.27
7.27
7.27
7.25
7.25
7.24
7.22
7.18
7.18
7.17
7.16
7.16
7.14
7.14
7.11
7.10
7.09
6.98
6.97
6.96
6.94
6.94
5.39
5.37
5.37
5.31
5.31
5.29
5.28
5.25
5.24
5.23
3.61
3.59
3.58
2.57
2.56
2.55
2.54
2.53
2.52
2.27
2.27
2.25
2.23
2.21
1.61
1.61
1.60
1.60
1.32
1.31
F
S
Ph
:
F
Ph
=
1.5 : 1
4z
4z'
7.20
5.18
3.43
3.43
1.00
0.63
1.37
2.01
2.03
1.38
1.95
3.12
f1 (ppm)





4aa (400 MHz, $CDCl_3$)


143.75
137.11
132.99
131.70
129.11
128.57
128.46
128.14
127.38
126.29
77.48
77.16
76.84
46.94
22.42
20.67
S
Ph
4aa (101 MHz, CDCl3)
f1 (ppm)