Supporting Information

Direct Trifluoromethylthiolation of Terminal Alkynes Mediated by a Hypervalent Trifluoromethylthio-Iodine(III) Reagent; Boosting Effect of Fluorinated Alcohol

Yu-Xin Cheng,‡ Xiao-Guang Yang,‡ Feng-Huan Du,‡ and Chi Zhang*

State Key Laboratory of Elemento-Organic Chemistry, The Research Institute of Elemento-Organic Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China

zhangchi@nankai.edu.cn

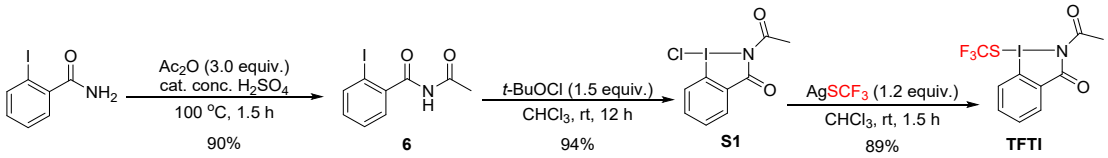
Table of Contents

General information. ^{1}H, ^{13}C, and ^{19}F NMR were recorded on the Bruker AV 400 (400 MHz, 100 MHz, and 376 MHz, respectively). ^{1}H NMR chemical shifts were determined relative to internal standard TMS (δ = 0.0 ppm), ^{13}C NMR chemical shifts were determined relative to the deuterated solvents, and ^{19}FNMR chemical shifts were determined relative to inter-standard $PhCF_3$ (δ = -62.8 ppm). Chemical shifts (δ) were reported in ppm, and coupling constants (*J*) were in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiple, br = broad. Mass spectra were acquired on Q Exactive GC-Orbitrap MS (EI), and Varian 7.0T FTMS (ESI). IR spectra were obtained on a Bruker Alpha FT-IR Spectrometer. Reactions were monitored by thin-layer chromatography (TLC) carried out on Huanghai HSGF254 plates. Preparative TLC was performed on Xincheng GF254 preparative TLC plates. Silica gel (200-300 mesh) was purchased from Anhui Liangchen Co., China.

Materials: All solvents were purified according to the purification handbook *Purification of Laboratory Chemicals* before use. Unless otherwise noted, other reagents and starting materials were purchased from commercial sources and used as received.

1. General procedure for the preparation of hypervalent trifluoromethylthio-iodine(III) reagent TFTI

$AgSCF_3$ was prepared according to the reported literature.[1]



2-iodobenzamide (11.86 g, 48 mmol, 1.0 equiv.), acetic anhydride (20 mL, 144 mmol, 3.0 equiv.), and 8 drops of conc. H_2SO_4 were placed into a high-pressure autoclave equipped with a stirring bar. The reaction mixture was stirred in an oil bath at 100 °C for 1.5 h. When the reaction was complete, EtOAc (200 mL) was added and the brown solution was washed with saturated $NaHCO_3$ aq. (3 × 50 mL). The combined organic phase was dried over $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The crude mixture was purified by flash column chromatography (Eluent: EtOAc: petroleum ether = 1:3) to give of *N*-acetyl-2-iodobenzamide **6** (12.5 g) in 90% yield as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (br, 1H), 7.86 (d, J = 7.9 Hz, 1H), 7.39 (d, J = 4.4 Hz, 2H), 7.15-7.11 (m, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 167.8, 140.1, 139.9, 132.0, 128.2, 128.1, 91.9, 25.3 ppm.

t-BuOCl (4.88 g, 45 mmol, 1.5 equiv.) was added to a solution of **6** (8.67 g, 30 mmol, 1.0 equiv.) in 40 mL $CHCl_3$. The reaction mixture was stirred at room temperature for 12 h in dark under air. When the reaction was complete, the precipitate was filtered and washed with Et_2O (4 × 10 mL) to give 2-acetyl-1-chloro-1,2-dihydro-3*H*-1λ^3-benzo[*d*][1,2]iodazol-3-one **S1** (9.1 g) in 94% yield as a colorless solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.43 (d, J = 8.3 Hz, 1H), 8.13-8.06 (m, 2H), 7.88 (t, J = 7.3 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 174.4, 161.9, 136.9, 134.4, 131.8, 131.6, 128.1, 115.0, 25.4 ppm.

$AgSCF_3$ (6.27 g, 30 mmol, 1.2 equiv.), **S1** (8.08 g, 25 mmol, 1.0 equiv.) were placed into an oven-dried two-necked 100 mL flask equipped with a stirring bar under an argon atmosphere. Then 50 mL of freshly distilled $CHCl_3$ was added and the reaction was stirred at room temperature in dark for 1.5 h. When the reaction was complete, the precipitate was filtered and washed with DCM (4 × 40 mL). The filtrate was collected and the solvent was removed under reduced pressure. The residue was washed with Et_2O (3 × 10 mL) to give 2-acetyl-1-((trifluoromethyl)thio)-1,2-dihydro-3*H*-1λ^3-

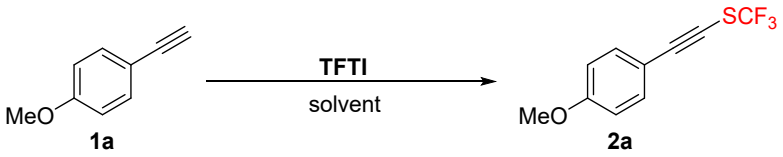
benzo[*d*][1,2]iodazol-3-one **TFTI** (8.7 g) in 89% yield as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.4 Hz, 1H), 8.26 (dd, *J* = 7.5 Hz, 1.6, 1H), 7.89 (dt, *J* = 7.2, 1.6 Hz, 1H), 7.79 (t, *J* = 7.2 Hz, 1H), 2.63 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -29.66 (s, 3 F); ^{13}C NMR (100MHz, $CDCl_3$) δ 176.7, 161.3, 136.2, 134.5, 132.4, 131.7, 130.5 (q, *J* = 309.1 Hz), 127.1, 113.1, 26.1 ppm.

2. Optimization of Reaction Conditions

2.1 Conditional Screening

These results showed that PFTB was the optimal solvent.

Table S1. Optimization of Reaction Conditions[a]



1a **2a**

Entry	TFTI (equiv.)	Solvent (2 mL)	Temp. (°C)	Time (h)	Yield (%)
1	1.5	DCE	80°C	24	10%
2	1.5	CH_3CN	rt	24	not detected[b]
3	1.5	TFE	rt	24	5[b]
4	1.5	HFIP	rt	1	71
5	1.2	PFTB	rt	1	99

[a]Reactions were conducted on 0.2 mmol scale. NMR yields are reported using $PhCF_3$ as an internal standard. [b]Reacovery of starting martial is 60%.

3. General procedure for direct trifluoromethylthiolation of terminal alkynes

3.1 General Procedure A (GP A)

Under an air atmosphere, PFTB (2 mL), terminal alkynes (0.2 mmol, 1.0 equiv.), and TFTI (0.24 mmol, 1.2 equiv.) were added sequentially to a 10 mL round bottom flask with a magnetic stirrer, after which the reaction was stirred at room temperature and monitored by TLC. When the reaction was complete, the solvent was concentrated under reduced pressure. The obtained residue was further purified by flash column chromatography to give the desired product.

3.2 General Procedure B (GP B)

Under an air atmosphere, HFIP (2 mL), terminal alkynes (0.2 mmol, 1.0 equiv.), and

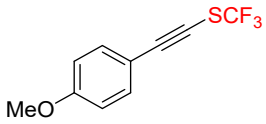
TFTI (0.3 mmol, 1.5 equiv.) were added sequentially to a 10 mL round bottom flask with a magnetic stirrer, after which the reaction was stirred at room temperature and monitored by TLC. When the reaction was complete, the solvent was concentrated under reduced pressure. The obtained residue was further purified by flash column chromatography to give the desired product.

3.2 General Procedure B (GP C)

Under an air atmosphere, PFTB (2 mL), terminal alkynes (0.2 mmol, 1.0 equiv.), and TFTI (0.6 mmol, 3 equiv.) were added sequentially to a 10 mL sealed tube with a magnetic stirrer, after which the reaction was stirred at 70˚C. TFTI (0.2 mmol, 1 equiv.) was added at 24 h intervals (6 equiv. in total) and monitored by TLC. When the reaction was complete, the solvent was concentrated under reduced pressure. The obtained residue was further purified by flash column chromatography to give the desired product.

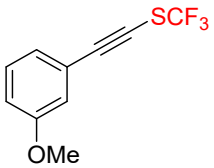
4. Characterization of the obtained products

((4-methoxyphenyl)ethynyl)(trifluoromethyl)sulfane 2a



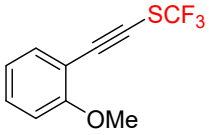
GP A. Colorless oil (99%, Eluent: petroleum ether); GP B. Colorless oil (71%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 9.2 Hz, 2H), 6.86 (d, J = 8.8 Hz, 2H), 3.82 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.10 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 134.4, 128.2 (q, J = 310.4 Hz), 114.1, 113.5, 101.5, 65.1 (q, J = 4.3 Hz), 55.3 ppm. The characterization data were in accordance with reported ones. [2]

((3-methoxyphenyl)ethynyl)(trifluoromethyl)sulfane 2b



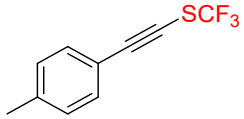
GP A (TFTI 2.0 equiv.) Pale yellow oil (99%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (t, J =7.9 Hz, 1 H), 7.08 (dt, J = 7.6, 1.1 Hz, 1 H), 6.99 (dd, J = 2.3, 1.5 Hz, 1 H), 6.94 (ddd, J = 8.4, 2.6, 0.9 Hz, 1 H), 3.79 (s, 3 H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -43.56 (s, 3 F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 129.6, 128.1 (q, J =312.5 Hz), 124.7, 122.4, 116.8, 116, 101.2, 66.5 (q, J =4.4 Hz), 55.3 ppm. The characterization data were in accordance with reported ones.[3]

((2-methoxyphenyl)ethynyl)(trifluoromethyl)sulfane 2c



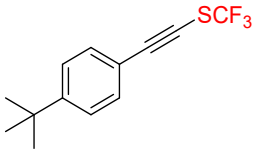
GP A (TFTI 1.5 equiv.) Pale yellow oil (99%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ7.45 (dd, *J* = 7.6, 1.7 Hz, 1 H), 7.36 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1 H), 6.93 (td, *J* = 7.5, 0.9 Hz, 1 H), 6.89 (d, *J* =8.4 Hz, 1 H), 3.89 (s, 3 H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.81 (s, 3 F); ^{13}C NMR (100 MHz, $CDCl_3$): 160.8, 134.2, 131.4, 128.1 (q, *J* =310.5 Hz), 120.5, 110.8, 97.9, 70.2 (q, *J* =4.2 Hz), 55.8 ppm. The characterization data were in accordance with reported ones.[3]

(*p*-tolylethynyl)(trifluoromethyl)sulfane 2d



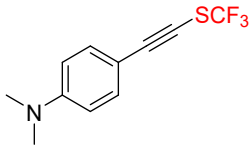
GP A. Colorless oil (99%, Eluent: petroleum ether); GP B. Colorless oil (62%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.76 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 132.3, 129.2, 128.1 (q, *J* = 310.8 Hz), 118.5, 101.5, 65.8 (q, *J* = 4.2 Hz), 21.6 ppm. The characterization data were in accordance with reported ones.[4]

((4-(*tert*-butyl)phenyl)ethynyl)(trifluoromethyl)sulfane 2e



GP A. Colorless oil (99%, Eluent: petroleum ether); GP B. Colorless oil (58%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.43 (m, 2H), 7.38-7.36 (m, 2H), 1.31 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.51 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 132.2, 128.2 (q, *J* = 310.5 Hz), 125.5, 118.5, 101.5, 65.8 (q, *J* = 4.2 Hz), 34.9, 31.1 ppm. The characterization data were in accordance with reported ones.[4]

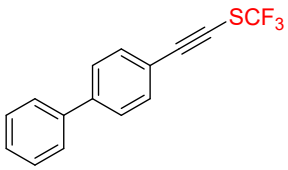
N, N-dimethyl-4-((trifluoromethylthio)ethynyl)aniline 2f



GP A. (TFTI 1.0 equiv., PFTB/DCE=2/3) white solid (80%, Eluent: petroleum ether/EtOAc = 100/3); GP B. (HFIP/DCE=1/2) white solid (68%, Eluent: petroleum ether/EtOAc = 100/3). A mixture of DCE and HFIP is used as the solvent, the solvent is DCE/HFIP = 2/1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.0 Hz, 2H), 6.61 (d, *J* =8.0 Hz, 2H), 3.00 (s, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.66 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 134.4, 128.2 (q, *J* = 310.6 Hz),111.4, 107.71, 103.2, 63.9 (q, *J* = 4.4 Hz), 40.0 ppm. The characterization data were in accordance with reported

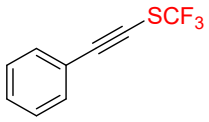
ones.[4]

(Biphenyl-4-ylethynyl)(trifluoromethyl)sulfane 2g



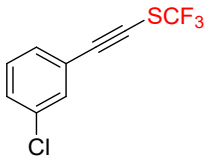
GP A (TFTI 2.0 equiv.) Yellow crystal (99%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.55 (m, 6H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.39-7.35 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.60 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 139.9, 132.7, 128.9, 128.1 (q, *J* = 311.0 Hz), 128.0, 127.1, 127.1, 120.3, 101.2, 67.3 (q, *J* = 4.0 Hz) ppm. The characterization data were in accordance with reported ones.[3]

(Phenylethynyl)(trifluoromethyl)sulfane 2h



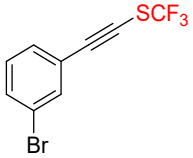
GP A. light yellow oil. (95%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.49 (m, 2H), 7.40-7.35 (m, 3H); ^{19}F NMR (376.1 MHz, $CDCl_3$): δ -43.64 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.2, 129.8, 128.5, 128.1 (q, *J* = 310.4 Hz), 121.6, 101.3 (d, *J* =1.5 Hz), 66.7 (q, *J* = 4.3 Hz) ppm. The characterization data were in accordance with reported ones.[4]

((3-Chlorophenyl)ethynyl)(trifluoromethyl)sulfane 2i



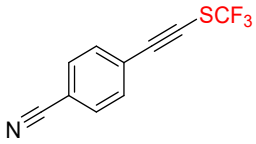
GP A (TFTI 2.0 equiv.) pale yellow oil (92%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.38-7.36 (m, 2H), 7.30-7.26 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.30 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.4, 131.9, 130.2, 130.0, 129.7, 128.0 (q, *J* = 310.8 Hz), 123.2, 99.8, 68.3 (q, *J* = 4.3 Hz) ppm. The characterization data were in accordance with reported ones. [5]

((3- Bromophenyl)ethynyl)(trifluoromethyl)sulfane 2j



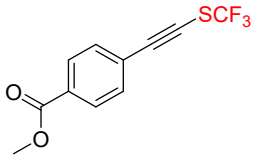
GP A (TFTI 2.3 equiv.) pale yellow oil (99%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.38-7.36 (m, 2H), 7.24-7.20 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.28 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.7, 131.8, 130.6, 129.9, 128.0 (q, *J* = 310.7 Hz), 123.4, 122.3, 99.6, 68.5 (q, *J* = 4.4 Hz) ppm.

4-(((Trifluoromethyl)thio)ethynyl)benzonitrile 2k



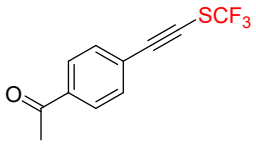
GP C.(80°C) Light yellow oil. (50%, Eluent: ethyl acetate/petroleum ether = 1/10) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 6.0 Hz, 2 H), 7.56 (d, *J* = 6.0 Hz, 2 H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.88 (s, 3 F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.2, 132.1, 127.8 (q, *J* = 311.0 Hz), 126.2, 118.1, 112.8, 99.5, 72.0 (q, *J* = 4.2 Hz) ppm. The characterization data were in accordance with reported ones. [6]

methyl 4-(2-((trifluoromethyl)sulfanyl)ethynyl)benzoate 2l



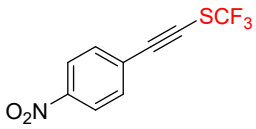
GP C. (60°C) Colorless oil. (85%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 2 H), 7.54 (d, *J* = 8.0 Hz, 2 H), 3.92 (s, 3 H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.21 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 131.7, 130.7, 129.6, 127.9 (q, *J* = 310.7 Hz), 126.0, 100.5, 70.2 (q, *J* = 4.2 Hz), 52.3 ppm. The characterization data were in accordance with reported ones. [7]

1-methoxy-4-(2-((trifluoromethyl)sulfanyl)ethynyl)benzene 2m



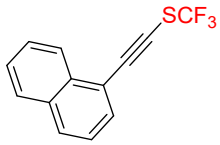
GP C. Colorless oil. (65%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.0 Hz, 2 H), 7.55 (d, *J* = 8.0 Hz, 2 H), 2.60 (s, 3 H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.16 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 137.1, 131.8, 128.3, 127.9 (q, *J* = 311.0 Hz), 126.1, 100.4, 70.4 (q, *J* = 4.5 Hz), 26.6 ppm. The characterization data were in accordance with reported ones. [7]

((4-Nitrophenyl)ethynyl)(trifluoromethyl)sulfane 2n



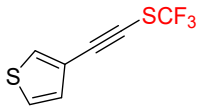
GP C. Light yellow liquid (55%, Eluent: ethyl acetate/petroleum ether = 1/ 10) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.0 Hz, 2 H), 7.63 (d, *J* = 8.0 Hz, 2 H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.75 (s, 3 F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 132.3, 128.1, 127.7 (q, *J* = 311.0 Hz), 123.7, 99.3, 73.0 (q, *J* = 4.2 Hz) ppm. The characterization data were in accordance with reported ones. [6]

(Naphthalen-1-ylethynyl)(trifluoromethyl)sulfane 2o



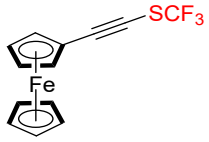
GP A (TFTI 2.0 equiv.) Colorless oil. (99%, Eluent: petroleum ether)^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.4 Hz, 1H), 7.86 (t, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.60-7.53 (m, 2H), 7.45-7.41 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.54 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.4, 133.1, 131.6, 130.3, 128.4, 128.2 (q, *J* = 310.2 Hz), 127.4,126.7, 125.7, 125.1, 119.1, 99.6, 71.2 (q, *J* = 4.4 Hz) ppm. The characterization data were in accordance with reported ones. [4]

3-((Trifluoromethylthio)ethynyl)thiophene 2p



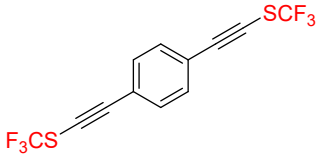
GP A (TFTI 1.5 equiv.) Yellow oil. (99%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.63 (m, 1H), 7.32-7.29 (m, 1H),7.20-7.16 (m, 1H); ^{19}F NMR (376.1 MHz, $CDCl_3$) δ -43.73 (s, 3F); ^{13}C NMR (100MHz, $CDCl_3$) δ 132.1, 130.1, 128.0 (q, *J* = 311.0 Hz), 125.7, 120.7, 96.4, 66.5 (q, *J* = 4.1 Hz) ppm. The characterization data were in accordance with reported ones. [6]

(Trifluoromethylthio)ethynylferrocene 2q



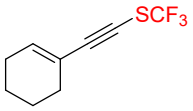
GP A (TFTI 1.5 equiv.) Red solid. (99%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.54 (s, 2H), 4.31 (s, 2H), 4.24 (s, 5H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.68 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 127.7 (q, *J* = 310.6 Hz), 102.4, 72.7, 70.1, 69.9, 62.3 (q, *J* = 4.1 Hz), 62.1 ppm. The characterization data were in accordance with reported ones.[8]

1,4-Bis-((trifluoromethylthio)ethynyl)benzene 2r



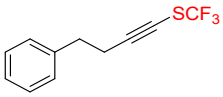
GP A (TFTI 2.5 equiv.) pale yellow solid. (99%, Eluent: petroleum ether) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.30 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.6, 127.9 (q, *J* = 310.7 Hz), 122.6, 100.4, 69.6 (q, *J* = 4.5 Hz) ppm. The characterization data were in accordance with reported ones. [8]

(cyclohex-1-en-1-ylethynyl)(trifluoromethyl)sulfane 2s



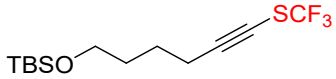
GP A (TFTI 1.0 equiv.) Colorless oil. (90%, Eluent: petroleum ether)^{1}H NMR (400 MHz, $CDCl_3$) δ 6.28 (m, 1H), 2.14 (m, 4H), 1.65-1.58 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.31 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 128.2 (q, J = 310.2 Hz),120.0, 103.2, 63.44 (q, J = 4.3 Hz), 28.5, 25.8, 22.0, 21.2 ppm. The characterization data were in accordance with reported ones.[8]

(4-phenylbut-1-yn-1-yl)(trifluoromethyl)sulfane 2t



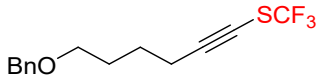
GP B. Colorless oil (81%, Eluent: petroleum ether.) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.28 (m, 2H), 7.23-7.20 (m, 3H), 2.87 (t, J = 7.2 Hz, 2H), 2.67 (t, J = 7.2 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.75 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 128.5, 128.4 (q, J = 309.7 Hz), 128.4, 126.5, 102.9, 57.9 (q, J = 4.3 Hz), 34.4, 22.4 ppm. The characterization data were in accordance with reported ones. [2]

***tert*-butyldimethyl((6-((trifluoromethyl)thio)hex-5-yn-1-yl)oxy)silane 2u**



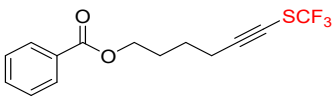
GP A. Colorless oil (99%, Eluent: petroleum ether/EtOAc = 4/1); GPB. (TFTI 2.5 equiv.) Colorless oil (75%, Eluent: petroleum ether/EtOAc = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (t, J = 6.0 Hz, 2H), 2.42 (t, J = 6.4 Hz, 2H), 1.62 (t, J = 3.6 Hz, 4H), 0.89 (s, 9H), 0.05 (s, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.32 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.5 (q, J = 309.5 Hz), 103.8, 62.4, 57.0 (q, J = 4.3 Hz), 31.7, 25.9, 24.6, 19.9, 18.3, -5.4 ppm.

(6-(benzyloxy)hex-1-yn-1-yl)(trifluoromethyl)sulfane 2v



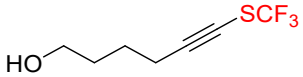
GP B. Colorless oil (82%, Eluent: petroleum ether/EtOAc = 100/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.31 (m, 4H), 7.30-7.27 (m, 1H), 4.50 (s, 2H), 3.49 (t, J = 6.0 Hz, 2H), 2.41 (t, J = 6.4 Hz, 2H), 1.76-1.62 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.44 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 128.5 (q, J = 309.4 Hz), 128.4, 127.6, 127.5, 103.6, 72.9, 69.5, 57.2 (q, J = 4.3 Hz), 28.7, 24.8, 19.4 ppm. HRMS (EI): *m/z* Calcd. for $C_{14}H_{15}F_3OS$ $[M]^+$: 288.0790, Found: 288.0793. IR(KBr): 2940, 2865, 1721, 1274, 1155, 1108, 739 cm^{-1}.

6-((trifluoromethyl)thio)hex-5-yn-1-yl benzoate 2w



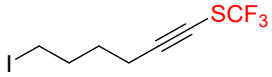
GP B. Colorless oil (80%, Eluent: DCM/petroleum ether = 1/4). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.03 (m, 2H), 7.59-7.54 (m, 1H), 7.47-7.43 (m, 2H), 4.35 (t, *J* = 6.4 Hz, 2H), 2.49 (t, *J* = 6.4 Hz, 2H), 1.91-1.86 (m, 2H), 1.78-1.70 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.41 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 132.9, 130.2, 129.5, 128.4 (q, *J* = 309.4 Hz), 128.3, 103.1, 64.2, 57.6 (q, *J* = 4.3 Hz), 27.7, 24.7, 19.8 ppm. HRMS (ESI): *m/z* Calcd. for $C_{14}H_{13}F_3O_2S$ $[M+Na]^+$: 325.0481, Found: 325.0485. IR(KBr): 2957, 1720, 1640, 1274, 1154, 1108, 711 cm^{-1}.

6-((trifluoromethyl)thio)hex-5-yn-1-ol 2x



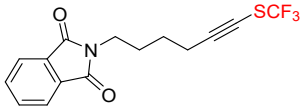
GP A Colorless oil (99%, Eluent: petroleum ether/EtOAc = 9/1). GP B Colorless oil (55%, Eluent: petroleum ether/EtOAc = 9/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.67 (t, *J* = 5.6 Hz, 2H), 2.44 (t, *J* = 6.0 Hz, 2H), 1.72-1.63 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.20 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.4 (q, *J* = 309.4 Hz), 103.4, 62.2, 57.3 (q, *J* = 4.3 Hz), 31.6, 24.4, 19.9 ppm. HRMS (EI): *m/z* Calcd. for $C_7H_9F_3OS$ $[M]^+$: 198.0321, Found: 198.0320. IR(KBr): 2949, 1721, 1276, 1156, 1108, 757, 713 cm^{-1}.

(6-iodohex-1-yn-1-yl)(trifluoromethyl)sulfane 2y



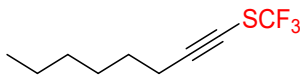
GP A (TFTI 1.5 equiv.) Colorless oil (99%, Eluent: petroleum ether). GP B (TFTI 2.5 equiv.) Colorless oil (63%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.21 (t, *J* = 6.8 Hz, 2H), 2.44 (t, *J* = 6.8 Hz, 2H), 1.97-1.90 (m 2H), 1.73-1.65 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.32 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.4 (q, *J* = 309.7 Hz), 102.8, 57.8 (q, *J* = 4.3 Hz), 32.1, 28.7, 19.1, 5.6 ppm. The characterization data were in accordance with reported ones. [2]

2-(6-((trifluoromethyl)thio)hex-5-yn-1-yl)isoindoline-1,3-dione 2z



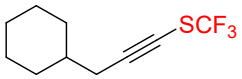
GP A. Colorless oil (99%, Eluent: petroleum ether/EtOAc = 20/1); GP B. (TFTI 2.5 equiv.) Colorless oil (72%, Eluent: petroleum ether/EtOAc = 20/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.84 (m, 2H), 7.74-7.71 (m, 2H), 3.72 (t, *J* = 7.2 Hz, 2H), 2.46 (t, *J* = 7.2 Hz, 2H), 1.84-1.77 (m, 2H), 1.65-1.58 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -43.92 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 133.9, 132.6, 128.4 (q, *J* = 309.4 Hz), 123.2, 102.9, 57.6 (q, *J* = 4.3 Hz), 37.2, 27.6, 25.2, 19.7 ppm. HRMS (ESI): *m/z* Calcd. for $C_{15}H_{12}F_3NO_2S$ $[M+H]^+$: 328.0614, Found: 328.0617. IR(KBr): 2949, 1773, 1714, 1397, 1154, 1108, 717 cm^{-1}.

oct-1-yn-1-yl(trifluoromethyl)sulfane 2aa



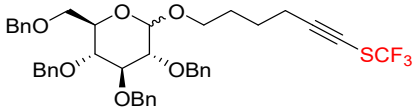
GP B. Colorless oil (94%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.38 (t, *J* = 7.2 Hz, 2H), 1.56-1.54 (m, 2H), 1.42-1.34 (m, 2H), 1.33-1.26 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.51 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.5 (q, *J* = 309.4 Hz), 104.0, 56.8 (q, *J* = 4.1 Hz), 31.2, 28.4, 27.9, 22.5, 20.2, 13.9 ppm.

(3-cyclohexylprop-1-yn-1-yl)(trifluoromethyl)sulfane 2ab



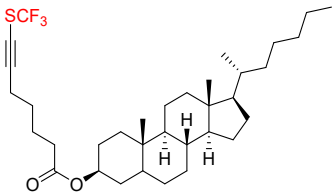
GP B. Colorless oil (85%, Eluent: petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (d, *J* = 6.8 Hz, 2H), 1.79-1.71 (m, 4H), 1.66 (d, *J* = 12.4 Hz, 1H), 1.58-1.48 (m, 1H), 1.28-1.12 (m, 4H), 1.05-0.99 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.53 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.5 (q, *J* = 309.5 Hz), 103.0, 57.5 (q, *J* = 4.2 Hz), 37.0, 32.6, 27.9, 26.1, 26.0 ppm. The characterization data were in accordance with reported ones.[2]

(2R,3R,4S,5R)-3,4,5-tris(benzyloxy)-2-((benzyloxy)methyl)-6-((6-((trifluoromethyl)thio)hex-5-yn-1-yl)oxy)tetrahydro-2H-pyran 2ac



GP B. Colorless oil (83%, Eluent: petroleum ether/EtOAc = 9/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.26 (m, 18H), 7.16-7.12 (m, 2H), 5.00-4.37 (m, 9H), 3.97 (t, *J* = 9.2 Hz, 1H), 3.73-3.41 (m, 7H), 2.40 (t, *J* = 6.8 Hz, 2H), 1.76-1.58 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.49 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8, 138.6, 138.4, 138.3, 138.2, 138.1, 138.0, 137.9, 128.4 (q, *J* = 309.4 Hz), 128.4, 128.4, 128.3, 128.3, 127.9, 127.9, 127.9, 127.9, 127.9, 127.9, 127.9, 127.8, 127.7, 127.7, 127.6, 127.6, 127.6, 127.5, 103.5, 96.9, 84.7, 82.2, 82.0, 80.1, 77.8, 77.7, 75.6, 75.6, 75.1, 74.9, 74.8, 73.4, 73.4, 73.2, 70.2, 69.0, 68.9, 68.5, 67.4, 57.3 (q, *J* = 4.3 Hz), 28.7, 28.4, 24.8, 24.8, 19.9, 19.8 ppm. HRMS (ESI): *m/z* Calcd. for $C_{41}H_{43}F_3O_6S$ $[M+Na]^+$: 743.2625, Found: 743.2628. IR(KBr): 3649, 3522, 3296, 3191, 2940, 1730, 1459, 1160, 1109 cm^{-1}.

(3*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-heptan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[a]phenanthren-3-yl 7-((trifluoromethyl)thio)hept-6-ynoate 2ad

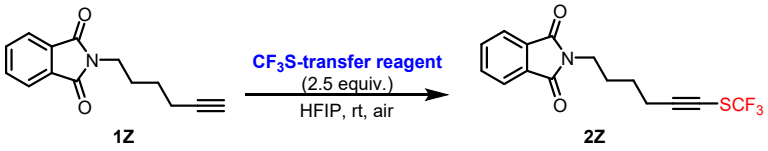


GP B. Colorless oil (87%, Eluent: petroleum ether/EtOAc = 50/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74-4.66 (m 1H), 2.41 (t, *J* = 6.8 Hz, 2H), 2.29 (t, *J* = 7.2 Hz, 2H), 1.98-1.94 (m, 1H), 1.83-1.43 (m, 14H), 1.40-0.94 (m, 20H), 0.91-0.85 (m, 10H), 0.82 (s, 3H), 0.65 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -44.40 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 127.4 (q, *J* = 309.6 Hz), 102.2, 72.7, 56.4 (q, *J* = 3.8 Hz), 55.4, 55.3,

53.2, 43.6, 41.6, 38.9, 38.5, 35.7, 35.2, 34.8, 34.5, 34.4, 33.0, 30.9, 27.6, 27.2, 26.9, 26.5, 26.4, 29.2, 23.1, 22.8, 21.8, 21.5, 20.2, 18.9, 17.6, 11.2, 11.0 ppm. HRMS (ESI): *m/z* Calcd. for $C_{34}H_{53}F_3O_2S$ $[M+K]^+$: 621.3350, Found: 621.3900. IR(KBr): 3612, 3562, 3464, 3410, 3296, 2948, 1732, 1160, 1110 cm^{-1}.

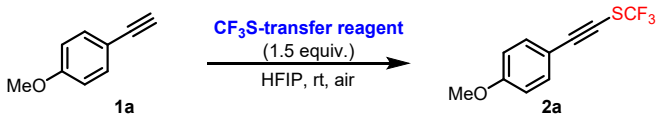
5. Comparative results of reactivity of other trifluoromethylthio transfer reagents

Table S2. Comparative results of reactivity of other trifluoromethylthio transfer reagents[a]



1Z 2Z

	Shen	Shen	Rueping	Billard Ⅰ	Billard Ⅱ	TFTI
Yield of **2z**	0%	0%	0%	0%	0%	72%
Recovery of starting material	100%	100%	100%	100%	100%	0%
Recovery of the reagent	100%	0%	100%	90%	100%	0%

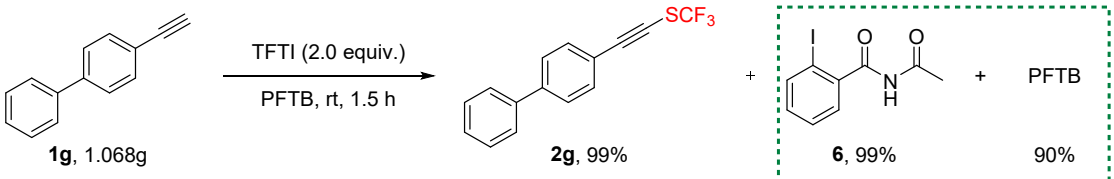


1a 2a

	Shen	Shen	Rueping	Billard Ⅰ	Billard Ⅱ	TFTI
Yield of **2a**	3%	0%	0%	0%	0%	71%
Recovery of starting material	0%[b]	0%[b]	100%	80%	100%	0%
Recovery of the reagent	85%	0%	100%	98%	100%	0%

[a]Reaction condition A: alkyne (0.2 mmol), CF_3S-transfer reagent, HFIP (2.0 mL), rt, 12 h. Isolated yields are reported. [b]The reaction time is 5 hours.

6. Recovery of PFTB and *N*-acetyl-2-iodobenzamide



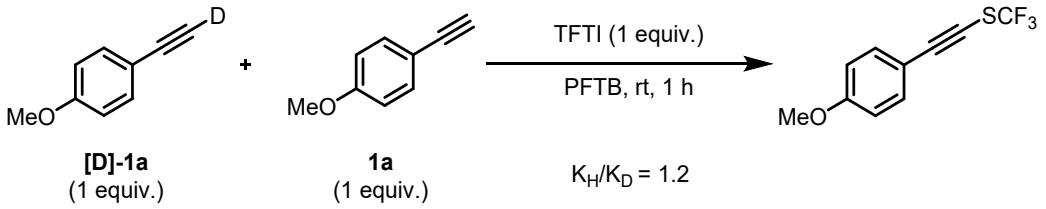
1g, 1.068g **2g**, 99% **6**, 99% 90%

Recovery

To a stirred solution of 4-ethynyl-1,1'-biphenyl **1g** (1.068 g, 6 mmol) and TFTI(4.668g, 12mmol) in PFTB (50.0 mL) at room temperature. After completion of the reaction (monitored by TLC) the solvent was recovered by distillation at atmospheric pressure (45.0 mL, 90%). The residue was purified by column chromatography on silica gel to give **2g** (1.658 g, 99%) as yellow crystal and **6** (3.449 g, 99%) as colorless solid. The recovered solvent was identified to NMR.

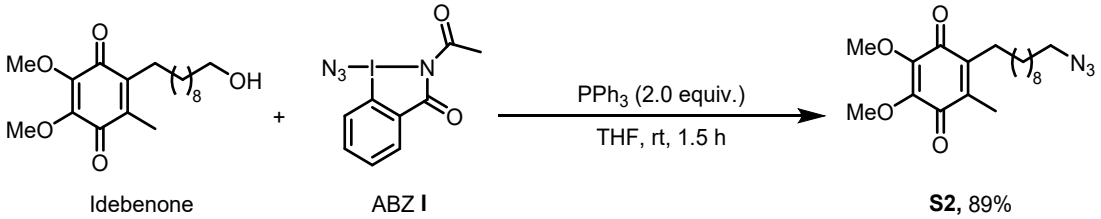
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.52 (d, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -74.42 (s, 9F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.1 (q, J = 288.0 Hz), 76.8 ppm. The characterization data were in accordance with reported ones.[9]

7. A KIE experiment



We carried out a competitive trifluoromethylthiolation reaction between **1a** and **[D]-1a** in the same pot. The general procedure for reaction monitoring by ^{1}H NMR was used, with the using 1,3,5-Trimethoxybenzene as an internal standard and using 0.09 equiv. of both **1a** and **[D]-1a**. The KIE value was obtained using the relative amount of unreacted starting materials recovered at the end of the reaction.

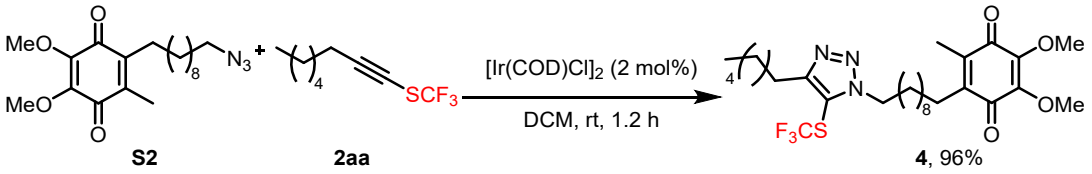
8. Transformations of Products



ABZ I (0.4 mmol, 2.0 equiv.) and PPh_3 (0.4 mmol, 2.0 equiv.) were placed into an oven-dried Schlenk flask equipped with a stirring bar under an argon atmosphere, and then 1.5 mL of freshly distilled THF and alcohol (0.2 mmol, 1.0 equiv.) were added in that order. The reaction mixture was stirred at room 50°C and monitored by thin-layer chromatography. When the reaction was complete, the solvent was evaporated under reduced pressure, and the residue was purified by flash column chromatography to give the azide product **S2**.

Red oil (64 mg, 89% yield, Eluent: EtOAc/petroleum ether = 1/9). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.99 (s, 3H), 3.98 (s, 3H), 3.26 (t, J = 6.8 Hz, 2H), 2.45 (t, J = 6.8 Hz, 2H),

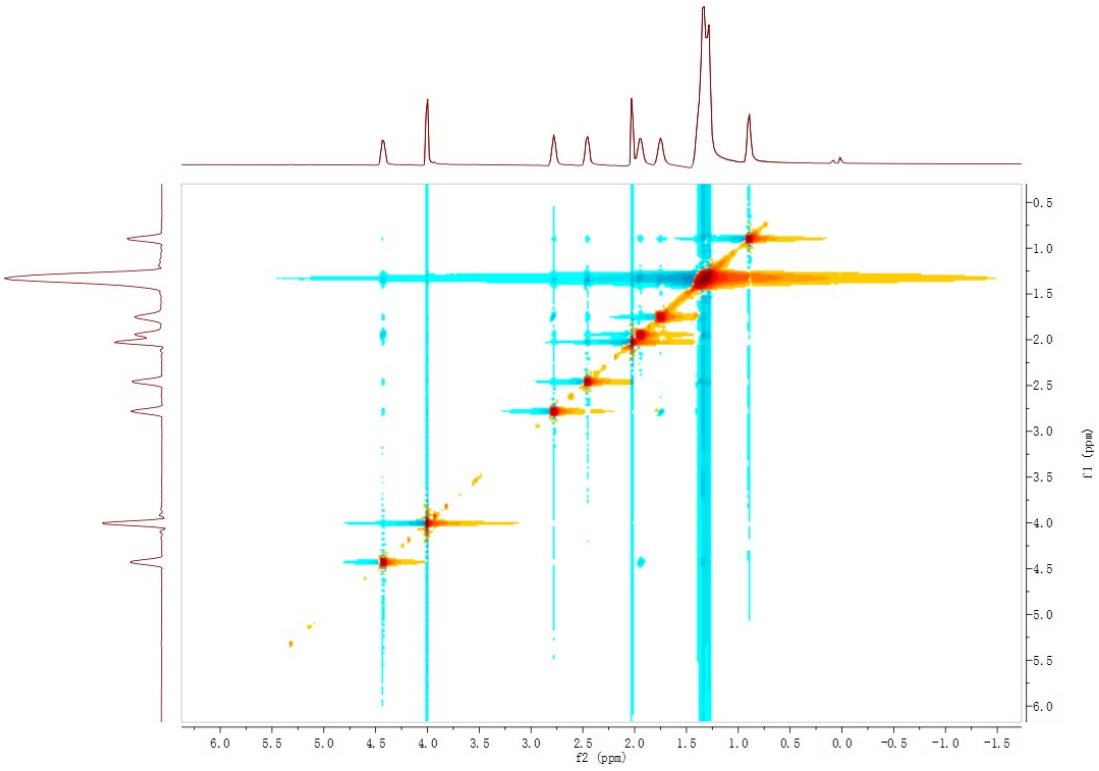
2.01 (s, 3H), 1.63-1.56 (m, 2H), 1.38-1.26 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.6, 184.0, 144.2, 144.2, 142.9, 138.6, 61.0, 51.4, 29.7, 29.3, 29.2, 29.2, 29.0, 28.7, 28.6, 26.6, 26.3, 11.8 ppm. The characterization data were in accordance with reported ones.[10]

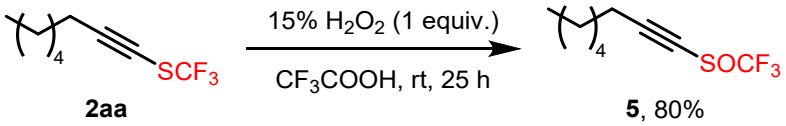


S2 **2aa** **4**, 96%

To an oven-dried 5-mL vial was added **2aa** (0.20 mmol), **S2** (0.30 mmol), $[Ir(COD)Cl]_2$ (2.7 mg, 4.0 μmol), and DCM (2.0 mL). The reaction mixture was stirred at room temperature for 1.2h. Subsequently, concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography to give the desired product.[11] Red oil (96% yield, Eluent: EtOAc/petroleum ether = 4:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.43 (d, J = 8.0 Hz, 2H), 4.00 (s, 6H), 2.78 (d, J = 8.0 Hz, 2H), 2.46 (m, 2H), 2.02 (s, 3H), 1.95 (m, 2H), 1.77-1.73 (m, 2H), 1.33-1.29 (m, 20H), 0.89 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -42.51 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4, 183.9, 155.3, 144.1, 142.8, 138.4, 127.4 (q, J = 311.0 Hz), 115.1, 60.9, 48.6, 31.3, 29.7, 29.5, 29.1, 28.8, 28.7, 28.6, 28.8, 26.7, 26.2, 26.1, 24.9, 22.3, 13.8, 11.6 ppm. HRMS (ESI): *m/z* Calcd. for $C_{28}H_{42}F_3N_3O_4S$ $[M+Na]^+$: 596.2749, Found: 596.2740.

Nuclear overhauser effect spectroscopy of 4





2aa **5**, 80%

To the solution of **1f** (0.5 mmol, 1.0 equiv.) in CF_3COOH (2 mL) in a 10 mL tube equipped with a stir bar, 15 % aqueous solution of H_2O_2 (0.5 mmol) was added dropwise very slowly. The reaction mixture was stirred at room temperature for 25 h. Subsequently, the mixture was poured into water (2 mL), and then neutralized with saturated aqueous solution of $NaHCO_3$ to pH = 7. After extraction with ether (8 mL × 3), the organic phase was washed with water (8 mL) and then brine (8 mL), and dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo. The residue was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate = 4:1 as the eluent to provide **5** as a colorless oil (80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 (t, J = 8.0 Hz, 2H), 1.66-1.60 (m, 2H), 1.43-1.40 (m, 2H), 1.33-1.28 (m, 4H), 0.90 (t, J = 8.0 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.63 (s, 3F); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.2 (q, J = 334.0 Hz), 110.8, 71.8, 31.0, 28.3, 27.1, 22.4, 19.8, 13.9 ppm. HRMS (ESI) calcd. for $C_9H_{13}F_3OS$ $(M+H)^+$: 227.0712, Found: 227.0715.

9. Details of DFT calculations for the mechanism

Quantum chemical calculations were performed using the Gaussian 16 suite of programs. [12] The B3LYP-D3(BJ) functional, i.e., the B3LYP functional[13] including the D3 dispersion correction with the Becke-Johnson damping function[14], was used for geometry optimizaions and frequencies calculations, and a mixed basis set of SDD[15] for I and 6-31G(d,p)[16] for other atoms in conjunction with the SMD[17] implicit solvation model to account for the solvation effects of the hexafluoroisopropanol (HFIP) on the computed Gibbs energy profile. Since HFIP solvent is not available in the list of default/prefined solvents in Gaussian 16 software, it is herein parametrised using a set of seven parameters raised by R. S. Paton.[18] These parameters include the static dielectric constant of the solvent at 25℃ (Eps = 16.7);[19] dynamic (optical) dielectric constant – using the square of the refractive index value of 1.275 at 20 ℃ [20] (EpsInf = 1.625625); hydrogen bond acidity (HbondAcidity = 1.96) and basicity (HbondBasicity = 0.00),[19(a)] which are Abraham's A and B values respectively; the surface tension of the solvent at interface (SurfaceTensionAtInterface = 23.23);[21] carbon aromaticity - the fraction of aromatic carbons (CarbonAromaticity = 0.00) and

electronegative halogenicity – the fraction of halogens (Electronnegative Halogencity = 0.60). These parameters were specified using the keyword "SCRF=(SMD,Solvent=Generic,Read)" in Gaussian 16. The recently corrected radius for iodine was used for SMD calculations.[22] Optimized geometries were verified by frequency computations as minima (zero imaginary frequencies) or transition structures (a single imaginary frequency) at the same level of theory. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connectivity between transition structure and intermediate.[23]

More accurate electronic energies were obtained by single point energy calculations at the SMD-M062X/6-311++G(2df,2p)+def2-TZVP(I)[24] level of theory. A factor of RTln(24.46) was added to free energy for each species to account for the 1 atm to 1 M standard state change. All Gibbs energies in solution reported throughout the text are in kilocalories per mole, and the bond lengths are in angstroms. The structures were generated by CYLview[25]. Multiwfn was utilized to perform the Hirshfeld charges calculation and analyze noncovalent interactions with an independent gradient model based on Hirshfeld partition(**IGMH**).[26]

9.1 Energy comparison and non-covalent interaction analysis of TS2 and TS2'

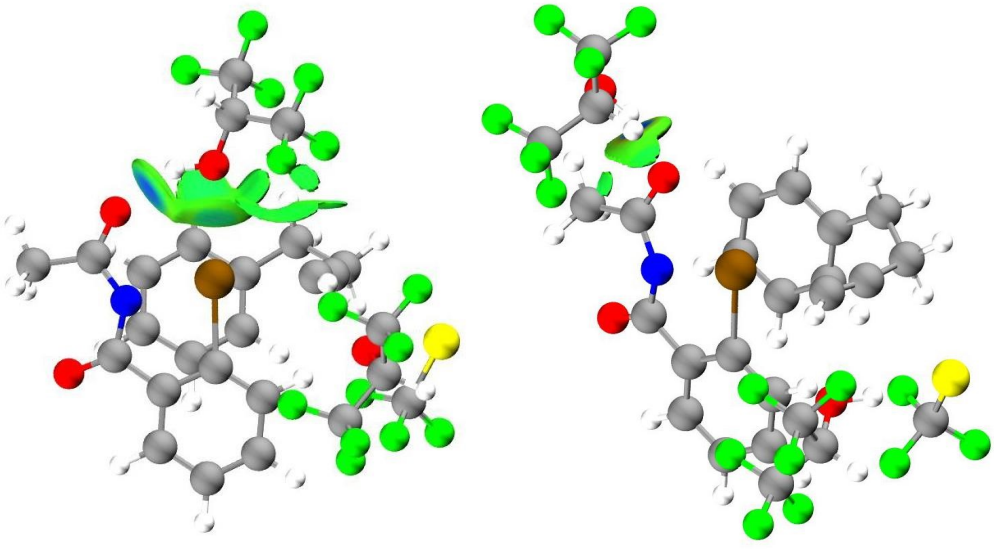


Figure S1. *Sign(λ_2)ρ* colored isosurfaces of δg^{inter}=0.005 a.u. corresponding to independent gradient model based on Hirshfeld partition (IGMH) analysis for the rate-limiting step **TS2** and **TS2'**.

SMD-B3LYP-D3(BJ)/6-31G(d,p)+SDD(I) Calculated Cartesian Coordinates and Single Point Energies Calculated Using the SMD-M062X/6-311++G(2df,2p)+def2-TZVP(I)// SMD-B3LYP-D3(BJ)/6-31G(d,p)+SDD(I).

TFTI

C	-0.33429900	3.60523800	-0.29776400
C	0.96680800	3.97370600	0.05028100
C	1.94233600	3.00011400	0.24254500
C	1.62078100	1.64728400	0.08888100
C	0.31082400	1.32688000	-0.25535300
C	-0.68420700	2.25819400	-0.45741300
H	-1.09589500	4.36384200	-0.44965800
H	1.21806500	5.02262500	0.17008900
H	2.96352100	3.25374000	0.51173400
H	-1.69251500	1.97172700	-0.72932600
I	-0.03624300	-0.82569500	-0.45090500
C	2.65129700	0.59735000	0.28799400
O	3.81582200	0.85215200	0.59274400
N	2.13785200	-0.65880700	0.08738100
C	2.75155300	-1.88938500	0.18122900
C	4.20571600	-1.96934100	0.54564800
H	4.80918100	-1.42824100	-0.18953600
H	4.38029200	-1.49347800	1.51522900
H	4.49142400	-3.02205000	0.57604500
O	2.06329500	-2.88890700	-0.04379900
S	-2.65016200	-0.49051200	-1.08705400
C	-3.28215400	-0.37663900	0.60486000
F	-2.72788600	0.64138700	1.30489300
F	-4.61213700	-0.16772300	0.58079700
F	-3.06446700	-1.49509500	1.32959500

Zero-point correction= 0.158364 (Hartree/Particle)

Thermal correction to Energy= 0.176161

Thermal correction to Enthalpy= 0.177105

Thermal correction to Gibbs Free Energy= 0.109634

SCF Done: E(RM062X) = -1585.75094508

$(HFIP)_2$

C	2.90937100	1.19209300	0.11511200
C	2.46306700	-0.13785400	0.72953100
O	1.38959900	0.05397700	1.61240500
H	0.62347500	0.44012700	1.13403600
F	3.99169900	1.04445700	-0.67265500
F	1.93474200	1.75852300	-0.63199000
F	3.22002900	2.06109100	1.09341300
C	2.14683000	-1.20867500	-0.32172300
F	1.16650000	-0.82923500	-1.17417800
F	3.23156900	-1.50380600	-1.06500100
F	1.73982500	-2.33607300	0.28530600
H	3.30994700	-0.51706900	1.30907200
C	-1.93032900	-1.17837200	0.30778800
C	-1.99871100	0.33617900	0.53629500
O	-0.78434400	0.95256800	0.17601400
H	-0.64153000	0.87718300	-0.78207700
F	-3.07295200	-1.78395300	0.67766900
F	-1.69883400	-1.47884300	-0.98604700
F	-0.92686900	-1.70148400	1.03512300
C	-3.15755700	1.01531400	-0.19805400
F	-3.03946000	0.86995500	-1.53534900
F	-4.34863100	0.51576900	0.17156100
F	-3.15156500	2.33215400	0.07003500
H	-2.14443300	0.49828600	1.60692700

Zero-point correction= 0.128517 (Hartree/Particle)
Thermal correction to Energy= 0.147883
Thermal correction to Enthalpy= 0.148827
Thermal correction to Gibbs Free Energy= 0.078335
SCF Done: E(RM062X) = -1579.71329273

TFTI-2HFIP

C	6.07154500	-1.98904000	-0.35937700

C	5.83585200	-3.32947600	-0.04814400
C	4.53448800	-3.78283800	0.14131100
C	3.45980300	-2.89545800	0.01969200
C	3.73645300	-1.56694200	-0.29365200
C	5.01302500	-1.08107400	-0.48688100
H	7.08617800	-1.63186000	-0.50626000
H	6.66886000	-4.01848400	0.04681500
H	4.31682500	-4.81840000	0.38551800
H	5.20118400	-0.04238100	-0.72705800
I	1.96137900	-0.30480700	-0.43321600
C	2.07155000	-3.36715400	0.23411700
O	1.79307700	-4.52851000	0.52243000
N	1.15521400	-2.35229800	0.06618400
C	-0.19467000	-2.36476400	0.29797800
C	-0.85454200	-3.59651700	0.84569100
H	-0.82008700	-4.39448500	0.09729700
H	-0.30874400	-3.95813100	1.72094500
H	-1.88694200	-3.36384800	1.10443300
O	-0.81298800	-1.31655600	0.05450100
S	3.45113100	1.90876500	-0.97247200
C	3.70915400	2.37933900	0.75712700
F	4.35414400	1.42709900	1.46598100
F	4.44795500	3.50087300	0.81982200
C	-4.36922800	-2.39927700	-0.67633000
C	-4.11067500	-0.99976000	-0.11333600
C	-5.37767000	-0.30659600	0.37769300
H	-3.70803200	-0.39709700	-0.93437400
O	-3.25564200	-1.07995900	0.99383400
H	-2.32155400	-1.13418500	0.66729700
F	-5.96337100	-0.99028200	1.38107300
F	-5.07288300	0.91940700	0.84348900
F	-6.28614300	-0.16007200	-0.60639200
F	-4.80432300	-3.25311900	0.26912100
F	-3.21628100	-2.90035400	-1.17532600
F	-5.27323200	-2.39088400	-1.67589900

F	2.55076900	2.62387400	1.41426000
C	-1.19523800	4.13832000	-0.58027200
C	-0.59205500	2.96599500	0.19879100
C	-1.64237500	1.94074600	0.62660900
H	-0.12308700	3.37322500	1.10155100
O	0.30604100	2.26588500	-0.62561200
H	1.08504300	2.81714600	-0.80956000
F	-2.09399900	1.25618300	-0.44295700
F	-1.10351600	1.06231800	1.49104200
F	-2.69425800	2.52113500	1.22750200
F	-1.90040500	3.72668400	-1.64950100
F	-0.19565400	4.92711800	-1.02920000
F	-2.00033100	4.89104500	0.18951600

Zero-point correction= 0.286952 (Hartree/Particle)
Thermal correction to Energy= 0.326321
Thermal correction to Enthalpy= 0.327266
Thermal correction to Gibbs Free Energy= 0.206734
SCF Done: E(RM062X) = -3165.48891619

1t

C	2.47712100	1.20647900	-0.13192600
C	1.12440200	1.20422500	0.20997600
C	0.43120400	0.00000800	0.38704300
C	1.12440500	-1.20421600	0.21003700
C	2.47712400	-1.20648400	-0.13186400
C	3.15795000	-0.00000600	-0.30450500
H	3.00012200	2.15030200	-0.26070700
H	0.59956700	2.14695400	0.34549100
H	0.59957200	-2.14693900	0.34560000
H	3.00012700	-2.15031200	-0.26059700
H	4.21194600	-0.00001200	-0.56794700
C	-1.04323600	0.00001500	0.70646800
H	-1.30313200	-0.88195700	1.30094300
H	-1.30313200	0.88201300	1.30090500
C	-1.89757400	-0.00001300	-0.58424700

H	-1.64054400	0.87871000	-1.18903600
H	-1.64054400	-0.87876300	-1.18899800
C	-3.33157900	-0.00000700	-0.30711700
C	-4.51380900	-0.00000100	-0.05250300
H	-5.56004100	0.00000300	0.16617300

Zero-point correction= 0.166626 (Hartree/Particle)
Thermal correction to Energy= 0.175799
Thermal correction to Enthalpy= 0.176743
Thermal correction to Gibbs Free Energy= 0.131395
SCF Done: E(RM062X) = -386.972517635

TS1

C	-5.67884200	-1.99122900	0.73303700
C	-5.98200800	-1.30959900	1.91422000
C	-5.02066000	-0.51282000	2.52856000
C	-3.75697000	-0.38502300	1.94464000
C	-3.50596800	-1.04163200	0.74042200
C	-4.42244800	-1.86776600	0.12351200
H	-6.42271600	-2.63037000	0.26733500
H	-6.96442500	-1.41548800	2.36245100
H	-5.21209500	0.00637300	3.46358400
H	-4.20552100	-2.38879800	-0.79959000
I	-1.49225800	-0.62969900	-0.03053200
C	-2.68239900	0.37316900	2.61066600
O	-2.80575200	1.05042100	3.62089000
N	-1.45915800	0.20314700	1.96321500
C	-0.22168800	0.78122500	2.18925500
C	0.03763500	1.45729900	3.50070600
H	-0.54796000	2.38044500	3.55432500
H	-0.28047500	0.81982800	4.32938300
H	1.10321700	1.67780400	3.56052700
O	0.61269800	0.67820400	1.29520200
C	-2.50757400	2.99996100	0.73488200
C	-3.55254500	2.61556200	-0.10584800
C	-3.34127800	2.44720700	-1.48217700

C	-2.05135300	2.63899300	-1.98929500
C	-1.00113800	3.02131300	-1.15167200
C	-1.22820100	3.21092800	0.21267800
H	-2.69709900	3.14526500	1.79527200
H	-4.54794000	2.46889700	0.30653900
H	-1.87054600	2.50234200	-3.05235900
H	-0.01387300	3.18474600	-1.57026700
H	-0.42085600	3.52705500	0.86354300
C	-4.48442600	2.06811300	-2.39193700
H	-5.35752200	2.69203500	-2.17094400
H	-4.20915500	2.25295300	-3.43465000
C	-4.92653200	0.59603900	-2.24177200
H	-5.24240500	0.40501700	-1.20891200
H	-5.80722100	0.41559100	-2.87134300
C	-3.89508900	-0.36759900	-2.60575200
C	-3.05175700	-1.19134200	-2.89058400
H	-2.34993400	-1.92984400	-3.20829200
S	0.40056200	-1.43767600	-2.44585300
C	0.19107300	-3.17814300	-2.13344100
F	0.36934200	-3.52914300	-0.82006800
F	-1.06249600	-3.63303400	-2.44563800
F	1.04857700	-3.95917100	-2.83367400
C	2.58562300	3.56104200	0.41803100
C	2.61343900	2.22343800	-0.31070100
C	3.15632900	2.32504000	-1.73635200
H	1.58186600	1.86579500	-0.38322800
O	3.43343300	1.37216900	0.44405300
H	3.13113200	0.45530900	0.26305100
F	4.41111800	2.80960000	-1.77533800
F	3.17749400	1.09347500	-2.28901400
F	2.38737700	3.11132600	-2.52230000
F	3.82222700	4.05218200	0.61793400
F	2.00823900	3.41686600	1.63002800
F	1.87808800	4.48800200	-0.26172700
C	4.47962800	-2.20795300	0.39721300

C	2.95045100	-2.20473500	0.45337500
C	2.40214400	-2.18883000	1.88376100
H	2.59778700	-3.11943900	-0.02992000
O	2.50737500	-1.04812000	-0.19659200
H	1.91938800	-1.24412900	-0.97273500
F	2.73335700	-1.05765700	2.53606800
F	1.05429000	-2.26028800	1.85746900
F	2.85232300	-3.23210400	2.60499500
F	5.00038700	-1.10266100	0.97130400
F	4.87869500	-2.22399900	-0.88708400
F	5.00725300	-3.28160500	1.01310600

Zero-point correction= 0.453683 (Hartree/Particle)
Thermal correction to Energy= 0.502941
Thermal correction to Enthalpy= 0.503885
Thermal correction to Gibbs Free Energy= 0.364225
SCF Done: E(RM062X) = -3552.46048197

IM1

C	-6.09296400	-1.40951400	1.18640900
C	-6.11506300	-0.75419100	2.42026900
C	-4.96076000	-0.15356000	2.91343400
C	-3.78630800	-0.19823000	2.15643000
C	-3.80544900	-0.82495400	0.91222900
C	-4.92704800	-1.45663100	0.41045800
H	-6.98916900	-1.89544000	0.81290100
H	-7.03075200	-0.72710400	3.00175100
H	-4.93612700	0.34056800	3.88040200
H	-4.92098000	-1.97266900	-0.54150000
I	-1.88373800	-0.69198100	-0.11993100
C	-2.52652100	0.36841500	2.67015300
O	-2.41501900	1.02307200	3.69740600
N	-1.43914600	0.05389200	1.85211600
C	-0.14175800	0.55351600	1.88127300
C	0.38121700	1.15092600	3.15126800
H	-0.16572000	2.07119600	3.37588600

H	0.21401600	0.46358500	3.98494600
H	1.44254700	1.35443900	3.01685000
O	0.51339800	0.43723600	0.85284100
C	-2.65770400	2.86368900	0.46294000
C	-3.60310100	2.44492100	-0.47461200
C	-3.23685500	2.22499400	-1.81099200
C	-1.90342500	2.42923000	-2.18249200
C	-0.95630400	2.85932400	-1.25098800
C	-1.33143500	3.07799000	0.07544800
H	-2.95341900	3.02764600	1.49654600
H	-4.63387100	2.29031500	-0.16485700
H	-1.60458200	2.25550700	-3.21297000
H	0.06678000	3.03239600	-1.56884800
H	-0.60062500	3.41806700	0.80078000
C	-4.25275800	1.75846400	-2.82679300
H	-5.10860000	2.44272100	-2.84406200
H	-3.81077900	1.76758000	-3.82707300
C	-4.81912100	0.35107000	-2.53691300
H	-5.32514300	0.33681800	-1.56389500
H	-5.58774800	0.10595600	-3.28181300
C	-3.83754900	-0.72399500	-2.56571400
C	-3.04409800	-1.65057400	-2.56015900
H	-2.40313700	-2.48990600	-2.74106600
S	0.49037900	-1.18723000	-2.34196500
C	0.43182400	-2.95569500	-2.23085000
F	0.06068500	-3.43205100	-1.00188800
F	-0.45755300	-3.53192500	-3.10579100
F	1.62589300	-3.56584100	-2.49312900
C	2.49336600	3.62807100	0.51086800
C	2.66912400	2.27339500	-0.16584200
C	3.43953600	2.36953700	-1.48440200
H	1.67166100	1.89235300	-0.40185000
O	3.35749100	1.44852800	0.73665300
H	3.13624000	0.52047900	0.49580800
F	4.66541800	2.90415600	-1.32635000

F	3.59917000	1.13634100	-2.00477200
F	2.77836500	3.11529000	-2.39701400
F	3.66850700	4.16312900	0.88838600
F	1.73541300	3.50072200	1.62219500
F	1.87473800	4.51272600	-0.29822500
C	4.59677500	-2.20261900	0.57834600
C	3.08035400	-2.19444300	0.38101300
C	2.30875100	-2.30611900	1.70192300
H	2.81945200	-3.06574700	-0.22769800
O	2.78223600	-0.98560200	-0.25326100
H	2.03432400	-1.07623700	-0.90987100
F	2.53300200	-1.24866000	2.50846300
F	0.98231300	-2.35454300	1.45901900
F	2.63680000	-3.42114100	2.38164600
F	5.00592000	-1.13023800	1.28905200
F	5.20691200	-2.15321600	-0.61866600
F	5.02113600	-3.30842600	1.21676900

Zero-point correction= 0.454721 (Hartree/Particle)
Thermal correction to Energy= 0.504183
Thermal correction to Enthalpy= 0.505127
Thermal correction to Gibbs Free Energy= 0.365478
SCF Done: E(RM062X) = -3552.46670962

IM2

C	3.23451400	2.04907500	1.68544500
C	3.49114800	3.19299200	0.92575600
C	2.64304800	3.54859800	-0.11856500
C	1.53194100	2.75006100	-0.40371300
C	1.31087700	1.61903400	0.37847400
C	2.12508600	1.23525400	1.42134300
H	3.90181000	1.76651000	2.49085200
H	4.35794300	3.80580900	1.15039000
H	2.81485700	4.43239700	-0.72601200
H	1.93858900	0.34828300	2.01135700
I	-0.48162400	0.57585300	-0.19113700

C	0.58777700	3.10934900	-1.47673200
O	0.64039900	4.13265300	-2.14318300
N	-0.41675400	2.14950500	-1.64277200
C	-1.60806400	2.23850900	-2.34135800
C	-1.80141400	3.34463600	-3.32926900
H	-1.81572100	4.30525900	-2.80457400
H	-0.97138100	3.37562300	-4.03973300
H	-2.75005600	3.17487700	-3.84021800
O	-2.46273300	1.37932600	-2.11492700
C	-2.94206300	3.35399400	0.51199200
C	-3.22790900	2.28090500	1.35617200
C	-2.34978200	1.92150300	2.38835200
C	-1.19978900	2.69756700	2.58530600
C	-0.90923600	3.77135400	1.74109400
C	-1.77040000	4.09541000	0.69104000
H	-3.62227200	3.59491300	-0.30056300
H	-4.12022300	1.68603800	1.18615800
H	-0.50117800	2.45251600	3.37954500
H	0.00167700	4.34279700	1.89433100
H	-1.52544100	4.91289200	0.01790500
C	-2.64233800	0.69081700	3.22139800
H	-3.12868300	0.98122000	4.16080800
H	-3.34738500	0.04913400	2.68595200
C	-1.40415200	-0.14533400	3.61910600
H	-0.68718300	0.45592100	4.18785100
H	-1.73443900	-0.94755800	4.29269100
C	-0.70033700	-0.80599000	2.52846700
C	-0.09528000	-1.40142000	1.64936400
H	0.45052200	-2.06165300	1.00397900
S	3.90646600	-2.90612800	1.80247600
C	4.67968500	-1.37853600	2.22893100
F	4.88055400	-0.53492700	1.16524400
F	3.96572300	-0.61748500	3.13493100
F	5.91136500	-1.51432000	2.80603300
C	-3.06162800	-2.78488500	-0.15303900

C	-3.96570600	-1.61600600	-0.54428500
C	-5.31902900	-1.64145500	0.17054000
H	-4.15590500	-1.70029900	-1.61909900
O	-3.30816400	-0.42867100	-0.19643500
H	-3.39423500	0.21431600	-0.92228800
F	-6.04977600	-0.58064000	-0.22468600
F	-5.18344400	-1.56109400	1.50976300
F	-6.01546100	-2.75837900	-0.10788400
F	-3.59758100	-3.96214600	-0.51929700
F	-1.86817600	-2.65901400	-0.77265400
F	-2.82822700	-2.82925500	1.17144000
C	1.86576300	-2.49855200	-2.32201900
C	2.82063100	-1.65453900	-1.47492100
C	3.18586800	-0.32565100	-2.14239400
H	3.75346400	-2.22340400	-1.37999600
O	2.22034500	-1.41192100	-0.24268000
H	2.73823600	-1.91484600	0.45924100
F	3.95816100	0.40988900	-1.32606200
F	2.09331500	0.41935700	-2.44140700
F	3.86025500	-0.52156700	-3.29209800
F	2.36722700	-2.77064000	-3.54225700
F	1.62964000	-3.66784000	-1.69627800
F	0.67007500	-1.89312800	-2.49807900

Zero-point correction= 0.453301 (Hartree/Particle)
Thermal correction to Energy= 0.503078
Thermal correction to Enthalpy= 0.504022
Thermal correction to Gibbs Free Energy= 0.361726
SCF Done: E(RM062X) = -3552.46227044

TS2

C	2.83820500	2.68438800	0.58905300
C	2.58739100	4.01327200	0.24151900
C	1.40938000	4.35570800	-0.41726600
C	0.47291000	3.36490000	-0.72699300
C	0.75839200	2.05261200	-0.35604000

C	1.91638800	1.67365200	0.28846400
H	3.75020700	2.41352800	1.10879300
H	3.31163800	4.78294000	0.48787700
H	1.18305400	5.38104500	-0.69474500
H	2.12424100	0.64978900	0.55544700
I	-0.86233200	0.68350000	-0.76540200
C	-0.81791500	3.71476200	-1.36007700
O	-1.17500900	4.86930500	-1.57264500
N	-1.57975300	2.59444500	-1.65620800
C	-2.92582700	2.54856900	-1.95426800
C	-3.62991200	3.78938600	-2.41558400
H	-3.65936000	4.52016900	-1.60121900
H	-3.09205000	4.25611400	-3.24473000
H	-4.64222900	3.51120300	-2.71277800
O	-3.51398000	1.46750400	-1.84265900
C	-3.41654000	2.60341300	1.36050000
C	-3.30863200	1.29638500	1.83322600
C	-2.13706000	0.85265300	2.46390100
C	-1.08800900	1.76329700	2.64333400
C	-1.19401100	3.07343500	2.17045100
C	-2.35280000	3.49685700	1.51788000
H	-4.32360600	2.91676900	0.85059800
H	-4.12381500	0.59701700	1.67360700
H	-0.16361800	1.45378600	3.11968700
H	-0.35874000	3.75650000	2.29527500
H	-2.41945400	4.50836200	1.12593400
C	-2.03513000	-0.59841900	2.88235500
H	-2.38743800	-0.72053800	3.91397700
H	-2.69046100	-1.20386700	2.25284300
C	-0.60813900	-1.20583000	2.85691200
H	0.05683100	-0.70361800	3.56223600
H	-0.68252800	-2.25262600	3.17654600
C	0.01426100	-1.21169500	1.54944400
C	0.36991200	-1.14911200	0.36197900
H	1.09757100	-1.48841100	-0.35902600

S	2.79698300	-2.19113200	2.70288900
C	3.22273200	-0.52186000	3.11738400
F	4.12640800	0.05309800	2.25818800
F	2.15859400	0.35369100	3.11740900
F	3.77681800	-0.38381700	4.35554200
C	-2.69151500	-3.09616000	-0.78950300
C	-3.86117900	-2.11587500	-0.87997100
C	-5.06151100	-2.53888300	-0.02907000
H	-4.18729800	-2.09516700	-1.92491500
O	-3.40172000	-0.87667100	-0.42099900
H	-3.75550100	-0.15354600	-0.97349000
F	-6.03242400	-1.61168600	-0.13787200
F	-4.74407400	-2.63907700	1.27774400
F	-5.56578700	-3.72249200	-0.42383200
F	-3.03766600	-4.32056900	-1.22251500
F	-1.67253100	-2.65555100	-1.55919300
F	-2.22462400	-3.21709000	0.46791800
C	3.97204700	-2.42294500	-2.09735200
C	4.30600100	-1.48301500	-0.93753700
C	4.80367500	-0.11444500	-1.40491400
H	5.11101200	-1.94508100	-0.35579600
O	3.13920100	-1.27787300	-0.20291500
H	3.17316300	-1.72788200	0.68699100
F	5.16816100	0.62782000	-0.34189600
F	3.84388800	0.56664900	-2.06465500
F	5.87076100	-0.21684000	-2.22109700
F	5.03874500	-2.68110600	-2.87688900
F	3.52137000	-3.59391600	-1.60750800
F	2.99924000	-1.91393600	-2.88387500

Zero-point correction= 0.453072 (Hartree/Particle)
Thermal correction to Energy= 0.501981
Thermal correction to Enthalpy= 0.502926
Thermal correction to Gibbs Free Energy= 0.362854
SCF Done: E(RM062X) = -3552.44866309

IM3

C	-2.94338200	2.20562300	1.98918900
C	-2.26343400	3.12876100	2.78502000
C	-0.87225400	3.14016400	2.80185000
C	-0.13551900	2.21901300	2.04448800
C	-0.85741200	1.31602500	1.27055000
C	-2.23683100	1.28760900	1.20787900
H	-4.02866700	2.18594100	1.95949800
H	-2.81777400	3.84388200	3.38491900
H	-0.31627100	3.86507100	3.38844900
H	-2.77627000	0.59480300	0.58078400
I	0.28649100	-0.09638200	0.05970500
C	1.35851200	2.31899000	2.01506800
O	1.91974300	3.31862200	2.48643600
N	1.92397100	1.25380700	1.39238000
C	3.18356300	1.23428600	0.89124700
C	4.24194900	2.21629200	1.31895700
H	3.99106300	3.21548300	0.94715300
H	4.28441700	2.29167000	2.40830700
H	5.20921800	1.90814800	0.91654000
O	3.44546800	0.35336100	0.03774900
C	0.98466700	4.07659400	-0.63186100
C	1.02510800	2.99622600	-1.51022900
C	-0.15458000	2.46189300	-2.05459200
C	-1.37706100	3.03000000	-1.68113500
C	-1.42001100	4.11141200	-0.79545500
C	-0.24290100	4.63898100	-0.26937600
H	1.90543800	4.46933000	-0.21033500
H	1.98087700	2.53948500	-1.76099600
H	-2.30992800	2.62760900	-2.06137400
H	-2.38067200	4.52893800	-0.50710000
H	-0.27736100	5.46966500	0.42939500
C	-0.05061100	1.30975700	-3.03408400
H	0.21524100	1.72201600	-4.01678300
H	0.79434000	0.66865100	-2.76258000

C	-1.30625600	0.46680000	-3.27701500
H	-2.10348800	1.11132500	-3.66159100
H	-1.09178100	-0.22185600	-4.10463300
C	-1.90374500	-0.38725500	-2.18576300
C	-1.51970600	-0.74820900	-0.96009600
H	-2.10944900	-1.42185500	-0.35356700
S	-3.45775900	-1.20460500	-2.68473300
C	-4.56959700	0.23543000	-2.59456300
F	-4.29603000	1.04896300	-1.55628800
F	-4.53784600	1.00545800	-3.70193700
F	-5.82731600	-0.21716600	-2.45507800
C	5.61083500	-2.36883200	-0.81573200
C	6.08866500	-1.13707500	-0.04321100
C	7.58301700	-1.15932200	0.25674700
H	5.55859500	-1.13455500	0.91778000
O	5.84501800	0.01435700	-0.80563100
H	4.90138300	0.27834900	-0.59907500
F	7.91129600	-0.08775300	1.00511200
F	8.32074700	-1.10862200	-0.86931300
F	7.94587900	-2.26493800	0.93770800
F	5.80808500	-3.51279700	-0.12939700
F	4.28595000	-2.26036900	-1.05698200
F	6.22831500	-2.48999500	-2.00661600
C	-4.78853900	-3.04265600	0.70771800
C	-4.88330200	-1.74193900	1.51339900
C	-3.84311600	-1.66121100	2.63165300
H	-5.86757400	-1.73241300	1.99190300
O	-4.67744900	-0.64691000	0.66307200
H	-5.53248100	-0.27432000	0.40725100
F	-4.02389000	-0.53538100	3.34332900
F	-2.57922100	-1.63977800	2.15264800
F	-3.94299100	-2.70865600	3.46948400
F	-5.08860400	-4.11566800	1.46297900
F	-5.65587200	-2.99781500	-0.31928900
F	-3.55595900	-3.24100500	0.19184100

Zero-point correction= 0.457886 (Hartree/Particle)
Thermal correction to Energy= 0.506389
Thermal correction to Enthalpy= 0.507333
Thermal correction to Gibbs Free Energy= 0.367393
SCF Done: E(RM062X) = -3552.50383871

TS3

C	-3.18157700	2.88133500	0.92197000
C	-2.49821500	4.08469400	1.09858100
C	-1.25972300	4.28681500	0.49454100
C	-0.66591900	3.28713700	-0.28899300
C	-1.40798700	2.12359100	-0.47000400
C	-2.64691000	1.88362100	0.10471900
H	-4.14205100	2.71239600	1.39865400
H	-2.92787100	4.86778300	1.71530800
H	-0.71094900	5.21218600	0.64149800
H	-3.18086800	0.95662600	-0.05424000
I	-0.70923500	0.61217700	-1.86036600
C	0.72986600	3.55029100	-0.80006300
O	0.95304700	4.58374800	-1.43814400
N	1.63549500	2.61684500	-0.40184200
C	2.96432300	2.60069500	-0.73705900
C	3.52187400	3.48357200	-1.81557800
H	2.89700900	3.46312600	-2.71284800
H	3.53633800	4.52172500	-1.46679800
H	4.53799100	3.15526600	-2.04256500
O	3.69674800	1.81418200	-0.10962400
C	-5.16501600	0.77825500	-2.16049300
C	-4.19058500	-0.08362100	-2.66217700
C	-3.75965600	-1.19744400	-1.92579600
C	-4.33260400	-1.42307800	-0.66793000
C	-5.31018300	-0.56109300	-0.16225700
C	-5.72976000	0.54295500	-0.90435800
H	-5.47890800	1.63662900	-2.74804700
H	-3.75479600	0.10969200	-3.63961400

H	-4.03214100	-2.27695300	-0.07393200
H	-5.73725700	-0.75454200	0.81795500
H	-6.48394100	1.21653700	-0.50758200
C	-2.72092700	-2.12509800	-2.52414200
H	-3.23052600	-2.86906400	-3.15034600
H	-2.08726100	-1.56880100	-3.22323800
C	-1.86685000	-2.93214700	-1.53820800
H	-2.49867500	-3.65996800	-1.02163200
H	-1.14190400	-3.53235800	-2.10384600
C	-1.09350100	-2.19867000	-0.47690600
C	-0.60866400	-0.97538600	-0.33408800
H	-0.03977000	-0.49809400	0.47128700
S	-0.54800800	-3.18286900	0.95254200
C	-2.01835300	-2.98947900	2.01317100
F	-2.39757200	-1.71071600	2.14586700
F	-3.08979000	-3.67806200	1.56402600
F	-1.70301400	-3.47373100	3.22341300
C	0.58546300	2.00042800	3.09455600
C	1.48420300	0.95222100	2.41916100
C	1.42995200	-0.38356100	3.16621300
H	2.52029300	1.32063700	2.50847500
O	1.08477300	0.75364700	1.11917800
H	1.34042000	1.70469800	0.40256100
F	2.14801300	-1.31397300	2.50822100
F	0.16382600	-0.85175600	3.27282600
F	1.93115000	-0.29557000	4.41645800
F	0.82316300	2.12672900	4.41865400
F	0.79811000	3.21346300	2.53513400
F	-0.72404800	1.71577700	2.94102500
C	2.83150500	-0.97984300	-2.35570800
C	3.28653400	-1.11816400	-0.89992800
C	3.36540000	-2.57542000	-0.45435400
H	2.55867500	-0.60973200	-0.25619400
O	4.58164000	-0.58391800	-0.78797600
H	4.48446400	0.36087000	-0.52865300

F	4.24736600	-3.27979400	-1.19010000
F	3.75721500	-2.64866000	0.82739500
F	2.16572700	-3.19355800	-0.56012700
F	3.68655900	-1.56092500	-3.21195600
F	2.75274300	0.32745900	-2.68919200
F	1.60666700	-1.52367900	-2.57178900

Zero-point correction= 0.451879 (Hartree/Particle)
Thermal correction to Energy= 0.500045
Thermal correction to Enthalpy= 0.500989
Thermal correction to Gibbs Free Energy= 0.362859
SCF Done: E(RM062X) = -3552.48982744

IM4

C	-3.18146000	2.88105300	0.92285500
C	-2.49840100	4.08426200	1.10006300
C	-1.25977300	4.28690300	0.49636700
C	-0.66718400	3.28719600	-0.28714800
C	-1.40778900	2.12250900	-0.46943800
C	-2.64665300	1.88351100	0.10529400
H	-4.14193500	2.71191100	1.39943700
H	-2.92791500	4.86713300	1.71701200
H	-0.71085800	5.21192800	0.64445700
H	-3.18066400	0.95659100	-0.05387700
I	-0.70915100	0.61278900	-1.86018600
C	0.72397000	3.55268400	-0.79772800
O	0.95470500	4.58107600	-1.43519900
N	1.63669000	2.61730600	-0.40106900
C	2.97009700	2.59942400	-0.73583100
C	3.52105200	3.48430300	-1.81351000
H	2.89589600	3.46280400	-2.71040200
H	3.53578500	4.52208400	-1.46387300
H	4.53691200	3.15529900	-2.03938400
O	3.69594200	1.81429900	-0.10840500
C	-5.16486600	0.77901300	-2.16051100
C	-4.19040400	-0.08269700	-2.66244500

C	-3.75954100	-1.19680900	-1.92646100
C	-4.33260000	-1.42290900	-0.66871500
C	-5.31020700	-0.56110400	-0.16279800
C	-5.72971400	0.54324100	-0.90451000
H	-5.47873600	1.63759500	-2.74778300
H	-3.75455200	0.11094400	-3.63978900
H	-4.03211800	-2.27694800	-0.07497600
H	-5.73733300	-0.75490800	0.81731800
H	-6.48393500	1.21666600	-0.50753600
C	-2.72078700	-2.12426000	-2.52505400
H	-3.23037400	-2.86793300	-3.15164000
H	-2.08706800	-1.56765600	-3.22391100
C	-1.86677100	-2.93162300	-1.53936000
H	-2.49869700	-3.65949600	-1.02299100
H	-1.14190900	-3.53166500	-2.10525200
C	-1.09333700	-2.19815900	-0.47774200
C	-0.60744000	-0.97551500	-0.33192300
H	-0.03315700	-0.48892400	0.47236700
S	-0.54815800	-3.18328400	0.95137800
C	-2.01844100	-2.99022000	2.01195500
F	-2.39784500	-1.71167600	2.14513800
F	-3.09002800	-3.67877300	1.56248500
F	-1.70337900	-3.47510100	3.22208200
C	0.58601600	1.99727100	3.09469800
C	1.48212700	0.94862200	2.41500500
C	1.42978700	-0.38370200	3.16672200
H	2.51967600	1.31966000	2.51374000
O	1.08292500	0.74924300	1.12223200
H	1.36225900	1.82521300	0.30465100
F	2.14790400	-1.31556200	2.50858300
F	0.16338700	-0.85360900	3.27299300
F	1.93110800	-0.29826900	4.41796000
F	0.82258200	2.12533600	4.42007900
F	0.79791200	3.21260600	2.53638700
F	-0.72469700	1.71489700	2.94203600

C	2.83163700	-0.97934900	-2.35556300
C	3.28620600	-1.11791000	-0.89974000
C	3.36525200	-2.57538000	-0.45482400
H	2.55867400	-0.60878700	-0.25495300
O	4.58188100	-0.58433900	-0.78802500
H	4.48778500	0.35815500	-0.52530600
F	4.24738800	-3.27954100	-1.19091700
F	3.75711900	-2.64919700	0.82675500
F	2.16570000	-3.19353900	-0.56107700
F	3.68674200	-1.55986300	-3.21214300
F	2.75290600	0.32840800	-2.68874900
F	1.60683800	-1.52283500	-2.57214200

Zero-point correction= 0.455299 (Hartree/Particle)
Thermal correction to Energy= 0.503697
Thermal correction to Enthalpy= 0.504641
Thermal correction to Gibbs Free Energy= 0.364438
SCF Done: E(RM062X) = -3552.48899379

TS4

C	-3.53075000	2.30250500	1.38468000
C	-3.02790600	3.45303300	1.99155700
C	-1.77779900	3.94655300	1.62544300
C	-1.01060000	3.29583900	0.65049100
C	-1.57264900	2.18601100	0.01682800
C	-2.81078800	1.66798100	0.37007600
H	-4.49440300	1.89801000	1.67845900
H	-3.60198000	3.95959600	2.76099100
H	-1.35730000	4.82129300	2.11269900
H	-3.20974100	0.79105400	-0.11985200
I	-0.60893200	1.31735500	-1.70154100
C	0.38541700	3.80118900	0.43813400
O	0.61030300	4.98014400	0.18244400
N	1.35509500	2.84898500	0.65814800
C	2.72546100	2.98113400	0.53074900
C	3.32000300	4.23435300	-0.02927700

H	2.85558000	4.49794300	-0.98392800
H	3.13578200	5.07038600	0.65334700
H	4.39302100	4.07778100	-0.15065100
O	3.41419200	2.02558800	0.90328900
C	-5.16000800	0.94636000	-2.11283000
C	-4.07553100	0.38934900	-2.78867100
C	-3.51770300	-0.83266500	-2.38264800
C	-4.07355300	-1.47806900	-1.27102900
C	-5.15894100	-0.92003500	-0.58858300
C	-5.70795300	0.29205400	-1.00629800
H	-5.57266200	1.89478800	-2.44565600
H	-3.65343400	0.90764700	-3.64614000
H	-3.67848700	-2.42752900	-0.93191600
H	-5.57042400	-1.43753900	0.27370200
H	-6.54900200	0.72657100	-0.47359000
C	-2.37352100	-1.41863800	-3.18419000
H	-2.78792800	-1.95033300	-4.05104500
H	-1.77465100	-0.60924600	-3.61208900
C	-1.47206200	-2.43220800	-2.47236200
H	-2.04416800	-3.33288600	-2.23247600
H	-0.68520200	-2.75779600	-3.16434900
C	-0.78975000	-2.00598200	-1.20478800
C	-0.38154200	-0.95732200	-0.53607500
H	0.18472600	-0.43227900	0.45390700
S	-0.13262300	-3.27445300	-0.08127700
C	-1.63753300	-3.60920200	0.91010300
F	-2.18121100	-2.49592800	1.41187000
F	-2.59147400	-4.24018900	0.19526000
F	-1.27908100	-4.41466100	1.91893000
C	-0.32349700	0.44063200	3.31768200
C	0.99447600	0.04979300	2.63276600
C	1.35906600	-1.40475900	2.97567400
H	1.78179500	0.66446000	3.09856200
O	0.92422500	0.28221700	1.28136900
H	1.07352000	1.87743800	0.95099600

F	2.31295300	-1.86104600	2.14579800
F	0.30090700	-2.24697200	2.88088400
F	1.82943100	-1.51299400	4.23745400
F	-0.37236700	0.05865600	4.61433500
F	-0.47777500	1.78211900	3.29162700
F	-1.39294700	-0.09682200	2.69464800
C	3.12276400	0.15944700	-2.25216900
C	3.47602200	-0.45835500	-0.89639300
C	3.69738700	-1.96556900	-0.98882300
H	2.64167600	-0.28185400	-0.20645700
O	4.68537700	0.10517700	-0.45181800
H	4.45983400	0.87435200	0.11391400
F	4.69342800	-2.27957100	-1.84017800
F	4.02324300	-2.46345000	0.21426900
F	2.58291800	-2.60475200	-1.41679800
F	4.10956000	0.00715700	-3.15198700
F	2.91252400	1.48671800	-2.11070500
F	1.99870500	-0.37703500	-2.78606000

Zero-point correction= 0.452342 (Hartree/Particle)
Thermal correction to Energy= 0.500488
Thermal correction to Enthalpy= 0.501432
Thermal correction to Gibbs Free Energy= 0.365161
SCF Done: E(RM062X) = -3552.47644512

IM5

C	-2.12920800	-1.06367000	1.34119400
C	-1.68941700	0.25735200	1.24560300
C	-1.80655300	0.96490300	0.04319800
C	-2.38645500	0.32390800	-1.05926300
C	-2.83156100	-0.99413100	-0.96618700
C	-2.69987600	-1.69405600	0.23507200
H	-2.02563500	-1.59952600	2.28074600
H	-1.24081800	0.74104000	2.10875500
H	-2.48611200	0.86249200	-1.99884600
H	-3.28087300	-1.47552000	-1.83065100

H	-3.04323700	-2.72221200	0.30872700
C	-1.24580000	2.35872400	-0.09479400
H	-1.86843800	2.95566100	-0.76936500
H	-1.23524600	2.86676500	0.87478900
C	0.18688300	2.35212400	-0.67791100
H	0.19415300	1.84437300	-1.64565200
H	0.53101900	3.37950100	-0.84448400
C	1.13486300	1.67332900	0.24400800
C	1.55331400	1.39733100	1.44937700
S	2.48100400	0.49306700	-0.09147200
C	1.57175400	-1.12232100	-0.19756500
F	1.11174400	-1.51883800	0.99148100
F	0.53835700	-1.05143900	-1.04606400
F	2.44006100	-2.03668000	-0.65617700

Zero-point correction= 0.172560 (Hartree/Particle)
Thermal correction to Energy= 0.186492
Thermal correction to Enthalpy= 0.187436
Thermal correction to Gibbs Free Energy= 0.130647
SCF Done: E(RM062X) = -1122.16947679

6-2HFIP

C	4.78265000	-0.76127700	-1.41946100
C	5.16281300	-0.67837000	-0.08020000
C	4.23771900	-0.96554700	0.91814000
C	2.91954600	-1.31830100	0.59391900
C	2.56508500	-1.42205800	-0.75577100
C	3.48697100	-1.15078900	-1.76369900
H	5.49548300	-0.53847500	-2.20769300
H	6.17533200	-0.39188400	0.18588300
H	4.51138300	-0.90342900	1.96735800
H	3.20884300	-1.24723300	-2.80713000
I	0.62595300	-2.15575800	-1.35421000
C	1.99363900	-1.50095100	1.75652700
O	2.25328800	-2.25377700	2.68642400
N	0.89894300	-0.65874100	1.72946500

C	-0.10962300	-0.50225700	2.66607300
C	-0.20728200	-1.44313600	3.82243100
H	-0.19460900	-2.48270100	3.48375700
H	0.65829600	-1.31294500	4.48048900
H	-1.12802100	-1.22078400	4.36366600
O	-0.89079200	0.43715400	2.49383700
C	1.84695300	2.96127600	-0.12871900
C	0.47284900	2.48594300	0.34920900
C	-0.65245700	3.49728800	0.11957700
H	0.53334800	2.31818100	1.42794600
H	0.81459000	-0.02037600	0.93574600
F	-1.77406300	3.07042700	0.72374700
F	-0.92073800	3.64592200	-1.19302500
F	-0.34252200	4.70689400	0.62161000
F	2.25771400	4.05238600	0.53718600
F	2.75408100	1.98429800	0.06531500
F	1.84054000	3.25322500	-1.44685000
C	-3.07528600	-1.73645000	0.41462300
C	-2.72927700	-0.27014600	0.14764400
C	-3.31833000	0.25792800	-1.15593000
H	-1.64341800	-0.18971300	0.05982200
O	-3.24995100	0.51614500	1.18874800
H	-2.55238500	0.59562600	1.87001800
F	-2.92526900	1.52920600	-1.35799200
F	-4.66455000	0.24202500	-1.14388200
F	-2.90515400	-0.47057300	-2.21495100
F	-2.66303400	-2.55509500	-0.57845400
F	-2.46654300	-2.14154900	1.55171700
F	-4.39708200	-1.92089600	0.57455500
O	0.15056400	1.25605500	-0.24816700
H	0.15193100	1.33014000	-1.21669800

Zero-point correction= 0.283352 (Hartree/Particle)

Thermal correction to Energy= 0.317393

Thermal correction to Enthalpy= 0.318337

Thermal correction to Gibbs Free Energy= 0.210622

SCF Done: E(RM062X) = -2430.31659262

TS5

C	-2.00779500	-1.21634500	1.33900100
C	-1.73955600	0.14966500	1.24596600
C	-1.94800400	0.83840800	0.04449700
C	-2.44020700	0.13194200	-1.05989300
C	-2.71478100	-1.23211900	-0.96857600
C	-2.49533000	-1.91120600	0.23147900
H	-1.83709000	-1.73670100	2.27741400
H	-1.35729400	0.68506800	2.11042000
H	-2.60735500	0.65560500	-1.99831200
H	-3.09964300	-1.76514200	-1.83377400
H	-2.70640900	-2.97454500	0.30346100
C	-1.58138800	2.29487900	-0.08329600
H	-2.24425000	2.80052700	-0.79214000
H	-1.67917400	2.80490500	0.87948300
C	-0.13136100	2.50089800	-0.61208400
H	-0.02202200	2.00132500	-1.58165200
H	0.07826100	3.56545200	-0.76531500
C	0.84405500	1.92340300	0.29668600
C	1.50870500	1.42823900	1.25949200
S	2.56244600	0.59850900	-0.07541400
C	1.70255900	-1.01350000	-0.19079200
F	1.37900900	-1.51491800	1.00892600
F	0.57652300	-0.94925100	-0.91875800
F	2.54385300	-1.86674500	-0.80214800

Zero-point correction= 0.171481 (Hartree/Particle)
Thermal correction to Energy= 0.185202
Thermal correction to Enthalpy= 0.186146
Thermal correction to Gibbs Free Energy= 0.128968
SCF Done: E(RM062X) = -1122.15874954

TS5-1

C	2.47609500	-0.63955000	-1.41546200

C	1.96826900	0.61159500	-1.06655000
C	1.69802300	0.92634900	0.27125400
C	1.94971900	-0.03969200	1.25222200
C	2.45607600	-1.29282300	0.90726600
C	2.72018100	-1.59661300	-0.42898100
H	2.68146200	-0.86690700	-2.45801200
H	1.77792400	1.35261300	-1.83786400
H	1.74731200	0.19245000	2.29503000
H	2.64631900	-2.03045300	1.68216300
H	3.11637600	-2.57143500	-0.69963400
C	1.12889200	2.27254600	0.64745700
H	1.48167500	2.55567400	1.64706000
H	1.48225800	3.03817300	-0.04745400
C	-0.40267200	2.32260900	0.71544200
H	-0.75872900	1.63983000	1.49408000
H	-0.77664000	3.31327900	0.96927000
C	-1.36085600	1.49711100	-0.47853300
C	-0.90490600	2.46601000	-1.16911400
S	-2.54710800	0.28837000	-0.17447500
C	-1.49915700	-1.20116300	0.07469000
F	-0.59713000	-1.36532800	-0.89584700
F	-0.85120400	-1.17948400	1.24879600
F	-2.33191200	-2.25467800	0.07914100

Zero-point correction= 0.170741 (Hartree/Particle)
Thermal correction to Energy= 0.184608
Thermal correction to Enthalpy= 0.185552
Thermal correction to Gibbs Free Energy= 0.128184
SCF Done: E(RM062X) = -1122.13093622

2t

C	5.36012800	-0.89590800	-0.02597600
C	4.01109100	-1.09588100	-0.32049300
C	3.12032100	-0.01606900	-0.37034000
C	3.61137400	1.27051600	-0.11404300
C	4.95967500	1.47471500	0.18085700

C	5.83868900	0.39106700	0.22604200
H	6.03811700	-1.74465200	0.00334700
H	3.64414500	-2.10024500	-0.51835400
H	2.93144000	2.11843500	-0.15020300
H	5.32441400	2.48033900	0.37204600
H	6.88945000	0.54876500	0.45267900
C	1.65274100	-0.24053400	-0.63832600
H	1.22175300	0.62660200	-1.14897100
H	1.51303900	-1.10745400	-1.29204000
C	0.87334700	-0.47943300	0.67755400
H	1.29477100	-1.34588800	1.20330700
H	1.00730300	0.37951900	1.34747200
C	-0.55041100	-0.70112400	0.46699600
C	-1.73506700	-0.86495600	0.25909500
S	-3.36017700	-1.23812000	-0.01819100
C	-4.04867900	0.46536600	-0.05112600
F	-5.36730600	0.35187700	-0.26747100
F	-3.85737600	1.11565700	1.10442000
F	-3.51541300	1.21112600	-1.02802300

Zero-point correction= 0.173248 (Hartree/Particle)
Thermal correction to Energy= 0.187710
Thermal correction to Enthalpy= 0.188655
Thermal correction to Gibbs Free Energy= 0.126539
SCF Done: E(RM062X) = -1122.22067822

TS2'

C	3.05794800	-1.19619400	2.25103200
C	2.49839800	-1.74559200	3.40575400
C	1.11588800	-1.84857200	3.53609000
C	0.28525500	-1.40490200	2.50249100
C	0.88942200	-0.87474800	1.36581300
C	2.24878300	-0.74135700	1.20053100
H	4.13351800	-1.12024500	2.14156500
H	3.14336400	-2.09621300	4.20487900
H	0.65091500	-2.27656100	4.41929300

H	2.69184500	-0.30872200	0.31794500
I	-0.54611600	-0.37527600	-0.19121700
C	-1.18080200	-1.57210100	2.58350800
O	-1.74952400	-2.17003100	3.48918600
N	-1.83457000	-1.00222700	1.49873500
C	-3.12093900	-1.23448500	1.07392900
C	-4.13973600	-1.77981300	2.02659400
H	-3.91427900	-2.83405000	2.22032300
H	-4.09516600	-1.26016100	2.98538100
H	-5.12798500	-1.68330400	1.57561800
O	-3.37236300	-0.96829200	-0.11049200
C	-1.88565600	-3.96088300	-0.36031400
C	-1.36201000	-3.56810500	-1.59153600
C	0.02070600	-3.42459800	-1.77564100
C	0.87086700	-3.69950200	-0.69674200
C	0.34842300	-4.08618400	0.53941900
C	-1.03055400	-4.21406300	0.71595700
H	-2.96174100	-4.04840700	-0.23805600
H	-2.03603000	-3.34101000	-2.41367000
H	1.94523900	-3.58516800	-0.79818300
H	1.02282600	-4.27033900	1.37062100
H	-1.43293200	-4.49217100	1.68635100
C	0.54021500	-2.95138700	-3.11616200
H	0.79496500	-3.81303600	-3.74521600
H	-0.24933200	-2.40435600	-3.63988300
C	1.81890000	-2.07646700	-3.07234800
H	2.66399400	-2.61755000	-2.64310100
H	2.09341200	-1.82585000	-4.10444100
C	1.66195200	-0.82089600	-2.36685800
C	1.34615200	0.20368600	-1.74348000
H	1.62601400	1.21050400	-1.47515800
S	4.78098600	-0.19870800	-2.61259400
C	5.13027000	-1.24332200	-1.22552600
F	5.39278600	-0.55879900	-0.06446000
F	4.10362700	-2.09845000	-0.88278100

F	6.20668800	-2.06026600	-1.40467200
C	-6.49510700	1.75821200	-1.66087000
C	-5.53460500	1.13871400	-0.64810800
C	-5.62983600	1.78142200	0.73789200
H	-4.51507500	1.30366600	-1.01505700
O	-5.86793400	-0.22256900	-0.54811700
H	-5.01985800	-0.72143600	-0.53184400
F	-4.69058000	1.24897100	1.55440600
F	-6.82779500	1.56315000	1.30841000
F	-5.42140600	3.11169100	0.69986800
F	-6.26991100	3.07522700	-1.83378500
F	-6.34263300	1.15363900	-2.85429400
F	-7.78029300	1.60378200	-1.28683900
C	3.49770900	4.02980900	-0.42853200
C	4.16519500	2.72720800	0.01643500
C	4.13423000	2.53118300	1.53301000
H	5.21602400	2.77033000	-0.28985100
O	3.46427100	1.66748600	-0.55891700
H	3.99384000	1.22300600	-1.27834600
F	4.84353800	1.43653100	1.86864800
F	2.87604900	2.35236600	1.98549800
F	4.66336200	3.58134800	2.19045900
F	4.11197600	5.12070400	0.06628800
F	3.52838400	4.11029200	-1.77302700
F	2.20229500	4.07764000	-0.05056500

Zero-point correction= 0.453753 (Hartree/Particle)
Thermal correction to Energy= 0.502617
Thermal correction to Enthalpy= 0.503561
Thermal correction to Gibbs Free Energy= 0.361621
SCF Done: E(RM062X) = -3552.44147326

References

[1] J. Zhu, C. Xu, C. Xu and Q. Shen, Preparation of N-Trifluoromethylthiosaccharin: A Shelf-Stable Electrophilic Reagent for Trifluoromethylthiolation, *Org. Synth.*, **2017**, *94*, 217–223.

[2] S. Alazet, L. Zimmer and T. Billard, Base-Catalyzed Electrophilic

Trifluoromethylthiolation of Terminal Alkynes, *Angew. Chem. Int. Ed.*, **2013**, *52*, 10814-10817.

[3] G. He, Y. H. Jiang, X. Xiao, J. H. Lin, X. Zheng, R. B. Du, Y. C. Cao and J. C. Xiao, Difluorocarbene-Based Trifluoromethylthiolation of Terminal Alkynes, *J. Fluor. Chem.*, **2020**, *230*, 109437-106442.

[4] S. Q. Zhu, X. H. Xu and F. L. Qing, Oxidative Trifluoromethylthiolation of Terminal Alkynes with $AgSCF_3$: A Convenient Approach to Alkynyl Trifluoromethyl Sulfides, *Eur. J. Org. Chem.*, **2014**, 4453-4456.

[5] C. Chen, L. L. Chu and F. L. Qing, Metal-Free Oxidative Trifluoromethylthiolation of Terminal Alkynes with CF_3SiMe_3 and Elemental Sulfur, *J. Am. Chem. Soc.*, **2012**, *134*, 12454−12457.

[6] X. Shao, C. Xu, L. Lu and Q. Shen, Structure-Reactivity Relationship of Trifluoromethanesulfenates: Discovery of an Electrophilic Trifluoromethylthiolating Reagent, *J. Org. Chem.*, **2015**, *80*, 3012-3021.

[7] A. Tlili, S. Alazet, Q. Glenadel, T. Billard, Copper-Catalyzed Perfluoroalkylthiolation of Alkynes with Perfluoroalkanesulfenamides, *Chem. Eur. J.*, **2016**, 22, 10230-10234.

[8] R. Pluta, P. Nikolaienko, and M. Rueping, Direct Catalytic Trifluoromethylthiolation of Boronic Acids and Alkynes Employing Electrophilic Shelf-Stable N-(trifluoromethylthio)phthalimide, *Angew. Chem. Int. Ed.*, **2014**, 53, 1650-1653.

[9] N. Walker, W. B. Fox, R. A. De Marco, and W. B. Moniz, Carbon-13 NMR Spectra: Halocarbons vs Hydrocarbons, *Journal of Magnetic Resonance (1969)*, **1979**, *34*, 295-299.

[10] X. G. Yang, F. H. Du, J. J. Li and C. Zhang, Late-Stage Dehydroxyazidation of Alcohols Promoted by Trifunctional Hypervalent Azido-Iodine(III) Reagents, *Chem. Eur. J.*, **2022**, *28*, e202200272 (1 of 7).

[11] S. Ding, G. Jia and J. Sun, Iridium-Catalyzed Intermolecular Azide–Alkyne Cycloaddition of Internal Thioalkynes under Mild Conditions, *Angew. Chem. Int. Ed.*, **2014**, *53*, 1877-1880.

[12] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N.

Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[13] P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields, *J. Phys. Chem*., **1994**, *98*, 11623-11627.

[14] (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys.*, **2010**, *132*, 154104; (b) S. Grimme, S. Ehrlich and L. Goerigk, Effect of the damping function in dispersion corrected density functional theory, *J. Comput. Chem*., **2011**, *32*, 1456-1465.

[15] (a) G. Igel-Mann, H. Stoll and H. Preuss, Pseudopotentials for main group elements (IIIa through VIIa), *Mol. Phys.*, **1988**, *65*, 1321−1328; (b) D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, Energy-adjusted ab initio pseudopotentials for the second and third row transition elements, *Theor. Chim. Acta.*, **1990**, *77*, 123-141.

[16] P. C. Hariharan and J. A. Pople, The influence of polarization functions on molecular orbital hydrogenation energies, *Theor. Chim. Acta.*, **1973**, *28*, 213-222.

[17] A. V. Marenich, C. J. Cramer and D. G. Truhlar, Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions, *J. Phys. Chem. B,* **2009**, *113*, 6378-6396.

[18] X. Zhang and R. S. Paton, Stereoretention in styrene heterodimerisation promoted by one-electron oxidants, *Chem. Sci.*, **2020**, *11*, 9309-9324.

[19] (a) L. Eberson, M. Hartshorn, O. Persson and F. Radner, Making radical cations

live longer, *Chem. Commun*., **1996**, *18*, 2105-2112;(b) X. Gu, X. Song, C. Shao, P. Zeng, X. Lu, X. Shen and Q. Yang, Electrospinning of poly(butylene-carbonate): Effect of Solvents on the Properties of the Nanofibers Film, *Int. J. Electrochem. Sci.*, **2014**, *9*, 8045-8056;(c) M. Carraro, M. Gardan, A. Sartorel, C. Maccato and M. Bonchio, Hydrogen peroxide activation by fluorophilic polyoxotungstates for fast and selective oxygen transfer catalysis, *Dalton Trans.*, **2016**, *45*, 14544-14548.

[20] Sigma-Aldrich, 1,1,1,3,3,3-Hexafluoro-2-propanol.

[21] (a) R. C. Weast, *CRC Handbook of Chemistry and Physics*, 76th, ed.; CRC Press: Boca Raton, FL, 1995;(b) E. Richmond, J. Yi, V. D. Vuković, F. Sajadi, C. N. Rowley and J. Moran, Ring-opening hydroarylation of monosubstituted cyclopropanes enabled by hexafluoroisopropanol, *Chem. Sci*., **2018**, *9*, 6411-6416.

[22] E. Engelage, N. Schulz, F. Heinen, S. M. Huber, D. G. Truhlar and C. J. Cramer, Refined SMD Parameters for Bromine and Iodine Accurately Model Halogen-Bonding Interactions in Solution, *Chem. Eur. J.*, **2018**, *24*, 15983-15987.

[23] (a) K. Fukui, The path of chemical reactions - the IRC approach, *Acc. Chem. Res.,* **1981**, *14*, 363–368;(b) K. Fukui, Formulation of the reaction coordinate, *J. Phys. Chem.*, **1970**, *74*, 4161–4163.

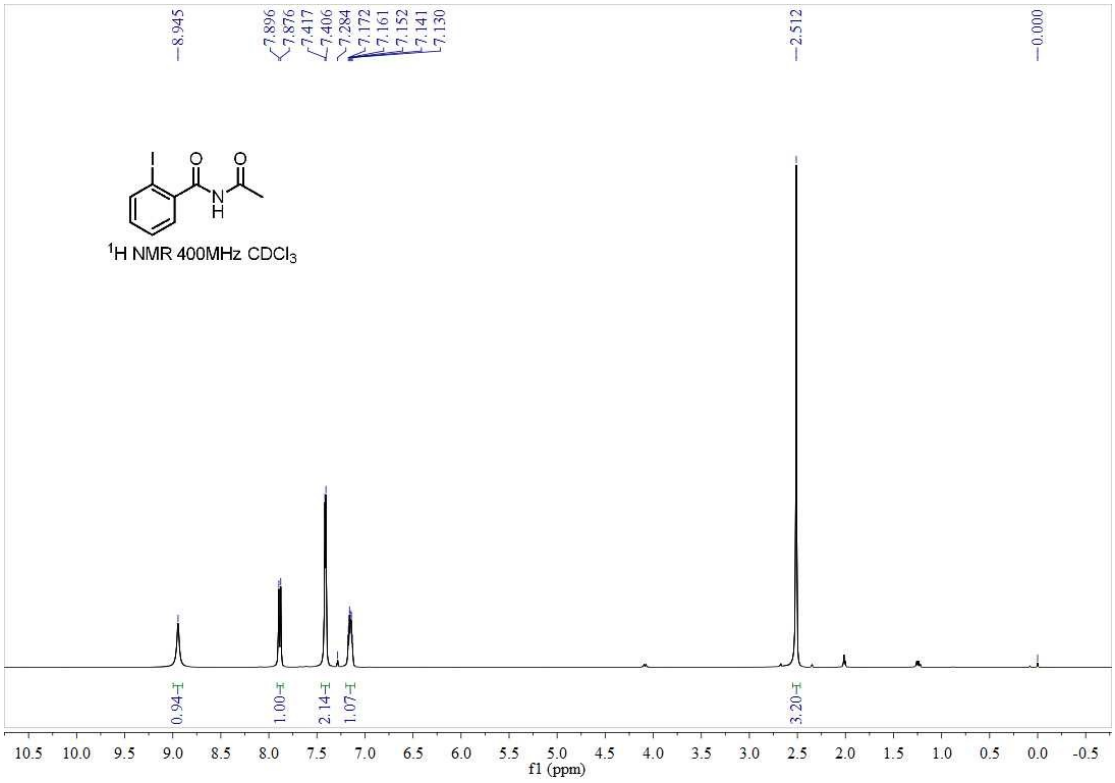
[24] (a) Y. Zhao and D. G. Truhlar, The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals, *Theor. Chim. Acta.*, **2008**, *120*, 215-241;(b) A. D. McLean and G. S. Chandler, Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11-18, *J. Chem. Phys*., **1980**, *72*, 5639-5648;(c) R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions, *J. Chem. Phys*., **1980**, *72*, 650-654;(d) G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Al-Laham and W. A. Shirley, A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row

elements, *J. Chem. Phys.*, **1988**, *89*, 2193-2218;(e) M. J. Frisch, J. A. Pople and J. S. Binkley, Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets, *J. Chem. Phys.*, **1984**, *80*, 3265-3269;(f) F. Weigend and R. Ahlrichs, Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy, *Phys. Chem. Chem. Phys*., **2005**, *7*, 3297-3305;(g) T.-Y. Sun, K. Chen, H. Zhou, T. You, P. Yin and X. Wang, Revisiting the effect of f-functions in predicting the right reaction mechanism for hypervalent iodine reagents, *J. Comput. Chem.*, **2021**, *42*, 470-474.

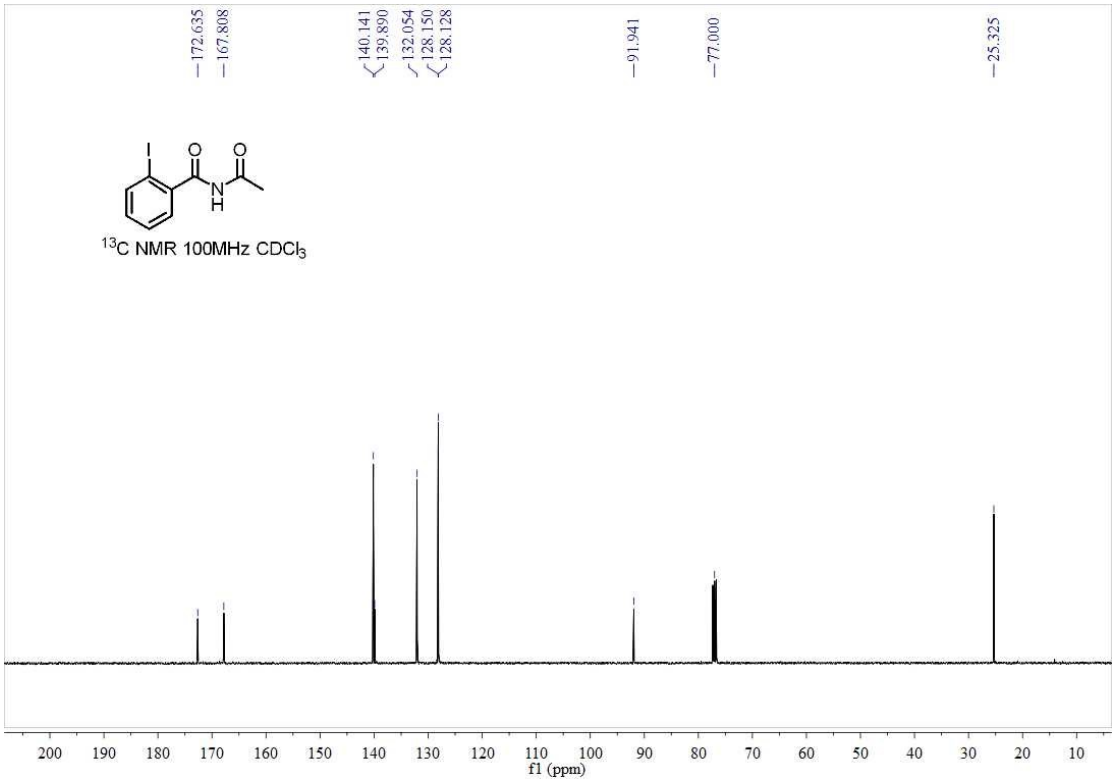
[25] CYLview, 1.0b; C. Y. Legault, Université de Sherbrooke: Quebec, Canada, **2009** (http://www.cylview.org).

[26] (a) B. Wang, C. Rong, P. K. Chattaraj and S. Liu, A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge, *Theor. Chem. Acc.*, **2019**, *138*: 124;(b) T. Lu, Q. Chen, in *Conceptual Density Functional Theory: Towards a New Chemical Reactivity Theory*, Vol. 2 (Ed: S. Liu,), WILEY-VCH, Weinheim, Germany **2022**, Ch. 31;(c) T. Lu and Q. Chen, Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems, *J. Comput. Chem.*, **2022**, *43*, 539-555.

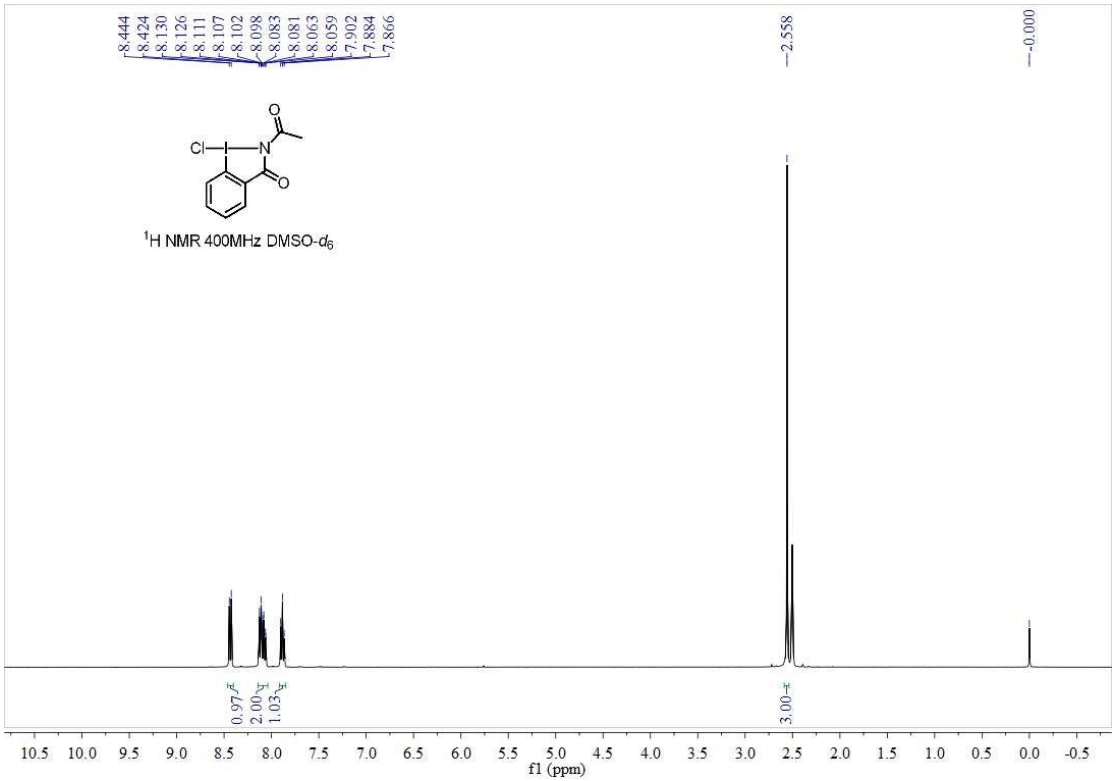
NMR Spectra of Corresponding Compounds

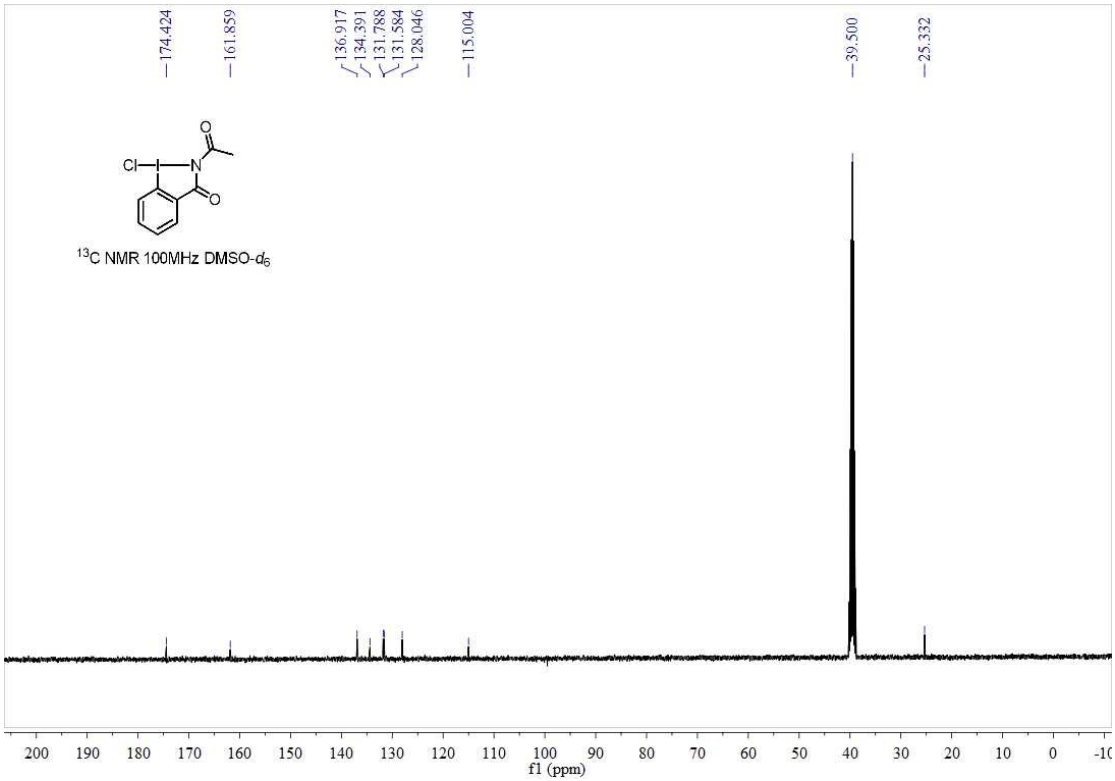


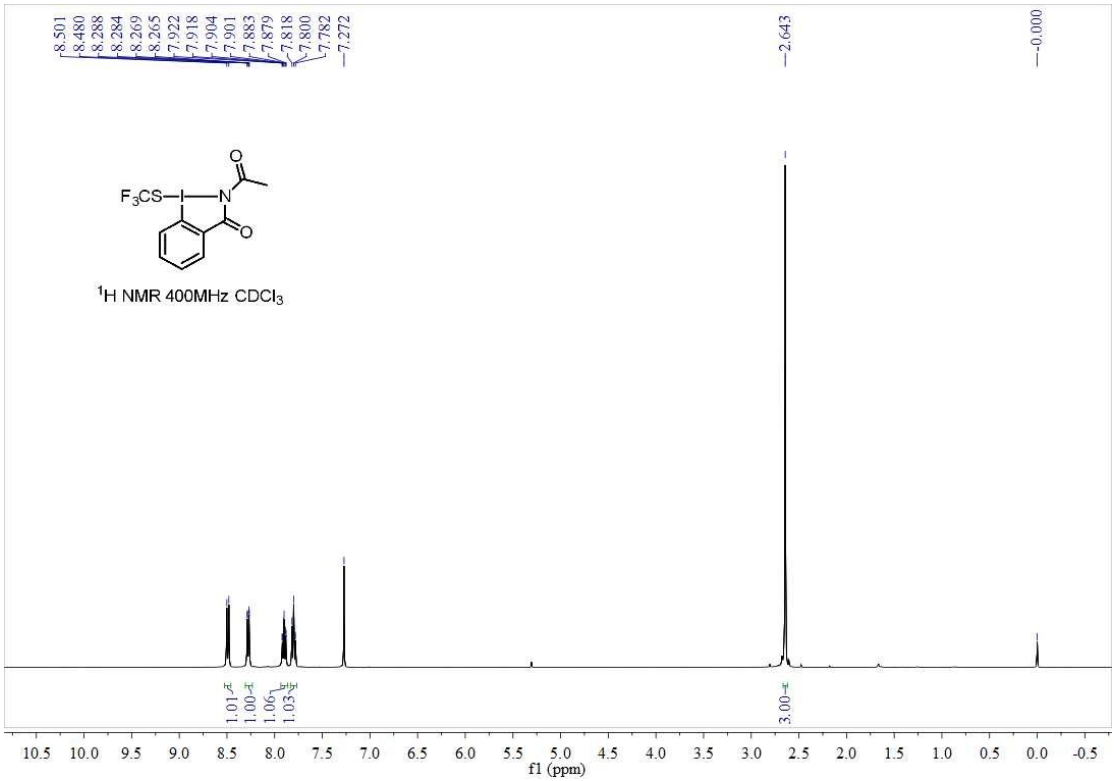
^{1}H NMR 400MHz $CDCl_3$

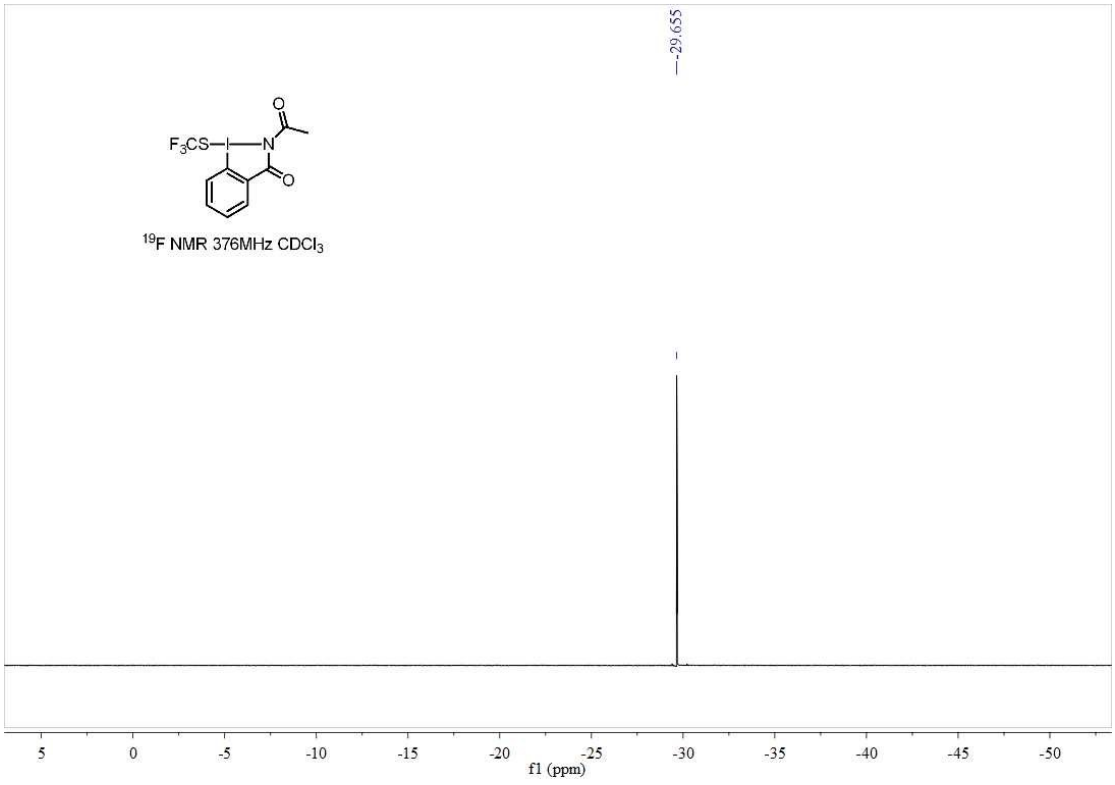


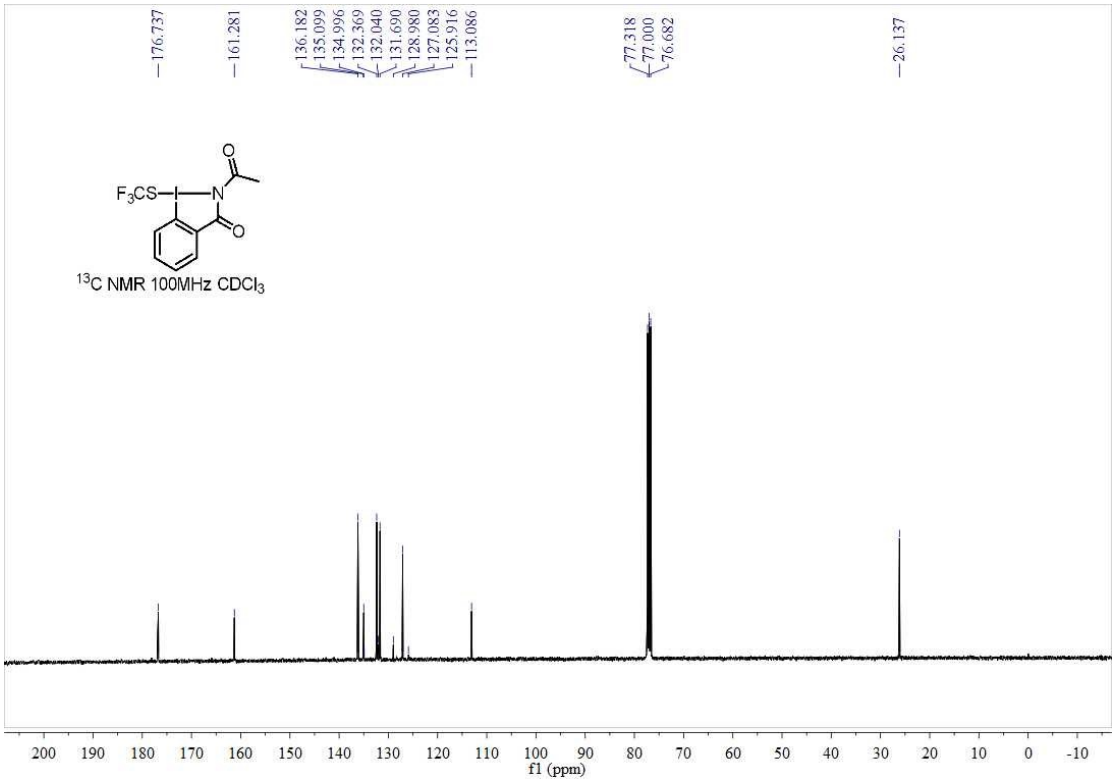
^{13}C NMR 100MHz $CDCl_3$

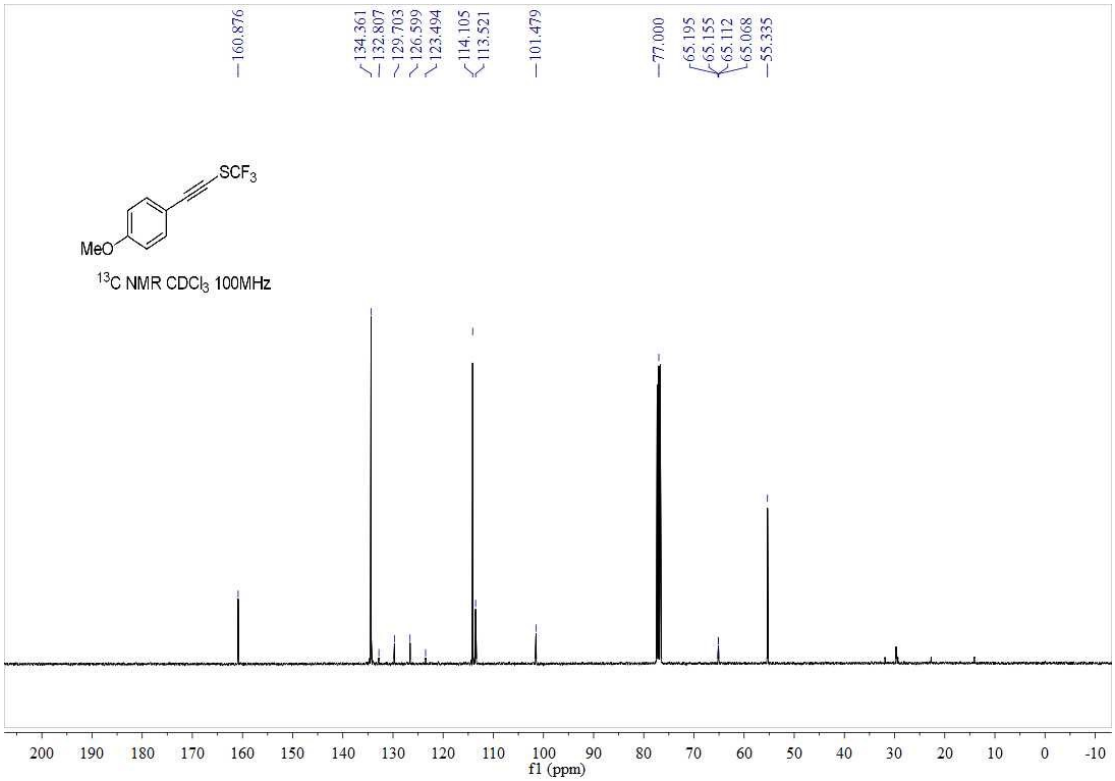

8.444
8.424
8.130
8.126
8.111
8.107
8.102
8.098
8.083
8.081
8.063
8.059
7.902
7.884
7.866
2.558
0.000
Cl
I
N
O
O
O
^{1}H NMR 400MHz DMSO-d_6
0.97
2.00
1.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

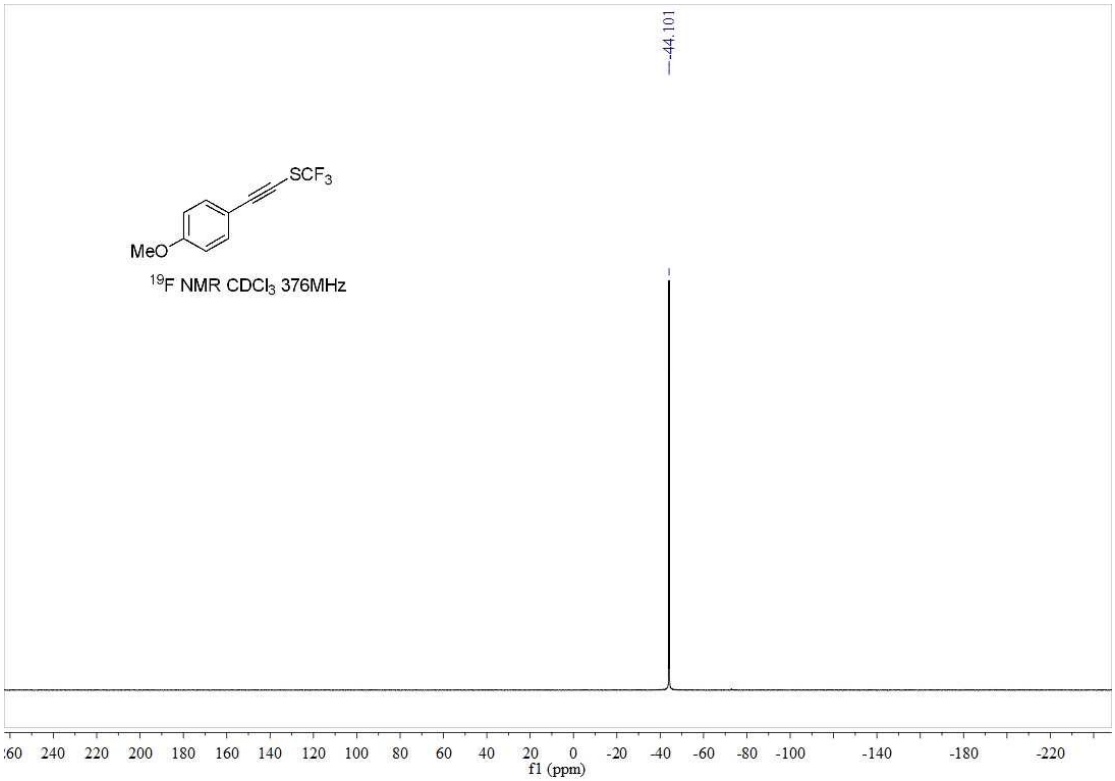

174.424
161.859
136.917
134.391
131.788
131.584
128.046
115.004
39.500
25.332
Cl
I
N
O
O
O
^{13}C NMR 100MHz DMSO-d_6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

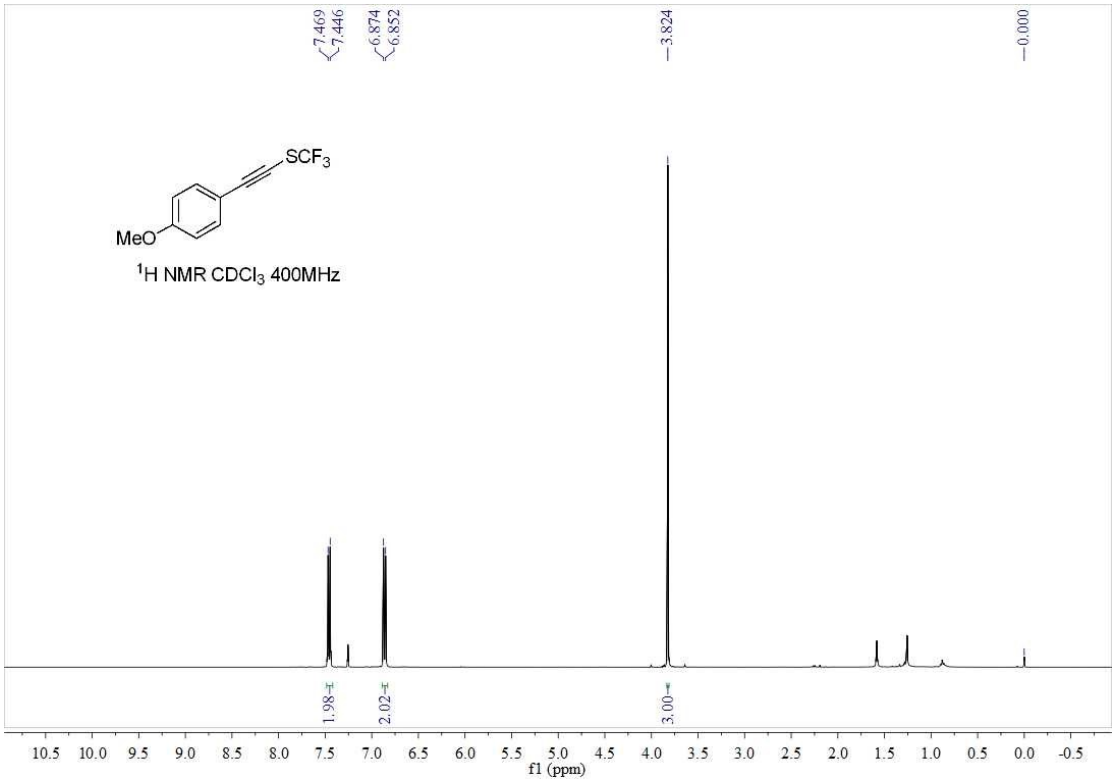

8.501
8.480
8.288
8.284
8.269
8.265
7.922
7.918
7.904
7.901
7.883
7.879
7.818
7.800
7.782
7.272
2.643
0.000
F3CS
I
N
O
O
1H NMR 400MHz CDCl3
1.01
1.00
1.06
1.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

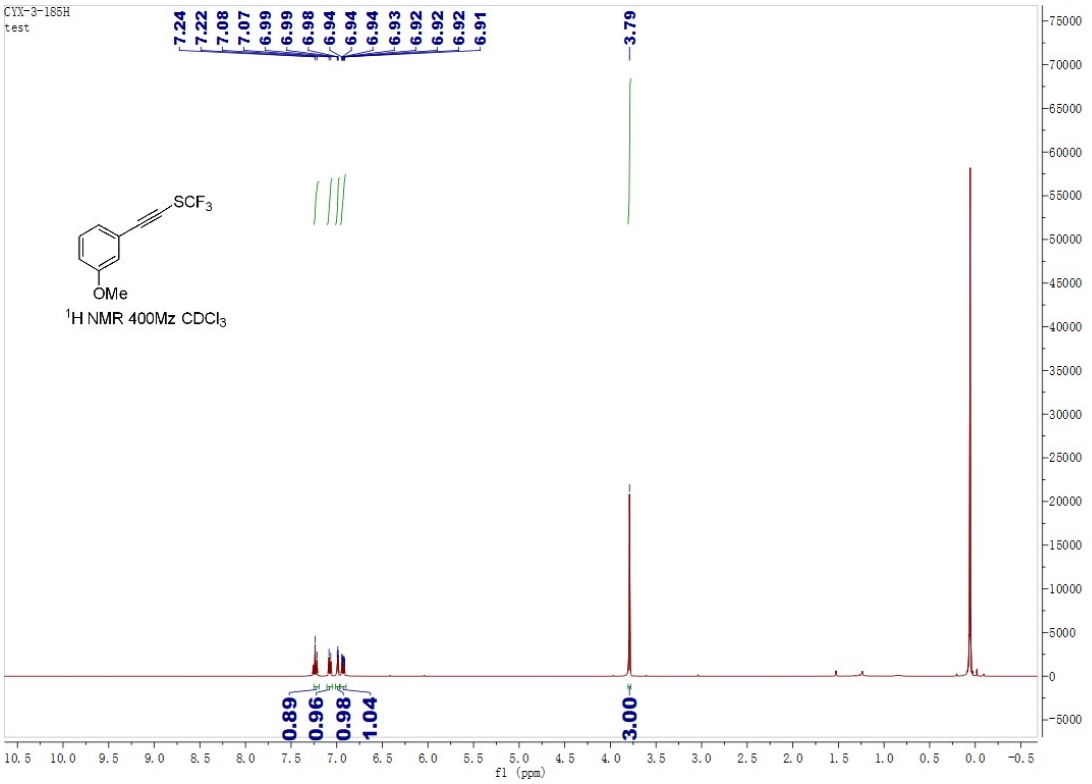

29.655
F3CS
I
N
O
O
19F NMR 376MHz CDCl3
5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50
f1 (ppm)

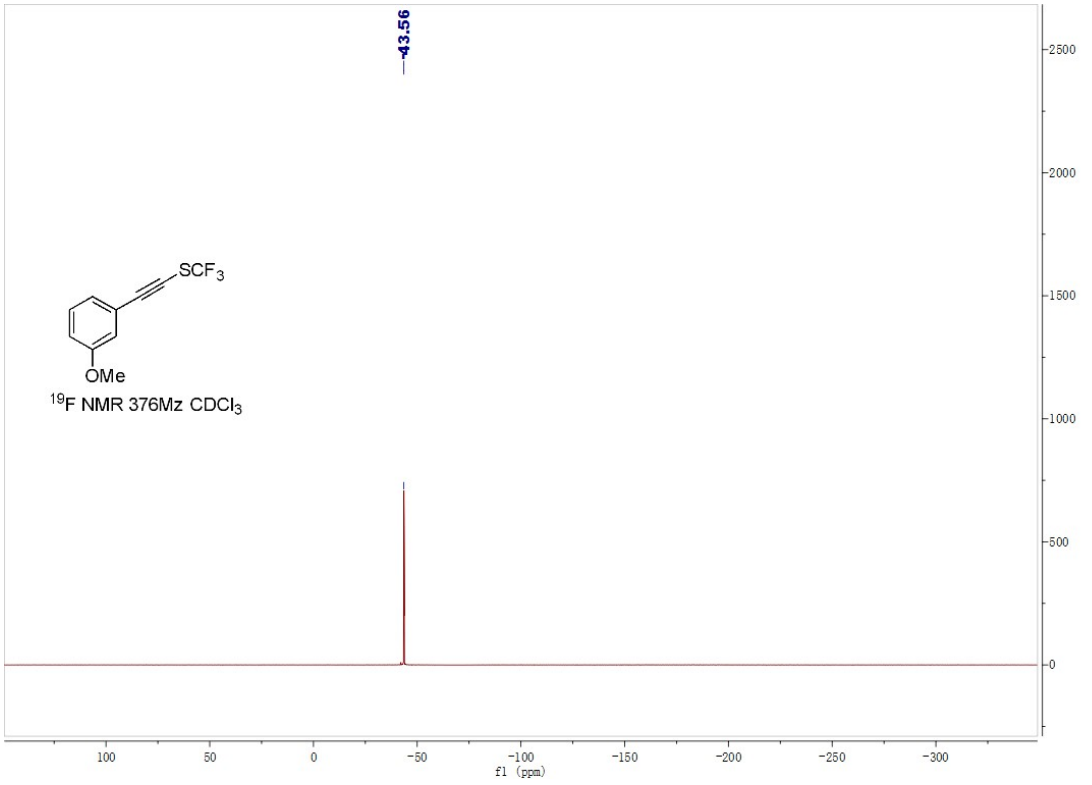

176.737
161.281
136.182
135.099
134.996
132.369
132.040
131.690
128.980
127.083
125.916
113.086
77.318
77.000
76.682
26.137
F3CS
I
N
O
O
13C NMR 100MHz CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

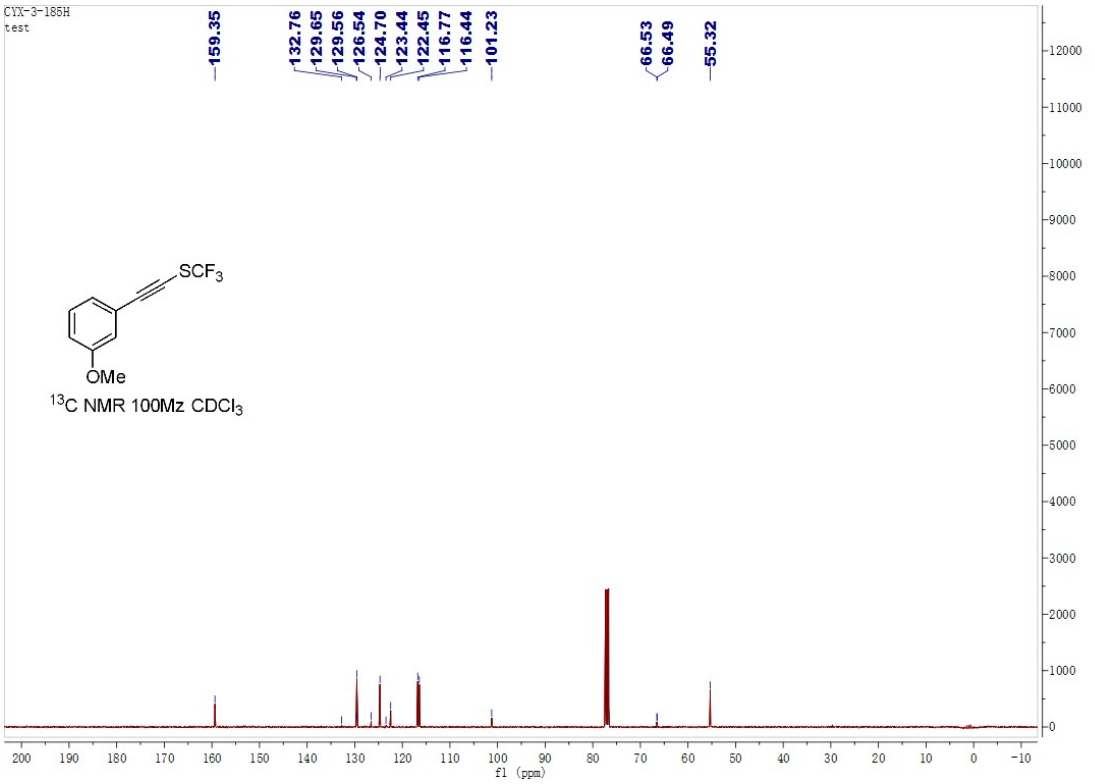

160.876
134.361
132.807
129.703
126.599
123.494
114.105
113.521
101.479
77.000
65.195
65.155
65.112
65.068
55.335
SCF3
MeO
13C NMR CDCl3 100MHz
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

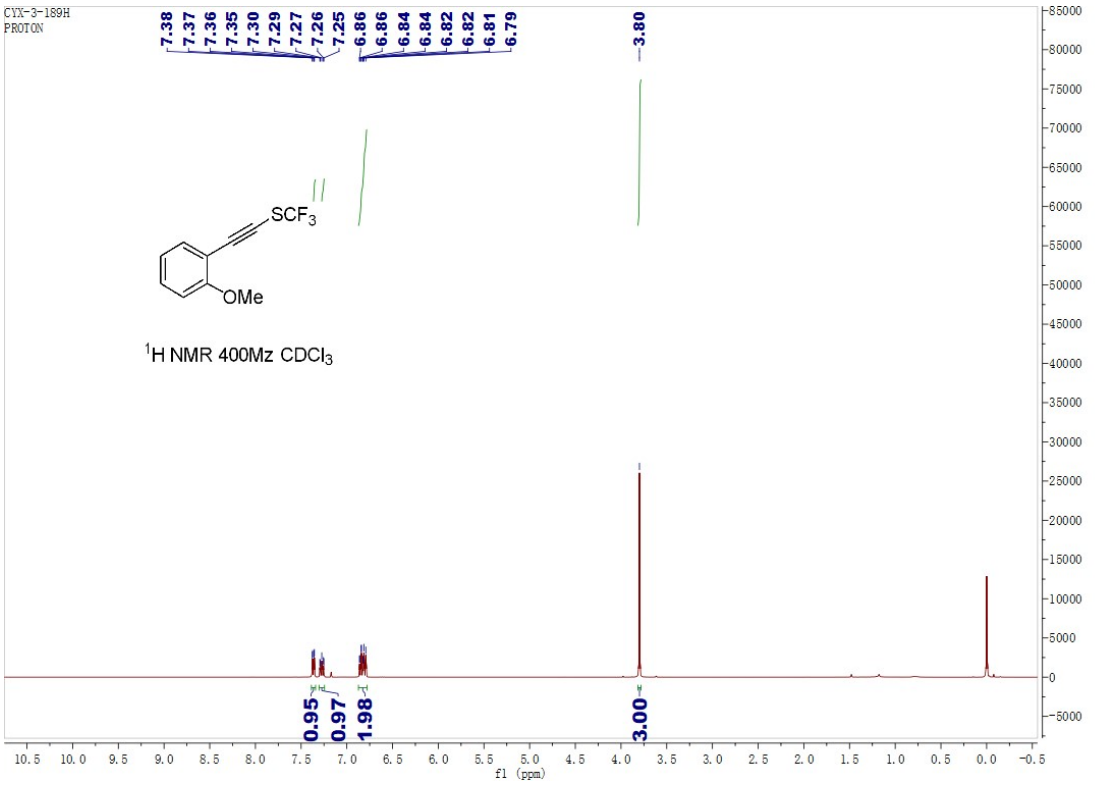

-44.101
SCF3
MeO
19F NMR CDCl3 376MHz
f1 (ppm)

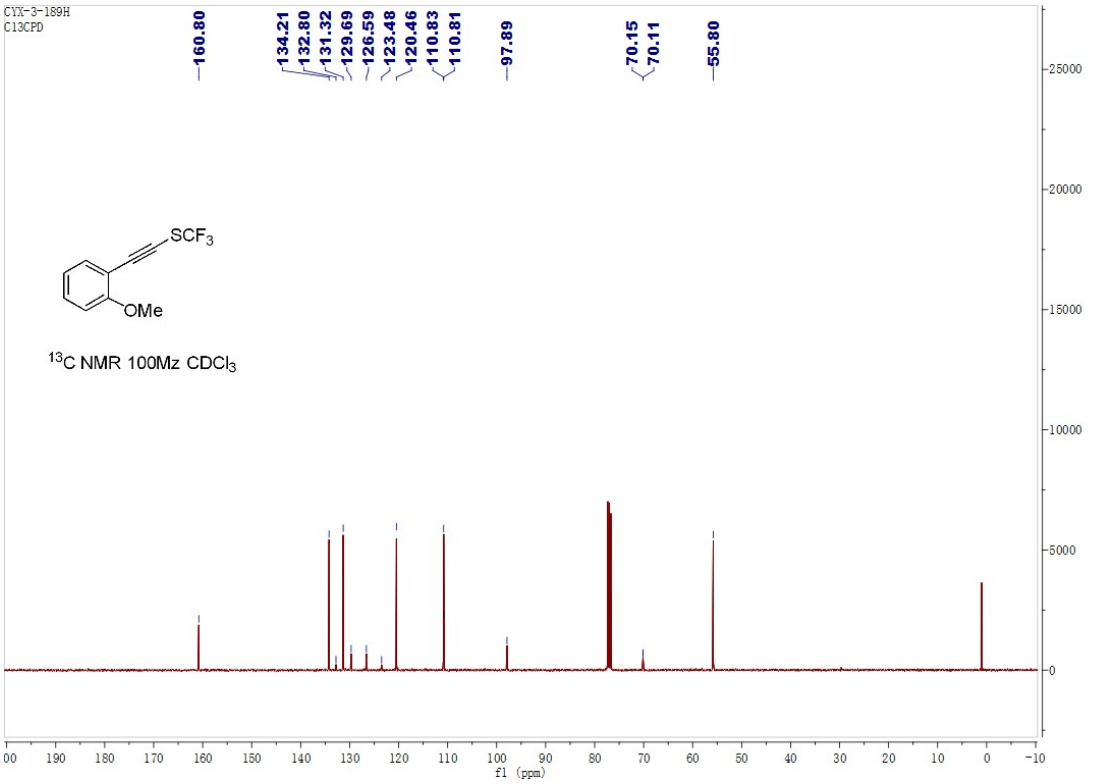

7.469
7.446
6.874
6.852
3.824
0.000
SCF3
MeO
1H NMR CDCl3 400MHz
1.98
2.02
3.00
f1 (ppm)

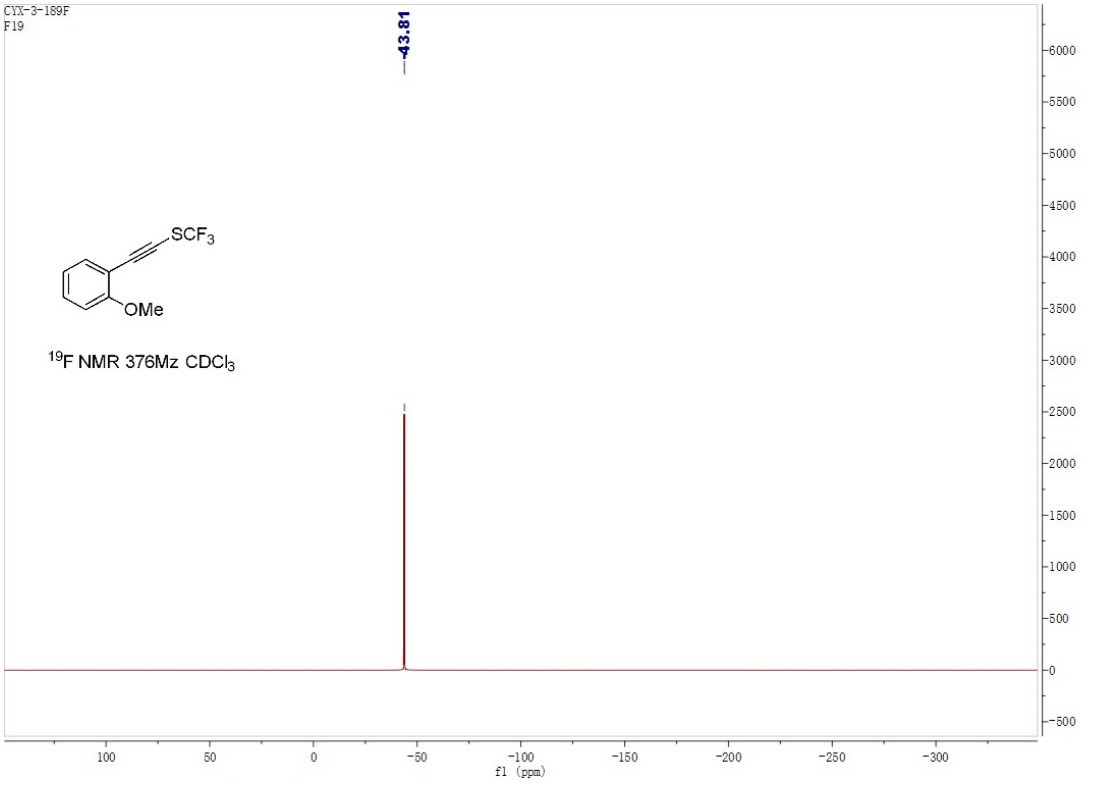

CYX-3-185H
test
7.24
7.22
7.08
7.07
6.99
6.99
6.98
6.94
6.94
6.94
6.93
6.92
6.92
6.92
6.91
3.79
SCF3
OMe
1H NMR 400Mz CDCl3
0.89
0.96
0.98
1.04
3.00
f1 (ppm)

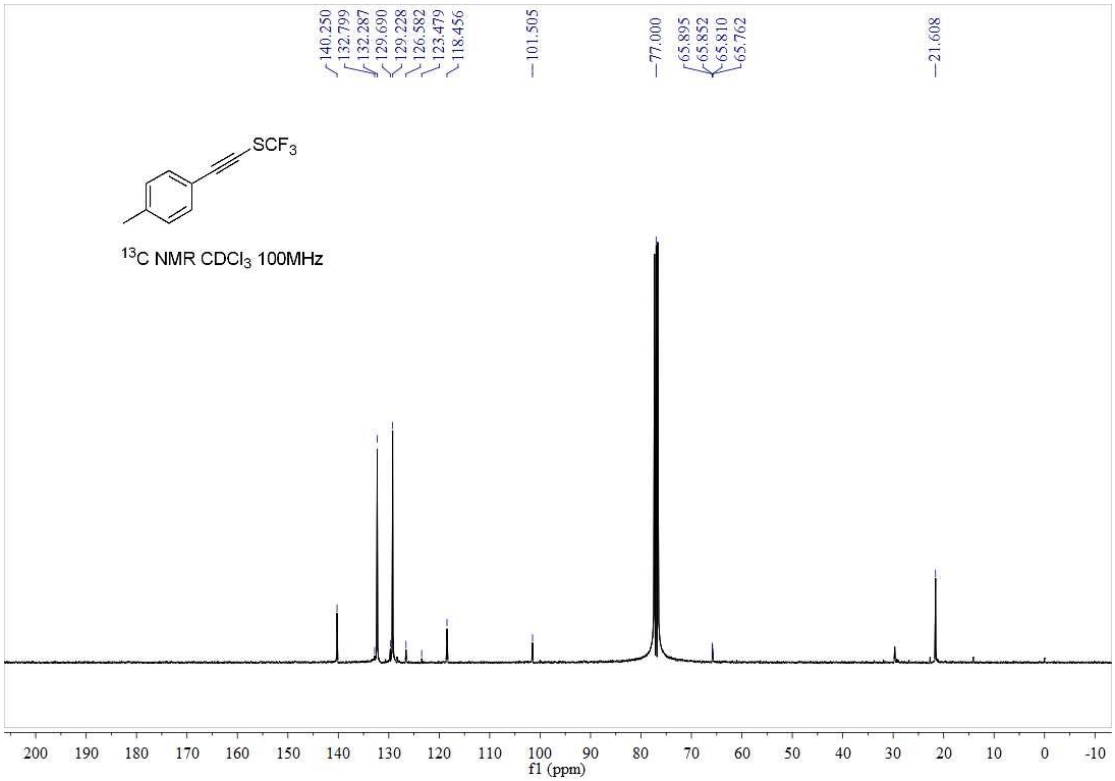

-43.56
SCF3
OMe
19F NMR 376Mz CDCl3
f1 (ppm)

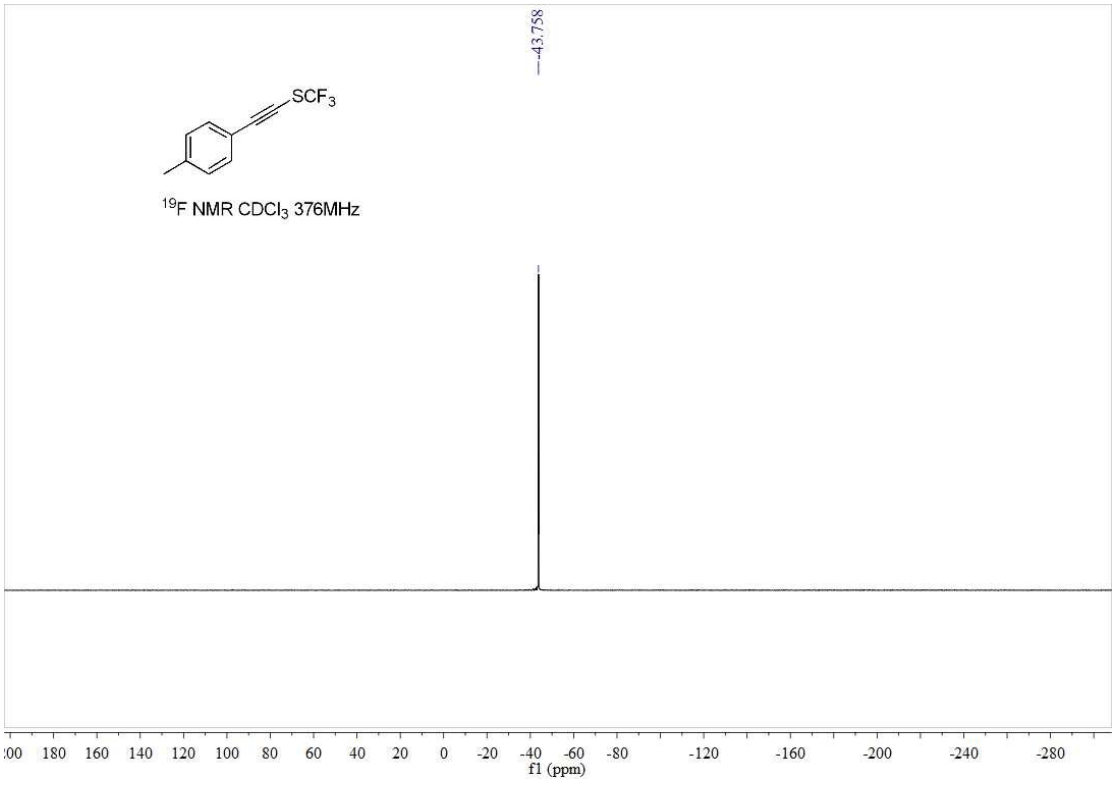

CYX-3-185H
test
159.35
132.76
129.65
129.56
126.54
124.70
123.44
122.45
116.77
116.44
101.23
66.53
66.49
55.32
SCF3
OMe
13C NMR 100Mz CDCl3
f1 (ppm)

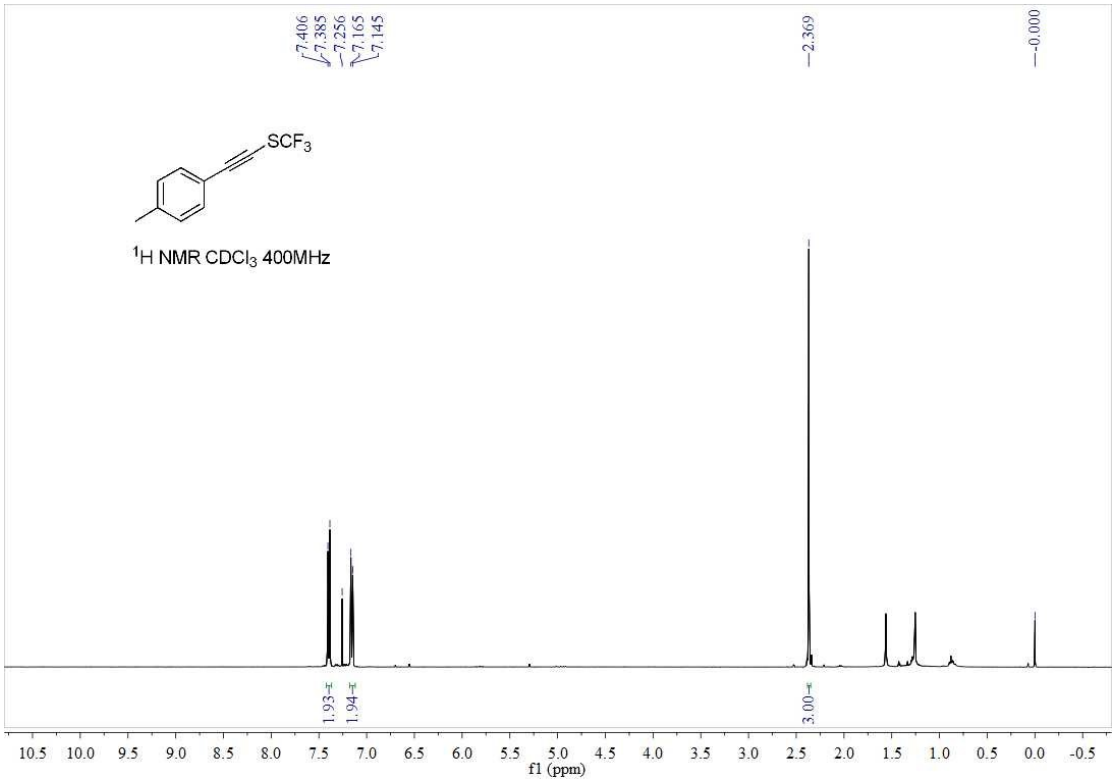

CYX-3-189H
PROTON
7.38
7.37
7.36
7.35
7.30
7.29
7.27
7.26
7.25
6.86
6.84
6.84
6.82
6.81
6.79
3.80
SCF3
OMe
1H NMR 400Mz CDCl3
0.95
0.97
1.98
3.00
f1 (ppm)

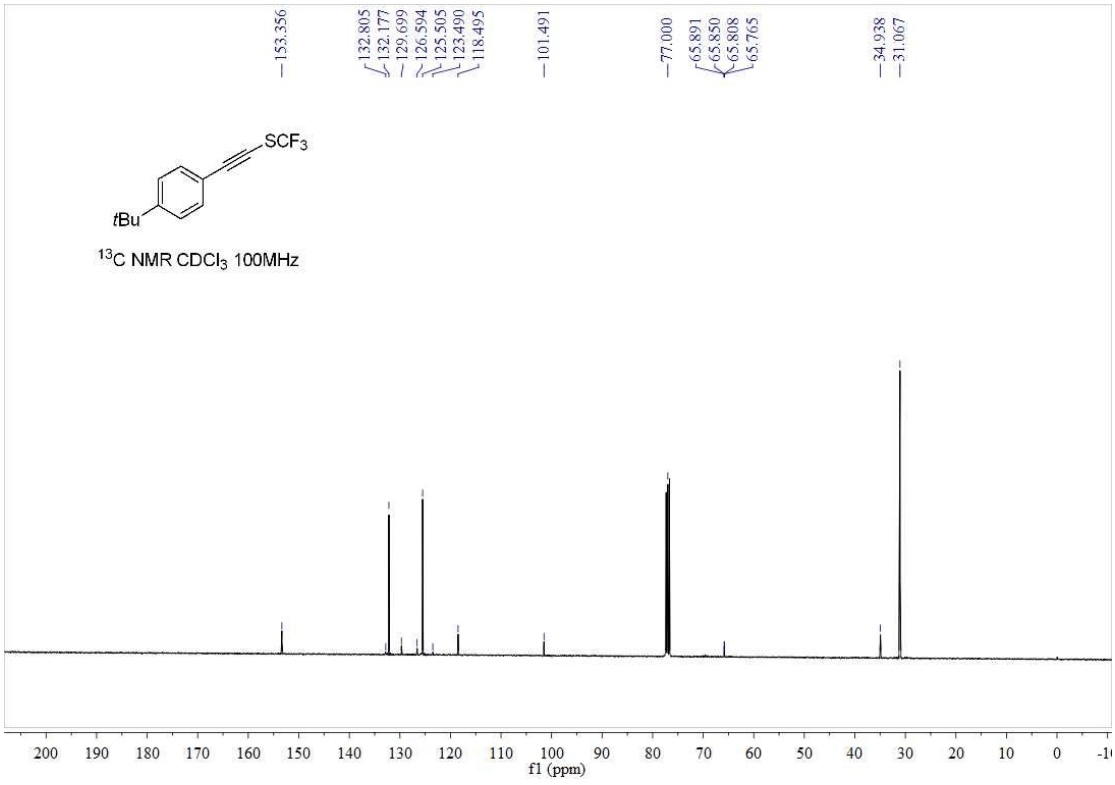

CYX-3-189H
C13CPD
160.80
134.21
132.80
131.32
129.69
126.59
123.48
120.46
110.83
110.81
97.89
70.15
70.11
55.80
SCF3
OMe
13C NMR 100Mz CDCl3
f1 (ppm)

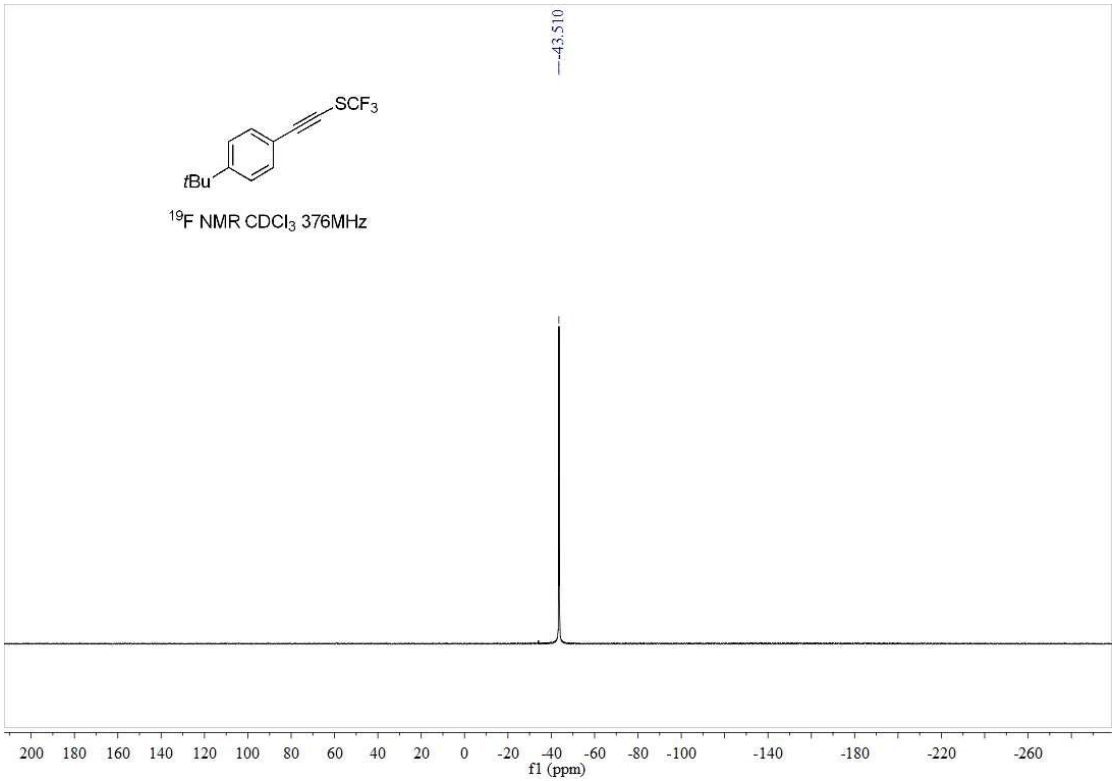

CYX-3-189F
F19
-43.81
SCF3
OMe
19F NMR 376Mz CDCl3
f1 (ppm)

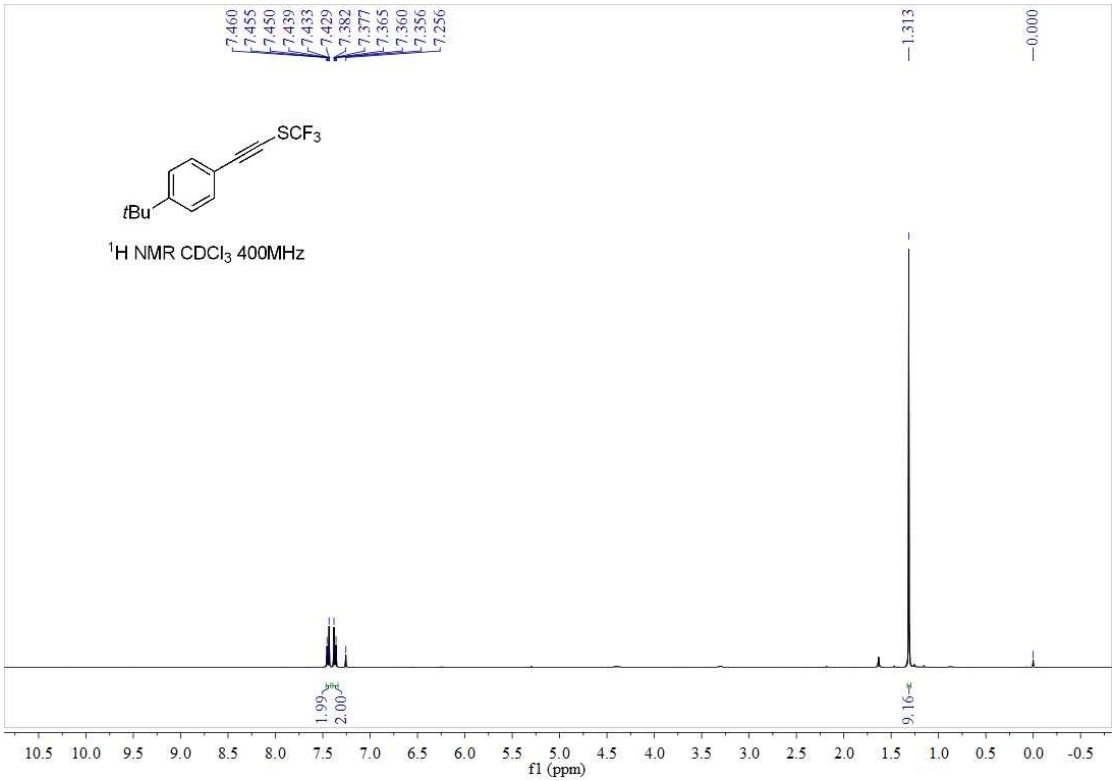

140.250
132.799
132.287
129.690
129.228
126.582
123.479
118.456
101.505
77.000
65.895
65.852
65.810
65.762
21.608
SCF3
13C NMR CDCl3 100MHz
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

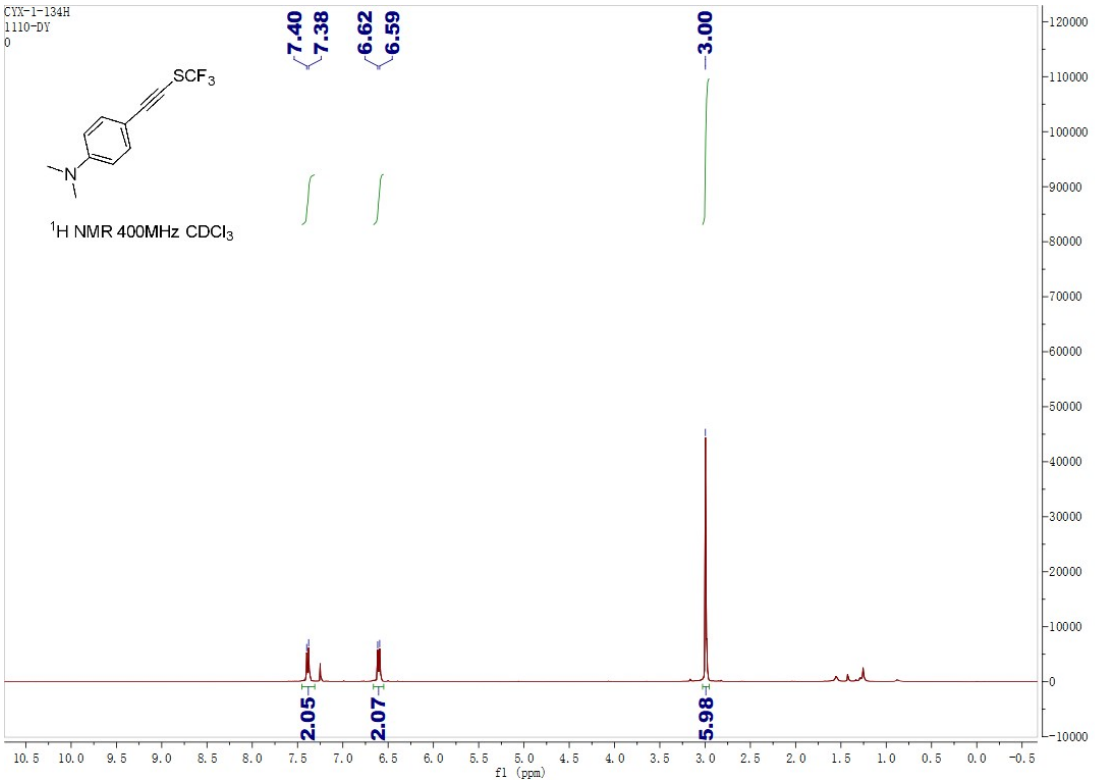

-43.758
SCF3
19F NMR CDCl3 376MHz
:00 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -120 -160 -200 -240 -280
f1 (ppm)

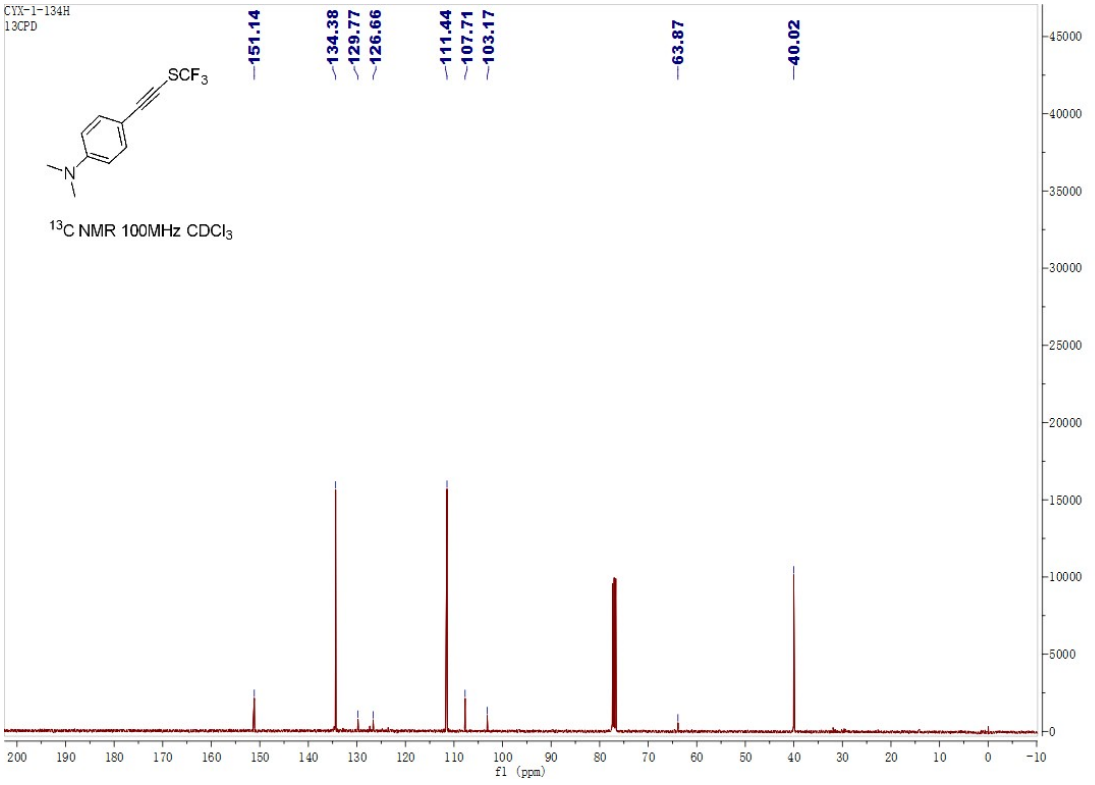

7.406
7.385
7.256
7.165
7.145
2.369
0.000
SCF3
1H NMR CDCl3 400MHz
1.93
1.94
3.00
f1 (ppm)

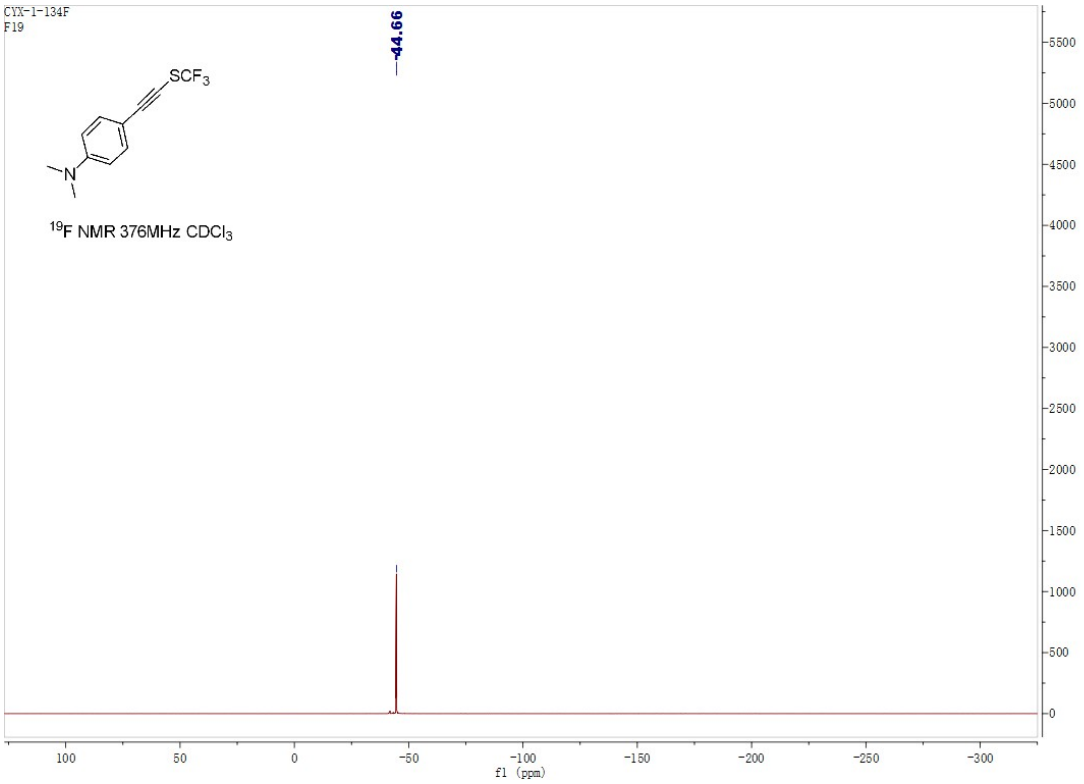

153.356
132.805
132.177
129.699
126.594
125.505
123.490
118.495
101.491
77.000
65.891
65.850
65.808
65.765
34.938
31.067
SCF3
tBu
13C NMR CDCl3 100MHz
f1 (ppm)

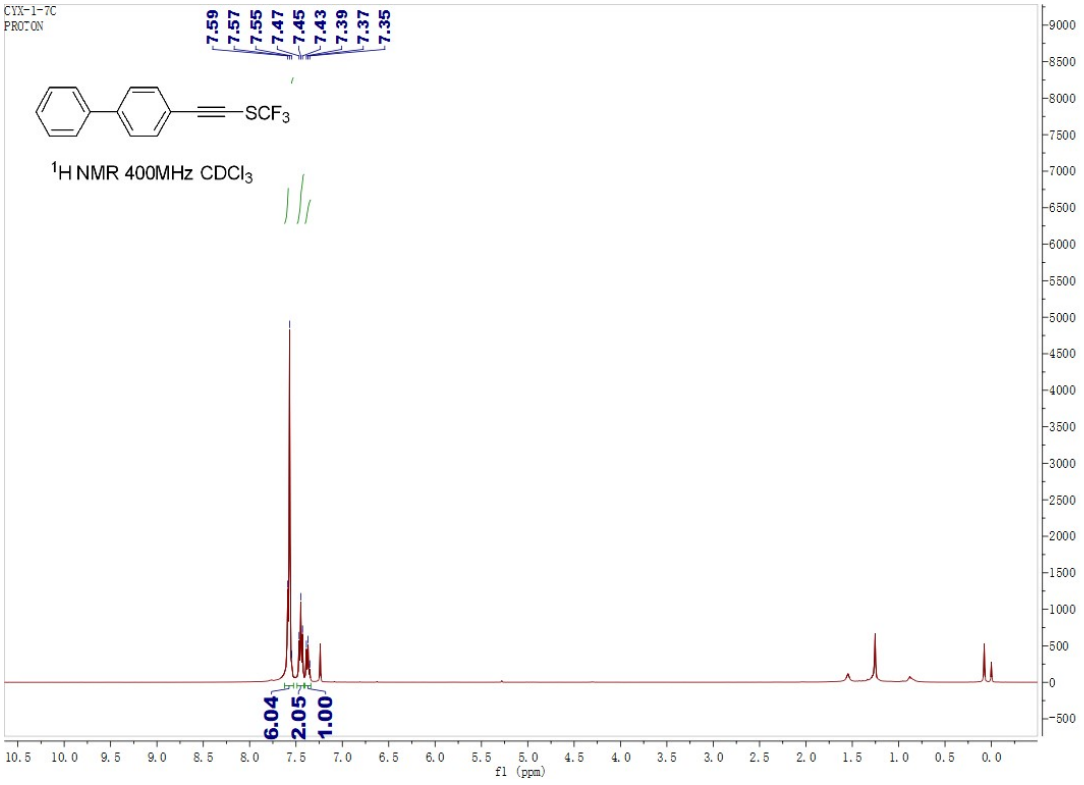

-43.510
SCF3
tBu
19F NMR CDCl3 376MHz
200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -140 -180 -220 -260
f1 (ppm)

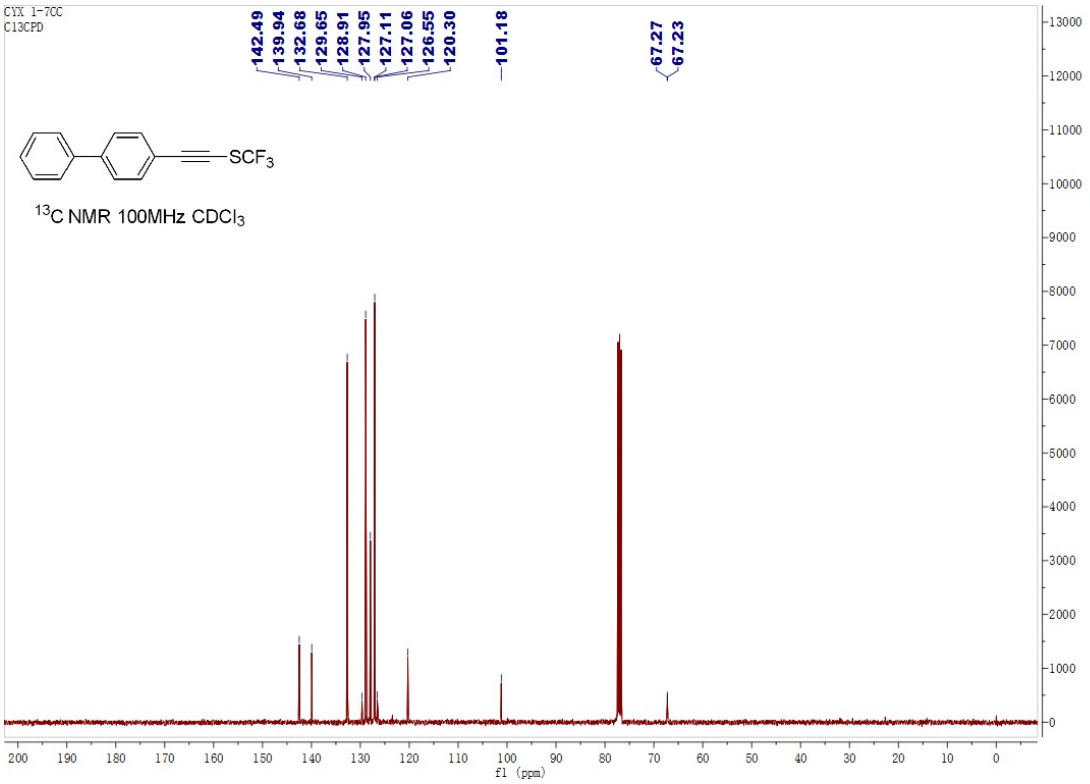

7.460
7.455
7.450
7.439
7.433
7.429
7.382
7.377
7.365
7.360
7.356
7.256
1.313
0.000
SCF3
tBu
1H NMR CDCl3 400MHz
1.99
2.00
9.16
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

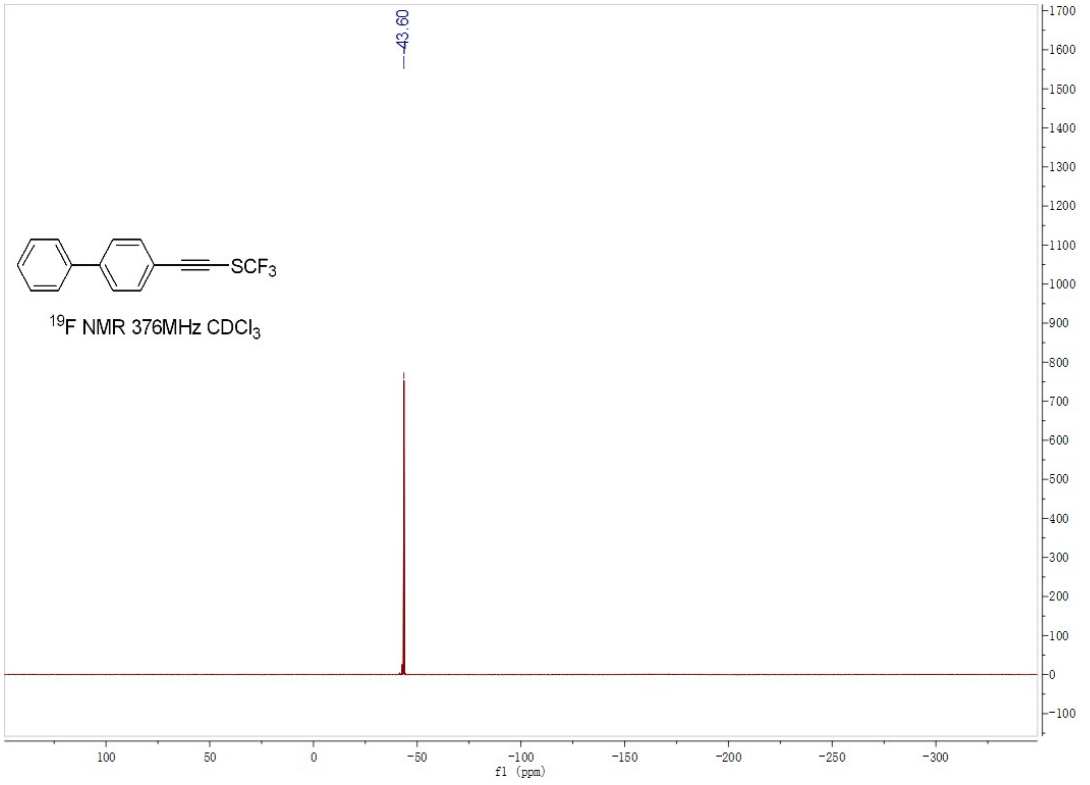

CYX-1-134H
1110-DY
0
7.40
7.38
6.62
6.59
3.00
SCF3
N
1H NMR 400MHz CDCl3
2.05
2.07
5.98
f1 (ppm)

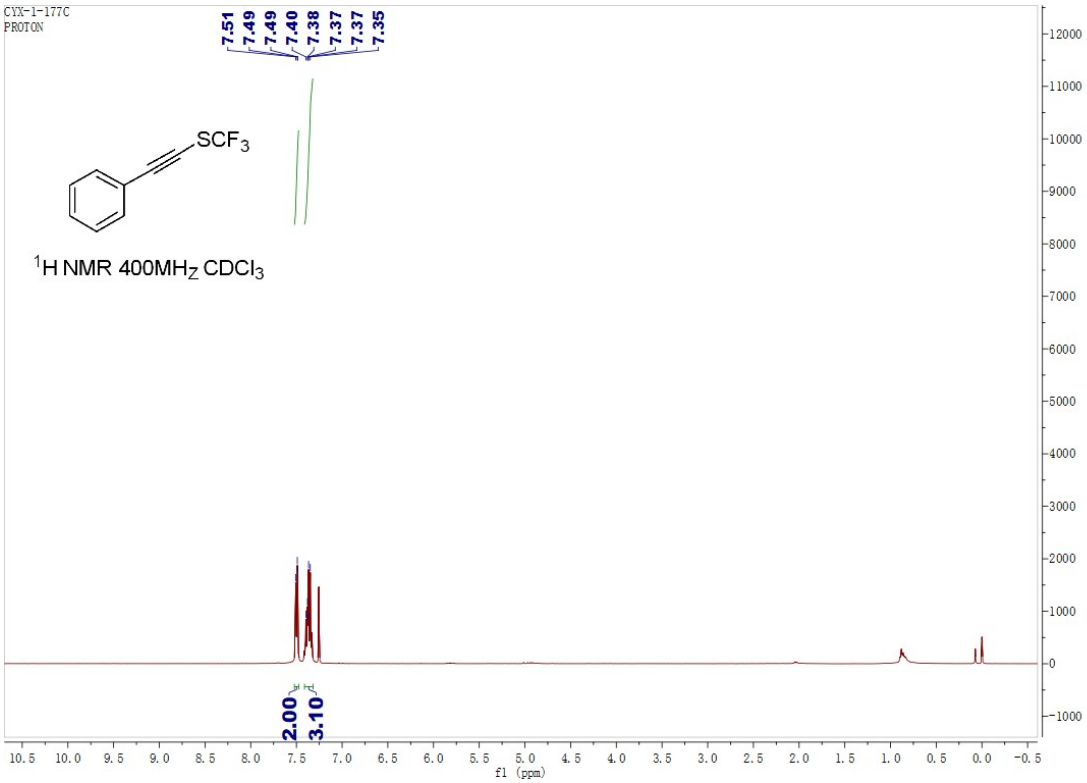

CYX-1-134H
13CPD
151.14
134.38
129.77
126.66
111.44
107.71
103.17
63.87
40.02
SCF3
N
13C NMR 100MHz CDCl3
f1 (ppm)

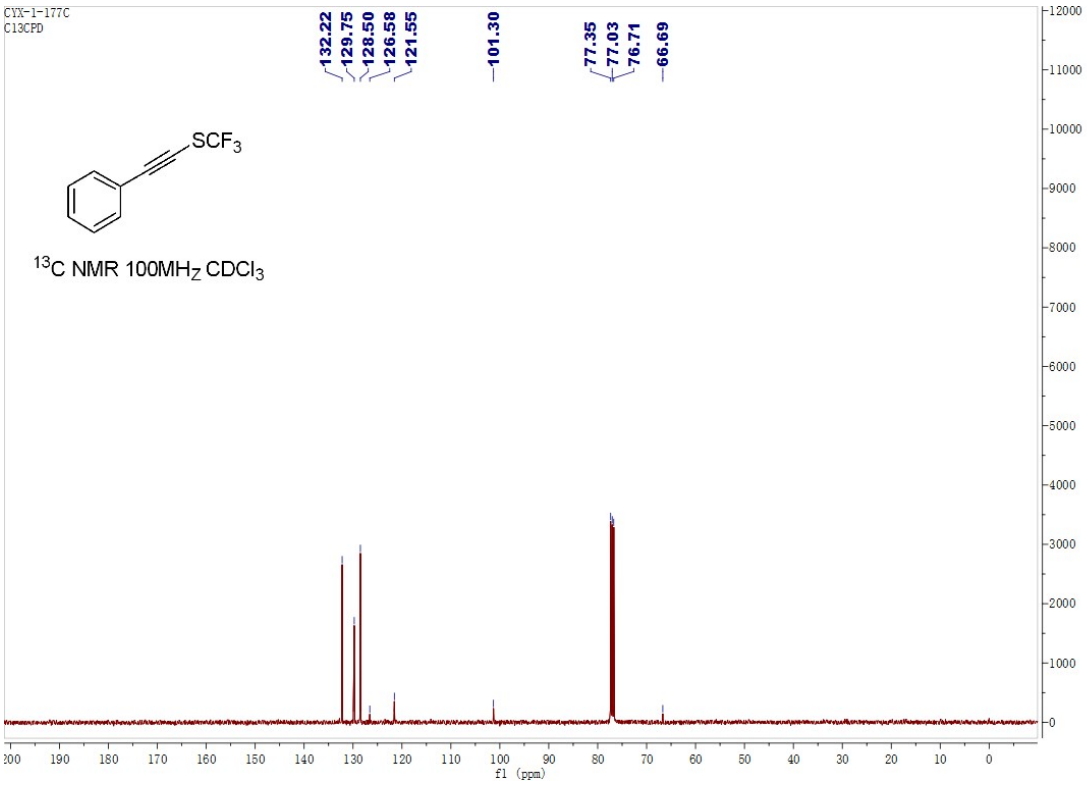

CYX-1-134F
F19
-44.66
SCF3
N
19F NMR 376MHz CDCl3
f1 (ppm)

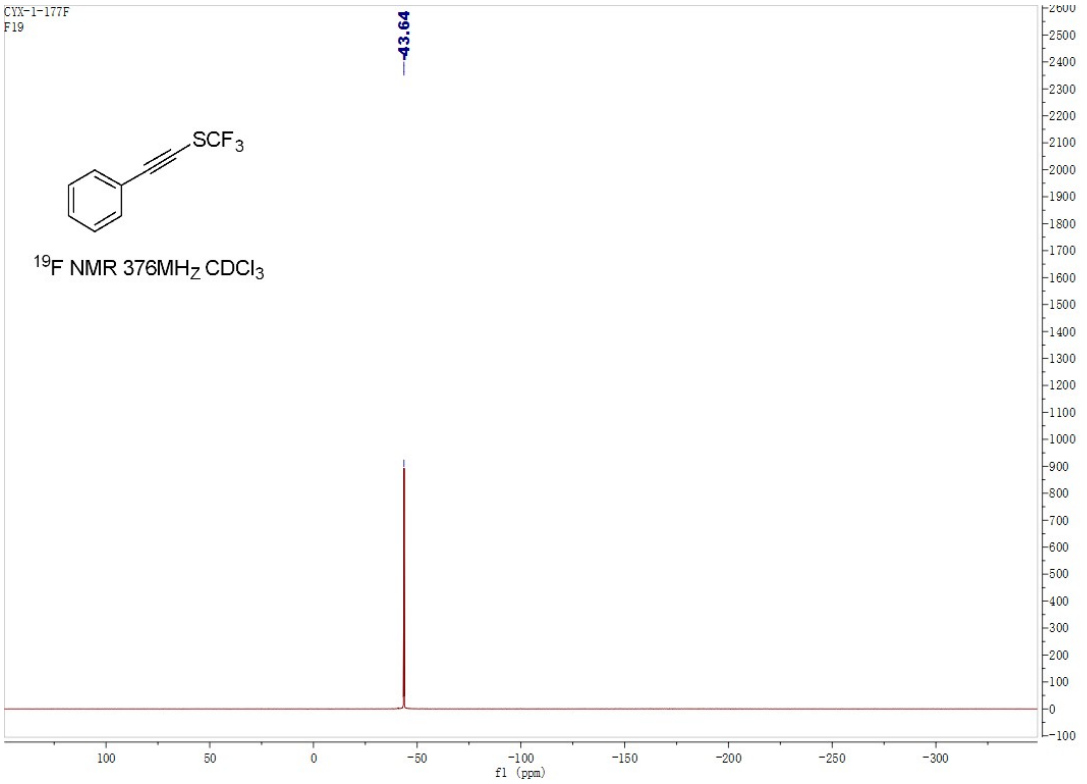

CYX-1-7C
PROTON
7.59
7.57
7.55
7.47
7.45
7.43
7.39
7.37
7.35
SCF3
1H NMR 400MHz CDCl3
6.04
2.05
1.00
f1 (ppm)

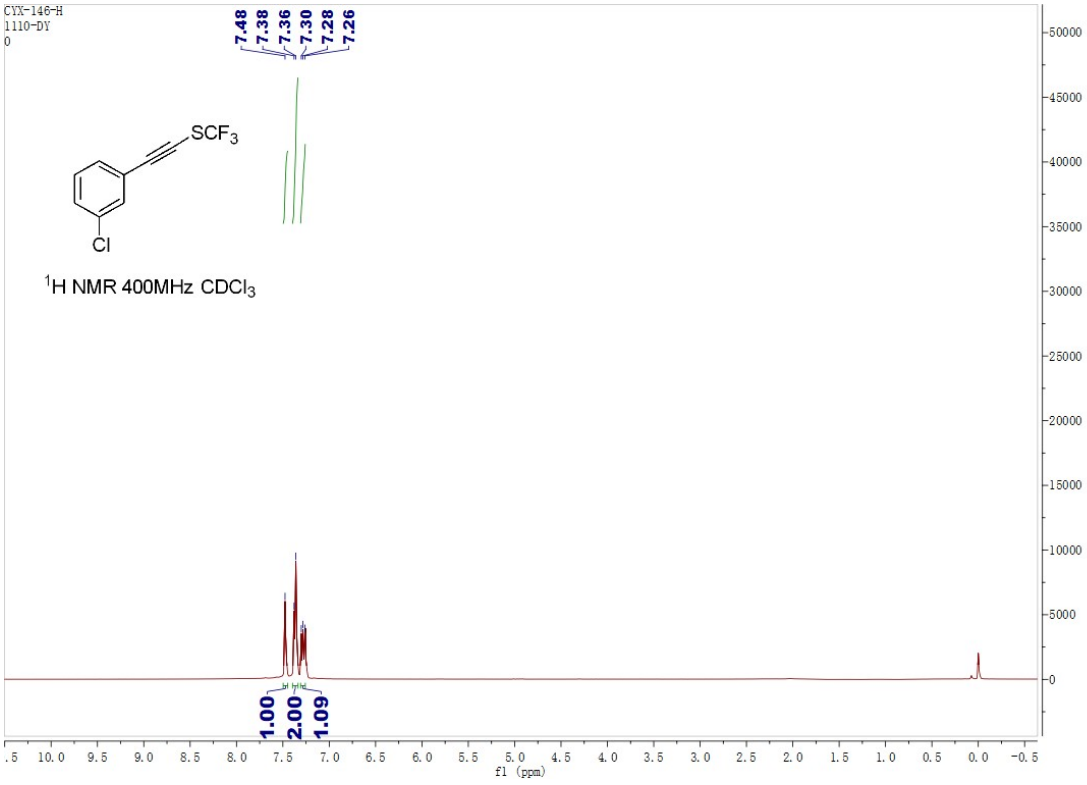

CYX 1-7CC
C13CPD
142.49
139.94
132.68
129.65
128.91
127.95
127.11
127.06
126.55
120.30
101.18
67.27
67.23
SCF3
13C NMR 100MHz CDCl3
f1 (ppm)

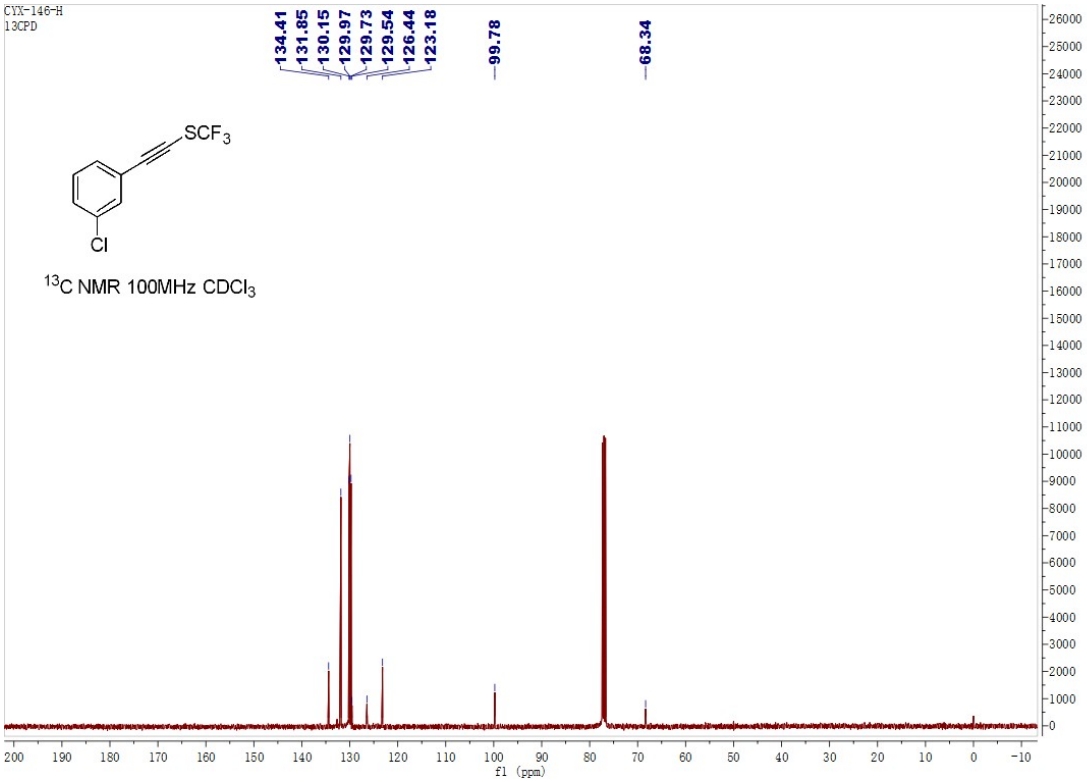

-43.60
SCF3
19F NMR 376MHz CDCl3
f1 (ppm)

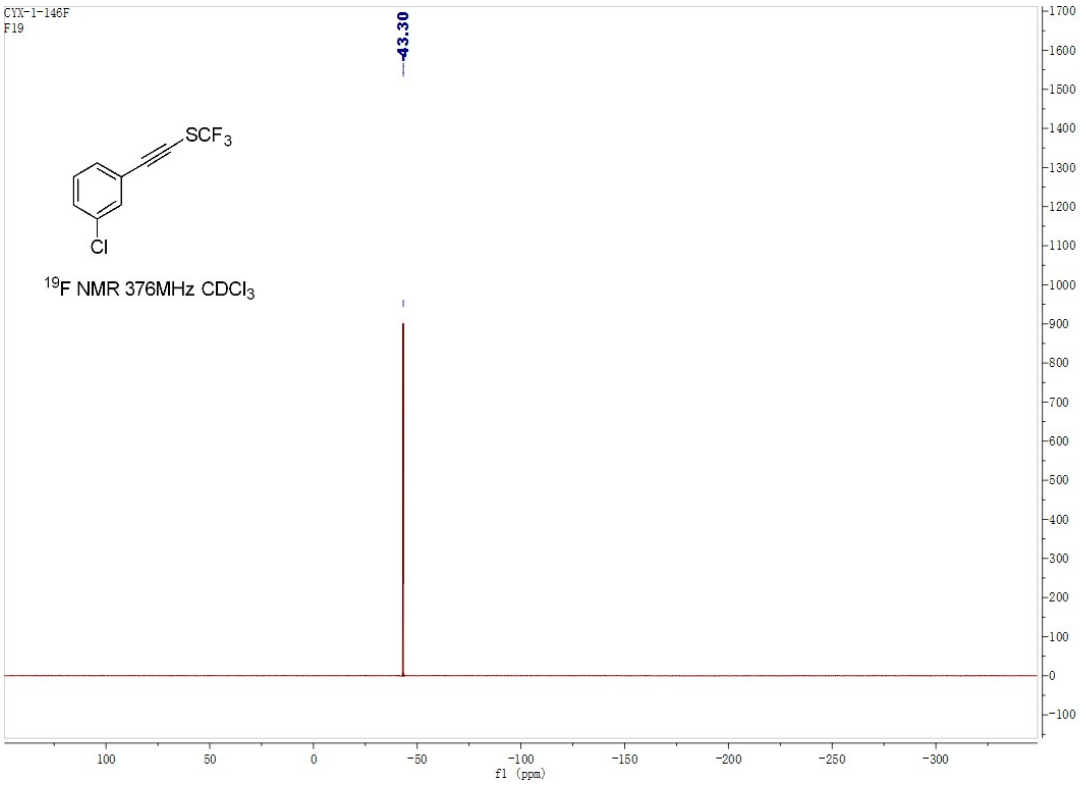

CYX-1-177C
PROTON
7.51
7.49
7.49
7.40
7.38
7.37
7.37
7.35
SCF3
1H NMR 400MHZ CDCl3
2.00
3.10
f1 (ppm)

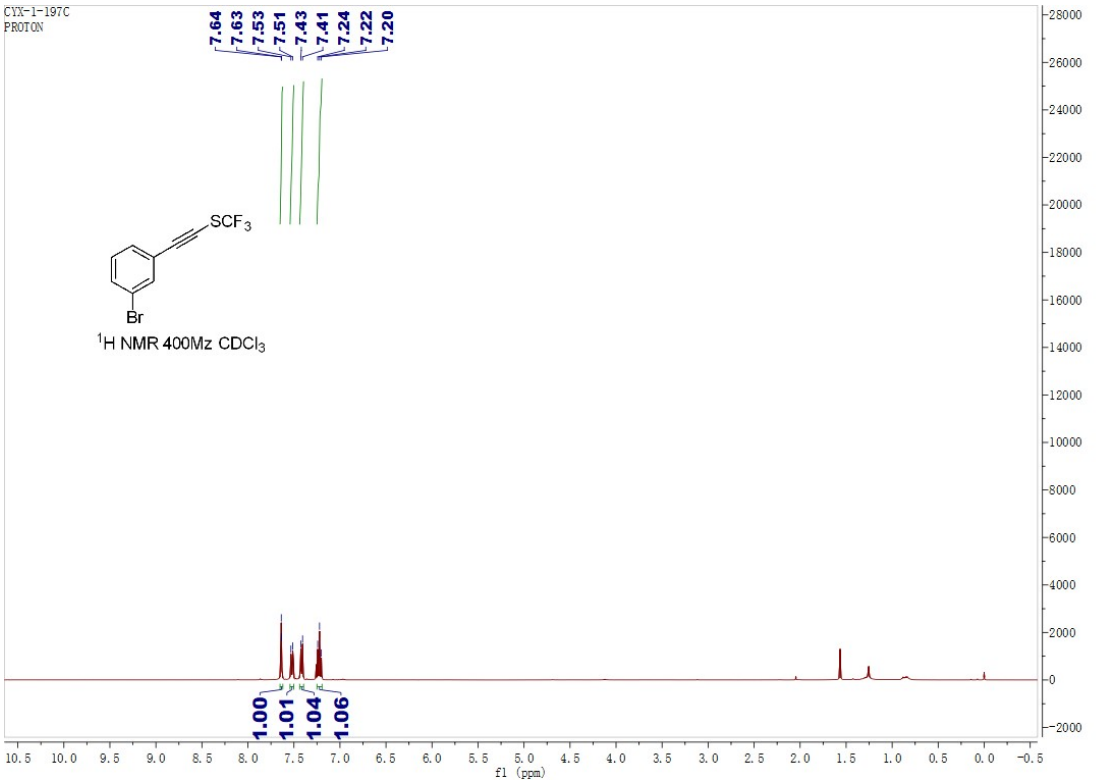

CYX-1-177C
C13CPD
132.22
129.75
128.50
126.58
121.55
101.30
77.35
77.03
76.71
66.69
SCF3
13C NMR 100MHZ CDCl3
f1 (ppm)

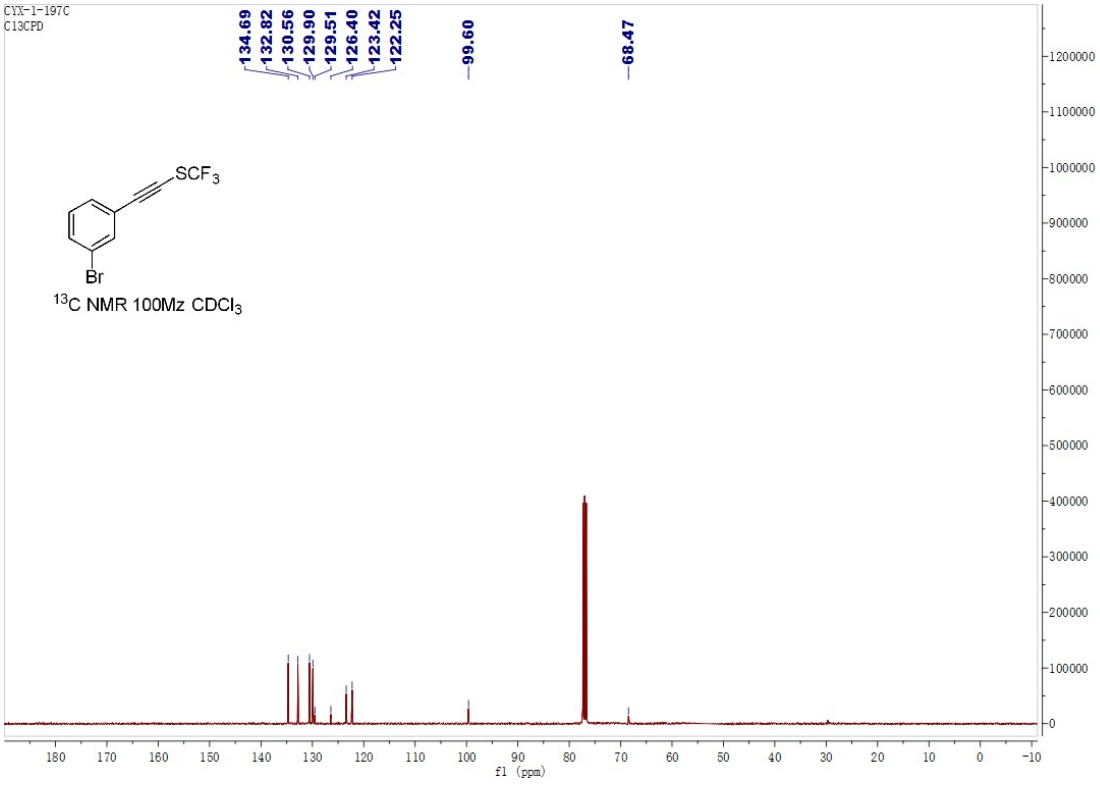

CYX-1-177F
F19
-43.64
SCF3
19F NMR 376MHz CDCl3
f1 (ppm)

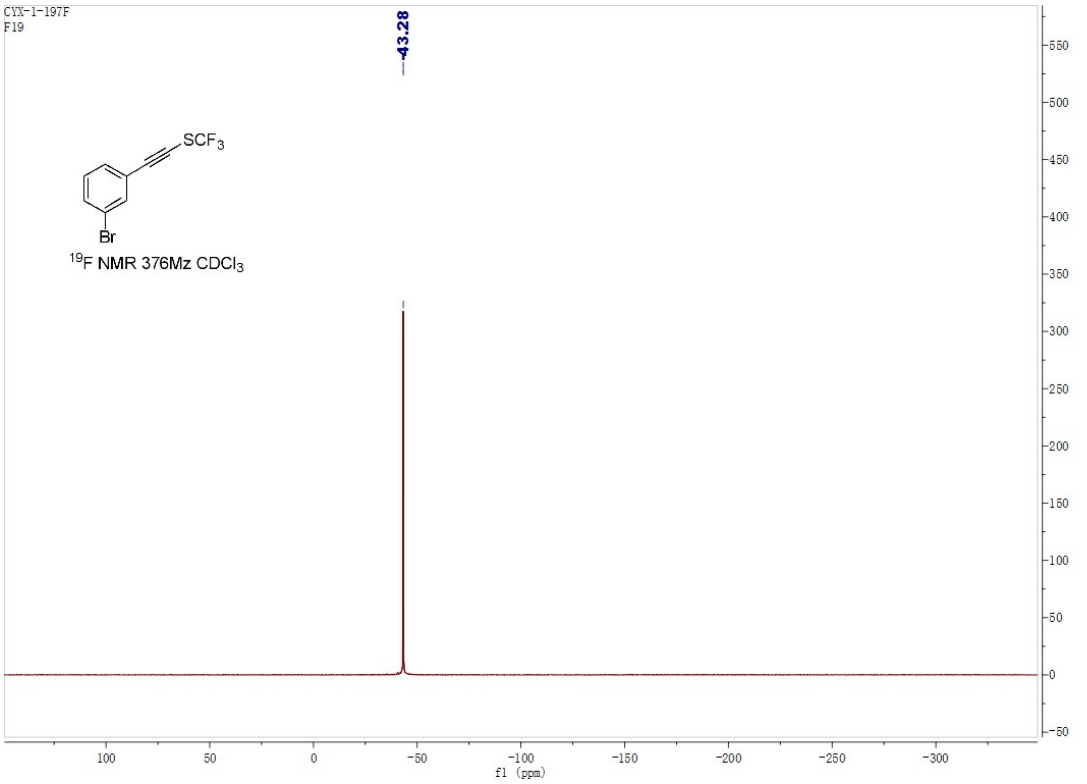

CYX-146-H
1110-DY
0
7.48
7.38
7.36
7.30
7.28
7.26
SCF3
Cl
1H NMR 400MHz CDCl3
1.00
2.00
1.09
f1 (ppm)

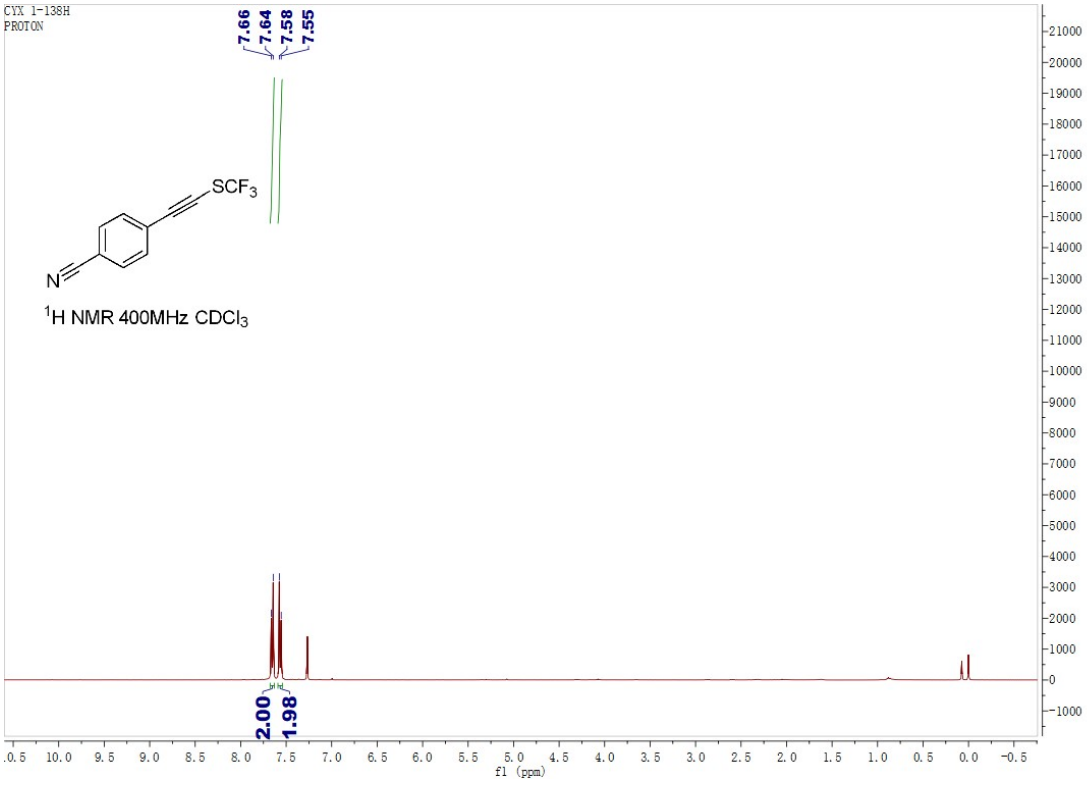

CYX-146-H
13CPD
134.41
131.85
130.15
129.97
129.73
129.54
126.44
123.18
99.78
68.34
SCF3
Cl
13C NMR 100MHz CDCl3
f1 (ppm)

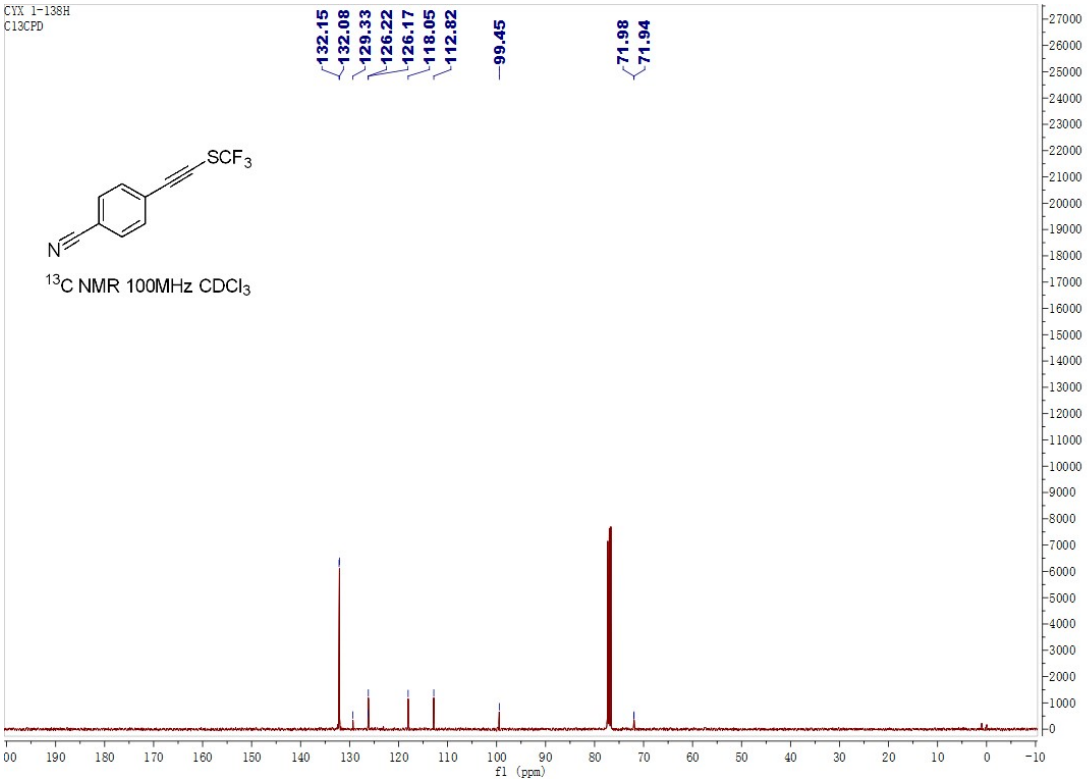

CYX-1-146F
F19
-43.30
SCF3
Cl
19F NMR 376MHz CDCl3
f1 (ppm)

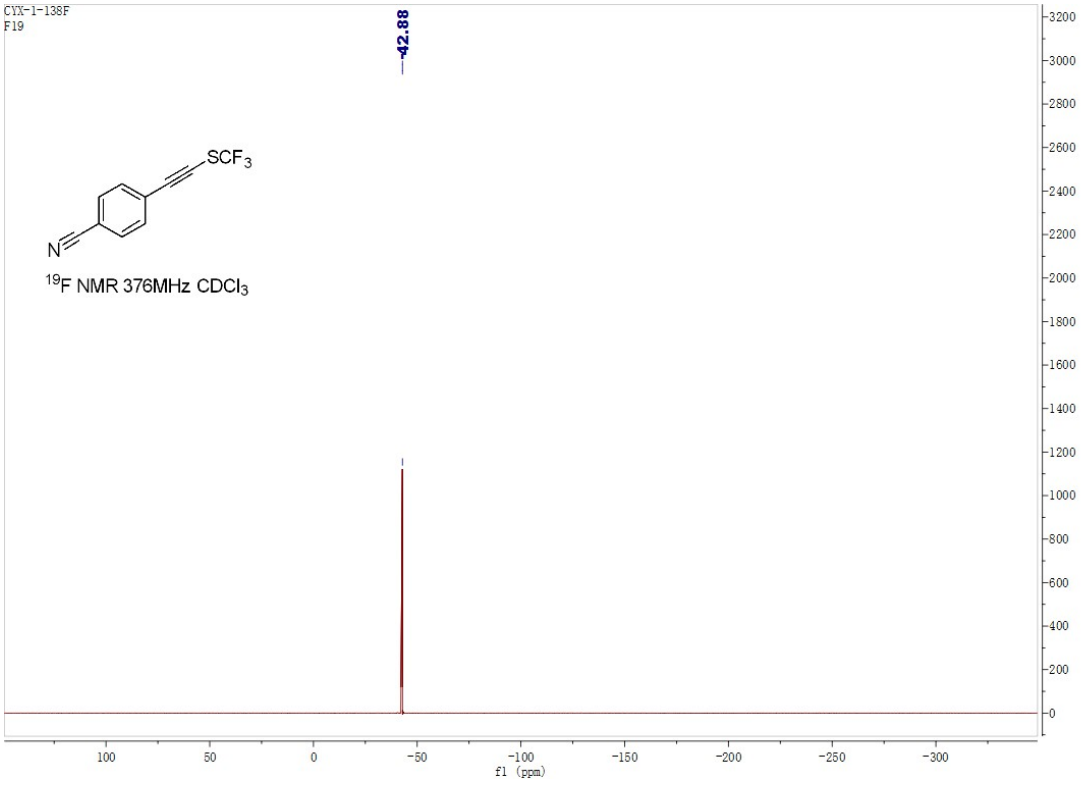

CYX-1-197C
PROTON
7.64
7.63
7.53
7.51
7.43
7.41
7.24
7.22
7.20
SCF3
Br
1H NMR 400Mz CDCl3
1.00
1.01
1.04
1.06
f1 (ppm)

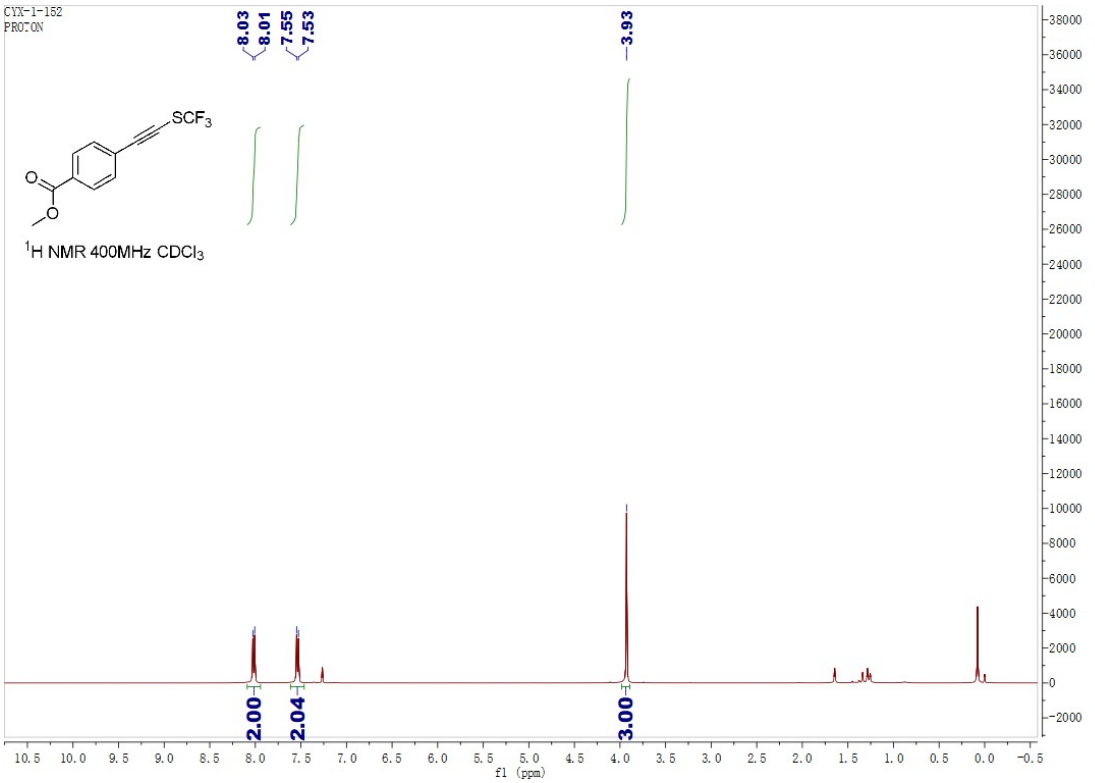

CYX-1-197C
C13CPD
134.69
132.82
130.56
129.90
129.51
126.40
123.42
122.25
99.60
68.47
SCF3
Br
13C NMR 100Mz CDCl3
f1 (ppm)

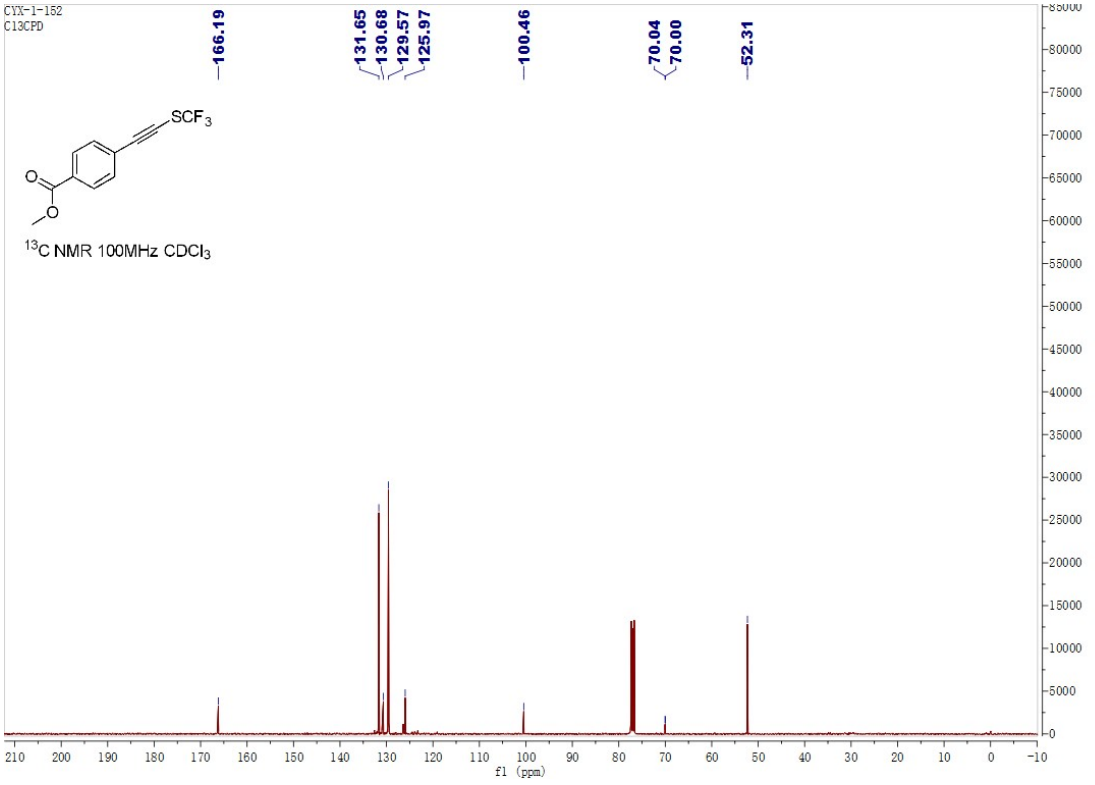

CYX-1-197F
F19
-43.28
SCF3
Br
19F NMR 376Mz CDCl3
f1 (ppm)

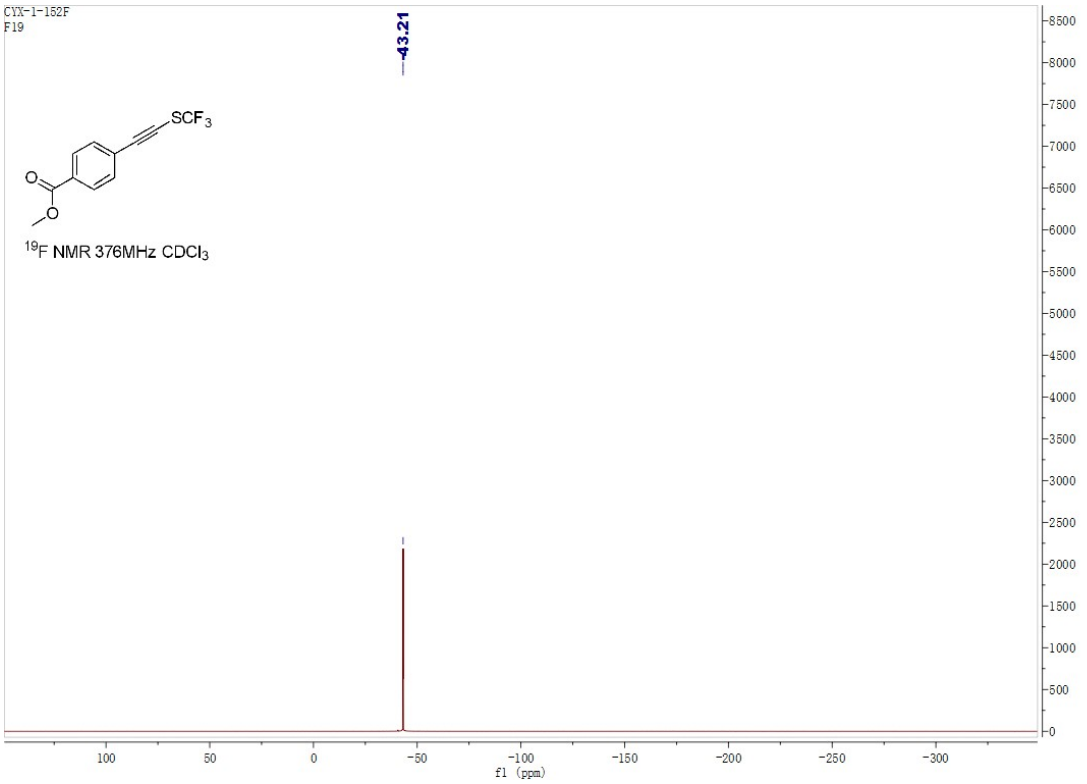

CYX 1-138H
PROTON
7.66
7.64
7.58
7.55
SCF3
N
1H NMR 400MHz CDCl3
2.00
1.98
f1 (ppm)

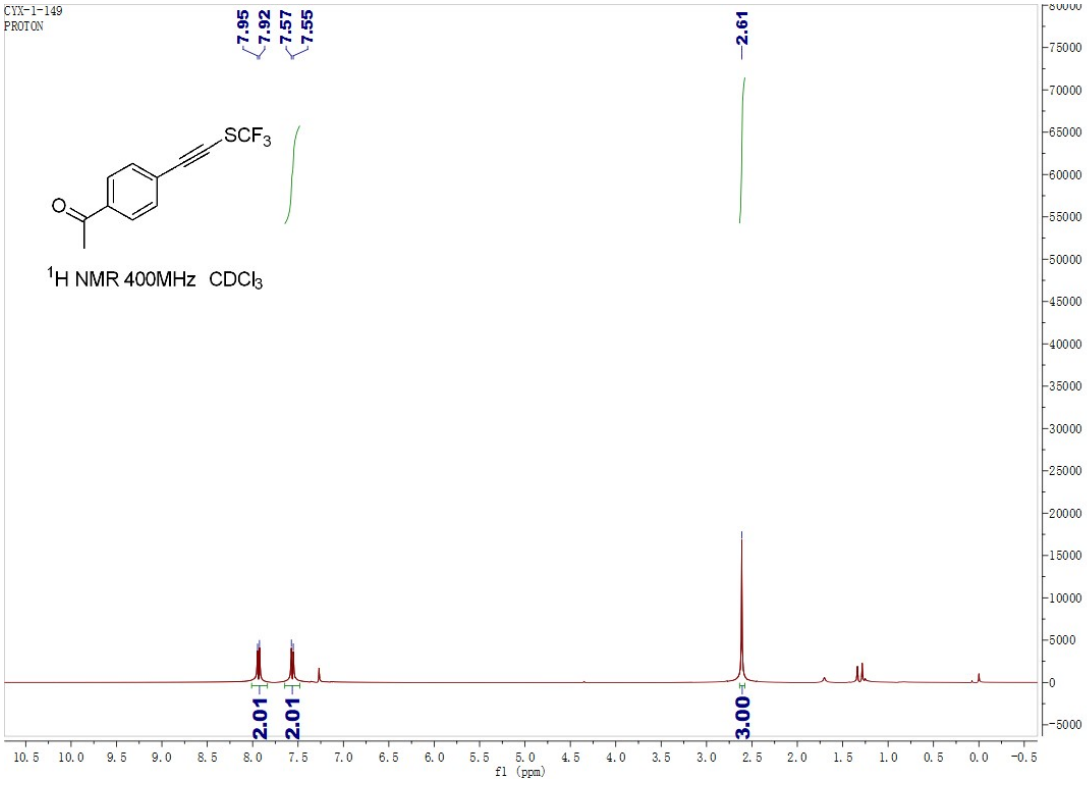

CYX 1-138H
C13CPD
132.15
132.08
129.33
126.22
126.17
118.05
112.82
99.45
71.98
71.94
SCF3
N
13C NMR 100MHz CDCl3
f1 (ppm)

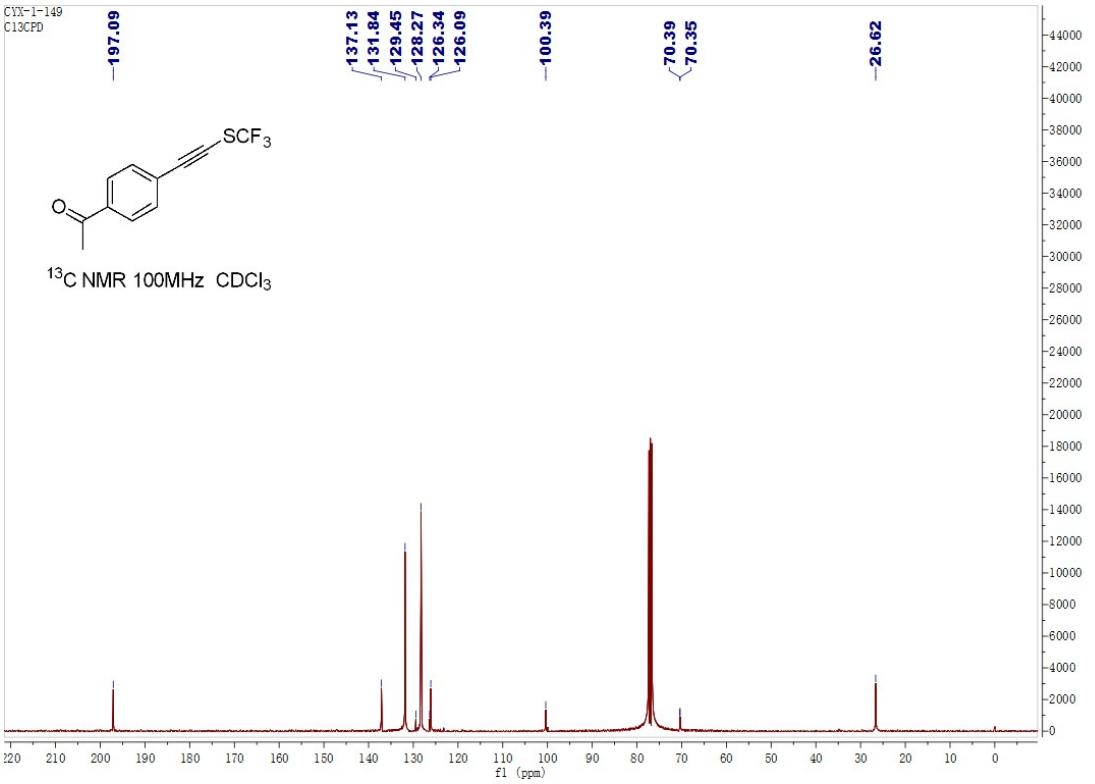

CYX-1-138F
F19
-42.88
SCF3
N
19F NMR 376MHz CDCl3
f1 (ppm)

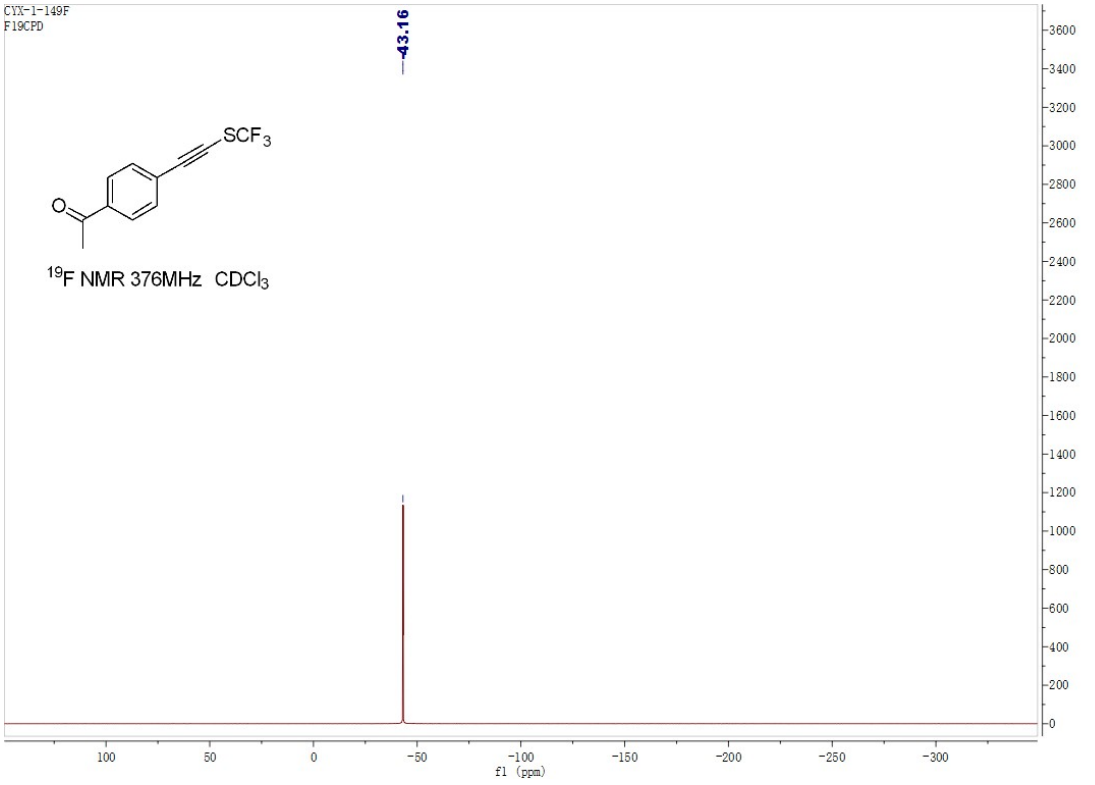

CYX-1-162
PROTON
8.03
8.01
7.55
7.53
3.93
SCF3
O
O
1H NMR 400MHz CDCl3
2.00
2.04
3.00
f1 (ppm)

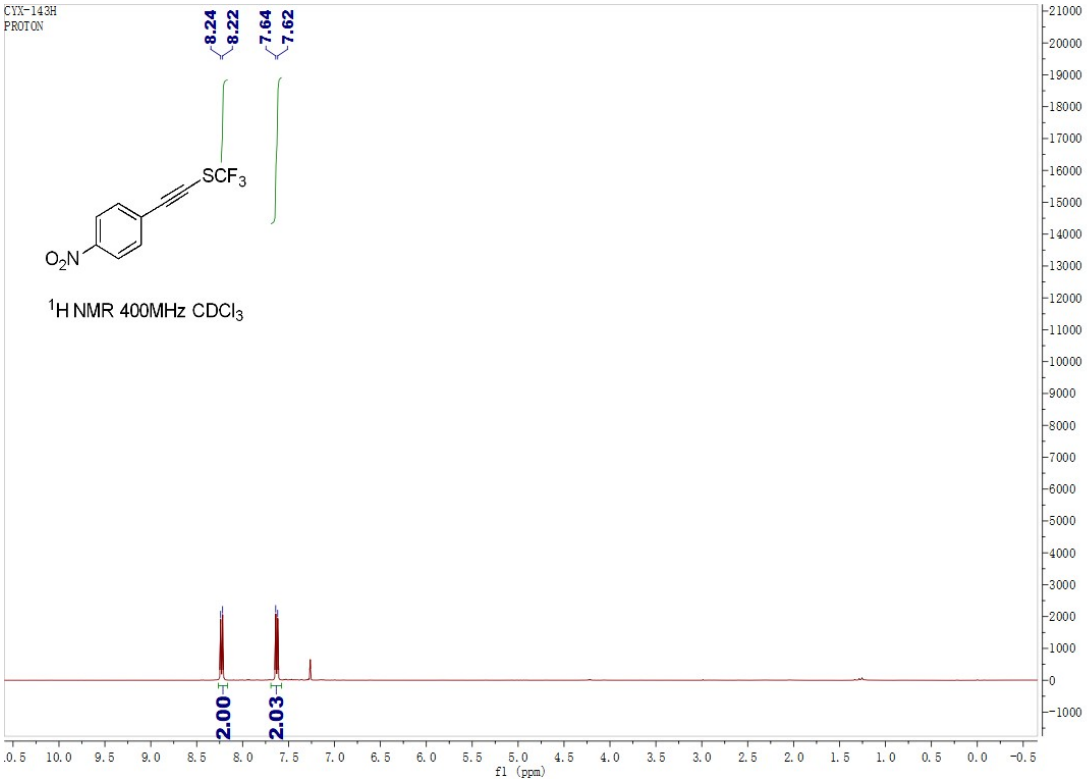

CYX-1-162
C13CPD
166.19
131.65
130.68
129.57
125.97
100.46
70.04
70.00
52.31
SCF3
O
O
13C NMR 100MHz CDCl3
f1 (ppm)

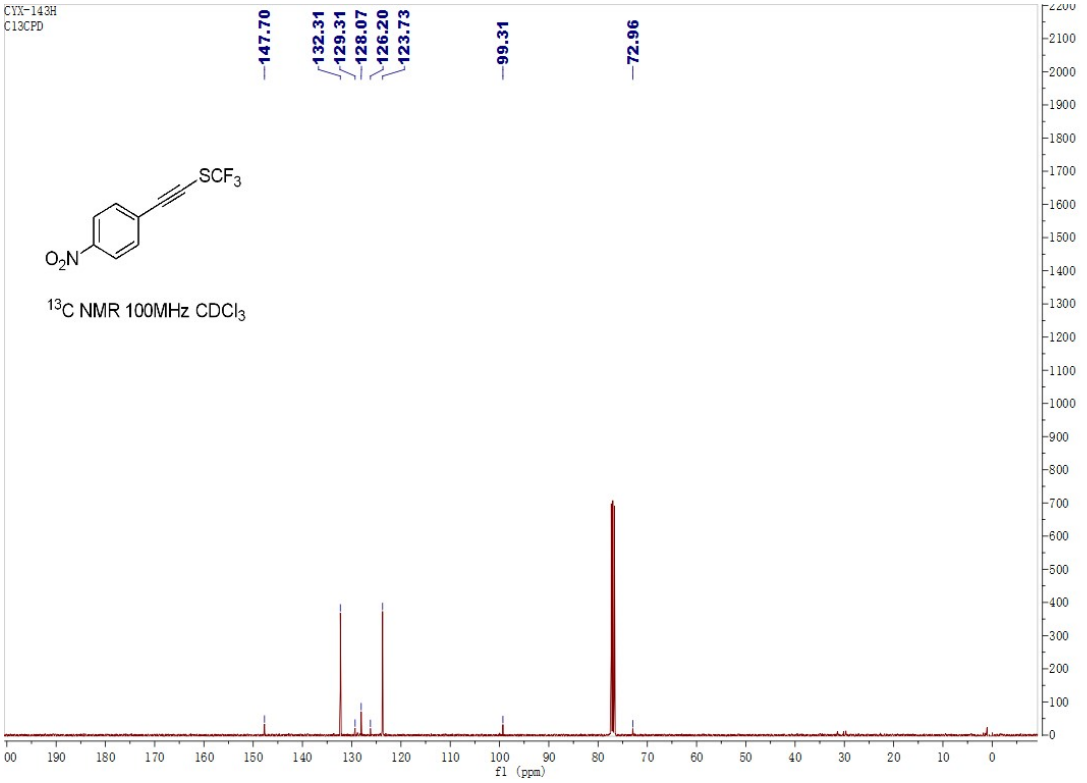

CYX-1-162F
F19
-43.21
SCF3
O
O
19F NMR 376MHz CDCl3
f1 (ppm)

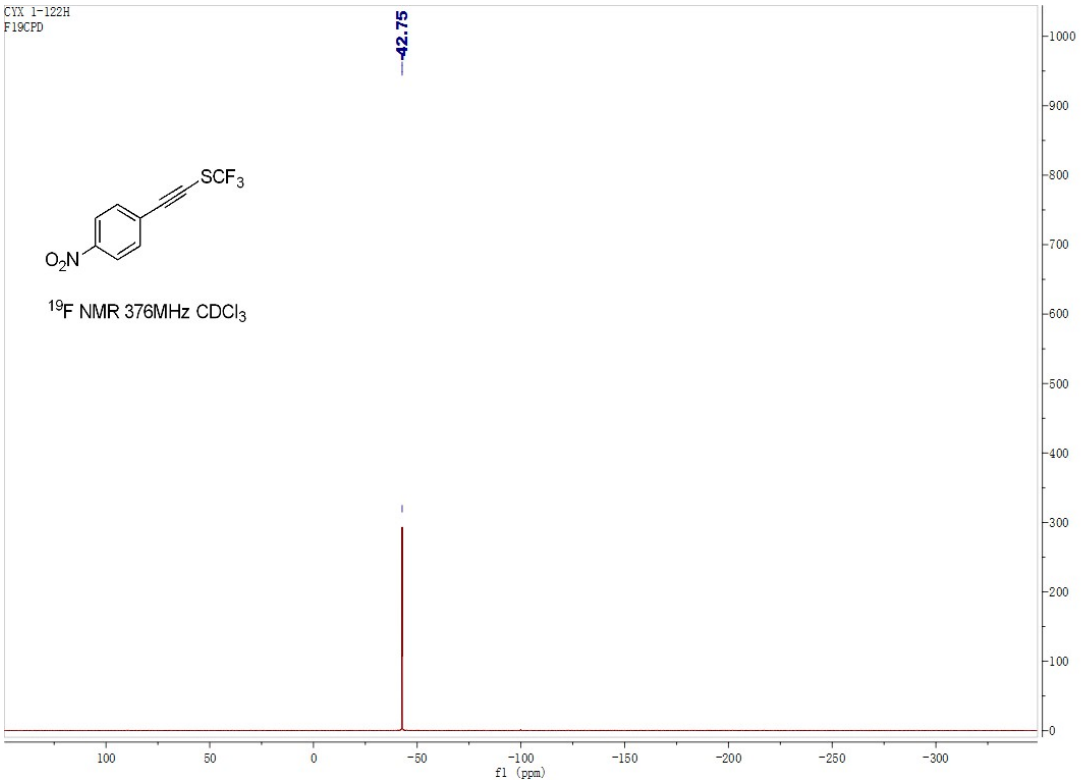

CYX-1-149
PROTON
7.95
7.92
7.57
7.55
2.61
SCF3
O
1H NMR 400MHz CDCl3
2.01
2.01
3.00
f1 (ppm)

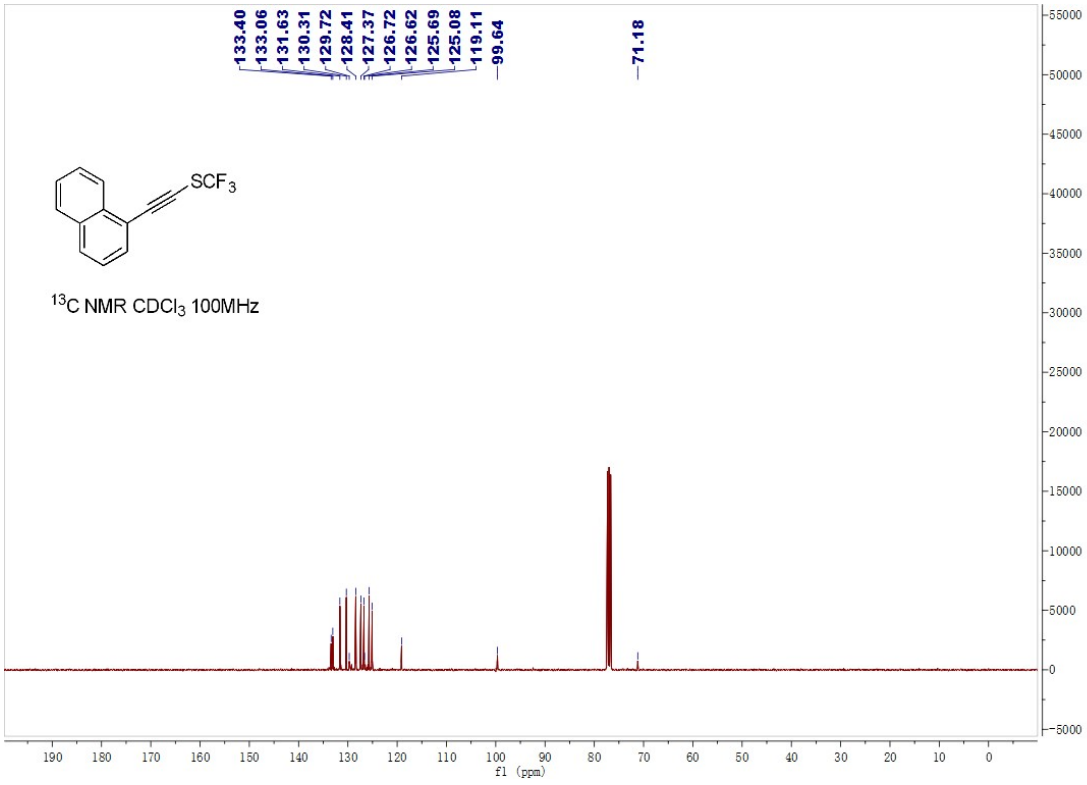

CYX-1-149
C13CPD
197.09
137.13
131.84
129.45
128.27
126.34
126.09
100.39
70.39
70.35
26.62
SCF3
O
13C NMR 100MHz CDCl3
f1 (ppm)

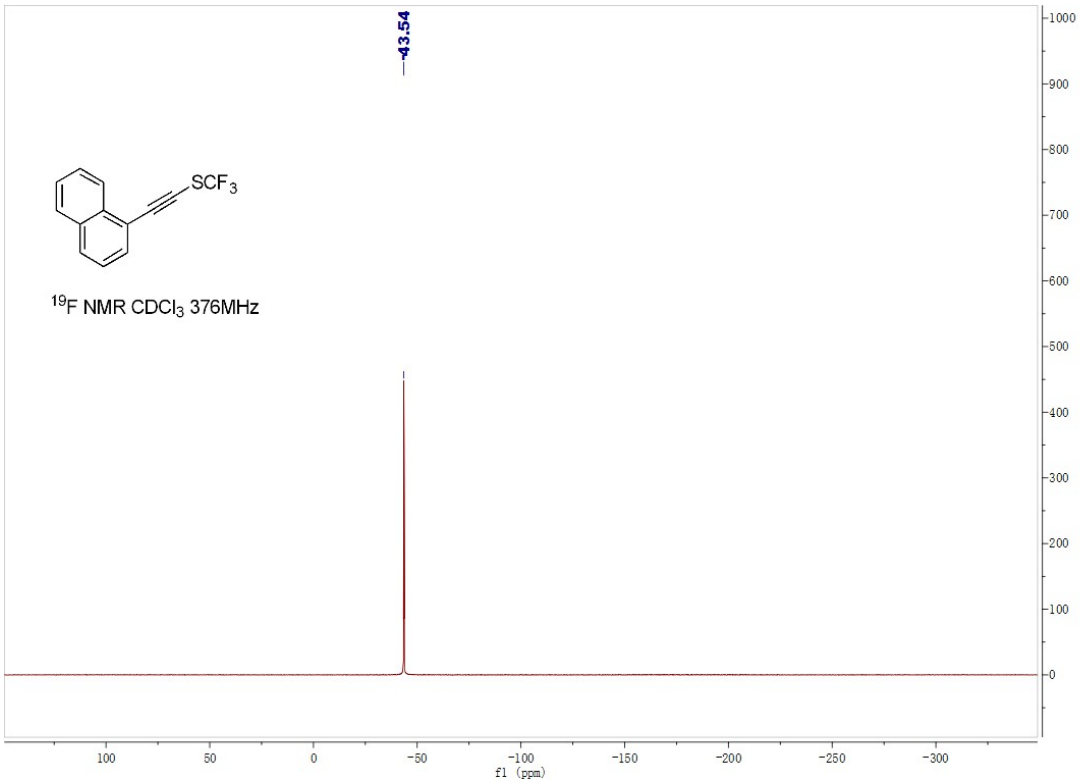

CYX-1-149F
F19CPD
43.16
SCF3
O
19F NMR 376MHz CDCl3
f1 (ppm)

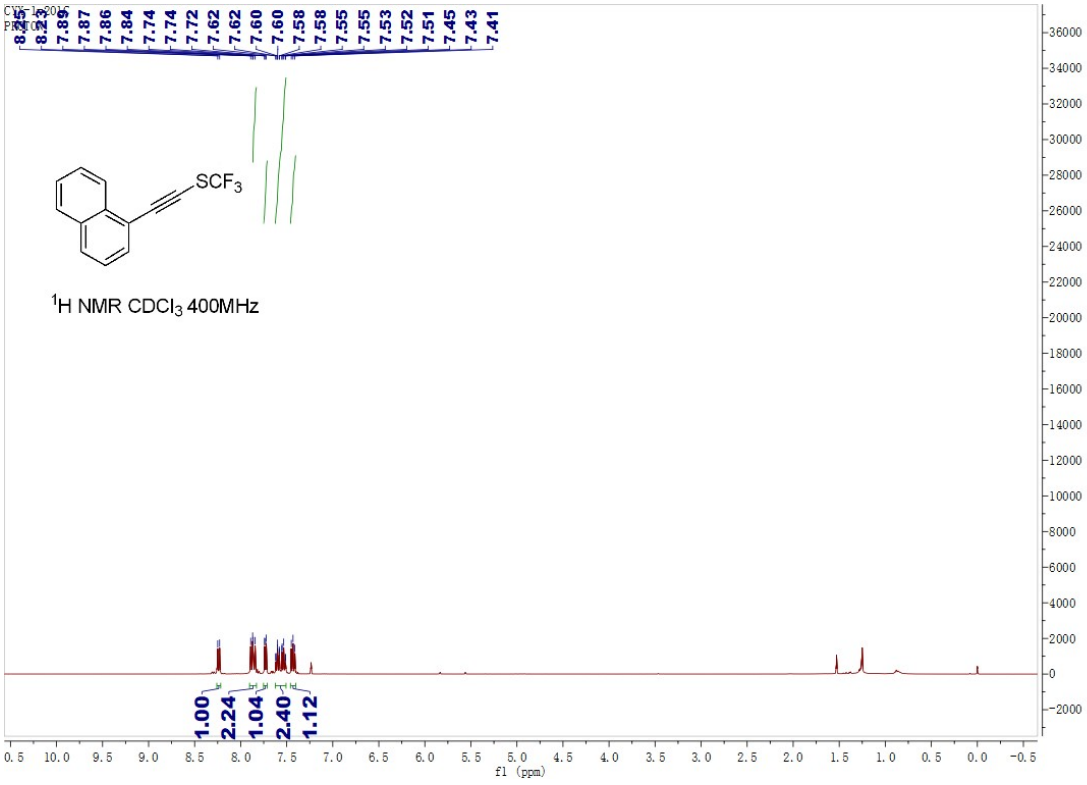

CYX-143H
PROTON
8.24
8.22
7.64
7.62
SCF3
O2N
1H NMR 400MHz CDCl3
2.00
2.03
f1 (ppm)

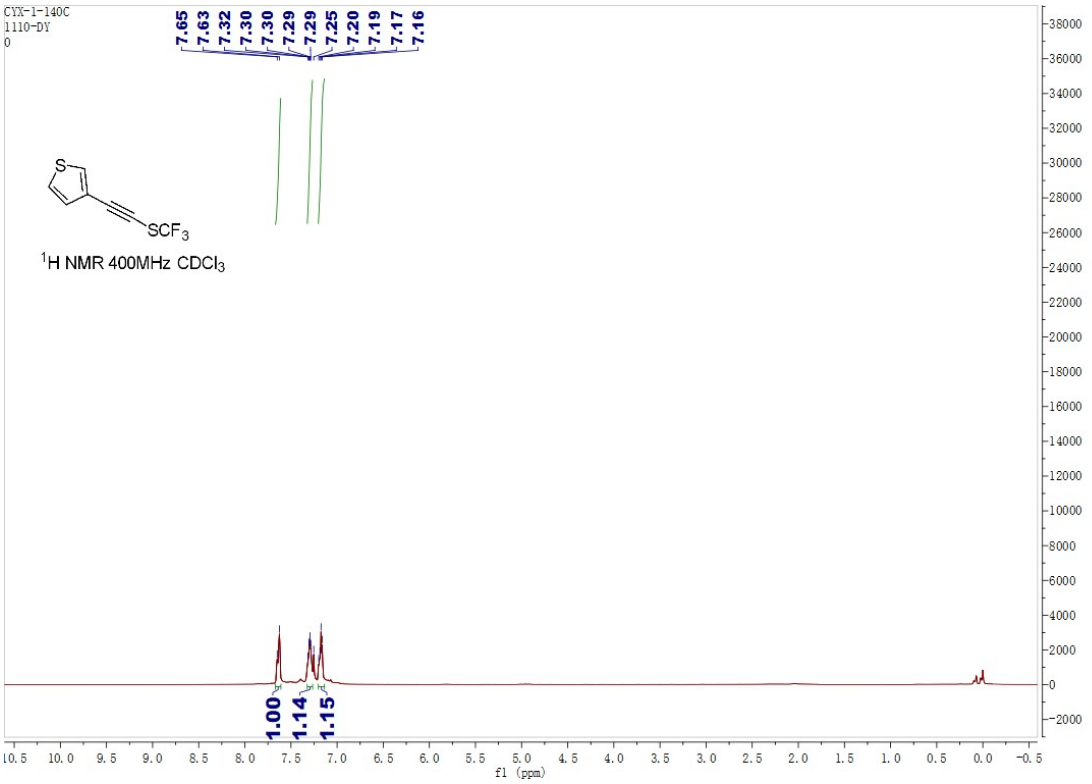

CYX-143H
C13CPD
147.70
132.31
129.31
128.07
126.20
123.73
99.31
72.96
SCF3
O2N
13C NMR 100MHz CDCl3
f1 (ppm)

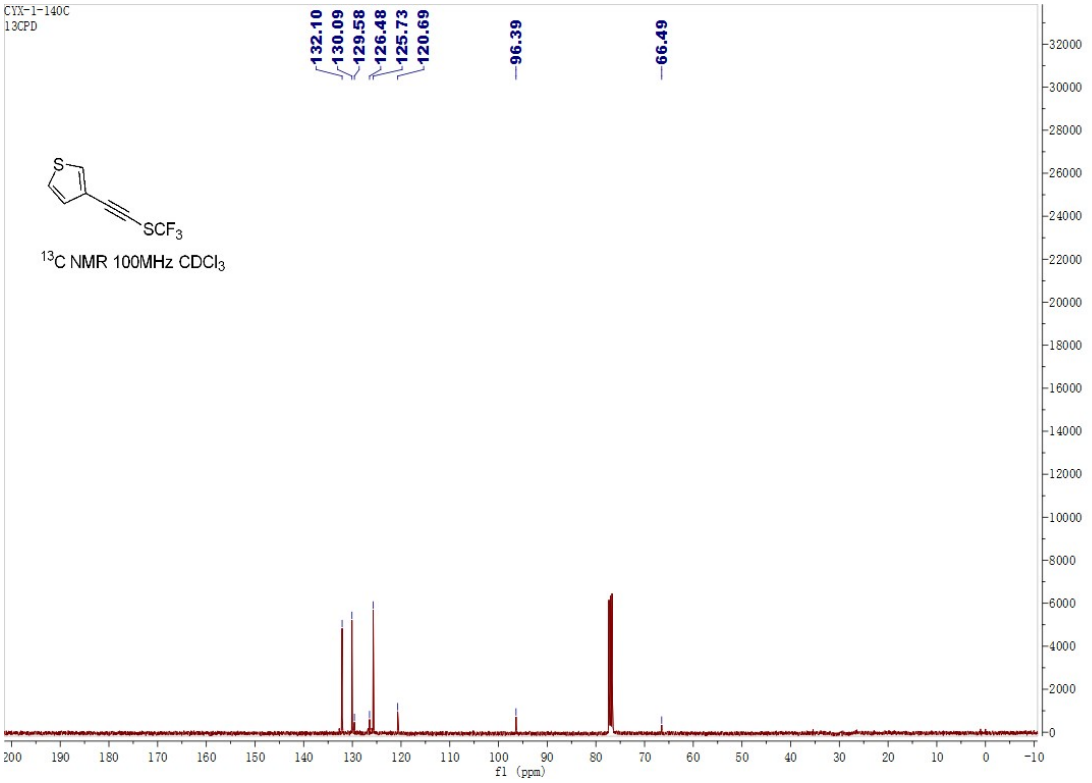

CYX 1-122H
F19CPD
-42.75
SCF3
O2N
19F NMR 376MHz CDCl3
f1 (ppm)

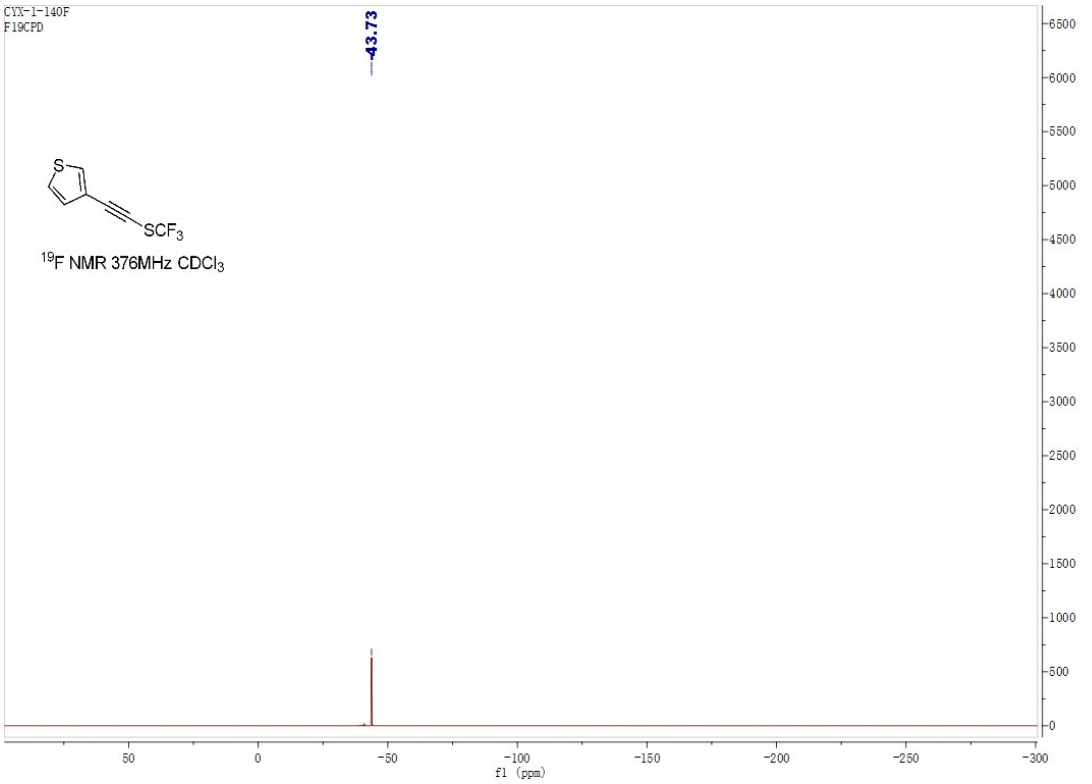

133.40
133.06
131.63
130.31
129.72
128.41
127.37
126.72
126.62
125.69
125.08
119.11
99.64
71.18
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

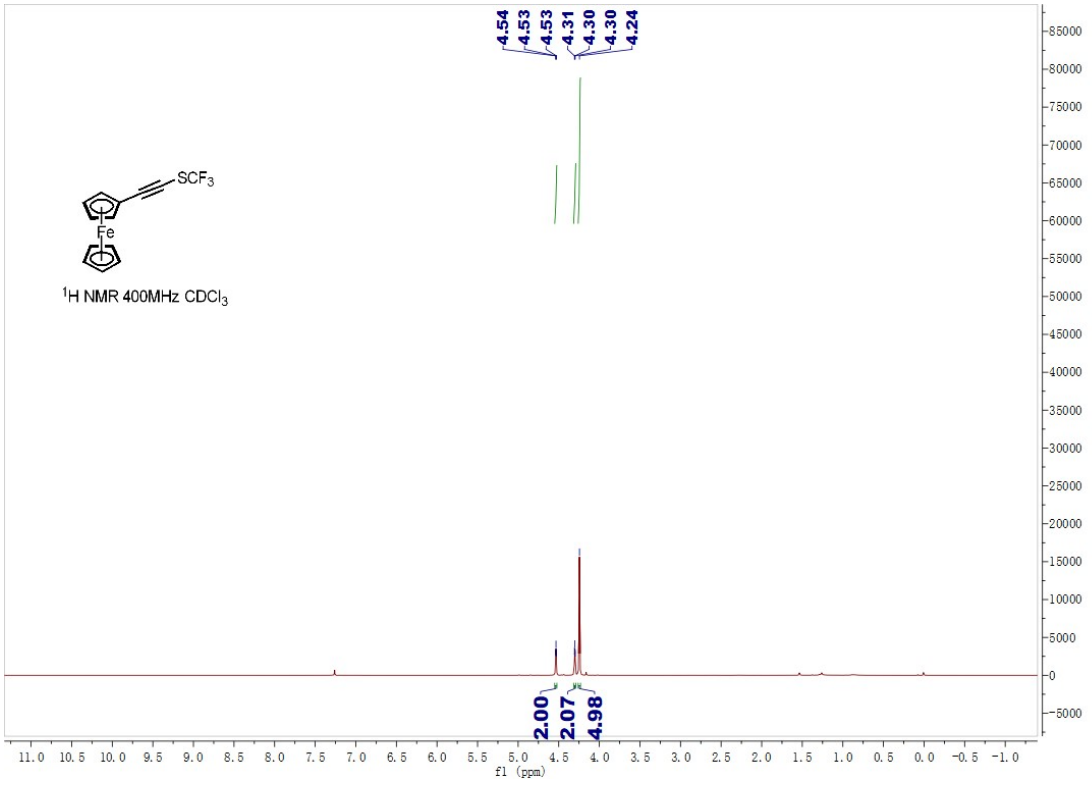

-43.54
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

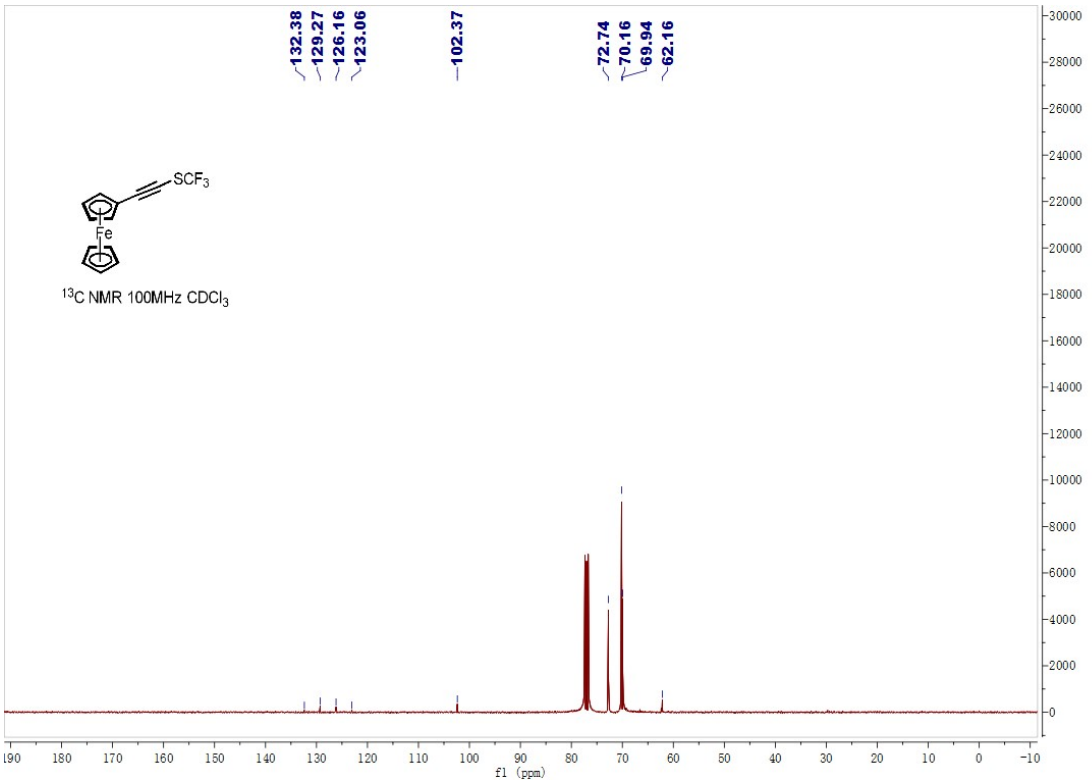

8.25
8.23
7.89
7.87
7.86
7.84
7.74
7.74
7.72
7.62
7.62
7.60
7.60
7.58
7.58
7.55
7.55
7.53
7.52
7.51
7.45
7.43
7.41
SCF3
1H NMR CDCl3 400MHz
1.00
2.24
1.04
2.40
1.12
f1 (ppm)

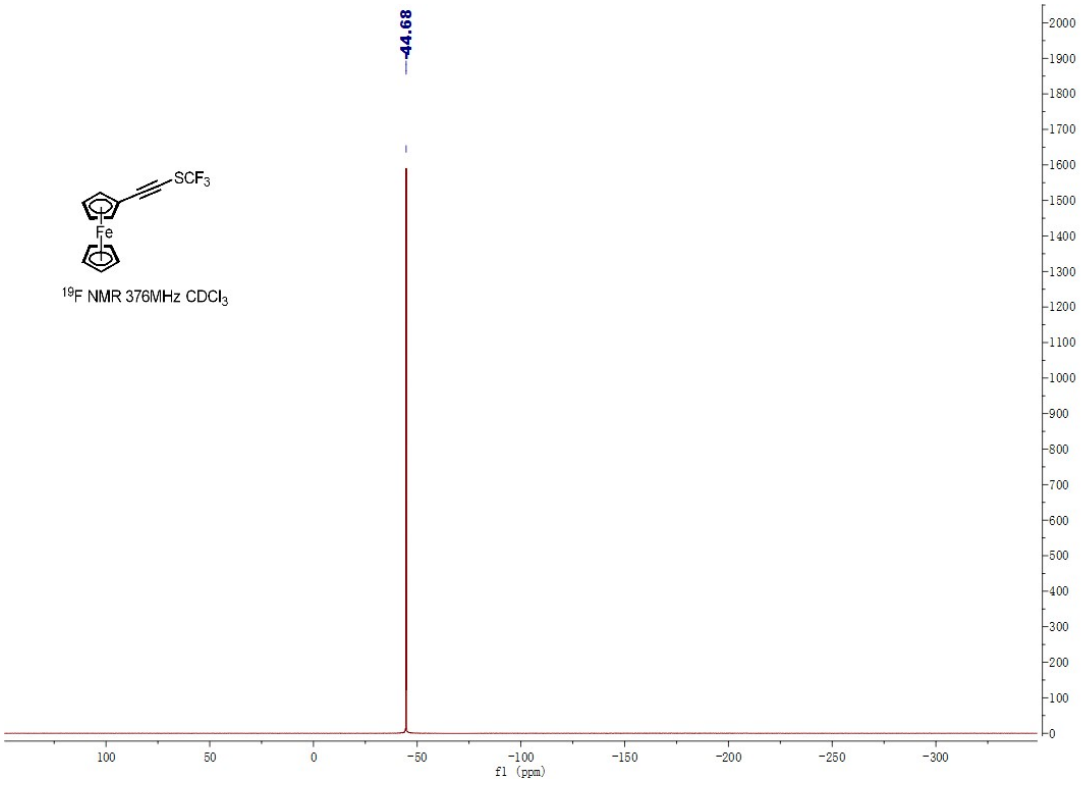

CYX-1-140C
1110-DY
0
7.65
7.63
7.32
7.30
7.30
7.29
7.29
7.25
7.20
7.19
7.17
7.16
S
SCF3
1H NMR 400MHz CDCl3
1.00
1.14
1.15
f1 (ppm)

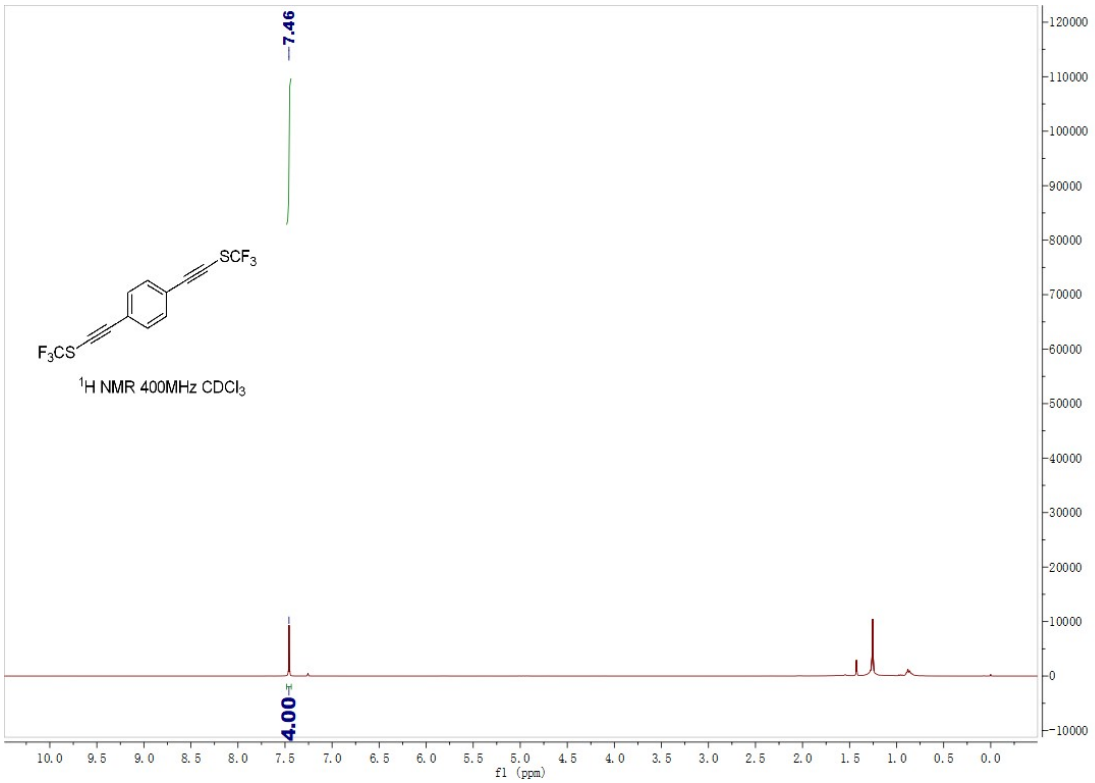

CYX-1-140C
13CPD
132.10
130.09
129.58
126.48
125.73
120.69
96.39
66.49
S
SCF3
13C NMR 100MHz CDCl3
f1 (ppm)

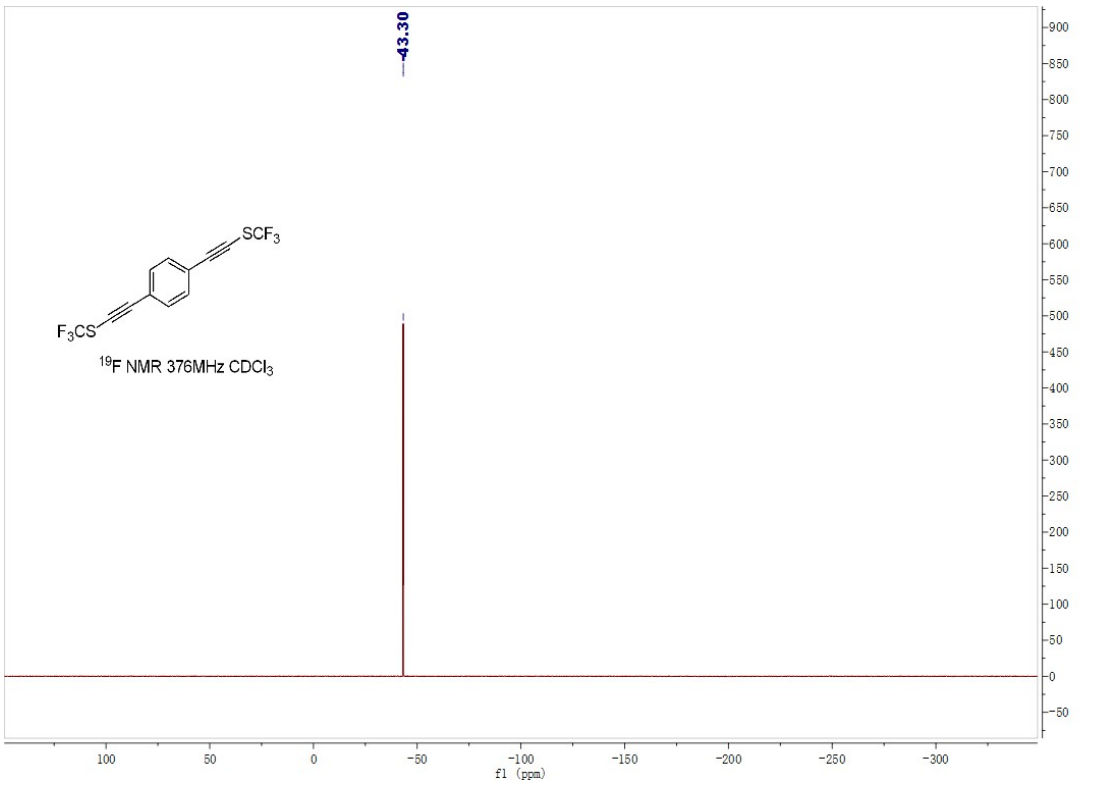

CYX-1-140F
F19CPD
-43.73
S
SCF3
19F NMR 376MHz CDCl3
f1 (ppm)

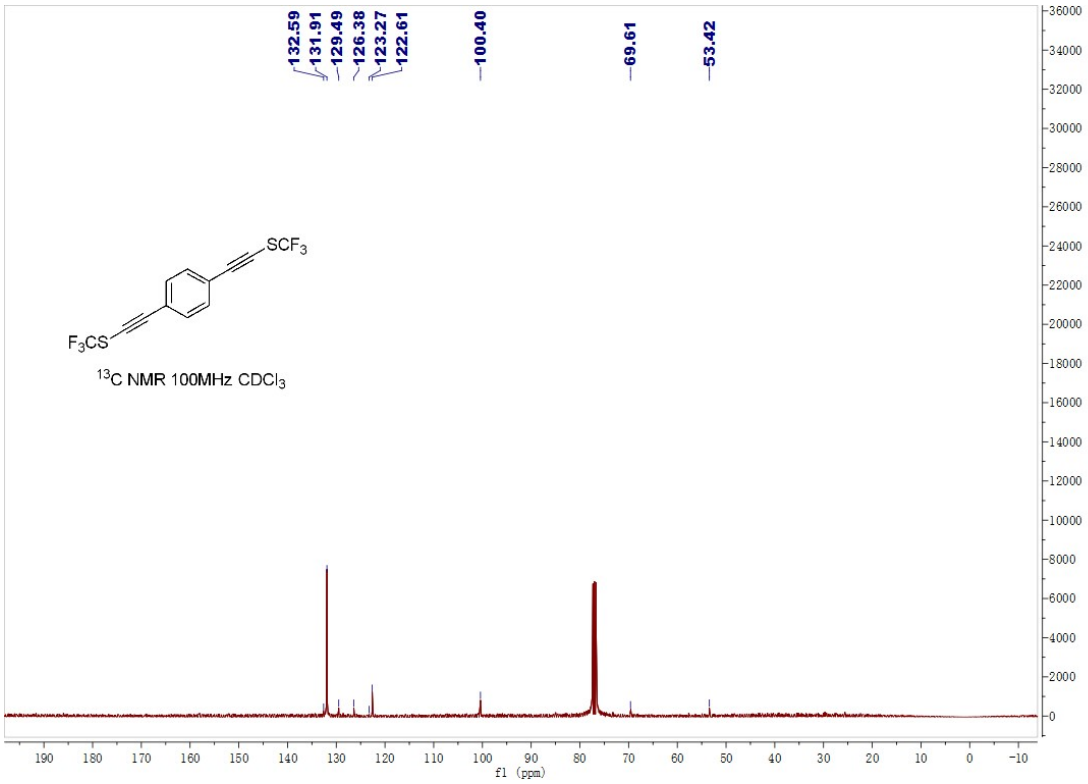

4.54
4.53
4.53
4.31
4.30
4.30
4.24
SCF3
Fe
1H NMR 400MHz CDCl3
2.00
2.07
4.98
f1 (ppm)

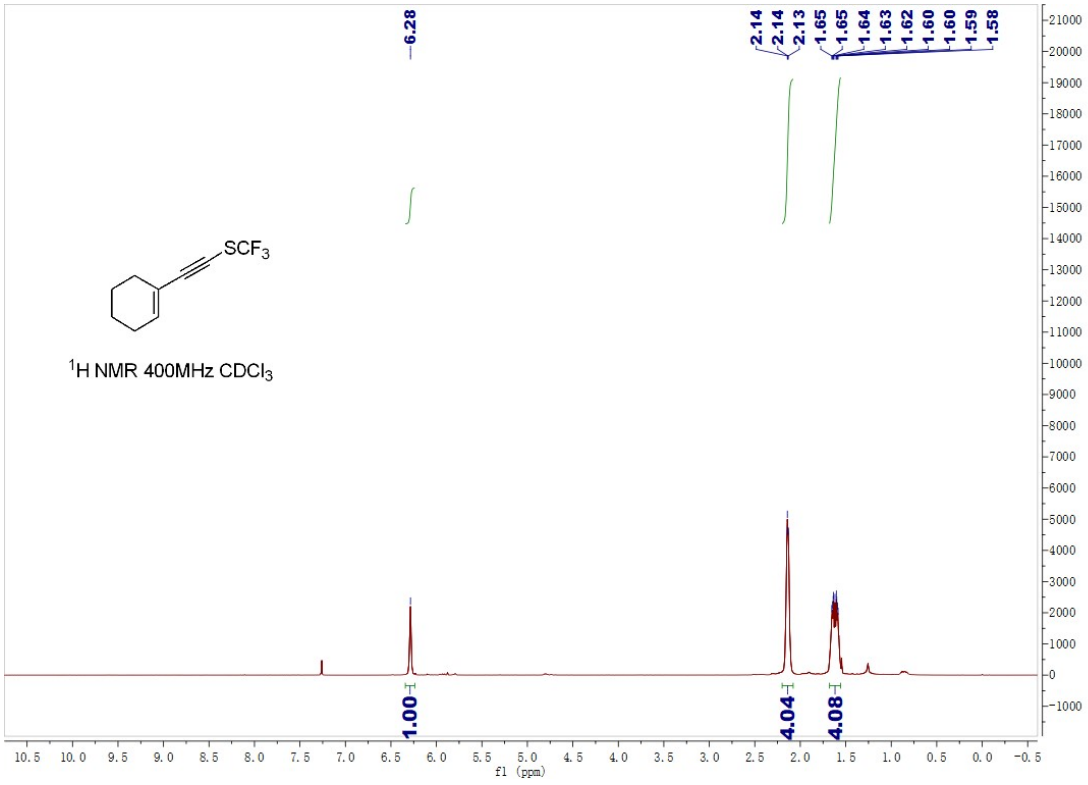

132.38
129.27
126.16
123.06
102.37
72.74
70.16
69.94
62.16
SCF3
Fe
13C NMR 100MHz CDCl3
f1 (ppm)

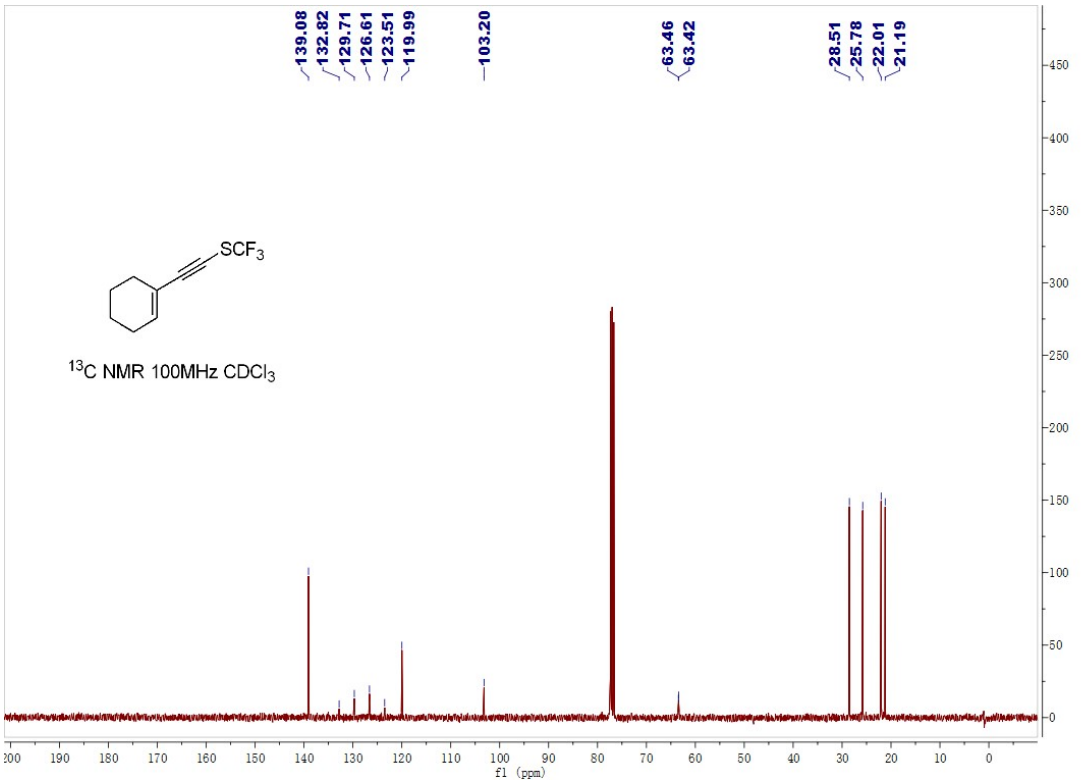

-44.68
SCF3
Fe
19F NMR 376MHz CDCl3
f1 (ppm)

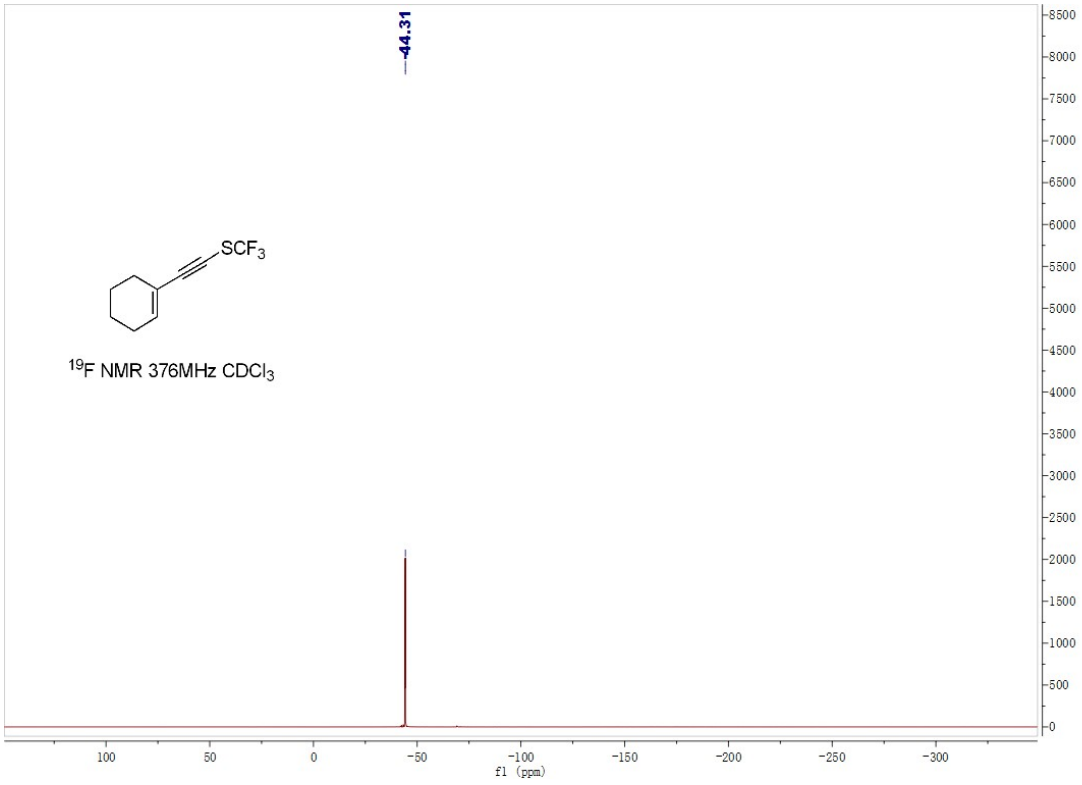

7.46
4.00
SCF3
F3CS
1H NMR 400MHz CDCl3
f1 (ppm)

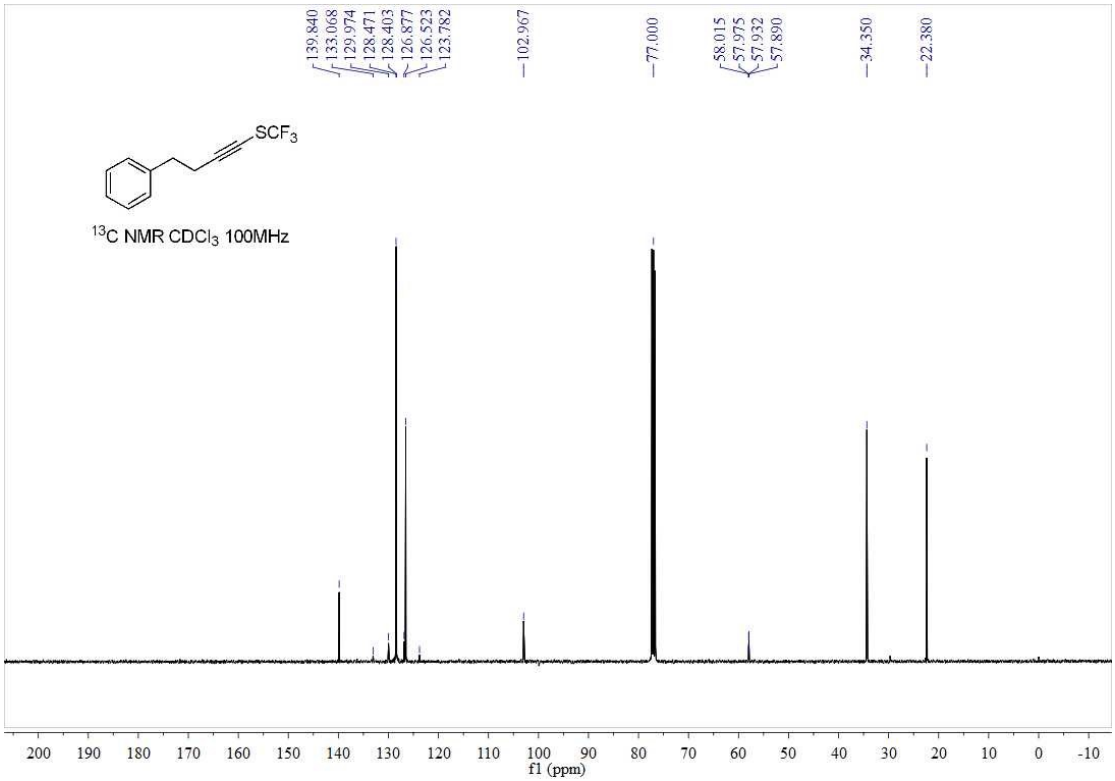

-43.30
SCF3
F3CS
19F NMR 376MHz CDCl3
f1 (ppm)

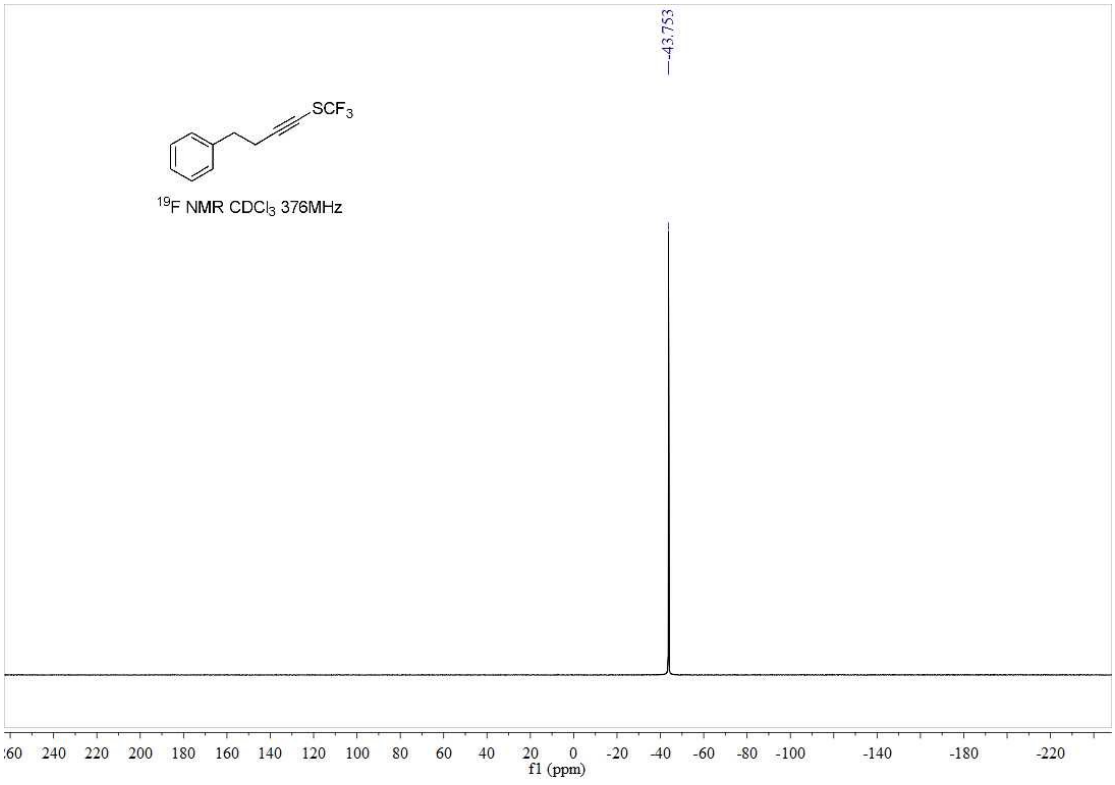

132.59
131.91
129.49
126.38
123.27
122.61
100.40
69.61
53.42
SCF3
F3CS
13C NMR 100MHz CDCl3
f1 (ppm)

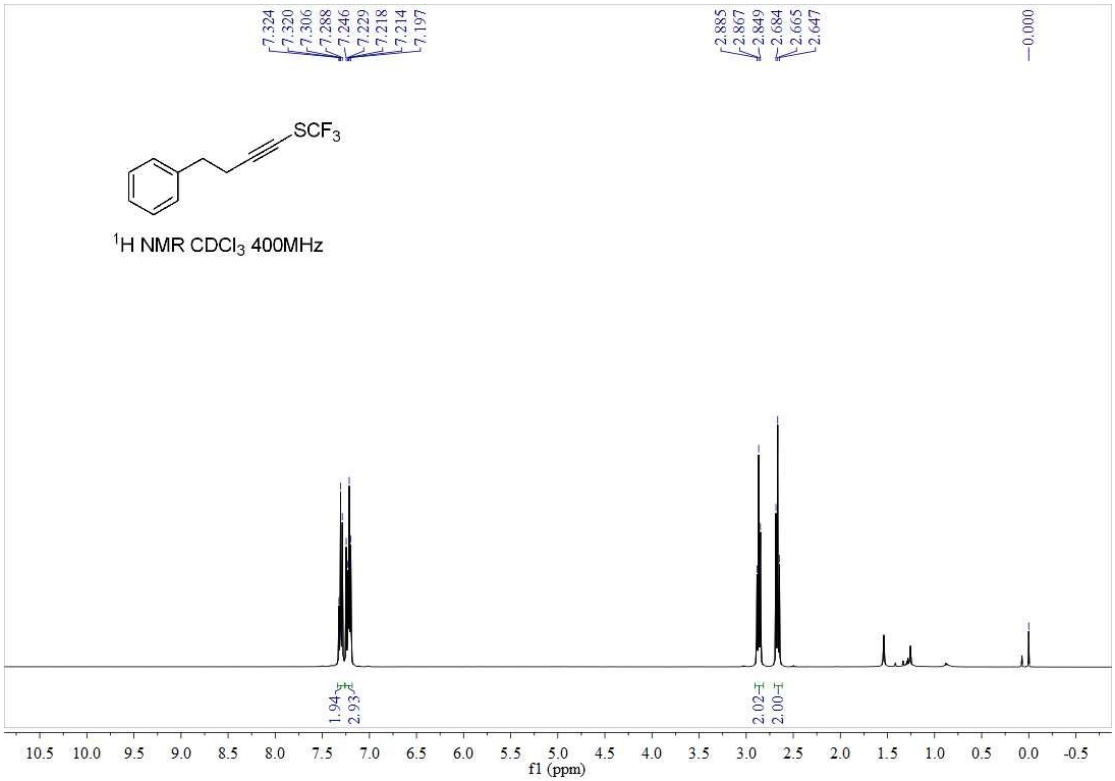

6.28
2.14
2.14
2.13
1.65
1.65
1.64
1.63
1.62
1.60
1.60
1.59
1.58
SCF3
1H NMR 400MHz CDCl3
1.00
4.04
4.08
f1 (ppm)

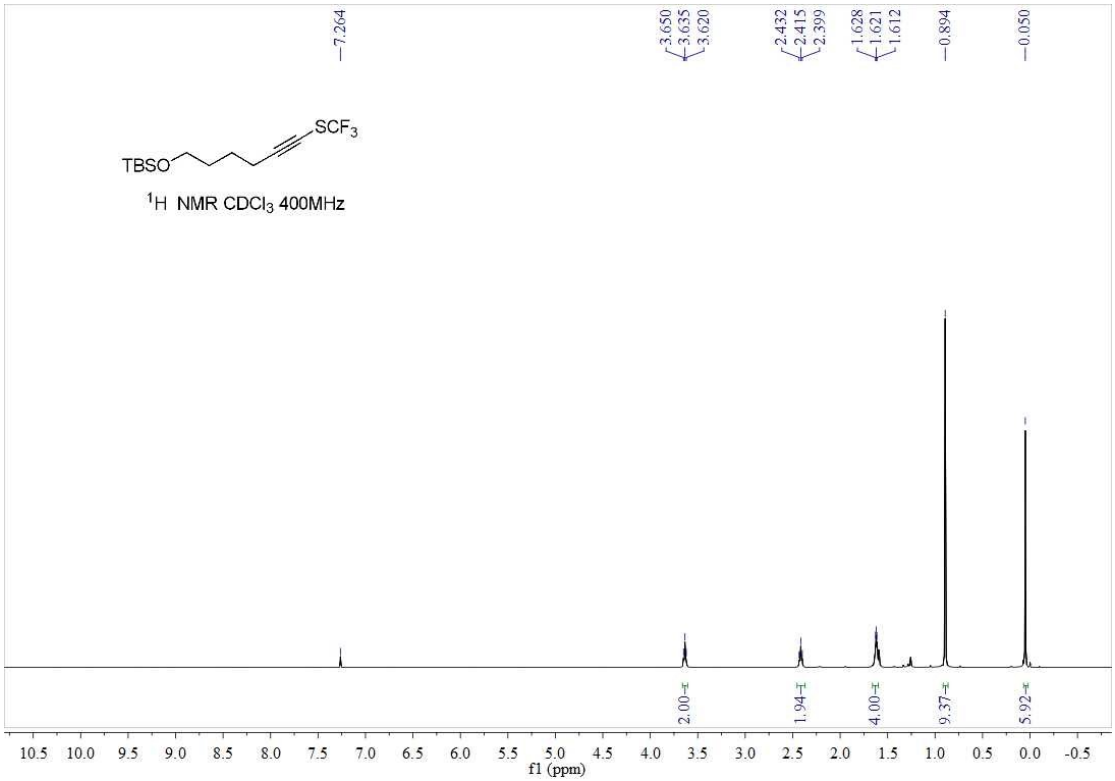

139.08
132.82
129.71
126.61
123.51
119.99
103.20
63.46
63.42
28.51
25.78
22.01
21.19
SCF3
13C NMR 100MHz CDCl3
f1 (ppm)

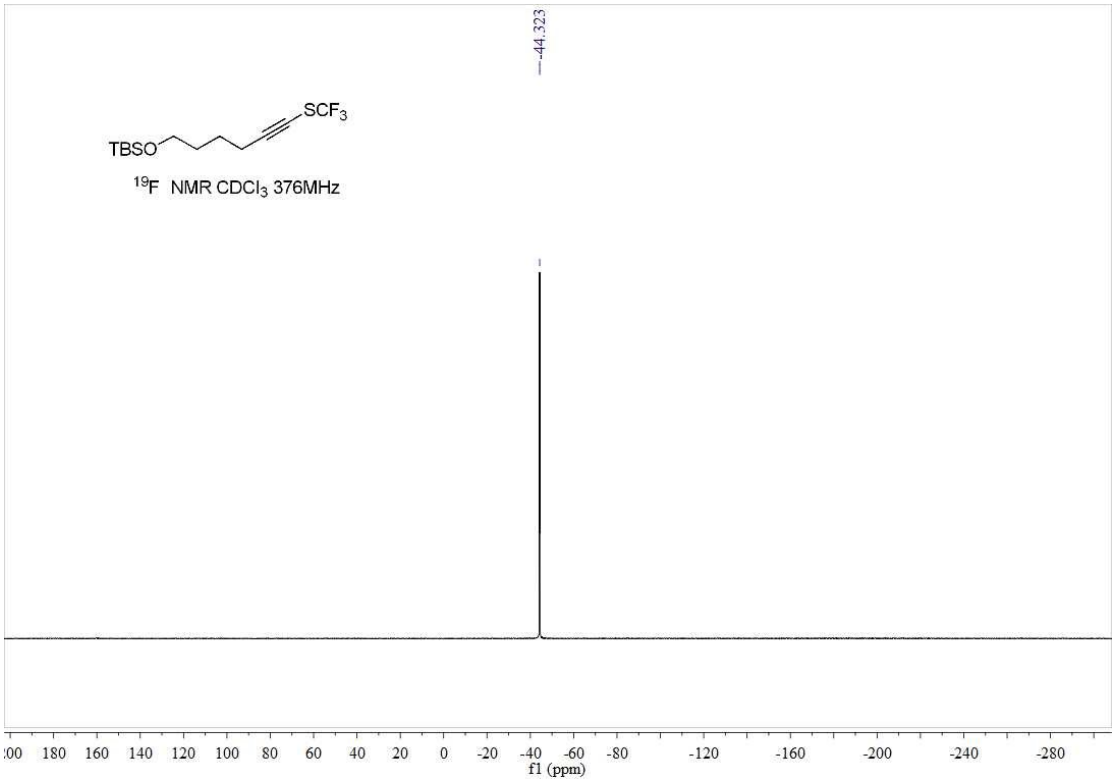

-44.31
SCF3
19F NMR 376MHz CDCl3
f1 (ppm)

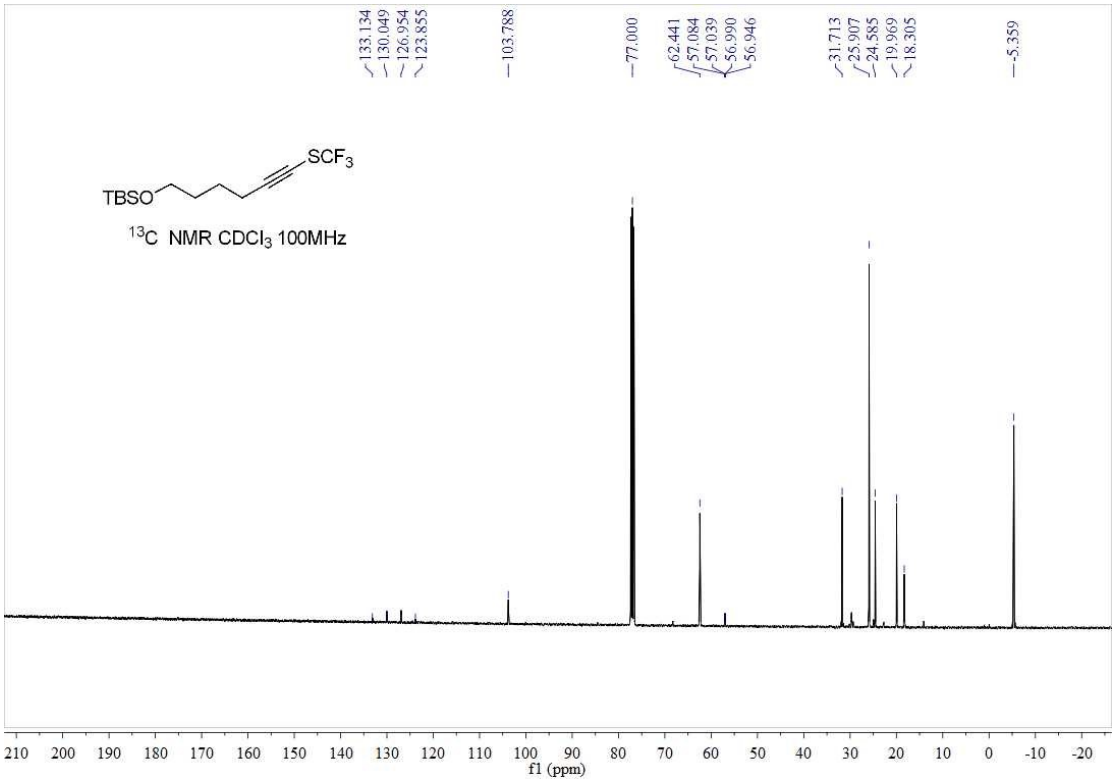

139.840
133.068
129.974
128.471
128.403
126.877
126.523
123.782
102.967
77.000
58.015
57.975
57.932
57.890
34.350
22.380
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

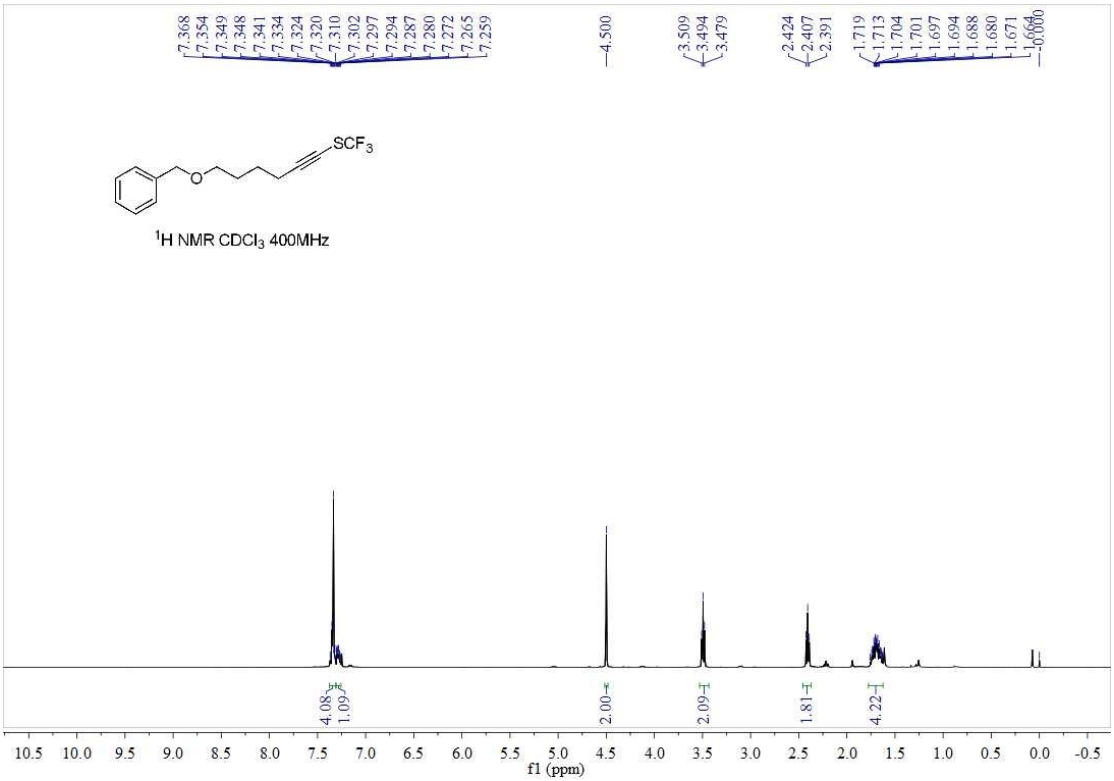

-43.753
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

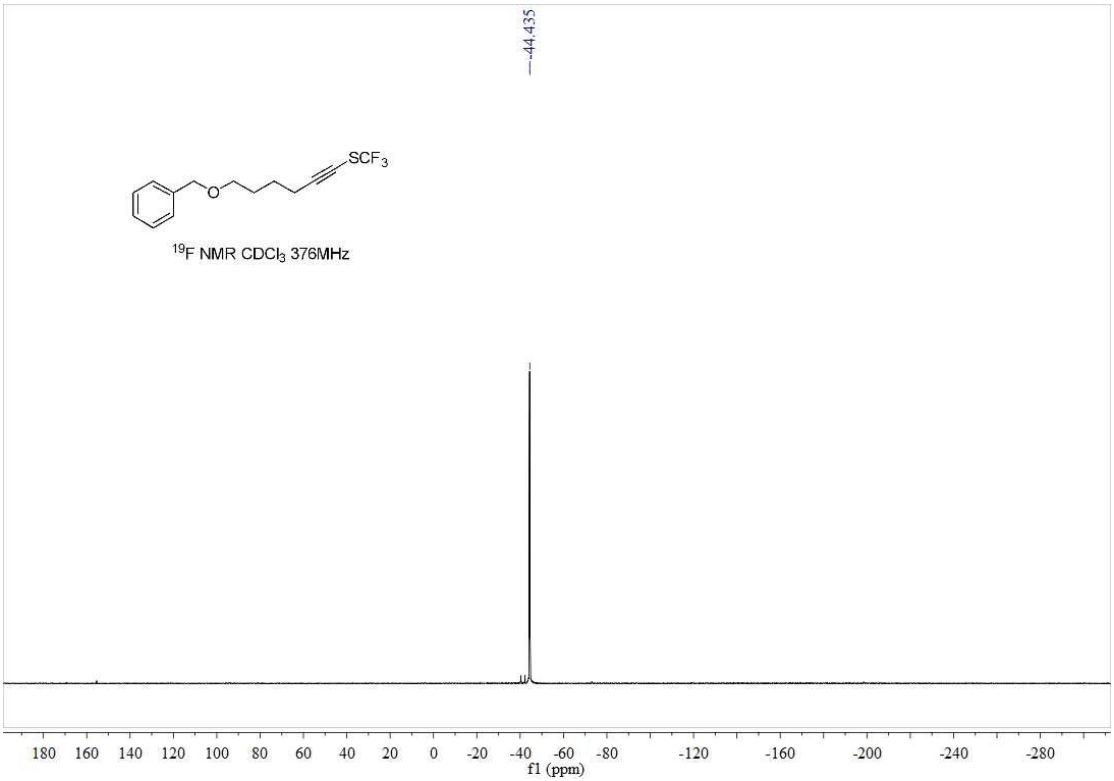

7.324
7.320
7.306
7.288
7.246
7.229
7.218
7.214
7.197
2.885
2.867
2.849
2.684
2.665
2.647
0.000
SCF3
1H NMR CDCl3 400MHz
1.94
2.93
2.02
2.00
f1 (ppm)

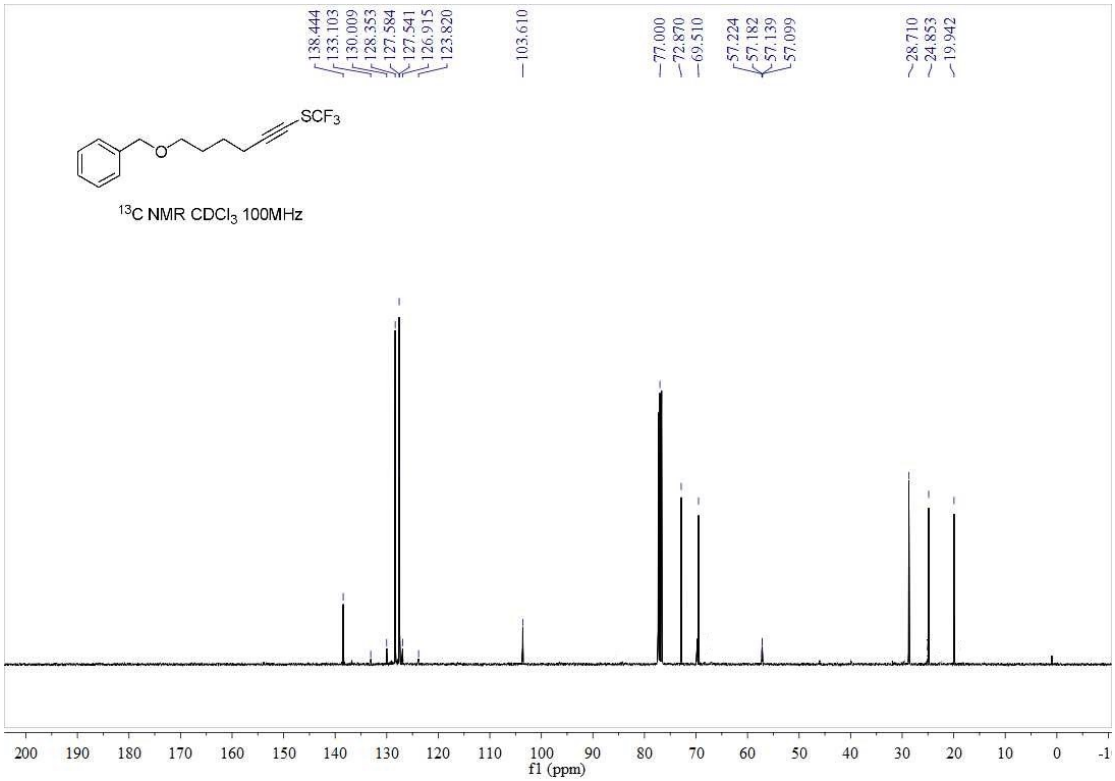

7.264
3.650
3.635
3.620
2.432
2.415
2.399
1.628
1.621
1.612
0.894
0.050
SCF3
TBSO
1H NMR CDCl3 400MHz
2.00
1.94
4.00
9.37
5.92
f1 (ppm)

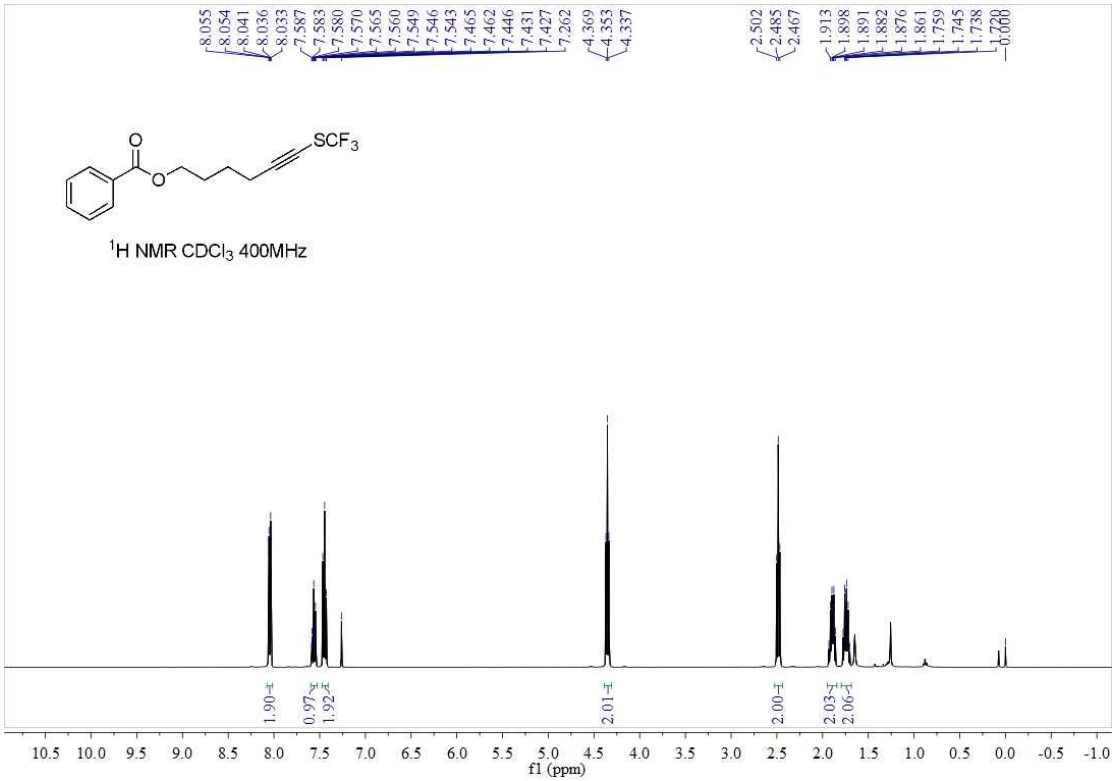

-44.323
SCF3
TBSO
19F NMR CDCl3 376MHz
f1 (ppm)

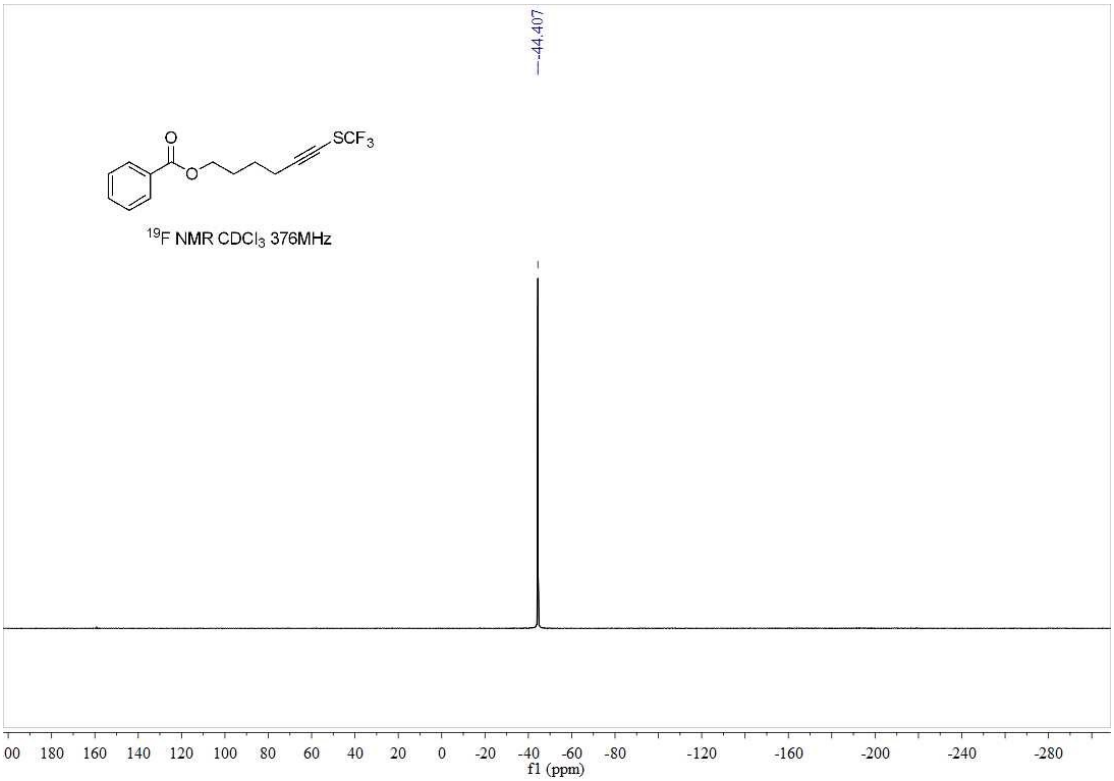

133.134
130.049
126.954
123.855
103.788
77.000
62.441
57.084
57.039
56.990
56.946
31.713
25.907
24.585
19.969
18.305
-5.359
SCF3
TBSO
13C NMR CDCl3 100MHz
f1 (ppm)

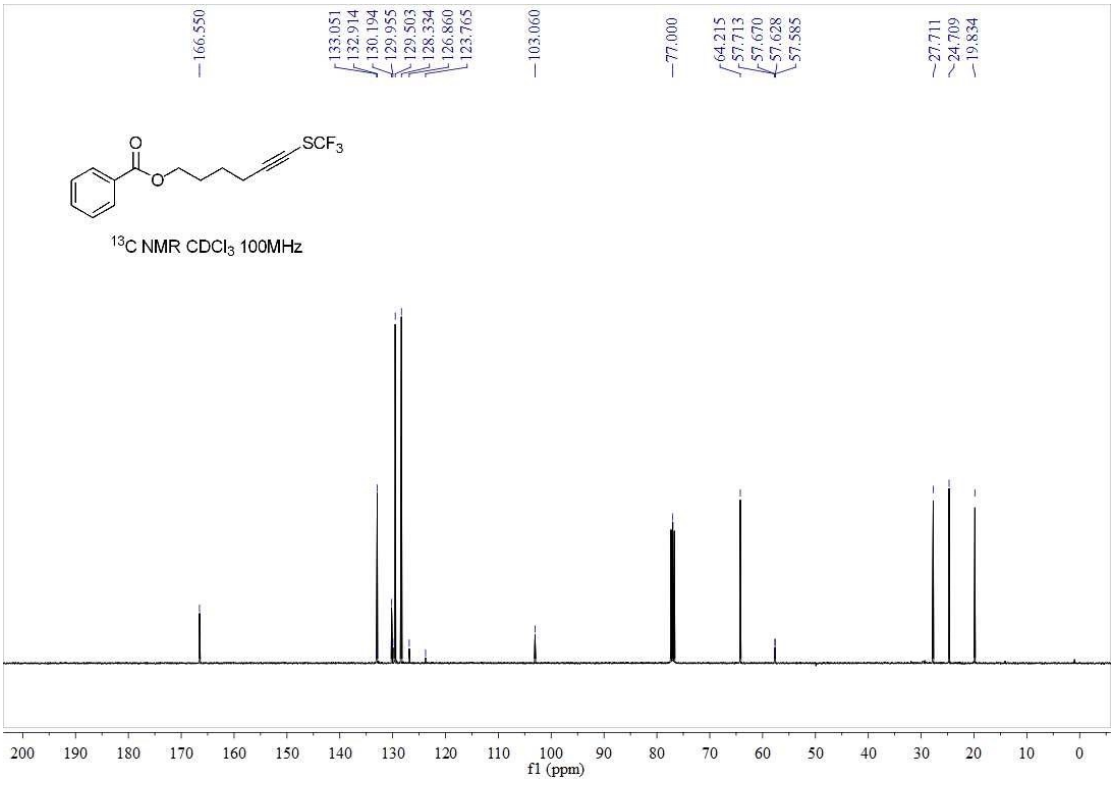

7.368
7.354
7.349
7.348
7.341
7.334
7.324
7.320
7.310
7.302
7.297
7.294
7.287
7.280
7.272
7.265
7.259
4.500
3.509
3.494
3.479
2.424
2.407
2.391
1.719
1.713
1.704
1.701
1.697
1.694
1.688
1.680
1.671
1.664
0.000
SCF3
O
1H NMR CDCl3 400MHz
4.08
1.09
2.00
2.09
1.81
4.22
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

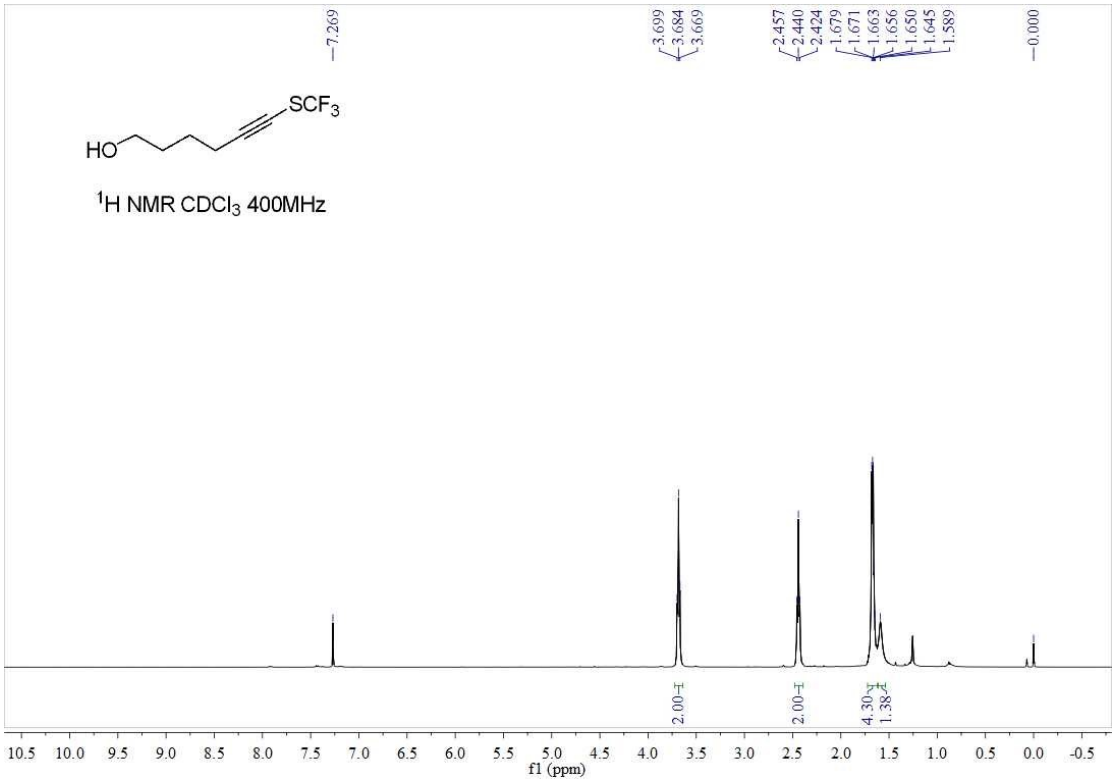

-44.435
SCF3
O
19F NMR CDCl3 376MHz
180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -120 -160 -200 -240 -280
f1 (ppm)

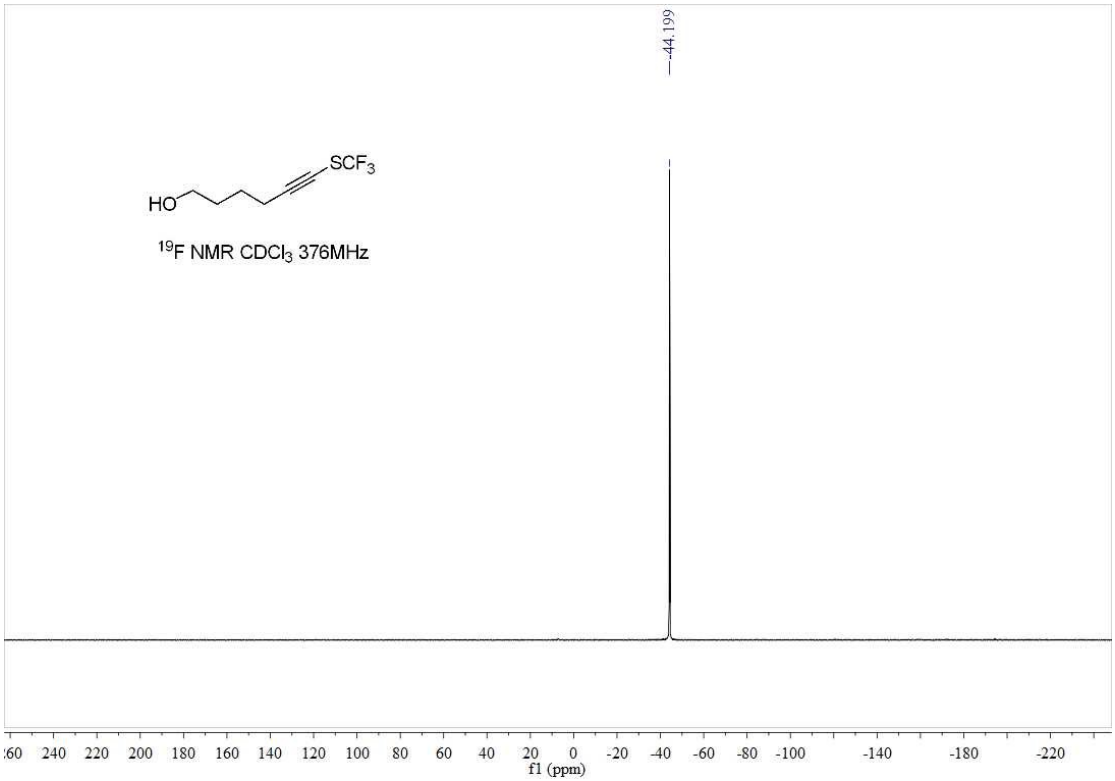

138.444
133.103
130.009
128.353
127.584
127.541
126.915
123.820
103.610
77.000
72.870
69.510
57.224
57.182
57.139
57.099
28.710
24.853
19.942
SCF3
O
13C NMR CDCl3 100MHz
f1 (ppm)

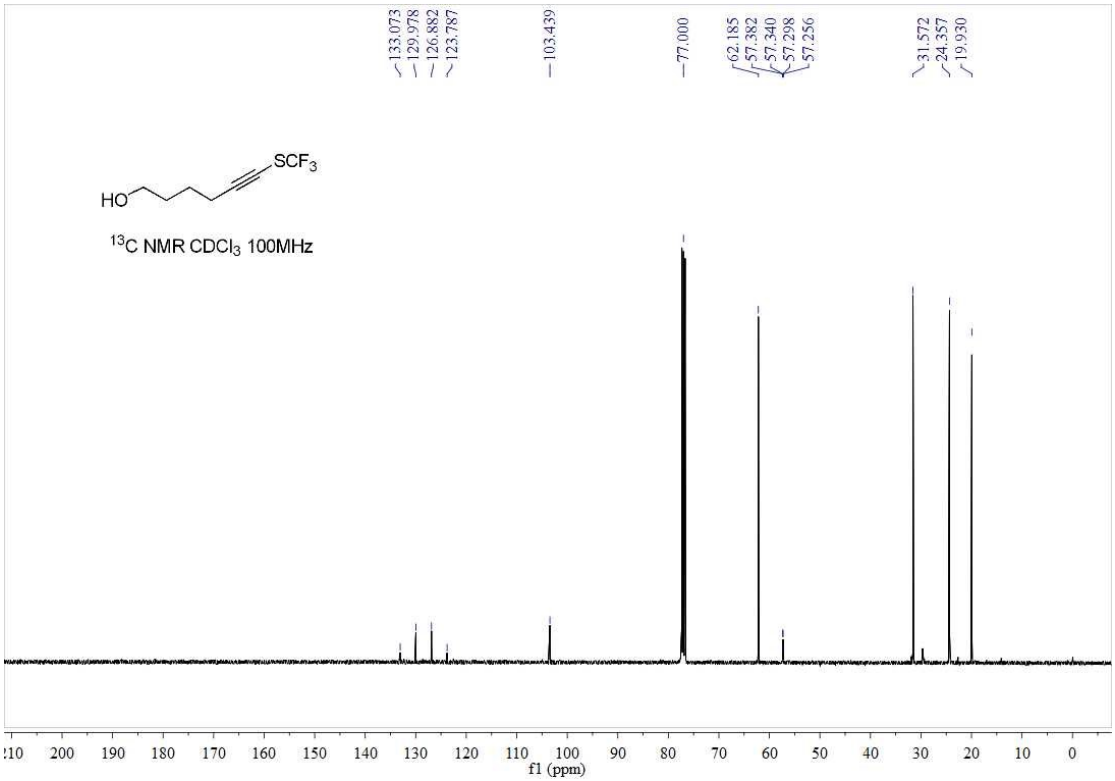

8.055
8.054
8.041
8.036
8.033
7.587
7.583
7.580
7.570
7.565
7.560
7.549
7.546
7.543
7.465
7.462
7.446
7.431
7.427
7.262
4.369
4.353
4.337
2.502
2.485
2.467
1.913
1.898
1.891
1.882
1.876
1.861
1.759
1.745
1.738
1.720
0.000
O
O
SCF3
1H NMR CDCl3 400MHz
1.90
0.97
1.92
2.01
2.00
2.03
2.06
f1 (ppm)

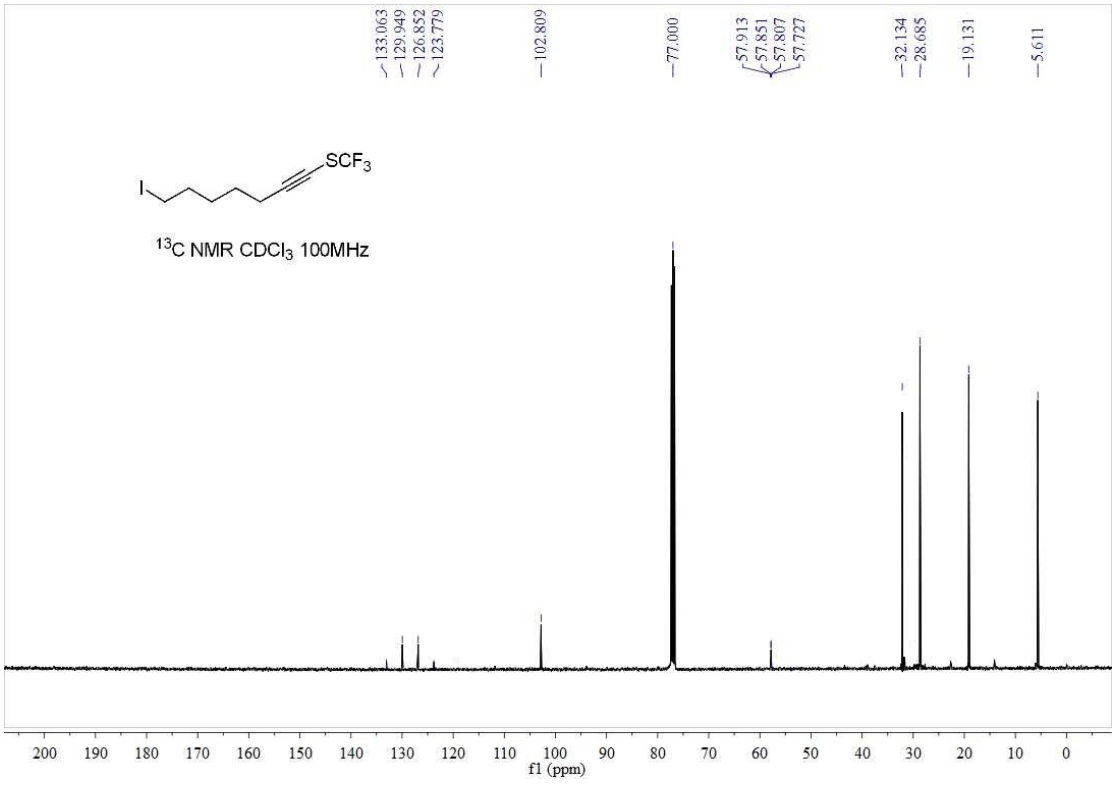

-44.407
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

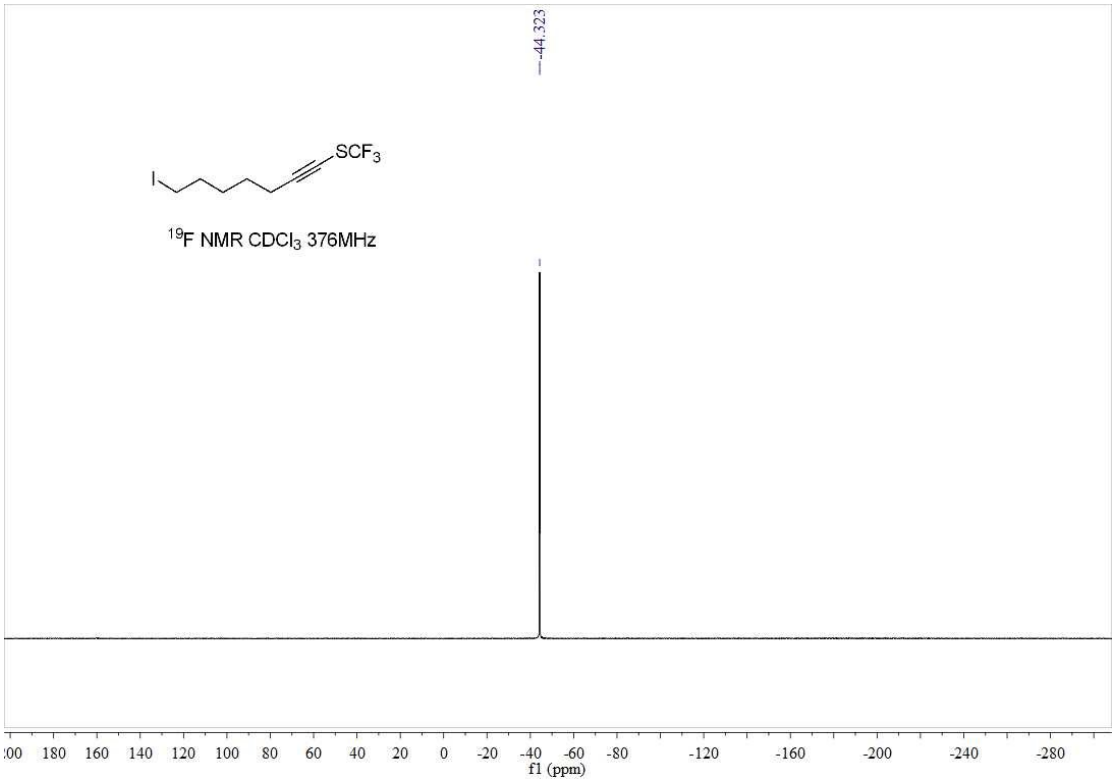

166.550
133.051
132.914
130.194
129.955
129.503
128.334
126.860
123.765
103.060
77.000
64.215
57.713
57.670
57.628
57.585
27.711
24.709
19.834
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

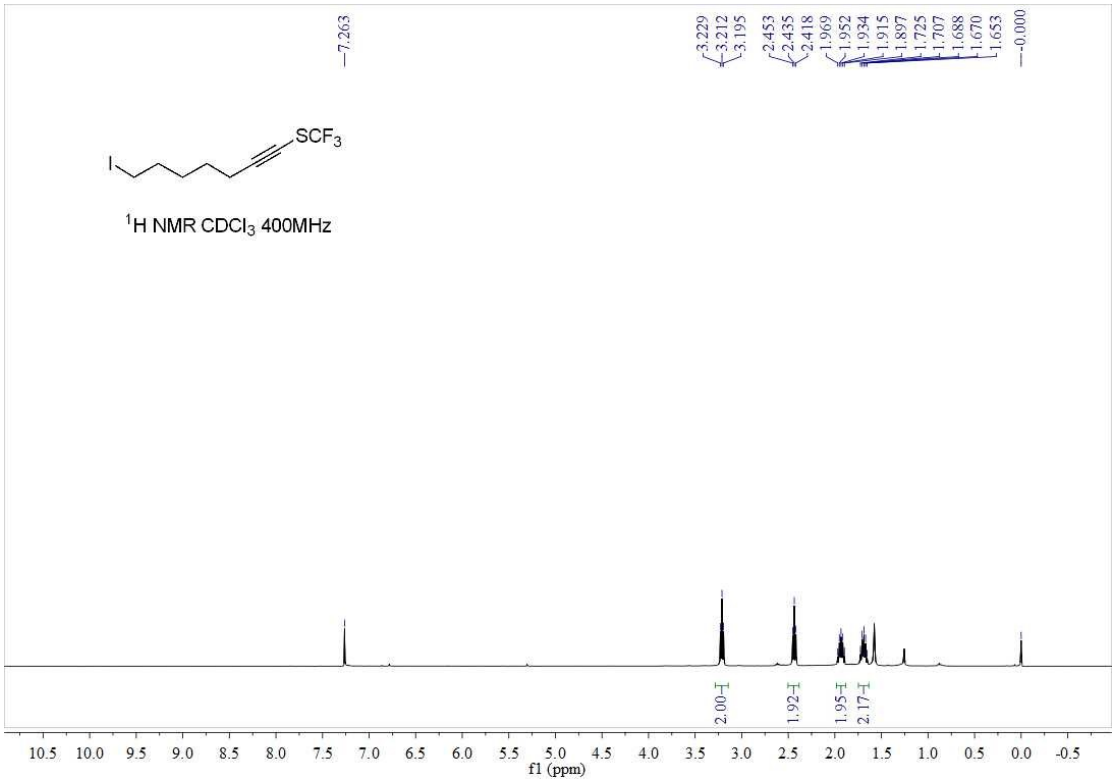

7.269
3.699
3.684
3.669
2.457
2.440
2.424
1.679
1.671
1.663
1.656
1.650
1.645
1.589
0.000
SCF3
HO
1H NMR CDCl3 400MHz
2.00
2.00
4.30
1.38
f1 (ppm)

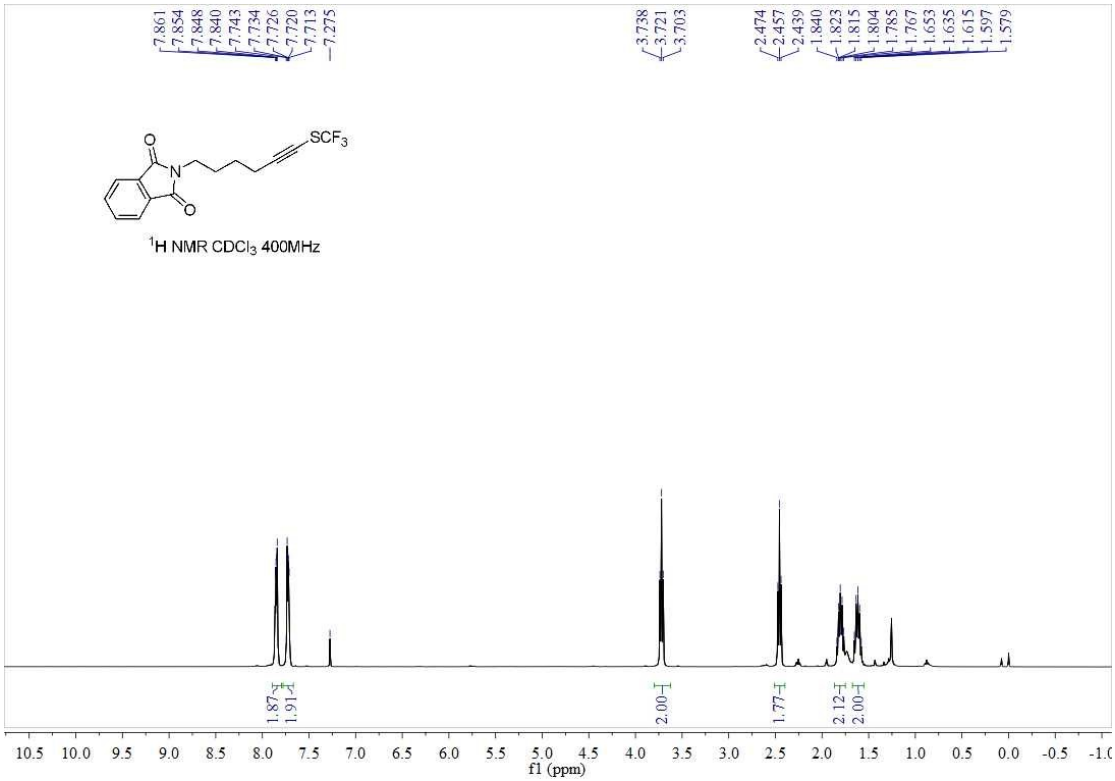

-44.199
SCF3
HO
19F NMR CDCl3 376MHz
f1 (ppm)

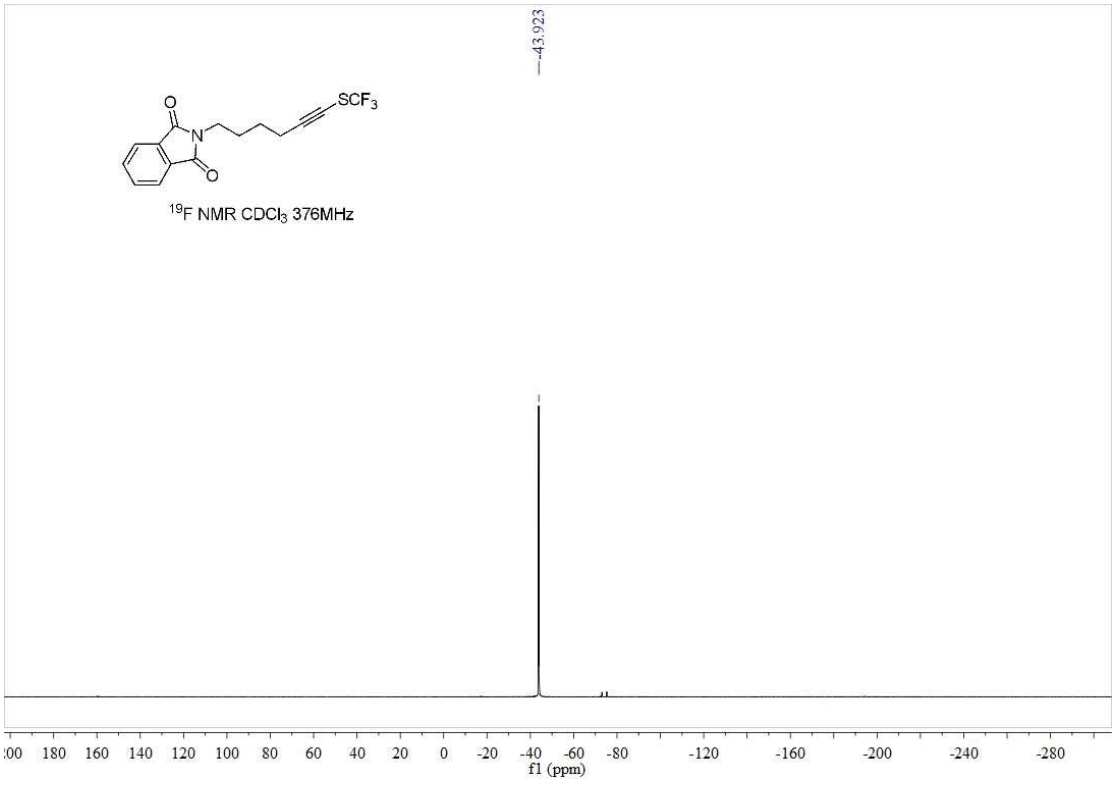

133.073
129.978
126.882
123.787
103.439
77.000
62.185
57.382
57.340
57.298
57.256
31.572
24.357
19.930
SCF3
HO
13C NMR CDCl3 100MHz
f1 (ppm)

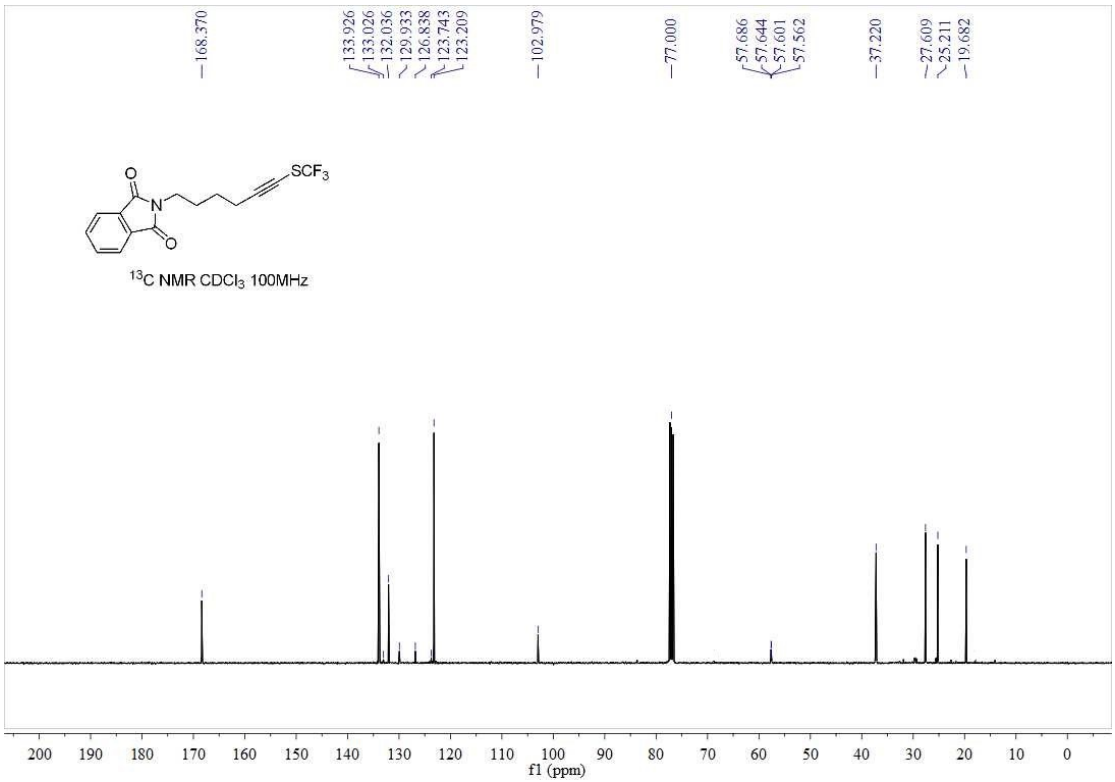

133.063
129.949
126.852
123.779
102.809
77.000
57.913
57.851
57.807
57.727
32.134
28.685
19.131
5.611
SCF3
I
13C NMR CDCl3 100MHz
f1 (ppm)

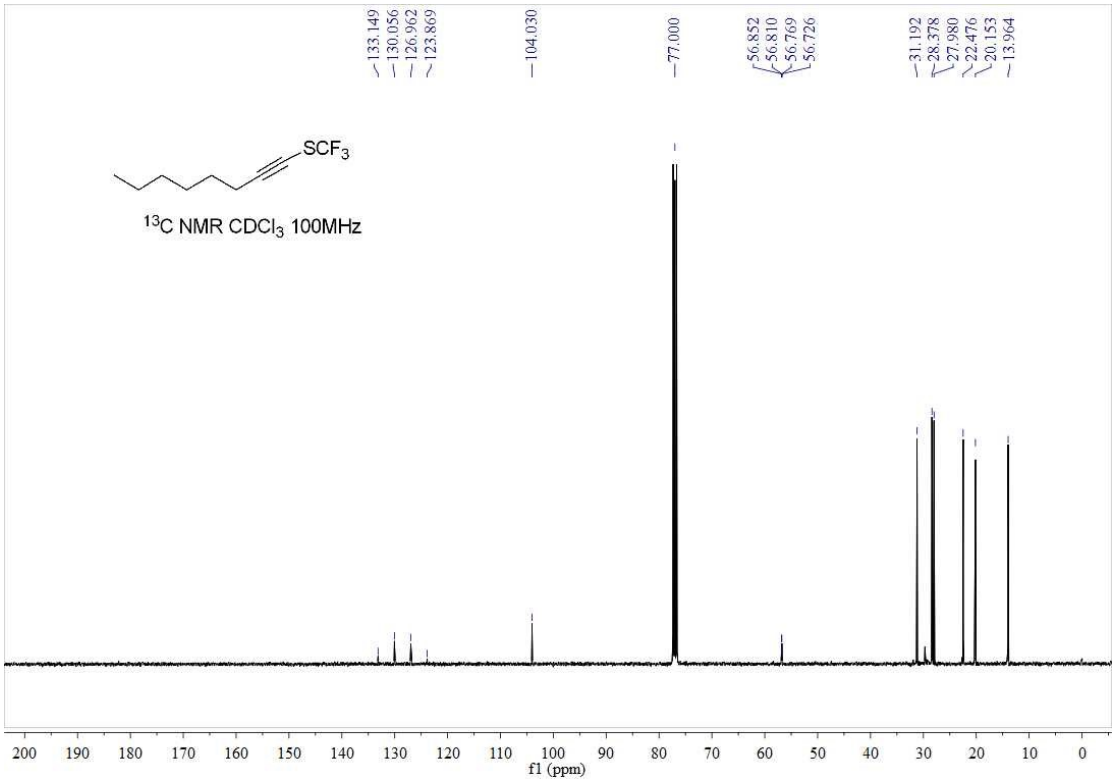

-44.323
SCF3
I
19F NMR CDCl3 376MHz
f1 (ppm)

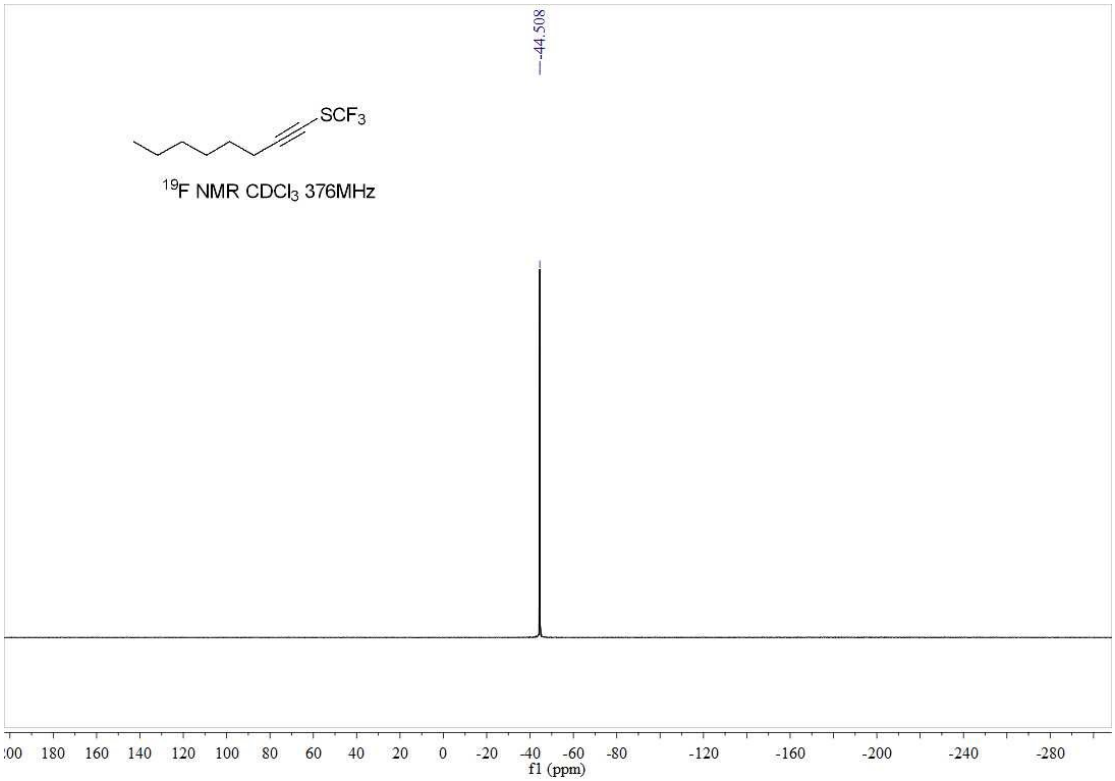

7.263
3.229
3.212
3.195
2.453
2.435
2.418
1.969
1.952
1.934
1.915
1.897
1.725
1.707
1.688
1.670
1.653
0.000
SCF3
I
1H NMR CDCl3 400MHz
2.00
1.92
1.95
2.17
f1 (ppm)

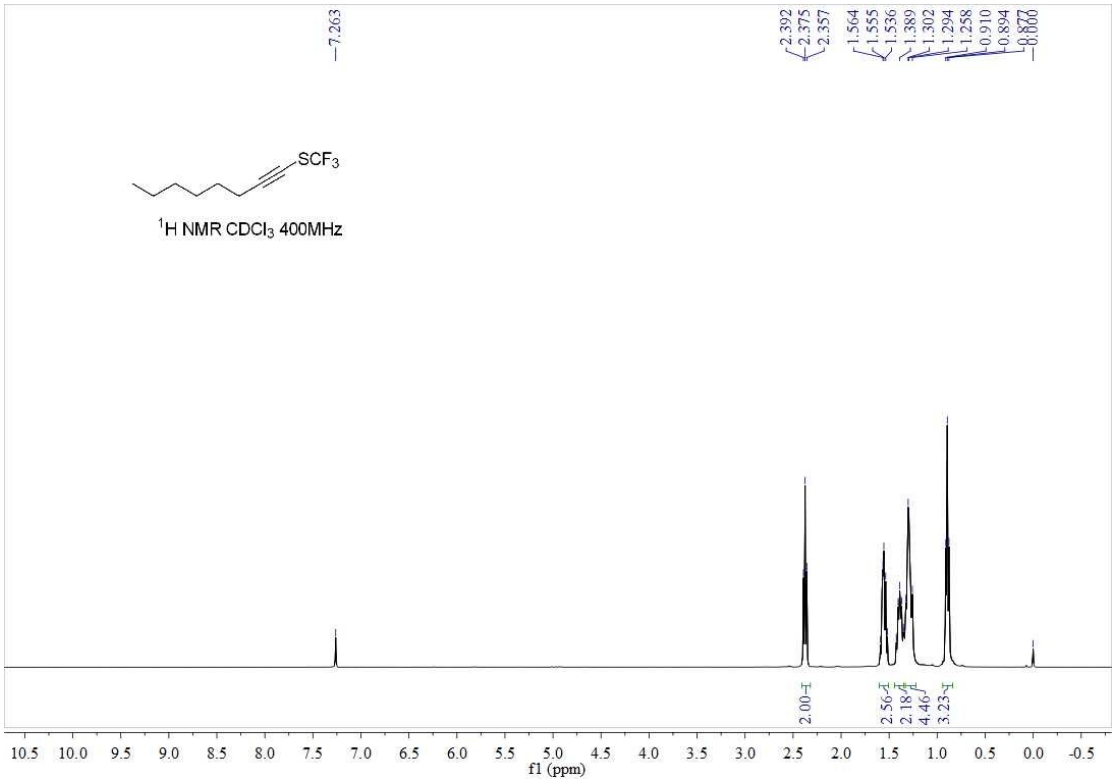

7.861
7.854
7.848
7.840
7.743
7.734
7.726
7.720
7.713
7.275
3.738
3.721
3.703
2.474
2.457
2.439
1.840
1.823
1.815
1.804
1.785
1.767
1.653
1.635
1.615
1.597
1.579
SCF3
O
N
O
1H NMR CDCl3 400MHz
1.87
1.91
2.00
1.77
2.12
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

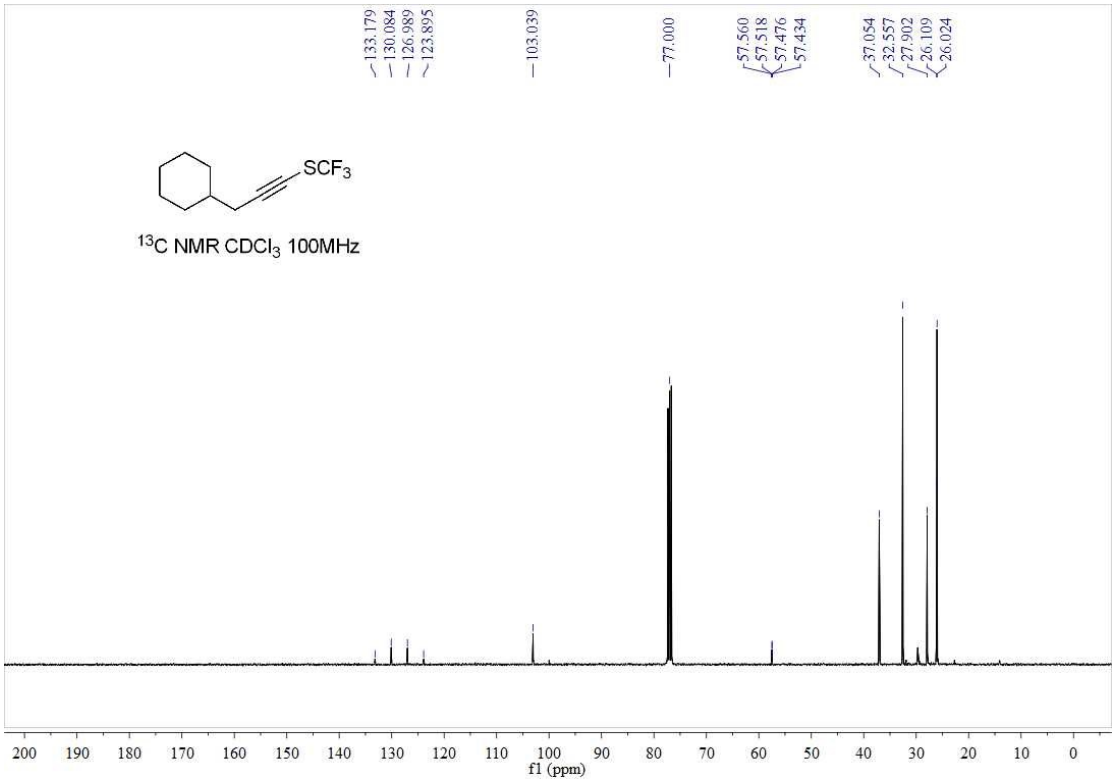

-43.923
SCF3
O
N
O
19F NMR CDCl3 376MHz
200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -120 -160 -200 -240 -280
f1 (ppm)

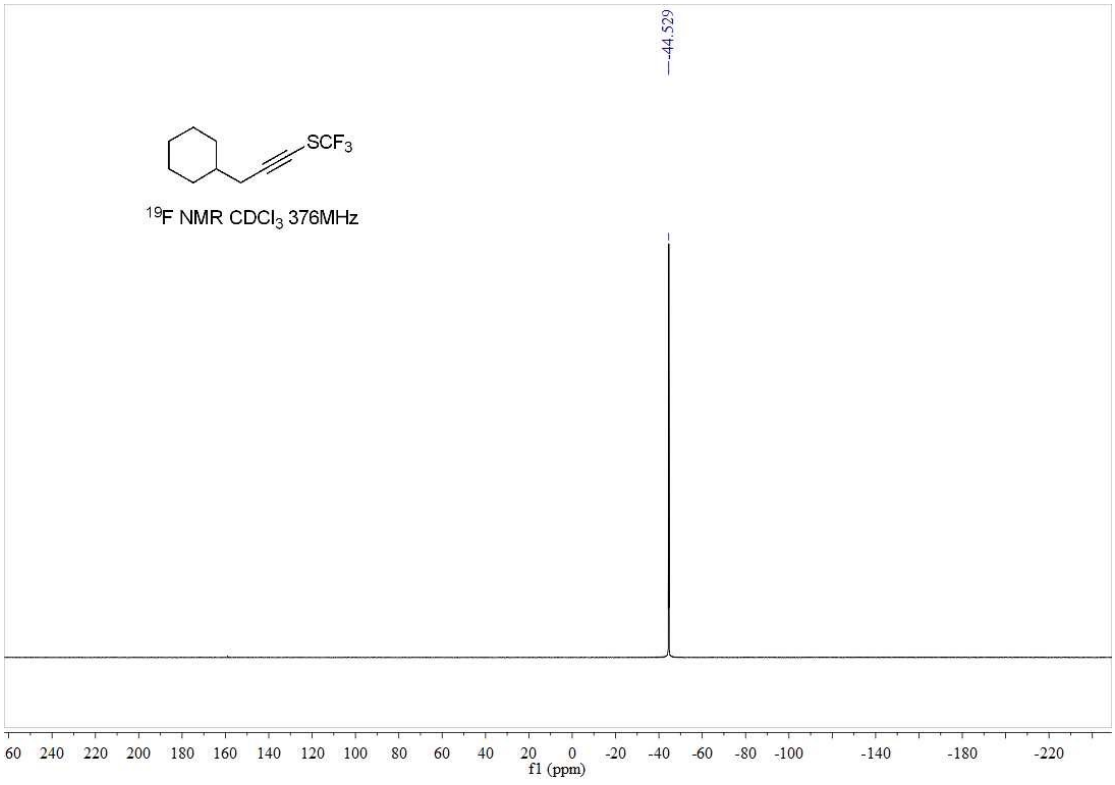

168.370
133.926
133.026
132.036
129.933
126.838
123.743
123.209
102.979
77.000
57.686
57.644
57.601
57.562
37.220
27.609
25.211
19.682
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

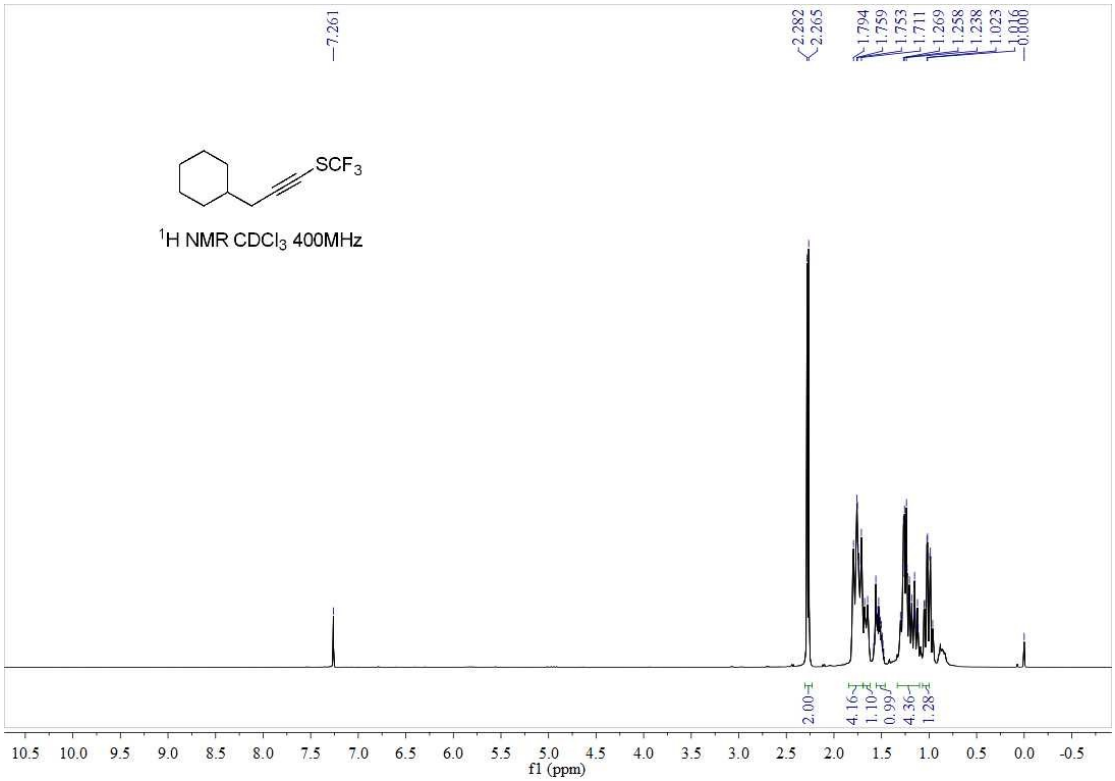

133.149
130.056
126.962
123.869
104.030
77.000
56.852
56.810
56.769
56.726
31.192
28.378
27.980
22.476
20.153
13.964
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

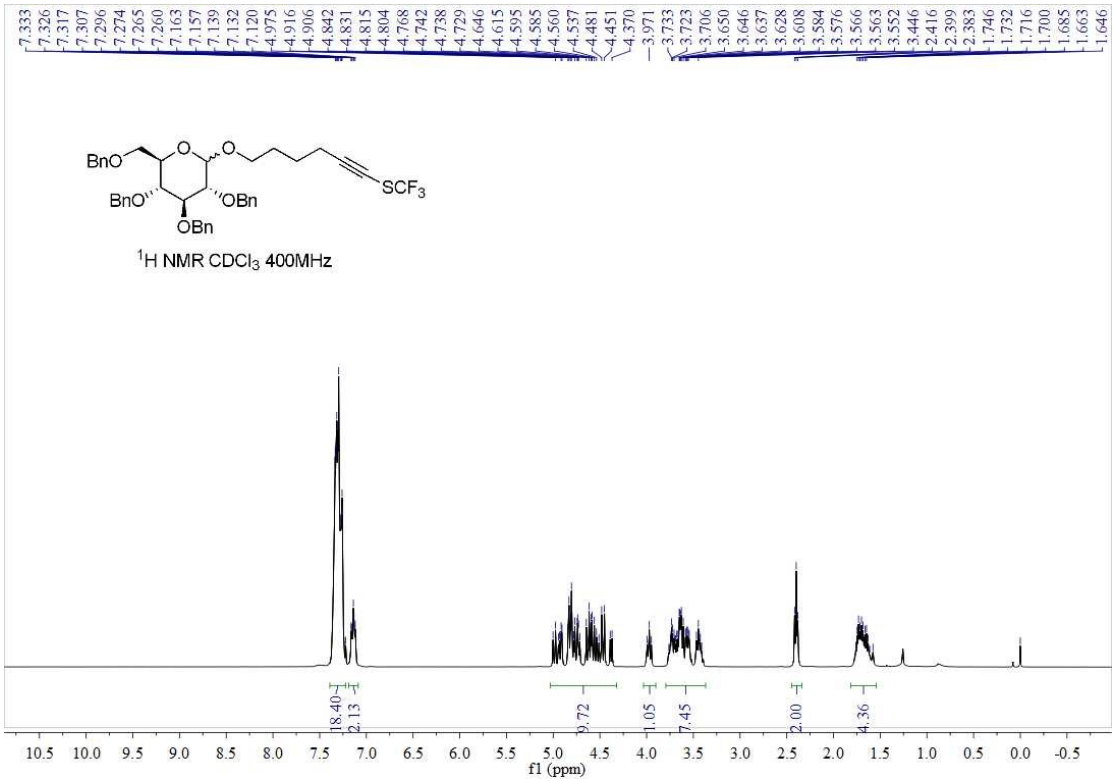

-44.508
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

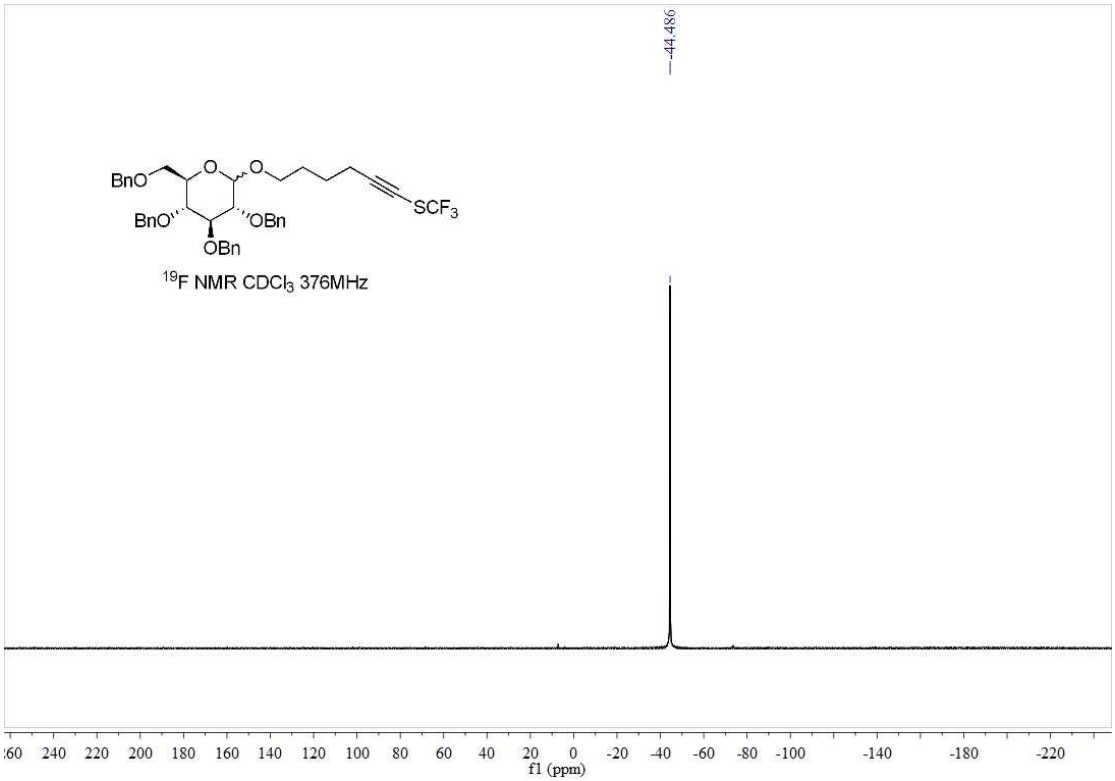

7.263
2.392
2.375
2.357
1.564
1.555
1.536
1.389
1.302
1.294
1.258
0.910
0.894
0.877
0.860
SCF3
1H NMR CDCl3 400MHz
2.00
2.56
2.18
4.46
3.23
f1 (ppm)

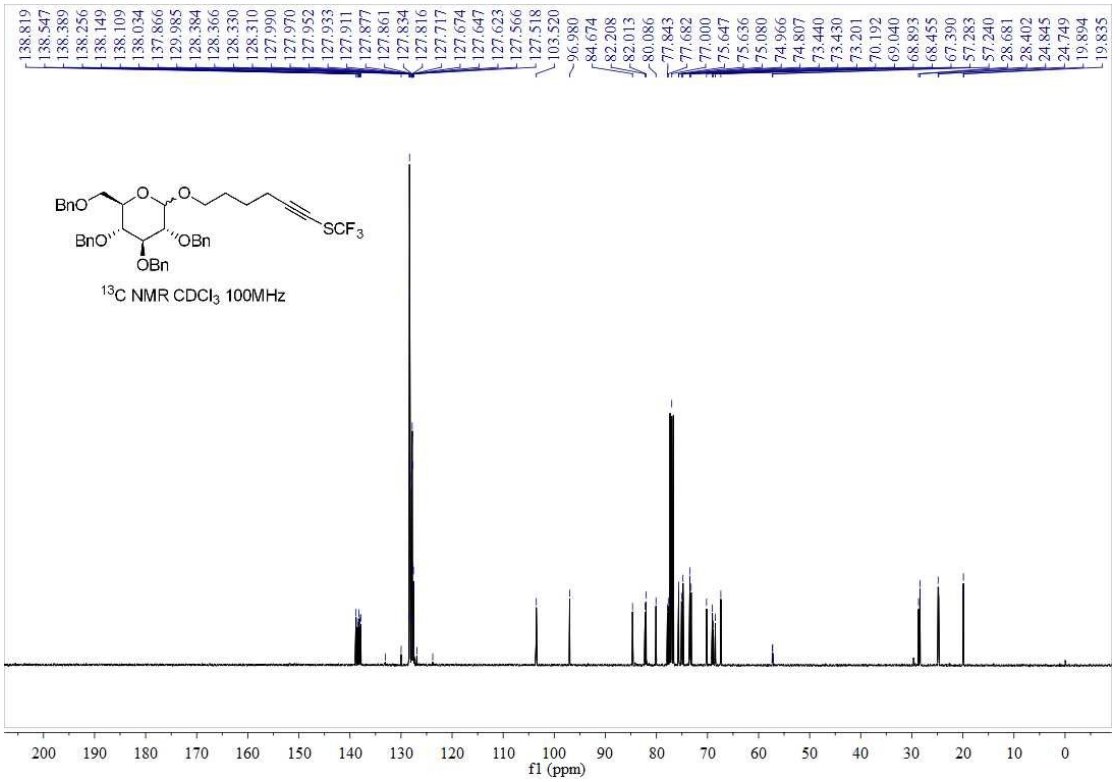

133.179
130.084
126.989
123.895
103.039
77.000
57.560
57.518
57.476
57.434
37.054
32.557
27.902
26.109
26.024
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

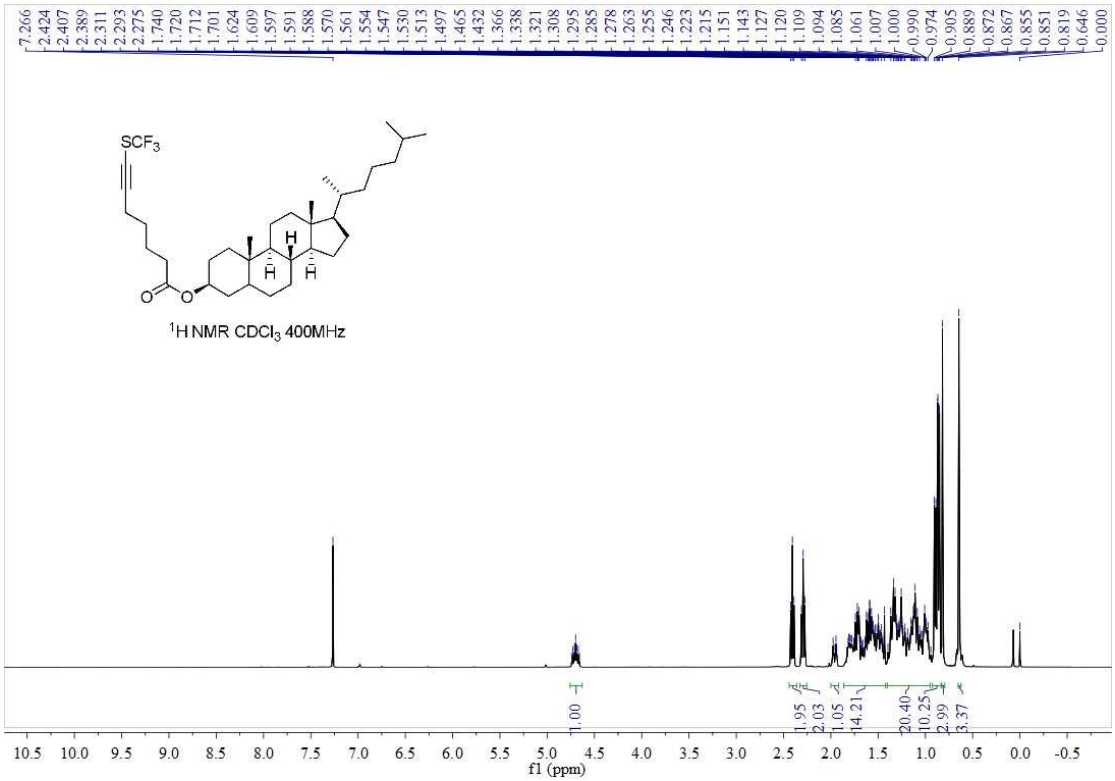

-44.529
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

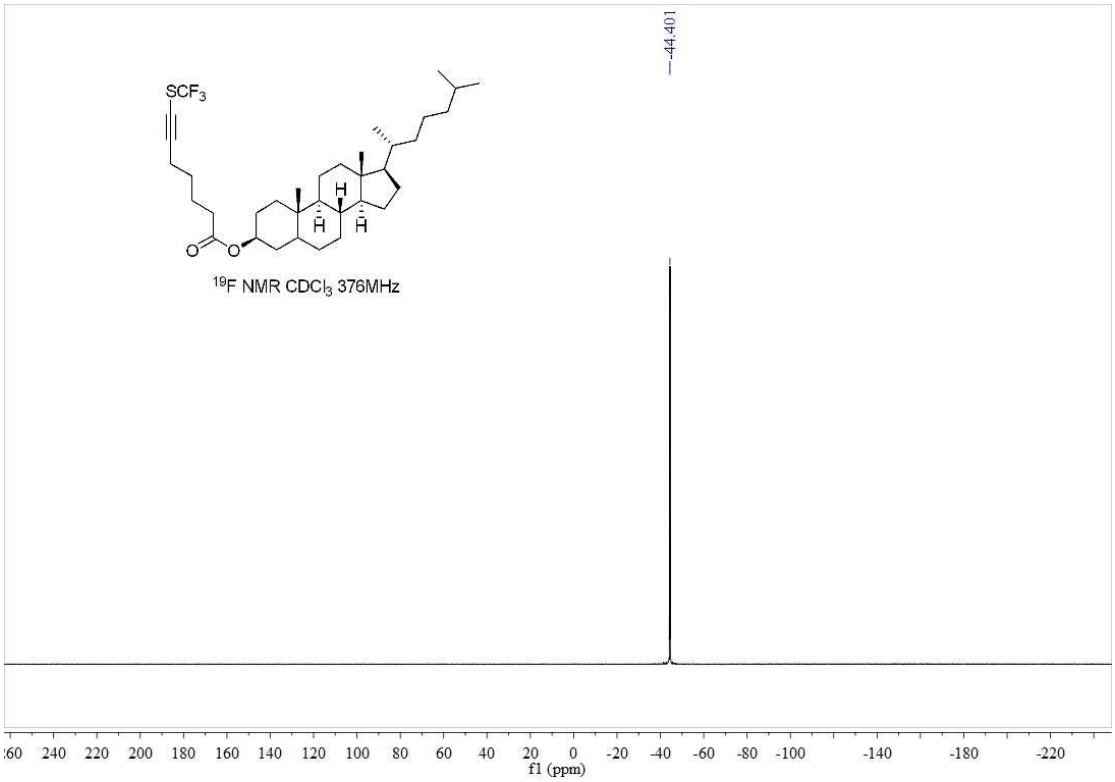

SCF3
1H NMR CDCl3 400MHz
f1 (ppm)

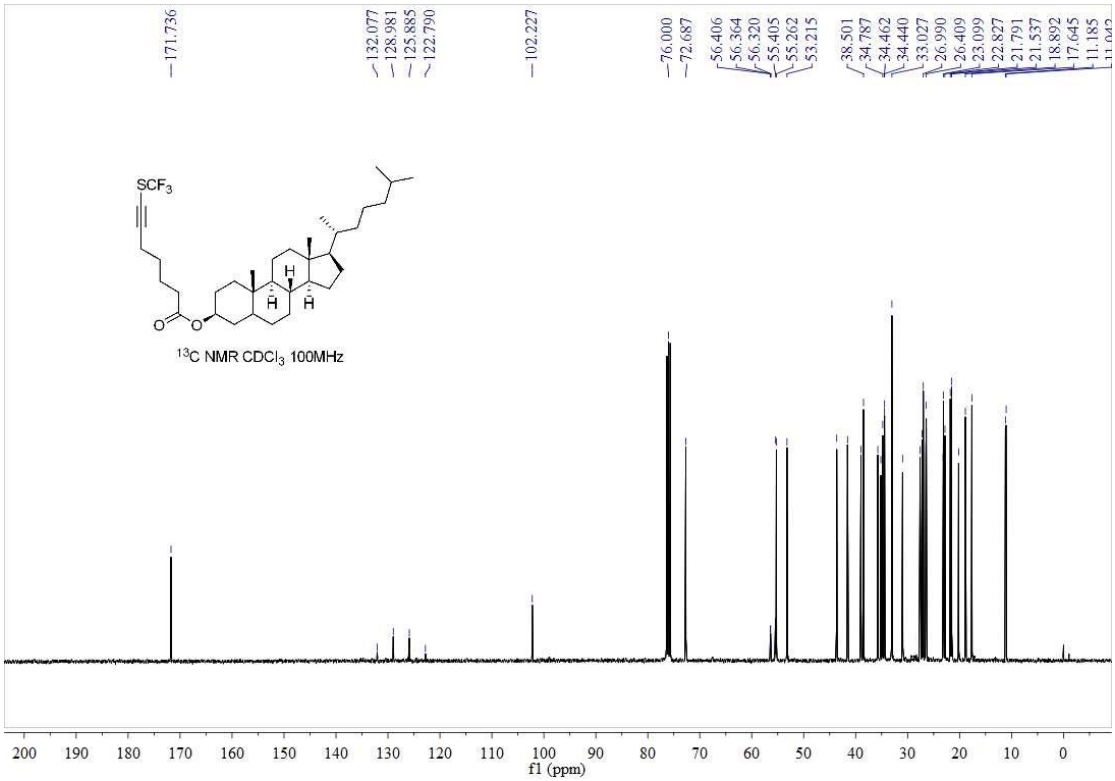

BnO
BnO
OBn
OBn
O
O
SCF3
1H NMR CDCl3 400MHz
f1 (ppm)

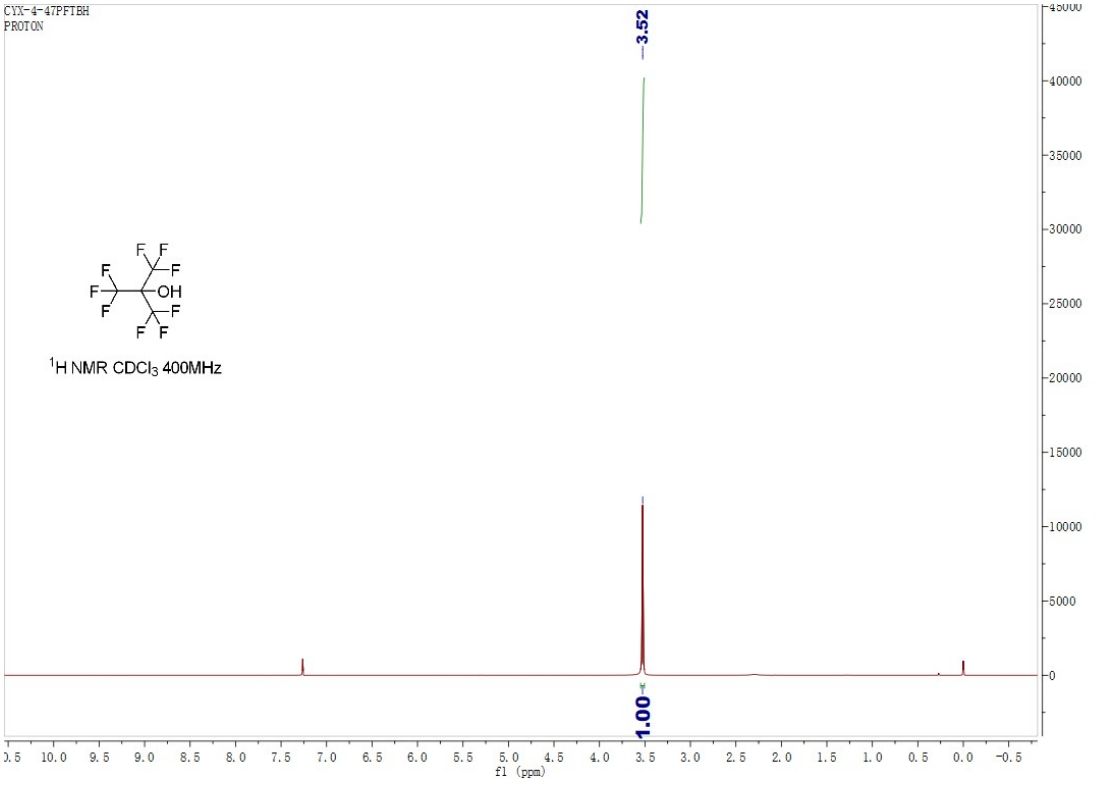

-44.486
BnO
BnO
OBn
OBn
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

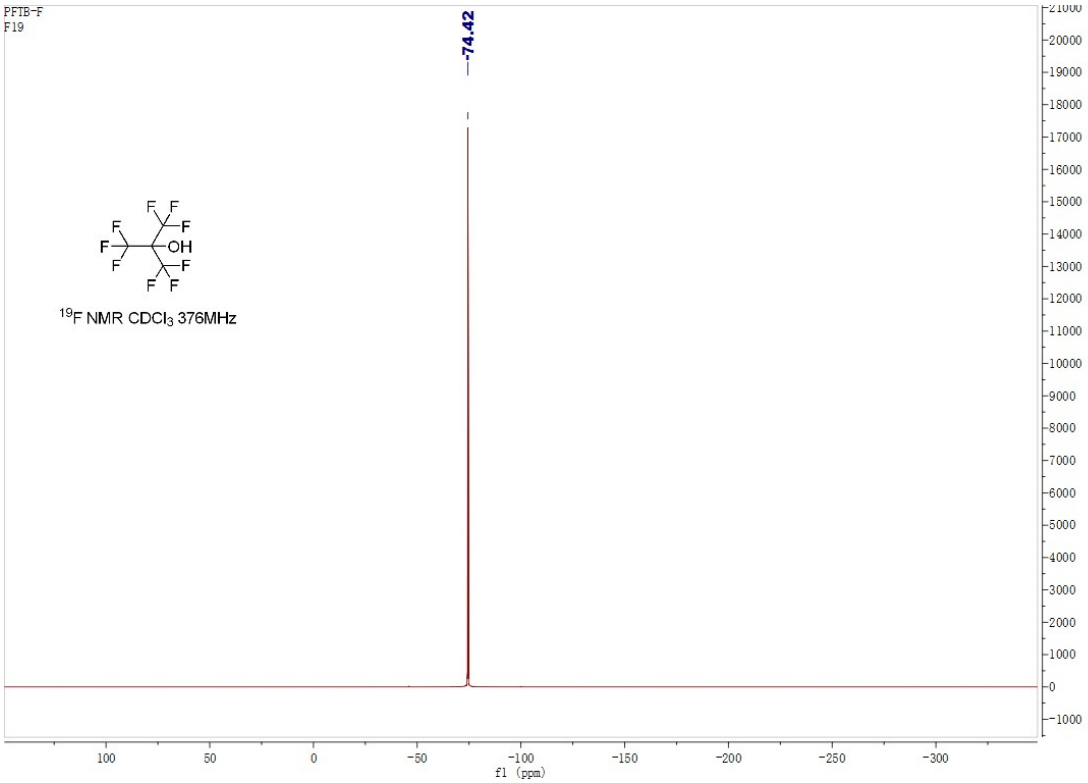

138.819
138.547
138.389
138.256
138.149
138.109
138.034
137.866
129.985
128.384
128.366
128.330
128.310
127.990
127.970
127.952
127.933
127.911
127.877
127.861
127.834
127.816
127.717
127.674
127.647
127.623
127.566
127.518
103.520
96.980
84.674
82.208
82.013
80.086
77.843
77.682
77.000
75.647
75.636
75.080
74.966
74.807
73.440
73.430
73.201
70.192
69.040
68.893
68.455
67.390
57.283
57.240
28.681
28.402
24.845
24.749
19.894
19.835
BnO
BnO
OBn
OBn
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

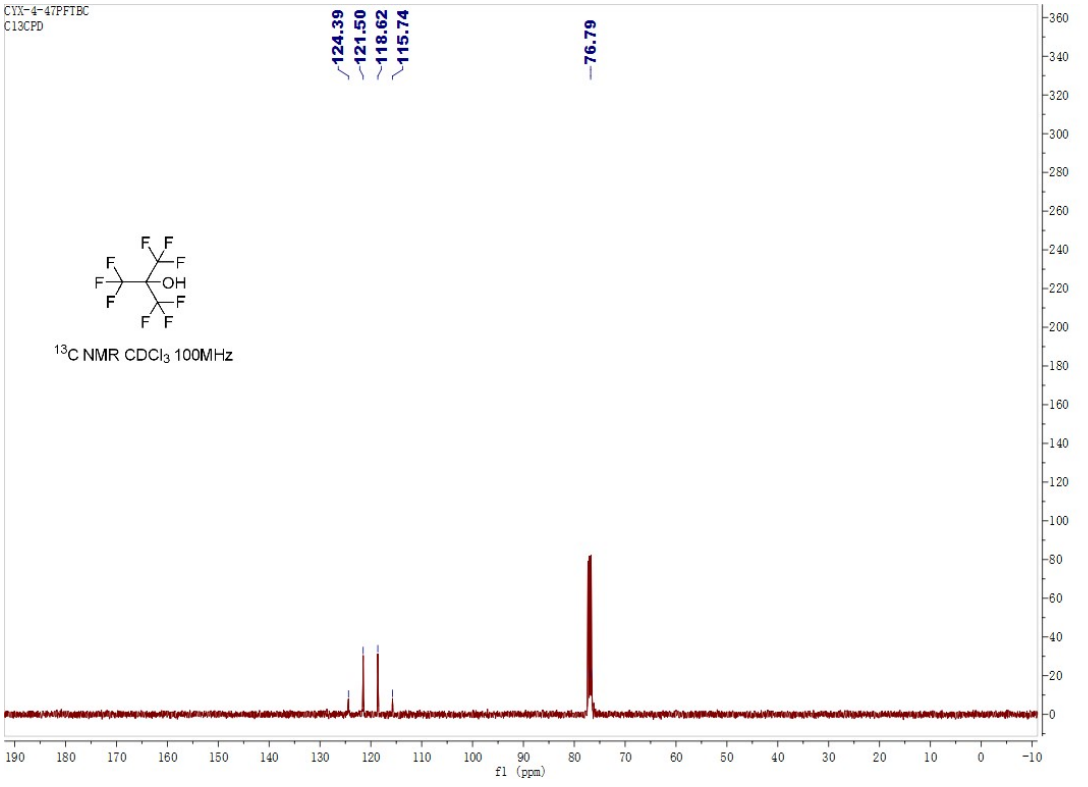

SCF3
1H NMR CDCl3 400MHz
f1 (ppm)

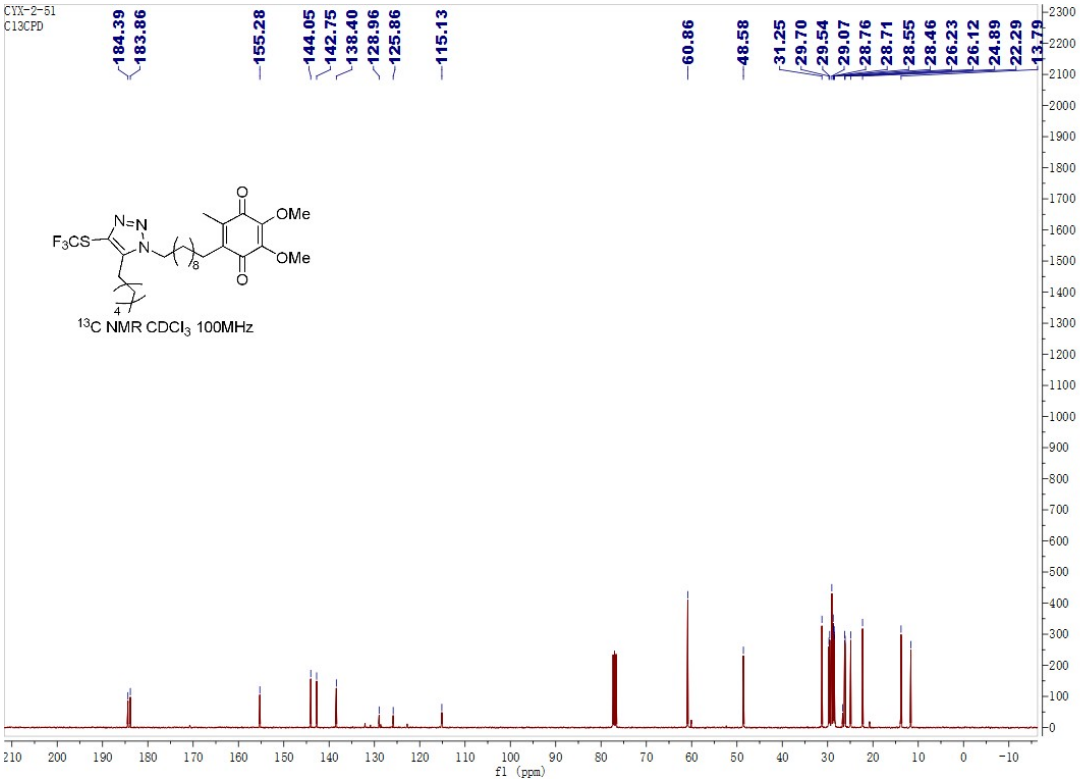

-44.401
SCF3
19F NMR CDCl3 376MHz
f1 (ppm)

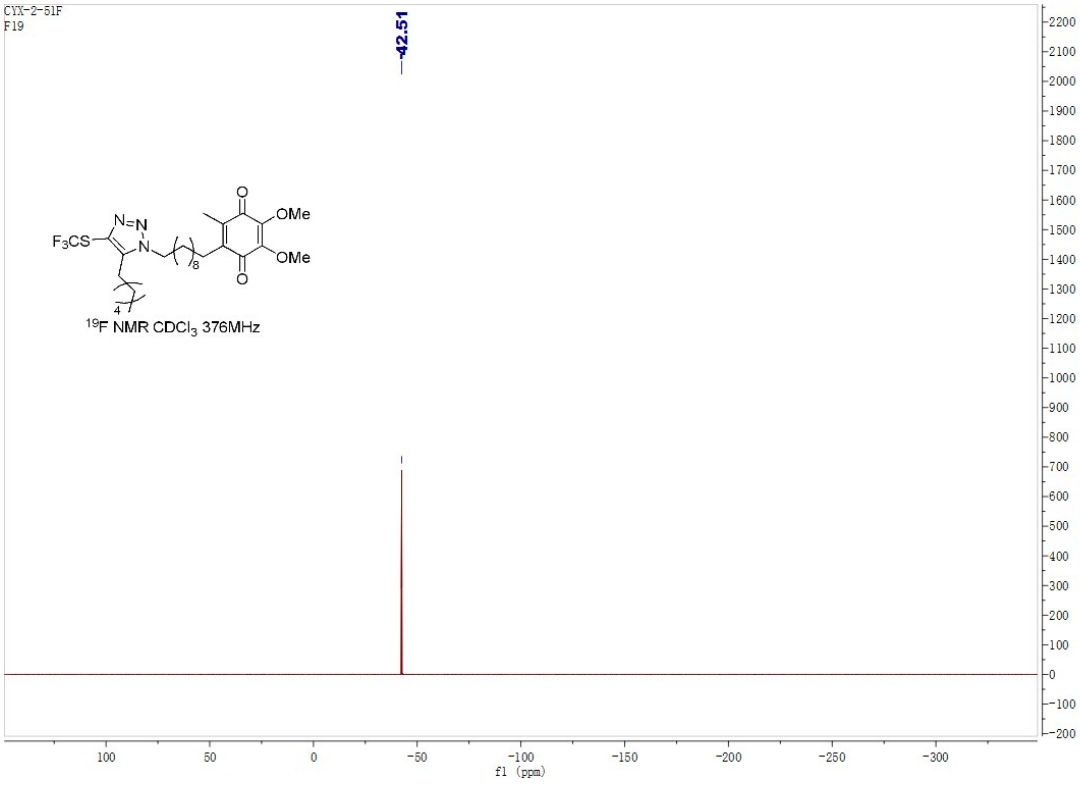

171.736
132.077
128.981
125.885
122.790
102.227
76.000
72.687
56.406
56.364
56.320
55.405
55.262
53.215
38.501
34.787
34.462
34.440
33.027
26.990
26.409
23.099
22.827
21.791
21.537
18.892
17.645
11.185
SCF3
13C NMR CDCl3 100MHz
f1 (ppm)

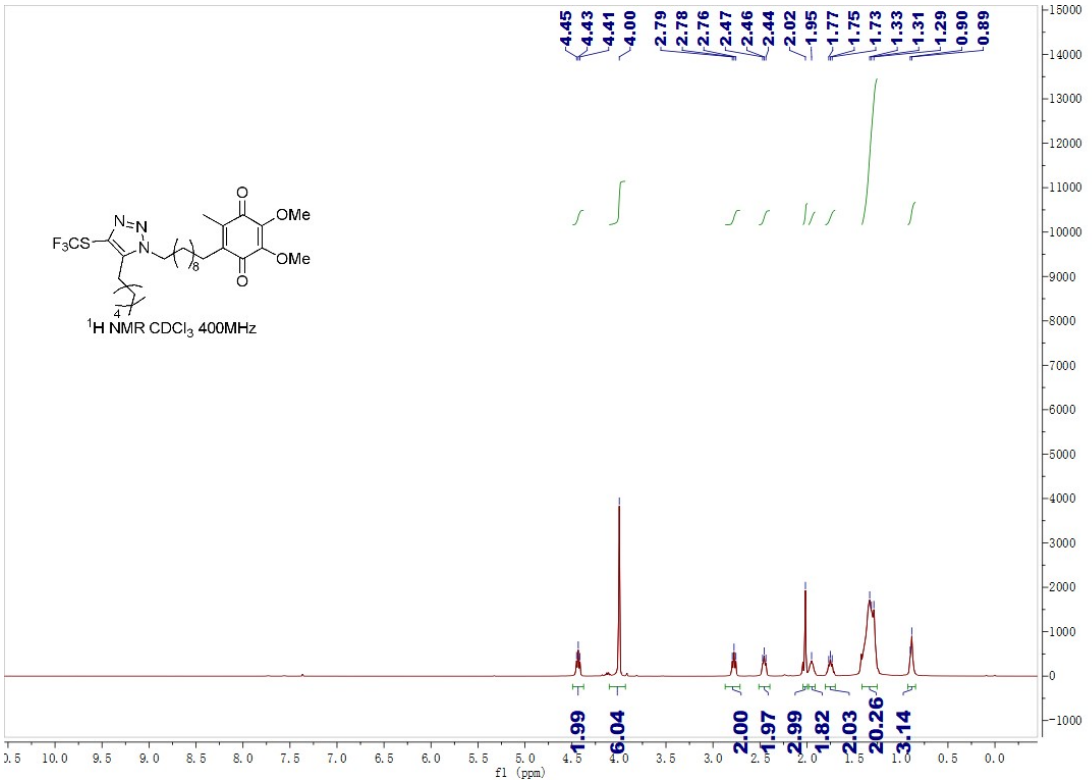

CYX-4-47PFTEH
PROTON
3.52
1.00
OH
1H NMR CDCl3 400MHz
f1 (ppm)

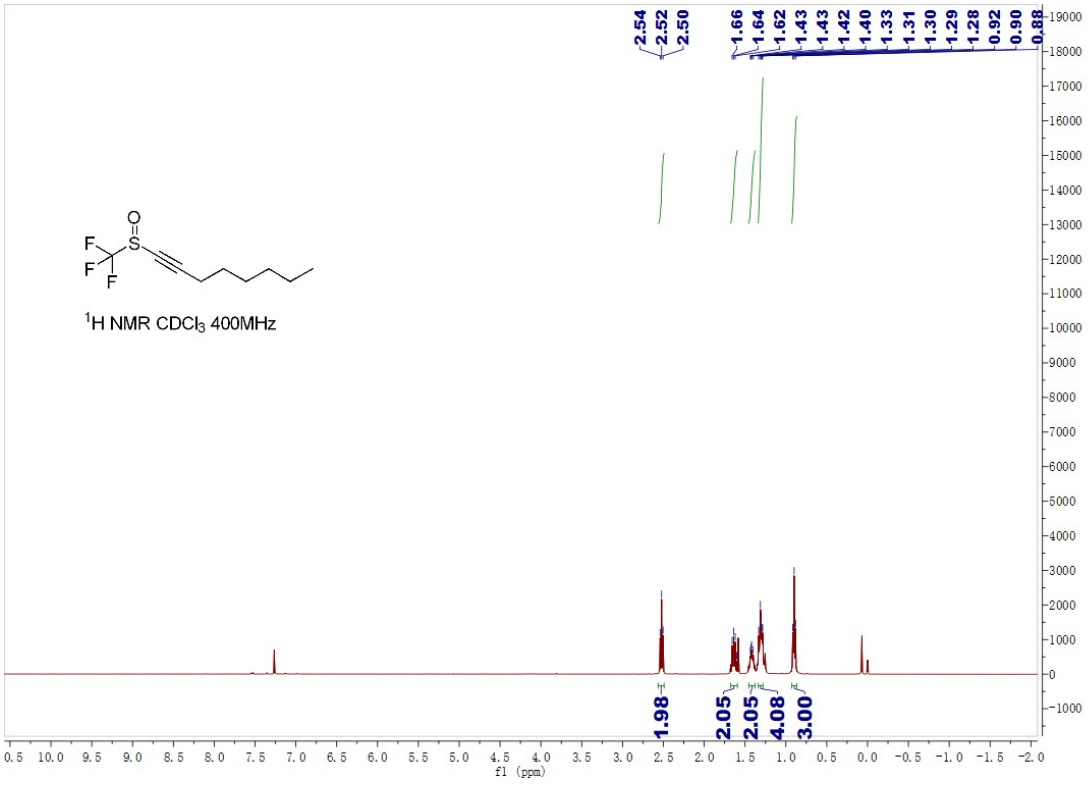

PFTB-F
F19
-74.42
^{19}F NMR $CDCl_3$ 376MHz
f1 (ppm)

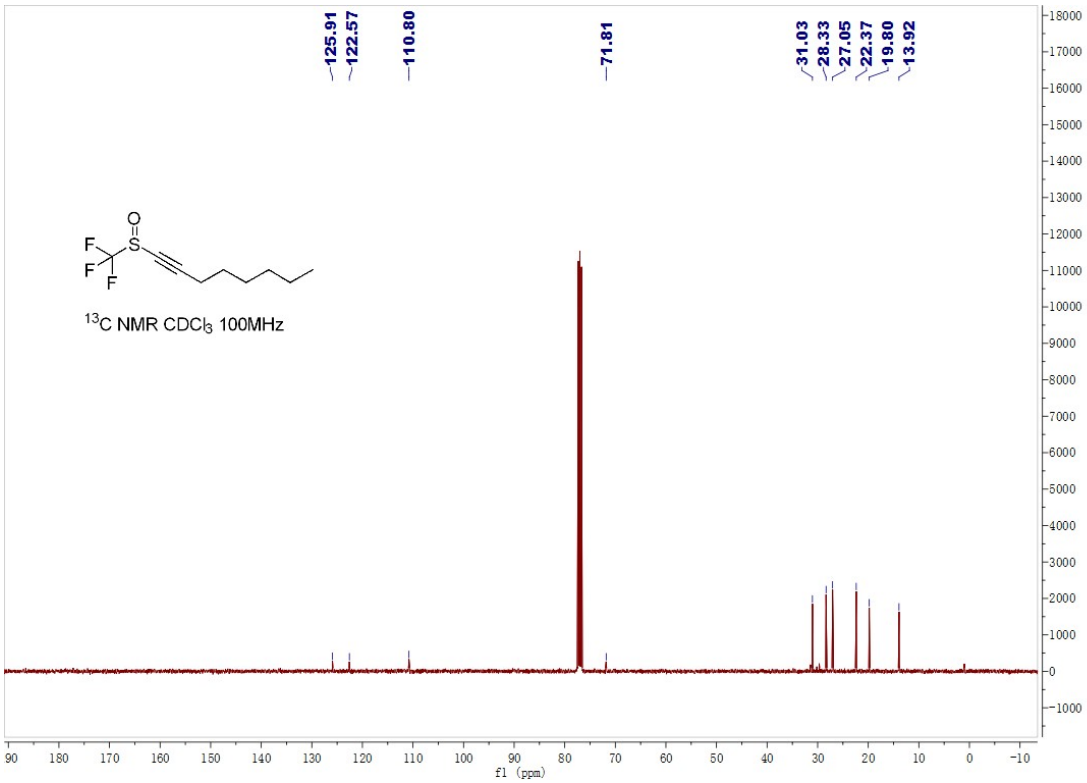

CYX-4-47PFTBC
C13CPD
124.39
121.50
118.62
115.74
76.79
^{13}C NMR $CDCl_3$ 100MHz
f1 (ppm)

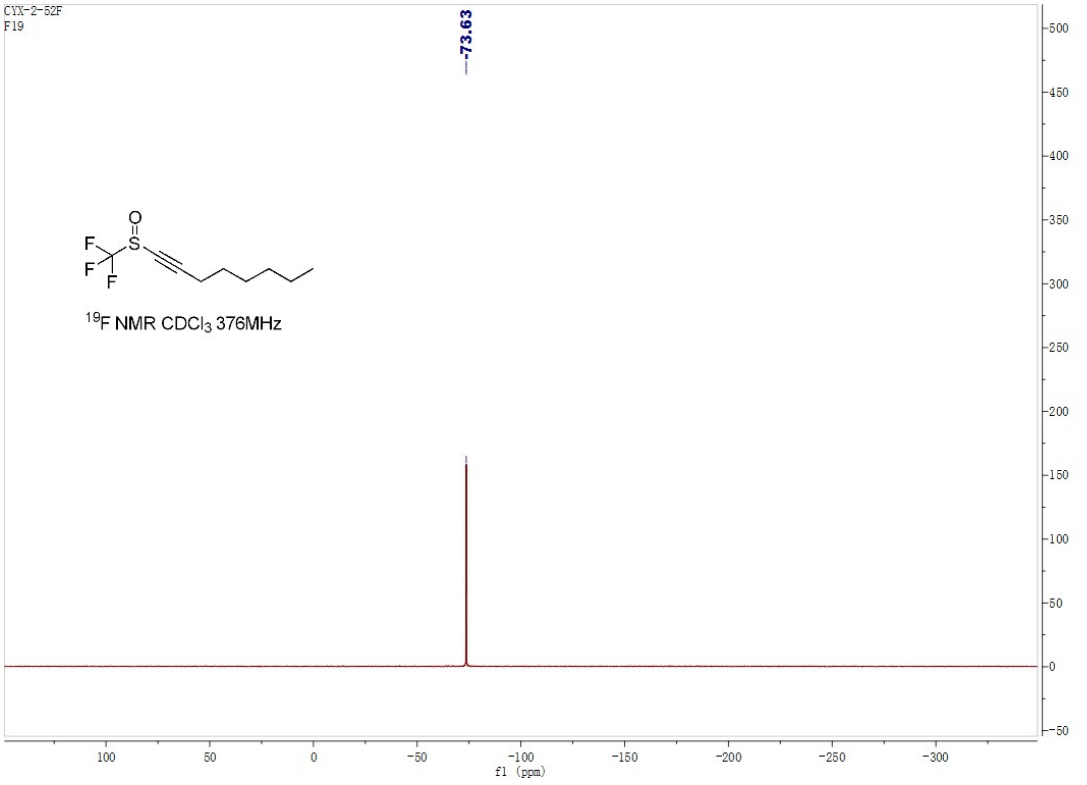

CYX-2-51
C13CPD
184.39
183.86
155.28
144.05
142.75
138.40
128.96
125.86
115.13
60.86
48.58
31.25
29.70
29.54
29.07
28.76
28.71
28.55
28.46
26.23
26.12
24.89
22.29
13.79
OMe
OMe
F3CS
N=N
8
4
13C NMR CDCl3 100MHz
f1 (ppm)


CYX-2-51F
F19
-42.51
OMe
OMe
F3CS
N=N
8
4
19F NMR CDCl3 376MHz
f1 (ppm)


4.45
4.43
4.41
4.00
2.79
2.78
2.76
2.47
2.46
2.44
2.02
1.95
1.77
1.75
1.73
1.33
1.31
1.29
0.90
0.89
OMe
OMe
F3CS
1H NMR CDCl3 400MHz
1.99
6.04
2.00
1.97
2.99
1.82
2.03
20.26
3.14
f1 (ppm)


2.54
2.52
2.50
1.66
1.64
1.62
1.43
1.43
1.42
1.40
1.33
1.31
1.30
1.29
1.28
0.92
0.90
0.88
F
F
F
O
S
1H NMR CDCl3 400MHz
1.98
2.05
2.05
4.08
3.00
f1 (ppm)


125.91
122.57
110.80
71.81
31.03
28.33
27.05
22.37
19.80
13.92
F
F
F
O
S
13C NMR CDCl3 100MHz
f1 (ppm)


CYX-2-52F
F19
-73.63
F
F
F
O
S
19F NMR CDCl3 376MHz
f1 (ppm)