

Supporting Information

Dual Gold and Photoredox Catalysis: Visible Light-Mediated Intermolecular Atom Transfer Thiosulfonylation of Alkenes

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General information

Unless otherwise noted, all the reagents were obtained commercially and used without further purification and reactions were monitored by TLC. Solvents used directly. All NMR spectra were recorded on Bruker-400 MHz spectrometer and Bruker-400 MHz spectrometer. HRMS were measured on the Q-TOF6510 instruments. The light source for the reaction is 100W 400nm blue LED and the total light intensity irradiated on the reaction vial was measured using a light intensity meter (model CEL-NP2000-10; Au light, China) and the value is ca. 120 mW/ cm². Thermo Scientific Lumina Fluorescence Instrument was used for Emission Quenching Experiments. In the transient absorption spectra measurements, excitation was provided by using an Nd:YAG laser and the detector was a xenon lamp on the Edingburge LP920 apparatus from Analytical Instruments.

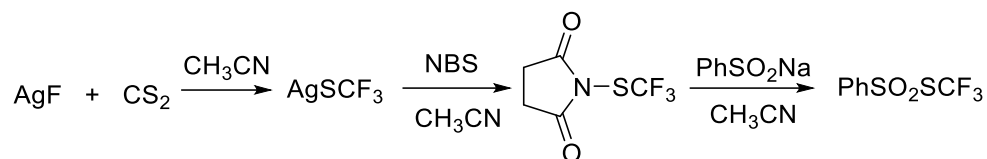
Synthesis of the starting materials

- 1) But-3-en-1-yn-1-ylbenzene **1m** was prepared according to reported procedures¹.

Typical procedure for the preparation of 4-Bromo- β -methylstyrene **1p**.

Ethyltriphenylphosphonium bromide (3.7g, 10mmol) was dissolved in 50mL anhydrous THF under N₂ atmosphere and the suspension was cooled to -78 °C. *n*-BuLi (2.5M in hexanes, 4.4mL, 11mmol) was added to the reaction mixture slowly and the mixture was stirred at 0 °C for an hour. After one hour, a solution of 4-bromobenzaldehyde (1.8g, 10mmol) in 10mL THF was slowly added to the flask at -78 °C and the mixture was stirred for two hours at room temperature. Brine (50mL) was added, and mixture was extracted with ethyl acetate (50mL, three times). The combined organic fractions were dried over NaSO₄. The reaction mixture was evaporated under reduced pressure and the residue was purified through column chromatography (petroleum ether: EtOAc = 50:1) afforded the desired product **1p** (1.4 g, 72% yield, (*Z*)-alkene: (*E*)-alkene = 7: 3) as a colourless oil. Known compound². ¹H NMR (400 MHz, CDCl₃) δ 7.52-7.37 (m, 2H), 7.21-7.12 (m, 2H), 6.41 – 6.30 (m, 1H), 6.28-6.17 (m, 0.3H), 5.87-5.74 (m, 0.7H), 1.91-1.83 (m, 3H).

2) Typical procedure for the preparation of S-(trifluoromethyl) benzenesulfonylthioate **2a**.



A mixture of AgF (10 g, mmol) and CS₂ 20 mL in dry CH₃CN (60 mL) was refluxed at 80 °C for 16 h under N₂ atmosphere. The reaction mixture was filtered on celite and evaporated under reduced pressure. Pale yellow crude product AgSCF₃ was obtained. Then NBS (3.9 g, 22mmol) and CH₃CN (30 mL) were added to the flask with AgSCF₃.

The mixture was stirred for 2h and filtered on celite. After evaporating under reduced pressure, white solid was obtained. Then PhSO₂Na (6.4 g, 40 mmol) and CH₃CN (30 mL) were added to the same flask and stirred at 10 °C for 1-3 h which was determined by TLC screening (PhSO₂SCF₃ was easy to decompose in the mixture). The reaction mixture was filtered on celite and evaporated under reduced pressure. The residue was purified through column chromatography (petroleum ether: EtOAc = 50:1) afforded the desired product **2a** (2.6 g, 54% yield) as a colourless oil. Known compound³. ¹H NMR (400 MHz, CDCl₃) δ 8.01 (d, *J* = 8.1 Hz, 2H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 2H).

Benzenesulfonylthioates **2b-2h** were prepared according to reported procedure⁴.

- (1) Cheng, J.; Loh, T. *J. Am. Chem. Soc.* **2015**, *137*, 42.
- (2) Zhang, L.; Dolbier, W. R.; Jr.; Sheeller, B.; Ingold, K. U. *J. Am. Chem. Soc.*, **2002**, *124*, 6362.
- (3) Shao, X.; Xu, C.; Lu, L.; Shen, Q. *J. Org. Chem.*, **2015**, *80*, 3012.
- (4) Wang, W.; Peng, X.; Wei, F.; Tung, C.; Xu, Z. *Angew. Chem. Int. Ed.* **2016**, *55*, 649.

General Procedure for the Thiosulfonylation of Alkenes

A mixture of alkene **1a** (0.4 mmol), thiosulfonylation reagent **2a** (0.2 mmol), IPrAuCl (10 mol%), AgSbF₆ (15 mol%), Ru(bpy)₃Cl₂ (2.5 mol%), DCE (1 mL) was stirred at room temperature under irradiation with 100 w blue LED at N₂ atmosphere for 1-3 h. The organic layer was filtered on celite and evaporated under reduced pressure. The crude reaction mixture was purified by silica gel flash chromatography to afford the desired product.

Optimization of light source

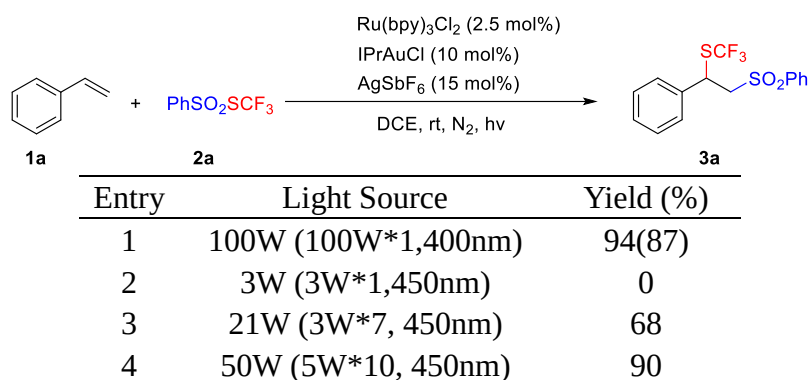
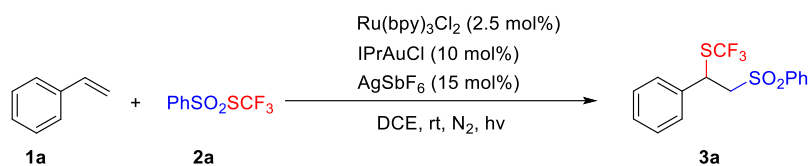


Table S1. Reaction conditions: a mixture of **1a** (0.4 mmol), **2a** (0.2 mmol), IPrAuCl (10 mol%), AgSbF₆ (15 mol%), Ru(bpy)₃Cl₂ (2.5 mol%), in DCE (1 mL) was stirred at room temperature under irradiation of LED at N₂ atmosphere.

Mechanism Study

Control Experiments



Variation from the		
Entry	“standard” conditions	Yield (%)
1	None	94 (87)
2	No IPrAuCl	<5
3	No Ru(bpy) ₃ Cl ₂	0.
4	No AgSbF ₆	<5
5	No light	0.

Table S2. Reaction conditions: a mixture of **1a** (0.4 mmol), **2a** (0.2 mmol), IPrAuCl (10 mol%), AgSbF₆ (15 mol%), Ru(bpy)₃Cl₂ (2.5 mol%), in DCE (1 mL) was stirred at rt under irradiation with 100 w 400nm LED at N₂ atmosphere.

Emission Quenching Experiments for Ru(bpy)₃(SbF₆)₂

Emission intensities were recorded using a HITACHI F-4500 Fluorescence Spectrometer. All Ru(bpy)₃(SbF₆)₂ solutions were excited at 450 nm and the emission intensity at 600 nm was observed. In the typical experiment, the Ru(bpy)₃(SbF₆)₂ solution was prepared by stirring the mixture of Ru(bpy)₃Cl₂•6H₂O (0.01 mmol) and AgSbF₆ (0.02 mmol) in DCE (200 mL) for 5 minutes and filtering the precipitate, and 5 × 10⁻⁵ M Ru(bpy)₃(SbF₆)₂ solution was obtained. Then the Ru(bpy)₃(SbF₆)₂ solution was degassed with a stream of N₂ for 30 minutes. The emission spectrum of a 5 × 10⁻⁵ M solution of Ru(bpy)₃(SbF₆)₂ in DCE was collected. Then, appropriate amount of quencher was added to the measured solution and the emission spectrum of the sample was collected.

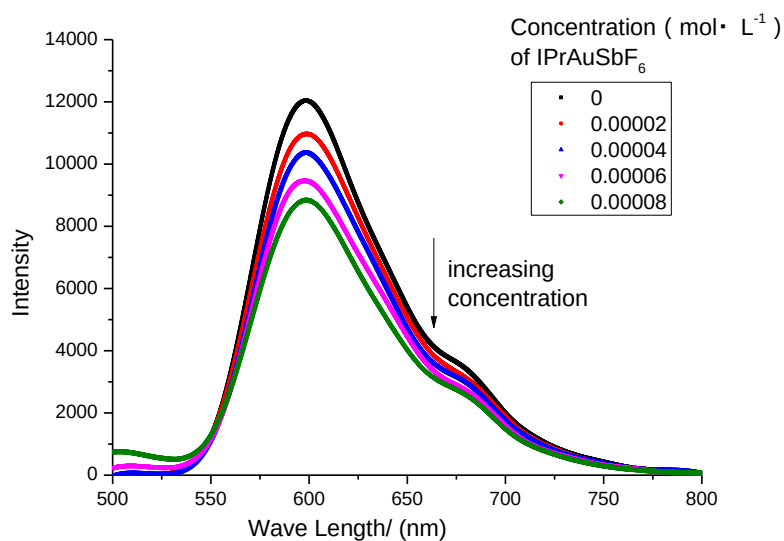


Figure S1. Ru(bpy)₃(SbF₆)₂ Emission Quenching by IPrAuSbF₆.

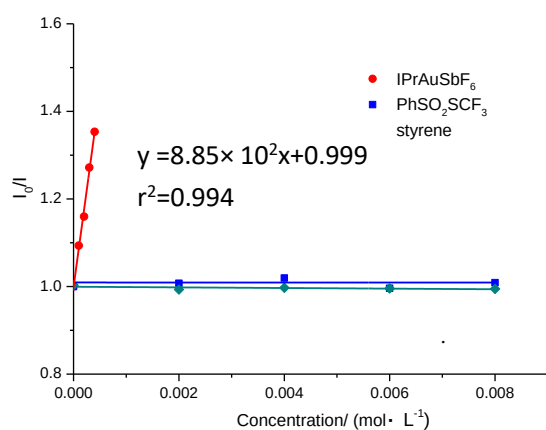


Figure S2. Ru(bpy)₃(SbF₆)₂ emission quenching with IPrAuSbF₆, PhSO₂SCF₃ and styrene; I₀ and I represent the intensities of the emission in the absence and presence of the quencher. Emission Quenching by IPrAuSbF₆, $k_q = 8.85 \times 10^2 \text{ mol}^{-1} \cdot \text{L}$; no quenching were observed by PhSO₂SCF₃ and styrene.

Light/dark Experiments

The reaction was done on the condition: styrene **1a** (0.4mmol), PhSO₂SCF₃ **2a** (0.2mmol), IPrAuCl (10 mol%), AgSbF₆ (15 mol%), Ru(bpy)₃Cl₂•6H₂O (2.5 mol%), DCE 1ml at N₂ atmosphere. Yields of the **3** was determined by ¹⁹F NMR and based on (trifluoromethyl)benzene as an internal standard.

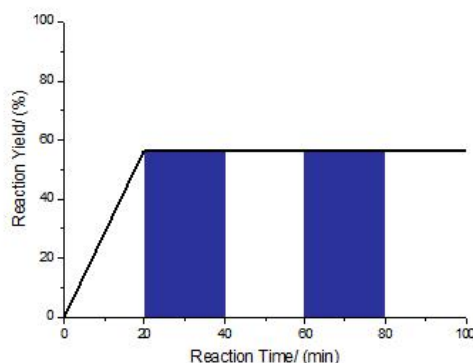


Figure S3. Light/dark experiments. The white area indicates the light irradiation, while the blue area indicates the dark treatment.

It was observed that the reaction completely ceased once the light source was removed. No more transformation was observed if irradiation was recommenced after a period of 20 minutes in the dark. This results may be caused by the altered reaction environment leading the aggregation of the active IPrAu(0) catalyst to inactive gold black.

Transient Absorption Experiments

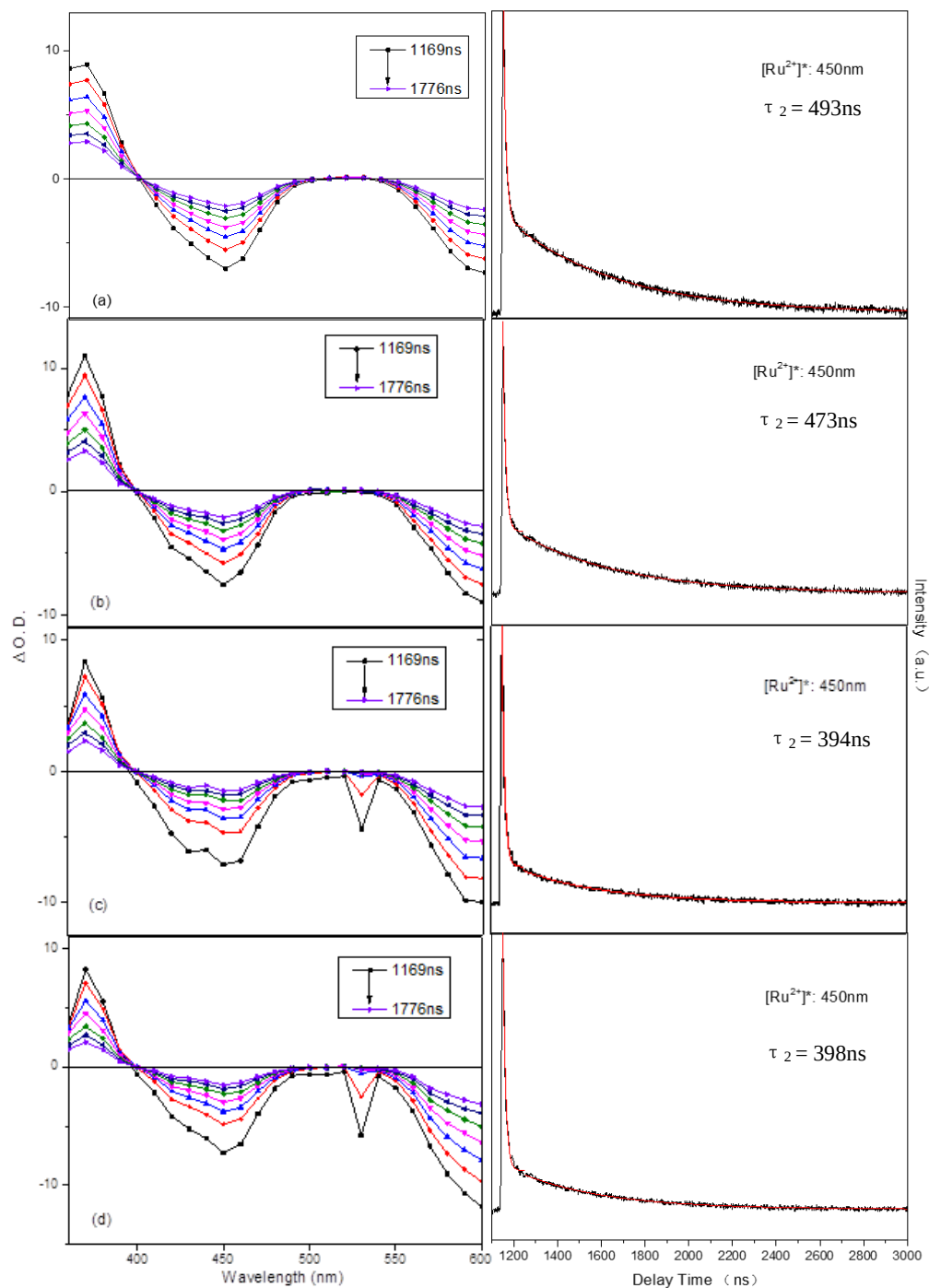


Figure S4. Transient absorption spectra (a) Ru(bpy)₃Cl₂ • 6H₂O = 8 × 10⁻⁵ M, AgSbF₆ = 1.6 × 10⁻⁴ M, τ₁ = 13 ns, τ₂ = 493 ns ; (b) Ru(bpy)₃Cl₂ • 6H₂O = 8 × 10⁻⁵ M, AgSbF₆ = 1.6 × 10⁻⁴ M, PhSO₂SCF₃ = 8 × 10⁻³ M, τ₁ = 12 ns, τ₂ = 473 ns; (c) Ru(bpy)₃Cl₂ • 6H₂O = 8 × 10⁻⁵ M, AgSbF₆ = 1.6 × 10⁻⁴ M, IPrAuSbF₆ = 1.5 × 10⁻³, τ₁ = 12 ns, τ₂ = 394 ns; (d) Ru(bpy)₃Cl₂ • 6H₂O = 8 × 10⁻⁵ M, AgSbF₆ = 1.6 × 10⁻⁴ M, IPrAuSbF₆ = 1.5 × 10⁻³ M, PhSO₂SCF₃ = 8 × 10⁻³ M, τ₁ = 12 ns, τ₂ = 398 ns; in dce at room temperature, excitation at 355 nm.

CV Experiments

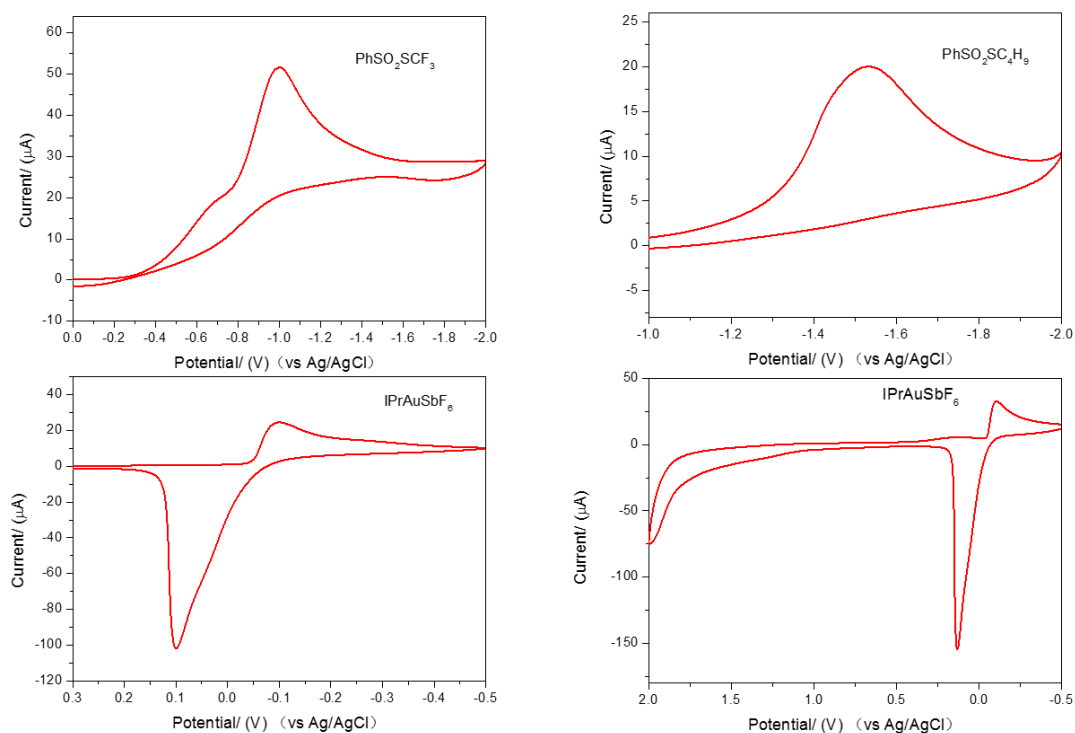
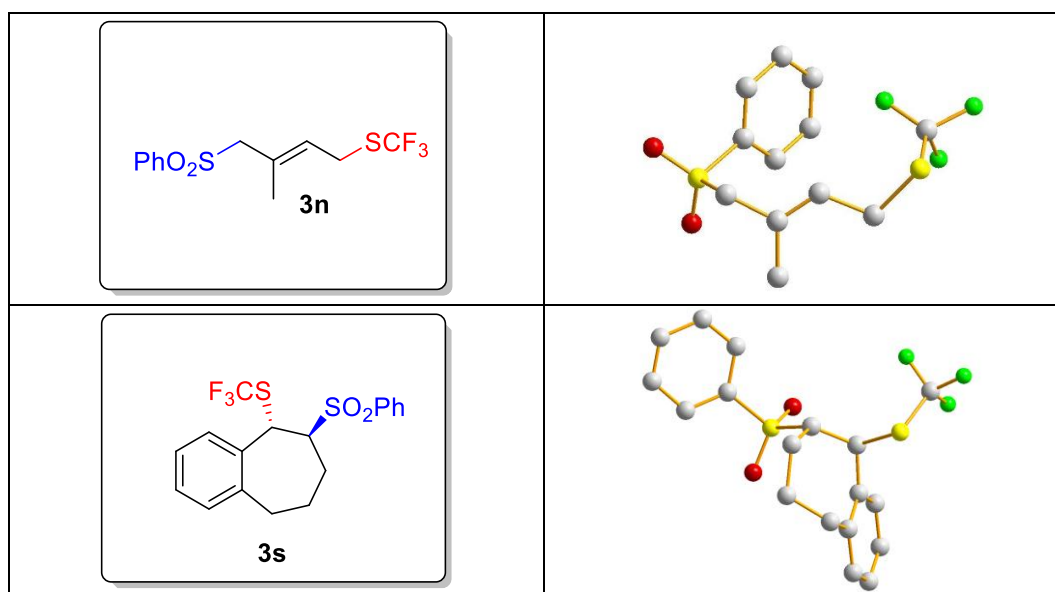
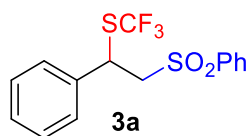


Figure S5. CV experiments condition: 10 mM sample in DCE, 0.1 M Bu₄NPF₆; scan rate, 100 mV s⁻¹. Potentials vs SCE results (Fc as a standard compound): PhSO₂SCF₃, E_{pa} = -1.11 V; PhSO₂SC₄H₉, E_{pa} = -1.64 V; IPrAuSbF₆, E_{pox} = 0.08 V, E_{pred} -0.11 V.

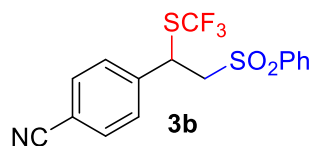
X-ray Crystallography Data



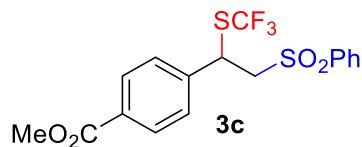
Characterization Data



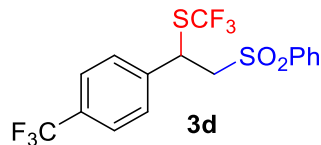
Yield: 87%. ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 7.3 Hz, 2H), 7.54-7.50 (m, 1H), 7.39-7.34 (m, 2H), 7.22-7.13 (m, 5H), 4.87 (dd, J = 10.2, 4.4 Hz, 1H), 3.99-3.90 (m, 1H), 3.85-3.79 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 139.07, 135.94, 133.73, 129.62 (q, J = 307.1 Hz, SCF_3), 129.14, 129.06, 128.90, 127.88, 127.65, 61.24, 43.60. ^{19}F NMR (282 MHz, CDCl_3) δ -40.05. HRMS (ESI, m/z) calcd for $\text{C}_{15}\text{H}_{13}\text{F}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{NH}_4]^+$ 364.0647, found 364.0630.



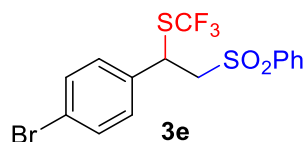
Yield: 69%. ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, J = 7.3 Hz, 2H), 7.62-7.57 (m, 1H), 7.55-7.51 (m, 2H), 7.49-7.41 (m, 2H), 7.39-7.31 (m, 2H), 4.90 (dd, J = 10.0, 4.5 Hz, 1H), 3.93-3.82 (m, 1H), 3.81-3.73 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 141.78, 138.82, 134.20, 132.73, 129.42, 129.31 (q, J = 307.1 Hz, SCF_3), 128.62, 127.85, 117.96, 112.84, 60.51, 42.92. ^{19}F NMR (282 MHz, CDCl_3) δ -39.26. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{12}\text{F}_3\text{NO}_2\text{S}_2$ $[\text{M}+\text{H}]^+$ 372.0334, found 372.0330.



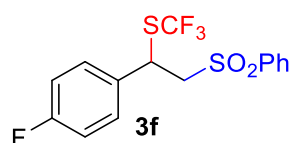
Yield: 76%. ^1H NMR (400 MHz, CDCl_3) δ 7.87 (d, J = 8.4 Hz, 2H), 7.65-7.62 (m, 2H), 7.56-7.52 (m, 1H), 7.40-7.36 (m, 2H), 7.29-7.22 (m, 2H), 4.89 (dd, J = 10.0, 4.5 Hz, 1H), 3.94-3.86 (m, 4H), 3.83-3.76 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 166.17, 141.17, 138.86, 133.97, 130.59, 130.26, 129.45 (q, J = 307.0 Hz, SCF_3), 129.25, 127.88, 127.78, 60.82, 52.32, 43.13. ^{19}F NMR (282 MHz, CDCl_3) δ -39.94. HRMS (ESI, m/z) calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{O}_4\text{S}_2$ $[\text{M}+\text{H}]^+$ 405.0437, found 405.0418.



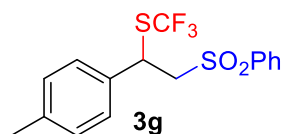
Yield: 67%. ^1H NMR (400 MHz, CDCl_3) δ 7.63-7.49 (m, 3H), 7.48-7.41 (m, 2H), 7.41-7.34 (m, 2H), 7.32-7.27 (m, 2H), 4.92 (dd, J = 10.4, 4.4 Hz, 1H), 3.98-3.87 (m, 1H), 3.87-3.77 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 140.11, 138.86, 133.95, 131.01 (q, J = 32.6 Hz), 129.40 (q, J = 307.0 Hz, SCF_3), 129.26, 128.22, 127.77, 125.98 (q, J = 3.8 Hz), 123.56 (q, J = 270.8 Hz, CF_3), 60.76, 42.99. ^{19}F NMR (282 MHz, CDCl_3) δ -39.89, -62.93. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{12}\text{F}_6\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 437.0075, found 437.0075.



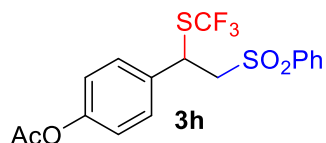
Yield: 90%. ^1H NMR (400 MHz, CDCl_3) δ 7.65-7.53 (m, 3H), 7.47-7.37 (m, 2H), 7.34-7.28 (m, 2H), 7.09-7.00 (m, 2H), 4.83 (dd, J = 10.3, 4.4 Hz, 1H), 3.94-3.84 (m, 1H), 3.83-3.74 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.99, 135.11, 133.79, 132.17, 129.45 (q, J = 307.1 Hz, SCF_3), 129.36, 129.25, 127.82, 123.04, 61.01, 42.98. ^{19}F NMR (282 MHz, CDCl_3) δ -39.89. HRMS (ESI, m/z) calcd for $\text{C}_{15}\text{H}_{12}\text{BrF}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 446.9306, found 446.9302.



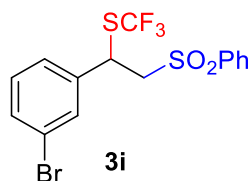
Yield: 77%. ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 7.3 Hz, 2H), 7.59-7.55 (m, 1H), 7.43-7.39 (m, 2H), 7.17-7.13 (m, 2H), 6.91-6.86 (m, 2H), 4.88 (dd, J = 10.3, 4.4 Hz, 1H), 3.92-3.86 (m, 1H), 3.82-3.77 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 163.92, 161.44, 139.13, 133.82, 131.88, 129.58, 129.50, 129.49 (q, J = 306.9 Hz, SCF_3), 129.20, 128.06, 127.85, 116.17, 115.95, 61.25, 42.87. ^{19}F NMR (282 MHz, CDCl_3) δ -39.97, -112.02. HRMS (ESI, m/z) calcd for $\text{C}_{15}\text{H}_{12}\text{F}_4\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 387.0107, found 387.0096.



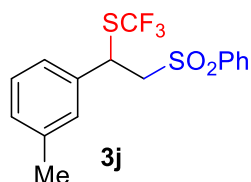
Yield: 63%. ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 7.5 Hz, 2H), 7.58-7.48 (m, 1H), 7.43-7.31 (m, 2H), 7.09-6.96 (m, 4H), 4.83 (dd, J = 10.3, 4.3 Hz, 1H), 3.97-3.76 (m, 2H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 139.16, 138.86, 133.52, 132.79, 129.69, 129.65 (q, J = 306.9 Hz, SCF_3), 129.06, 127.91, 127.55, 61.40, 43.37, 21.11. ^{19}F NMR (282 MHz, CDCl_3) δ -40.06. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{15}\text{F}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 383.0358, found 383.0360.



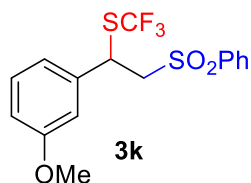
Yield: 70%. ^1H NMR (400 MHz, CDCl_3) δ 7.67-7.48 (m, 3H), 7.44-7.34 (m, 2H), 7.15 (d, J = 8.5 Hz, 2H), 6.92 (d, J = 8.5 Hz, 2H), 4.88 (dd, J = 10.0, 4.5 Hz, 1H), 3.97-3.85 (m, 1H), 3.85-3.76 (m, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 168.89, 150.88, 138.93, 133.88, 133.36, 129.53 (q, J = 306.9 Hz, SCF_3), 129.28, 128.78, 127.80, 122.22, 61.29, 43.04, 21.12. ^{19}F NMR (282 MHz, CDCl_3) δ -39.97. HRMS (ESI, m/z) calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{O}_4\text{S}_2$ $[\text{M}+\text{Na}]^+$ 427.0256, found 427.0257.



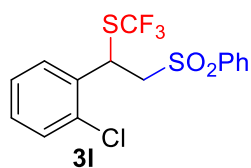
Yield: 69%. ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 7.8 Hz, 2H), 7.58-7.53 (m, 1H), 7.42-7.38 (m, 2H), 7.34-7.31 (m, 1H), 7.23 (s, 1H), 7.15-7.06 (m, 2H), 4.81 (dd, J = 10.2, 4.4 Hz, 1H), 3.92-3.85 (m, 1H), 3.80-3.76 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.80, 138.22, 132.06, 130.66, 130.56, 129.44 (q, J = 307.0 Hz, SCF_3), 129.18, 128.03, 127.80, 126.47, 122.96, 60.84, 42.96. ^{19}F NMR (282 MHz, CDCl_3) δ -39.94. HRMS (ESI, m/z) calcd for $\text{C}_{15}\text{H}_{12}\text{BrF}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 446.9306, found 446.9301.



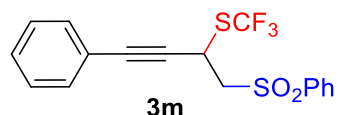
Yield: 86%. ^1H NMR (400 MHz, CDCl_3) δ 7.59 (d, J = 8.0 Hz, 2H), 7.54-7.47 (m, 1H), 7.40-7.32 (m, 2H), 7.10-7.05 (m, 1H), 7.03-6.95 (m, 2H), 6.88 (s, 1H), 4.83 (dd, J = 10.3, 4.2 Hz, 1H), 4.06-3.89 (m, 1H), 3.87-3.77 (m, 1H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 139.12, 138.83, 135.59, 133.61, 129.69, 129.65 (q, J = 306.9 Hz, SCF_3), 129.05, 128.97, 128.15, 127.85, 124.84, 61.27, 43.60, 21.22. ^{19}F NMR (282 MHz, CDCl_3) δ -40.08. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{15}\text{F}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 383.0358, found 383.0353.



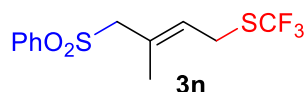
Yield: 76%. ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 7.3 Hz, 2H), 7.54-7.50 (m, 1H), 7.39-7.35 (m, 2H), 7.13-7.09 (m, 1H), 6.76-6.71 (m, 2H), 6.63-6.61 (m, 1H), 4.82 (dd, J = 10.2, 4.4 Hz, 1H), 3.98-3.90 (m, 1H), 3.83-3.76 (m, 1H), 3.71 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 159.86, 139.08, 137.27, 133.66, 130.16, 129.61 (q, J = 306.8 Hz, SCF_3), 129.06, 127.88, 119.92, 114.30, 113.26, 61.24, 55.22, 43.54. ^{19}F NMR (282 MHz, CDCl_3) δ -40.01. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{15}\text{F}_3\text{O}_3\text{S}_2$ $[\text{M}+\text{Na}]^+$ 399.0307, found 399.0299.



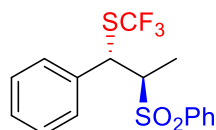
Yield: 72%. ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, J = 7.5 Hz, 2H), 7.61-7.51 (m, 1H), 7.48-7.38 (m, 2H), 7.27-7.23 (m, 2H), 7.21-7.12 (m, 2H), 5.28-5.08 (m, 1H), 4.28-4.08 (m, 1H), 3.88-3.78 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.57, 133.84, 133.66, 133.25, 130.42, 130.06, 129.65 (q, J = 306.9 Hz, SCF_3), 129.17, 128.25, 127.91, 127.33, 62.68, 60.02. ^{19}F NMR (282 MHz, CDCl_3) δ -40.72. HRMS (ESI, m/z) calcd for $\text{C}_{15}\text{H}_{12}\text{ClF}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 402.9812, found 402.9800.



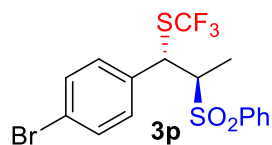
Yield: 31%. ^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, J = 7.2 Hz, 2H), 7.64-7.55 (m, 1H), 7.54-7.48 (m, 2H), 7.34-7.26 (m, 3H), 7.23-7.17 (m, 2H), 4.68 (dd, J = 9.9, 3.8 Hz, 1H), 3.87-3.78 (m, 1H), 3.74-3.65 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.94, 134.21, 132.78 (q, J = 306.9 Hz, SCF_3), 131.77, 129.36, 129.13, 128.51, 128.19, 121.28, 87.89, 82.54, 61.18, 30.50, 29.69. ^{19}F NMR (282 MHz, CDCl_3) δ -39.43. HRMS (ESI, m/z) calcd for $\text{C}_{17}\text{H}_{13}\text{F}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 393.0201, found 393.0200.



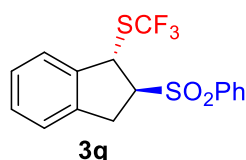
Yield: 55%. ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, J = 7.3 Hz, 2H), 7.72-7.62 (m, 1H), 7.61-7.53 (m, 2H), 5.20 (t, J = 7.8 Hz, 1H), 3.76 (s, 2H), 3.46 (d, J = 7.9 Hz, 2H), 1.85 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.16, 133.88, 130.60 (q, J = 306.8 Hz, SCF_3), 129.53, 129.19, 128.44, 128.28, 65.62, 27.36, 16.83. ^{19}F NMR (282 MHz, CDCl_3) δ -41.43. HRMS (ESI, m/z) calcd for $\text{C}_{12}\text{H}_{13}\text{F}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{H}]^+$ 311.0382, found 311.0394.



Yield: 67% / 61% (from *(E)*-alkene / from *(Z)*-alkene), d.r.=9:1 / d.r.=9:1. ^1H NMR (400 MHz, CDCl_3) δ 7.86 (d, J = 8.0 Hz, 2H), 7.70-7.62 (m, 1H), 7.58-7.49 (m, 2H), 7.35-7.27 (m, 5H), 5.04 (d, J = 3.8 Hz, 1H), 3.48 (m, 1H), 1.43 (d, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.75, 137.65, 134.01, 130.00 (q, J = 306.2 Hz, SCF_3), 129.24, 128.99, 128.86, 128.38, 127.78, 65.31, 48.13, 10.28. ^{19}F NMR (282 MHz, CDCl_3) δ -40.03. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{15}\text{F}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 383.0358, found 383.0357.

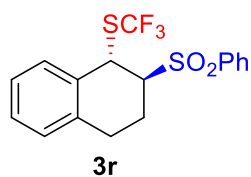


Yield: 65%, d.r.=7:1. ^1H NMR (400 MHz, CDCl_3) δ 7.79 (d, J = 7.8 Hz, 2H), 7.68-7.59 (m, 1H), 7.57-7.48 (m, 2H), 7.43-7.36 (d, J = 8.5 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 4.94 (d, J = 4.6 Hz, 1H), 3.51 – 3.39 (m, 1H), 1.44 (d, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 137.70, 133.99, 131.96, 130.03, 129.60, 129.85 (q, J = 305.9 Hz, SCF_3), 129.28, 128.81, 122.52, 64.94, 48.01, 10.79. ^{19}F NMR (282 MHz, CDCl_3) δ -40.01. HRMS (ESI, m/z) calcd for $\text{C}_{16}\text{H}_{14}\text{BrF}_3\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 460.9463, found 460.9468.

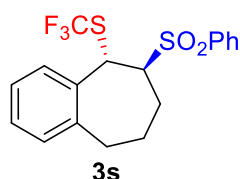


Yield: 63%, d.r.>20:1. ^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, J = 7.4 Hz, 2H), 7.70-7.59 (m, 1H), 7.57-7.48 (m, 2H), 7.38-7.14 (m, 4H), 5.33-5.21 (m, 1H), 4.24-4.14 (m, 1H), 3.64-3.45 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 140.20, 137.15, 137.11, 134.21, 129.65 (q, J = 307.2 Hz, SCF_3), 129.55, 129.35, 128.87, 128.00, 125.51, 124.70, 70.34, 49.24, 31.86. ^{19}F NMR (282 MHz, CDCl_3) δ -40.14. HRMS (ESI, m/z) calcd for

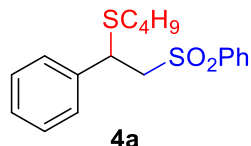
C₁₆H₁₃F₃O₂S₂ [M+Na]⁺ 381.0201, found 381.0206.



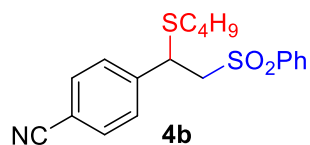
Yield: 56%, d.r.=10:1. ¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 7.7 Hz, 2H), 7.73-7.63 (m, 1H), 7.64-7.53 (m, 2H), 7.38-7.32 (m, 1H), 7.24-7.17 (m, 2H), 7.13-7.04 (m, 1H), 5.08-4.95 (m, 1H), 3.90-3.79 (m, 1H), 3.27-3.14 (m, 1H), 2.90-2.79 (m, 1H), 2.61-2.42 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 137.93, 136.65, 134.14, 130.74, 129.76 (q, *J* = 307.1 Hz, SCF₃), 129.41, 129.28, 129.15, 128.59, 128.57, 126.82, 64.58, 42.07, 24.37, 18.07. ¹⁹F NMR (282 MHz, CDCl₃) δ -41.05. HRMS (ESI, *m/z*) calcd for C₁₇H₁₅F₃O₂S₂ [M+Na]⁺ 395.0358, found 395.0367.



Yield: 52%, d.r.=9:1. ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 7.5 Hz, 2H), 7.72-7.64 (m, 1H), 7.58-7.51 (m, 2H), 7.26-7.17 (m, 3H), 7.12-7.05 (m, 1H), 5.13 (d, *J* = 4.3 Hz, 1H), 3.60-3.52 (m, 1H), 3.07-2.94 (m, 1H), 2.80-2.70 (m, 1H), 2.43-2.27 (m, 1H), 2.15-2.05 (m, 1H), 1.92-1.75 (m, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 140.90, 137.95, 134.87, 134.02, 130.75, 130.34, 130.12 (q, *J* = 306.1 Hz, SCF₃), 129.36, 129.30, 128.86, 126.85, 66.28, 48.36, 33.94, 25.02, 22.75. ¹⁹F NMR (282 MHz, CDCl₃) δ -40.58. HRMS (ESI, *m/z*) calcd for C₁₈H₁₇F₃O₂S₂ [M+Na]⁺ 409.0514, found 409.0514.

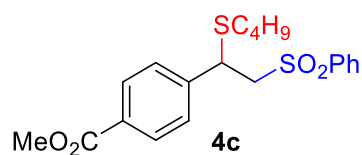


Yield: 84%. ¹H NMR (400 MHz, CDCl₃) δ 7.63 (d, *J* = 7.6 Hz, 2H), 7.51-7.47 (m, 1H), 7.37-7.33 (m, 2H), 7.14-7.12 (m, 5H), 4.32 (dd, *J* = 9.4, 4.6 Hz, 1H), 3.80-3.68 (m, 1H), 3.68-3.63 (m, 1H), 2.37-2.24 (m, 2H), 1.49-1.38 (m, 2H), 1.31-1.23 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 139.56, 138.95, 133.37, 128.95, 128.59, 127.91, 127.81, 127.79, 61.58, 43.30, 31.23, 31.04, 21.87, 13.58. HRMS (ESI, *m/z*) calcd for C₁₈H₂₂O₂S₂ [M+H]⁺ 335.1134, found 335.1136.

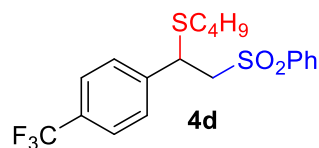


Yield: 71%. ¹H NMR (400 MHz, CDCl₃) δ 7.64 (d, *J* = 7.3 Hz, 2H), 7.58-7.54 (m, 1H), 7.48-7.46 (m, 2H), 7.42-7.38 (m, 2H), 7.30-7.28 (m, 2H), 4.35 (dd, *J* = 9.7, 4.5 Hz, 1H), 3.74-3.62 (m, 2H), 2.36-2.24 (m, 2H), 1.46-1.41 (m, 2H), 1.29-1.24 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 144.72, 139.32, 133.78, 132.34, 129.19, 128.71, 127.84, 118.37, 111.63, 60.98, 43.00, 31.36, 30.90, 21.80, 13.53. HRMS (ESI,

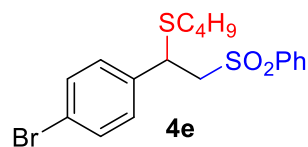
m/z) calcd for C₁₉H₂₁NO₂S₂ [M+H]⁺ 360.1086, found 360.1081.



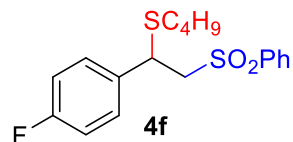
Yield: 40%. ¹H NMR (400 MHz, CDCl₃) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.52-7.48 (m, 1H), 7.37-7.33 (m, 2H), 7.23-7.21 (m, 2H), 4.35 (dd, *J* = 9.6, 4.4 Hz, 1H), 3.90 (s, 3H), 3.78-3.63 (m, 2H), 2.35-2.23 (m, 2H), 1.45-1.41 (m, 2H), 1.29-1.25 (m, 2H), 0.81 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 166.51, 144.27, 139.35, 133.58, 129.87, 129.55, 129.04, 127.90, 127.89, 61.20, 52.18, 43.01, 31.25, 30.95, 21.83, 13.55. HRMS (ESI, m/z) calcd for C₂₀H₂₄O₄S₂ [M+Na]⁺ 415.1008, found 415.0999.



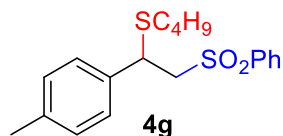
Yield: 48%. ¹H NMR (300 MHz, CDCl₃) δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.54-7.45 (m, 1H), 7.44-7.31 (m, 4H), 7.29-7.21 (m, 2H), 4.37 (dd, *J* = 9.7, 4.6 Hz, 1H), 3.85-3.62 (m, 2H), 2.41-2.24 (m, 2H), 1.51-1.41 (m, 2H), 1.35-1.25 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 143.01, 139.34, 133.54, 129.02, 128.26, 127.76, 125.52, 125.47, 122.01, 61.14, 42.97, 31.30, 30.95, 21.82, 13.53. ¹⁹F NMR (282 MHz, CDCl₃) δ -62.73. HRMS (ESI, m/z) calcd for C₁₉H₂₁F₃O₂S₂ [M+H]⁺ 403.1008, found 403.1003.



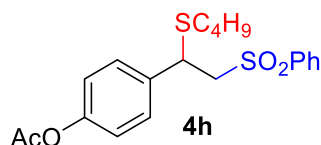
Yield: 66%. ¹H NMR (400 MHz, CDCl₃) δ 7.60 (d, *J* = 7.3 Hz, 2H), 7.56-7.52 (m, 1H), 7.39-7.35 (m, 2H), 7.26-7.24 (m, 2H), 7.02-7.00 (m, 2H), 4.28 (dd, *J* = 9.7, 4.6 Hz, 1H), 3.73-3.61 (m, 2H), 2.36-2.23 (m, 2H), 1.49-1.40 (m, 2H), 1.34-1.22 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 139.44, 138.01, 133.42, 131.66, 129.56, 129.05, 127.83, 121.68, 61.38, 42.76, 31.22, 30.99, 21.85, 13.58. HRMS (ESI, m/z) calcd for C₁₈H₂₁BrO₂S₂ [M+H]⁺ 413.0239, found 413.0236.



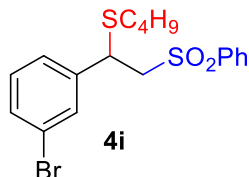
Yield: 68%. ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, *J* = 7.4 Hz, 2H), 7.55-7.51 (m, 1H), 7.40-7.35 (m, 2H), 7.14-7.09 (m, 2H), 6.86-6.81 (m, 2H), 4.32 (dd, *J* = 9.7, 4.5 Hz, 1H), 3.75-3.61 (m, 2H), 2.38-2.23 (m, 2H), 1.50-1.39 (m, 2H), 1.33-1.23 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.28, 160.83, 139.51, 134.71, 133.48, 129.54, 129.46, 129.01, 127.85, 115.60, 115.38, 61.55, 42.58, 31.21, 31.00, 21.87, 13.59. ¹⁹F NMR (282 MHz, CDCl₃) δ -114.10. HRMS (ESI, m/z) calcd for C₁₈H₂₁FO₂S₂ [M+H]⁺ 353.1040, found 353.1044.



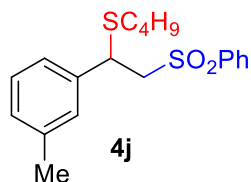
Yield: 60%. ^1H NMR (400 MHz, CDCl_3) δ 7.67-7.58 (m, 2H), 7.56-7.46 (m, 1H), 7.40-7.29 (m, 2H), 7.03 (d, $J = 8.1$ Hz, 2H), 6.95 (d, $J = 8.0$ Hz, 2H), 4.30 (dd, $J = 9.5, 4.6$ Hz, 1H), 3.80-3.60 (m, 2H), 2.37-2.30 (m, 2H), 2.26 (s, 3H), 1.50-1.40 (m, 2H), 1.32-1.26 (m, 2H), 0.84 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 139.65, 137.48, 135.85, 133.18, 129.24, 128.88, 127.94, 127.69, 61.72, 42.99, 31.19, 31.08, 21.89, 21.07, 13.60. HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{24}\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 371.1110, found 371.1115.



Yield: 52%. ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, $J = 7.3$ Hz, 2H), 7.53-7.49 (m, 1H), 7.39-7.35 (m, 2H), 7.14-7.11 (m, 2H), 6.88-6.85 (m, 2H), 4.33 (dd, $J = 9.3, 4.8$ Hz, 1H), 3.76-3.62 (m, 2H), 2.34-2.28 (m, 2H), 2.27 (s, 3H), 1.47-1.42 (m, 2H), 1.33-1.25 (m, 2H), 0.83 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 169.08, 150.05, 139.41, 136.46, 133.53, 129.08, 128.80, 127.83, 121.69, 61.66, 42.78, 31.27, 31.00, 21.87, 21.16, 13.59. HRMS (ESI, m/z) calcd for $\text{C}_{20}\text{H}_{24}\text{O}_4\text{S}_2$ $[\text{M}+\text{NH}_4]^+$ 410.1454, found 410.1458.

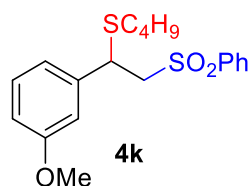


Yield: 57%. ^1H NMR (300 MHz, CDCl_3) δ 7.67-7.59 (m, 2H), 7.57-7.49 (m, 1H), 7.45-7.33 (m, 2H), 7.29-7.18 (m, 2H), 7.15-6.99 (m, 2H), 4.26 (dd, $J = 9.5, 4.7$ Hz, 1H), 3.79-3.57 (m, 2H), 2.41-2.24 (m, 2H), 1.53-1.39 (m, 2H), 1.39-1.23 (m, 2H), 0.84 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 141.26, 139.27, 133.63, 130.92, 130.80, 130.07, 128.96, 127.81, 126.60, 122.61, 61.19, 42.90, 31.31, 30.96, 21.83, 13.55. HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{21}\text{BrO}_2\text{S}_2$ $[\text{M}+\text{H}]^+$ 413.0239, found 413.0248.

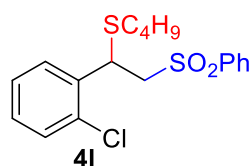


Yield: 70%. ^1H NMR (300 MHz, CDCl_3) δ 7.66-7.55 (m, 2H), 7.51-7.44 (m, 1H), 7.38-7.28 (m, 2H), 7.03 (d, $J = 7.5$ Hz, 1H), 6.97-6.89 (m, 2H), 6.86 (s, 1H), 4.27 (dd, $J = 9.4, 4.7$ Hz, 1H), 3.84-3.71 (m, 1H), 3.69-3.58 (m, 1H), 2.35-2.28 (m, 2H), 2.18 (s, 3H), 1.52-1.39 (m, 2H), 1.33-1.24 (m, 2H), 0.84 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 139.56, 138.68, 138.18, 133.27, 128.77, 128.57, 128.44, 128.28, 127.88, 125.01, 61.51, 43.29, 31.26, 31.06, 21.87, 21.26, 13.58. HRMS (ESI, m/z) calcd for

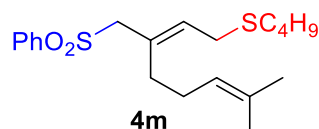
C₁₉H₂₄O₂S₂ [M+H]⁺ 349.1290, found 349.1296.



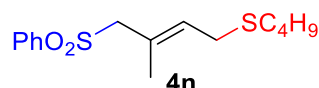
Yield: 41%. ¹H NMR (400 MHz, CDCl₃) δ 7.64 (d, *J* = 7.4 Hz, 2H), 7.52-7.48 (m, 1H), 7.38-7.34 (m, 2H), 7.09-7.05 (m, 1H), 6.74 (d, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 8.3 Hz, 1H), 6.62 (s, 1H), 4.28 (dd, *J* = 9.4, 4.7 Hz, 1H), 3.78-3.71 (m, 1H), 3.70 (s, 3H), 3.69-3.61 (m, 1H), 2.42-2.23 (m, 2H), 1.48-1.40 (m, 2H), 1.36-1.26 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 159.66, 140.50, 139.62, 133.30, 129.57, 128.86, 127.92, 120.32, 113.35, 113.22, 61.60, 55.14, 43.38, 31.29, 31.05, 21.86, 13.56. HRMS (ESI, *m/z*) calcd for C₁₉H₂₄O₃S₂ [M+H]⁺ 365.1240, found 365.1242.



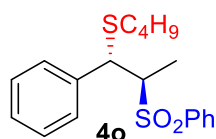
Yield: 71%. ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, *J* = 7.9 Hz, 2H), 7.55-7.48 (m, 1H), 7.43-7.35 (m, 2H), 7.24-7.20 (m, 2H), 7.10-7.05 (m, 2H), 4.88-4.76 (m, 1H), 3.94-3.81 (m, 1H), 3.69-3.64 (m, 1H), 2.47-2.32 (m, 2H), 1.53-1.41 (m, 2H), 1.33-1.26 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 139.01, 136.63, 133.57, 133.49, 129.82, 129.05, 129.01, 128.80, 128.01, 127.19, 60.62, 52.55, 31.54, 31.20, 21.87, 13.57. HRMS (ESI, *m/z*) calcd for C₁₈H₂₁ClO₂S₂ [M+H]⁺ 369.0744, found 369.0744.



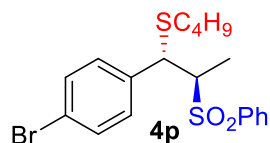
Yield: 51%. ¹H NMR (400 MHz, CDCl₃) δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.69-7.59 (m, 1H), 7.58-7.50 (m, 2H), 5.23 (t, *J* = 7.8 Hz, 1H), 5.04 (t, *J* = 7.1 Hz, 1H), 3.77 (s, 2H), 3.06 (d, *J* = 7.8 Hz, 2H), 2.41-2.31 (m, 2H), 2.28-2.13 (m, 2H), 2.12-2.01 (m, 2H), 1.66 (s, 3H), 1.58 (s, 3H), 1.55-1.44 (m, 2H), 1.43-1.31 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 138.59, 133.60, 132.79, 132.70, 130.12, 129.07, 128.50, 122.97, 63.14, 31.62, 31.35, 29.75, 29.10, 26.65, 25.65, 22.00, 17.73, 13.69. HRMS (ESI, *m/z*) calcd for C₂₀H₃₀O₂S₂ [M+H]⁺ 367.1760, found 367.1754.



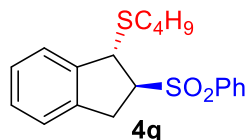
Yield: 55%. ¹H NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 7.2 Hz, 2H), 7.66-7.61 (m, 1H), 7.56-7.52 (m, 2H), 5.20 (t, *J* = 7.7 Hz, 1H), 3.76 (s, 2H), 3.04 (d, *J* = 7.5 Hz, 2H), 2.39-2.33 (m, 2H), 1.81 (s, 3H), 1.51-1.44 (m, 2H), 1.38-1.34 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 138.46, 133.68, 132.19, 129.09, 128.43, 126.01, 65.91, 31.58, 31.07, 29.13, 22.04, 16.85, 13.71. HRMS (ESI, *m/z*) calcd for C₁₅H₂₂O₂S₂ [M+H]⁺ 299.1134, found 299.1132.



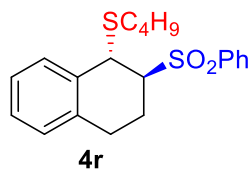
Yield: 45% / 48% (from (*E*)-alkene / from (*Z*)-alkene), d.r.>20:1 / d.r.>20:1. ^1H NMR (400 MHz, CDCl_3) δ 7.81 (d, J = 7.3 Hz, 2H), 7.63-7.55 (m, 1H), 7.51-7.43 (m, 2H), 7.36-7.29 (m, 2H), 7.28 -7.17 (m, 3H), 4.55 (d, J = 4.6 Hz, 1H), 3.52-3.41 (m, 1H), 2.26 (m, 2H), 1.53-1.38 (m, 5H), 1.31-1.23 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 140.15, 138.58, 133.40, 129.78, 128.87, 128.58, 128.38, 127.59, 66.06, 48.84, 31.42, 31.00, 21.89, 13.59, 10.50. HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{24}\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 371.1110, found 371.1110.



Yield: 51%, d.r.=12:1. ^1H NMR (400 MHz, CDCl_3) δ 7.72 (d, J = 8.0 Hz, 2H), 7.62-7.55 (m, 1H), 7.47-7.41 (m, 2H), 7.32 (d, J = 8.4 Hz, 2H), 7.16 (d, J = 8.4 Hz, 2H), 4.43 (d, J = 5.7 Hz, 1H), 3.50-3.39 (m, 1H), 2.32-2.17 (m, 2H), 1.48 (d, J = 7.1 Hz, 3H), 1.45-1.38 (m, 2H), 1.30-1.22 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 139.18, 138.62, 133.34, 131.61, 130.14, 128.95, 128.65, 121.50, 65.71, 48.65, 31.36, 30.95, 21.87, 13.58, 10.97. HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{23}\text{BrO}_2\text{S}_2$ $[\text{M}+\text{H}]^+$ 427.0396, found 427.0392.

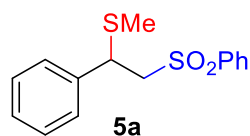


Yield: 57%, d.r.>20:1. ^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, J = 7.8 Hz, 2H), 7.63-7.58 (m, 1H), 7.53-7.49 (m, 2H), 7.29-7.26 (m, 1H), 7.18-7.08 (m, 3H), 4.78 (d, J = 2.9 Hz, 1H), 4.02 -3.96 (m, 1H), 3.46-3.44 (m, 2H), 2.52-2.34 (m, 2H), 1.55-1.43 (m, 2H), 1.37-1.27 (m, 2H), 0.88 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 140.51, 139.36, 137.59, 133.88, 129.18, 128.85, 128.34, 127.50, 125.14, 124.31, 71.18, 49.80, 32.49, 31.36, 31.16, 22.01, 13.65. HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{22}\text{O}_2\text{S}_2$ $[\text{M}+\text{H}]^+$ 347.1134, found 347.1135.

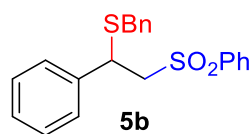


Yield: 56%, d.r.=14:1. ^1H NMR (400 MHz, CDCl_3) δ 7.87 (d, J = 7.6 Hz, 2H), 7.68-7.60 (m, 1H), 7.57-7.46 (m, 2H), 7.28-7.22 (m, 1H), 7.18-7.07 (m, 2H), 7.02 (d, J = 6.7 Hz, 1H), 4.52-4.41 (m, 1H), 3.68-3.62 (m, 1H), 3.05-2.94 (m, 1H), 2.90-2.76 (m, 1H), 2.55-2.42 (m, 1H), 2.37-2.16 (m, 3H), 1.48-1.36 (m, 2H), 1.31-1.23 (m, 2H), 0.85 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 138.09, 136.35, 133.80, 133.36, 130.04,

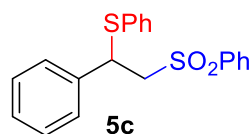
129.20, 128.76, 128.54, 127.35, 126.28, 64.97, 41.13, 31.89, 31.20, 25.19, 21.96, 19.71, 13.62. HRMS (ESI, m/z) calcd for C₂₀H₂₄O₂S₂ [M+Na]⁺ 383.1110, found 383.1122.



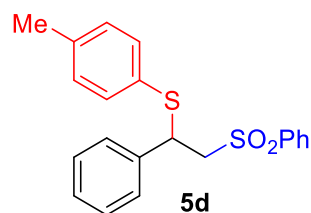
Yield: 90%. ¹H NMR (400 MHz, CDCl₃) δ 7.64 (d, *J* = 7.3 Hz, 2H), 7.52-7.48 (m, 1H), 7.38-7.33 (m, 2H), 7.18-7.11 (m, 5H), 4.24 (dd, *J* = 9.3, 4.8 Hz, 1H), 3.81-3.65 (m, 2H), 1.91 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 139.48, 138.43, 133.46, 129.00, 128.63, 127.92, 127.88, 127.82, 61.17, 44.98, 14.87. HRMS (ESI, m/z) calcd for C₁₅H₁₆O₂S₂ [M+H]⁺ 293.0664, found 293.0677.



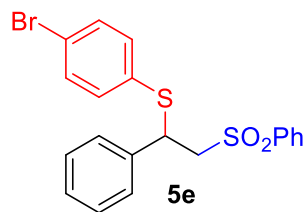
Yield: 66%. ¹H NMR (400 MHz, CDCl₃) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.53-7.48 (m, 1H), 7.38-7.26 (m, 5H), 7.23-7.15 (m, 5H), 7.16-7.06 (m, 2H), 4.20 (dd, *J* = 9.2, 4.8 Hz, 1H), 3.80-3.41 (m, 4H). ¹³C NMR (100 MHz, CDCl₃) δ 139.43, 138.64, 137.13, 133.40, 128.97, 128.95, 128.67, 128.62, 128.00, 127.93, 127.92, 127.31, 61.41, 43.06, 36.05. HRMS (ESI, m/z) calcd for C₂₁H₂₀O₂S₂ [M+H]⁺ 369.0977, found 369.0977.



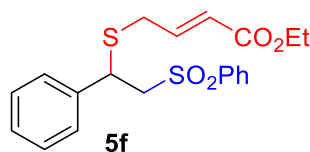
Yield: 92%. ¹H NMR (300 MHz, CDCl₃) δ 7.54 (d, *J* = 7.3 Hz, 2H), 7.50-7.44 (m, 1H), 7.33-7.25 (m, 6H), 7.16-6.98 (m, 6H), 4.65 (dd, *J* = 10.4, 3.8 Hz, 1H), 3.92-3.77 (m, 1H), 3.72-3.60 (m, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 139.28, 137.27, 133.34, 133.19, 132.74, 129.25, 128.91, 128.56, 128.36, 128.03, 127.91, 127.88, 60.54, 47.28. HRMS (ESI, m/z) calcd for C₂₀H₁₈O₂S₂ [M+H]⁺ 355.0821, found 355.0823.



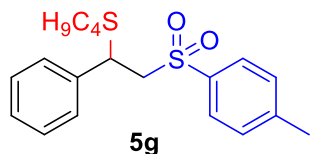
Yield: 84%. ¹H NMR (300 MHz, CDCl₃) δ 7.52 (d, *J* = 7.1 Hz, 2H), 7.47-7.42 (m, 1H), 7.32-7.25 (m, 3H), 7.20-7.16 (m, 2H), 7.12-7.05 (m, 6H), 4.57 (dd, *J* = 10.5, 3.8 Hz, 1H), 3.89-3.77 (m, 1H), 3.69-3.59 (m, 1H), 2.33 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 139.32, 138.78, 137.38, 133.82, 133.28, 130.04, 128.95, 128.86, 128.51, 127.95, 127.92, 127.88, 60.51, 47.68, 21.21. HRMS (ESI, m/z) calcd for C₂₁H₂₀O₂S₂ [M+H]⁺ 369.0977, found 369.0979.



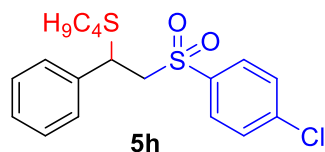
Yield: 65%. ^1H NMR (300 MHz, CDCl_3) δ 7.57 (d, $J = 7.3$ Hz, 2H), 7.51-7.47 (m, 1H), 7.39-7.30 (m, 4H), 7.15-7.04 (m, 7H), 4.63 (dd, $J = 10.1, 4.1$ Hz, 1H), 3.89-3.77 (m, 1H), 3.68-3.58 (m, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 139.69, 137.67, 135.22, 133.94, 132.79, 129.45, 129.10, 128.64, 128.64, 128.37, 128.35, 123.28, 60.99, 47.85. HRMS (ESI, m/z) calcd for $\text{C}_{20}\text{H}_{17}\text{BrO}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 454.9746, found 454.9743.



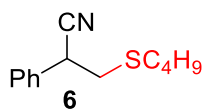
Yield: 53%. ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, $J = 7.4$ Hz, 2H), 7.56-7.48 (m, 1H), 7.42-7.33 (m, 2H), 7.20-7.12 (m, 5H), 6.78-6.66 (m, 1H), 5.74 (d, $J = 15.5$ Hz, 1H), 4.31-4.16 (m, 3H), 3.78-3.57 (m, 2H), 3.11-2.89 (m, 2H), 1.31 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 165.79, 142.61, 139.33, 138.21, 133.56, 129.06, 128.81, 128.18, 128.03, 127.95, 123.62, 61.34, 60.57, 42.85, 32.33, 14.28. HRMS (ESI, m/z) calcd for $\text{C}_{20}\text{H}_{22}\text{O}_4\text{S}_2$ $[\text{M}+\text{H}]^+$ 391.1032, found 391.1035.



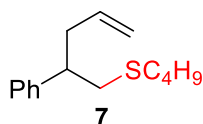
Yield: 72%. ^1H NMR (500 MHz, CDCl_3) δ 7.52 (d, $J = 8.3$ Hz, 2H), 7.20-7.05 (m, 7H), 4.30 (dd, $J = 9.4, 4.6$ Hz, 1H), 3.79-3.68 (m, 1H), 3.66-3.57 (m, 1H), 2.37 (s, 3H), 2.34-2.20 (m, 2H), 1.49-1.38 (m, 2H), 1.36-1.23 (m, 2H), 0.83 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 144.37, 139.11, 136.54, 129.57, 128.56, 127.97, 127.82, 127.62, 61.65, 43.29, 31.22, 31.05, 21.89, 21.58, 13.60. HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{24}\text{O}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 371.1110, found 371.1121.



Yield: 56%. ^1H NMR (500 MHz, CDCl_3) δ 7.56-7.46 (m, 2H), 7.32-7.27 (m, 2H), 7.21-7.13 (m, 3H), 7.12-7.08 (m, 2H), 4.30 (dd, $J = 9.7, 4.6$ Hz, 1H), 3.80-3.70 (m, 1H), 3.70-3.61 (m, 1H), 2.36-2.25 (m, 2H), 1.50-1.37 (m, 2H), 1.37-1.20 (m, 3H), 0.84 (d, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 140.09, 138.64, 137.95, 130.95, 129.40, 129.16, 128.67, 127.84, 61.59, 43.37, 31.24, 31.04, 21.88, 13.59. HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{21}\text{ClO}_2\text{S}_2$ $[\text{M}+\text{Na}]^+$ 391.0564, found 391.0562.



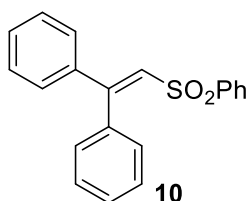
Yield: 80%. ^1H NMR (300 MHz, CDCl_3) δ 7.36-7.25 (m, 5H), 3.91 (dd, $J = 8.2, 6.4$ Hz, 1H), 3.01-2.82 (m, 2H), 2.54-2.40 (m, 2H), 1.51-1.44 (m, 2H), 1.37-1.25 (m, 2H), 0.83 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 134.71, 129.17, 128.56, 127.48, 119.97, 39.19, 37.64, 32.75, 31.55, 21.83, 13.59. HRMS (ESI, m/z) calcd for $\text{C}_{13}\text{H}_{17}\text{NS}$ $[\text{M}+\text{H}]^+$ 220.1154, found 220.1155.



Yield: 63%. ^1H NMR (400 MHz, CDCl_3) δ 7.33-7.25 (m, 2H), 7.21-7.09 (m, 3H), 5.63 (m, 1H), 5.03-4.87 (m, 2H), 2.88-2.68 (m, 3H), 2.62-2.52 (m, 1H), 2.45-2.32 (m, 3H), 1.53-1.44 (m, 2H), 1.38-1.28 (m, 2H), 0.86 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 143.76, 136.30, 128.38, 127.68, 126.57, 116.52, 46.00, 39.70, 38.54, 32.48, 31.76, 21.98, 13.68. HRMS (ESI, m/z) calcd for $\text{C}_{15}\text{H}_{22}\text{S}$ $[\text{M}+\text{H}]^+$ 235.1515, found 235.1514.

IPrAuSCF_3 (**8**)

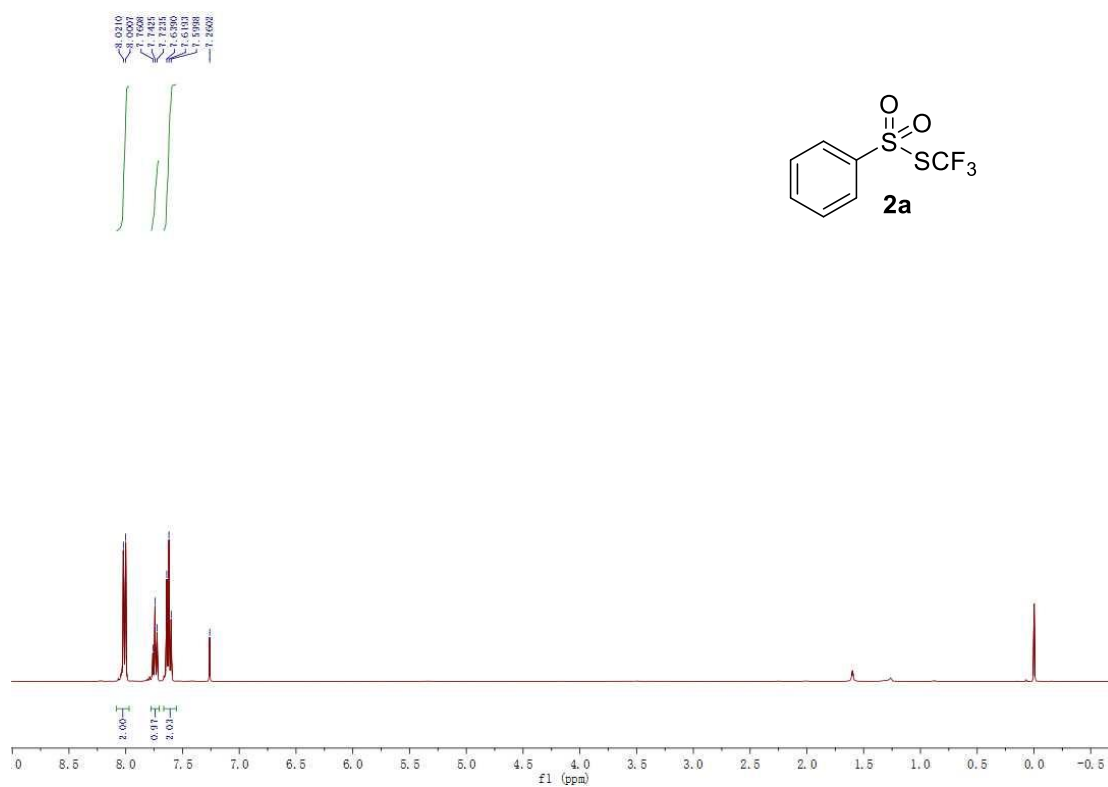
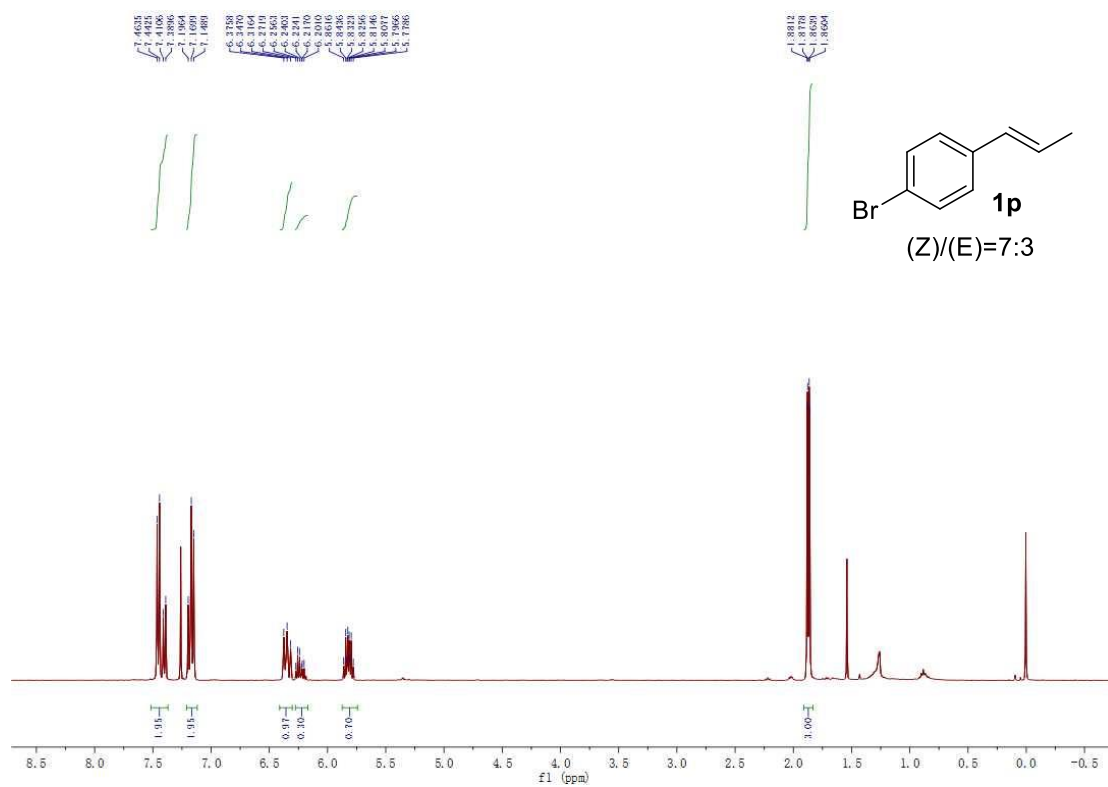
^1H NMR (400 MHz, CD_3CN) δ 7.62-7.48 (m, 4H), 7.45-7.32 (m, 4H), 2.56 (m, 4H), 1.29 (d, $J = 6.9$ Hz, 12H), 1.23 (d, $J = 6.9$ Hz, 12H). ^{13}C NMR (100 MHz, CD_3CN) δ 165.45, 145.94, 133.99, 130.63, 124.12, 117.32, 28.63, 23.54, 23.12 (SCF_3 was not observed). ^{19}F NMR (282 MHz, CDCl_3) δ -22.49. HRMS (ESI, m/z) calcd for $\text{C}_{28}\text{H}_{36}\text{AuF}_3\text{N}_2\text{S}$ $[\text{M}+\text{H}]^+$ 687.2290, found 687.2293.

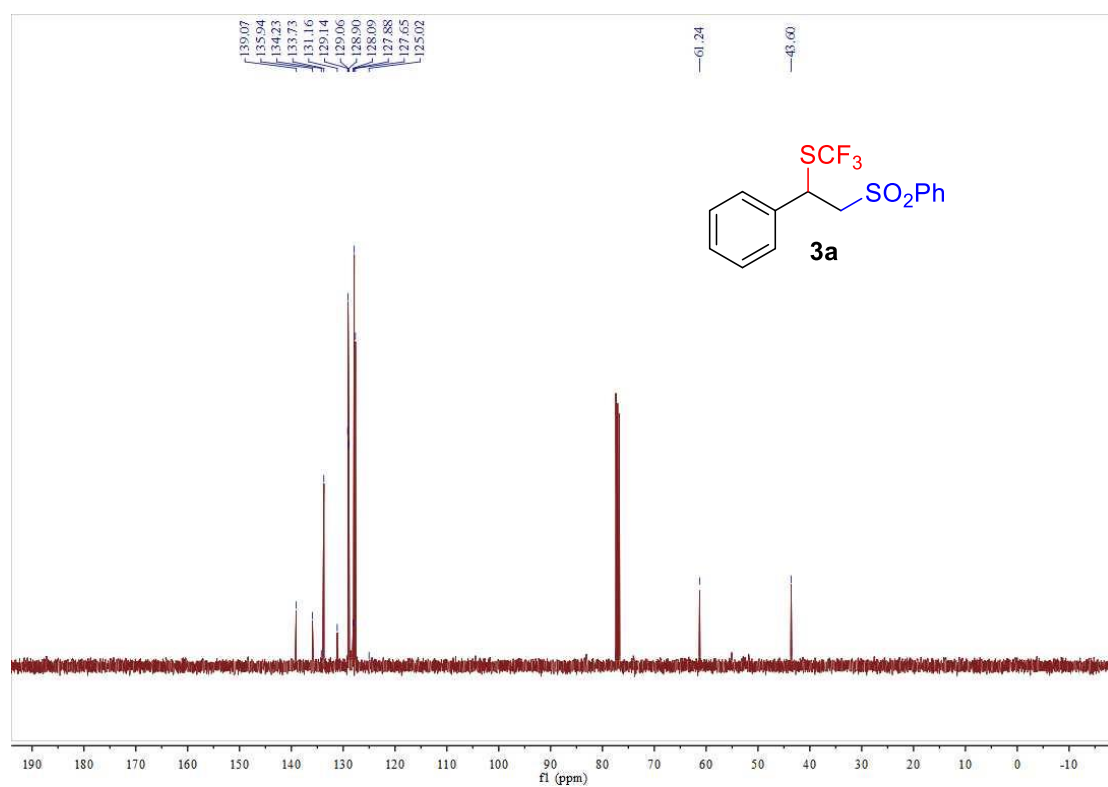
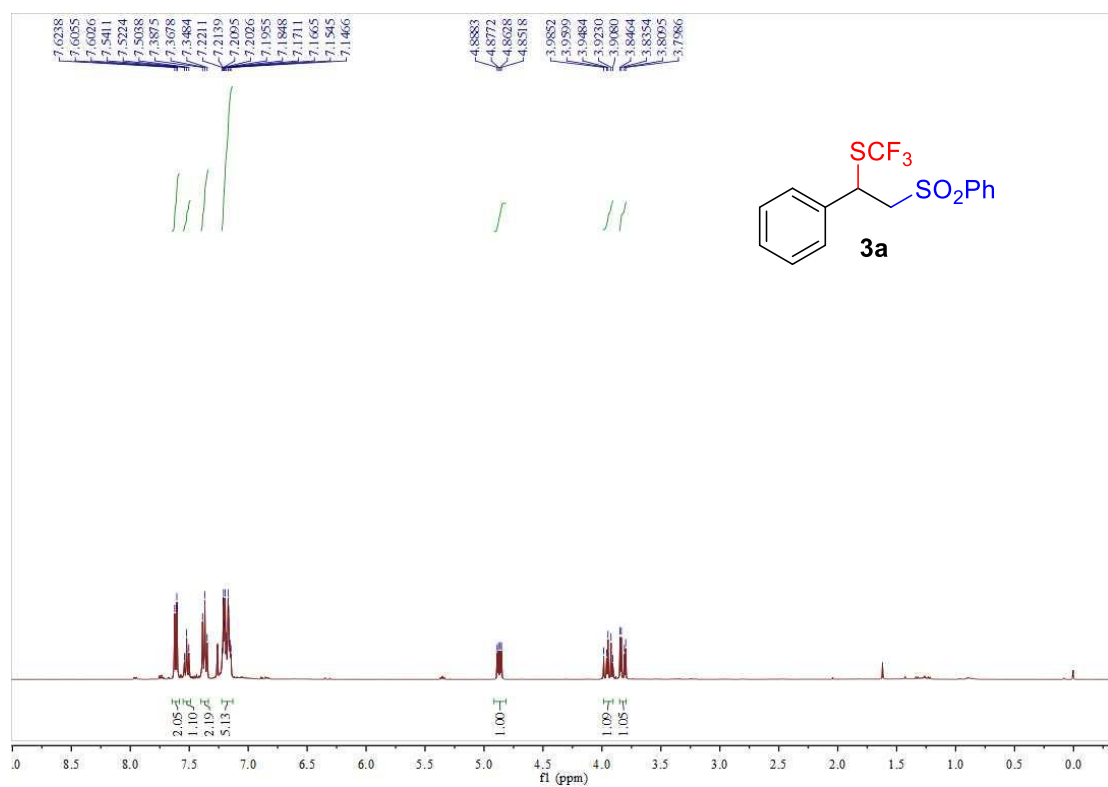


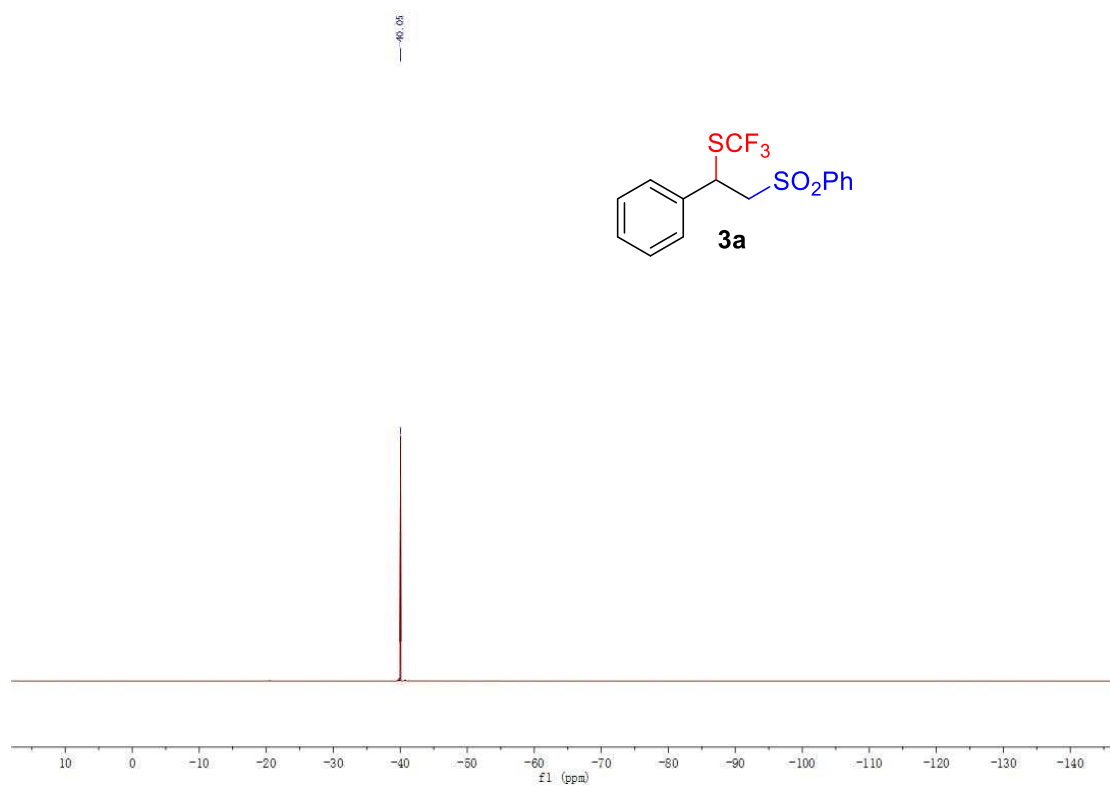
Known compound⁵. ^1H NMR (400 MHz, CDCl_3) δ 7.59 (d, $J = 7.5$ Hz, 2H), 7.53-7.45 (m, 1H), 7.40-7.25 (m, 8H), 7.24-7.19 (m, 2H), 7.12-7.06 (m, 2H), 7.04 (s, 1H).

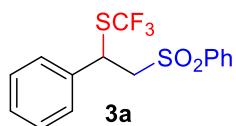
(5) Russell, G. A.; Ngoviwatchai, P.; Tashtoush, H. 1.; Pla-Dalmau, A.; Khanna, R. K. *J. Am. Chem. Soc.* **1988**, *110*, 3530.

NMR spectra for the products









Chemical Formula: $C_{15}H_{13}F_3O_2S_2$

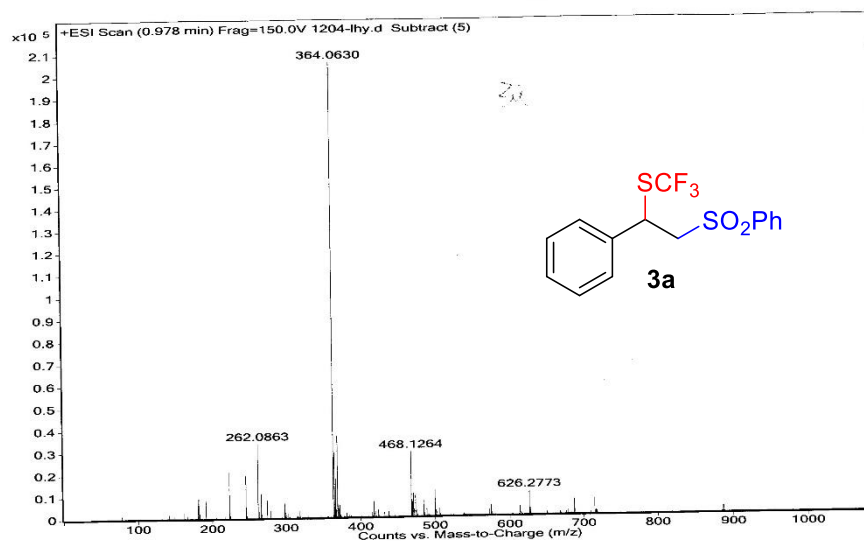
Exact Mass: 346.0309

Molecular Weight: 346.3822

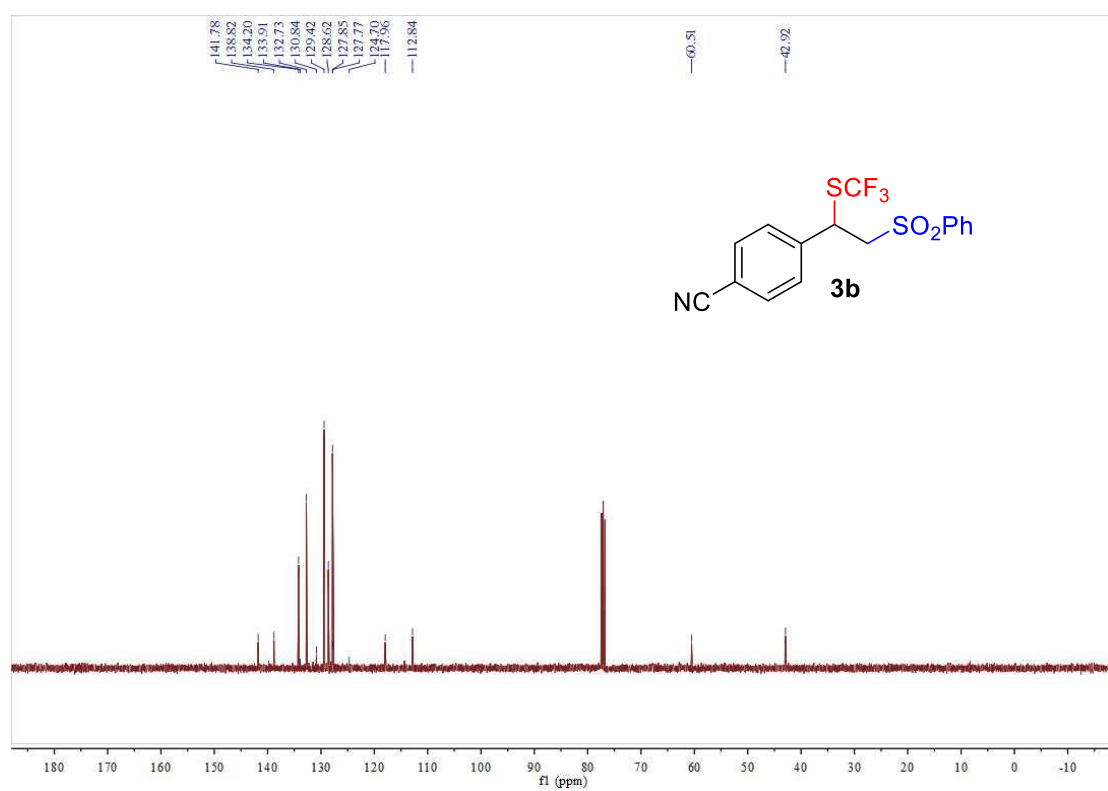
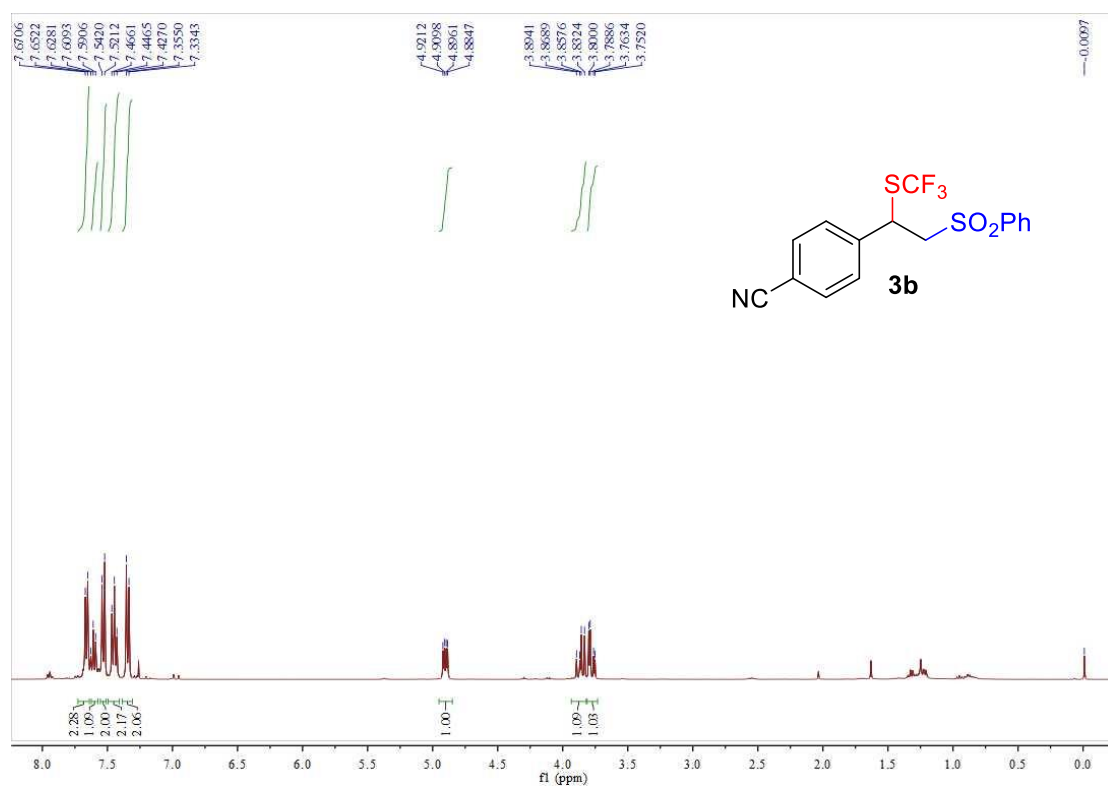
m/z: 346.0309 (100.0%), 347.0343 (16.2%), 348.0267 (9.0%),
347.0303 (1.6%), 349.0301 (1.5%), 348.0376 (1.2%)

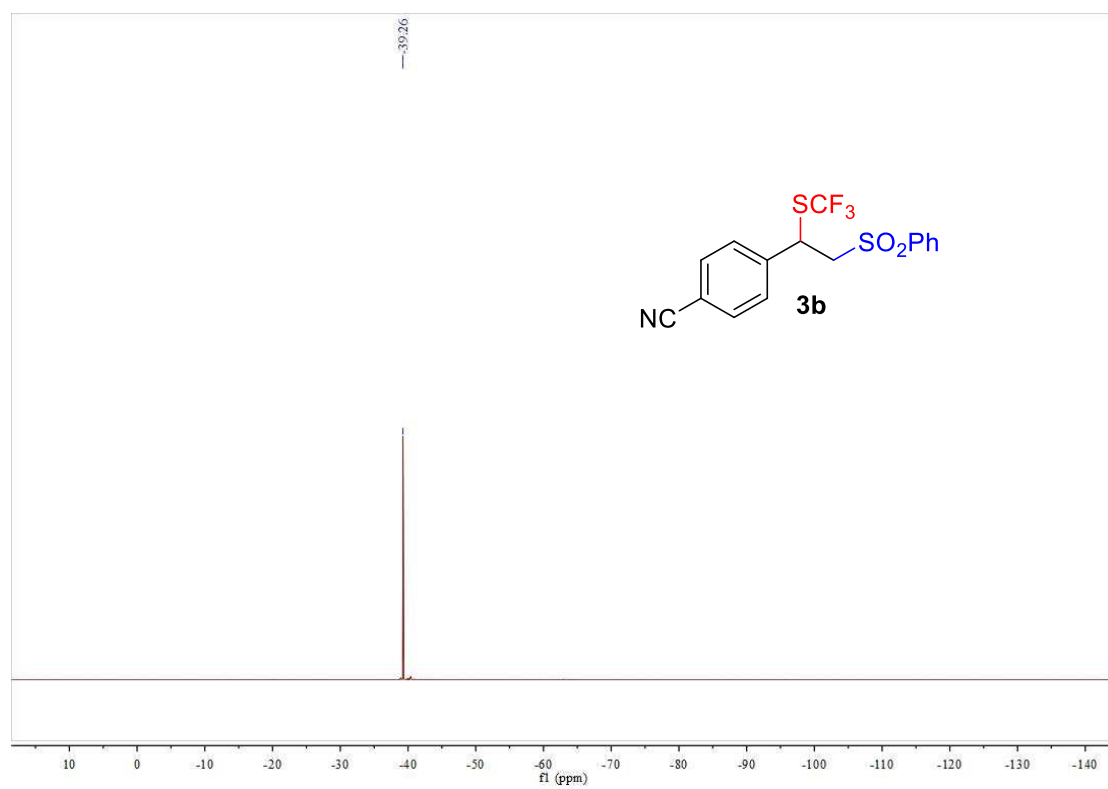
Elemental Analysis: C, 52.01; H, 3.78; F, 16.45; O, 9.24; S, 18.51

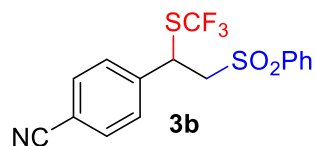
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	1204-lhy.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



HRMS (ESI, m/z) calcd for $C_{15}H_{13}F_3O_2S_2$ $[M+NH_4]^+$ 364.0647, found 364.0630.







Chemical Formula: $C_{16}H_{12}F_3NO_2S_2$

Exact Mass: 371.0262

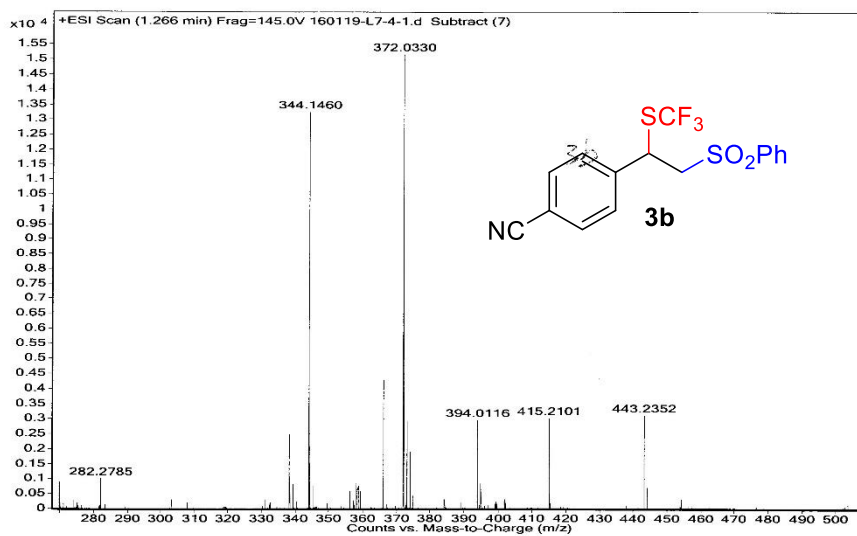
Molecular Weight: 371.3922

m/z : 371.0262 (100.0%), 372.0295 (17.3%), 373.0220 (9.0%), 372.0255 (1.6%),

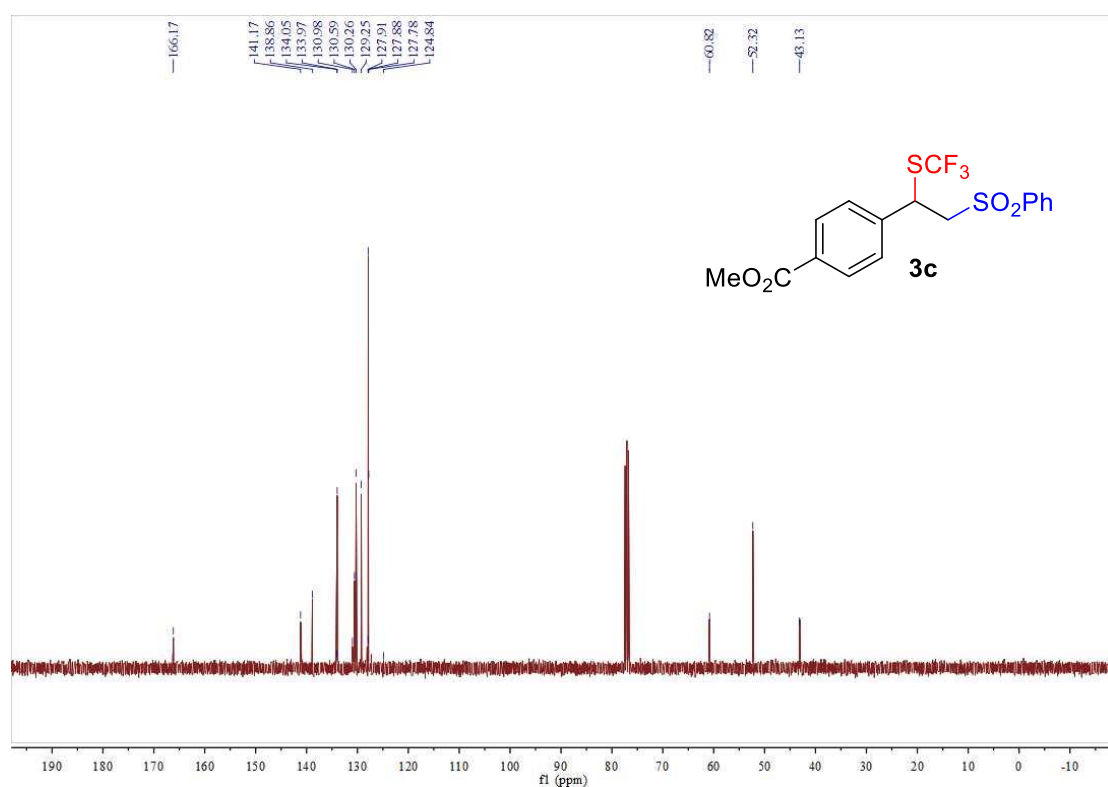
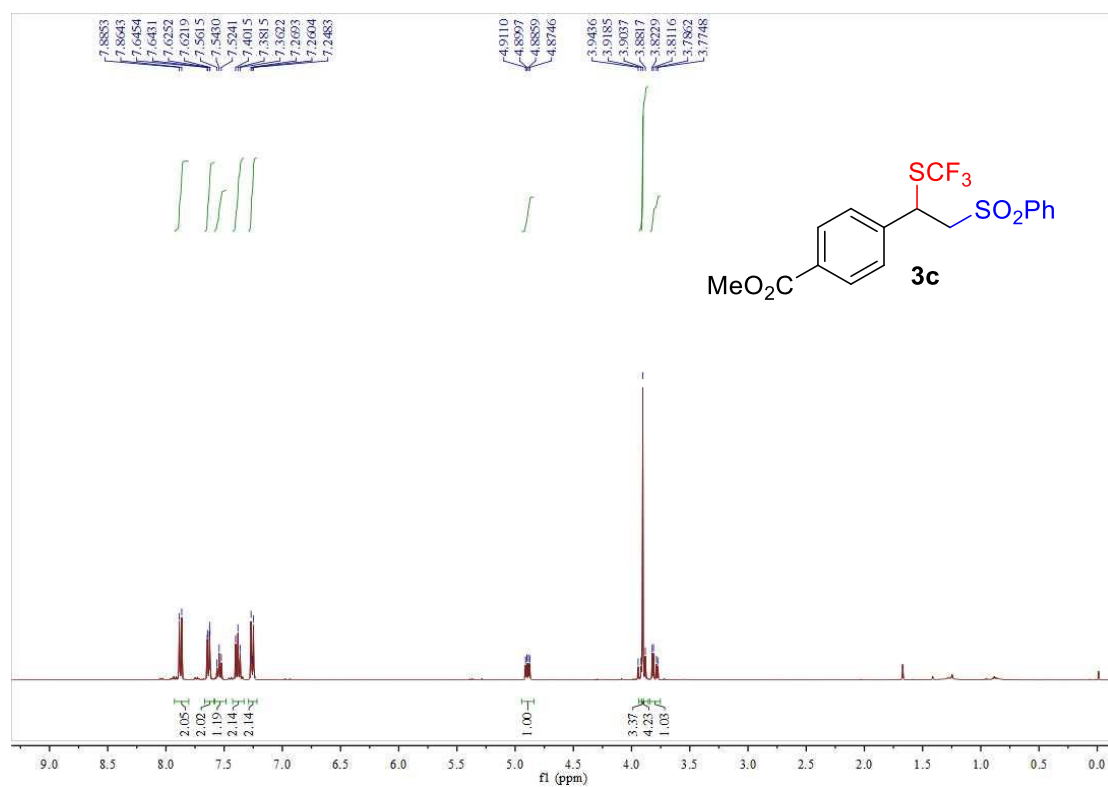
374.0253 (1.6%), 373.0329 (1.4%)

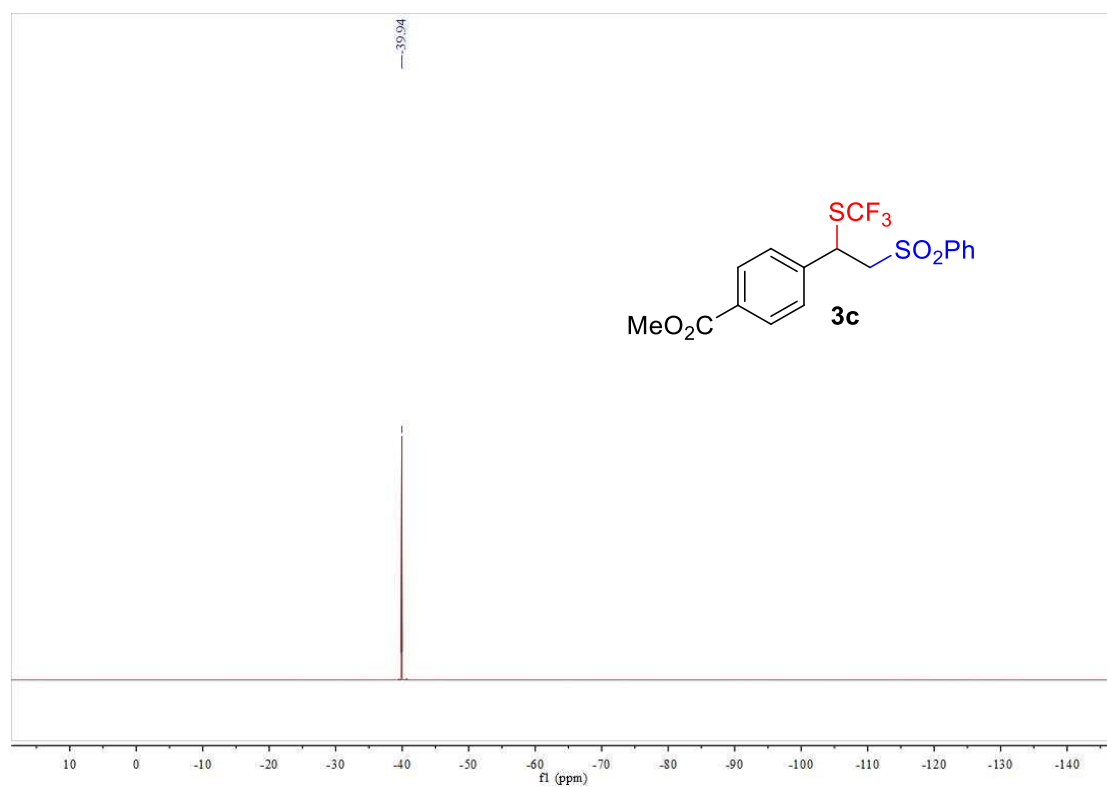
Elemental Analysis: C, 51.74; H, 3.26; F, 15.35; N, 3.77; O, 8.62; S, 17.26

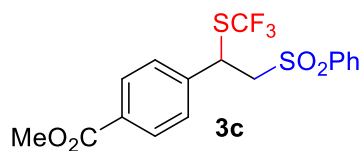
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	160119-L7-4-1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



HRMS (ESI, m/z) calcd for $C_{16}H_{12}F_3NO_2S_2$ $[M+H]^+$ 372.0334, found 372.0330.







Chemical Formula: $C_{17}H_{15}F_3O_4S_2$

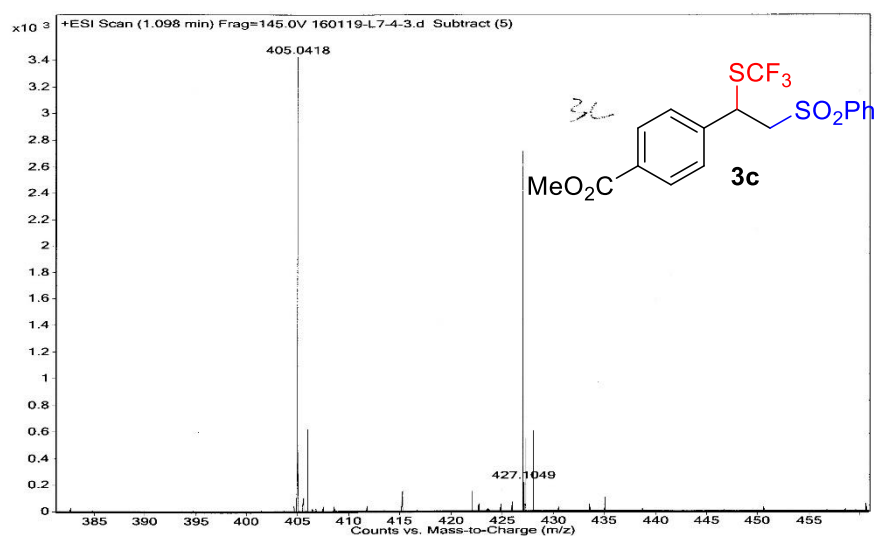
Exact Mass: 404.0364

Molecular Weight: 404.4182

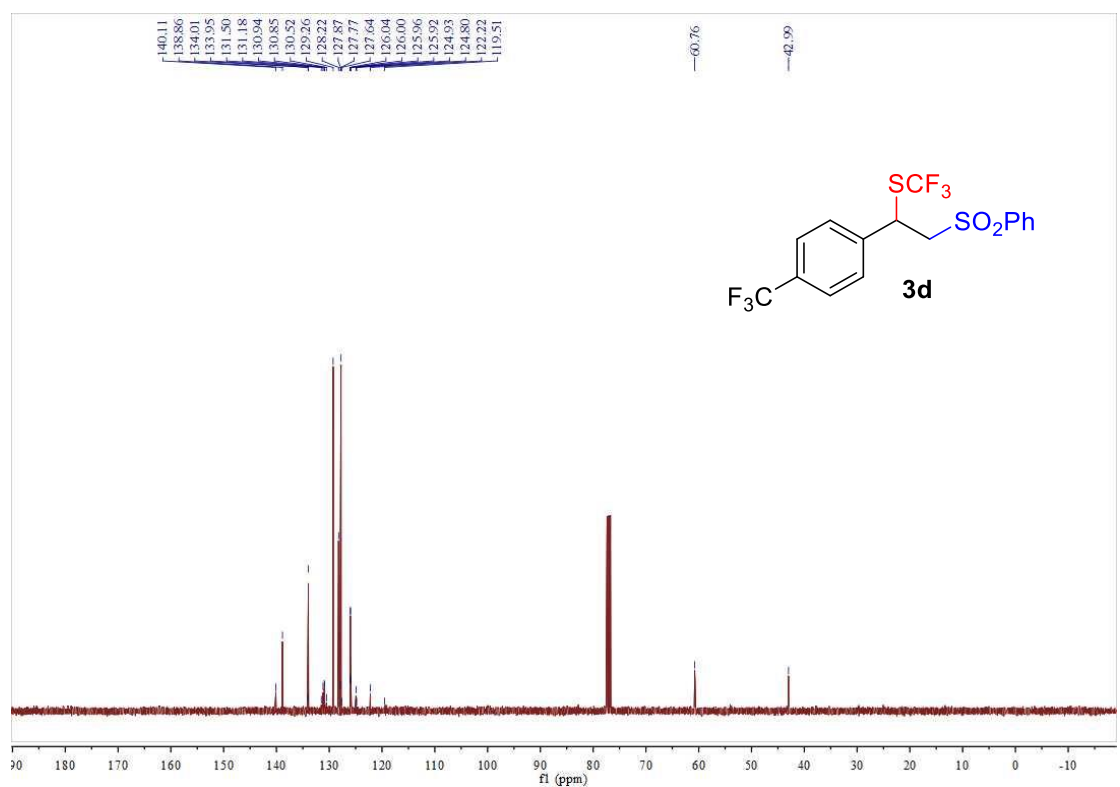
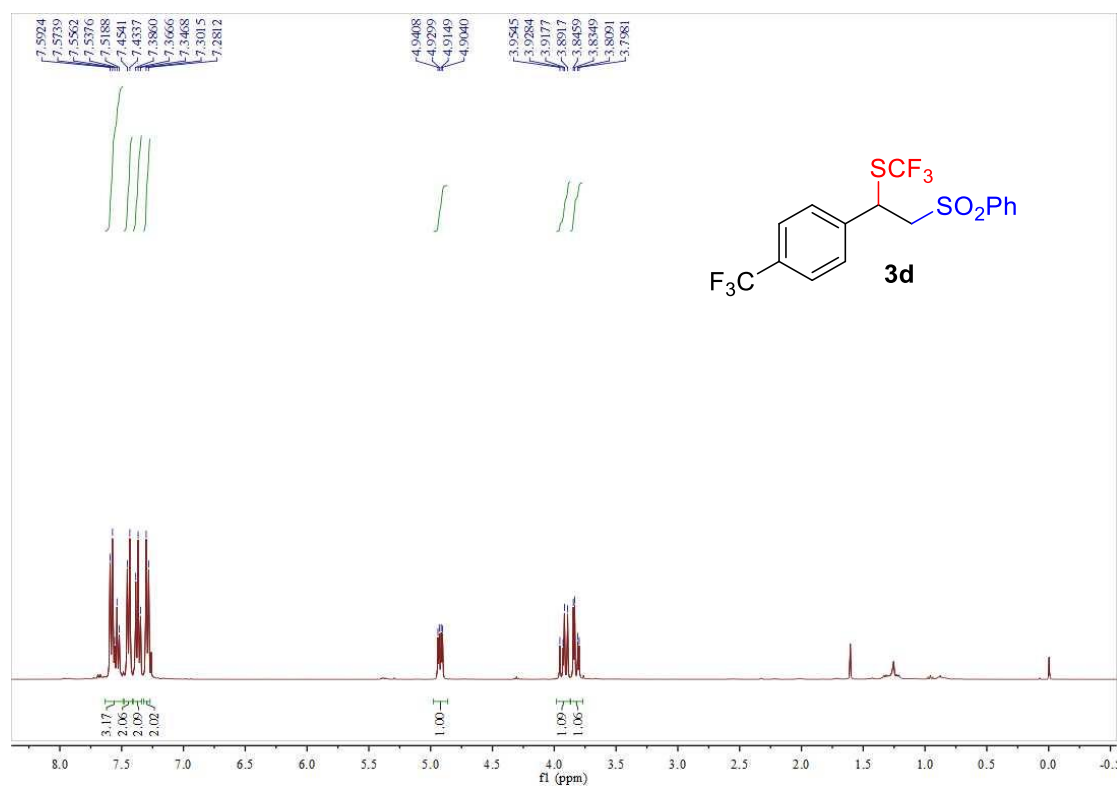
m/z : 404.0364 (100.0%), 405.0397 (18.4%), 406.0322 (9.0%),
407.0355 (1.7%), 405.0358 (1.6%), 406.0431 (1.6%)

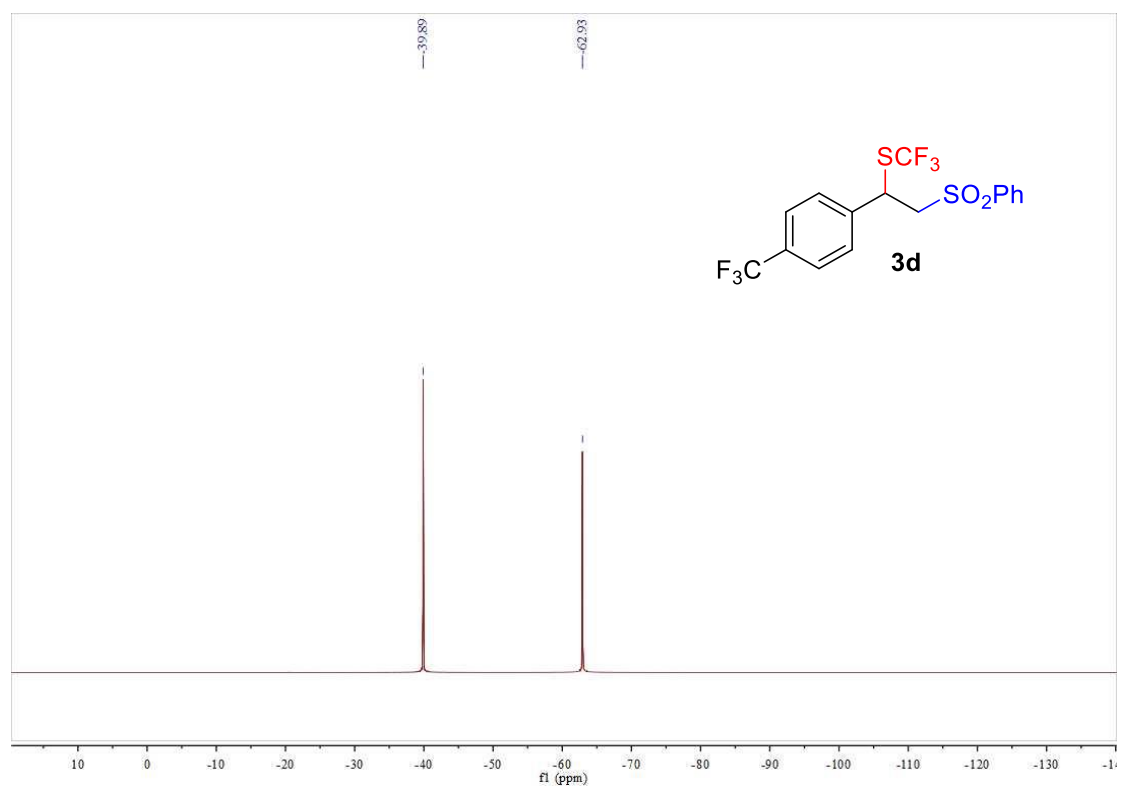
Elemental Analysis: C, 50.49; H, 3.74; F, 14.09; O, 15.82; S, 15.85

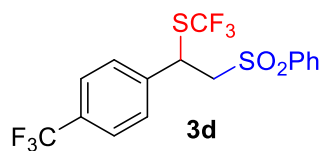
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	160119-L7-4-3.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



HRMS (ESI, m/z) calcd for $C_{17}H_{15}F_3O_4S_2$ $[M+H]^+$ 405.0437, found 405.0418.







Chemical Formula: C₁₆H₁₂F₆O₂S₂

Exact Mass: 414.0183

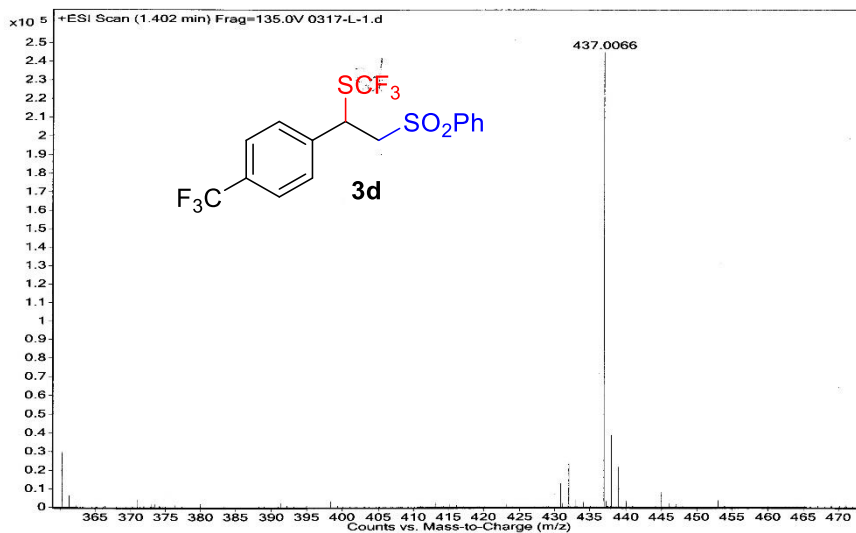
Molecular Weight: 414.3804

m/z: 414.0183 (100.0%), 415.0216 (17.3%), 416.0141 (9.0%), 415.0177 (1.6%), 417.0174 (1.6%), 416.0250 (1.4%)

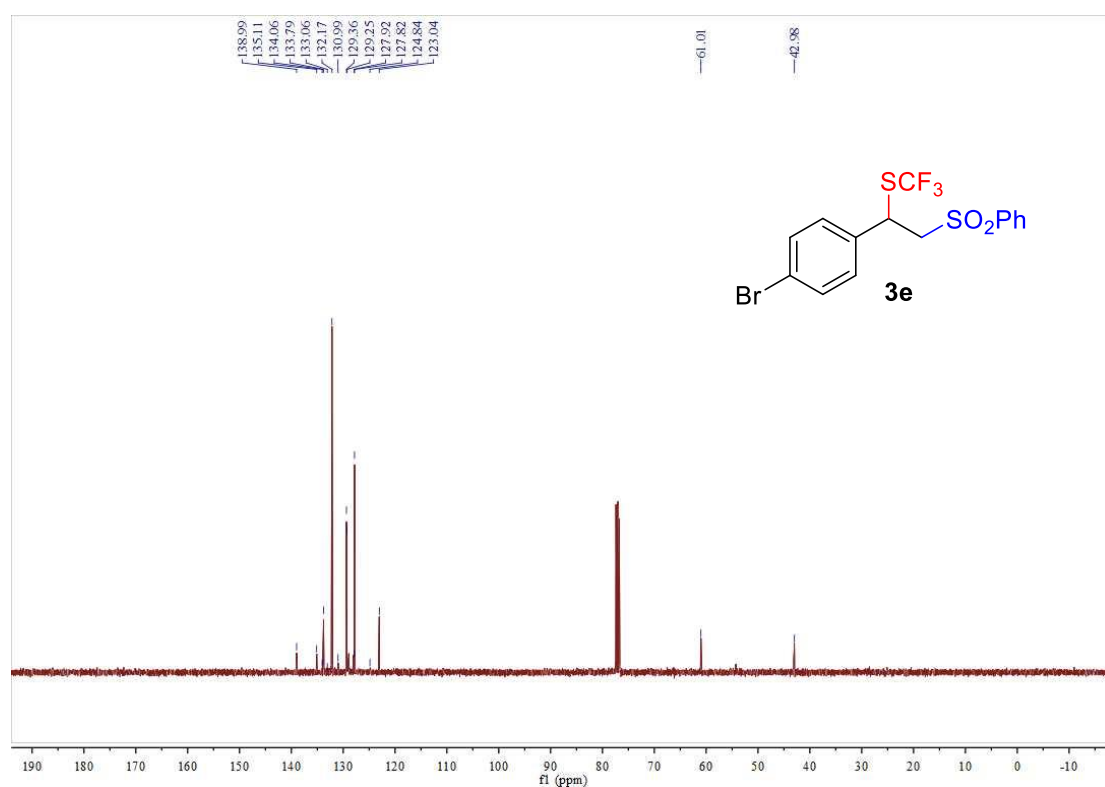
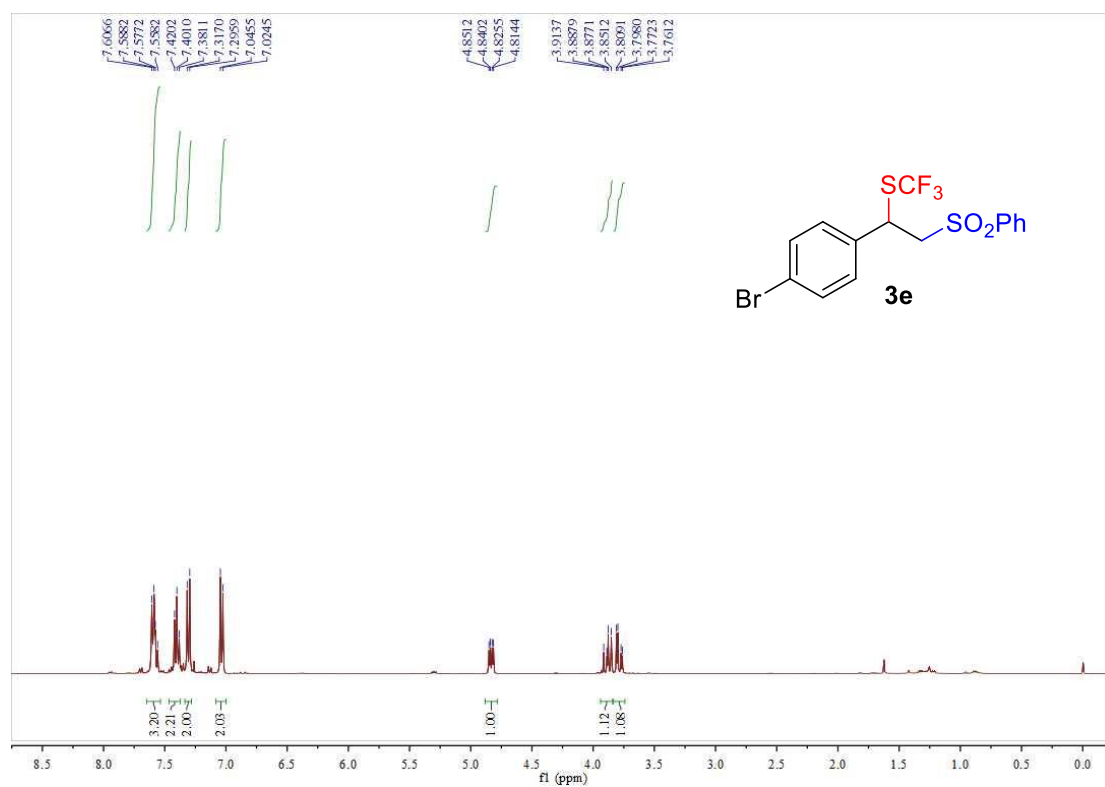
Elemental Analysis: C, 46.38; H, 2.92; F, 27.51; O, 7.72; S, 15.47

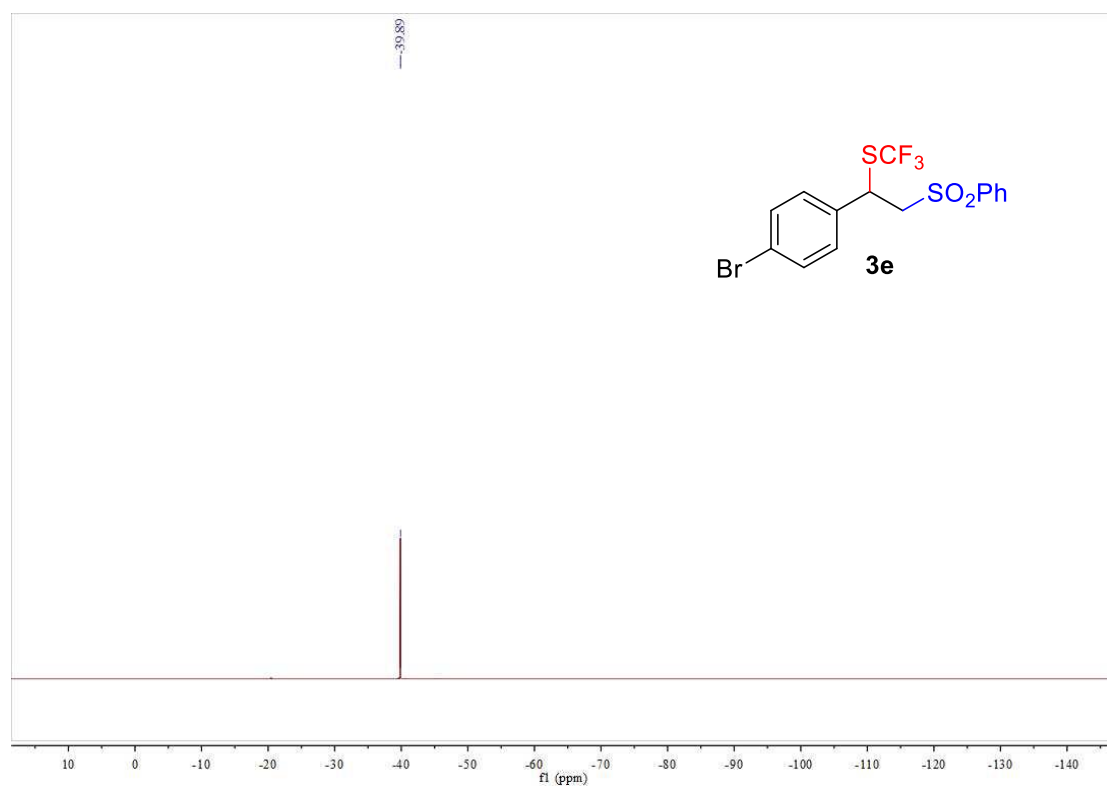
Sample Name	Position	Instrument Name	User Name
0317-L-1	P1-F2	Instrument 1	
Inj Vol	InjPosition	SampleType	IRM Calibration Status
0317-L-1.d	ACQ Method	Comment	Acquired Time

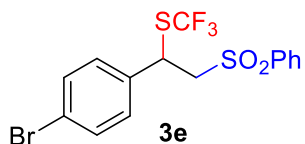
Success
3/14/2016 12:24:59 PM



HRMS (ESI, m/z) calcd for C₁₆H₁₂F₆O₂S₂ [M+Na]⁺ 437.0075, found 437.0075.







Chemical Formula: C₁₅H₁₂BrF₃O₂S₂

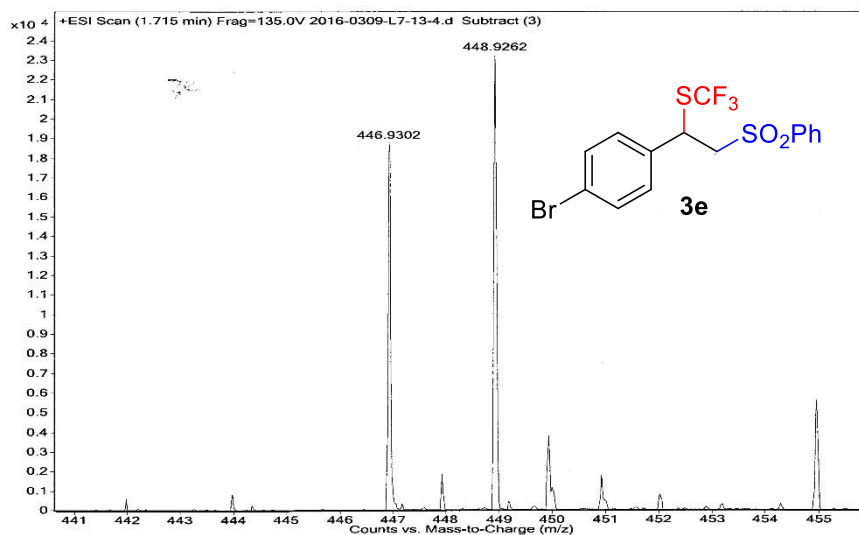
Exact Mass: 423.9414

Molecular Weight: 425.2782

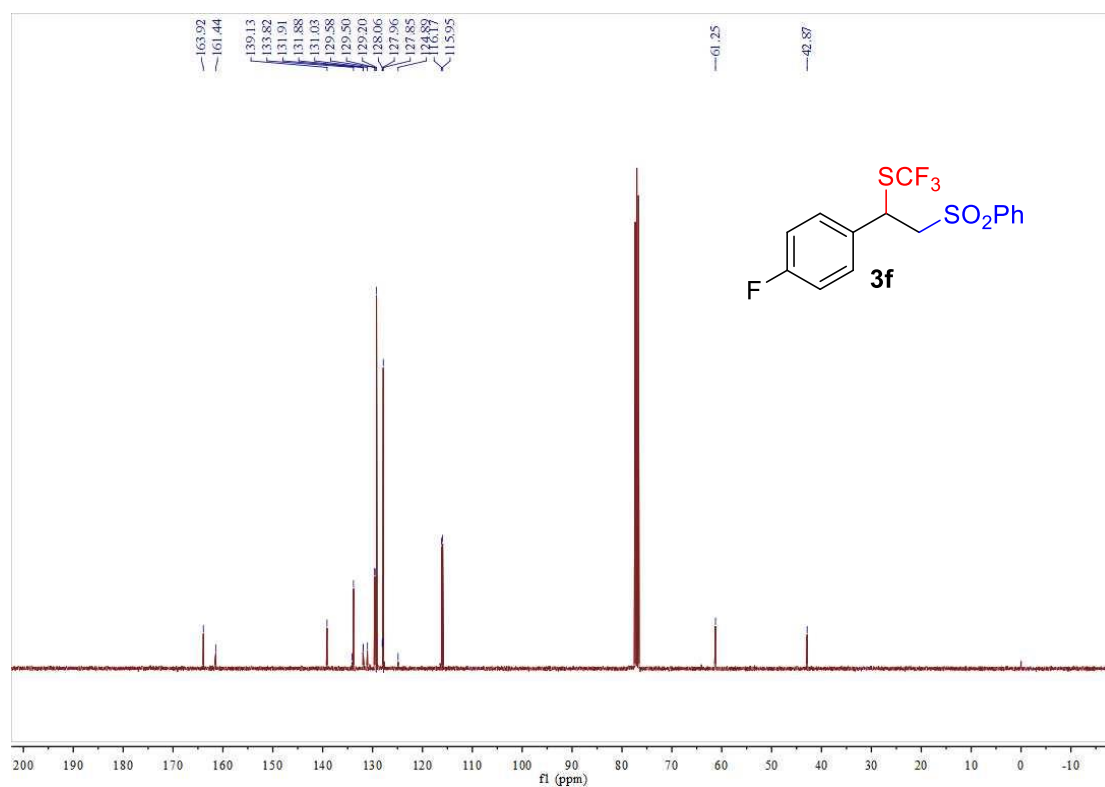
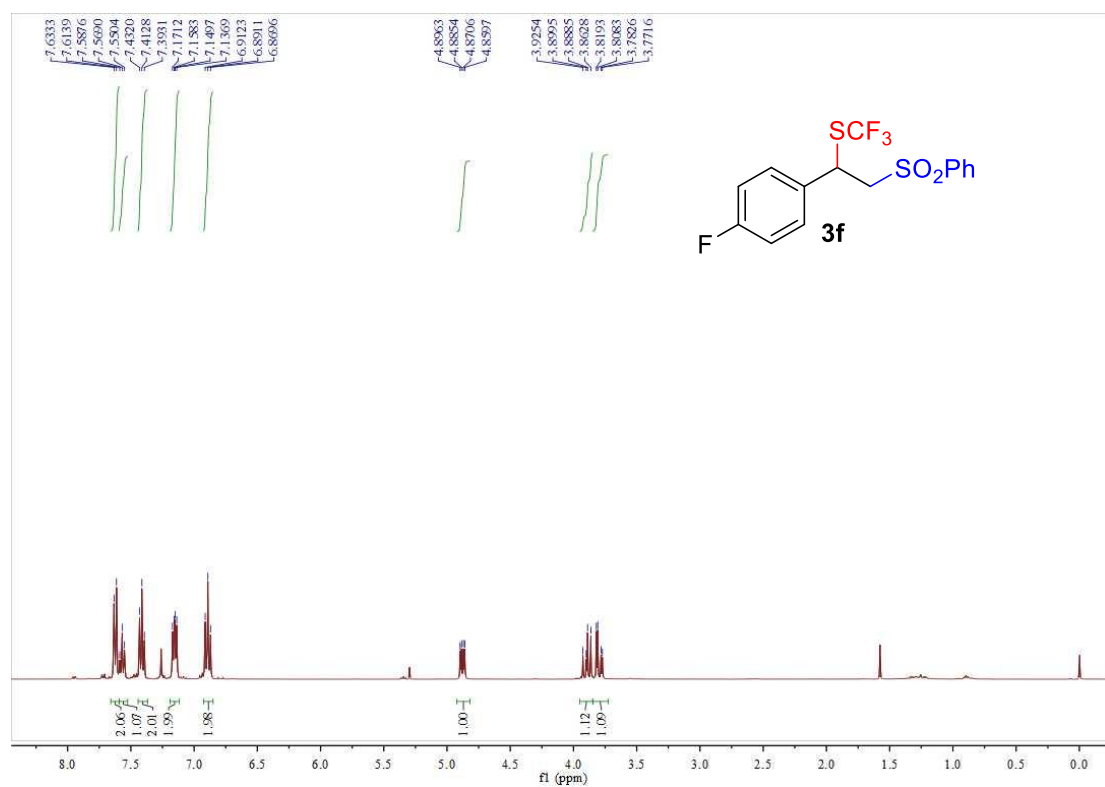
m/z: 423.9414 (100.0%), 425.9394 (97.3%), 424.9448 (16.2%), 426.9427 (15.8%),
425.9372 (9.0%), 427.9352 (8.8%), 424.9408 (1.6%), 426.9388 (1.6%),
426.9406 (1.5%), 428.9385 (1.4%), 425.9481 (1.2%), 427.9461 (1.2%)

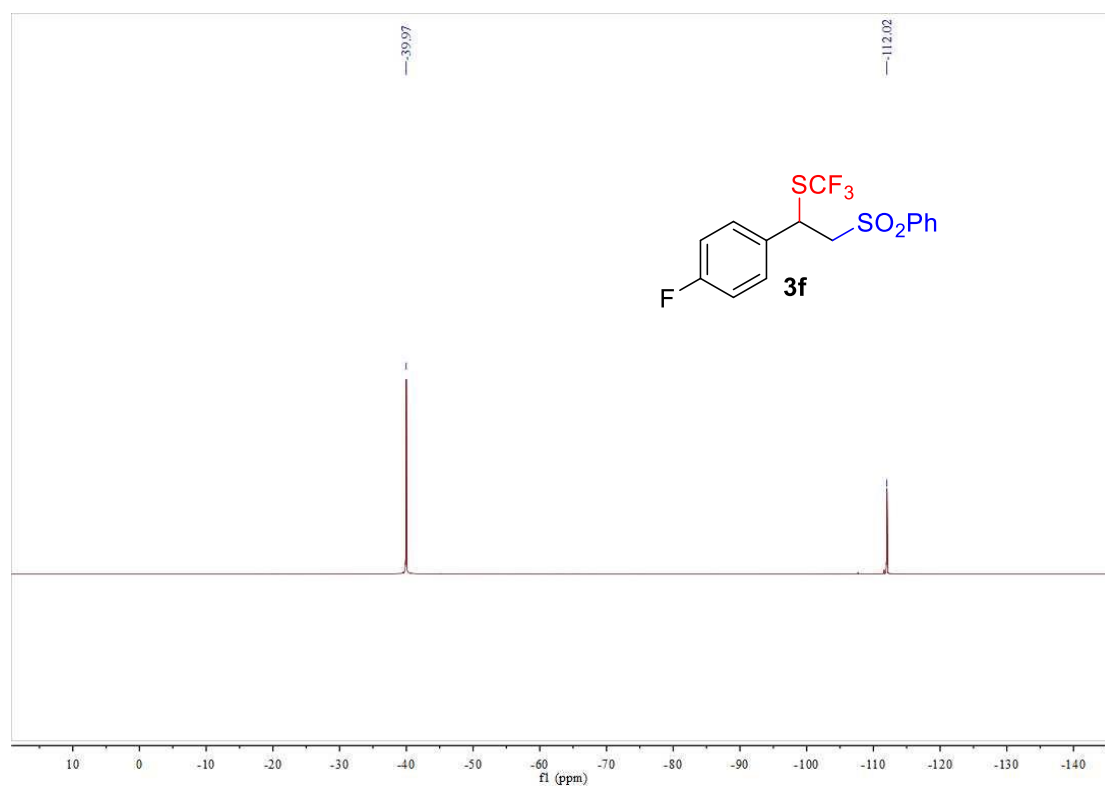
Elemental Analysis: C, 42.36; H, 2.84; Br, 18.79; F, 13.40; O, 7.52; S, 15.08

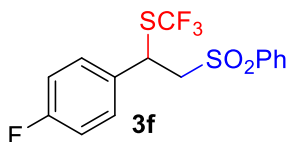
Sample Name	2016-0309-L7-13-4	Position	P1-D9	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	2016-0309-L7-13-4.d	ACQ Method	0103.m	Comment		Acquired Time	3/6/2016 2:48:37 PM



HRMS (ESI, m/z) calcd for C₁₅H₁₂BrF₃O₂S₂ [M+Na]⁺ 446.9306, found 446.9302.







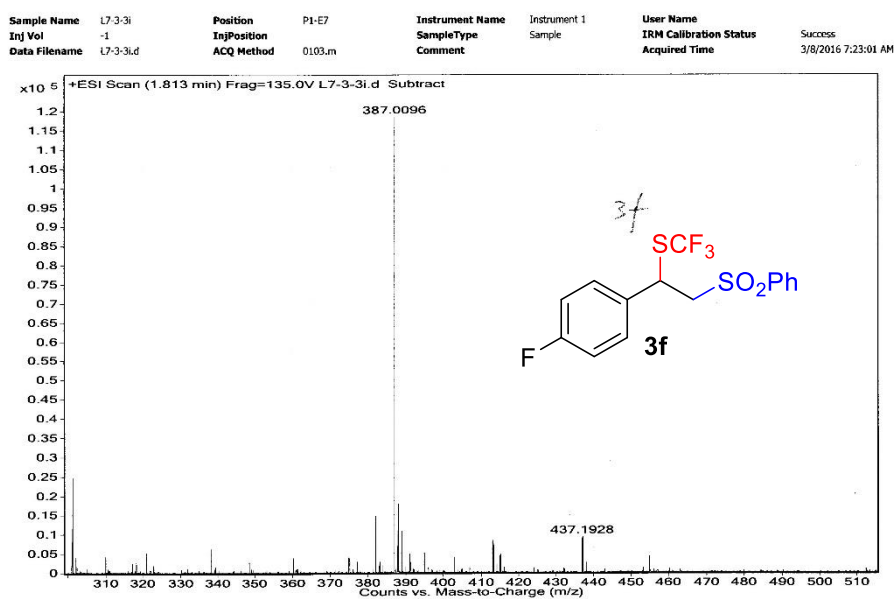
Chemical Formula: $C_{15}H_{12}F_4O_2S_2$

Exact Mass: 364.0215

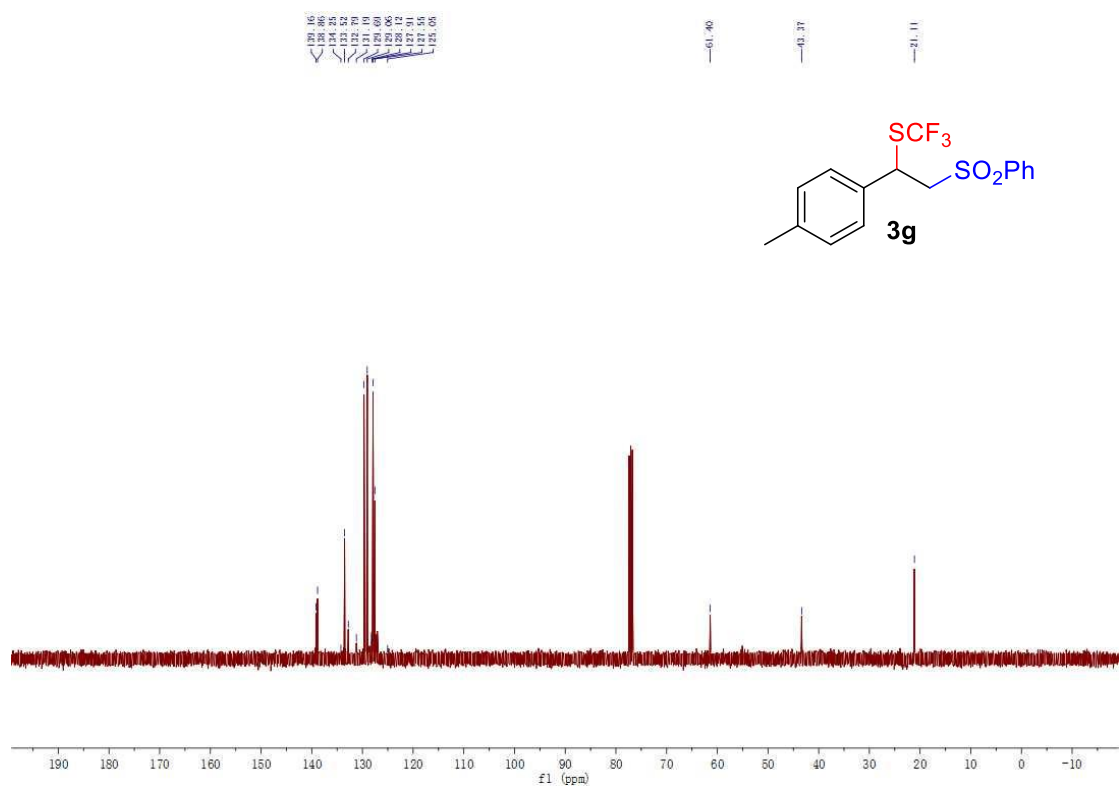
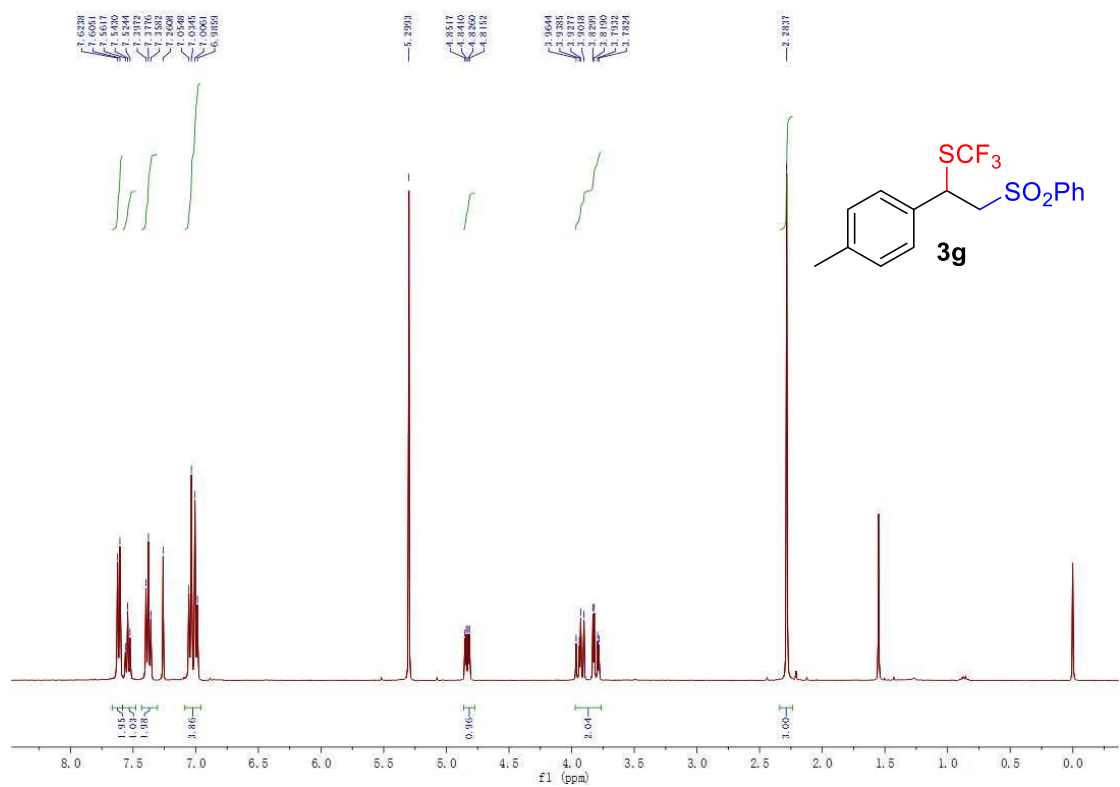
Molecular Weight: 364.3726

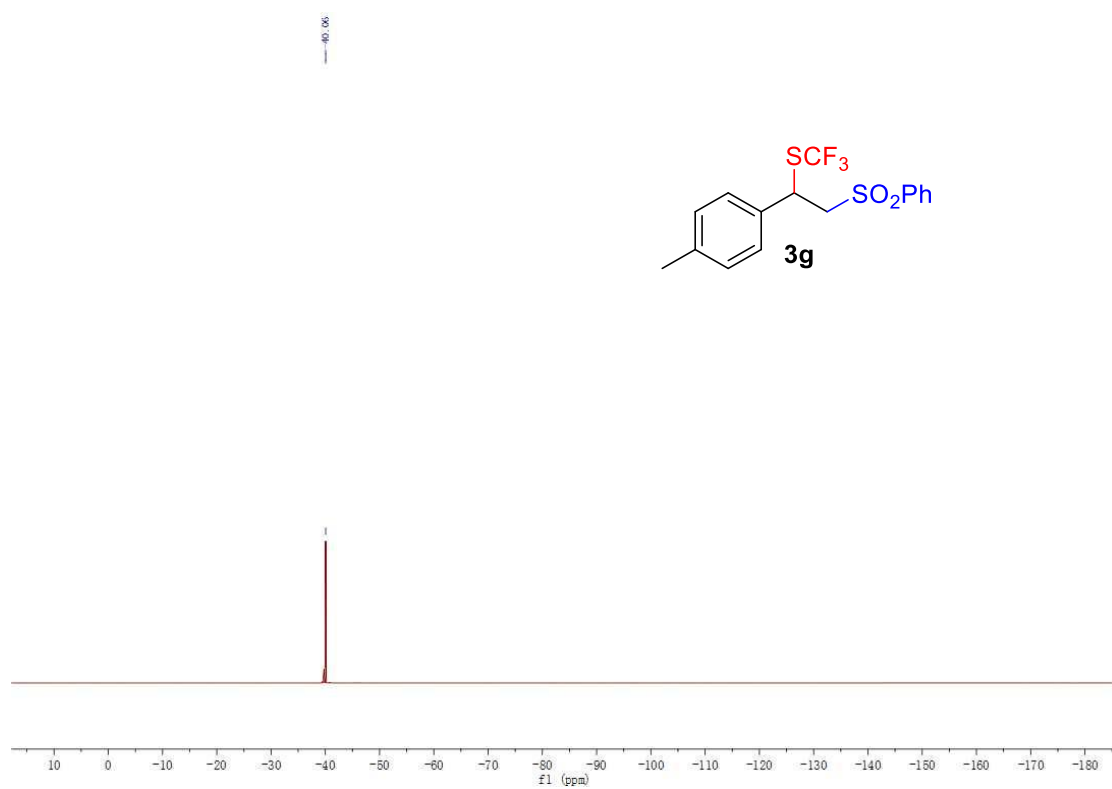
m/z: 364.0215 (100.0%), 365.0248 (16.2%), 366.0173 (9.0%), 365.0209 (1.6%),
367.0206 (1.5%), 366.0282 (1.2%)

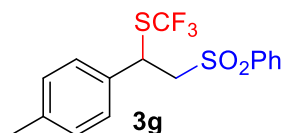
Elemental Analysis: C, 49.45; H, 3.32; F, 20.86; O, 8.78; S, 17.60



HRMS (ESI, m/z) calcd for $C_{15}H_{12}F_4O_2S_2$ $[M+Na]^+$ 387.0107, found 387.0096.







Chemical Formula: $C_{16}H_{15}F_3O_2S_2$

Exact Mass: 360.0466

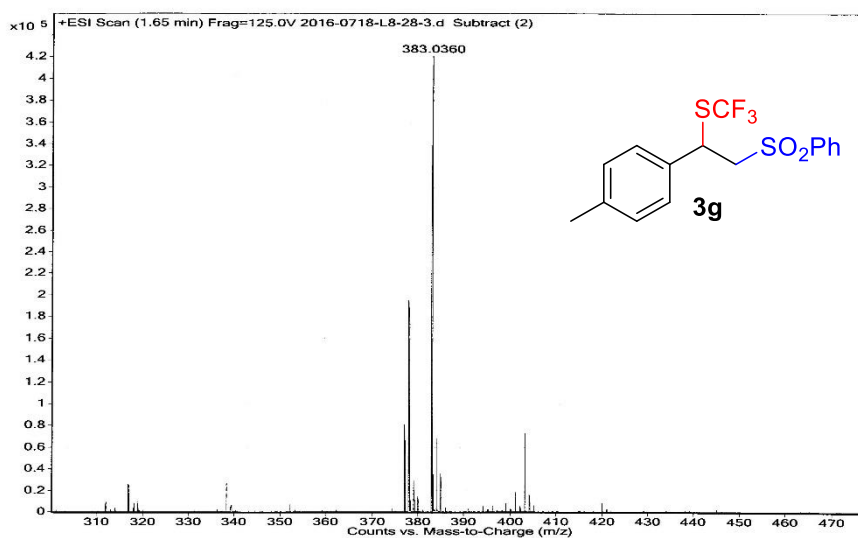
Molecular Weight: 360.4092

m/z: 360.0466 (100.0%), 361.0499 (17.3%), 362.0424 (9.0%), 361.0459 (1.6%),

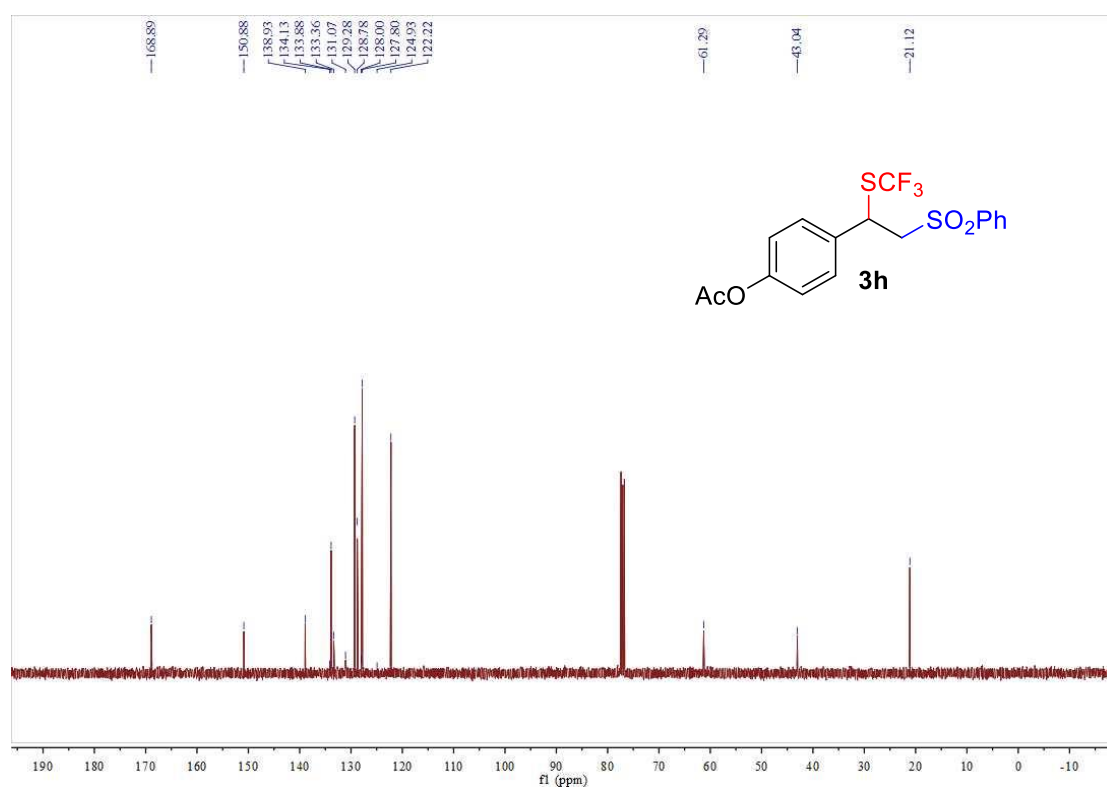
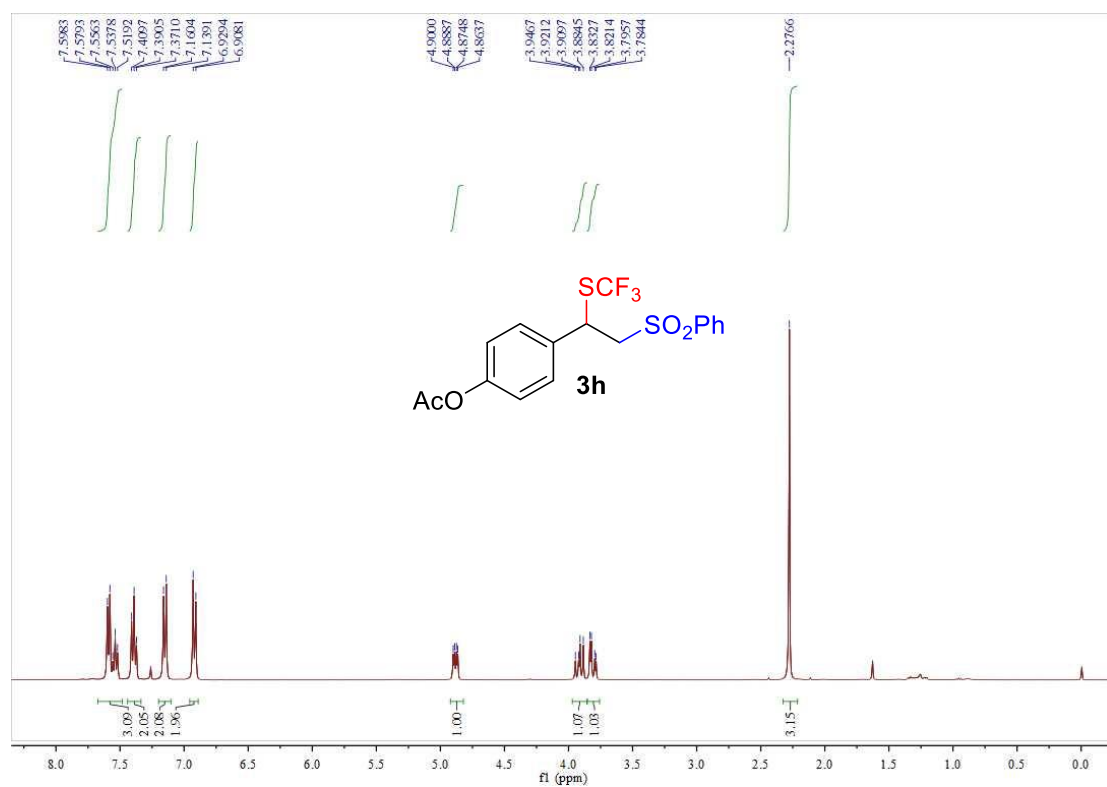
363.0457 (1.6%), 362.0533 (1.4%)

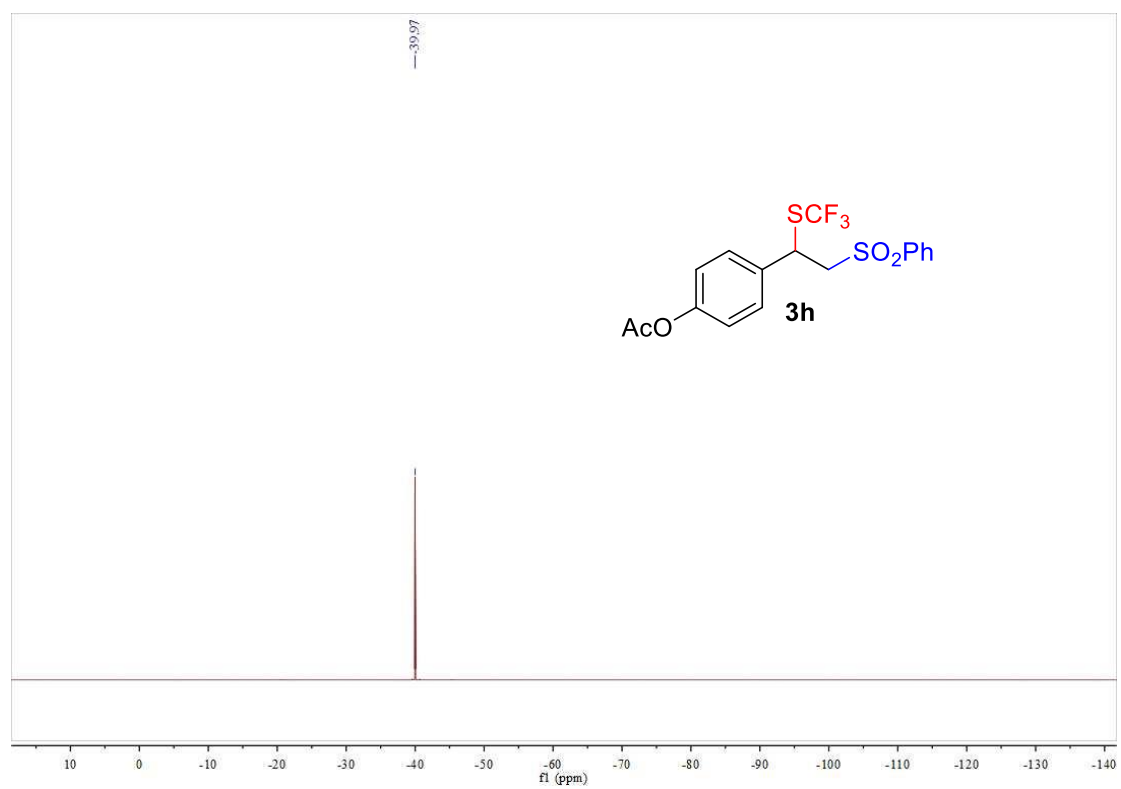
Elemental Analysis: C, 53.32; H, 4.20; F, 15.81; O, 8.88; S, 17.79

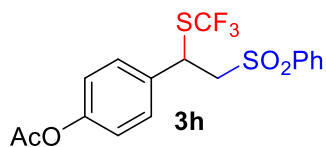
Sample Name	2016-0718-L8-28-3	Position	P1-F9	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	2016-0718-L8-28-3.d	ACQ Method	0103.m	Comment		Acquired Time	7/18/2016 3:41:36 PM



HRMS (ESI, m/z) calcd for $C_{16}H_{15}F_3O_2S_2$ $[M+Na]^+$ 383.0358, found 383.0360.







Chemical Formula: $C_{17}H_{15}F_3O_4S_2$

Exact Mass: 404.0364

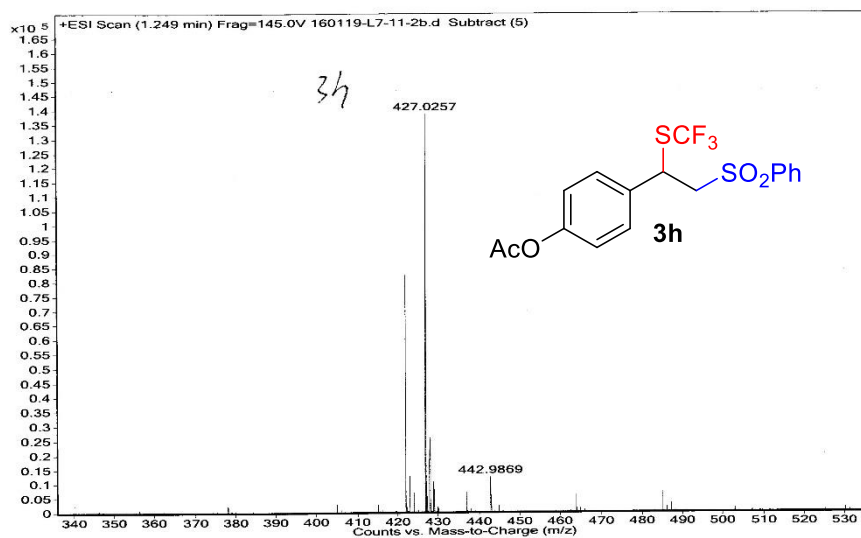
Molecular Weight: 404.4182

m/z : 404.0364 (100.0%), 405.0397 (18.4%), 406.0322 (9.0%),

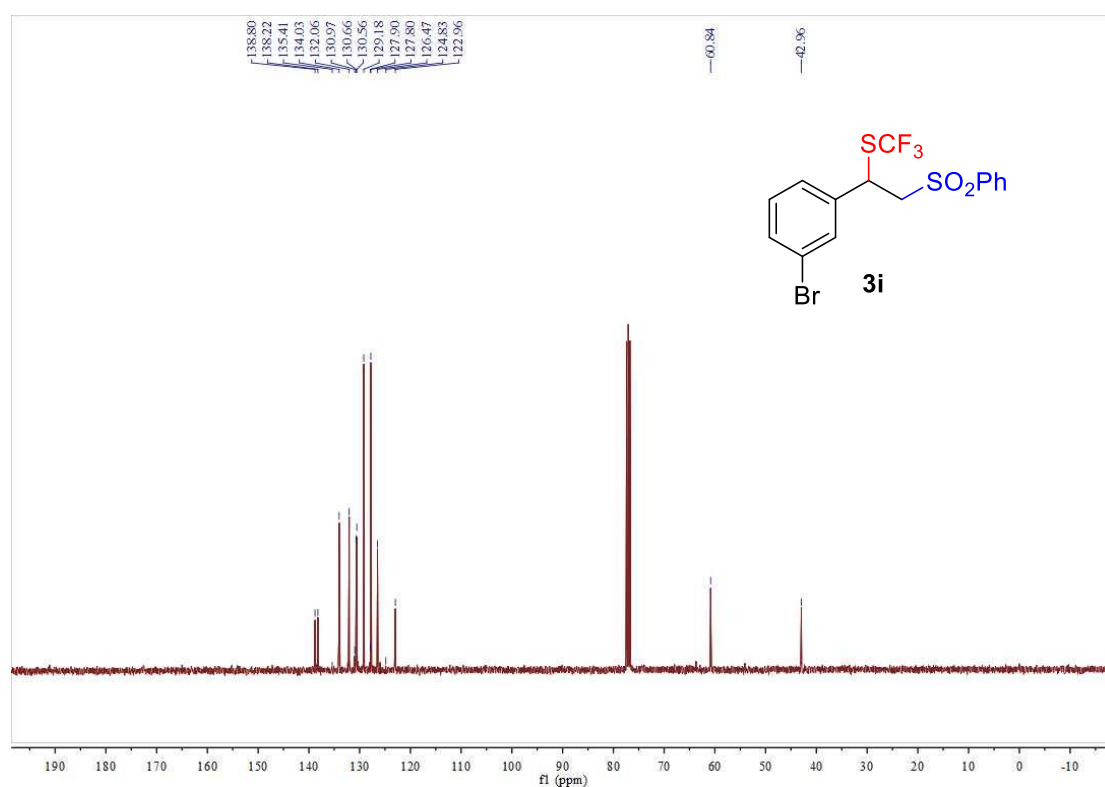
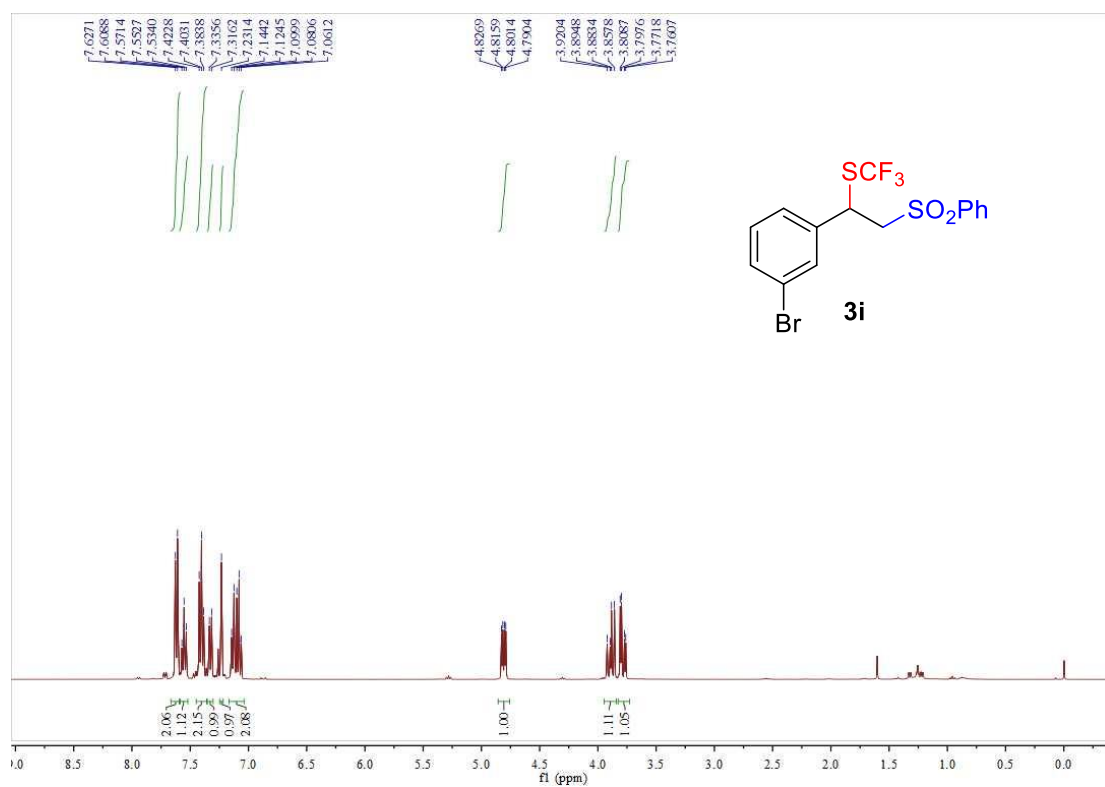
407.0355 (1.7%), 405.0358 (1.6%), 406.0431 (1.6%)

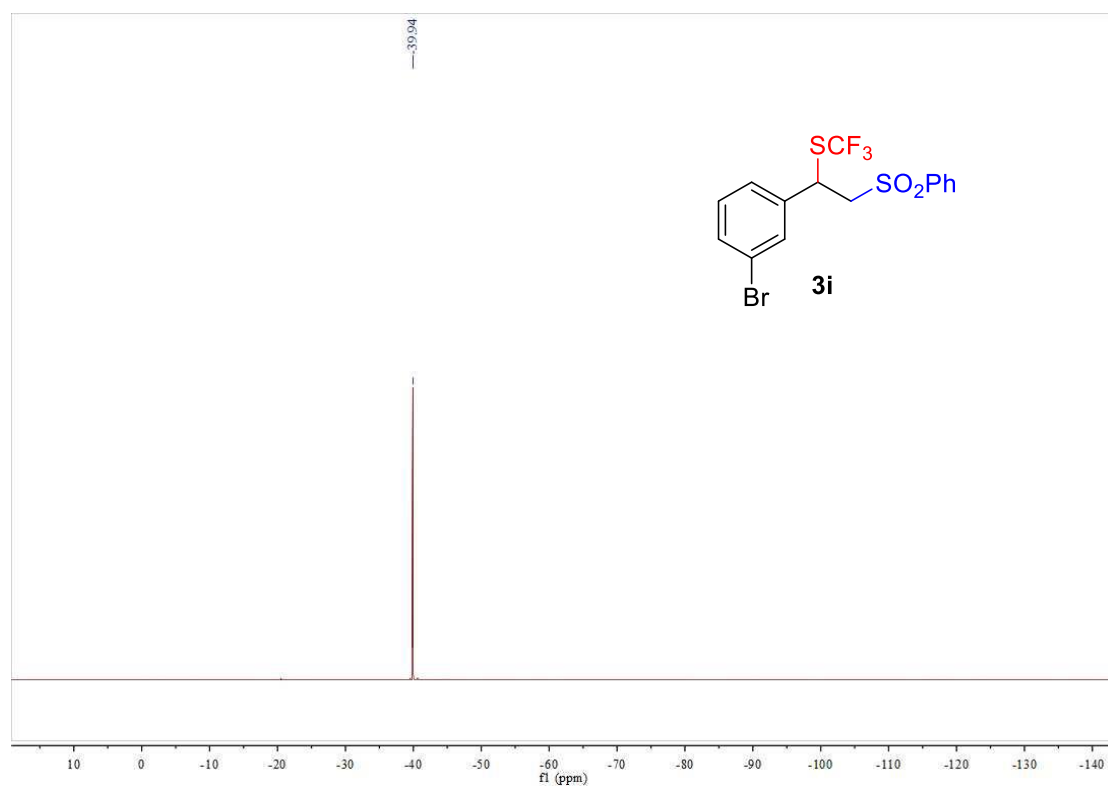
Elemental Analysis: C, 50.49; H, 3.74; F, 14.09; O, 15.82; S, 15.85

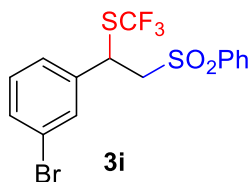
Sample Name	160119-L7-11-28	Position	P1-D4	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	160119-L7-11-2b.d	ACQ Method	0103.m	Comment		Acquired Time	1/19/2016 4:13:15 PM



HRMS (ESI, m/z) calcd for $C_{17}H_{15}F_3O_4S_2$ $[M+Na]^+$ 427.0256, found 427.0257.







Chemical Formula: C₁₅H₁₂BrF₃O₂S₂

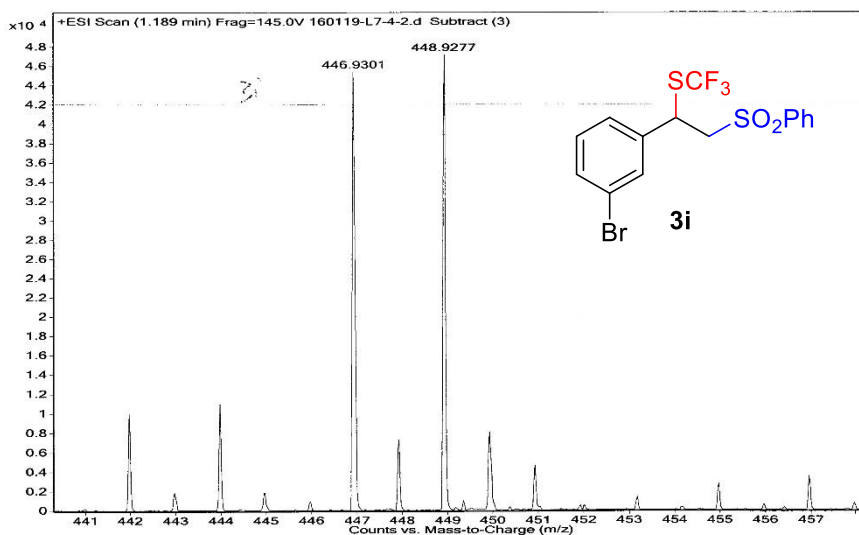
Exact Mass: 423.9414

Molecular Weight: 425.2782

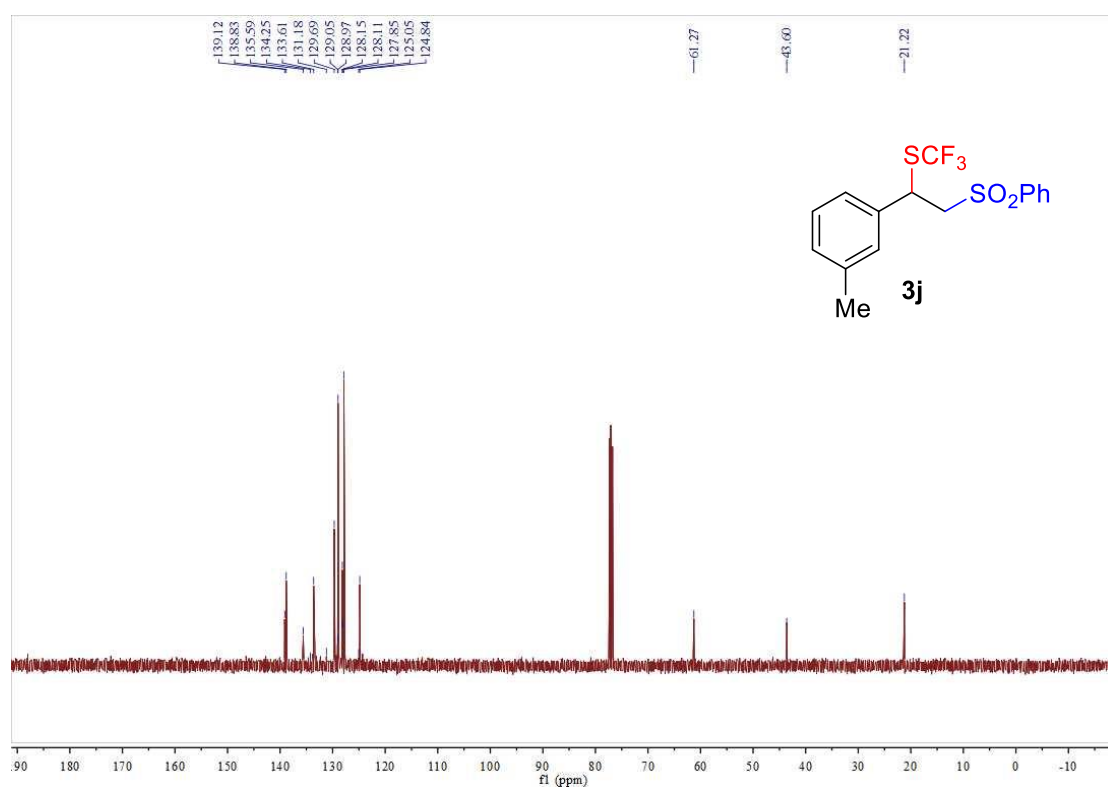
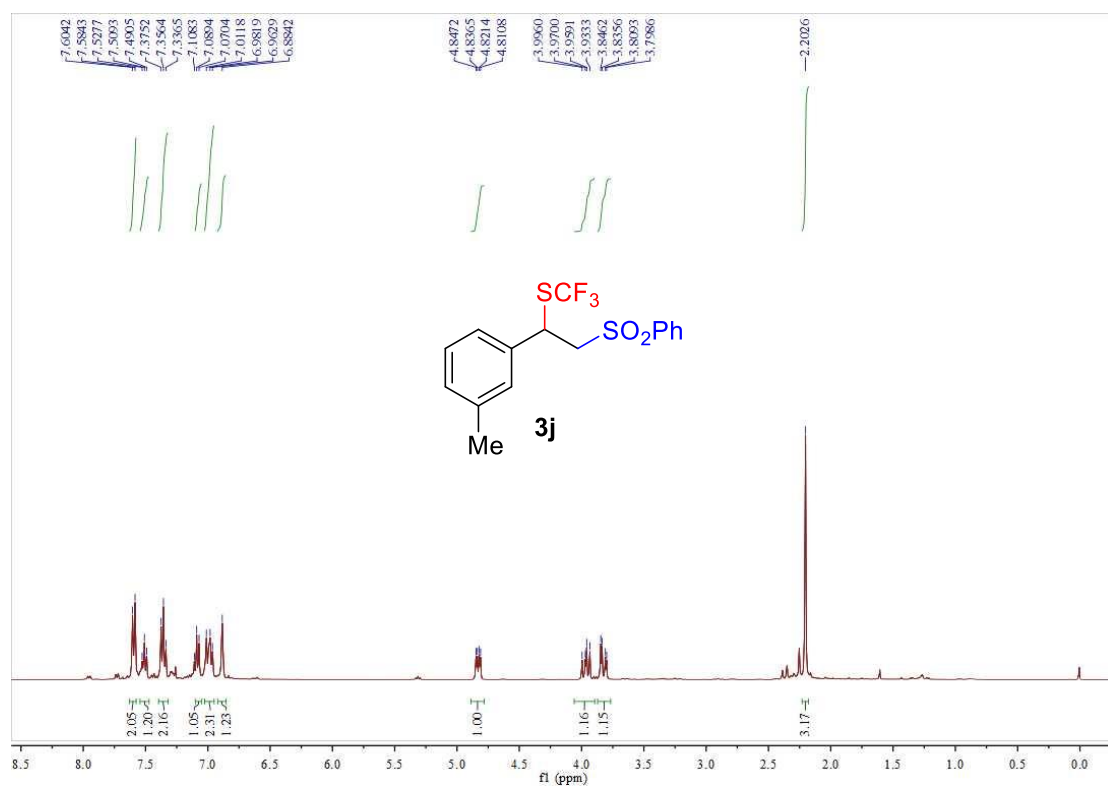
m/z: 423.9414 (100.0%), 425.9394 (97.3%), 424.9448 (16.2%), 426.9427 (15.8%),
425.9372 (9.0%), 427.9352 (8.8%), 424.9408 (1.6%), 426.9388 (1.6%),
426.9406 (1.5%), 428.9385 (1.4%), 425.9481 (1.2%), 427.9461 (1.2%)

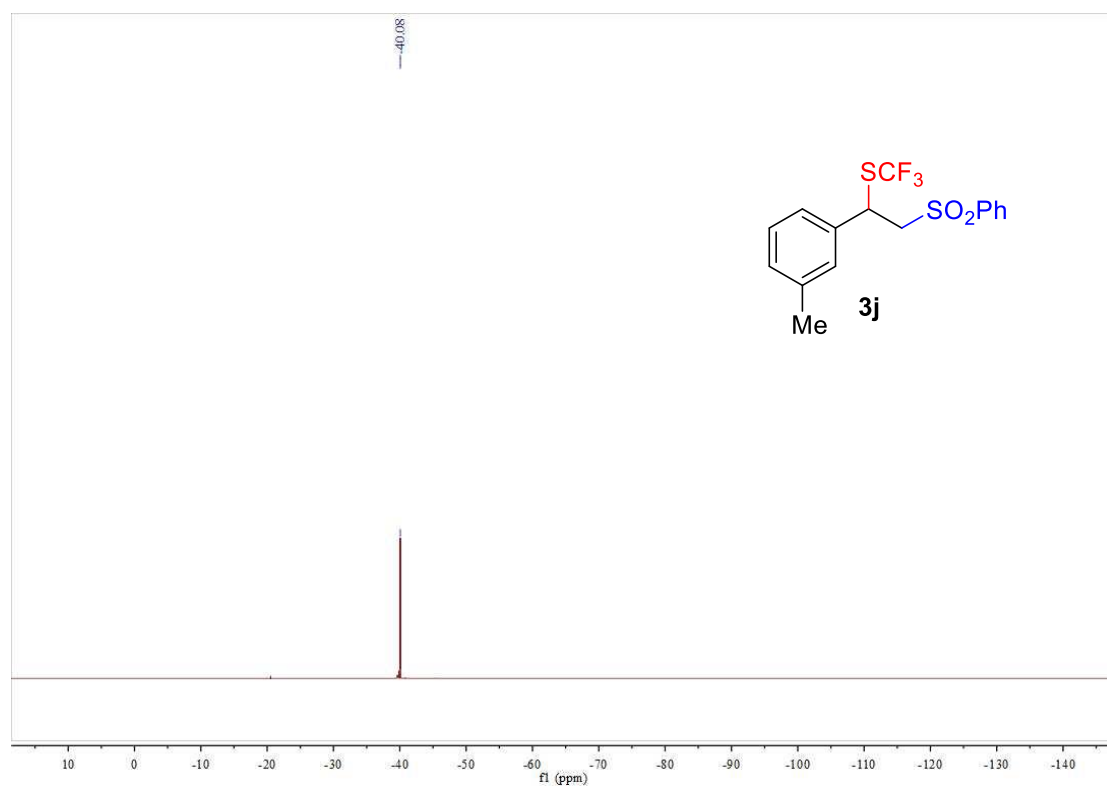
Elemental Analysis: C, 42.36; H, 2.84; Br, 18.79; F, 13.40; O, 7.52; S, 15.08

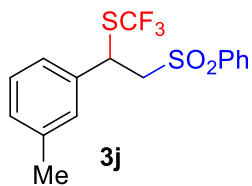
Sample Name	160119-L7-4-2	Position	P1-C3	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	Inj Position		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	160119-L7-4-2.d	Acq Method	0103.m	Comment		Acquired Time	1/19/2016 3:53:40 PM



HRMS (ESI, m/z) calcd for C₁₅H₁₂BrF₃O₂S₂ [M+Na]⁺ 446.9306, found 446.9301.







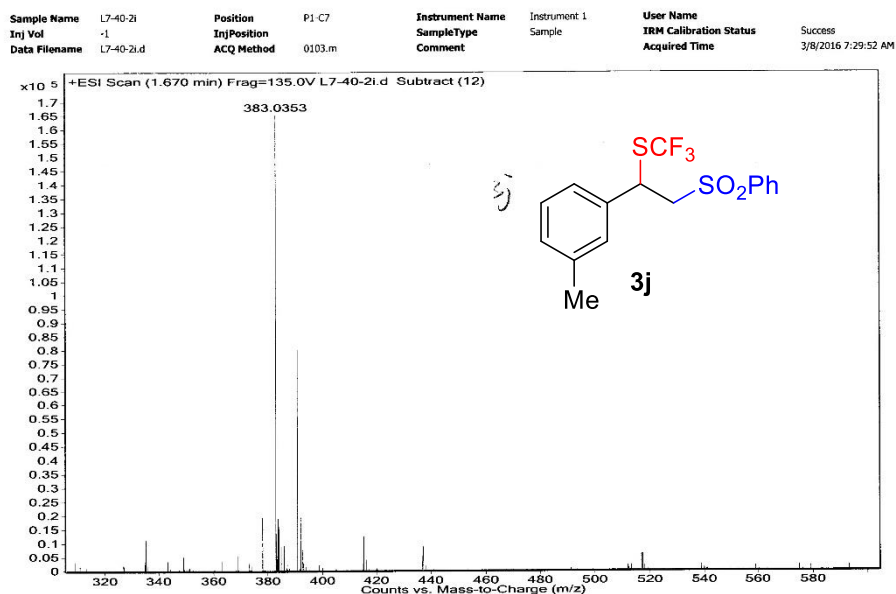
Chemical Formula: $C_{16}H_{15}F_3O_2S_2$

Exact Mass: 360.0466

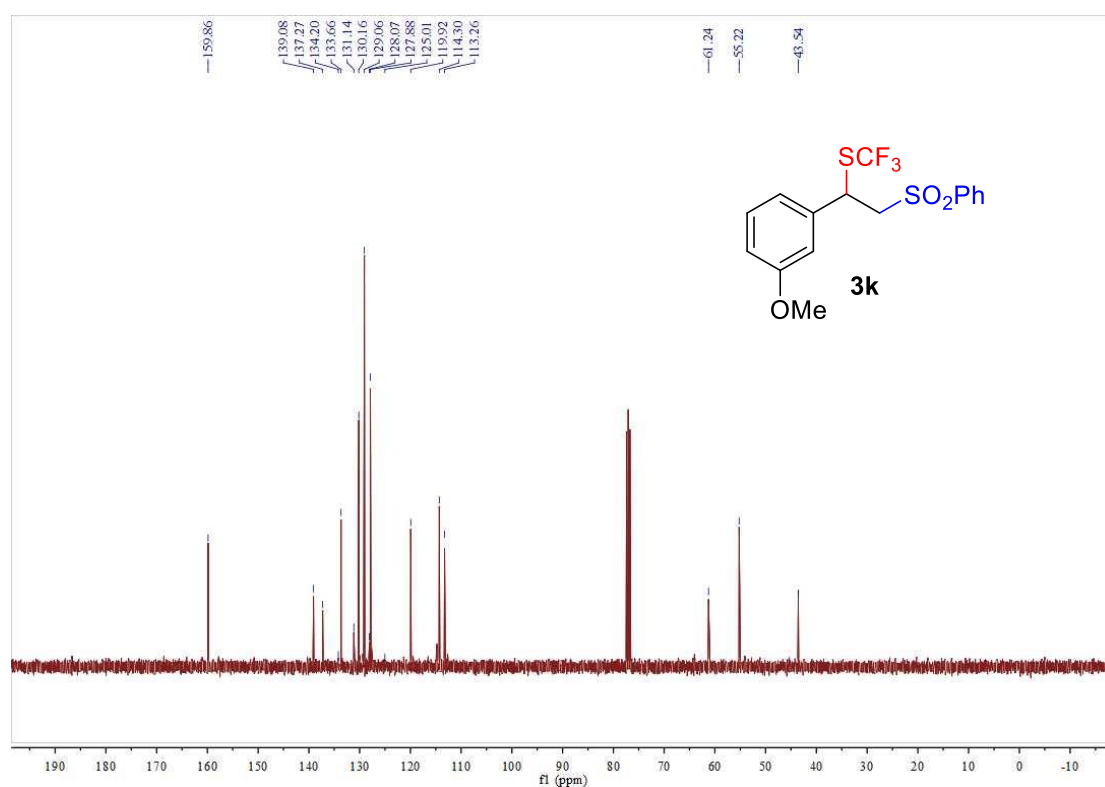
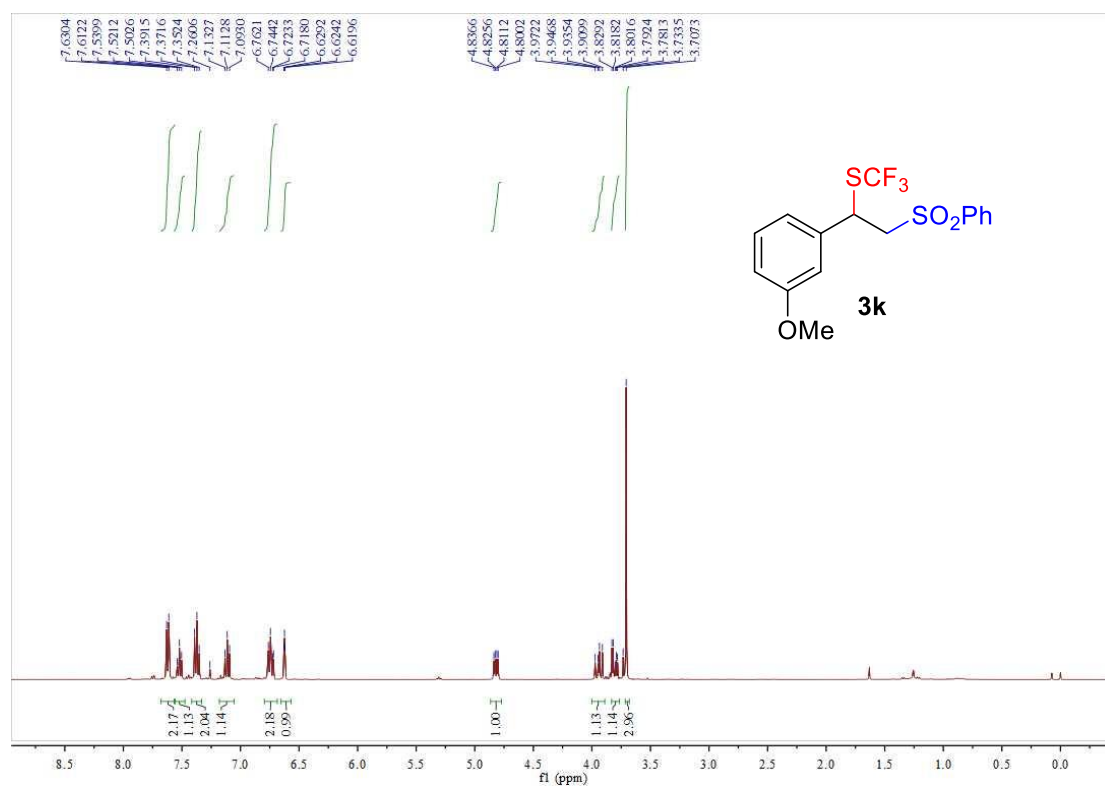
Molecular Weight: 360.4092

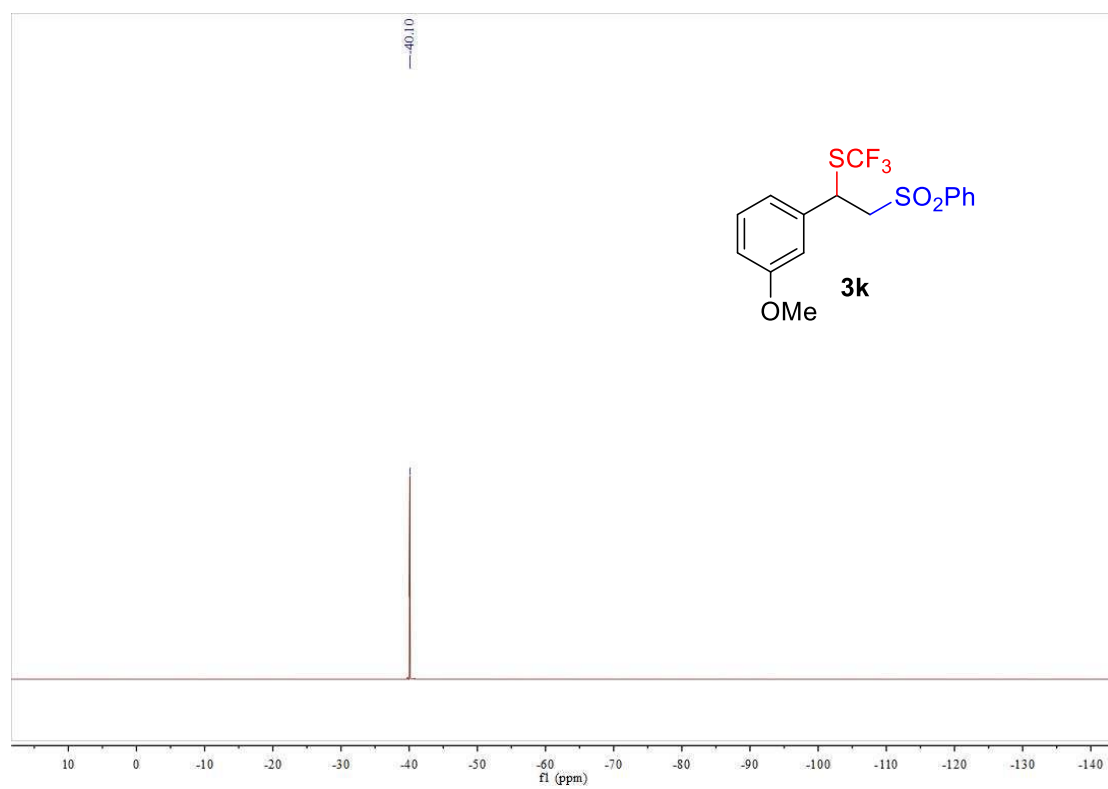
m/z : 360.0466 (100.0%), 361.0499 (17.3%), 362.0424 (9.0%), 361.0459 (1.6%),
363.0457 (1.6%), 362.0533 (1.4%)

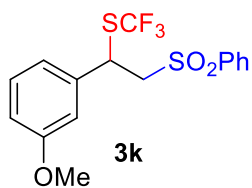
Elemental Analysis: C, 53.32; H, 4.20; F, 15.81; O, 8.88; S, 17.79



HRMS (ESI, m/z) calcd for $C_{16}H_{15}F_3O_2S_2$ $[M+Na]^+$ 383.0358, found 383.0353.







Chemical Formula: $C_{16}H_{15}F_3O_3S_2$

Exact Mass: 376.0415

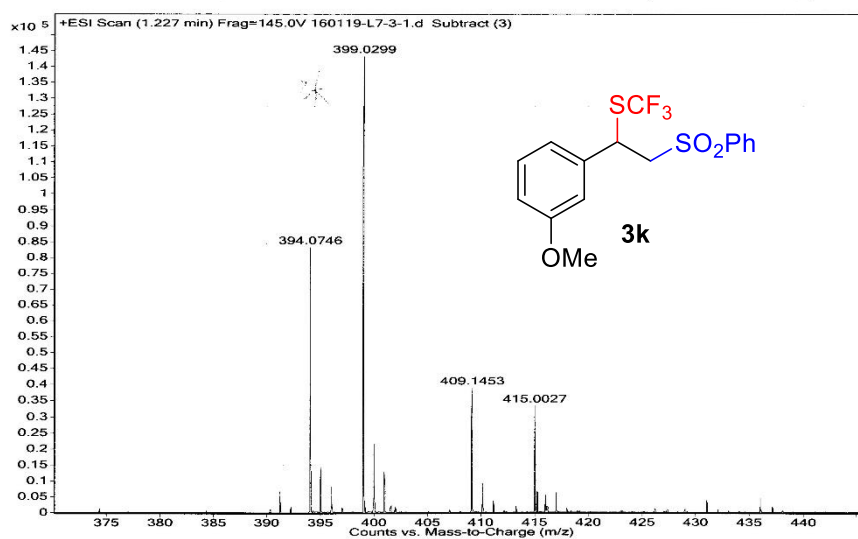
Molecular Weight: 376.4082

m/z: 376.0415 (100.0%), 377.0448 (17.3%), 378.0373 (9.0%), 377.0409 (1.6%),
379.0406 (1.6%), 378.0482 (1.4%)

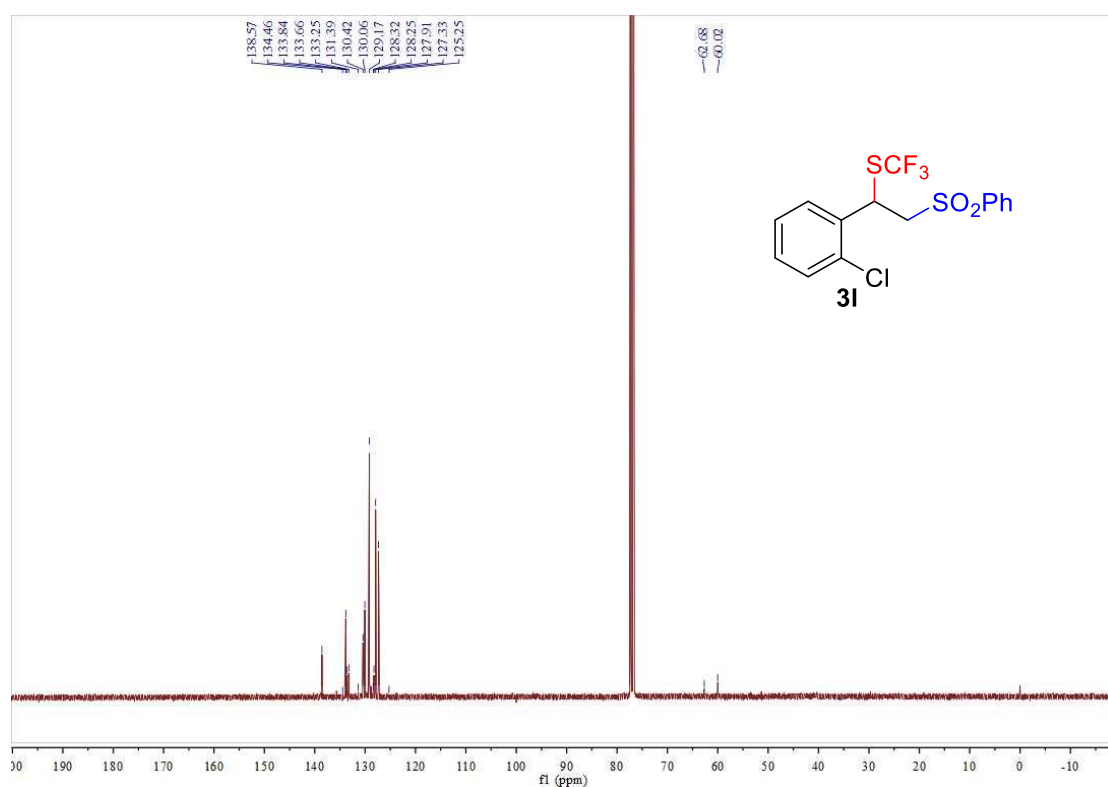
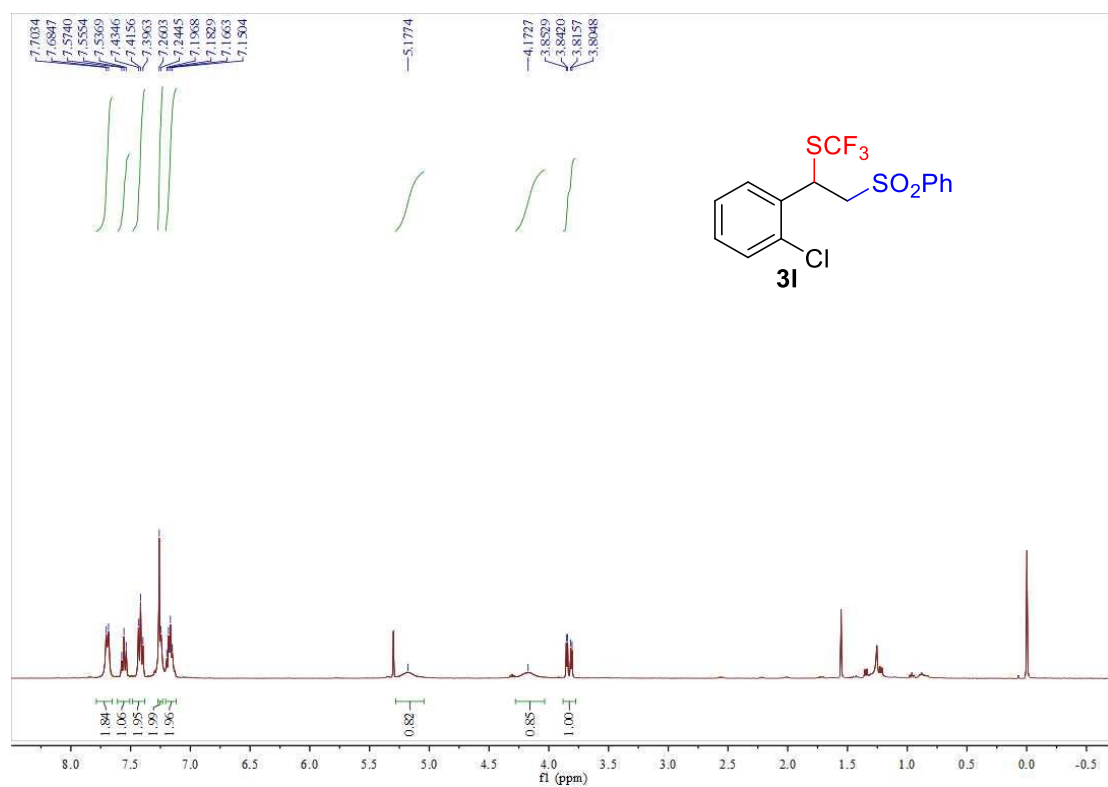
Elemental Analysis: C, 51.06; H, 4.02; F, 15.14; O, 12.75; S, 17.03

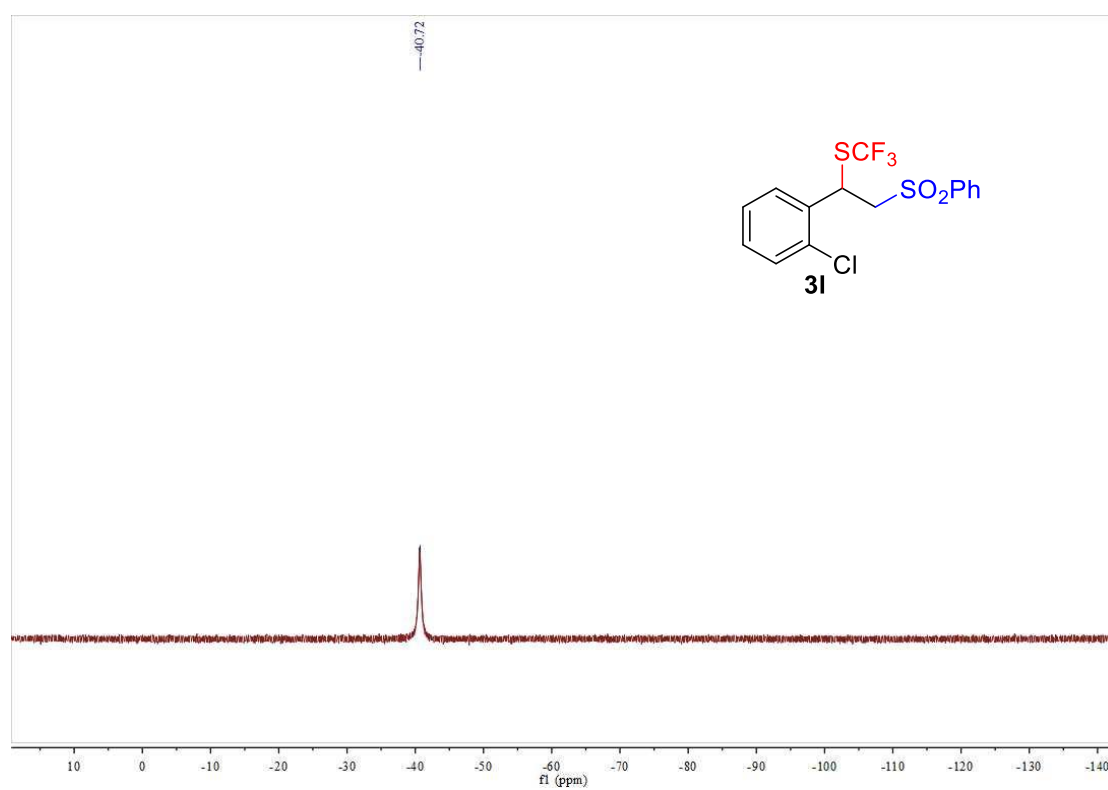
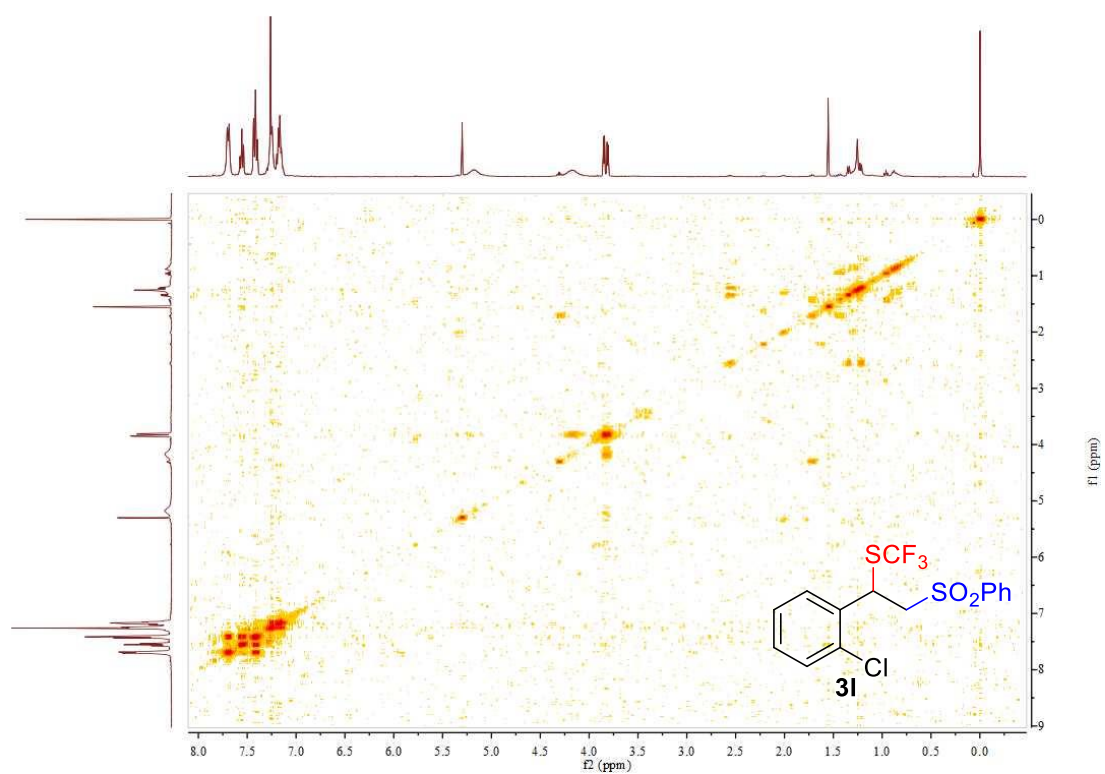
Sample Name	160119-L7-3-1	Position	P1-C2	Instrument Name	Instrument 1	User Name
Inj Vol	~1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	160119-L7-3-1.d	ACQ Method	0103.m	Comment		Acquired Time

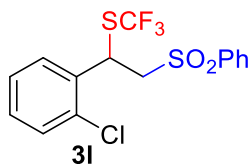
Success
1/19/2016 3:40:27 PM



HRMS (ESI, m/z) calcd for $C_{16}H_{15}F_3O_3S_2$ $[M+Na]^+$ 399.0307, found 399.0299.







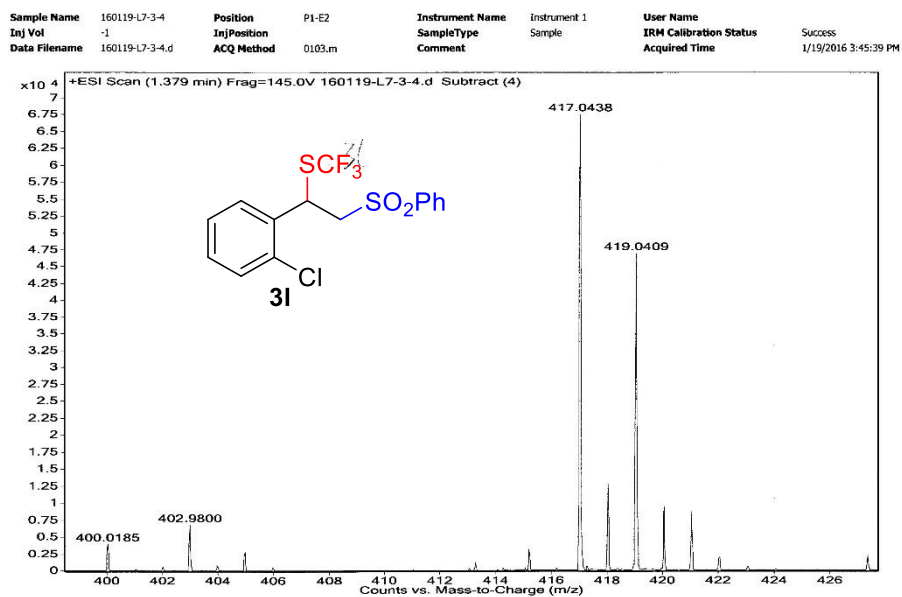
Chemical Formula: C₁₅H₁₂ClF₃O₂S₂

Exact Mass: 379.9919

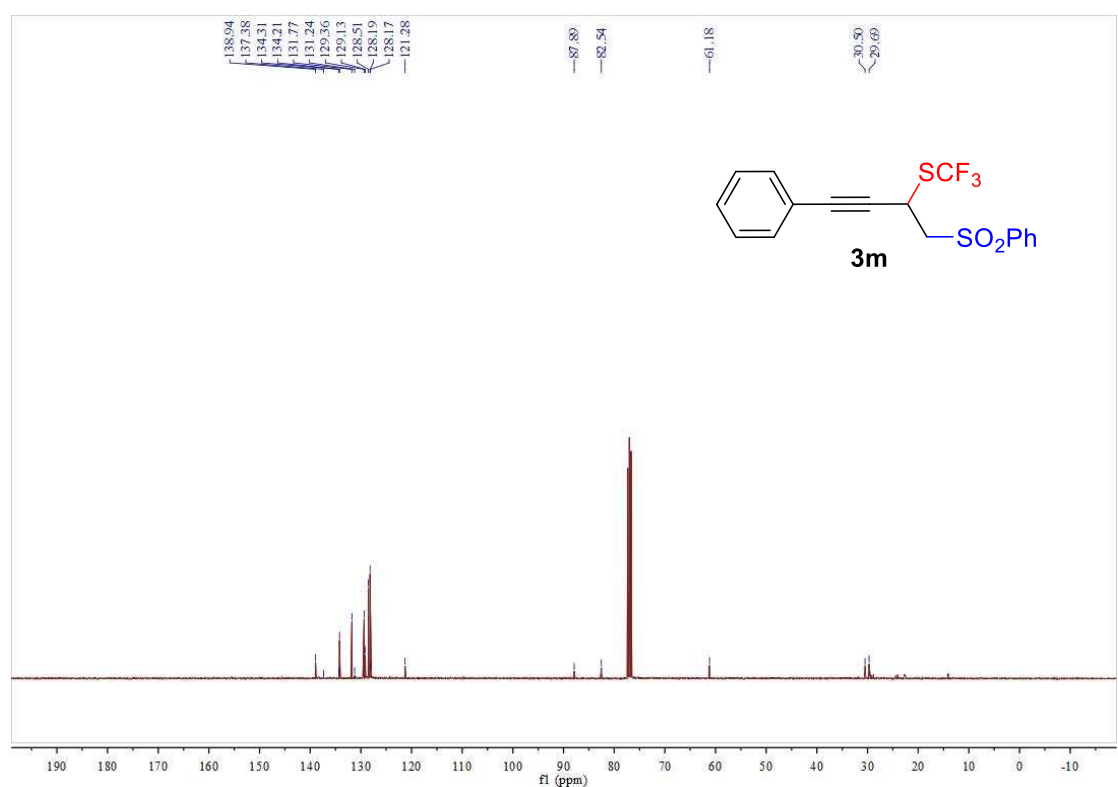
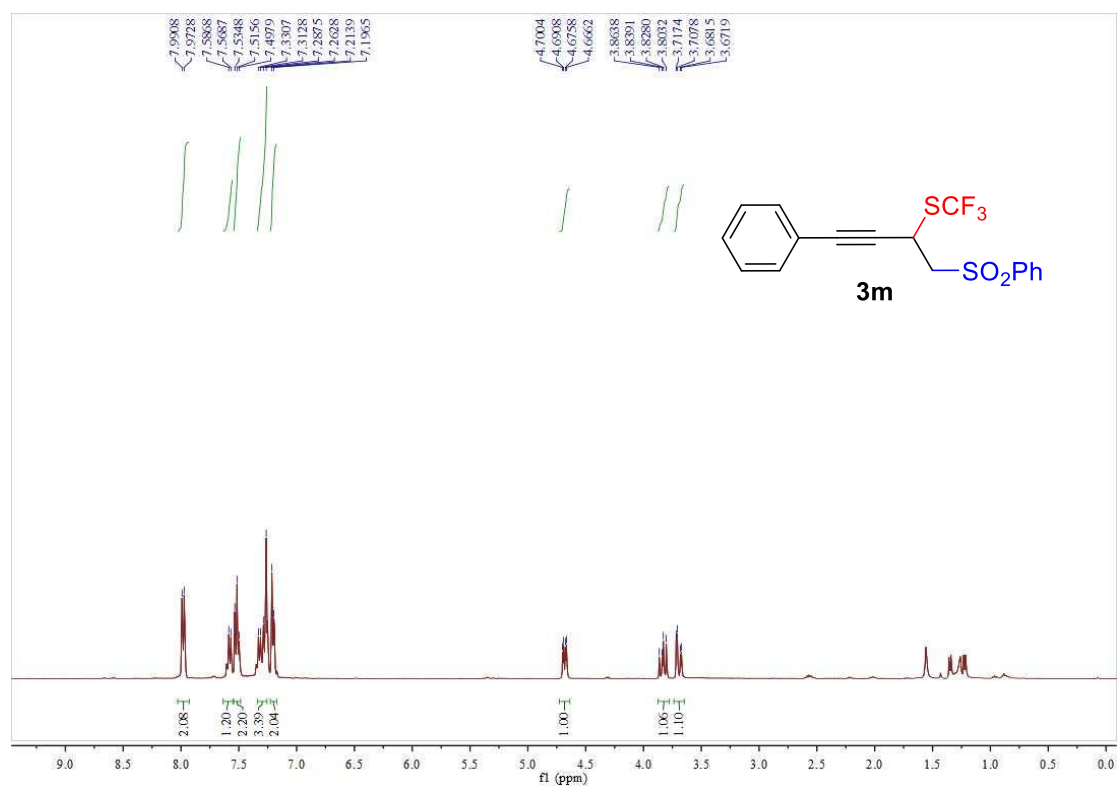
Molecular Weight: 380.8242

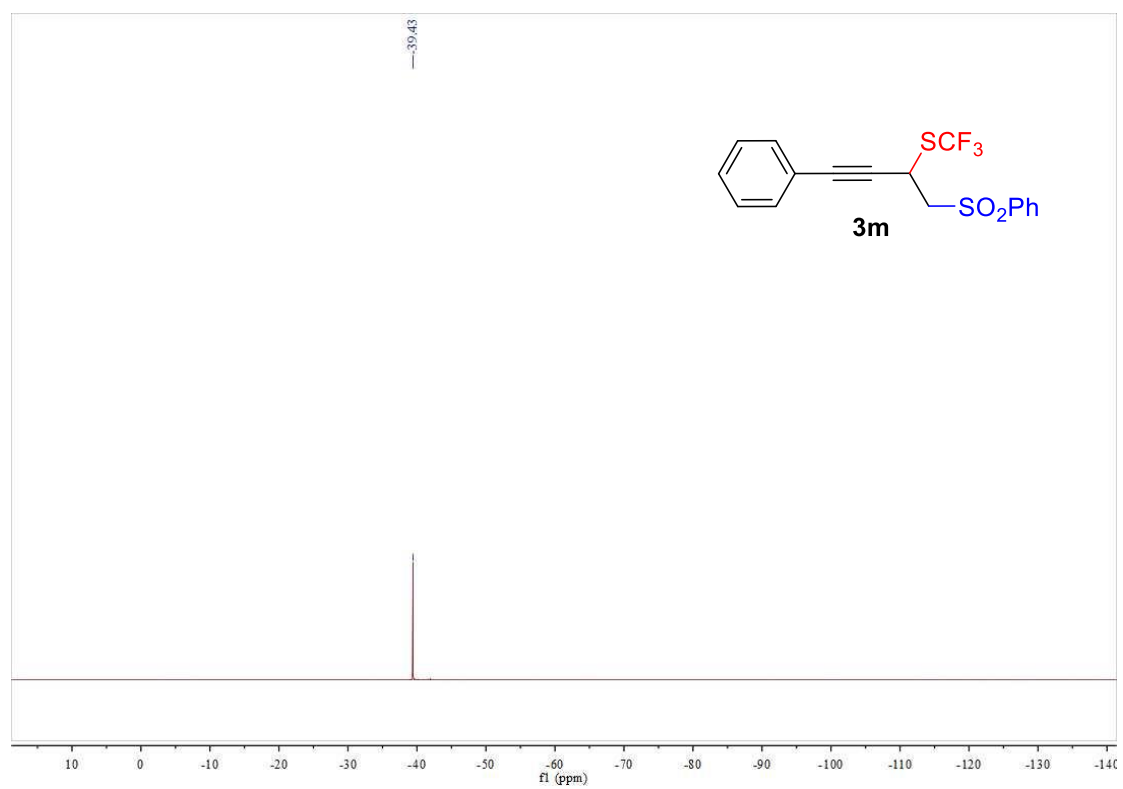
m/z: 379.9919 (100.0%), 381.9890 (32.0%), 380.9953 (16.2%), 381.9877 (9.0%),
382.9923 (5.2%), 383.9848 (2.9%), 380.9913 (1.6%), 382.9911 (1.5%), 381.9986 (1.2%)

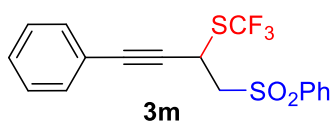
Elemental Analysis: C, 47.31; H, 3.18; Cl, 9.31; F, 14.97; O, 8.40; S, 16.84



HRMS (ESI, m/z) calcd for C₁₅H₁₂ClF₃O₂S₂ [M+Na]⁺ 402.9812, found 402.9800.







Chemical Formula: C₁₇H₁₃F₃O₂S₂

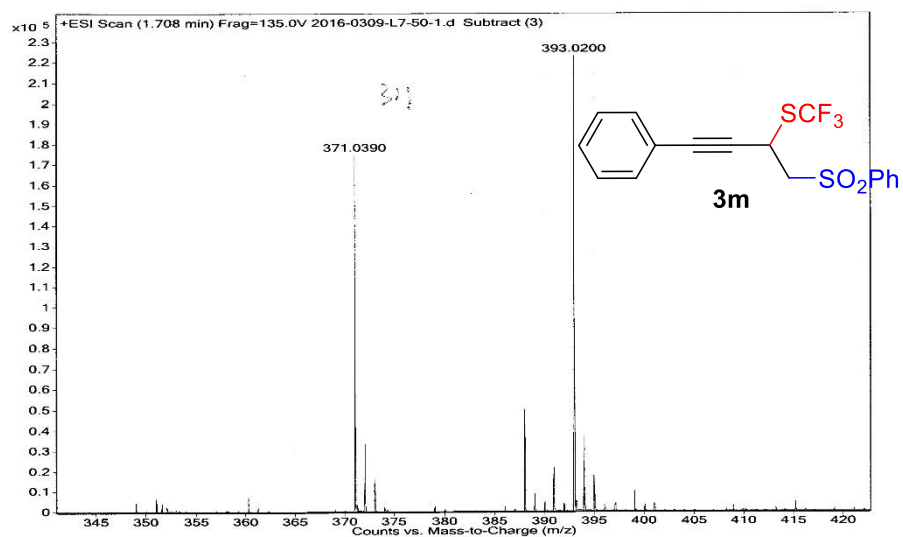
Exact Mass: 370.0309

Molecular Weight: 370.4042

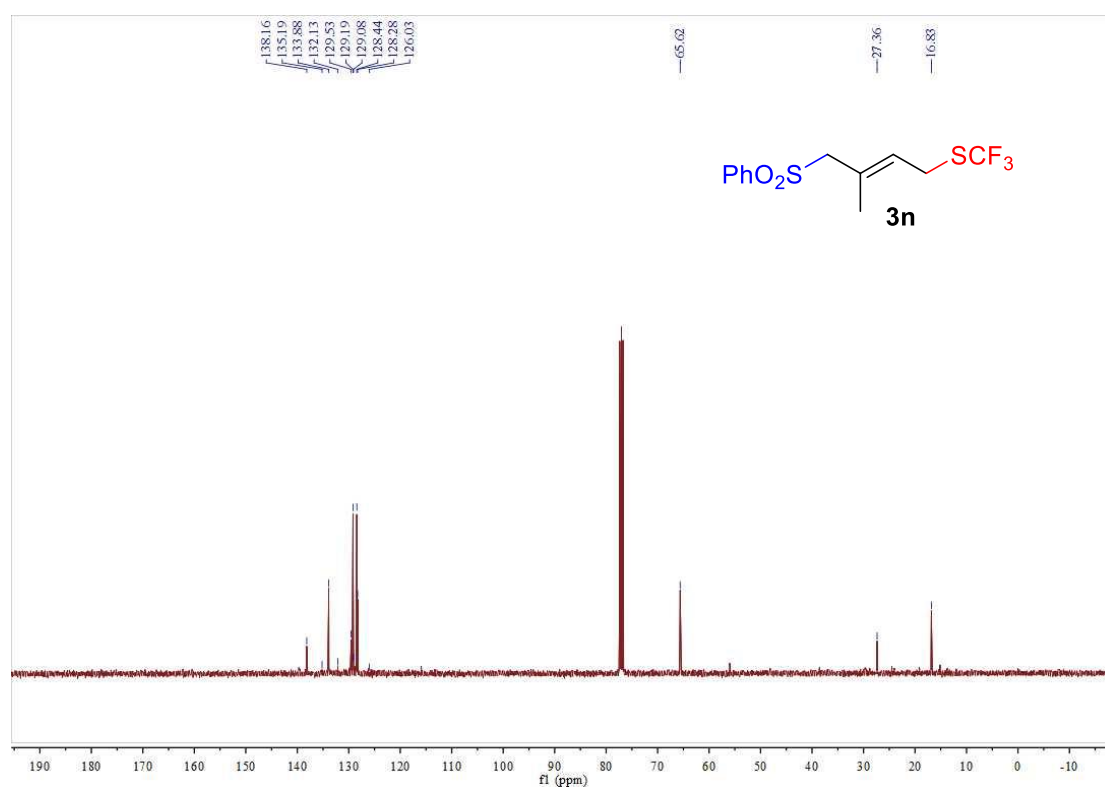
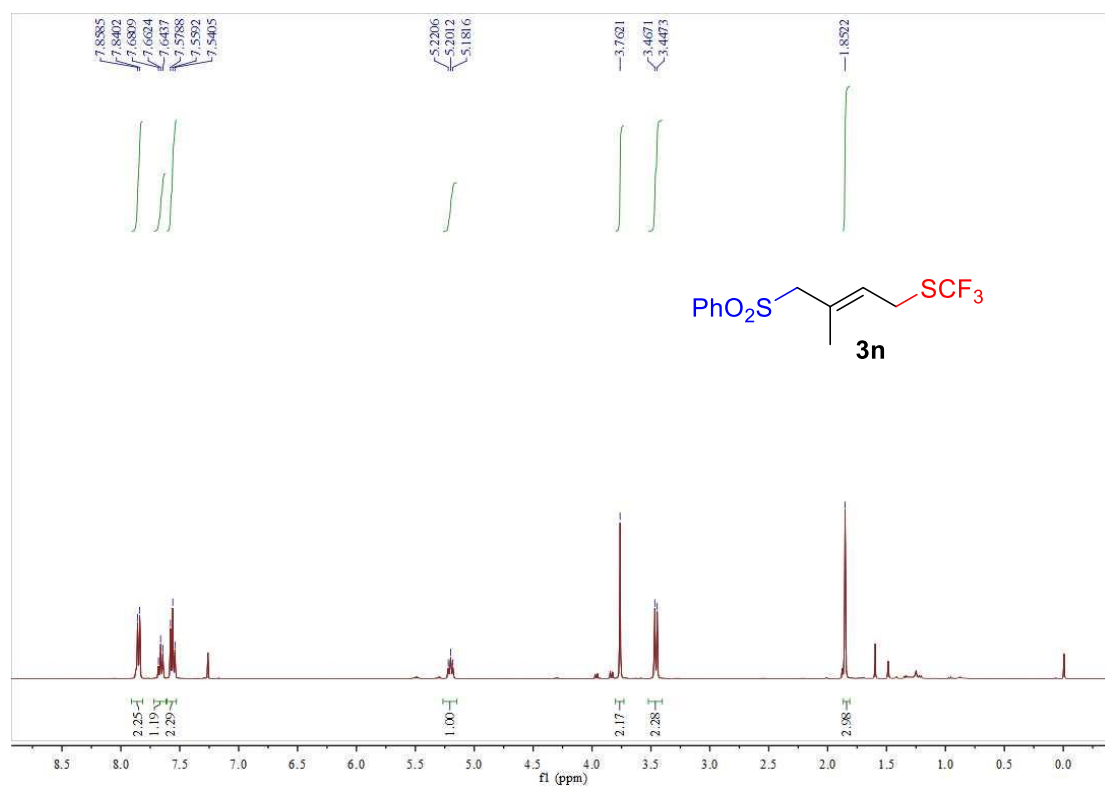
m/z: 370.0309 (100.0%), 371.0343 (18.4%), 372.0267 (9.0%), 373.0301 (1.7%),
371.0303 (1.6%), 372.0376 (1.6%)

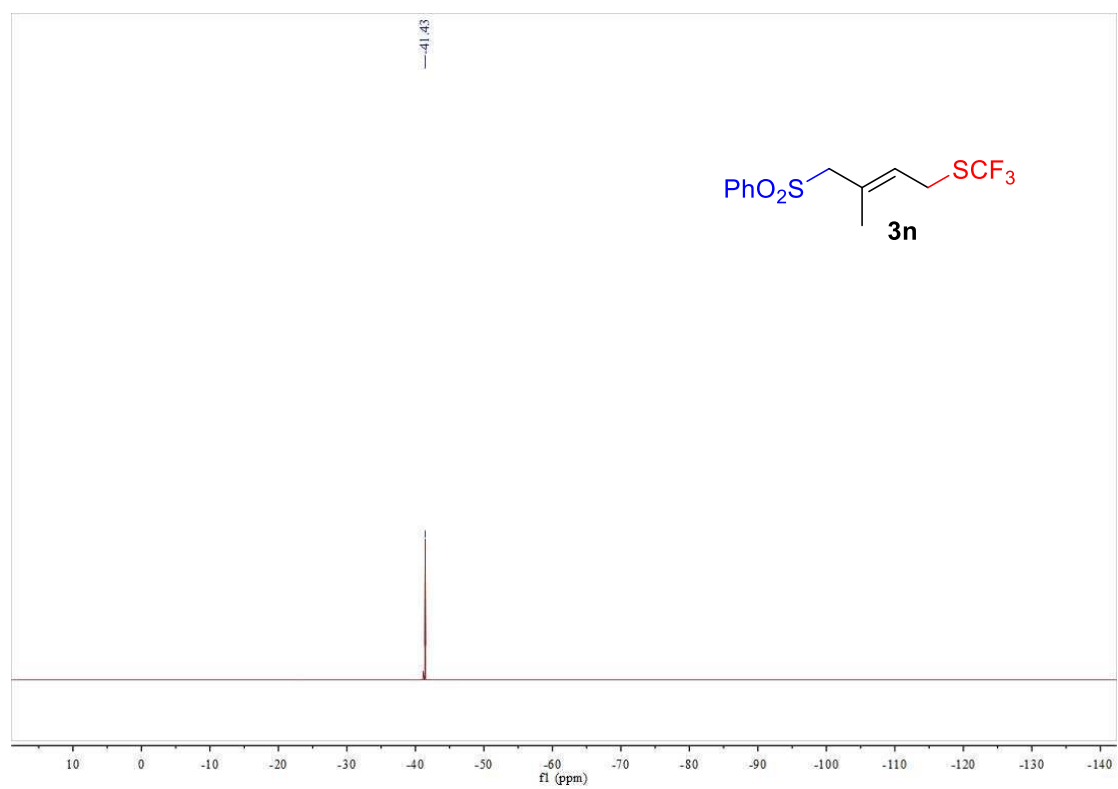
Elemental Analysis: C, 55.13; H, 3.54; F, 15.39; O, 8.64; S, 17.31

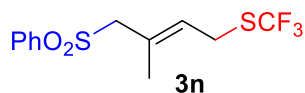
Sample Name	2016-0309-L7-50-1	Position	P1-C9	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	2016-0309-L7-50-1.d	ACQ Method	0103.m	Comment		Acquired Time	3/6/2016 2:55:14 PM



HRMS (ESI, m/z) calcd for C₁₇H₁₃F₃O₂S₂ [M+Na]⁺ 393.0201, found 393.0200.







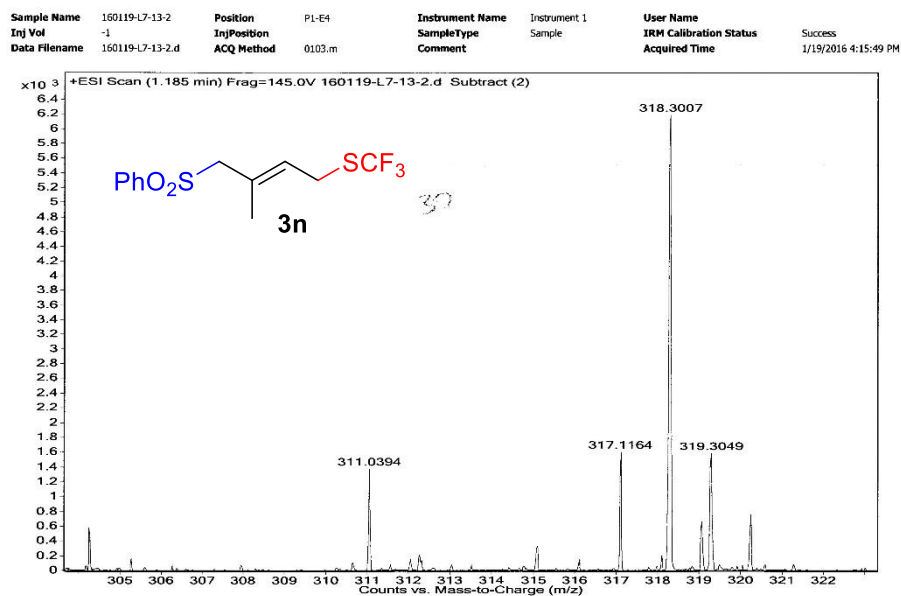
Chemical Formula: $C_{12}H_{13}F_3O_2S_2$

Exact Mass: 310.0309

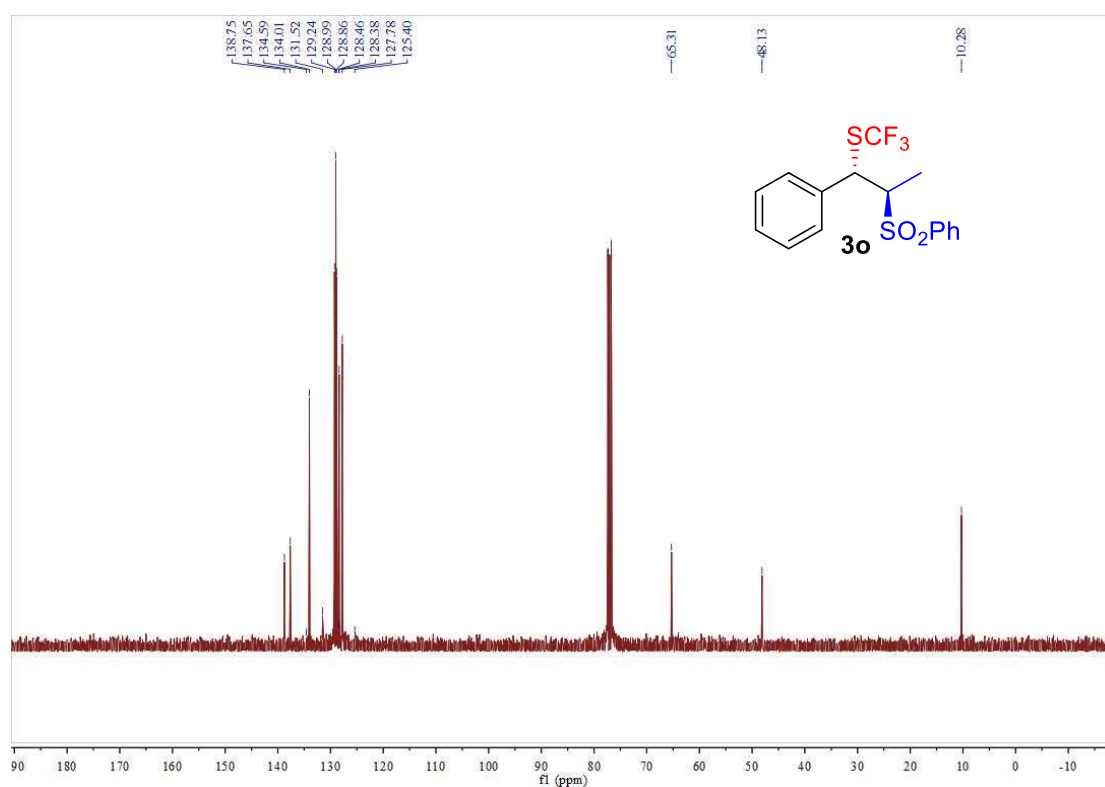
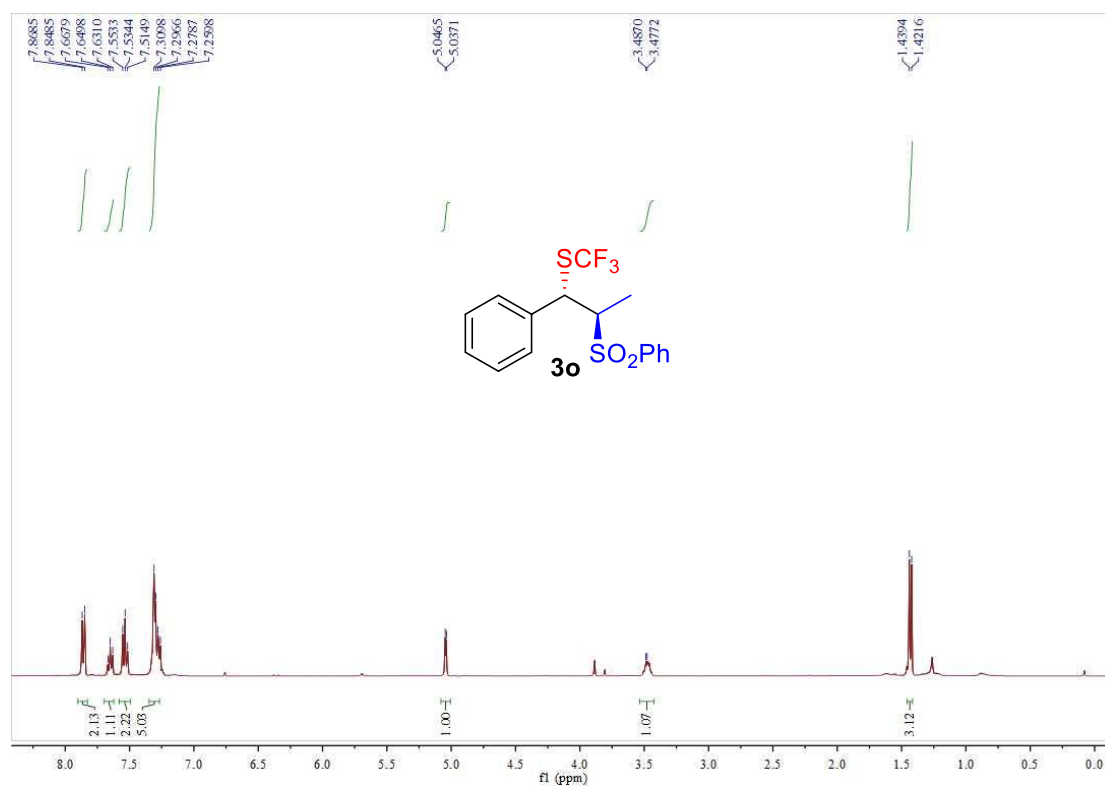
Molecular Weight: 310.3492

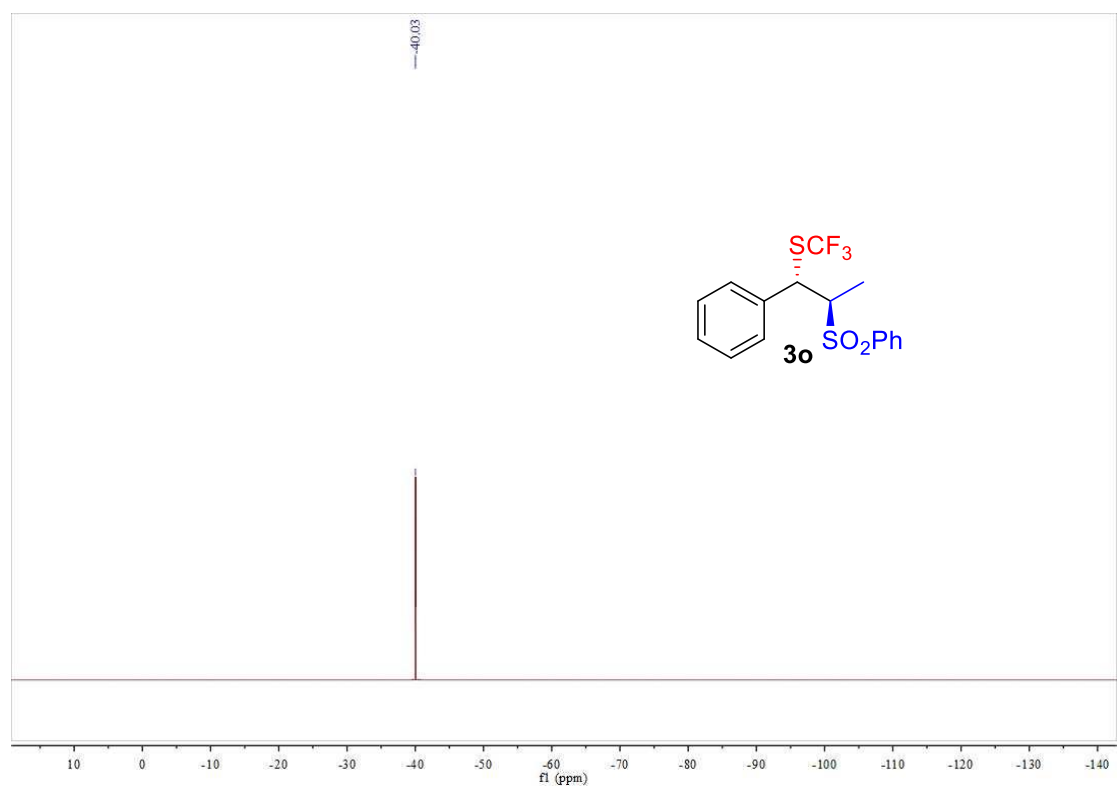
m/z: 310.0309 (100.0%), 311.0343 (13.0%), 312.0267 (4.5%), 312.0267 (4.5%)

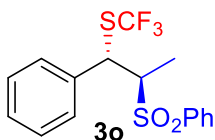
Elemental Analysis: C, 46.44; H, 4.22; F, 18.36; O, 10.31; S, 20.66



HRMS (ESI, m/z) calcd for $C_{12}H_{13}F_3O_2S_2$ $[M+H]^+$ 311.0382, found 311.0394.







Chemical Formula: $C_{16}H_{15}F_3O_2S_2$

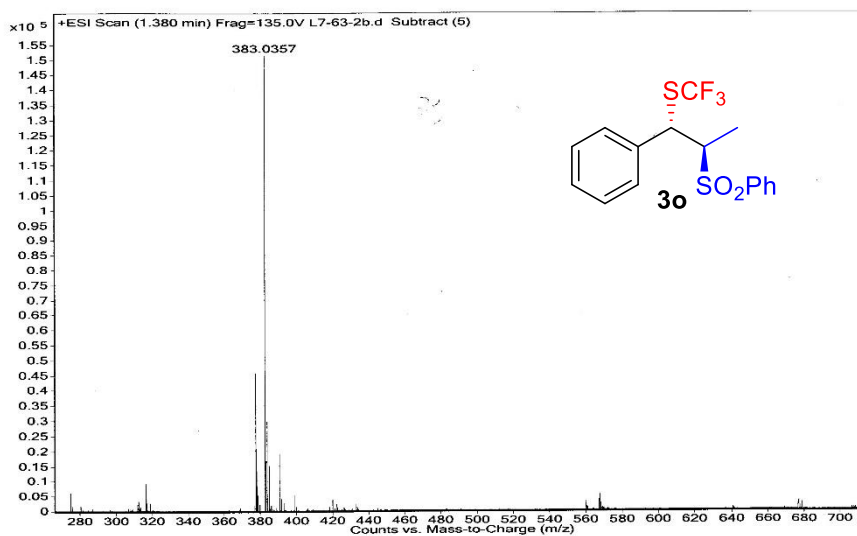
Exact Mass: 360.0466

Molecular Weight: 360.4092

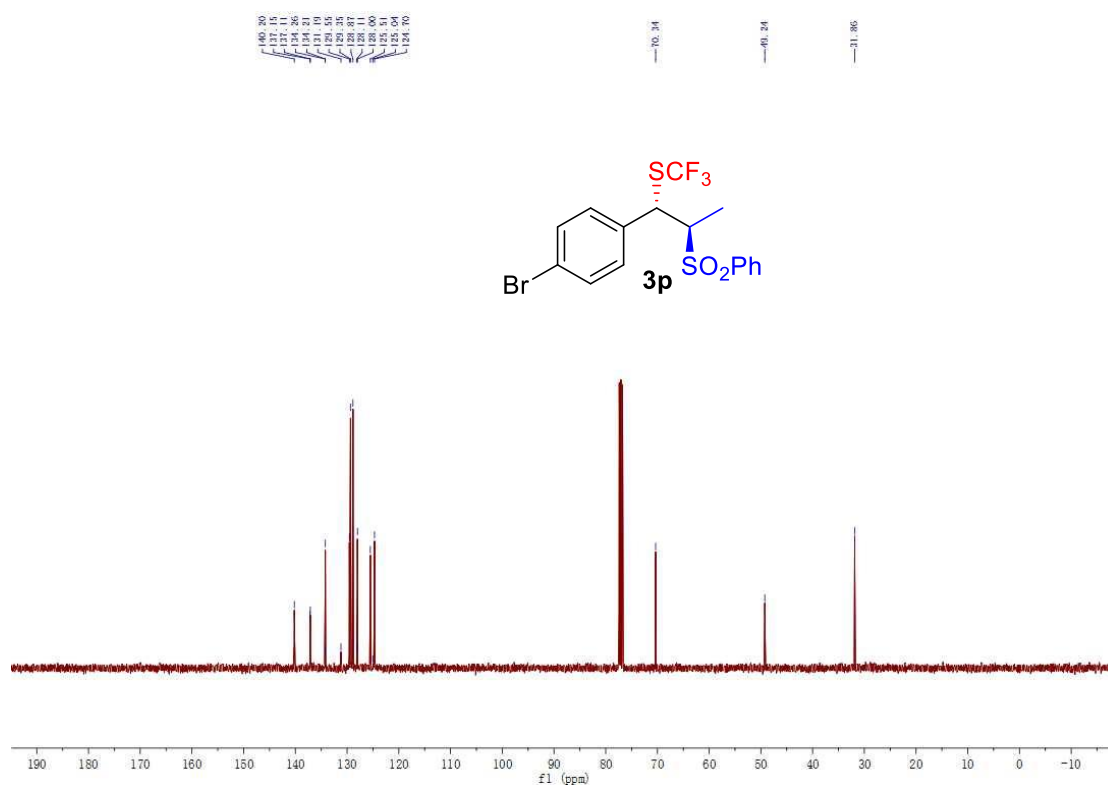
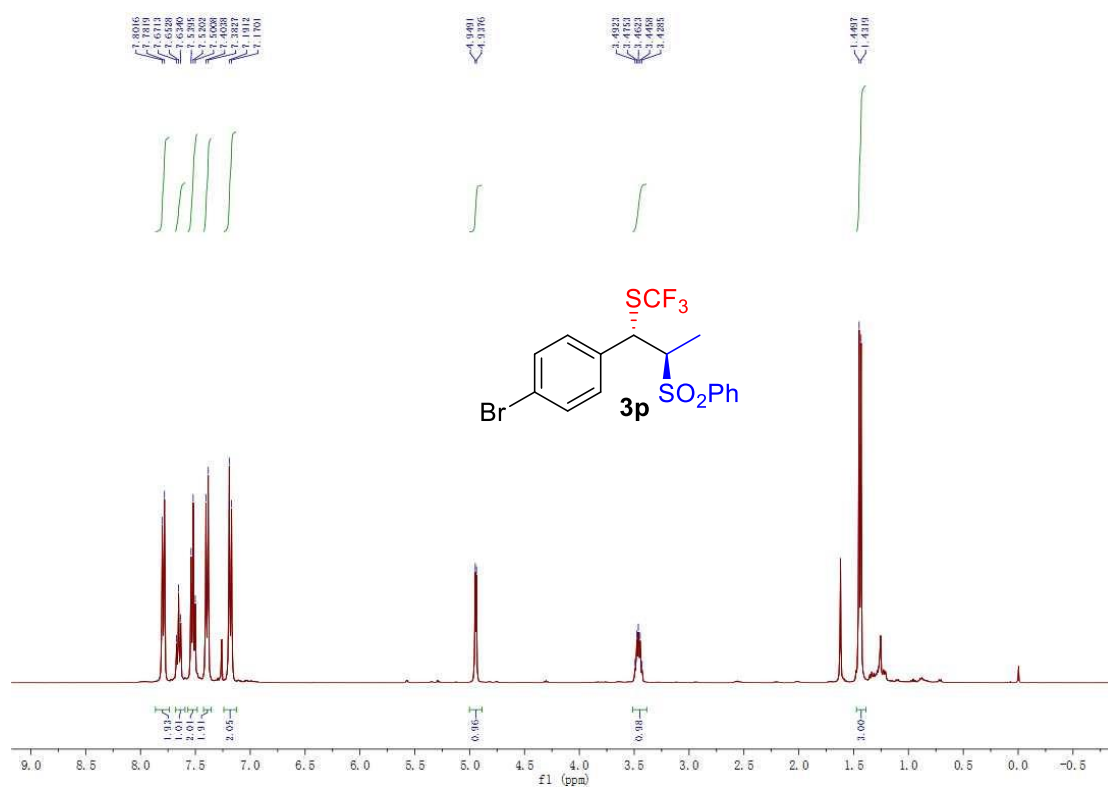
m/z : 360.0466 (100.0%), 361.0499 (17.3%), 362.0424 (9.0%), 361.0459 (1.6%),
363.0457 (1.6%), 362.0533 (1.4%)

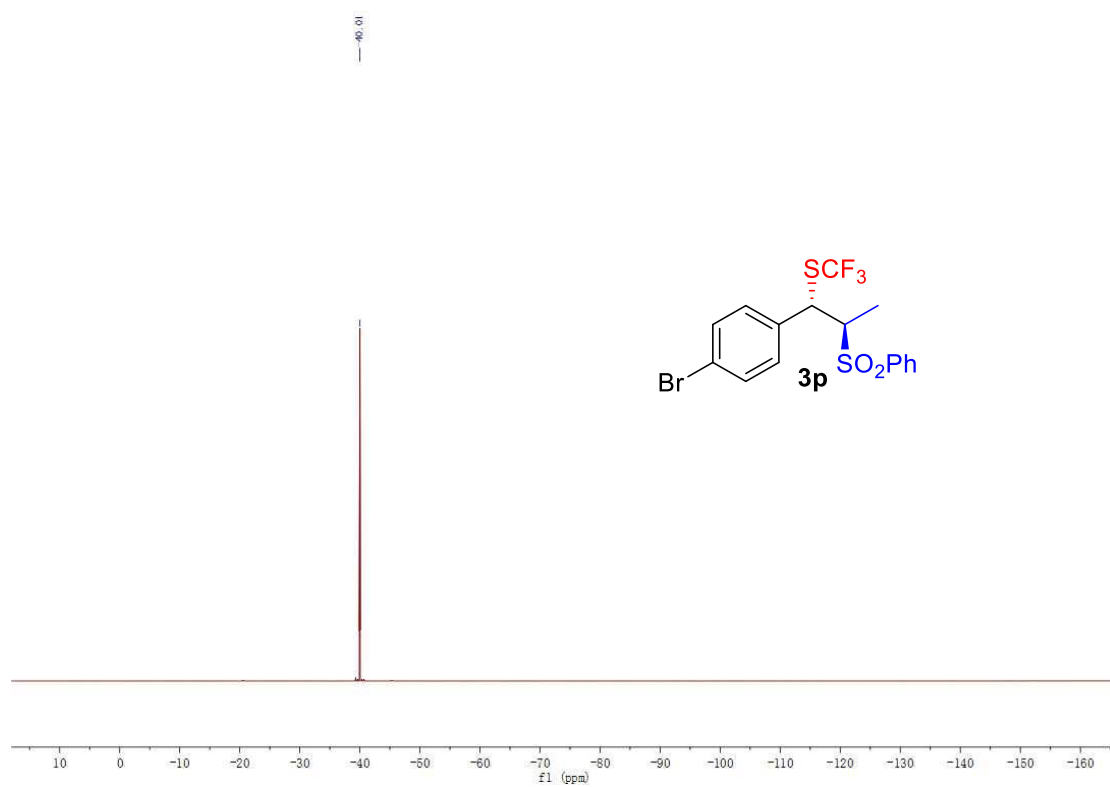
Elemental Analysis: C, 53.32; H, 4.20; F, 15.81; O, 8.88; S, 17.79

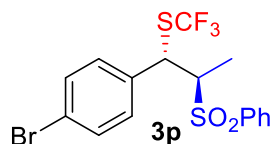
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	L7-63-2b.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



HRMS (ESI, m/z) calcd for $C_{16}H_{15}F_3O_2S_2$ $[M+Na]^+$ 383.0358, found 383.0357.







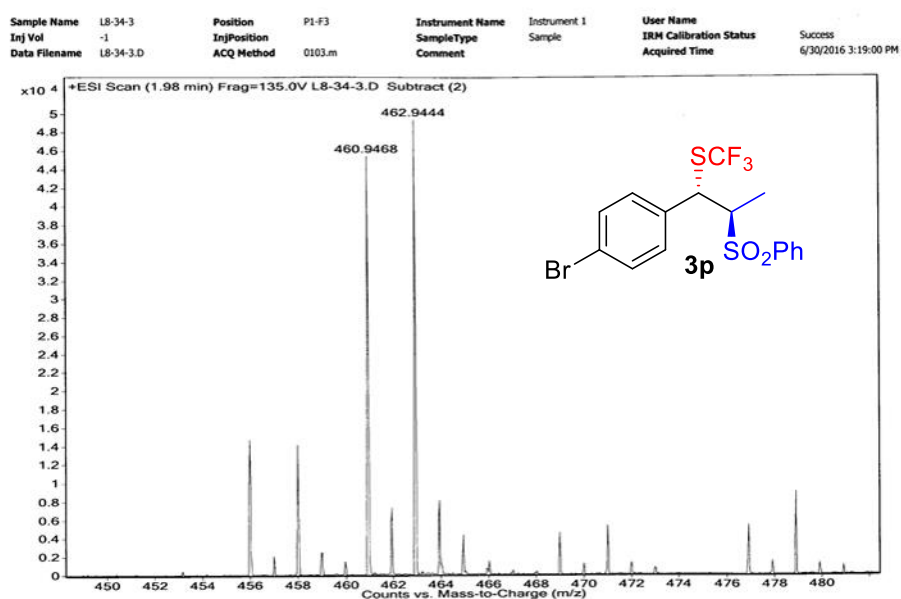
Chemical Formula: $C_{16}H_{14}BrF_3O_2S_2$

Exact Mass: 437.9571

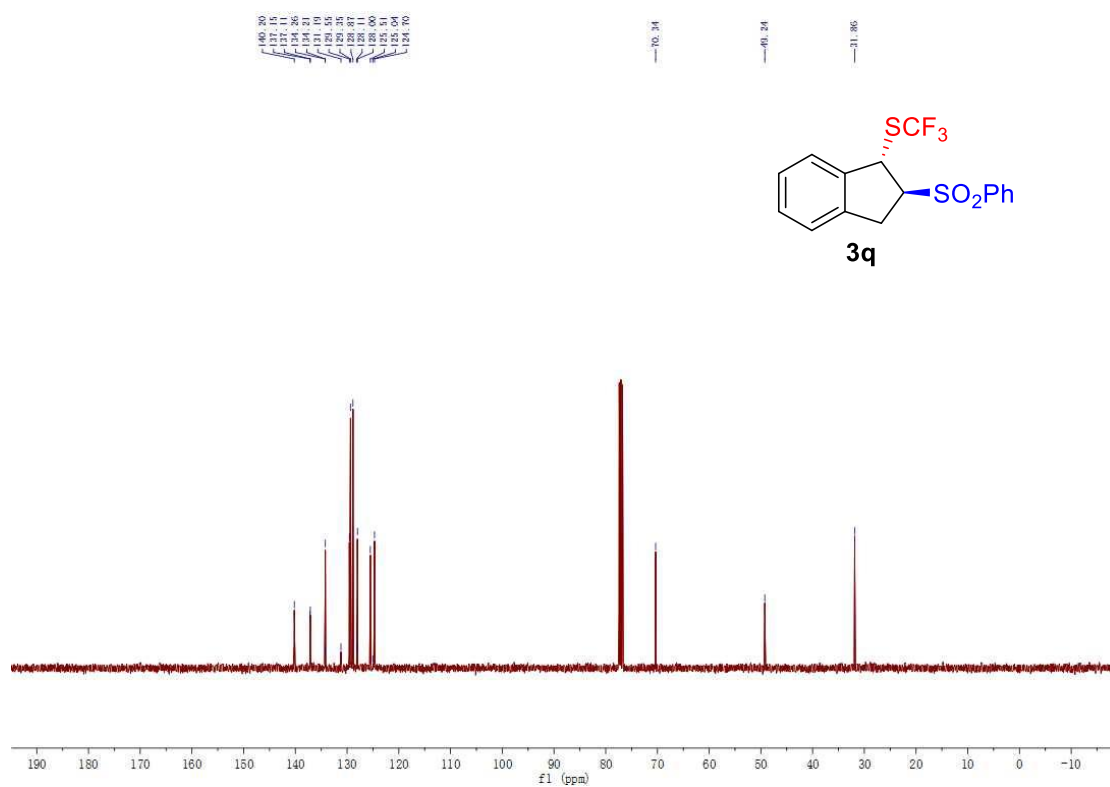
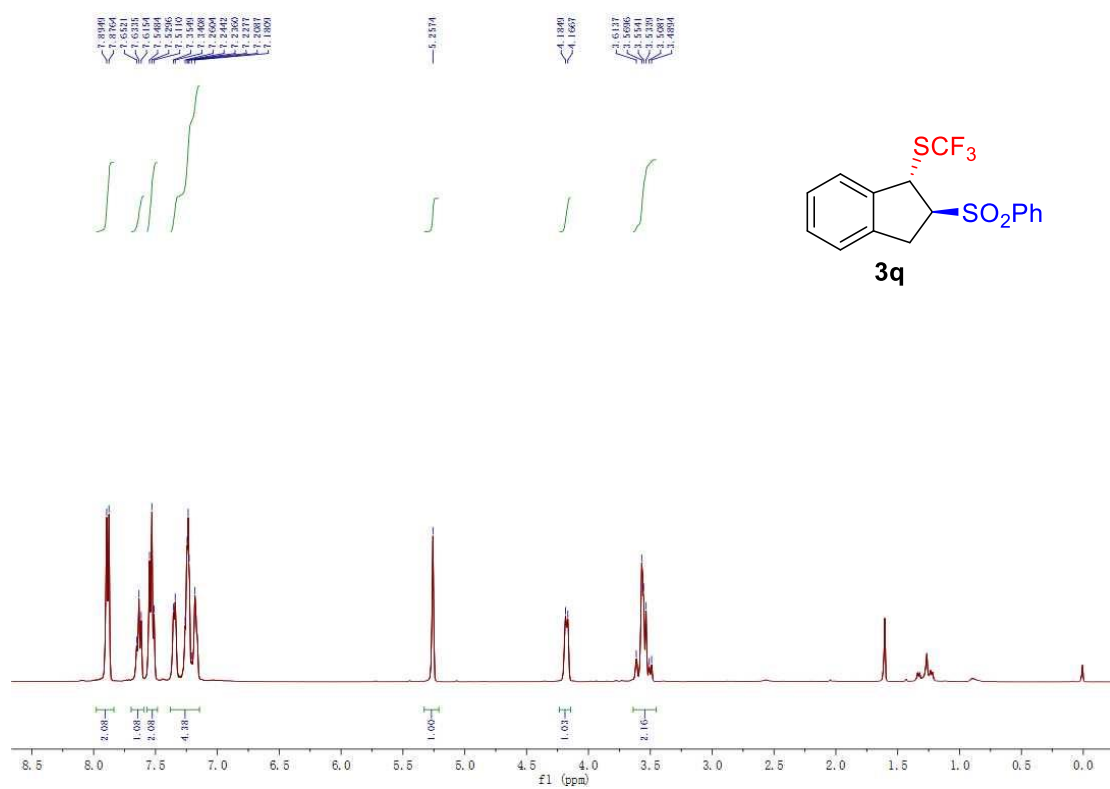
Molecular Weight: 439.3052

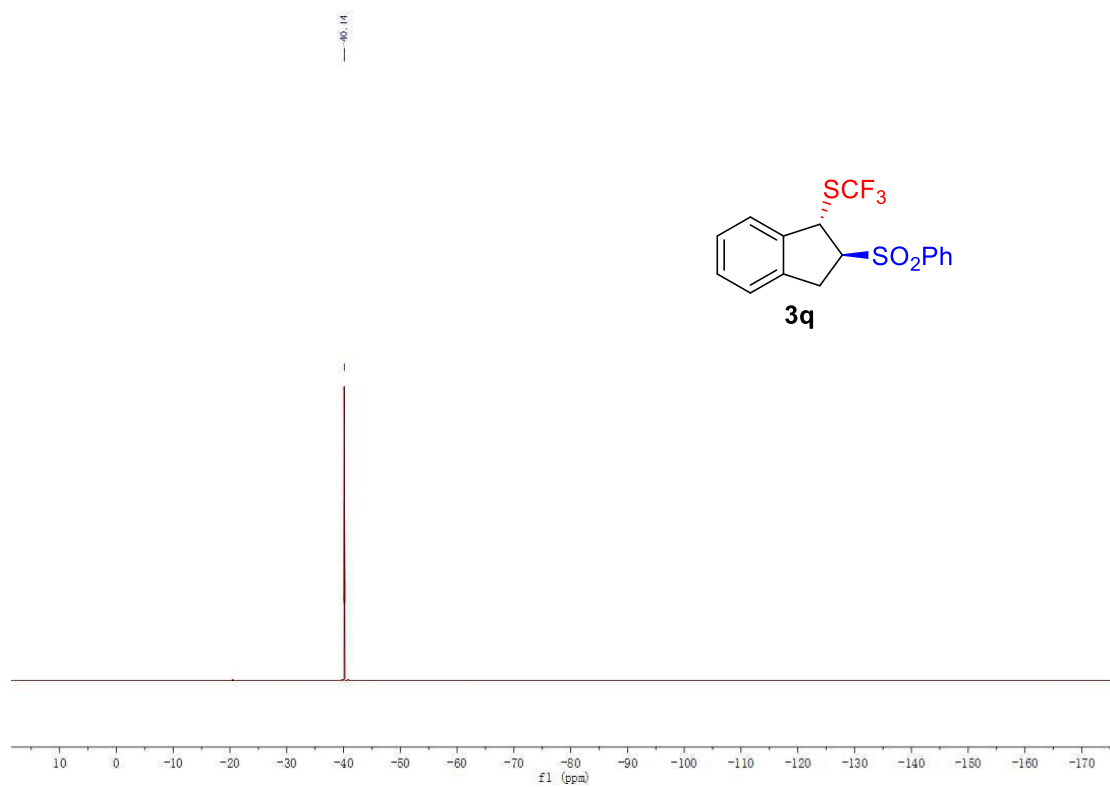
m/z : 437.9571 (100.0%), 439.9550 (97.3%), 438.9604 (17.3%), 440.9584 (16.8%),
439.9529 (9.0%), 441.9508 (8.8%), 438.9565 (1.6%), 440.9544 (1.6%),
442.9542 (1.5%), 440.9562 (1.5%), 441.9617 (1.4%), 439.9638 (1.1%)

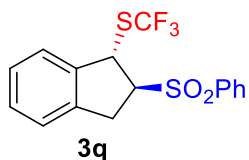
Elemental Analysis: C, 43.75; H, 3.21; Br, 18.19; F, 12.97; O, 7.28; S, 14.60



HRMS (ESI, m/z) calcd for $C_{16}H_{14}BrF_3O_2S_2$ $[M+Na]^+$ 460.9463, found 460.9468.







Chemical Formula: $C_{16}H_{13}F_3O_2S_2$

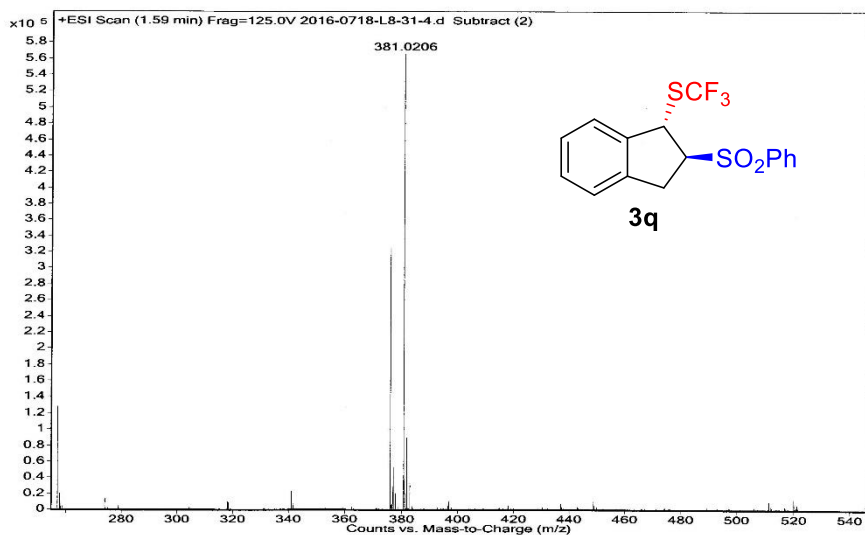
Exact Mass: 358.0309

Molecular Weight: 358.3932

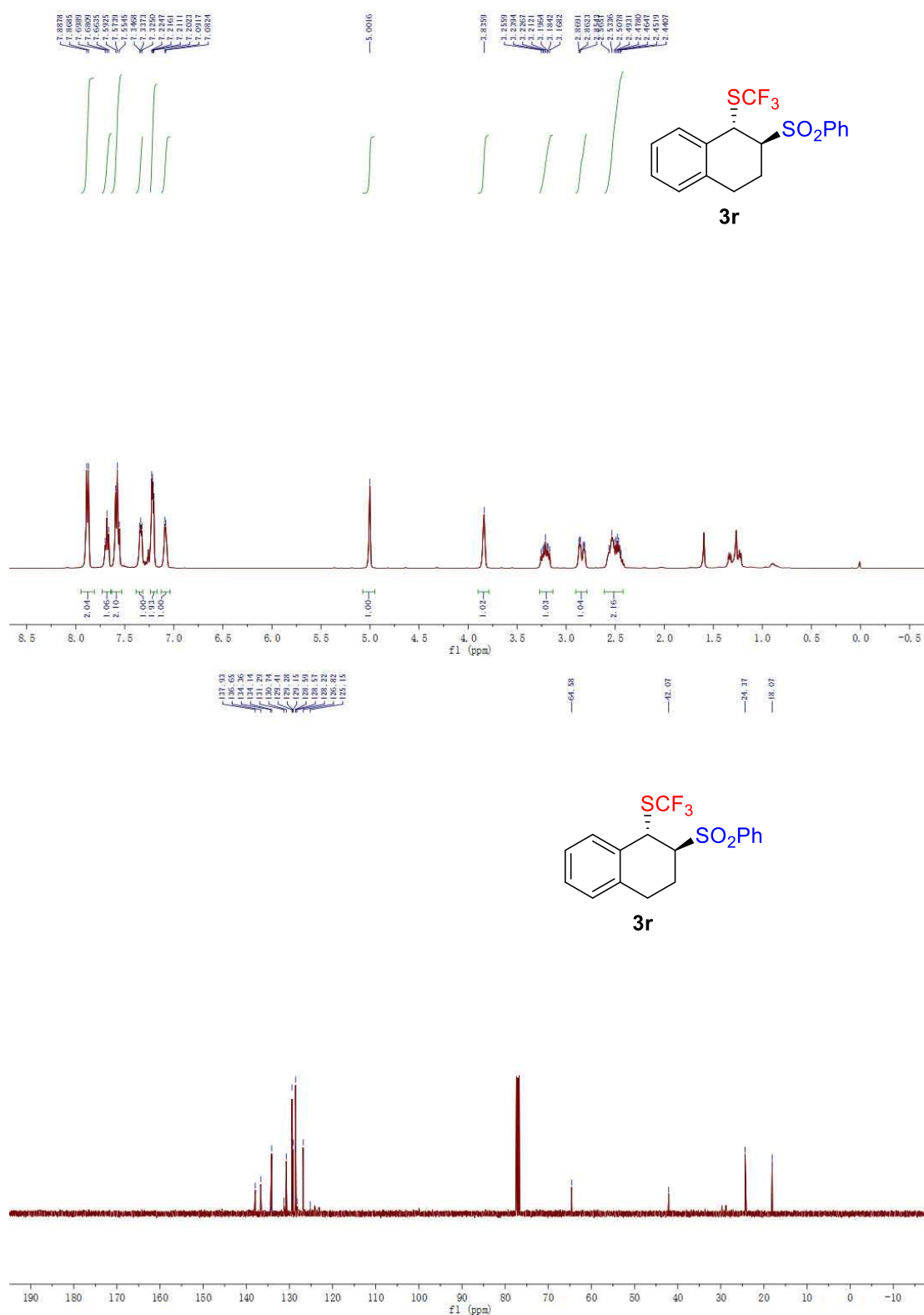
m/z: 358.0309 (100.0%), 359.0343 (17.3%), 360.0267 (9.0%), 359.0303 (1.6%),
361.0301 (1.6%), 360.0376 (1.4%)

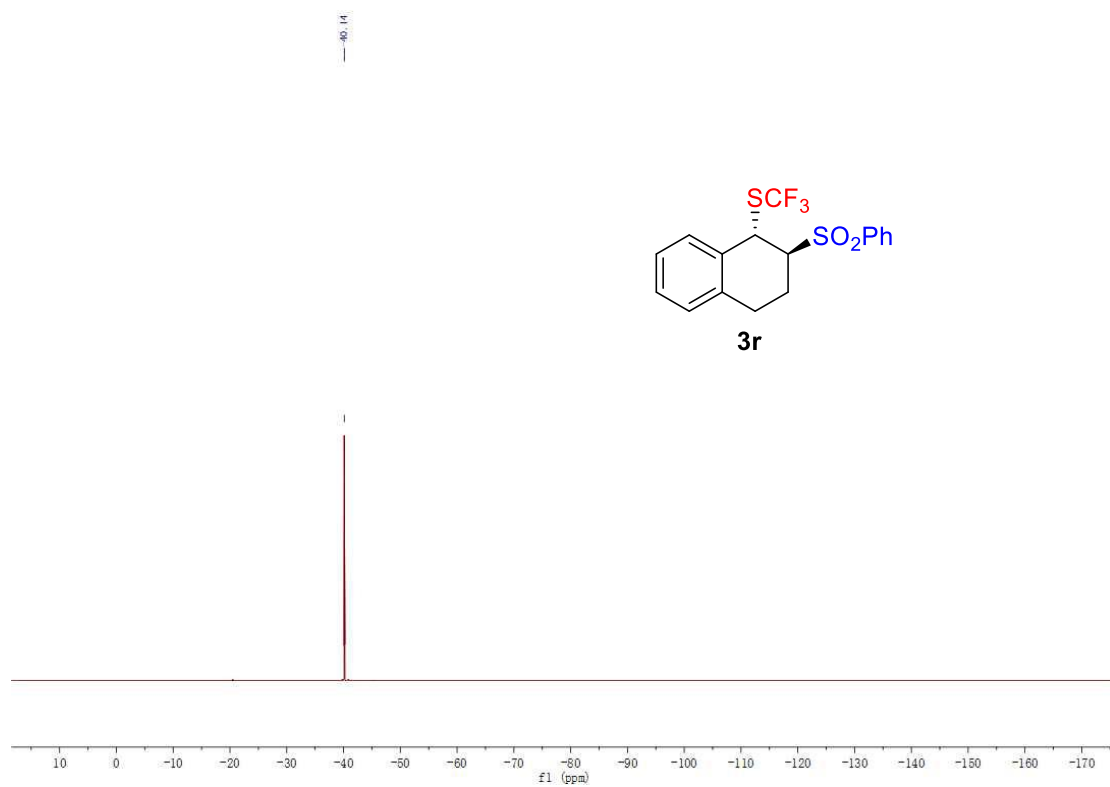
Elemental Analysis: C, 53.62; H, 3.66; F, 15.90; O, 8.93; S, 17.89

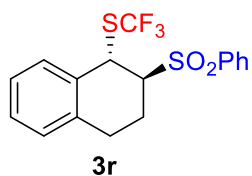
Sample Name	2016-0718-L8-31-4	Position	P1-E9	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	Inj Position		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	2016-0718-L8-31-4.d	ACQ Method	0103.m	Comment		Acquired Time	7/18/2016 3:44:55 PM



HRMS (ESI, m/z) calcd for $C_{16}H_{13}F_3O_2S_2$ $[M+Na]^+$ 381.0201, found 381.0206.







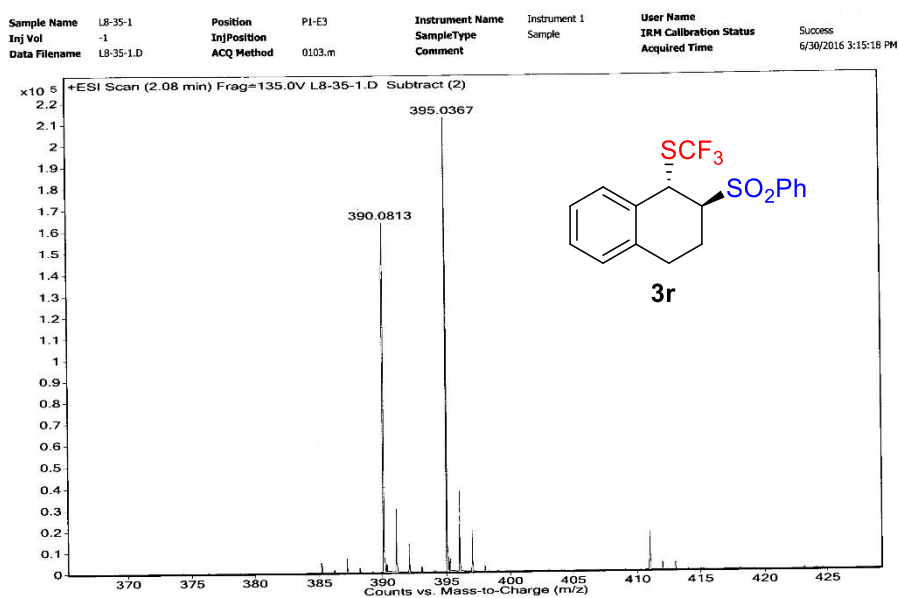
Chemical Formula: $C_{17}H_{15}F_3O_2S_2$

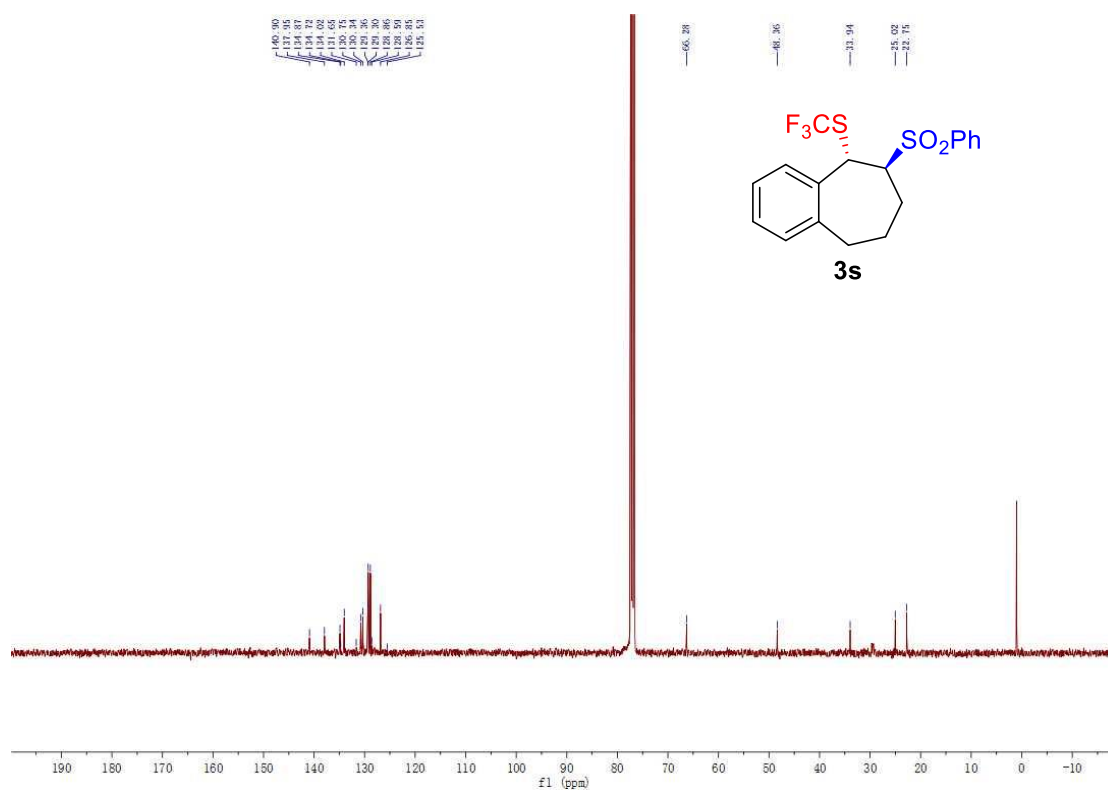
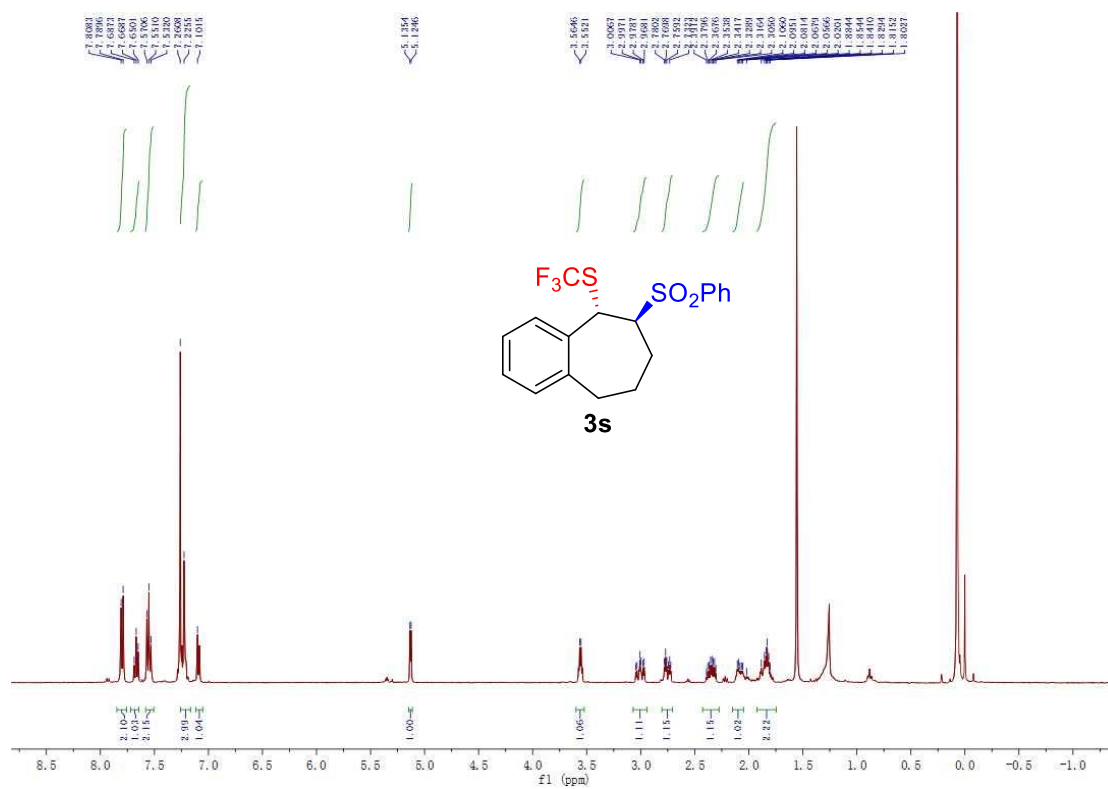
Exact Mass: 372.0466

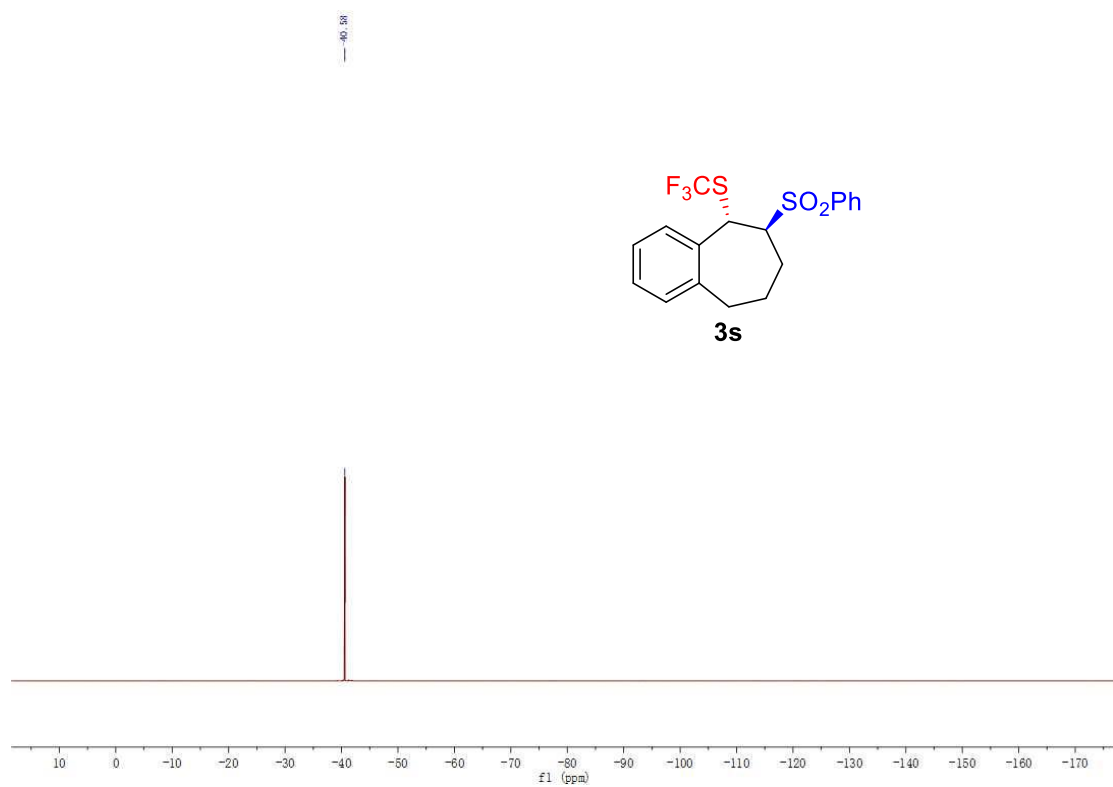
Molecular Weight: 372.4202

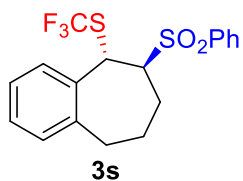
m/z: 372.0466 (100.0%), 373.0499 (18.4%), 374.0424 (9.0%), 375.0457 (1.7%),
373.0459 (1.6%), 374.0533 (1.6%)

Elemental Analysis: C, 54.83; H, 4.06; F, 15.30; O, 8.59; S, 17.22









Chemical Formula: $C_{18}H_{17}F_3O_2S_2$

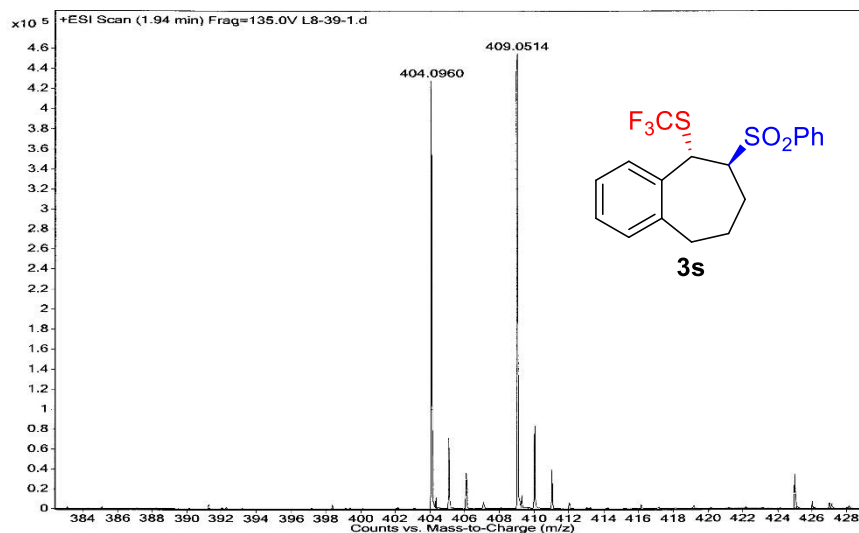
Exact Mass: 386.0622

Molecular Weight: 386.4472

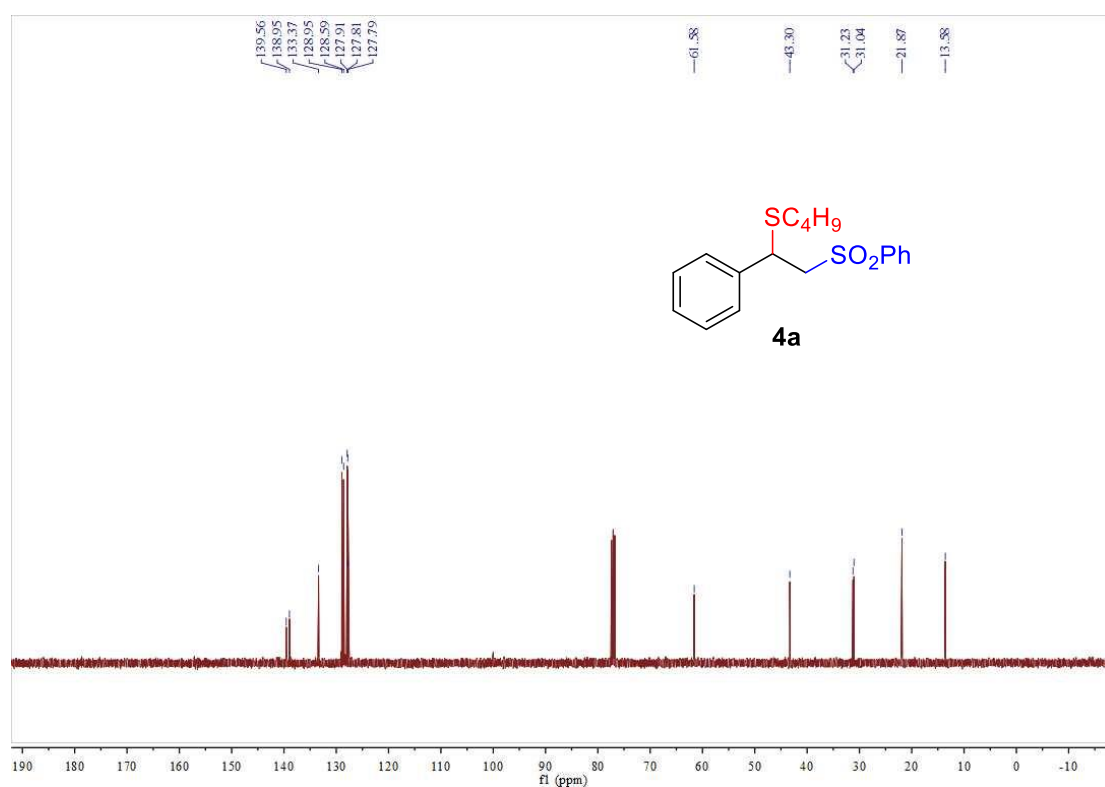
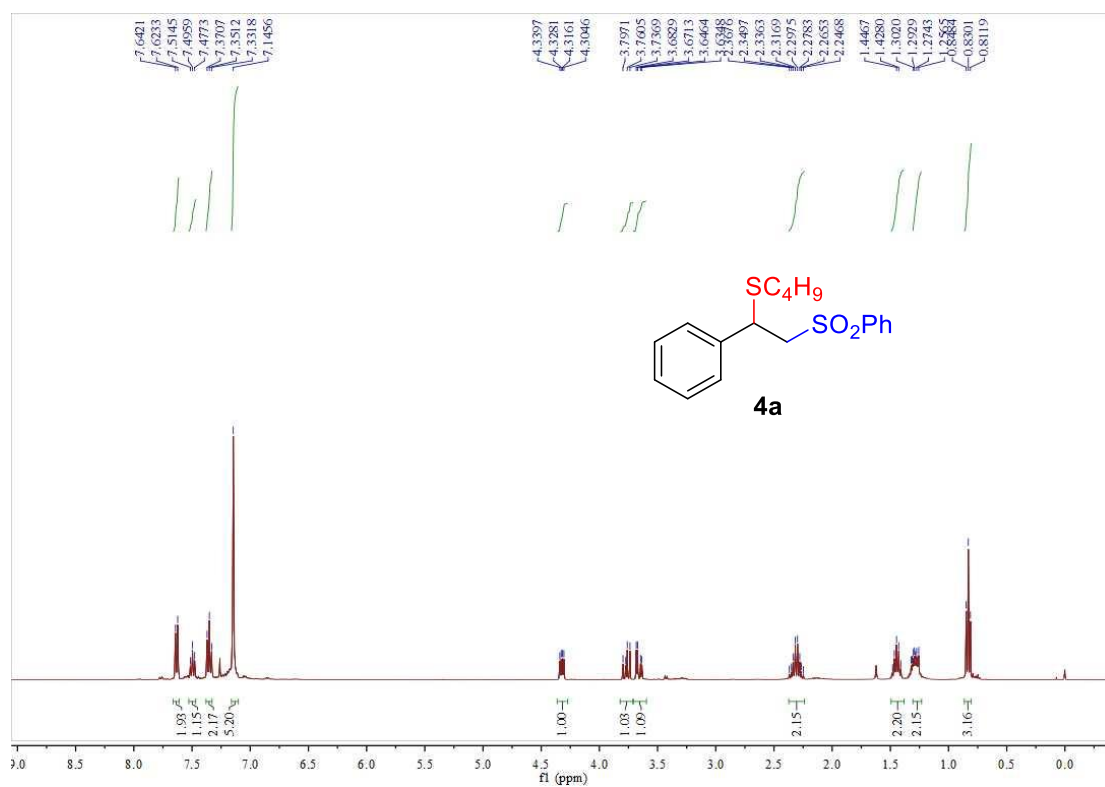
m/z: 386.0622 (100.0%), 387.0656 (19.5%), 388.0580 (9.0%), 388.0689 (1.8%),
389.0614 (1.8%), 387.0616 (1.6%)

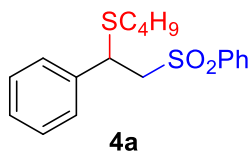
Elemental Analysis: C, 55.95; H, 4.43; F, 14.75; O, 8.28; S, 16.59

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	L8-39-1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



HRMS (ESI, m/z) calcd for $C_{18}H_{17}F_3O_2S_2$ $[M+Na]^+$ 409.0514, found 409.0514.





Chemical Formula: C₁₈H₂₂O₂S₂

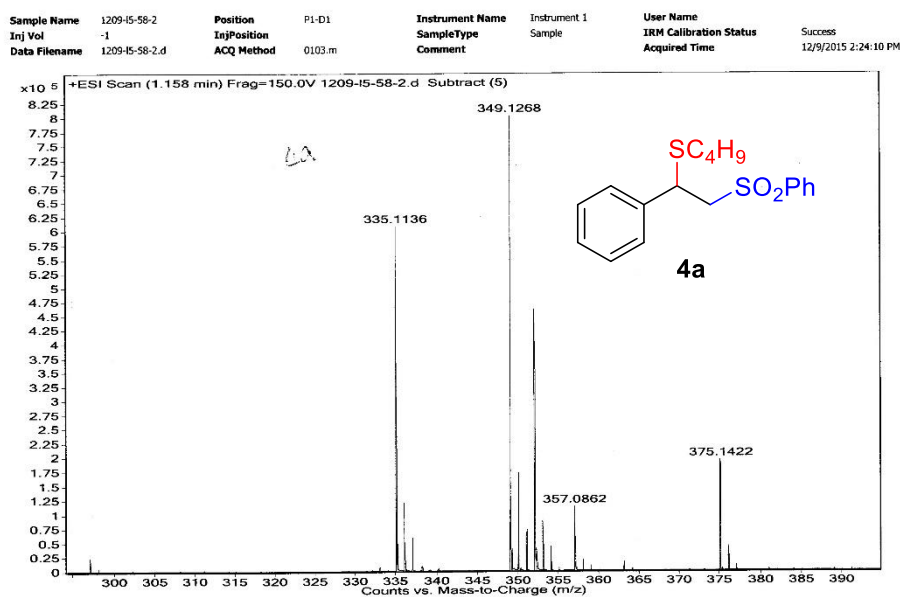
Exact Mass: 334.1061

Molecular Weight: 334.4920

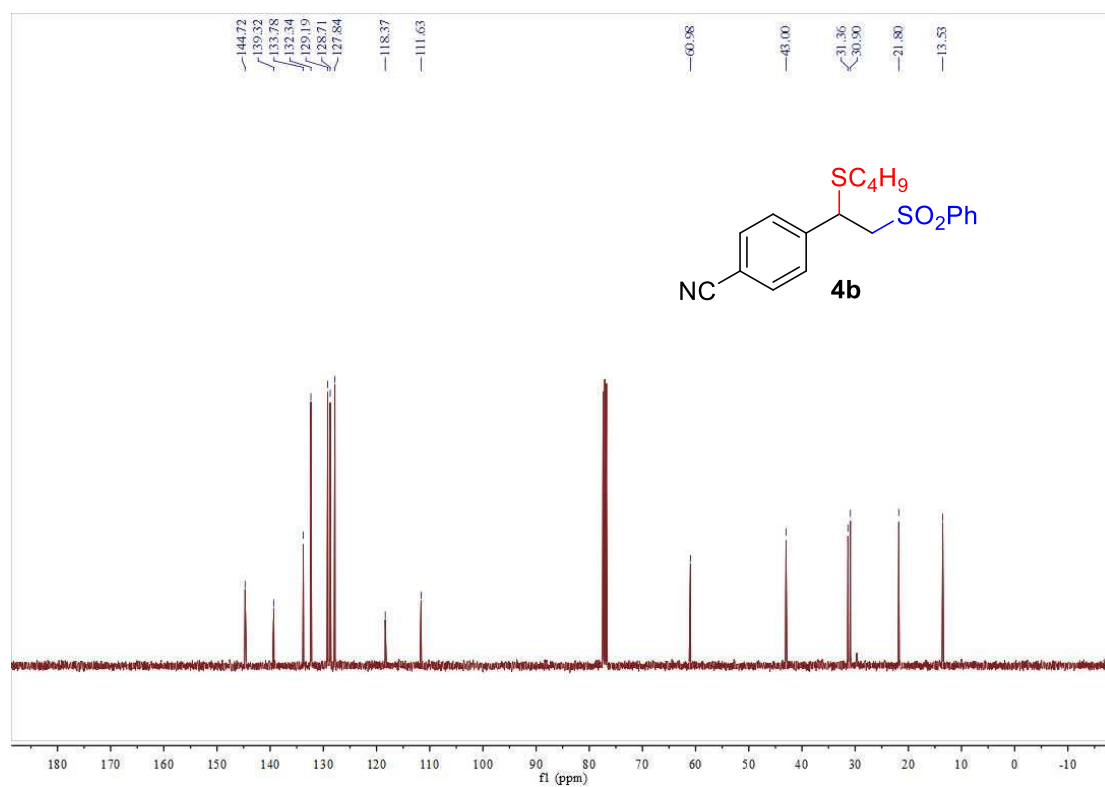
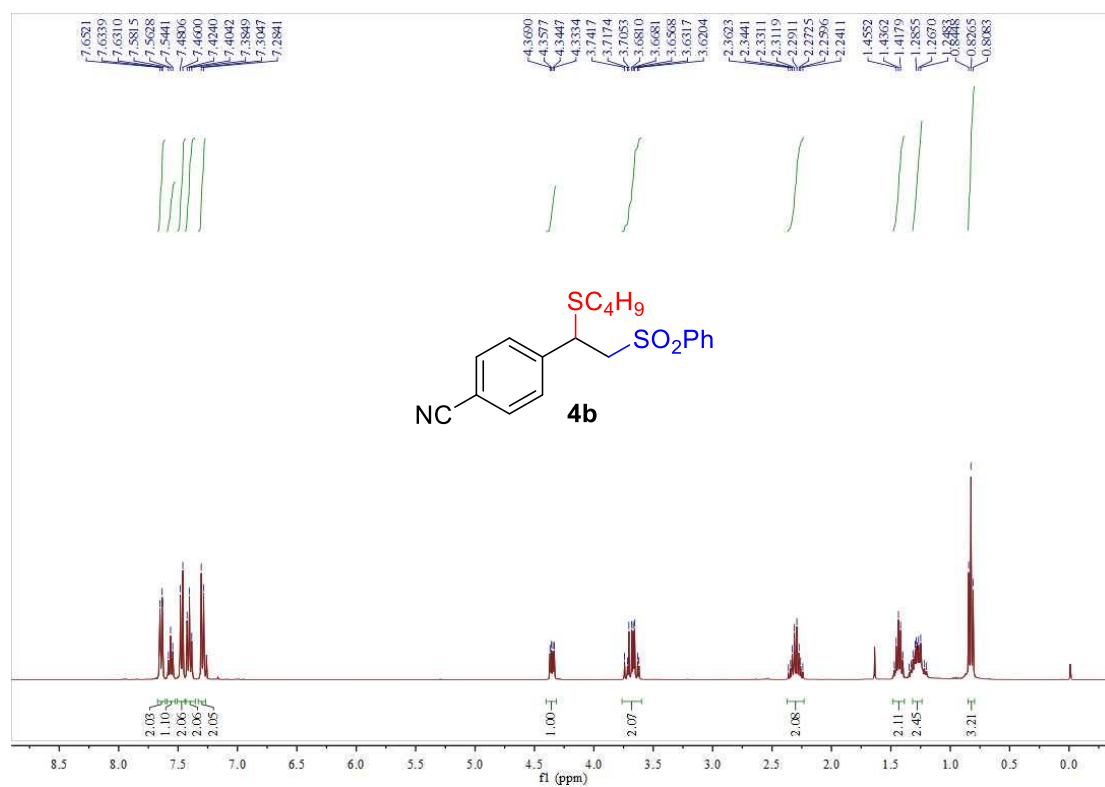
m/z: 334.1061 (100.0%), 335.1095 (19.5%), 336.1019 (9.0%), 336.1128 (1.8%),

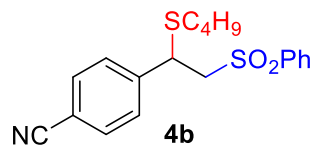
337.1053 (1.8%), 335.1055 (1.6%)

Elemental Analysis: C, 64.63; H, 6.63; O, 9.57; S, 19.17



HRMS (ESI, m/z) calcd for C₁₈H₂₂O₂S₂ [M+H]⁺ 335.1134, found 335.1136.





Chemical Formula: $C_{19}H_{21}NO_2S_2$

Exact Mass: 359.1014

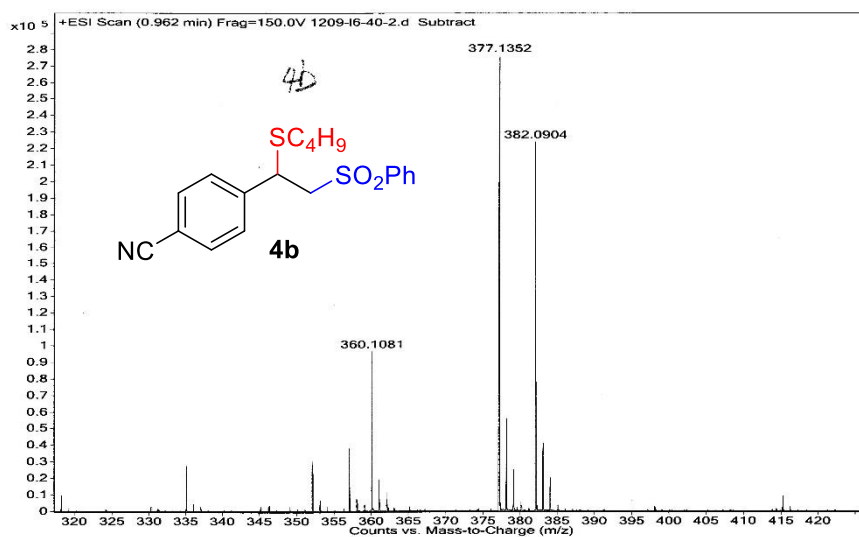
Molecular Weight: 359.5020

m/z: 359.1014 (100.0%), 360.1047 (20.5%), 361.0972 (9.0%), 361.1081 (2.0%),
362.1005 (1.9%), 360.1008 (1.6%)

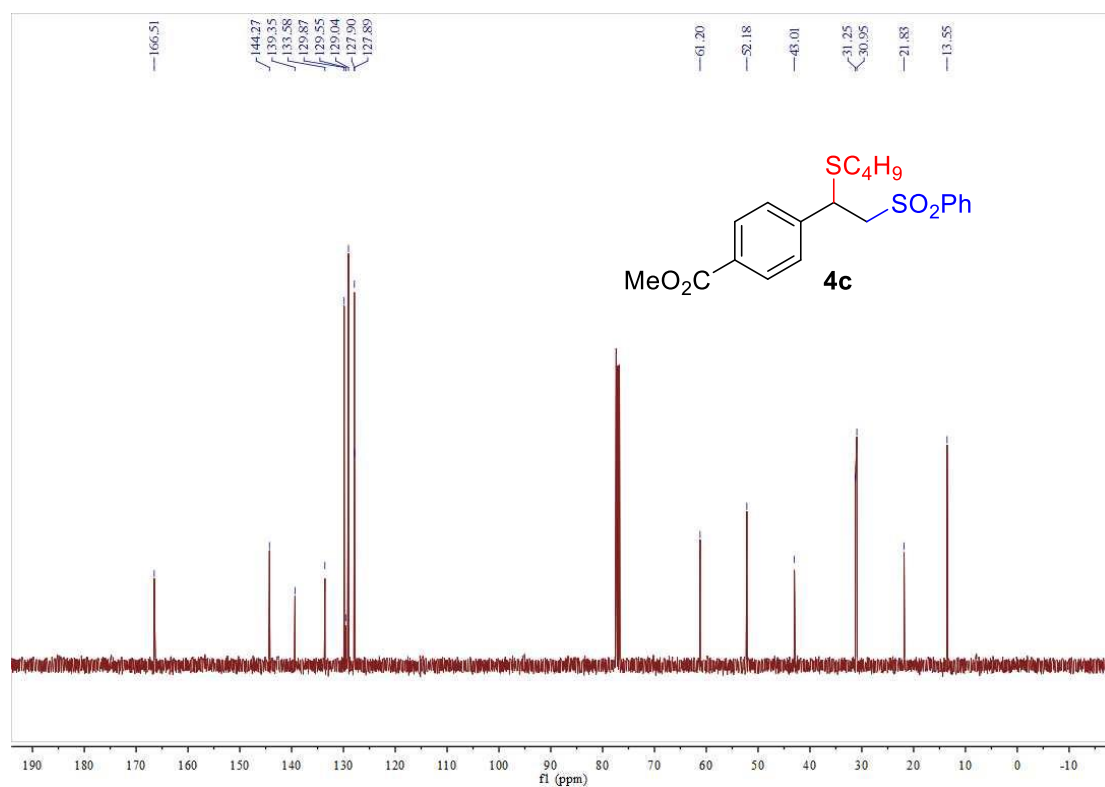
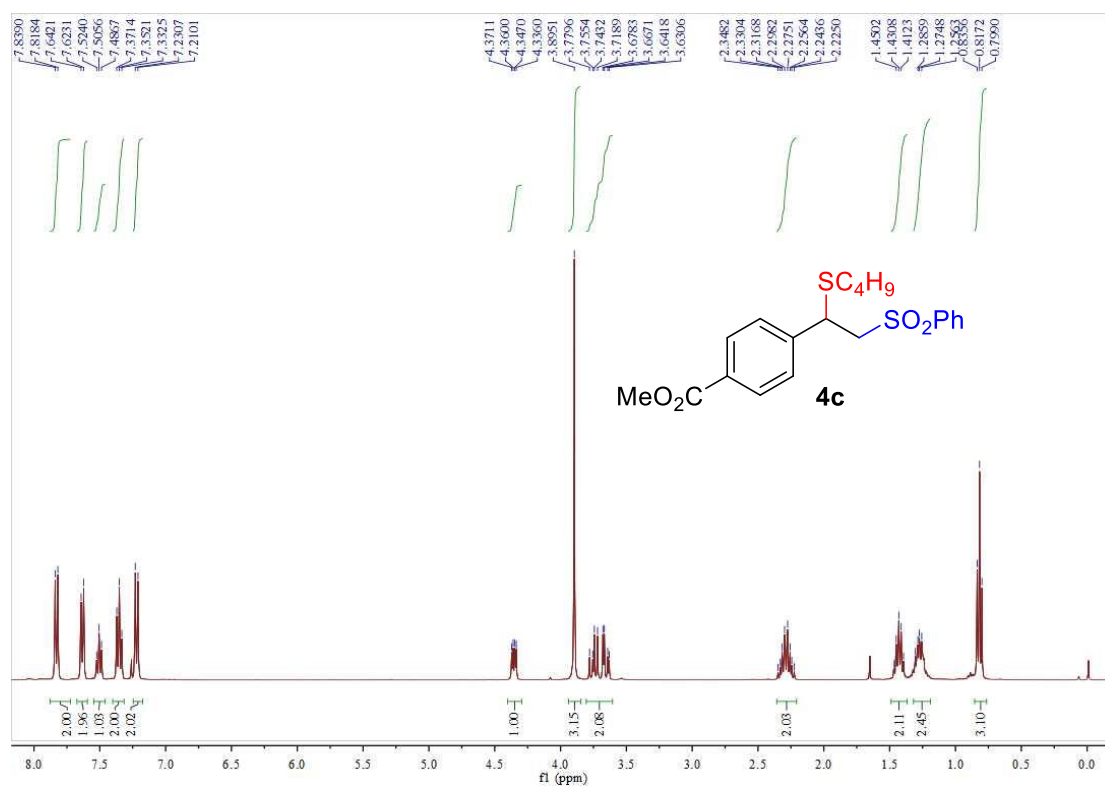
Elemental Analysis: C, 63.48; H, 5.89; N, 3.90; O, 8.90; S, 17.84

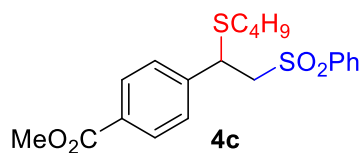
Sample Name	1209-I6-40-2	Position	P1-EI	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	1209-I6-40-2.d	ACQ Method	0103.m	Comment		Acquired Time

Success
12/9/2015 2:34:46 PM



HRMS (ESI, m/z) calcd for $C_{19}H_{21}NO_2S_2$ $[M+H]^+$ 360.1086, found 360.1081.





Chemical Formula: $C_{20}H_{24}O_4S_2$

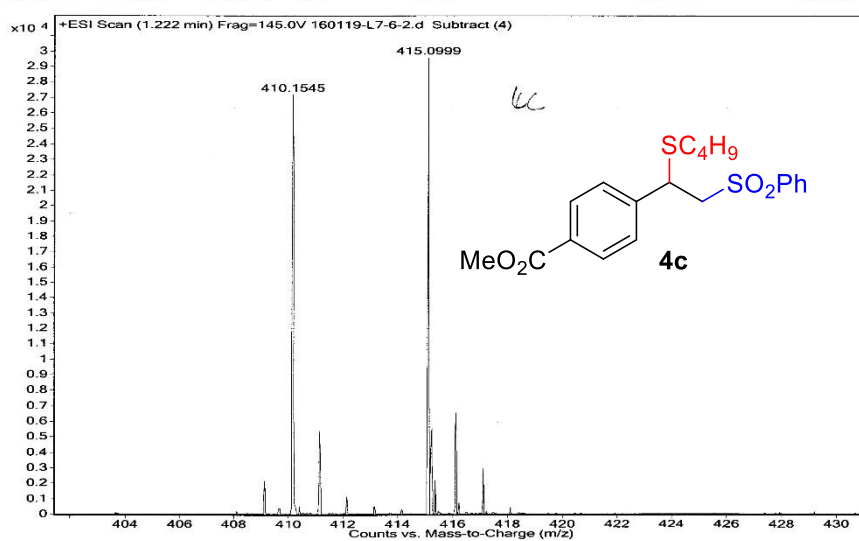
Exact Mass: 392.1116

Molecular Weight: 392.5280

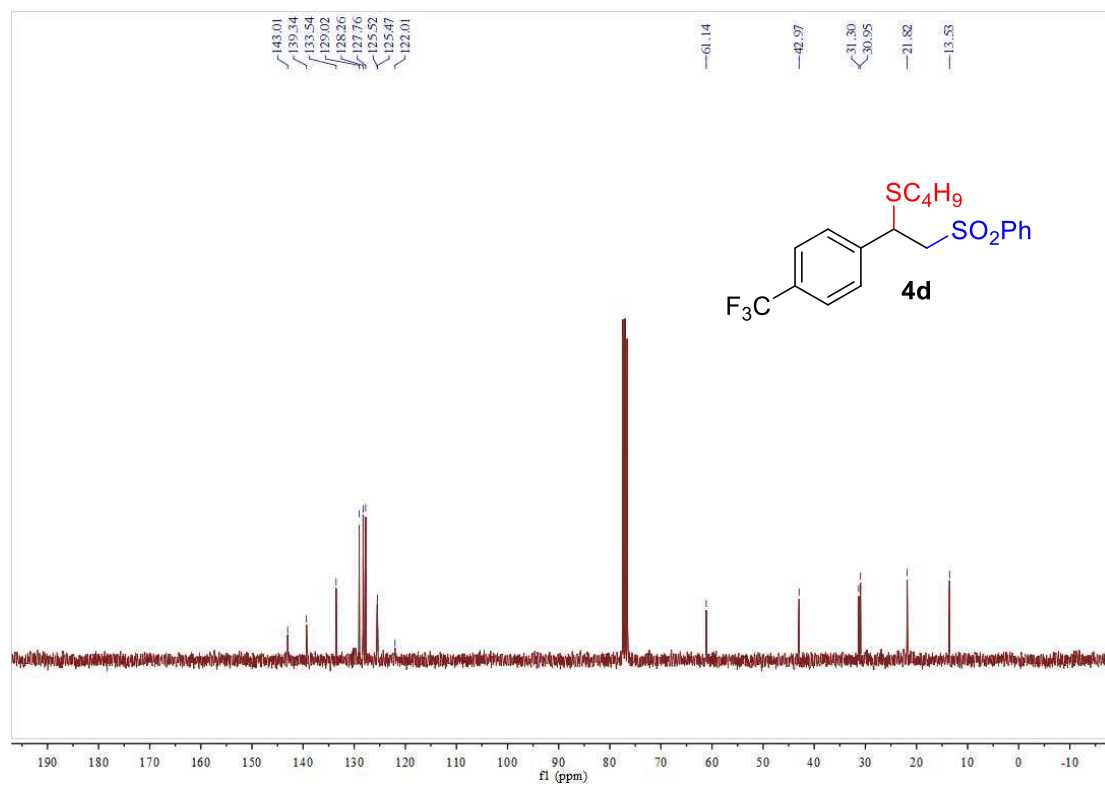
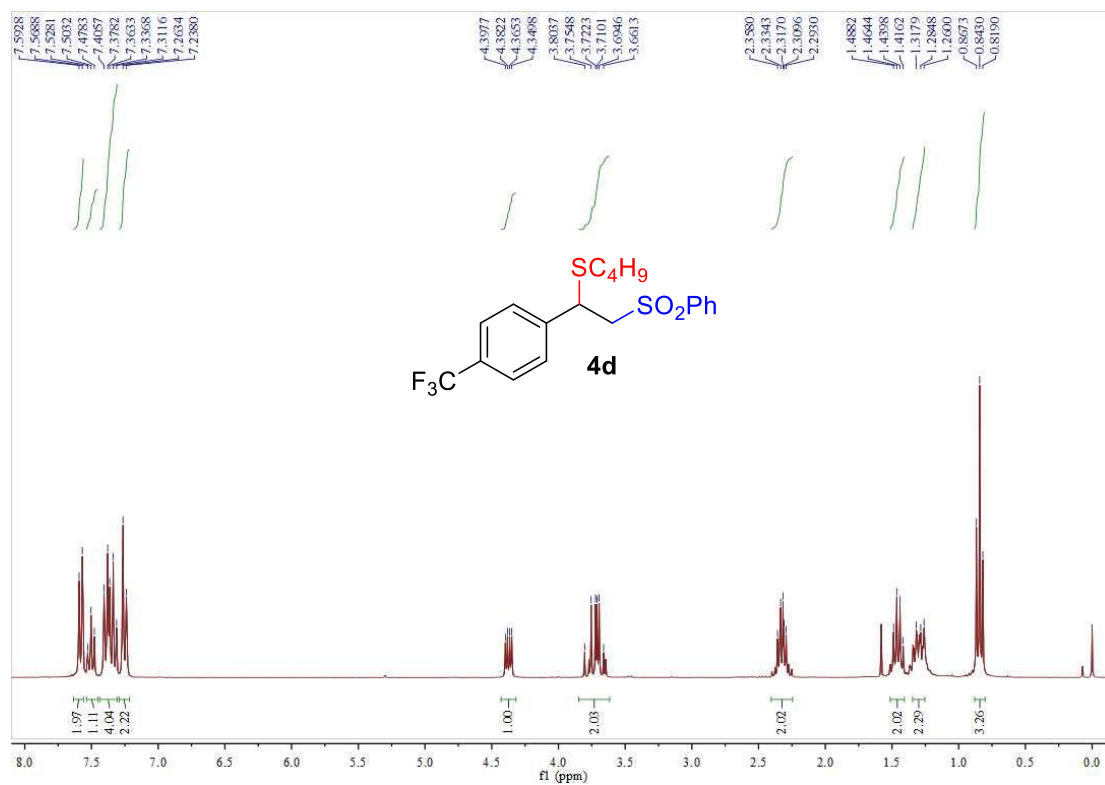
m/z : 392.1116 (100.0%), 393.1150 (21.6%), 394.1074 (9.0%), 394.1183 (2.2%),
395.1108 (2.0%), 393.1110 (1.6%)

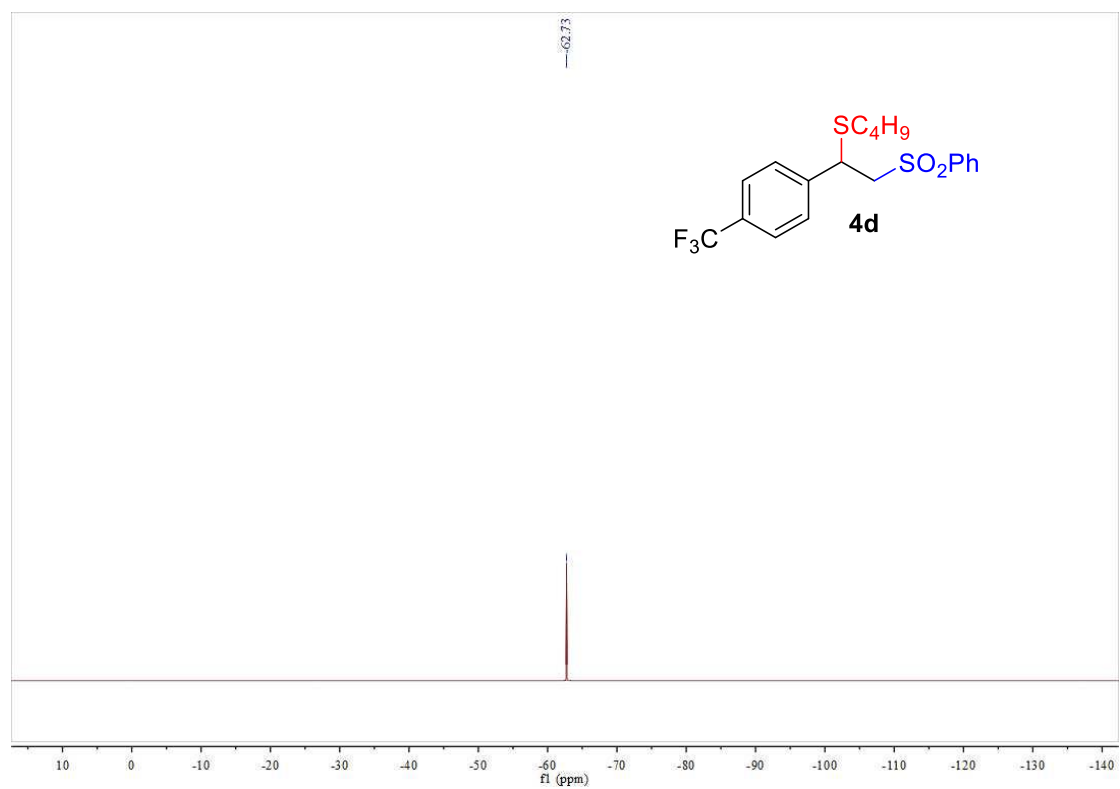
Elemental Analysis: C, 61.20; H, 6.16; O, 16.30; S, 16.34

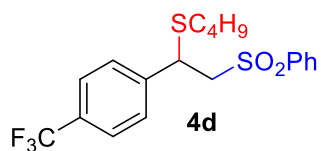
Sample Name	160119-L7-6-2	Position	P1-F3	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRN Calibration Status	Success
Data Filename	160119-L7-6-2.d	ACQ Method	0103.m	Comment		Acquired Time	3/19/2016 4:01:19 PM



HRMS (ESI, m/z) calcd for $C_{20}H_{24}O_4S_2$ $[M+Na]^+$ 415.1008, found 415.0999.







Chemical Formula: $C_{19}H_{21}F_3O_2S_2$

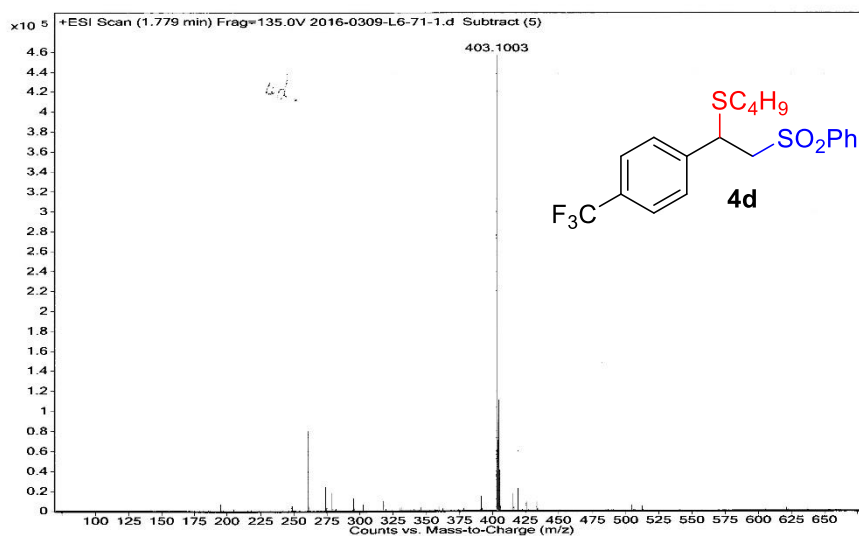
Exact Mass: 402.0935

Molecular Weight: 402.4902

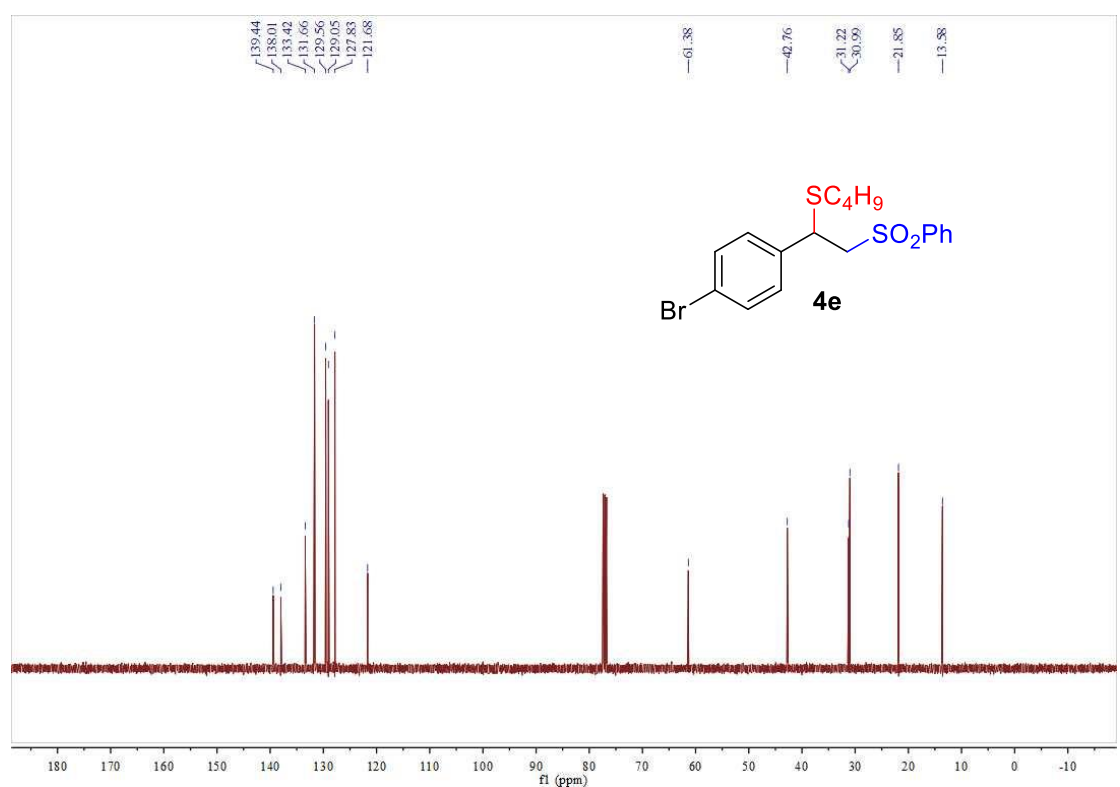
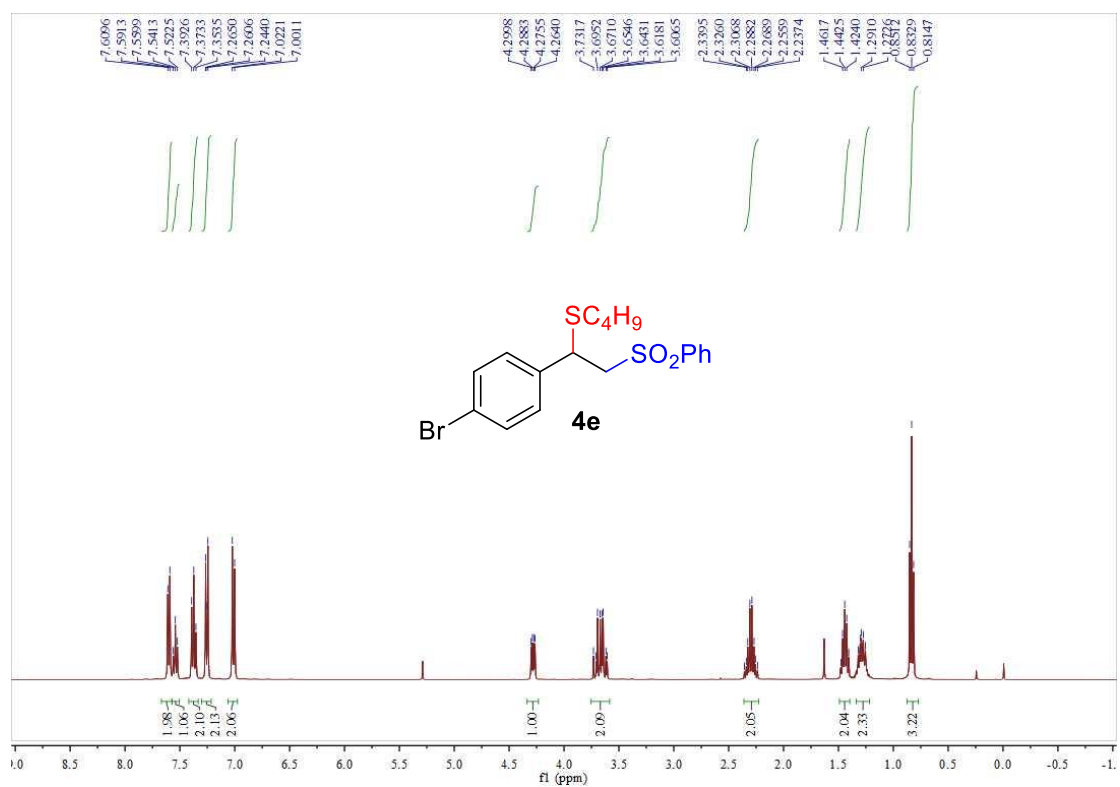
m/z: 402.0935 (100.0%), 403.0969 (20.5%), 404.0893 (9.0%), 404.1002 (2.0%),
405.0927 (1.9%), 403.0929 (1.6%)

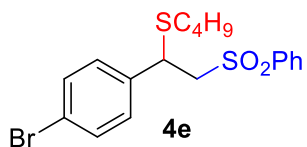
Elemental Analysis: C, 56.70; H, 5.26; F, 14.16; O, 7.95; S, 15.93

Sample Name	2016-0309-L6-71-1	Position	P1-E9	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	2016-0309-L6-71-1.d	ACQ Method	0103.m	Comment		Acquired Time	3/6/2016 2:45:23 PM



HRMS (ESI, m/z) calcd for $C_{19}H_{21}F_3O_2S_2$ $[M+H]^+$ 403.1008, found 403.1003.





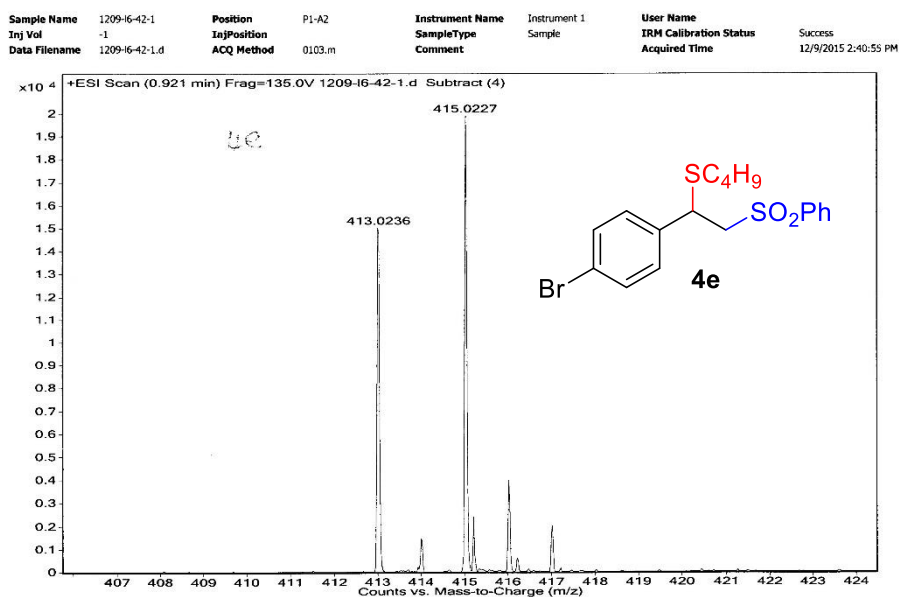
Chemical Formula: $C_{18}H_{21}BrO_2S_2$

Exact Mass: 412.0166

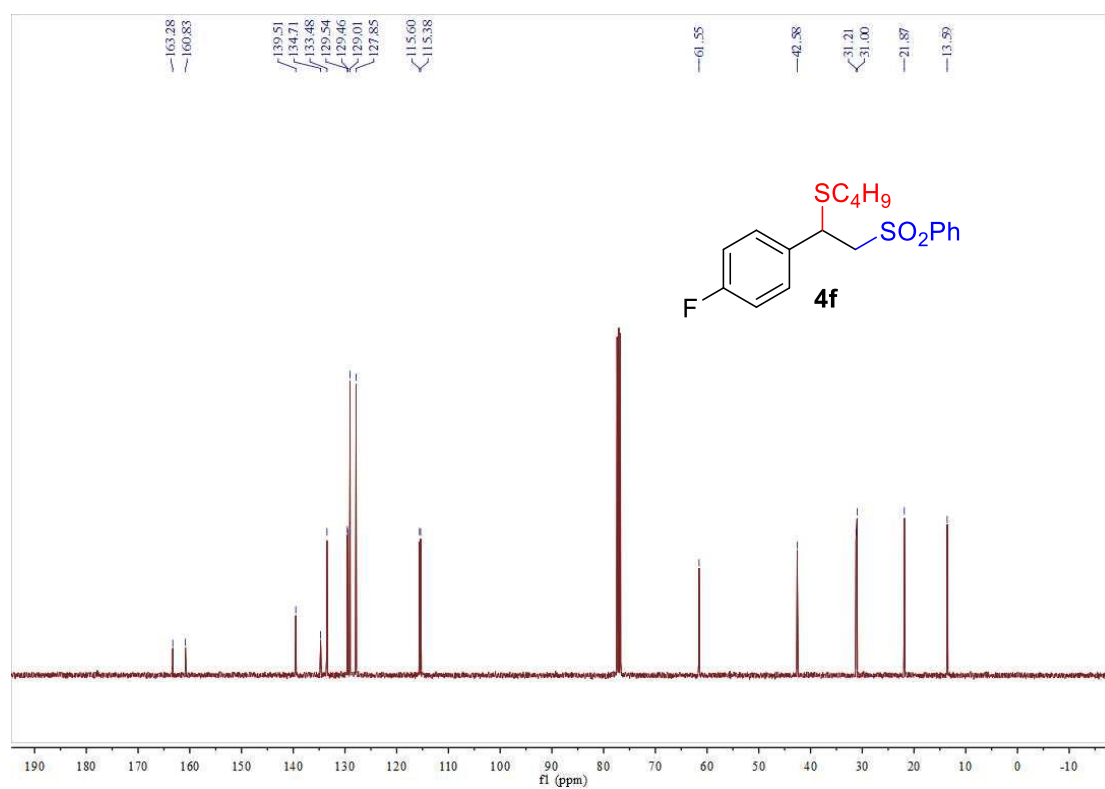
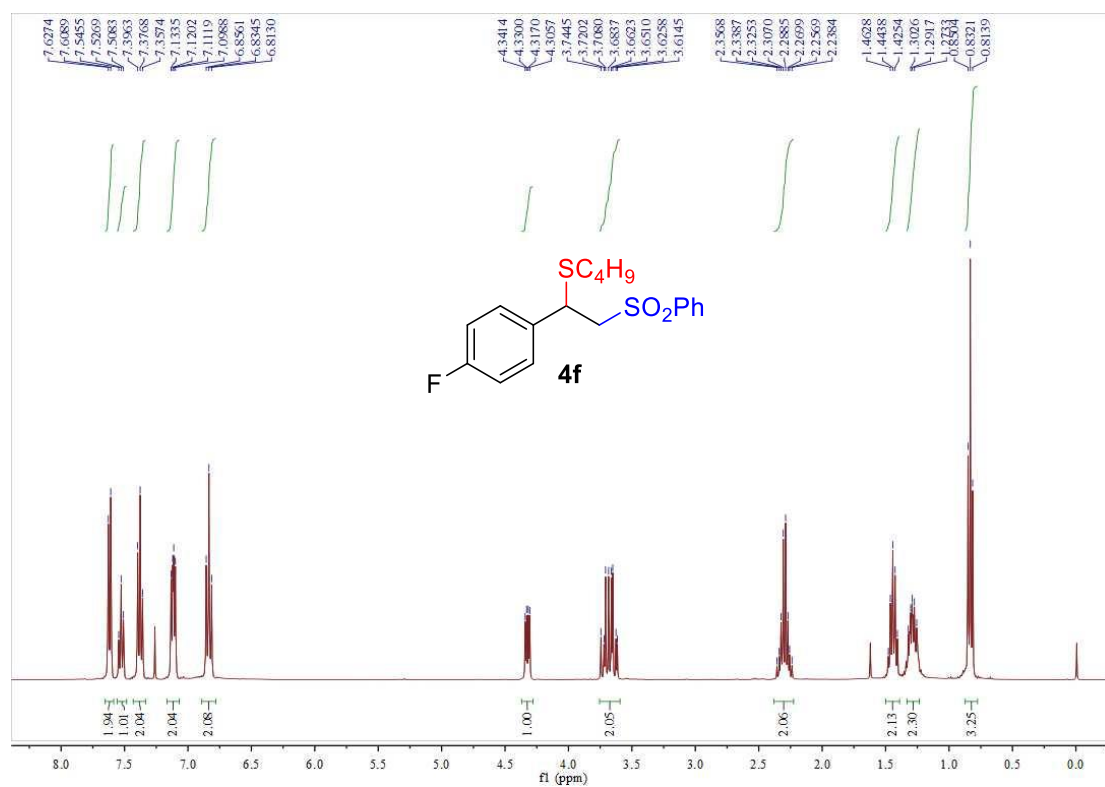
Molecular Weight: 413.3880

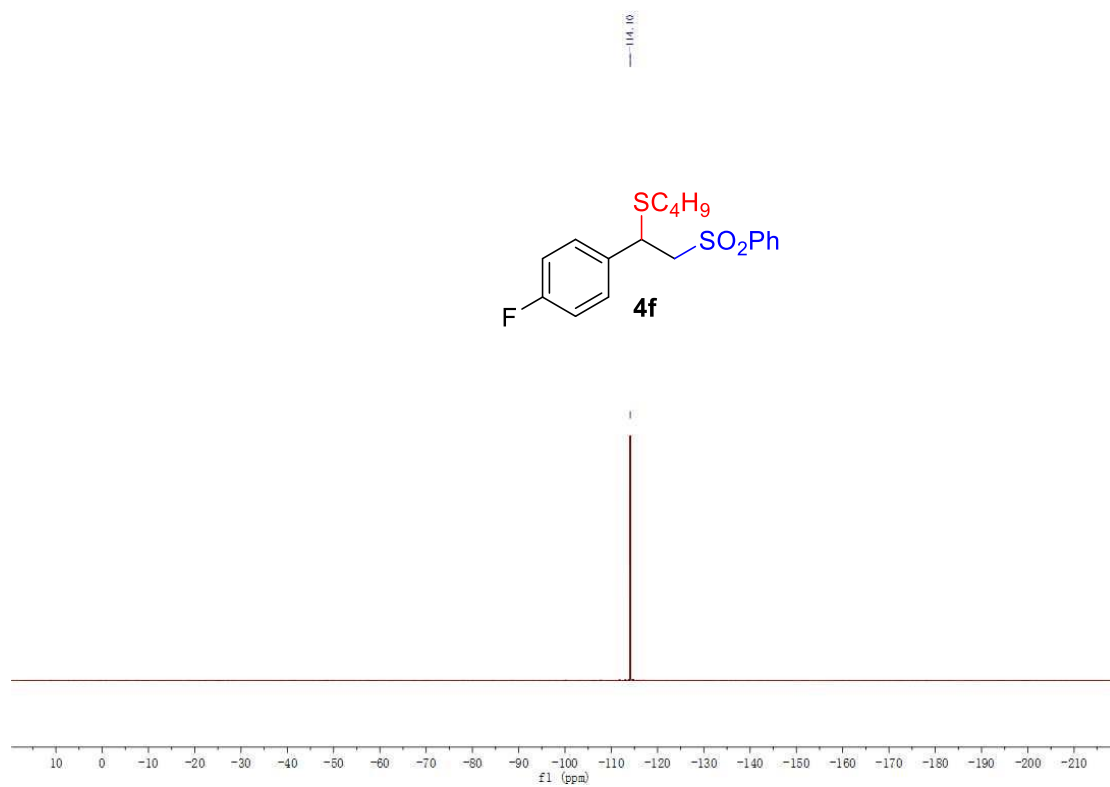
m/z: 412.0166 (100.0%), 414.0146 (97.3%), 413.0200 (19.5%), 415.0179 (18.9%),
414.0124 (9.0%), 416.0104 (8.8%), 416.0213 (1.7%), 417.0137 (1.7%),
413.0160 (1.6%), 415.0140 (1.6%), 415.0158 (1.5%), 414.0233 (1.1%)

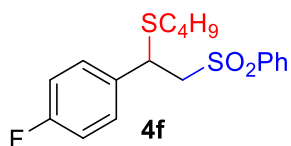
Elemental Analysis: C, 52.30; H, 5.12; Br, 19.33; O, 7.74; S, 15.51



HRMS (ESI, m/z) calcd for $C_{18}H_{21}BrO_2S_2$ $[M+H]^+$ 413.0239, found 413.0236.







Chemical Formula: $C_{18}H_{21}FO_2S_2$

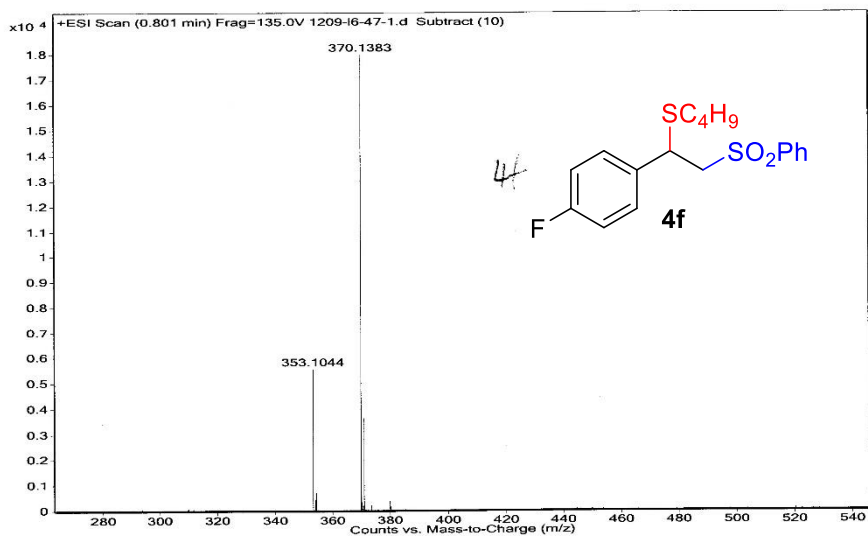
Exact Mass: 352.0967

Molecular Weight: 352.4824

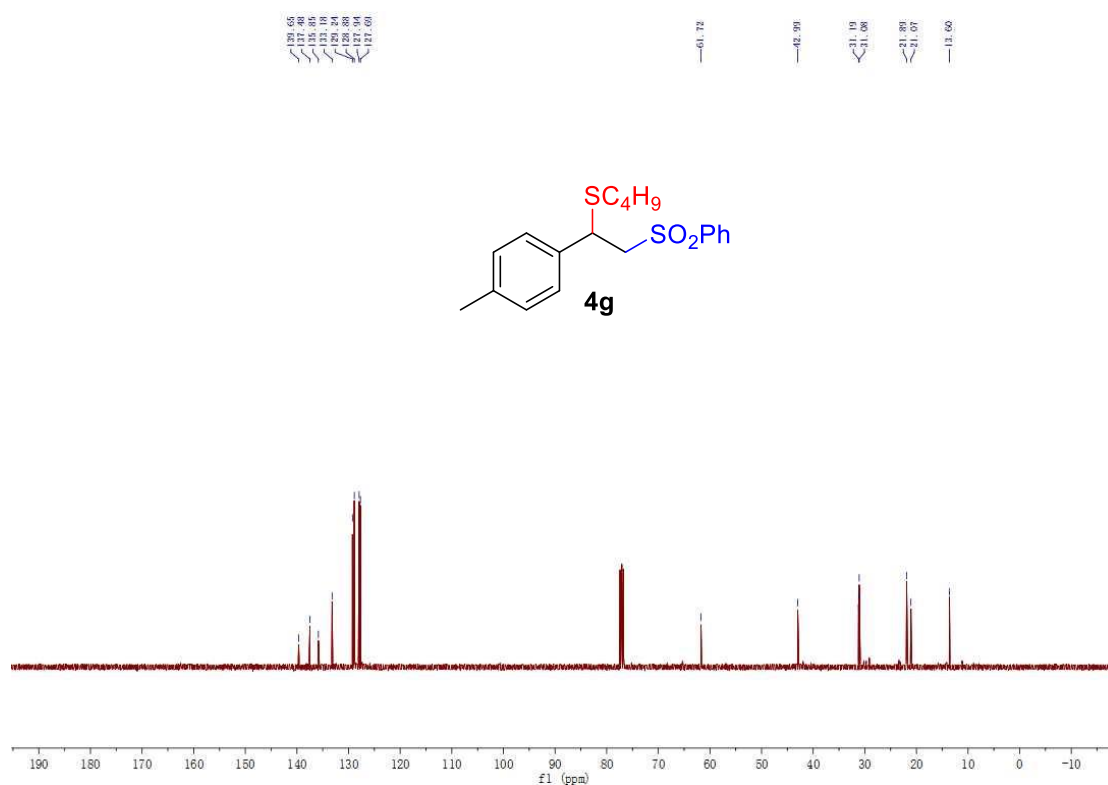
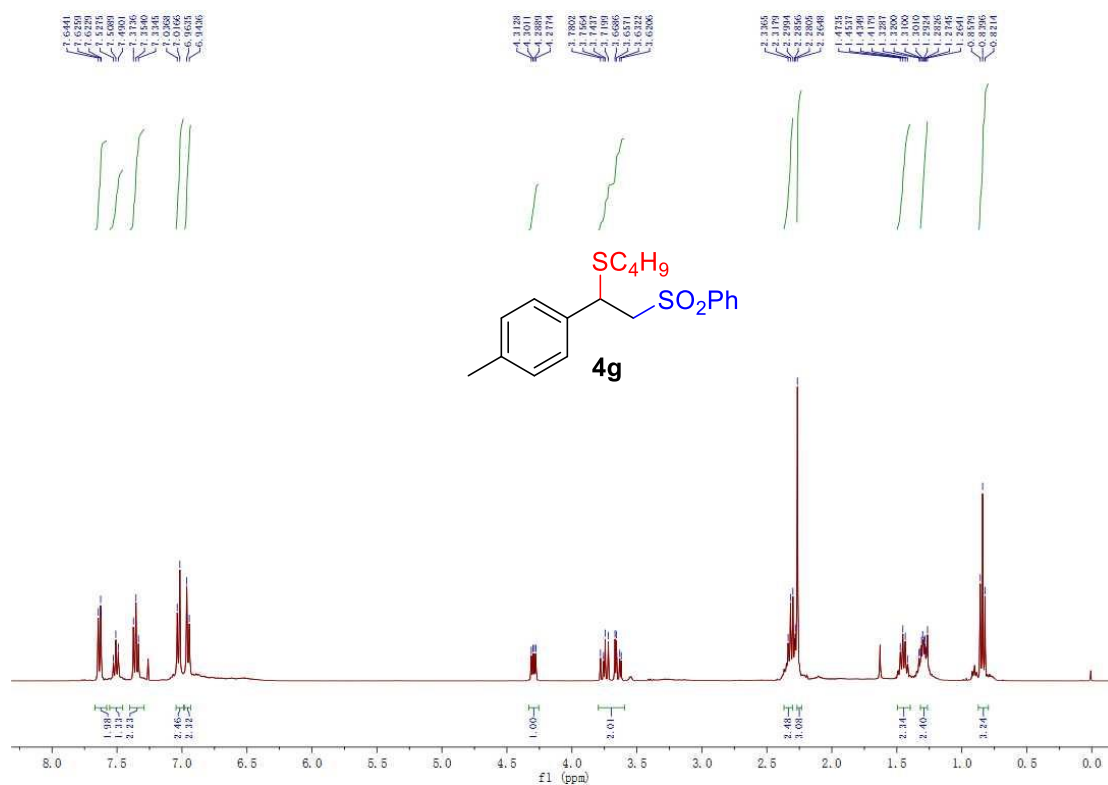
m/z: 352.0967 (100.0%), 353.1001 (19.5%), 354.0925 (9.0%), 354.1034 (1.8%),
355.0959 (1.8%), 353.0961 (1.6%)

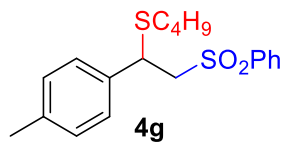
Elemental Analysis: C, 61.34; H, 6.01; F, 5.39; O, 9.08; S, 18.19

Sample Name	1209-16-47-1	Position	P1-A3	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	1209-16-47-1.d	ACQ Method	0103.m	Comment		Acquired Time	12/9/2015 2:58:23 PM



HRMS (ESI, m/z) calcd for $C_{18}H_{21}FO_2S_2$ $[M+H]^+$ 353.1040, found 353.1044.





Chemical Formula: C₁₉H₂₄O₂S₂

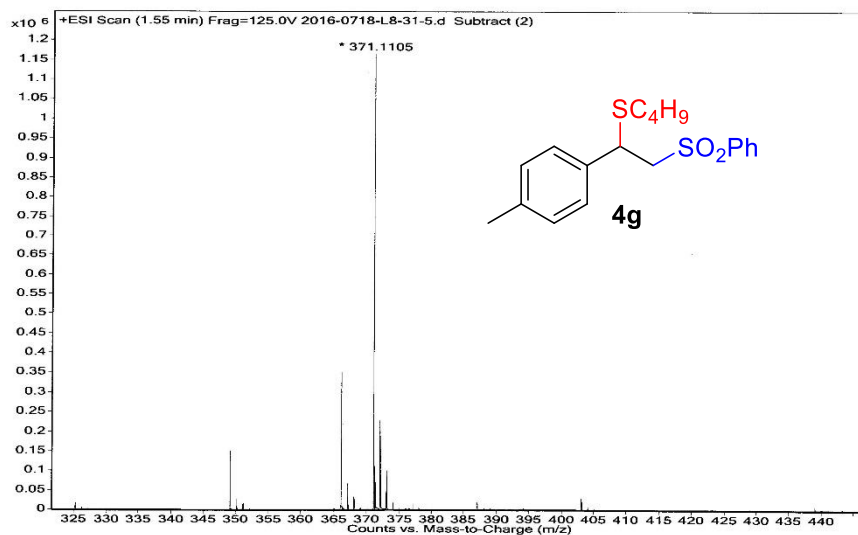
Exact Mass: 348.1218

Molecular Weight: 348.5190

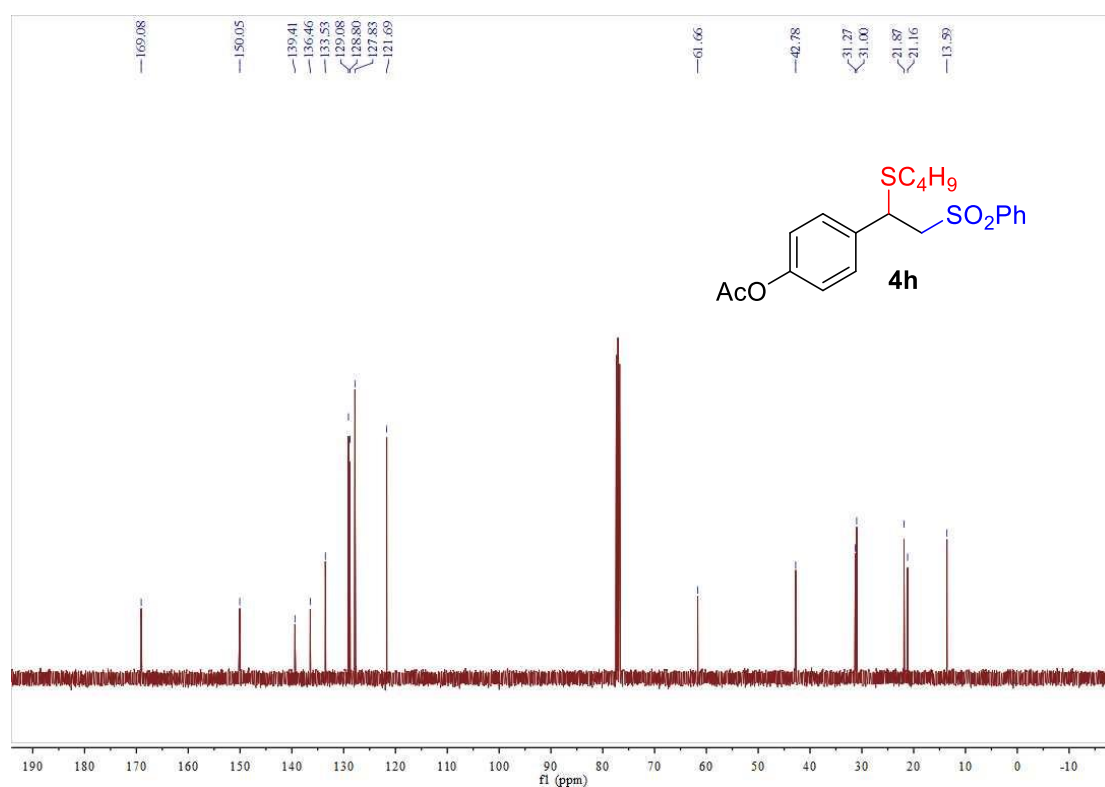
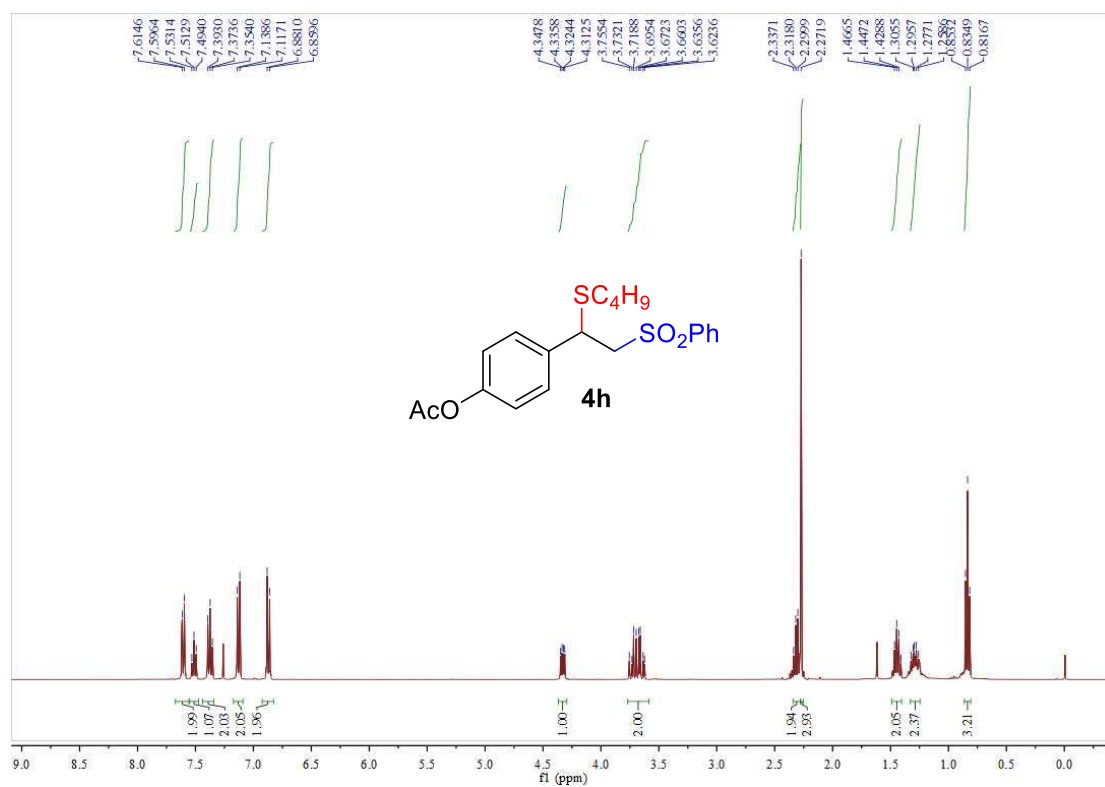
m/z: 348.1218 (100.0%), 349.1251 (20.5%), 350.1176 (9.0%), 350.1285 (2.0%),
351.1209 (1.9%), 349.1212 (1.6%)

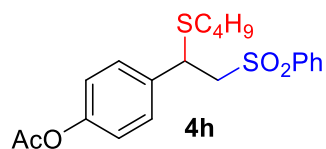
Elemental Analysis: C, 65.48; H, 6.94; O, 9.18; S, 18.40

Sample Name	2016-0718-L8-31-5	Position	P1-D9	Instrument Name	Instrument I	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	2016-0718-L8-31-5.d	ACQ Method	0103.m	Comment		Acquired Time	7/18/2016 3:48:20 PM



HRMS (ESI, m/z) calcd for C₁₉H₂₄O₂S₂ [M+Na]⁺ 371.1110, found 371.1115.





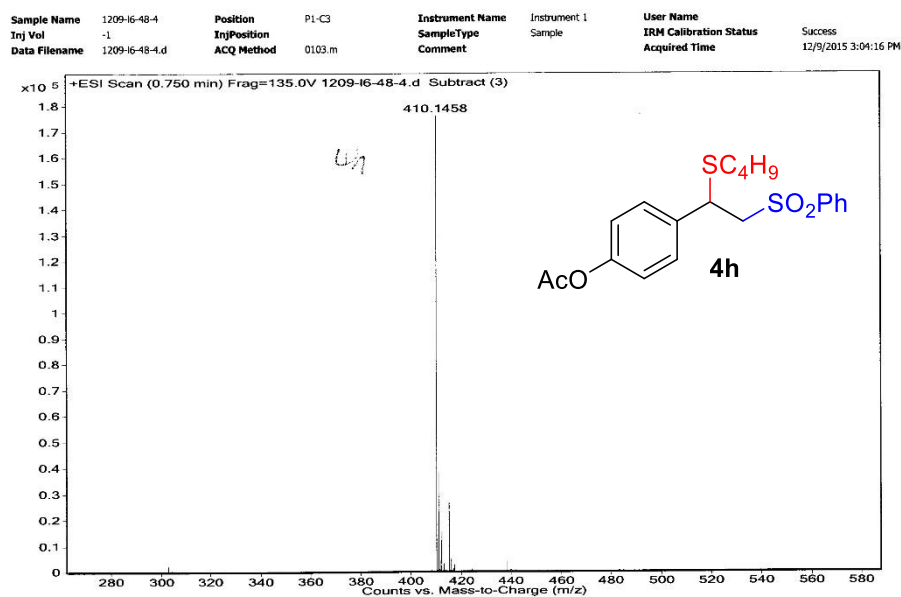
Chemical Formula: $C_{20}H_{24}O_4S_2$

Exact Mass: 392.1116

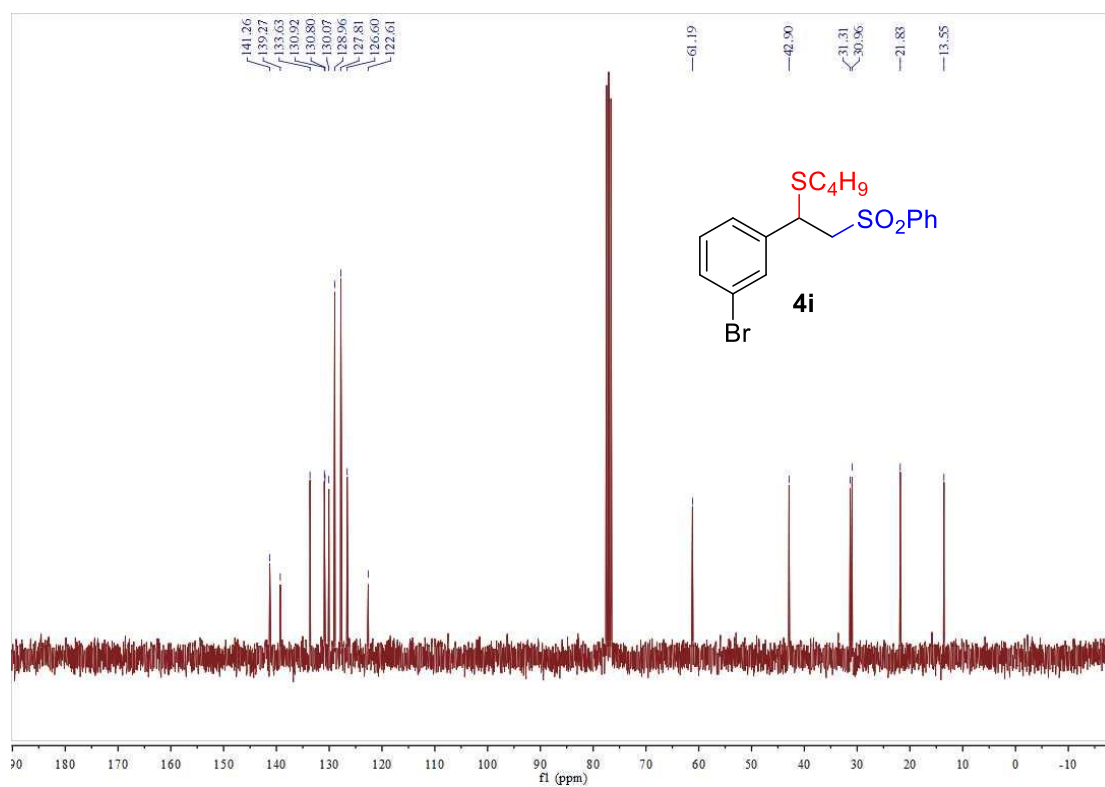
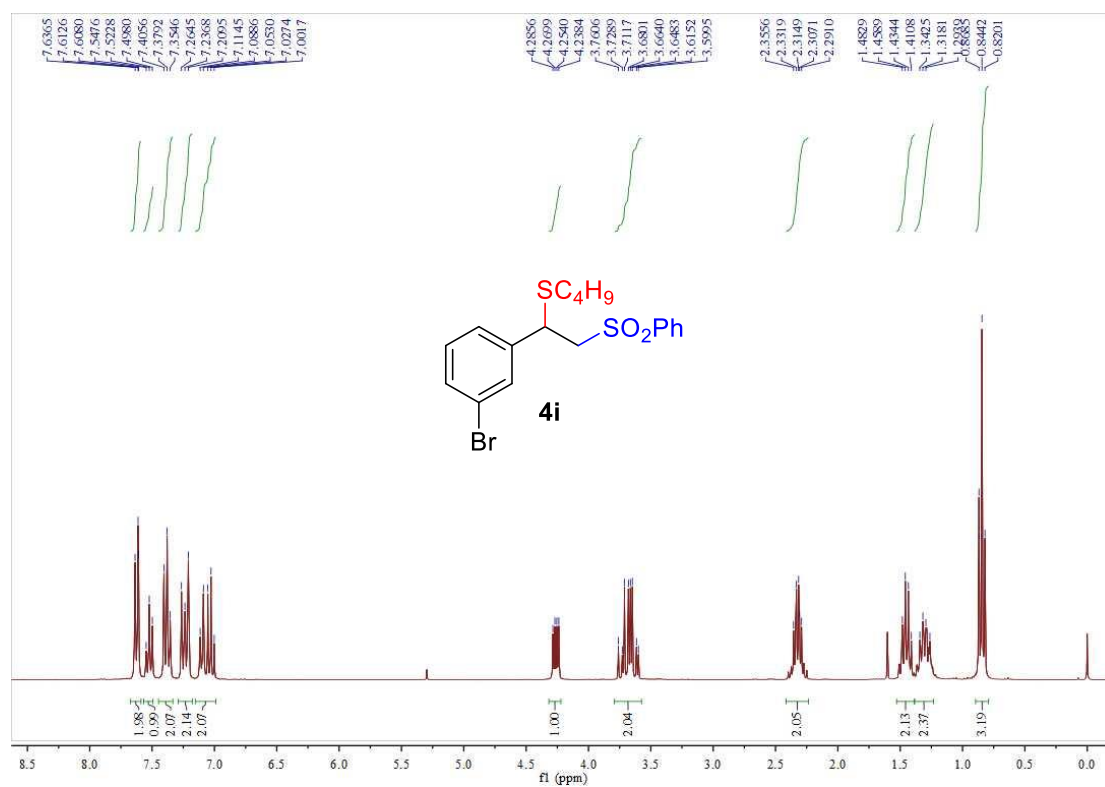
Molecular Weight: 392.5280

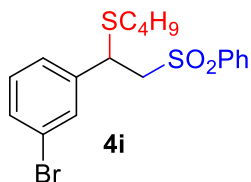
m/z : 392.1116 (100.0%), 393.1150 (21.6%), 394.1074 (9.0%),
394.1183 (2.2%), 395.1108 (2.0%), 393.1110 (1.6%)

Elemental Analysis: C, 61.20; H, 6.16; O, 16.30; S, 16.34



HRMS (ESI, m/z) calcd for $C_{20}H_{24}O_4S_2$ $[M+NH_4]^+$ 410.1454, found 410.1458.





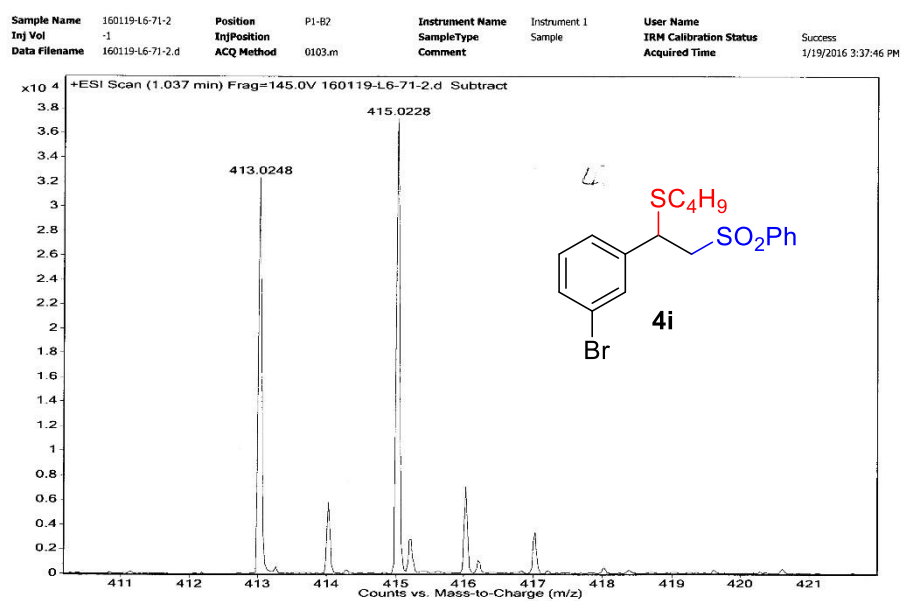
Chemical Formula: $C_{18}H_{21}BrO_2S_2$

Exact Mass: 412.0166

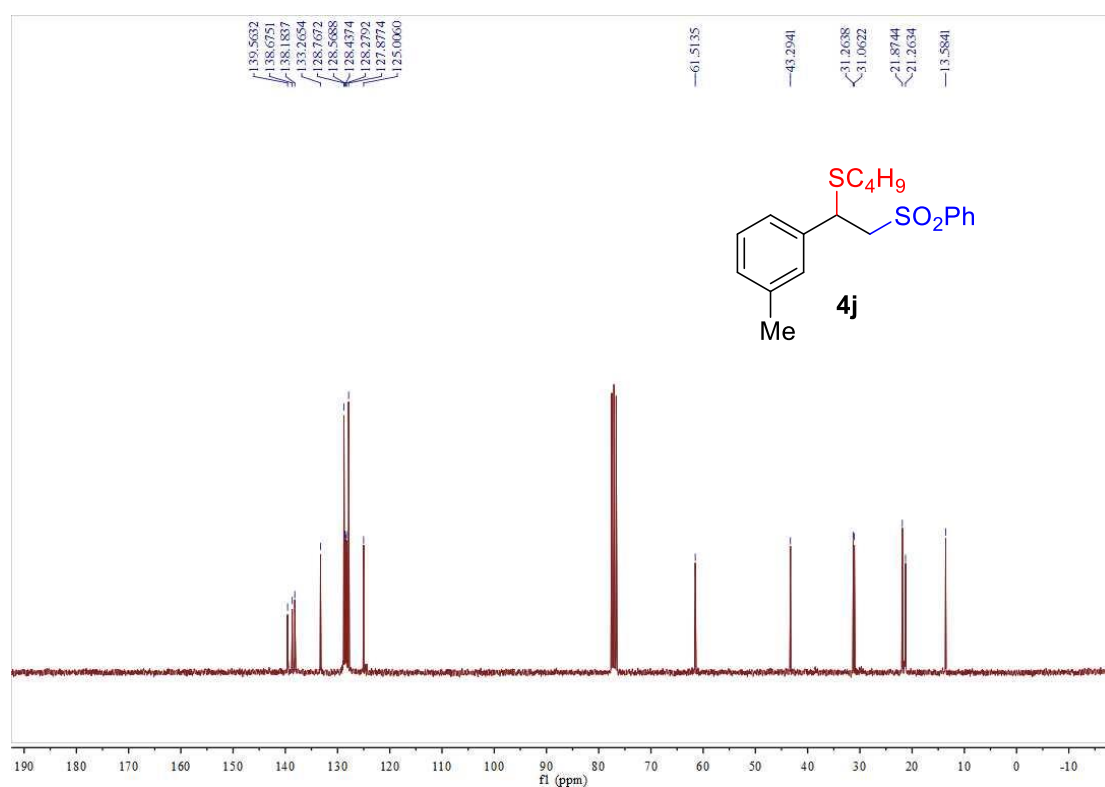
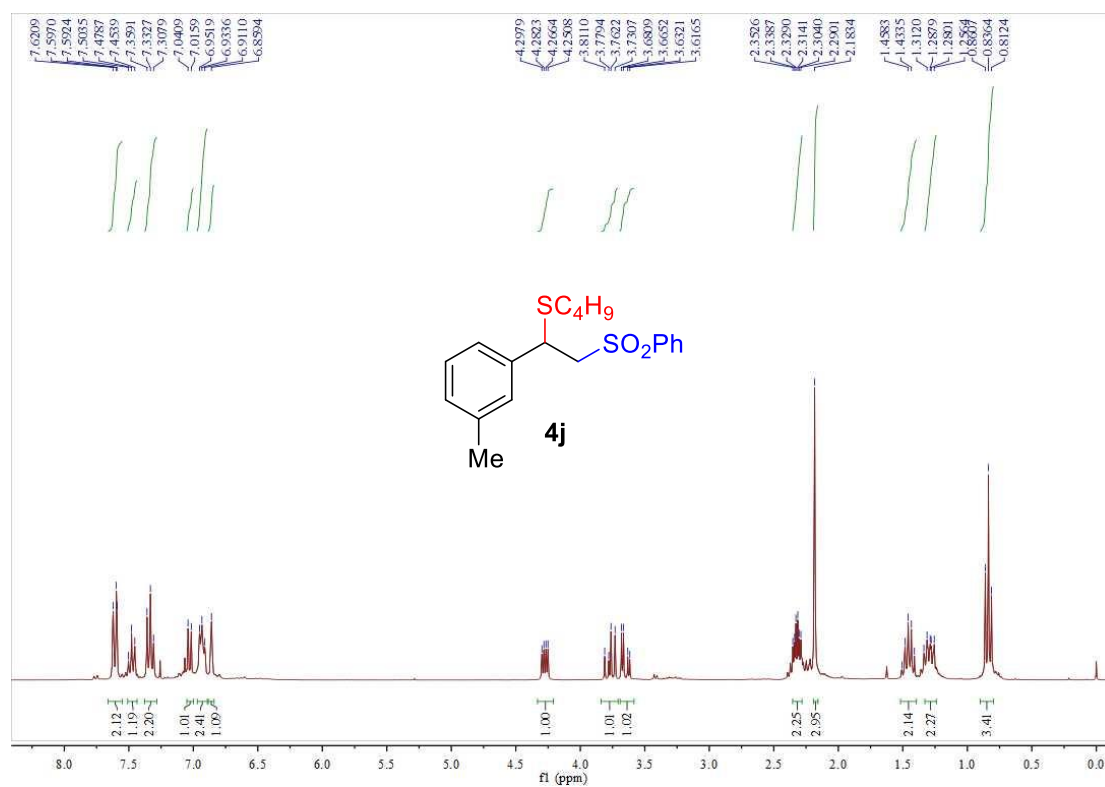
Molecular Weight: 413.3880

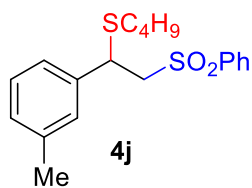
m/z: 412.0166 (100.0%), 414.0146 (97.3%), 413.0200 (19.5%), 415.0179 (18.9%), 414.0124 (9.0%), 416.0104 (8.8%), 416.0213 (1.7%), 417.0137 (1.7%), 413.0160 (1.6%), 415.0140 (1.6%), 415.0158 (1.5%), 414.0233 (1.1%)

Elemental Analysis: C, 52.30; H, 5.12; Br, 19.33; O, 7.74; S, 15.51



HRMS (ESI, m/z) calcd for $C_{18}H_{21}BrO_2S_2$ $[M+H]^+$ 413.0239, found 413.0248.





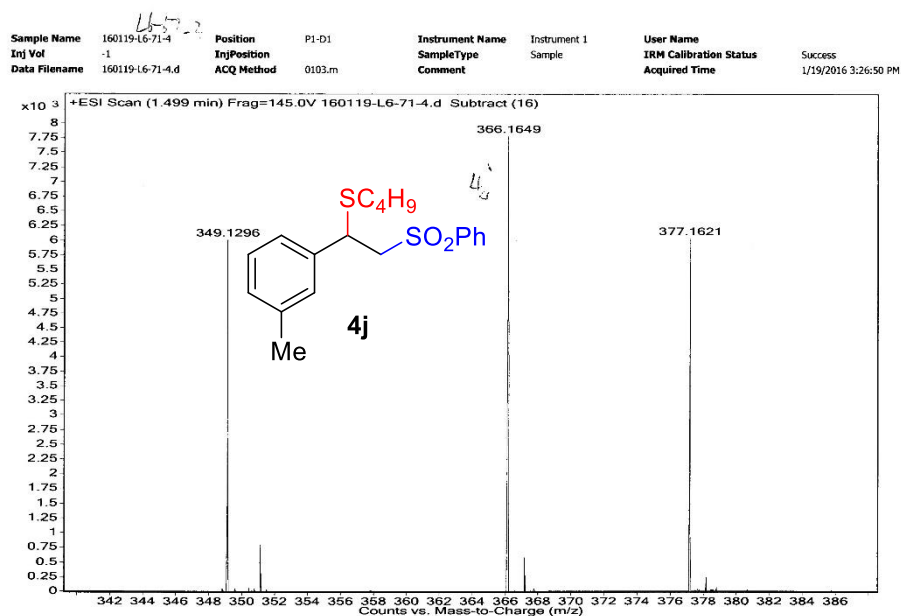
Chemical Formula: C₁₉H₂₄O₂S₂

Exact Mass: 348.1218

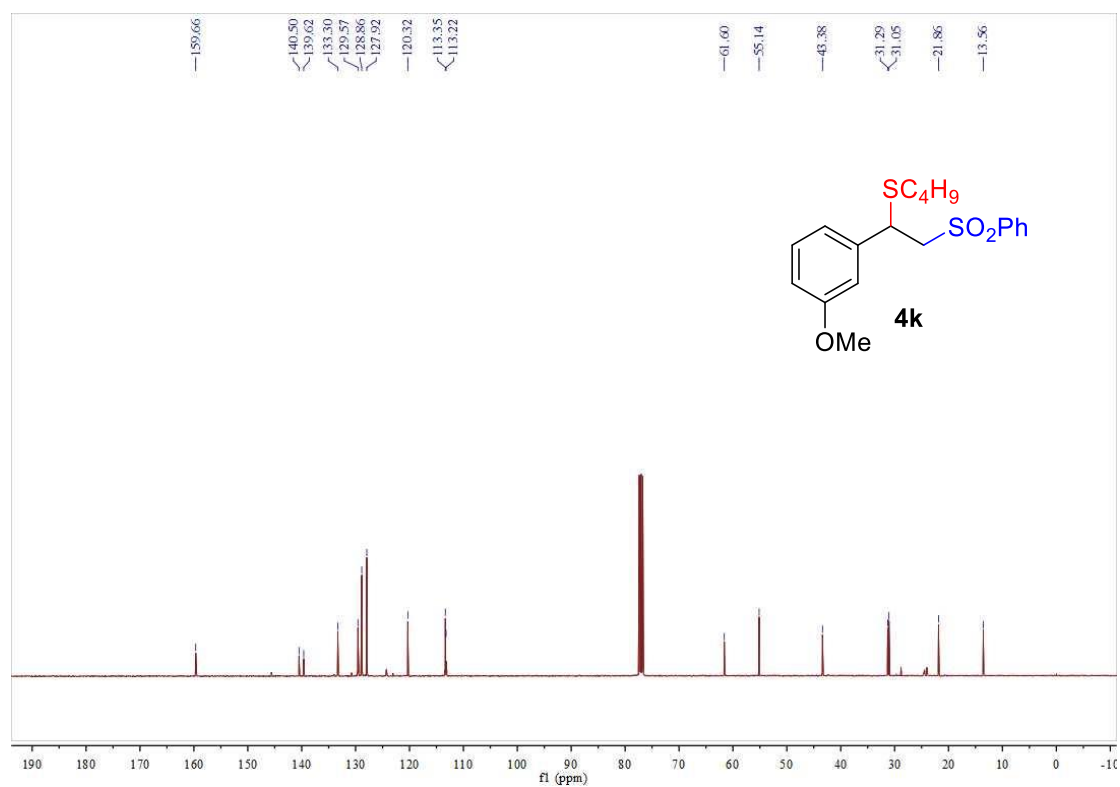
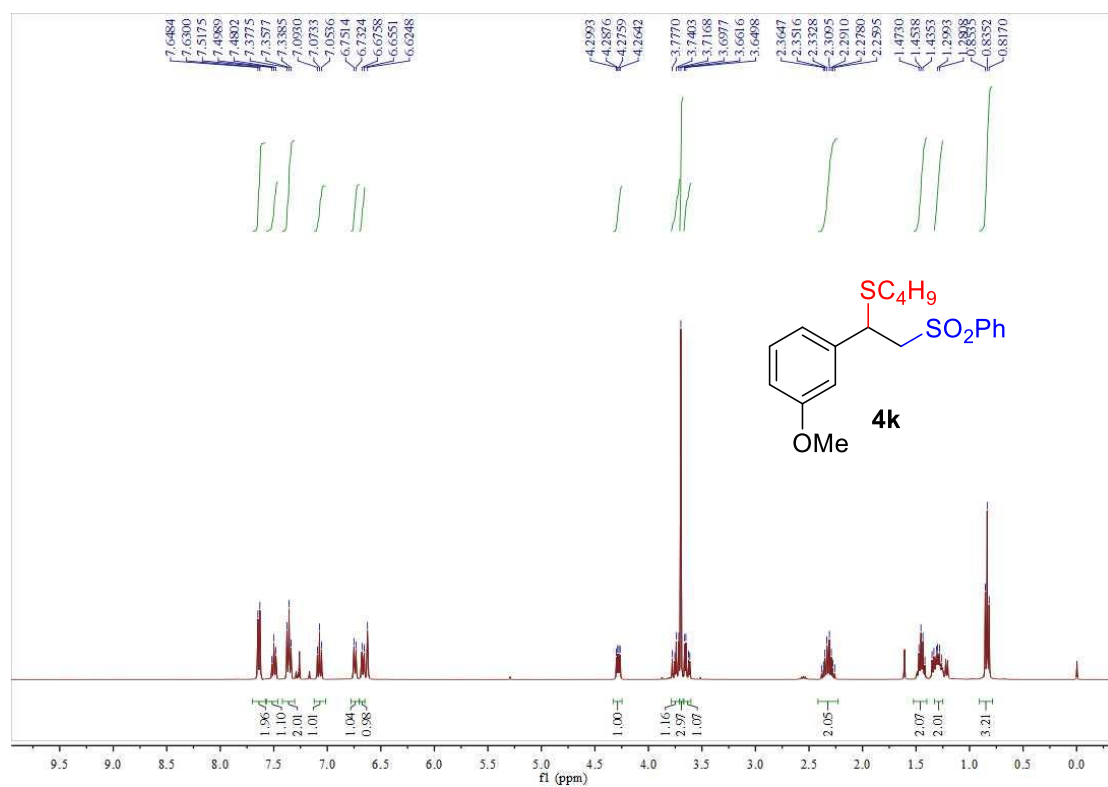
Molecular Weight: 348.5190

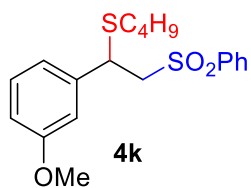
m/z: 348.1218 (100.0%), 349.1251 (20.5%), 350.1176 (9.0%), 350.1285 (2.0%),
351.1209 (1.9%), 349.1212 (1.6%)

Elemental Analysis: C, 65.48; H, 6.94; O, 9.18; S, 18.40



HRMS (ESI, m/z) calcd for C₁₉H₂₄O₂S₂ [M+H]⁺ 349.1290, found 349.1296.





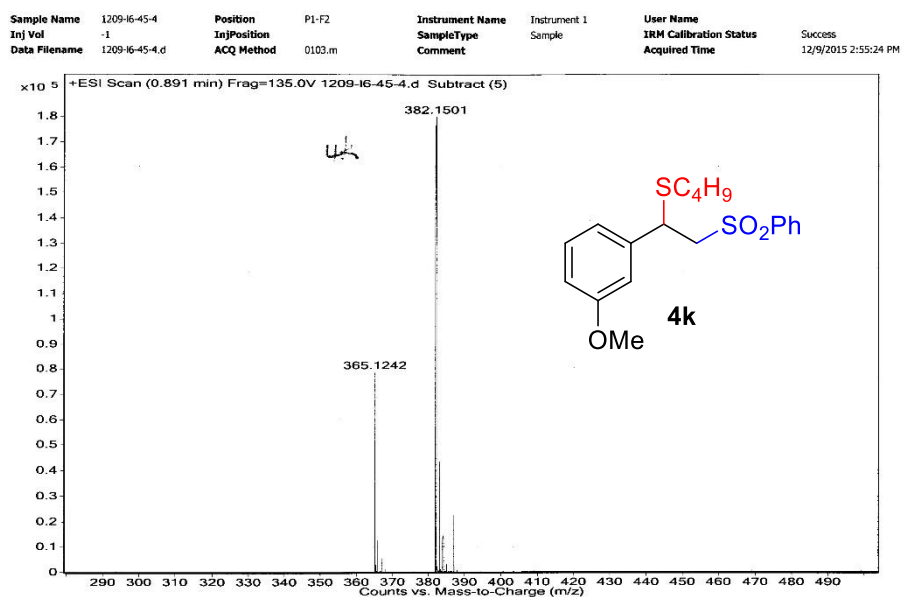
Chemical Formula: C₁₉H₂₄O₃S₂

Exact Mass: 364.1167

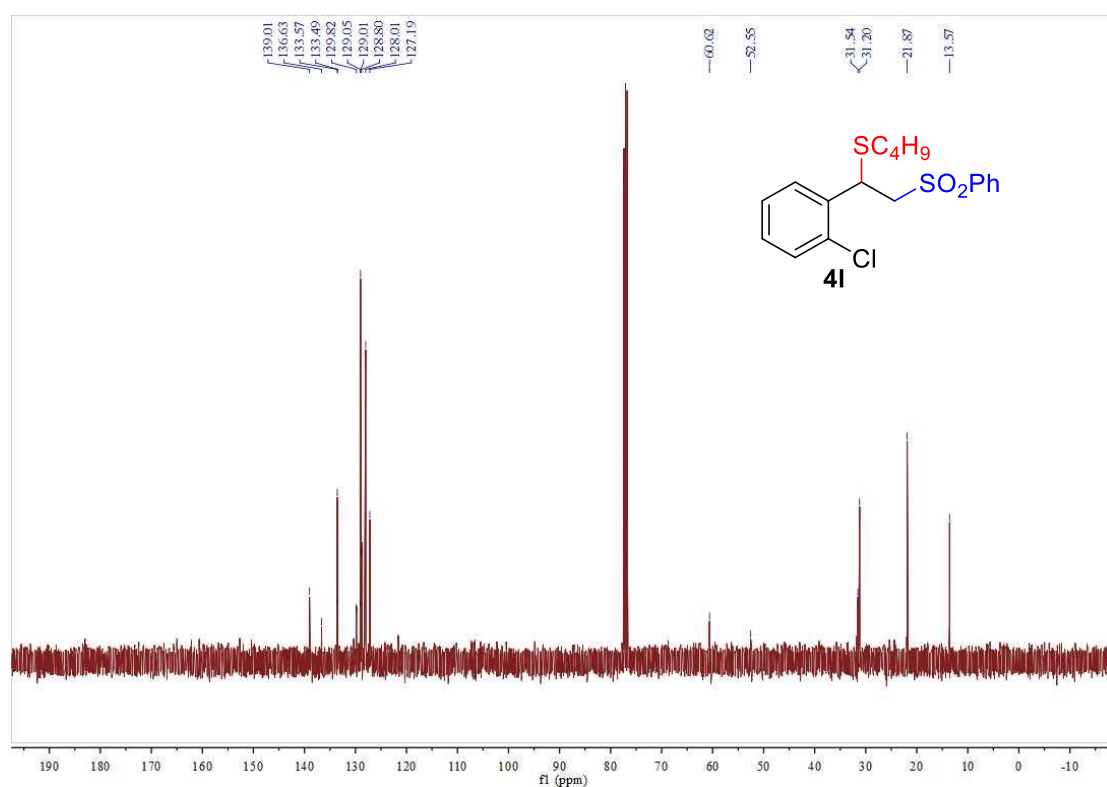
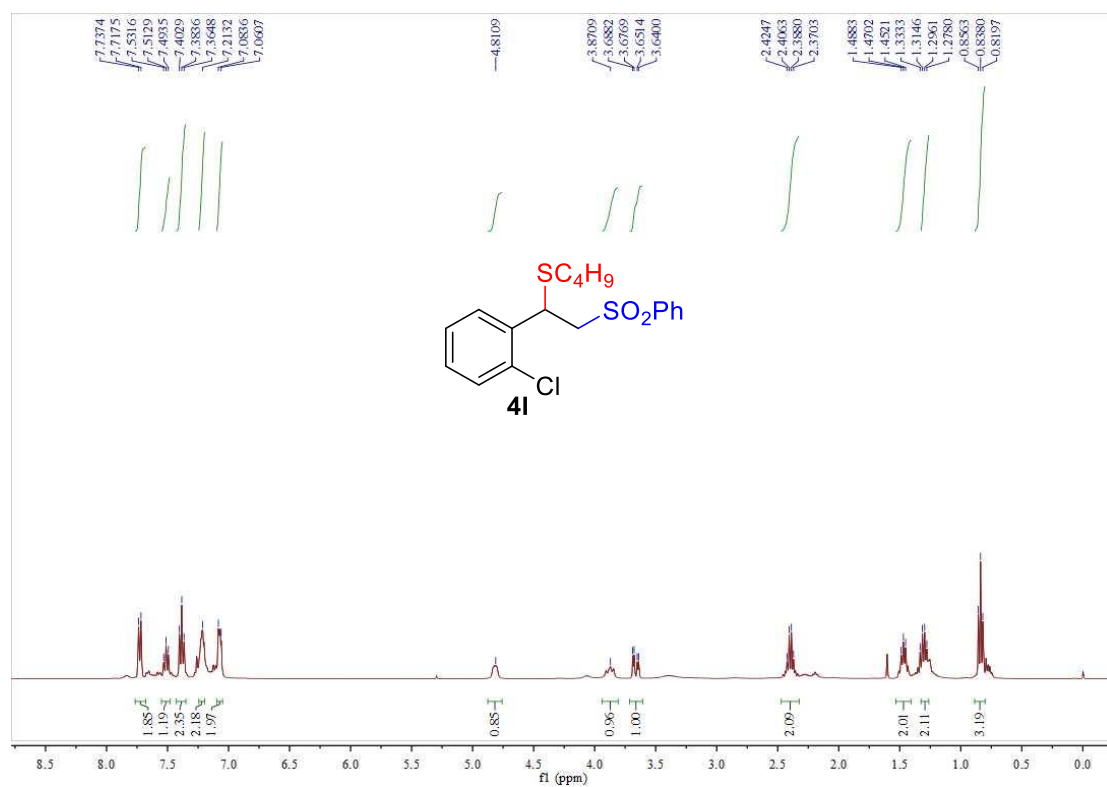
Molecular Weight: 364.5180

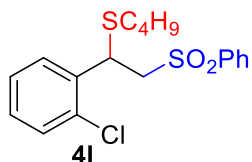
m/z: 364.1167 (100.0%), 365.1200 (20.5%), 366.1125 (9.0%), 366.1234 (2.0%),
367.1158 (1.9%), 365.1161 (1.6%)

Elemental Analysis: C, 62.61; H, 6.64; O, 13.17; S, 17.59



HRMS (ESI, m/z) calcd for C₁₉H₂₄O₃S₂ [M+H]⁺ 365.1240, found 365.1242.





Chemical Formula: $C_{18}H_{21}ClO_2S_2$

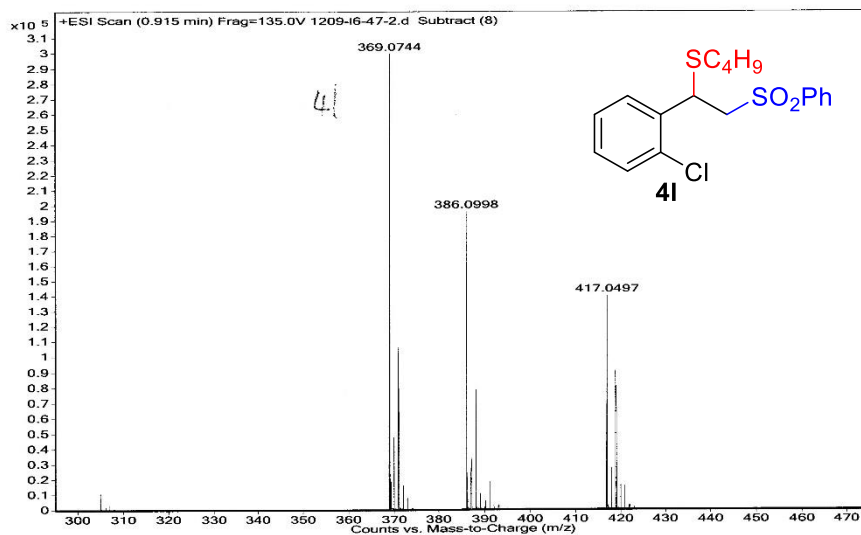
Exact Mass: 368.0671

Molecular Weight: 368.9340

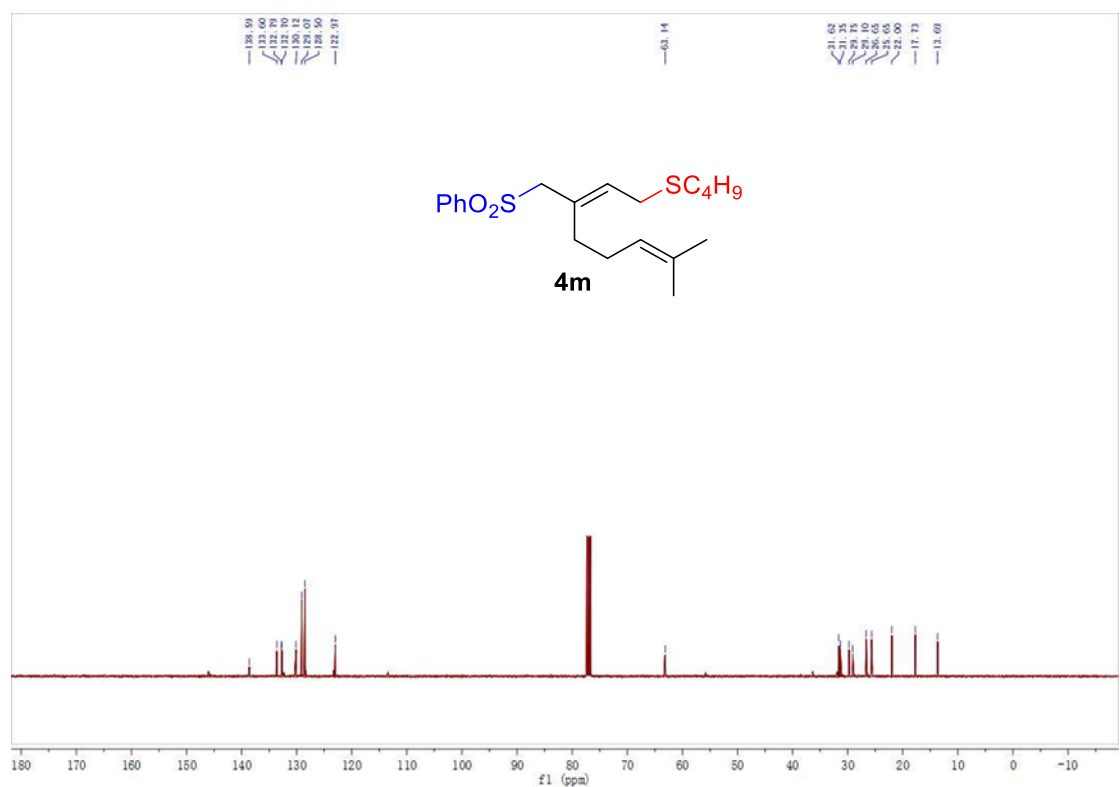
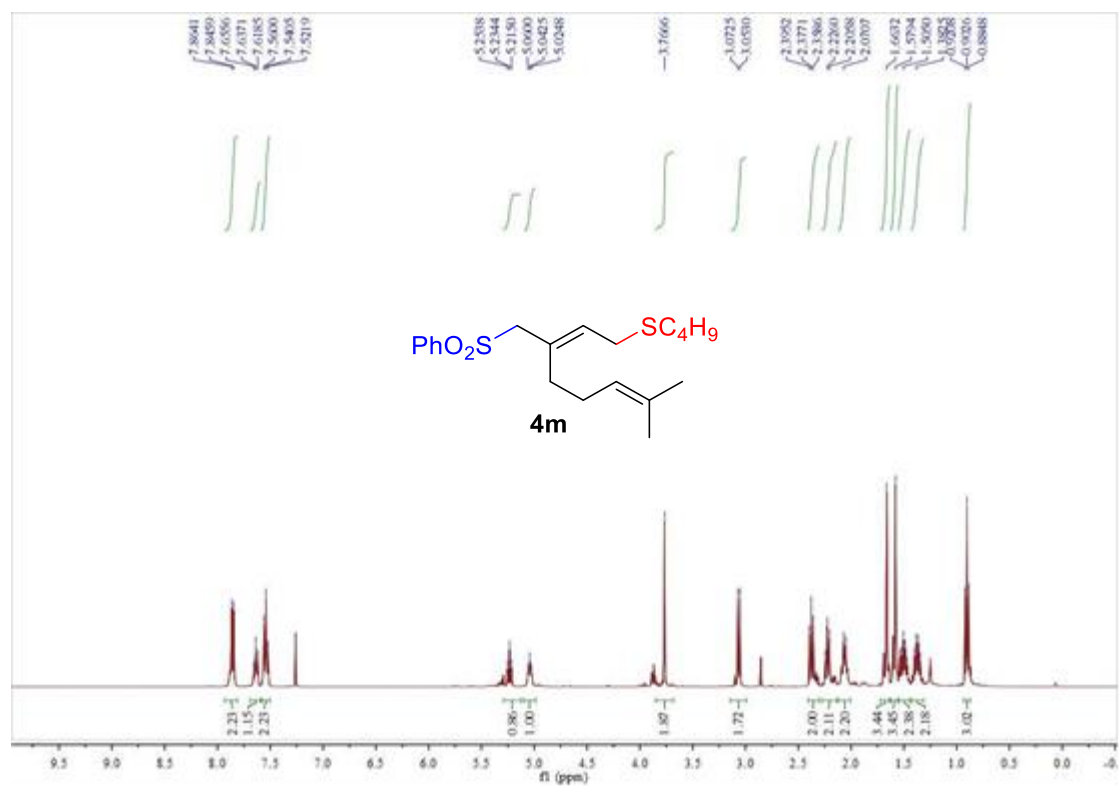
m/z : 368.0671 (100.0%), 370.0642 (32.0%), 369.0705 (19.5%), 370.0629 (9.0%), 371.0676 (6.2%), 372.0600 (2.9%), 370.0739 (1.8%), 371.0663 (1.8%), 369.0665 (1.6%)

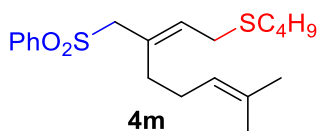
Elemental Analysis: C, 58.60; H, 5.74; Cl, 9.61; O, 8.67; S, 17.38

Sample Name	1209-I6-47-2	Position	P1-B3	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Success
Inj Vol	-1	InjPosition		SampleType	Sample	Acquired Time		12/9/2015 3:01:20 PM
Data Filename	1209-I6-47-2.d	ACQ Method	0103.m	Comment				



HRMS (ESI, m/z) calcd for $C_{18}H_{21}ClO_2S_2$ $[M+H]^+$ 369.0744, found 369.0744.





Chemical Formula: C₂₀H₃₀O₂S₂

Exact Mass: 366.1687

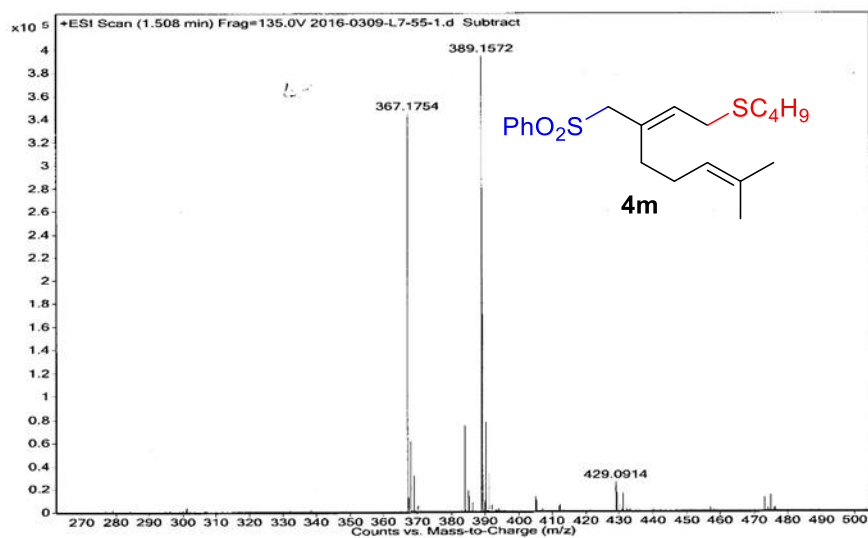
Molecular Weight: 366.5780

m/z: 366.1687 (100.0%), 367.1721 (21.6%), 368.1645 (9.0%),

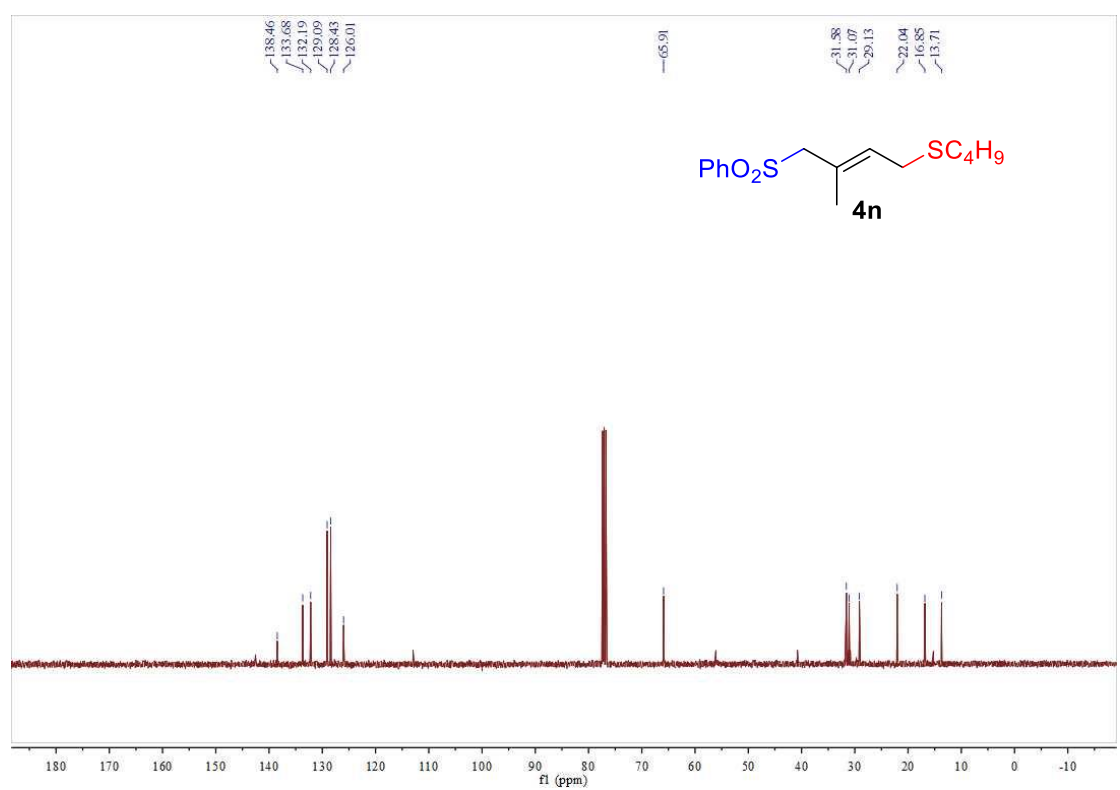
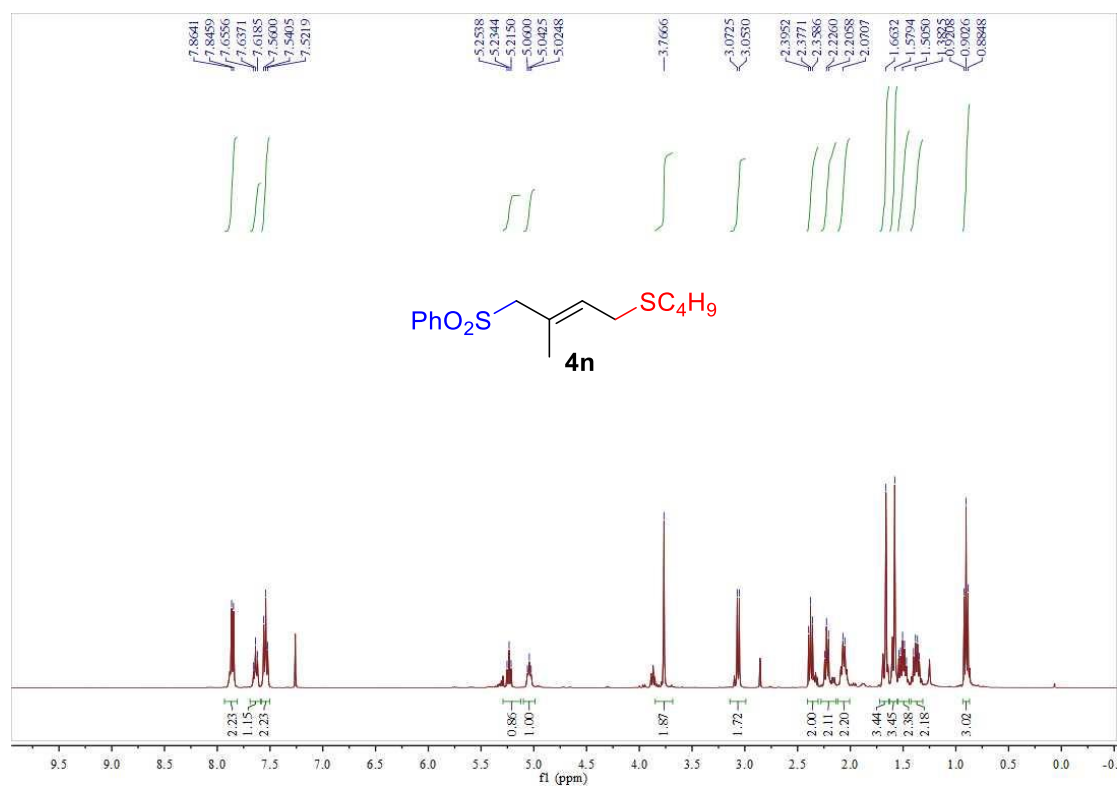
368.1754 (2.2%), 369.1679 (2.0%), 367.1681 (1.6%)

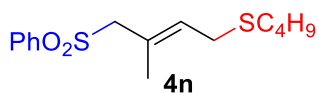
Elemental Analysis: C, 65.53; H, 8.25; O, 8.73; S, 17.49

Sample Name	2016-0309-L7-55-1	Position	P1-B9	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	2016-0309-L7-55-1.d	ACQ Method	0103.m	Comment		Acquired Time	3/6/2016 2:58:27 PM



HRMS (ESI, m/z) calcd for C₂₀H₃₀O₂S₂ [M+H]⁺ 367.1760, found 367.1754.





Chemical Formula: C₁₅H₂₂O₂S₂

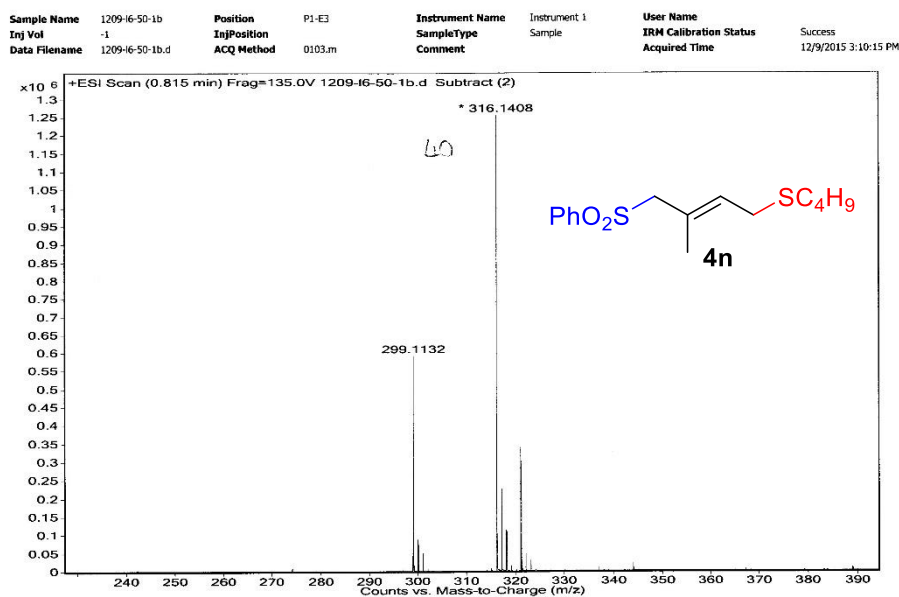
Exact Mass: 298.1061

Molecular Weight: 298.4590

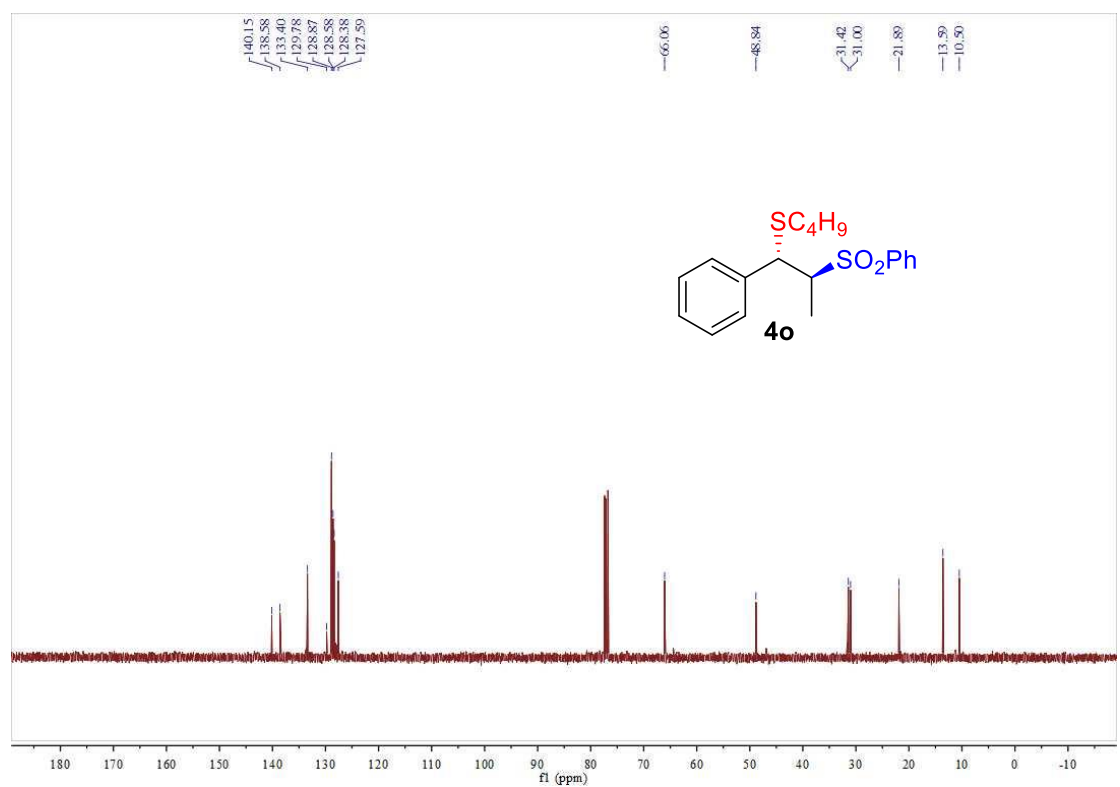
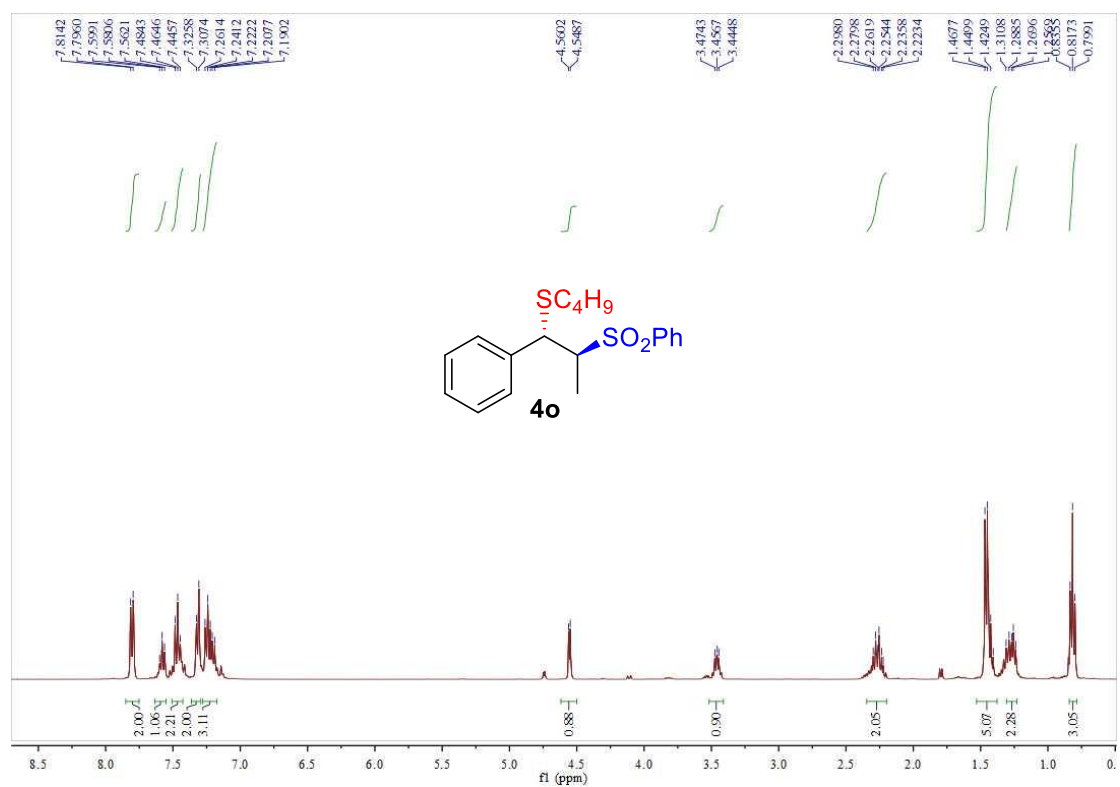
m/z: 298.1061 (100.0%), 299.1095 (16.2%), 300.1019 (9.0%),

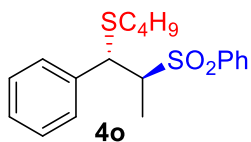
299.1055 (1.6%), 300.1128 (1.2%)

Elemental Analysis: C, 60.37; H, 7.43; O, 10.72; S, 21.48



HRMS (ESI, m/z) calcd for C₁₅H₂₂O₂S₂ [M+H]⁺ 299.1134, found 299.1132.





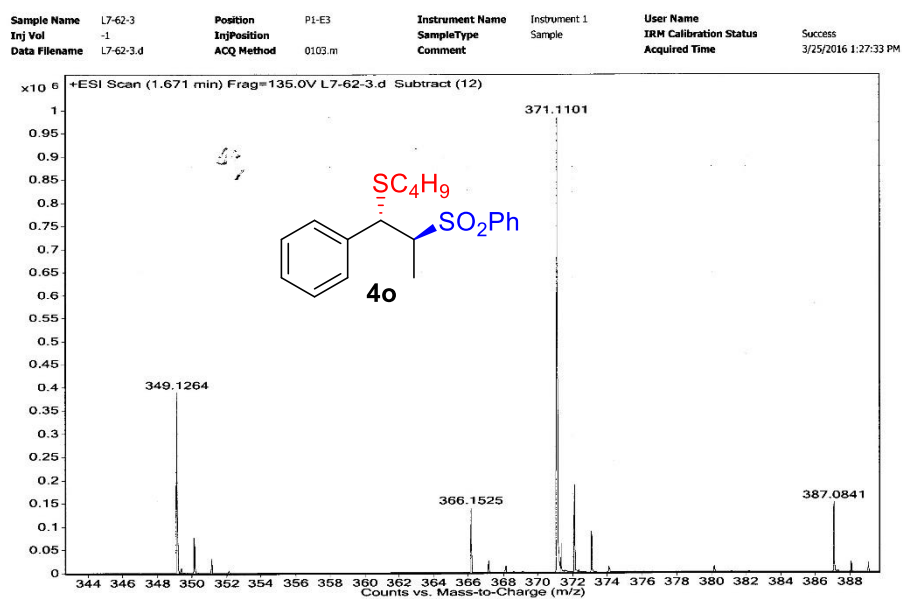
Chemical Formula: C₁₉H₂₄O₂S₂

Exact Mass: 348.1218

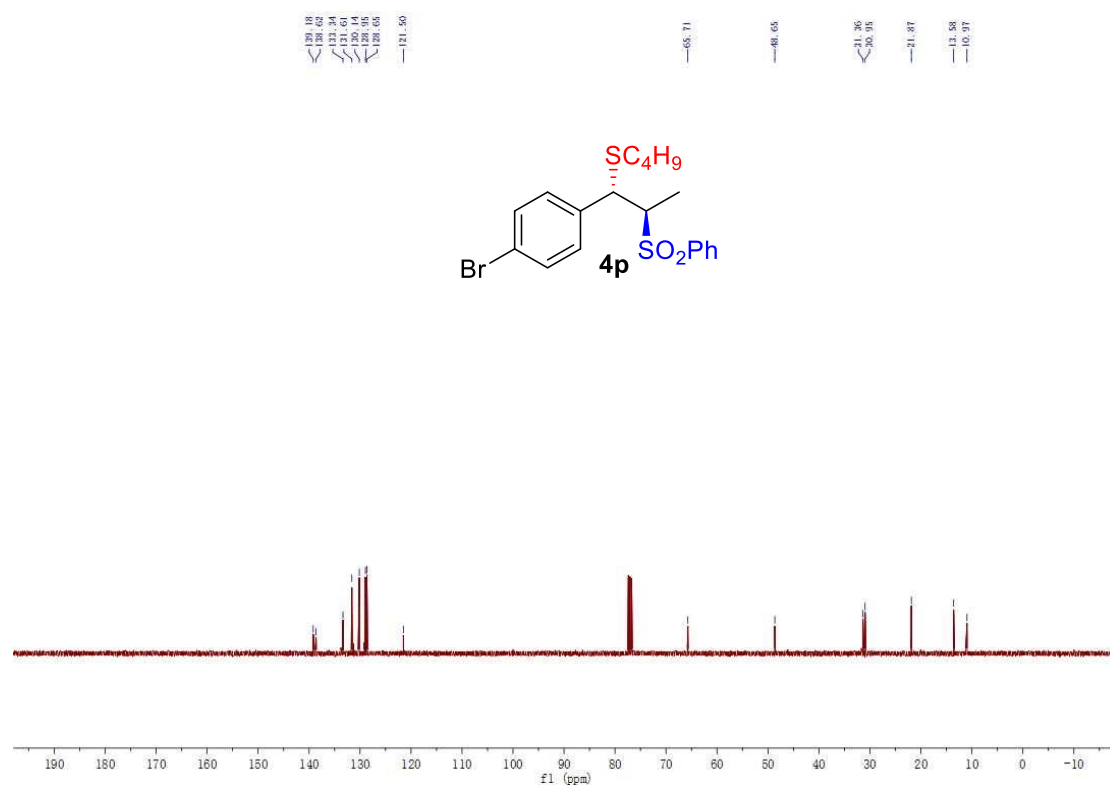
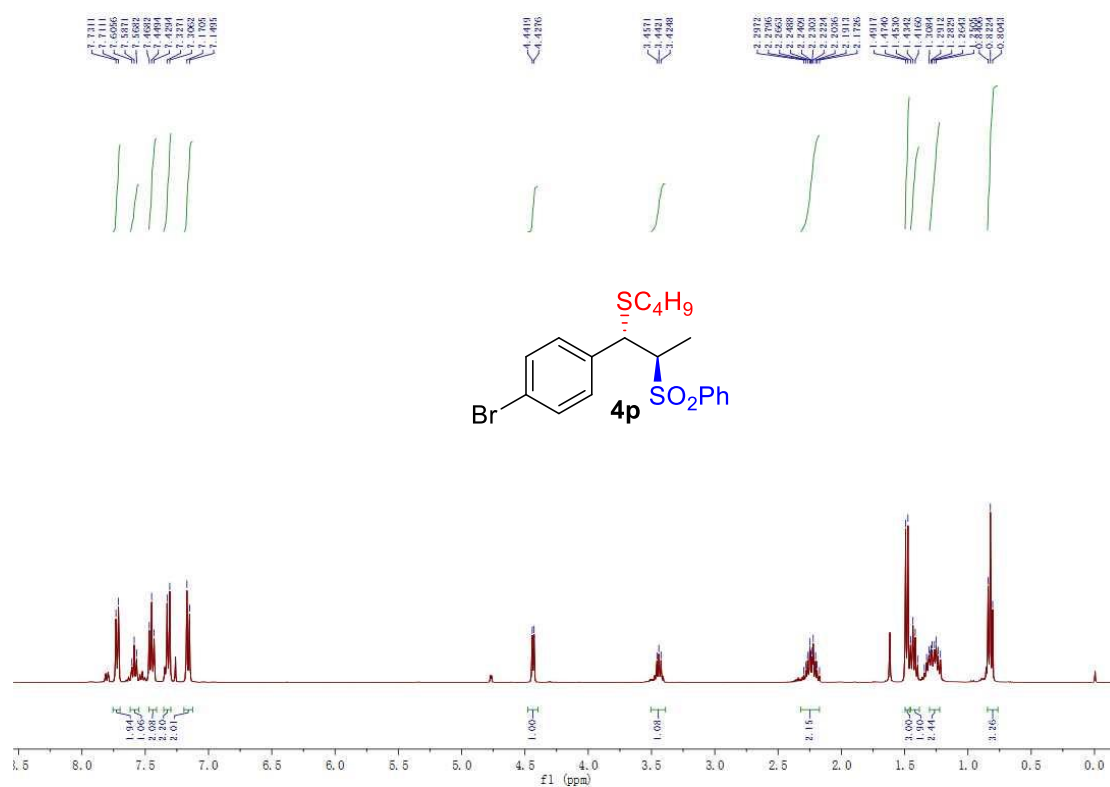
Molecular Weight: 348.5190

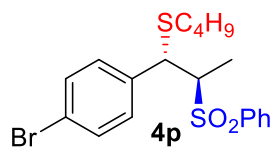
m/z: 348.1218 (100.0%), 349.1251 (20.5%), 350.1176 (9.0%), 350.1285 (2.0%),
351.1209 (1.9%), 349.1212 (1.6%)

Elemental Analysis: C, 65.48; H, 6.94; O, 9.18; S, 18.40



HRMS (ESI, m/z) calcd for C₁₉H₂₄O₂S₂ [M+Na]⁺ 371.1110, found 371.1110.





Chemical Formula: $C_{19}H_{23}BrO_2S_2$

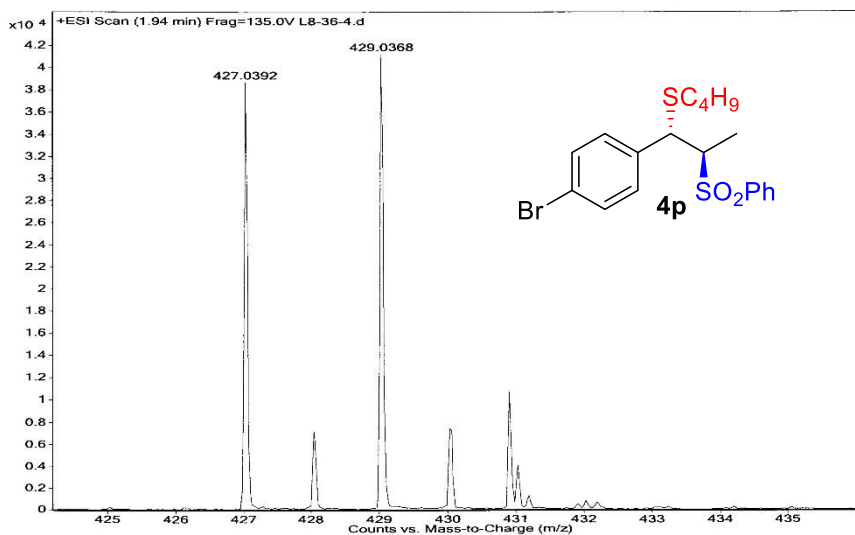
Exact Mass: 426.0323

Molecular Weight: 427.4150

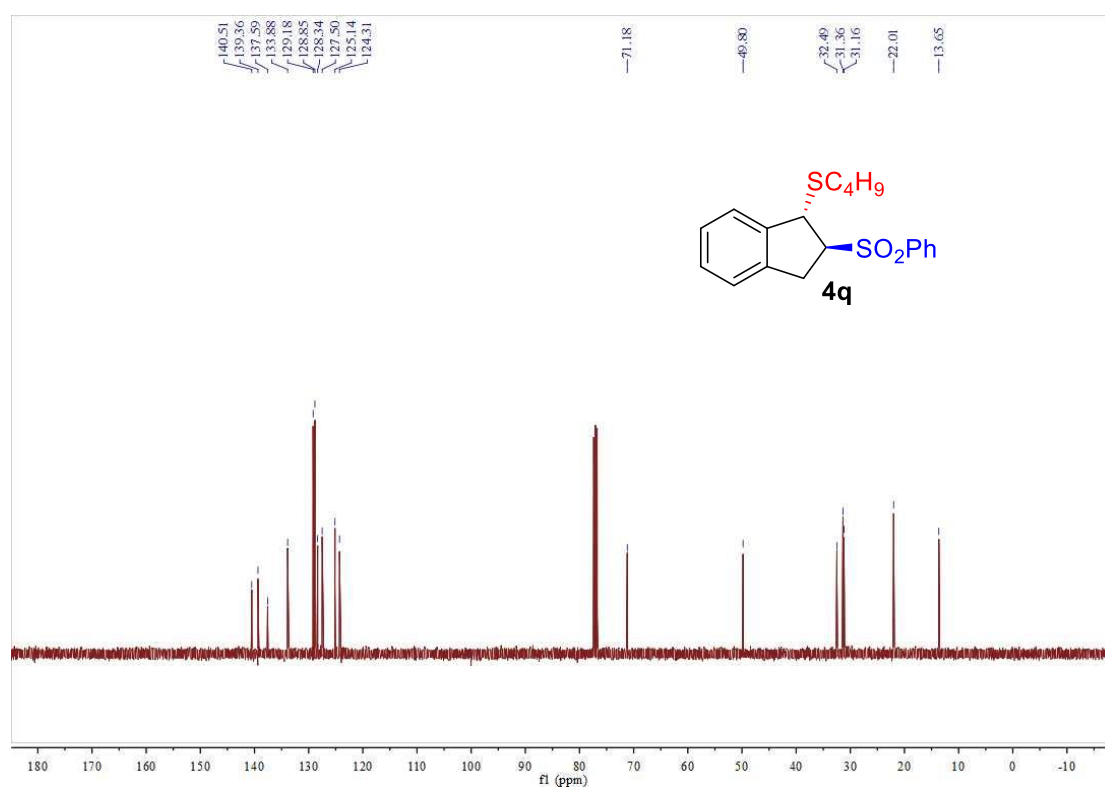
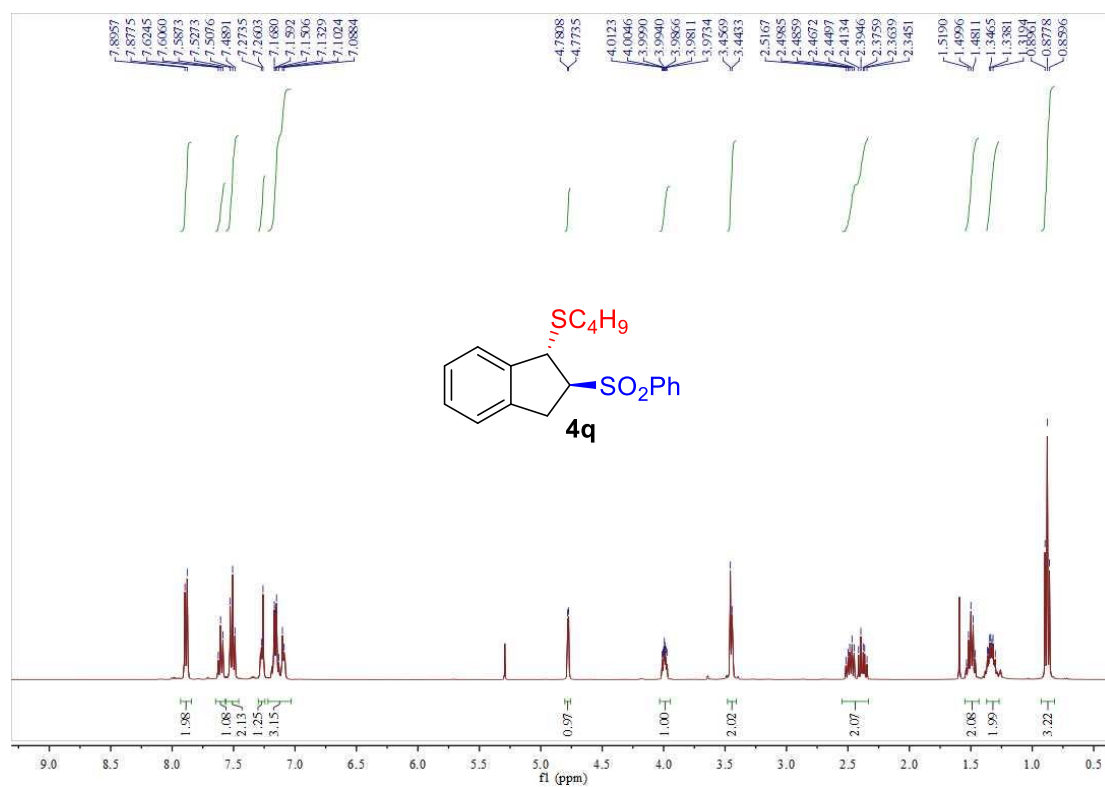
m/z: 426.0323 (100.0%), 428.0302 (97.3%), 429.0336 (20.0%), 427.0356 (16.2%),
428.0281 (9.0%), 430.0260 (8.8%), 427.0356 (4.3%), 431.0294 (1.8%),
427.0317 (1.6%), 429.0296 (1.6%), 429.0314 (1.5%), 430.0369 (1.2%),
428.0390 (1.1%)

Elemental Analysis: C, 53.39; H, 5.42; Br, 18.69; O, 7.49; S, 15.00

Sample Name	Position	Instrument Name	User Name
Unavailable	Unavailable	Unavailable	Unavailable
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Unavailable	Unavailable	Unavailable	Success
Data Filename	ACQ Method	Comment	Acquired Time
L8-36-4.d		Sample information is unavailable	Unavailable



HRMS (ESI, m/z) calcd for $C_{19}H_{23}BrO_2S_2$ $[M+H]^+$ 427.0396, found 427.0392.



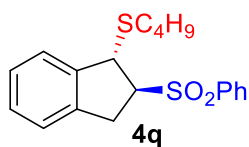
Chemical Formula: C₁₉H₂₂O₂S₂

Exact Mass: 346.1061

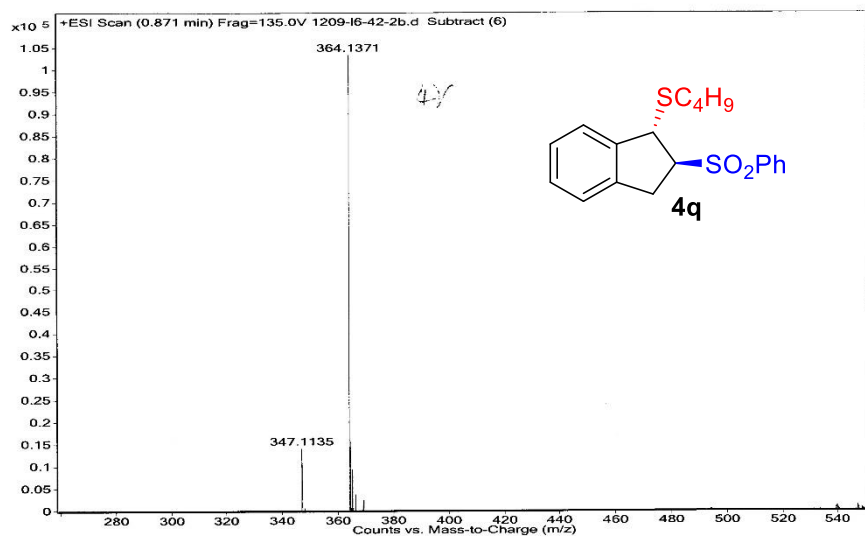
Molecular Weight: 346.5030

m/z: 346.1061 (100.0%), 347.1095 (20.5%), 348.1019 (9.0%), 348.1128 (2.0%), 349.1053 (1.9%), 347.1055 (1.6%)

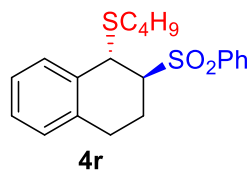
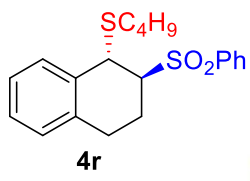
Elemental Analysis: C, 65.86; H, 6.40; O, 9.23; S, 18.50

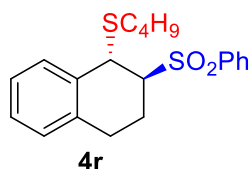


Sample Name	1209-I6-42-2b	Position	P1-C2	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	1209-I6-42-2b.d	ACQ Method	0103.m	Comment		Acquired Time



HRMS (ESI, m/z) calcd for C₁₉H₂₂O₂S₂ [M+H]⁺ 347.1134, found 347.1135.





Chemical Formula: C₂₀H₂₄O₂S₂

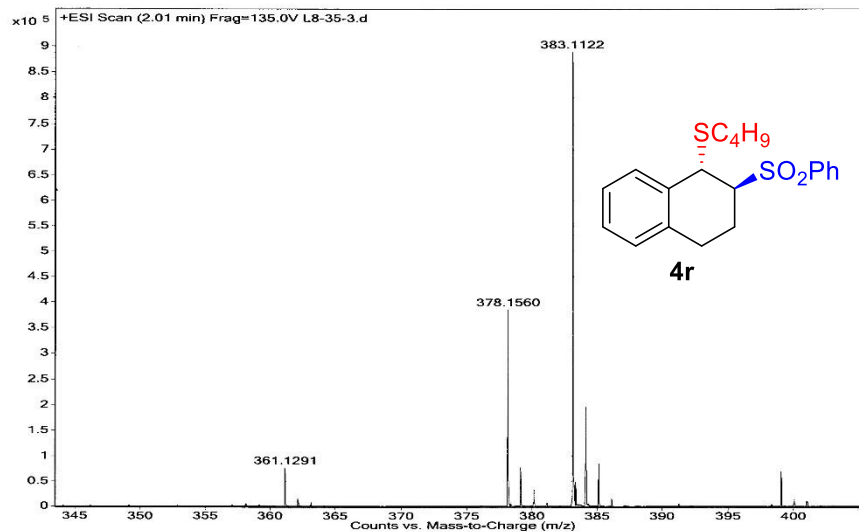
Exact Mass: 360.1218

Molecular Weight: 360.5300

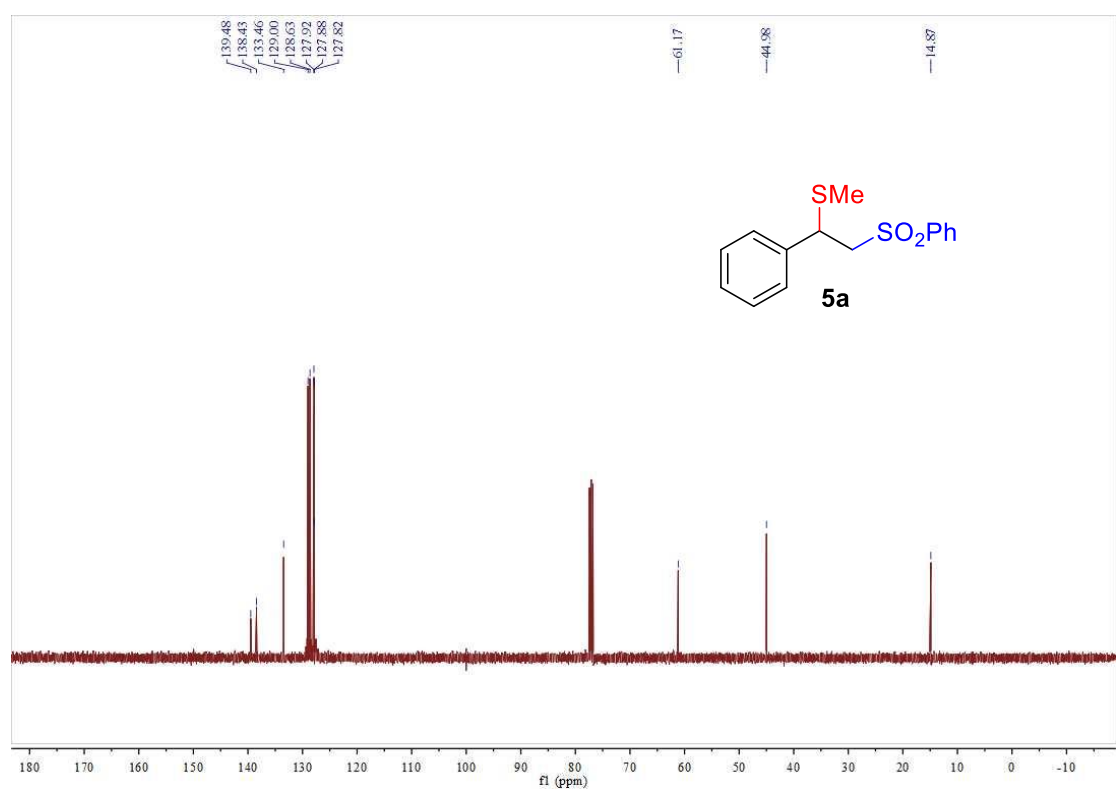
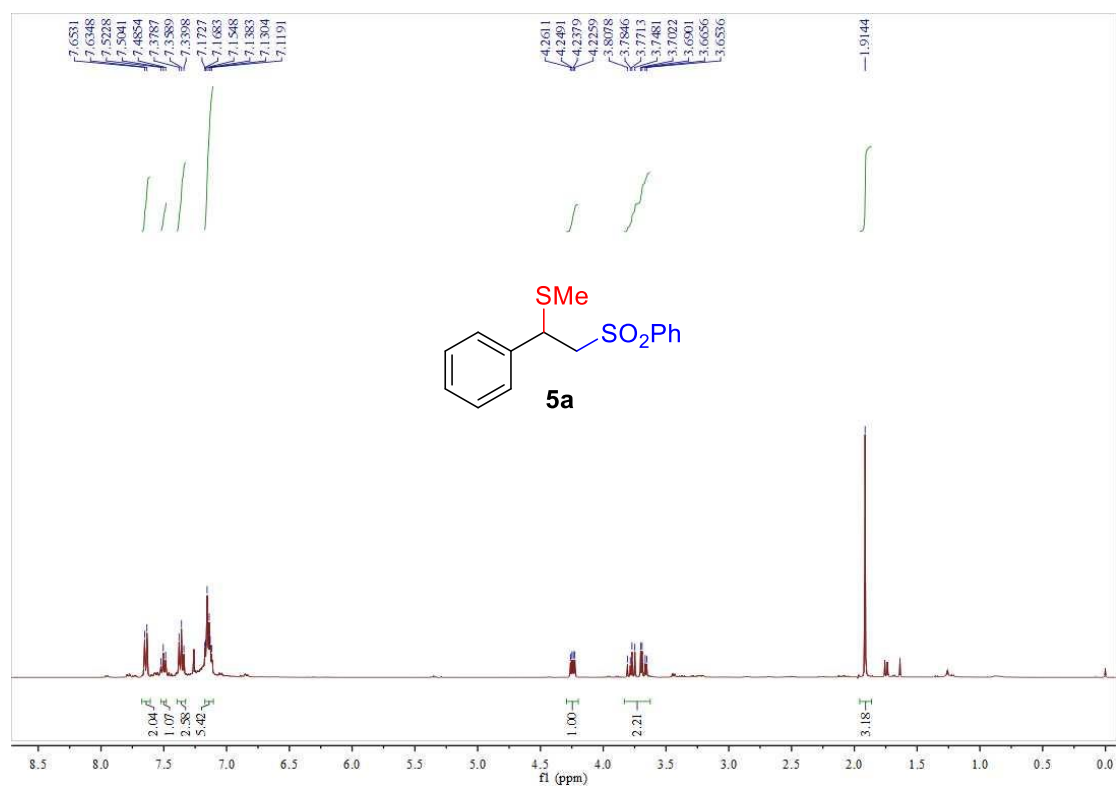
m/z: 360.1218 (100.0%), 361.1251 (21.6%), 362.1176 (9.0%), 362.1285 (2.2%),
363.1209 (2.0%), 361.1212 (1.6%)

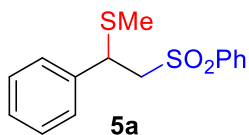
Elemental Analysis: C, 66.63; H, 6.71; O, 8.88; S, 17.78

Sample Name	Injection Volume	Position	Injection Position	Instrument Name	Sample Type	User Name	IRMS Calibration Status
Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Success
Data Filename	L8-35-3.d	ACQ Method	ACQ Method	Comment	Sample information is unavailable	Acquired Time	Unavailable



HRMS (ESI, m/z) calcd for C₂₀H₂₄O₂S₂ [M+Na]⁺ 383.1110, found 383.1122.





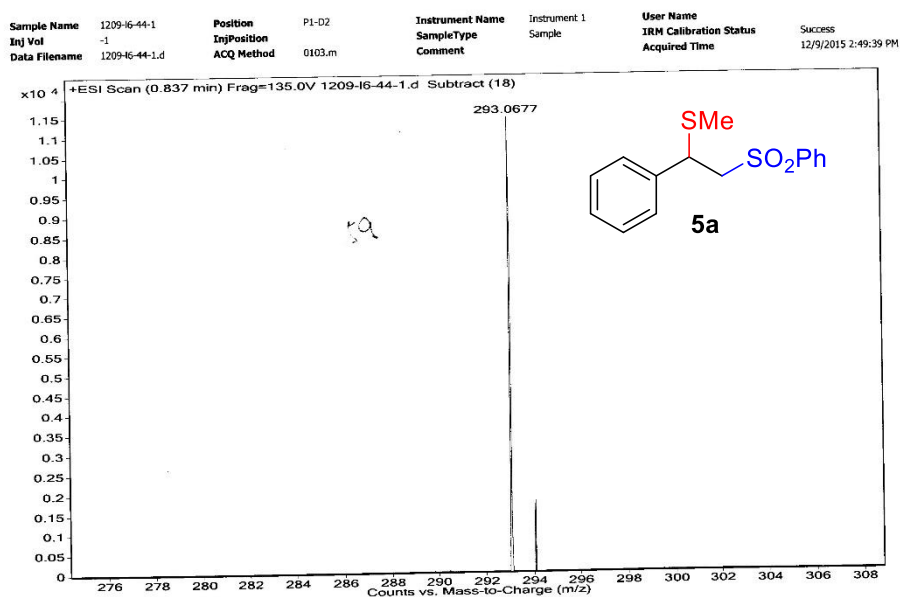
Chemical Formula: C₁₅H₁₆O₂S₂

Exact Mass: 292.0592

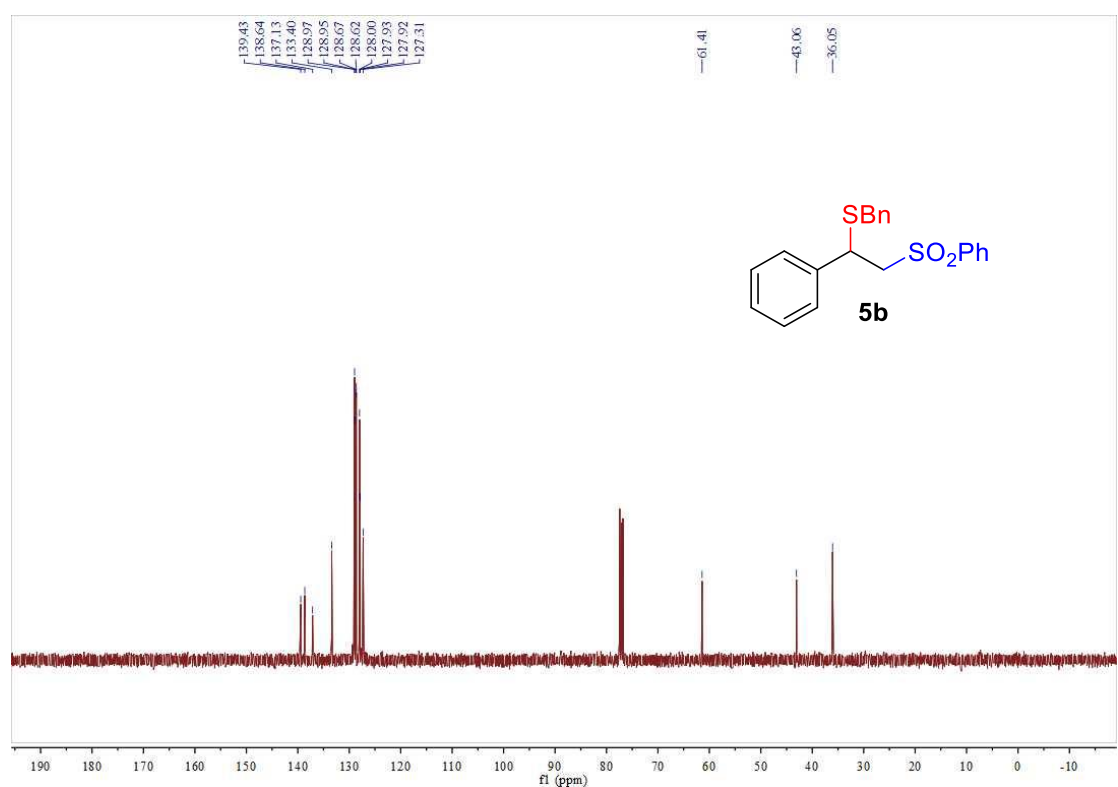
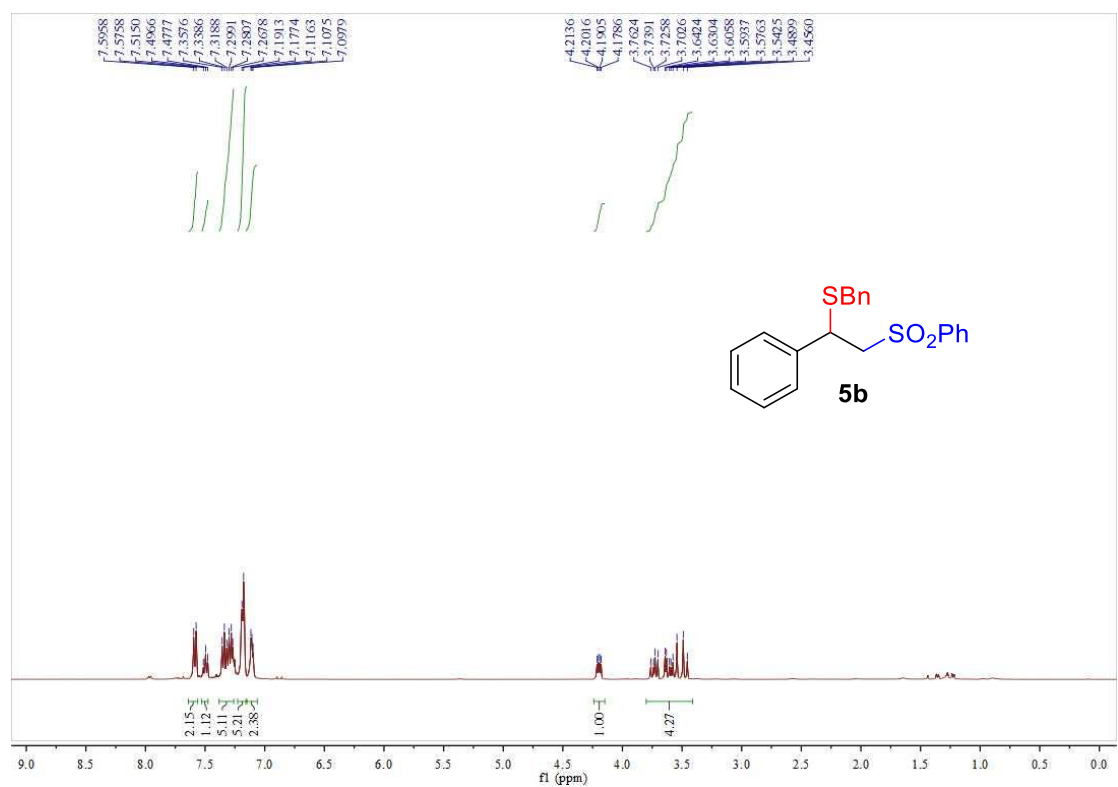
Molecular Weight: 292.4110

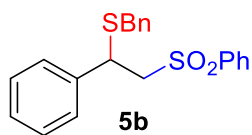
m/z: 292.0592 (100.0%), 293.0625 (16.2%), 294.0550 (9.0%), 293.0586 (1.6%),
294.0659 (1.2%)

Elemental Analysis: C, 61.61; H, 5.52; O, 10.94; S, 21.93



HRMS (ESI, m/z) calcd for C₁₅H₁₆O₂S₂ [M+H]⁺ 293.0664, found 293.0677.





Chemical Formula: $C_{21}H_{20}O_2S_2$

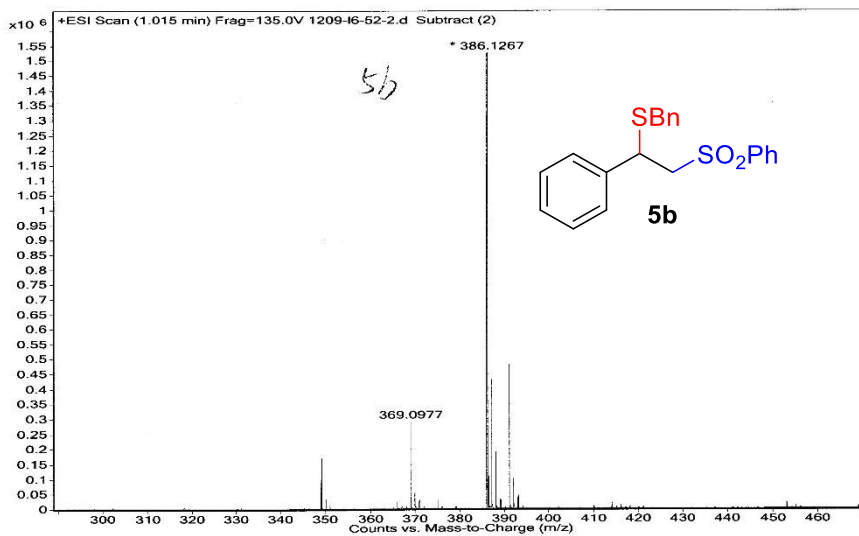
Exact Mass: 368.0905

Molecular Weight: 368.5090

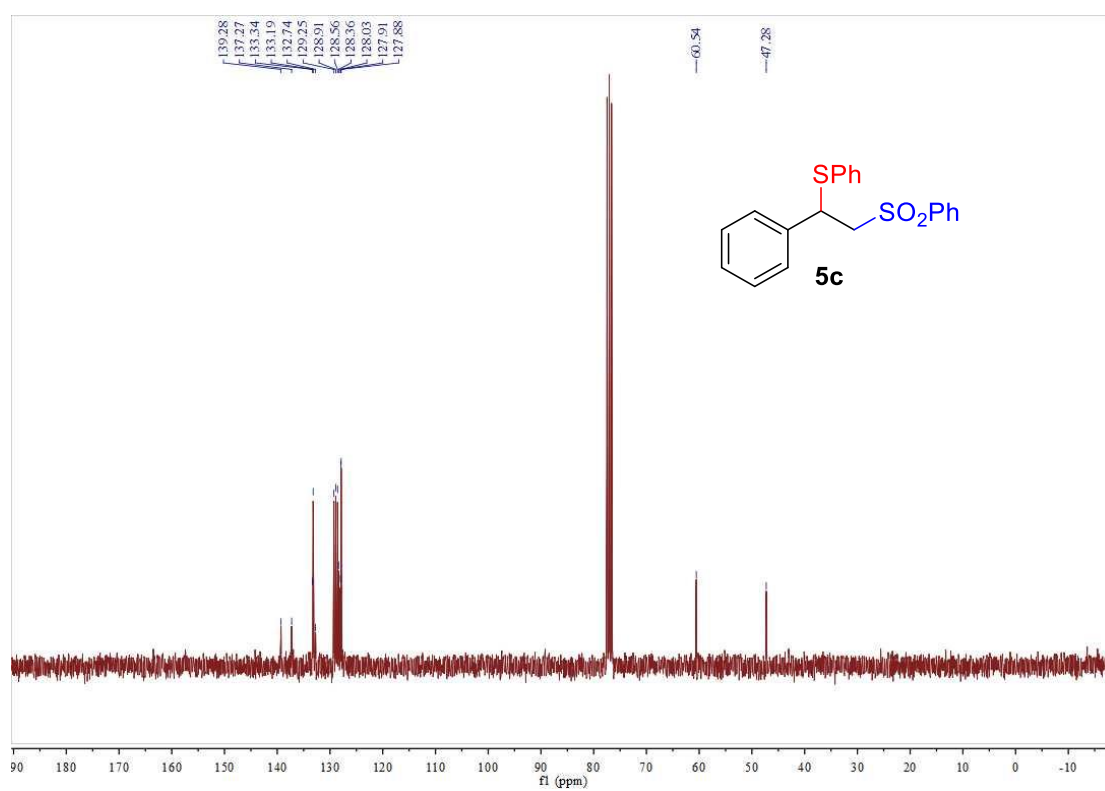
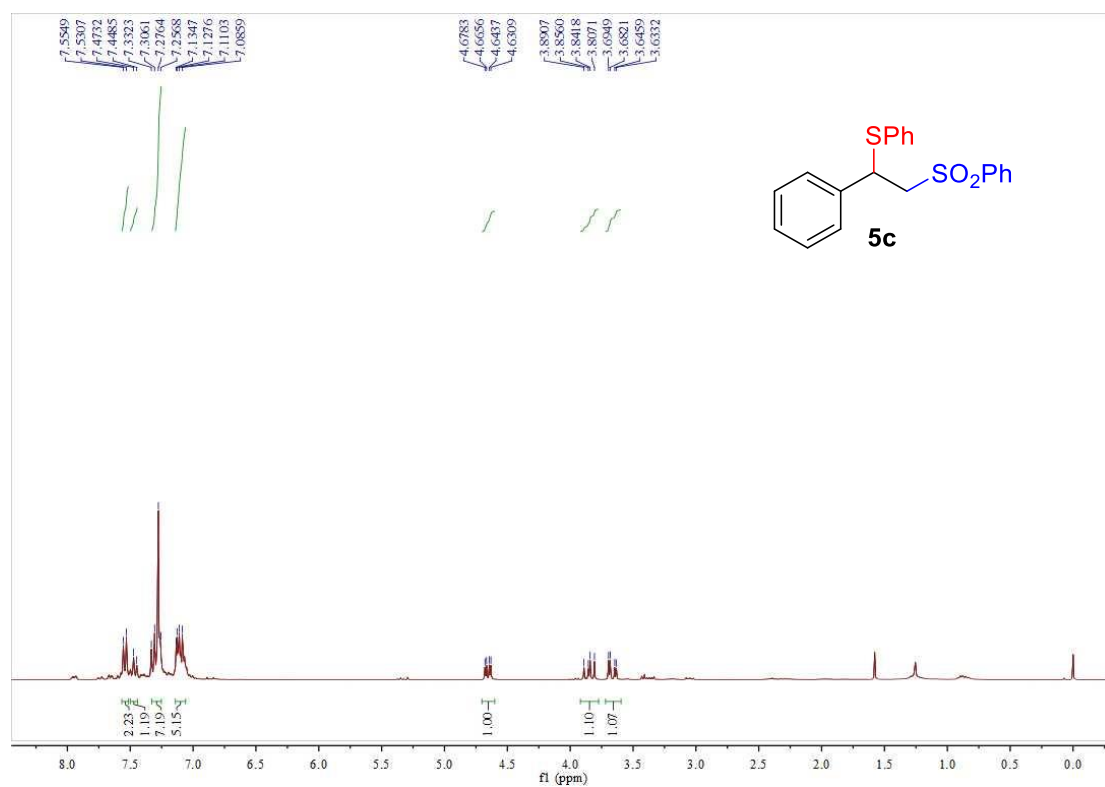
m/z: 368.0905 (100.0%), 369.0938 (22.7%), 370.0863 (9.0%), 370.0972 (2.5%),
371.0896 (2.1%), 369.0899 (1.6%)

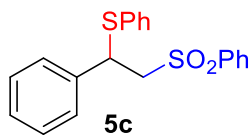
Elemental Analysis: C, 68.45; H, 5.47; O, 8.68; S, 17.40

Sample Name	1209-16-52-2	Position	P1-F3	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	1209-16-52-2.d	ACQ Method	0103.m	Comment		Acquired Time	12/8/2015 3:13:09 PM



HRMS (ESI, m/z) calcd for $C_{21}H_{20}O_2S_2$ $[M+H]^+$ 369.0977, found 369.0977.





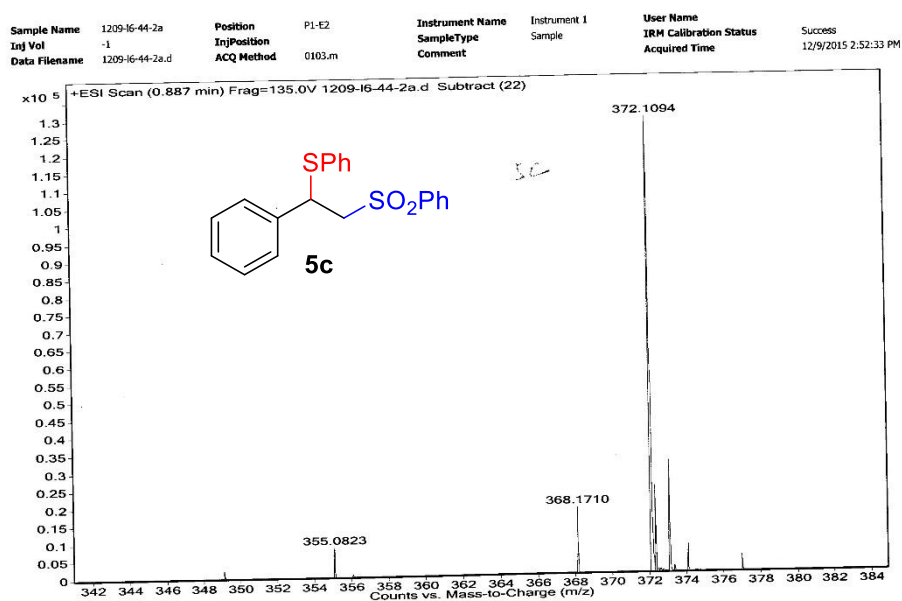
Chemical Formula: C₂₀H₁₈O₂S₂

Exact Mass: 354.0748

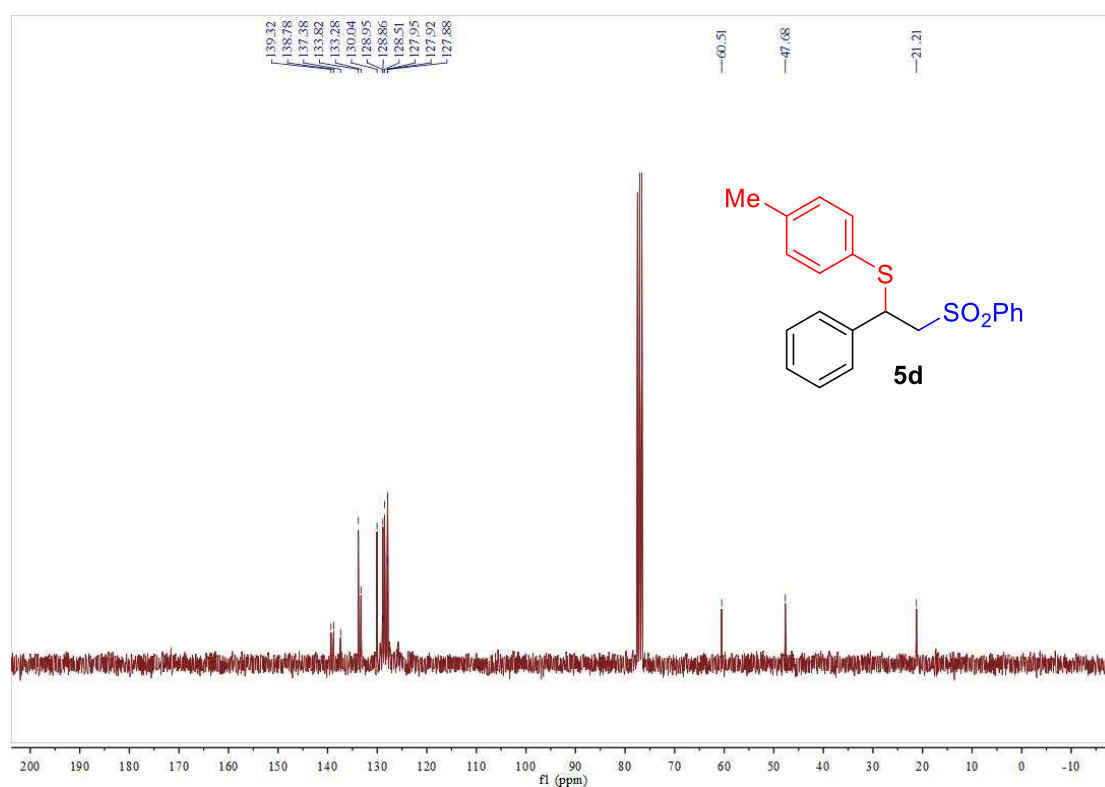
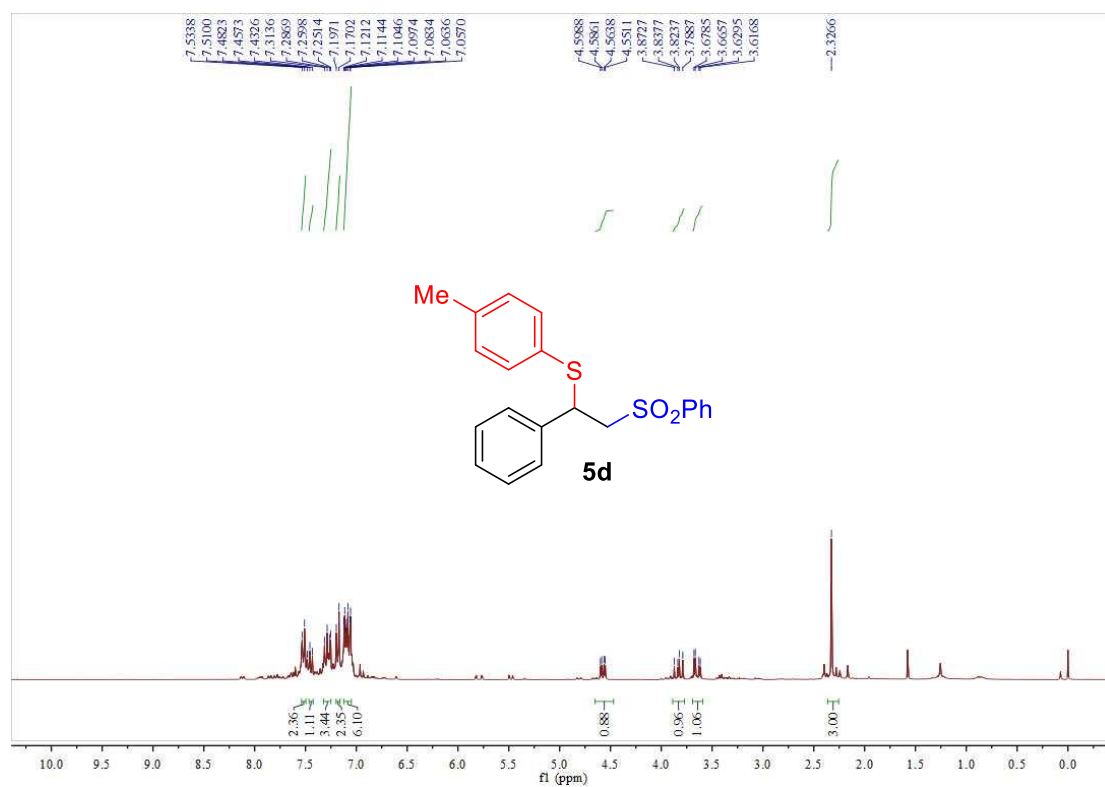
Molecular Weight: 354.4820

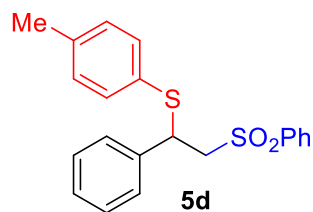
m/z: 354.0748 (100.0%), 355.0782 (21.6%), 356.0706 (9.0%), 356.0815 (2.2%),
357.0740 (2.0%), 355.0742 (1.6%)

Elemental Analysis: C, 67.77; H, 5.12; O, 9.03; S, 18.09



HRMS (ESI, m/z) calcd for C₂₀H₁₈O₂S₂ [M+H]⁺ 355.0821, found 355.0823.





Chemical Formula: $C_{21}H_{20}O_2S_2$

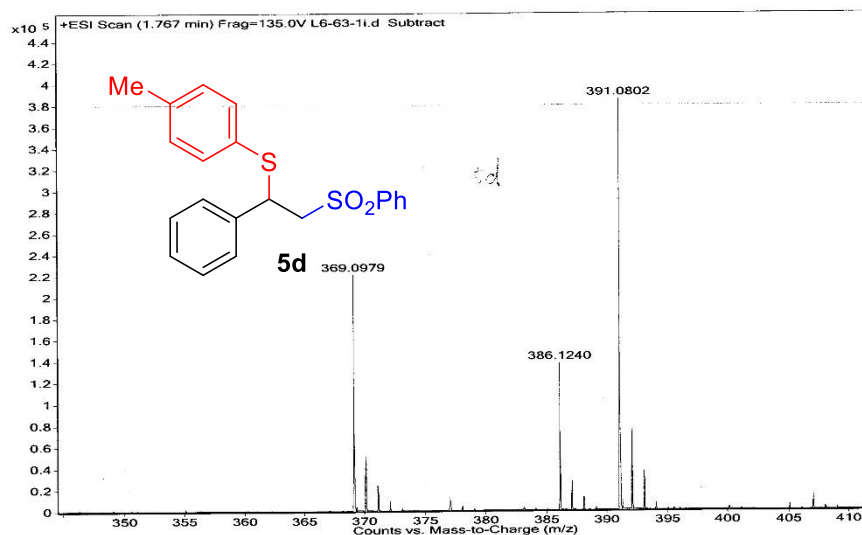
Exact Mass: 368.0905

Molecular Weight: 368.5090

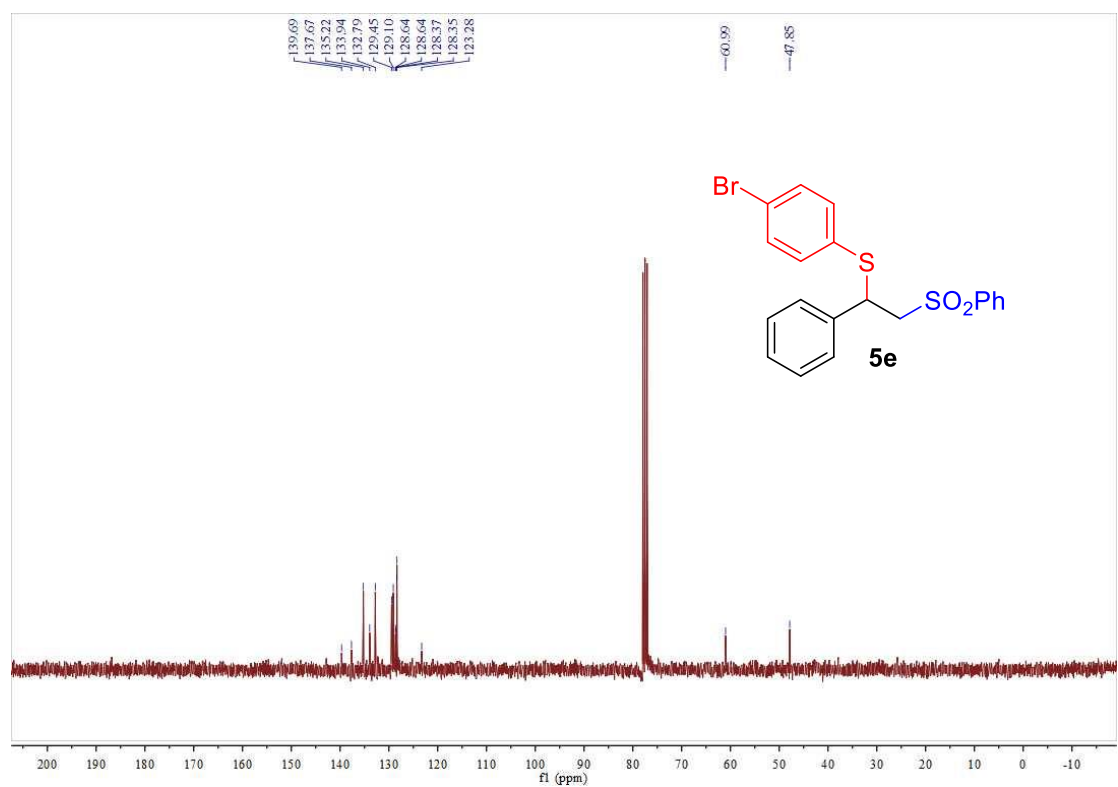
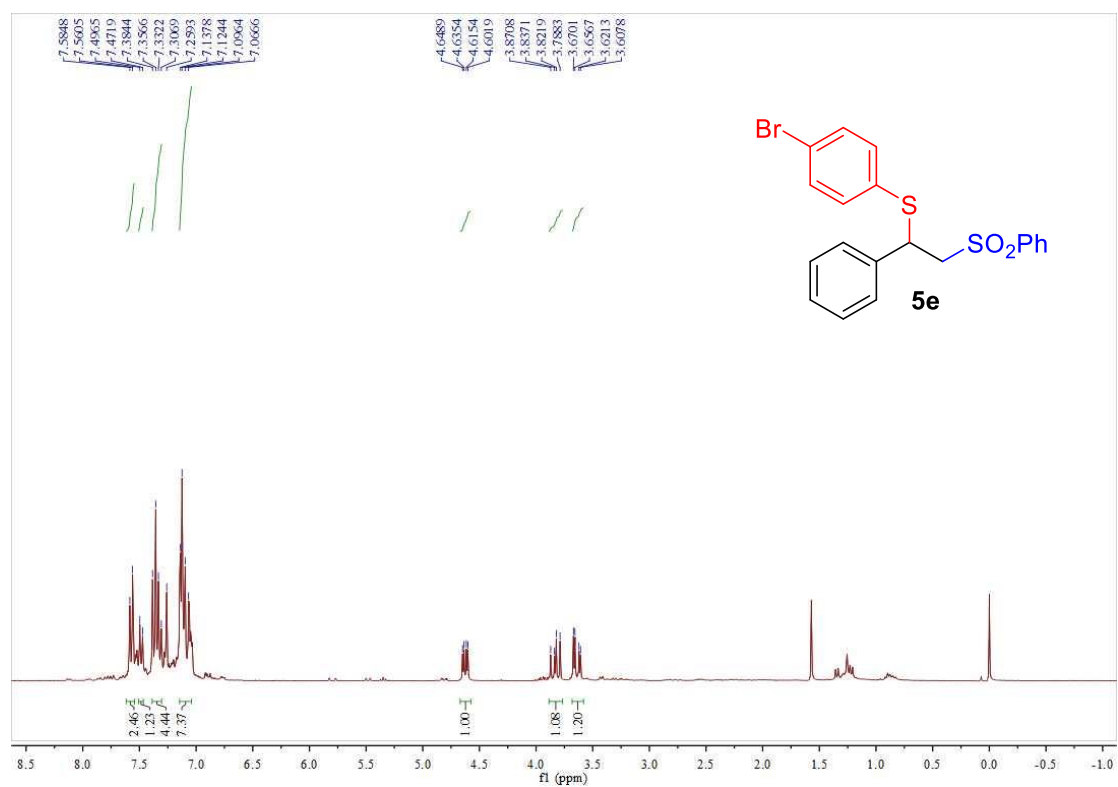
m/z: 368.0905 (100.0%), 369.0938 (22.7%), 370.0863 (9.0%), 370.0972 (2.5%),
371.0896 (2.1%), 369.0899 (1.6%)

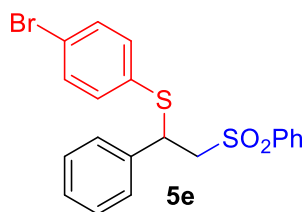
Elemental Analysis: C, 68.45; H, 5.47; O, 8.68; S, 17.40

Sample Name	Position	P1:47	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Success
L6-63-11	-1		SampleType	Sample			
Data Filename	L6-63-11.d	ACQ Method	0103.m	Comment		Acquired Time	3/8/2016 7:19:29 AM



HRMS (ESI, m/z) calcd for $C_{21}H_{20}O_2S_2$ $[M+H]^+$ 369.0977, found 369.0979.





Chemical Formula: $C_{20}H_{17}BrO_2S_2$

Exact Mass: 431.9853

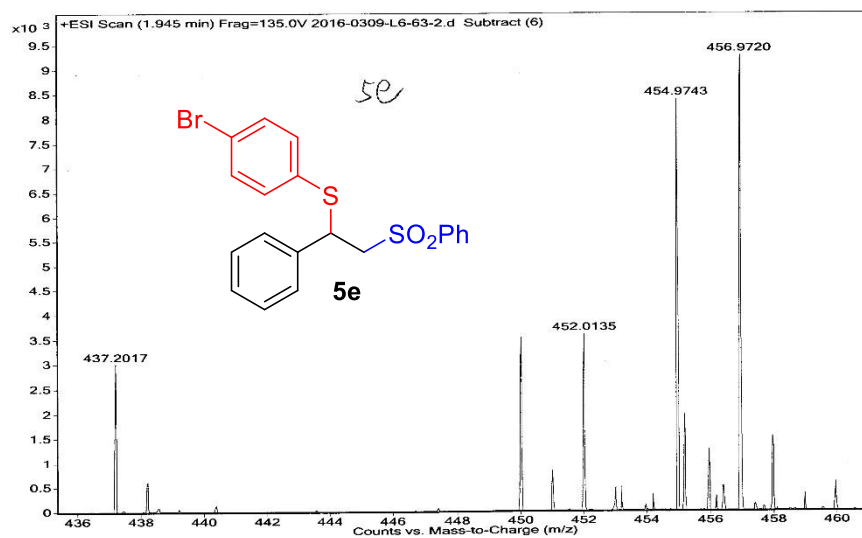
Molecular Weight: 433.3780

m/z: 431.9853 (100.0%), 433.9833 (97.3%), 432.9887 (21.6%), 434.9866 (21.0%),
 433.9811 (9.0%), 435.9791 (8.8%), 435.9900 (2.2%), 436.9824 (1.9%),
 432.9847 (1.6%), 434.9827 (1.6%), 434.9845 (1.5%), 433.9920 (1.1%),
 433.9920 (1.0%)

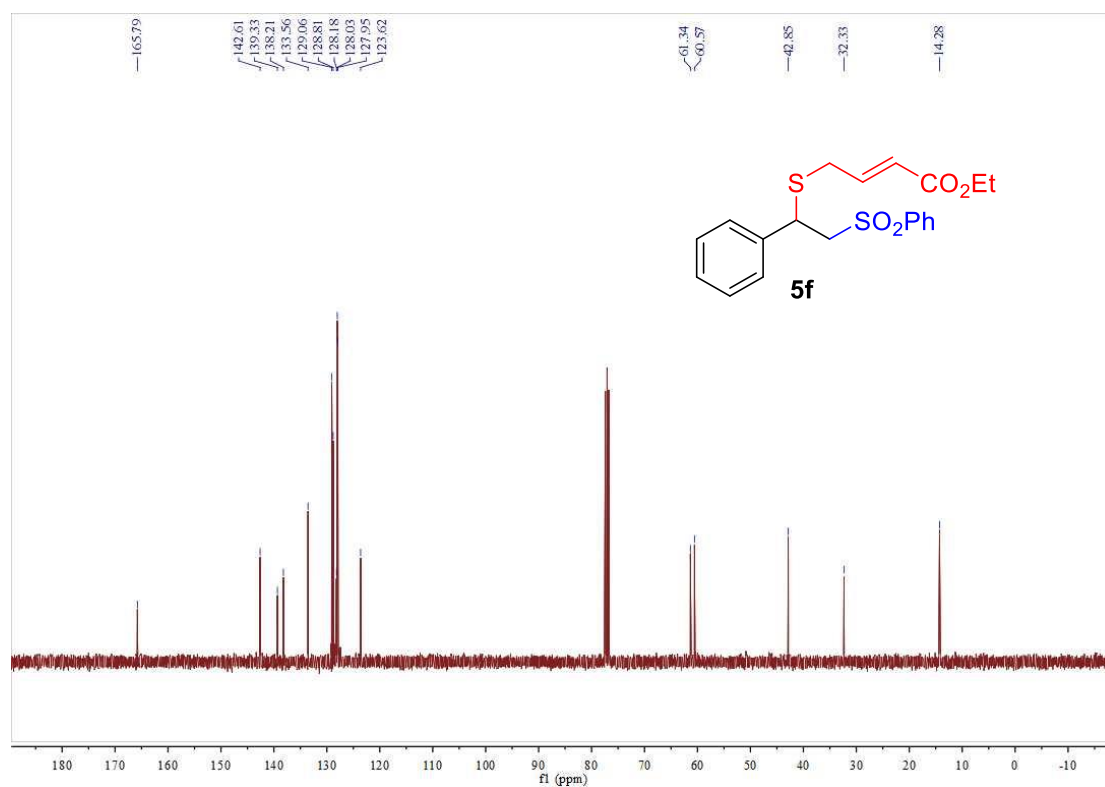
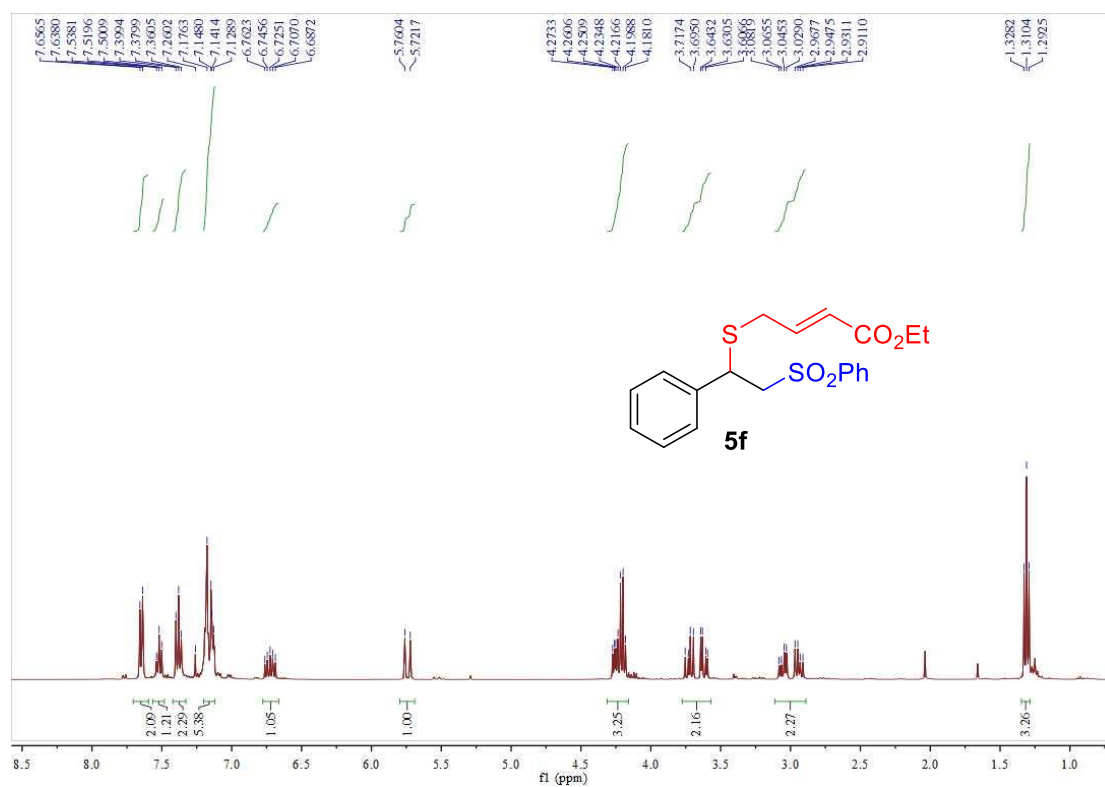
Elemental Analysis: C, 55.43; H, 3.95; Br, 18.44; O, 7.38; S, 14.80

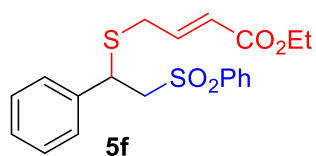
Sample Name	2016-0309-L6-63-2	Position	P1-F9	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	2016-0309-L6-63-2.d	Acq Method	0103.m	Comment		Acquired Time

Success
3/6/2016 2:42:12 PM



HRMS (ESI, m/z) calcd for $C_{20}H_{17}BrO_2S_2$ $[M+Na]^+$ 454.9746, found 454.9743.





Chemical Formula: C₂₀H₂₂O₄S₂

Exact Mass: 390.0960

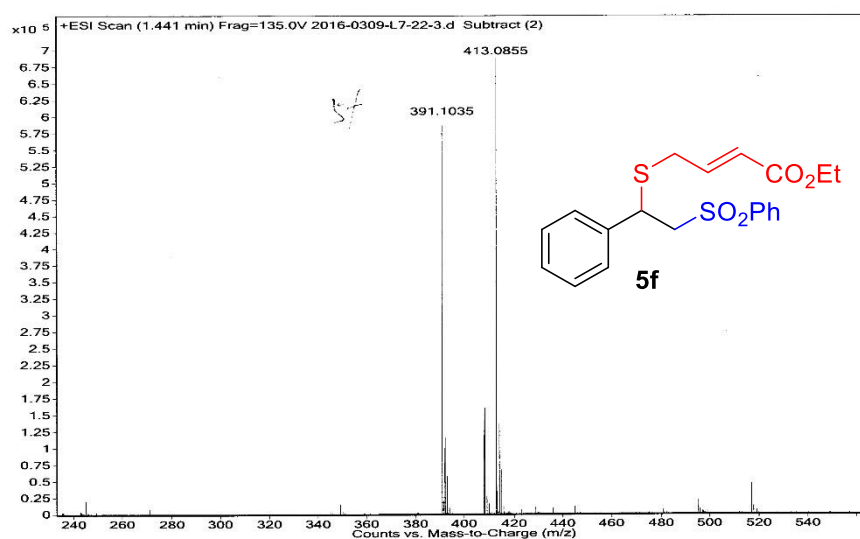
Molecular Weight: 390.5120

m/z: 390.0960 (100.0%), 391.0993 (21.6%), 392.0917 (9.0%), 392.1027 (2.2%),
393.0951 (2.0%), 391.0953 (1.6%)

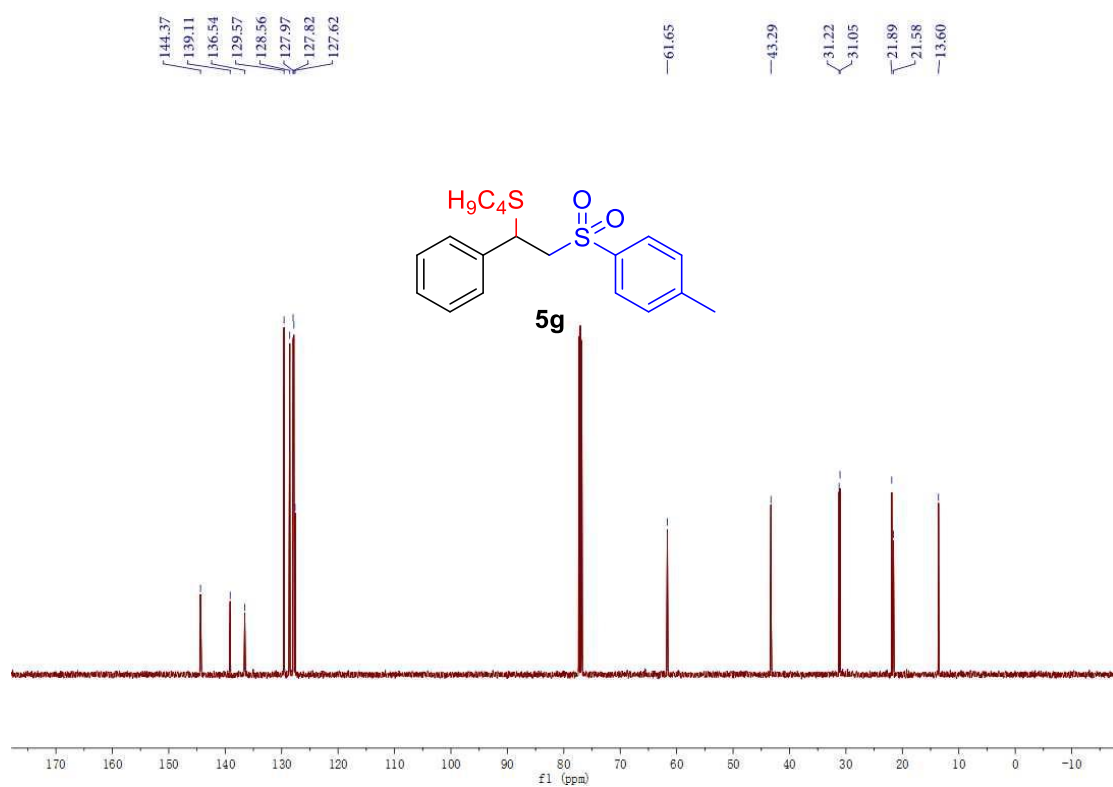
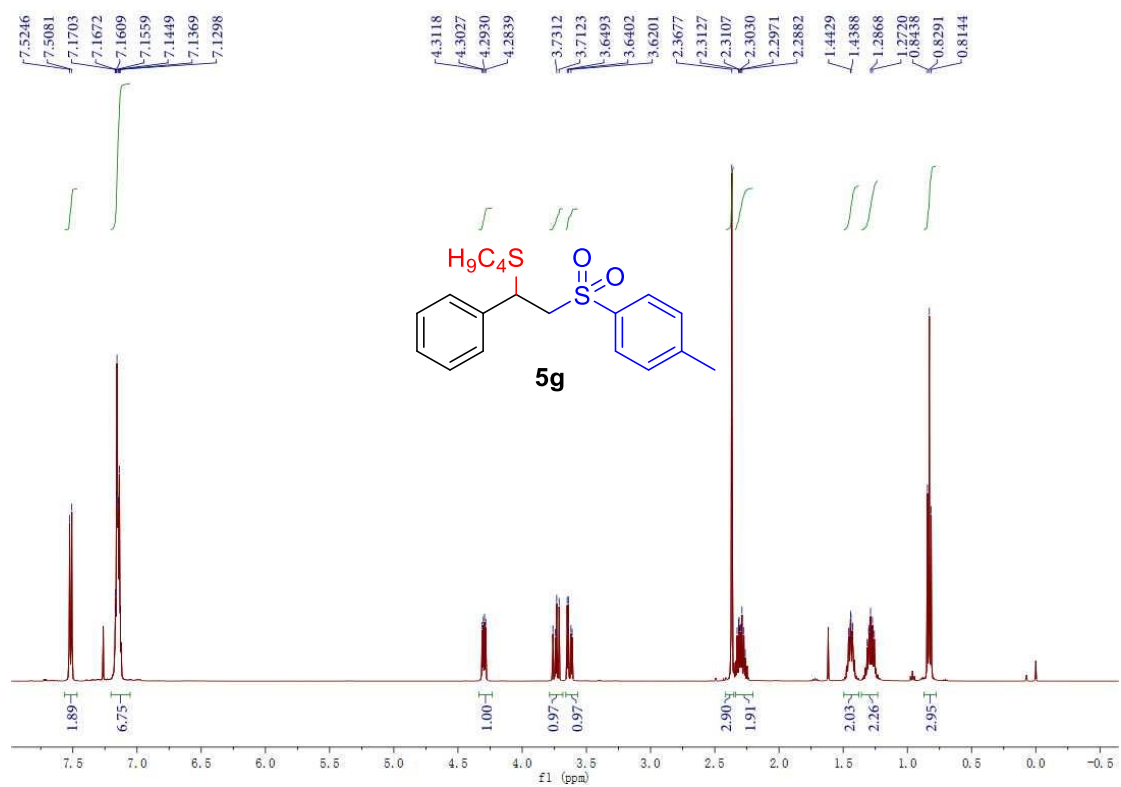
Elemental Analysis: C, 61.51; H, 5.68; O, 16.39; S, 16.42

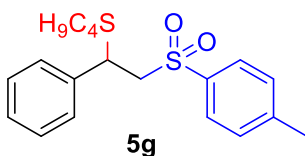
Sample Name	2016-0309-L7-22-3	Position	P1-F8	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	2016-0309-L7-22-3.d	ACQ Method	0103.m	Comment		Acquired Time

Success
3/6/2016 3:08:31 PM



HRMS (ESI, m/z) calcd for C₂₀H₂₂O₄S₂ [M+H]⁺ 391.1032, found 391.1035.





Chemical Formula: C₁₉H₂₄O₂S₂

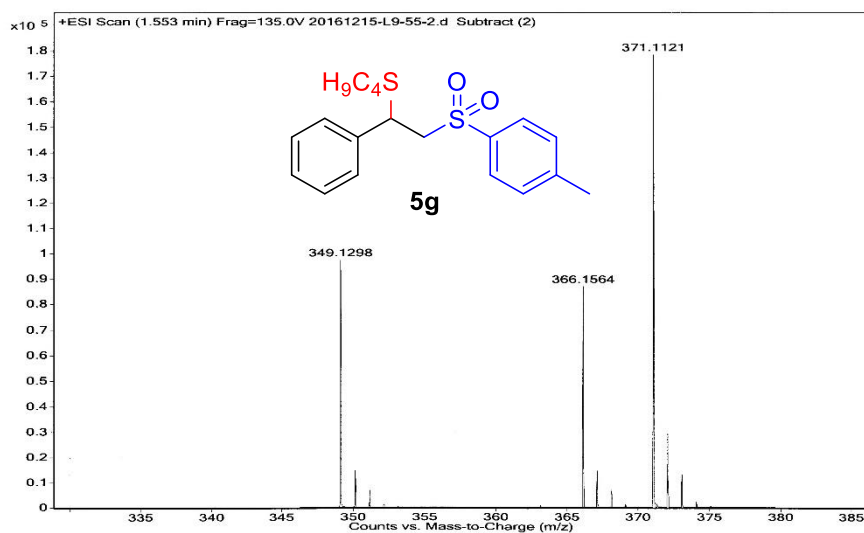
Exact Mass: 348.1218

Molecular Weight: 348.5190

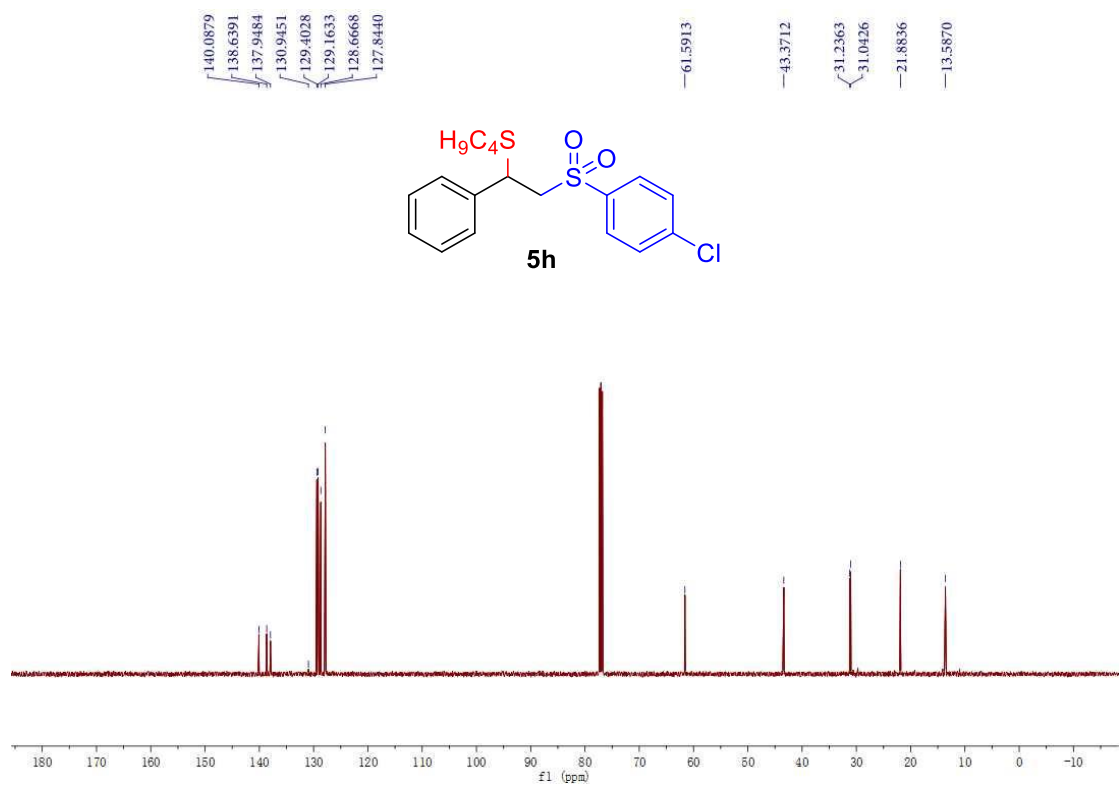
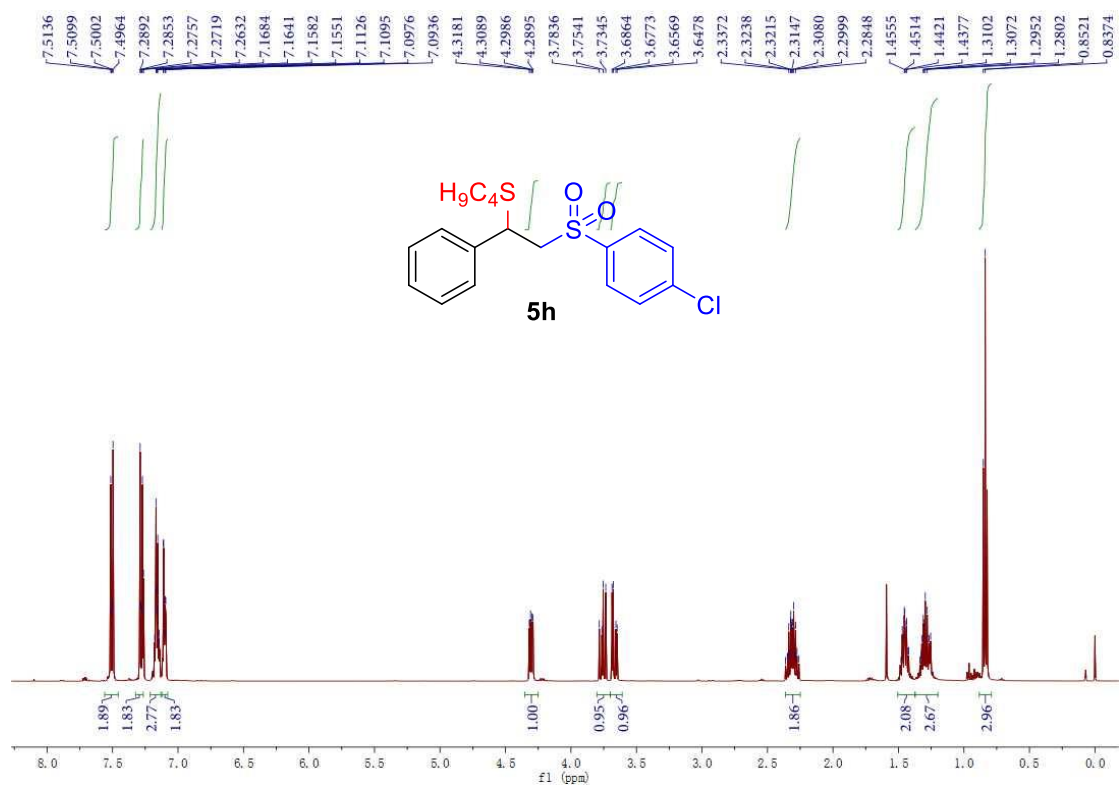
m/z: 348.1218 (100.0%), 349.1251 (20.5%), 350.1176 (9.0%), 350.1285 (2.0%),
351.1209 (1.9%), 349.1212 (1.6%)

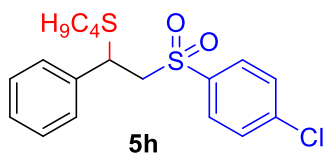
Elemental Analysis: C, 65.48; H, 6.94; O, 9.18; S, 18.40

Sample Name	20161215-L9-55-2	Position	P1-C8	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	Inj Position		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	20161215-L9-55-2.d	ACQ Method	0103.m	Comment		Acquired Time	12/15/2016 11:03:41 AM



HRMS (ESI, m/z) calcd for C₁₉H₂₄O₂S₂ [M+Na]⁺ 371.1110, found 371.1121.





Chemical Formula: $C_{18}H_{21}ClO_2S_2$

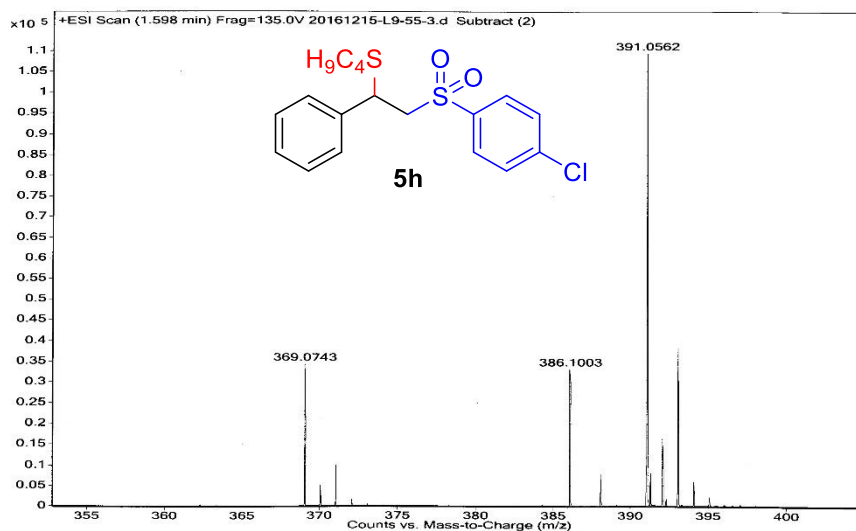
Exact Mass: 368.0671

Molecular Weight: 368.9340

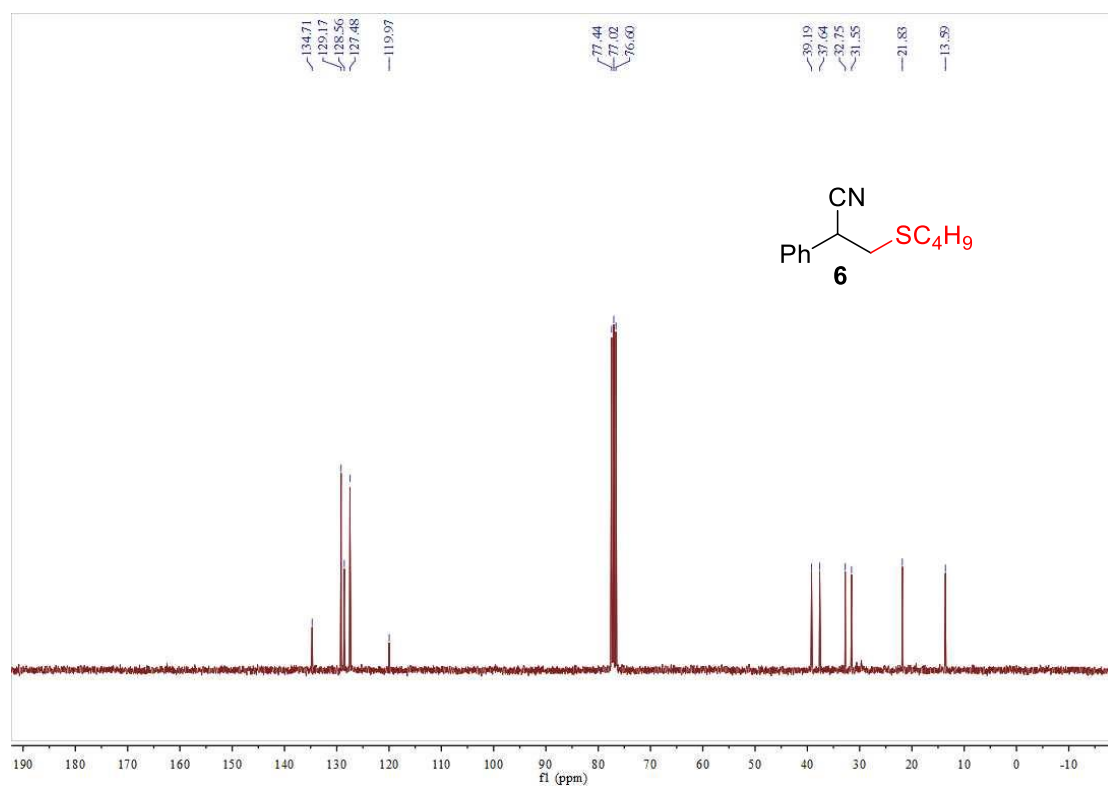
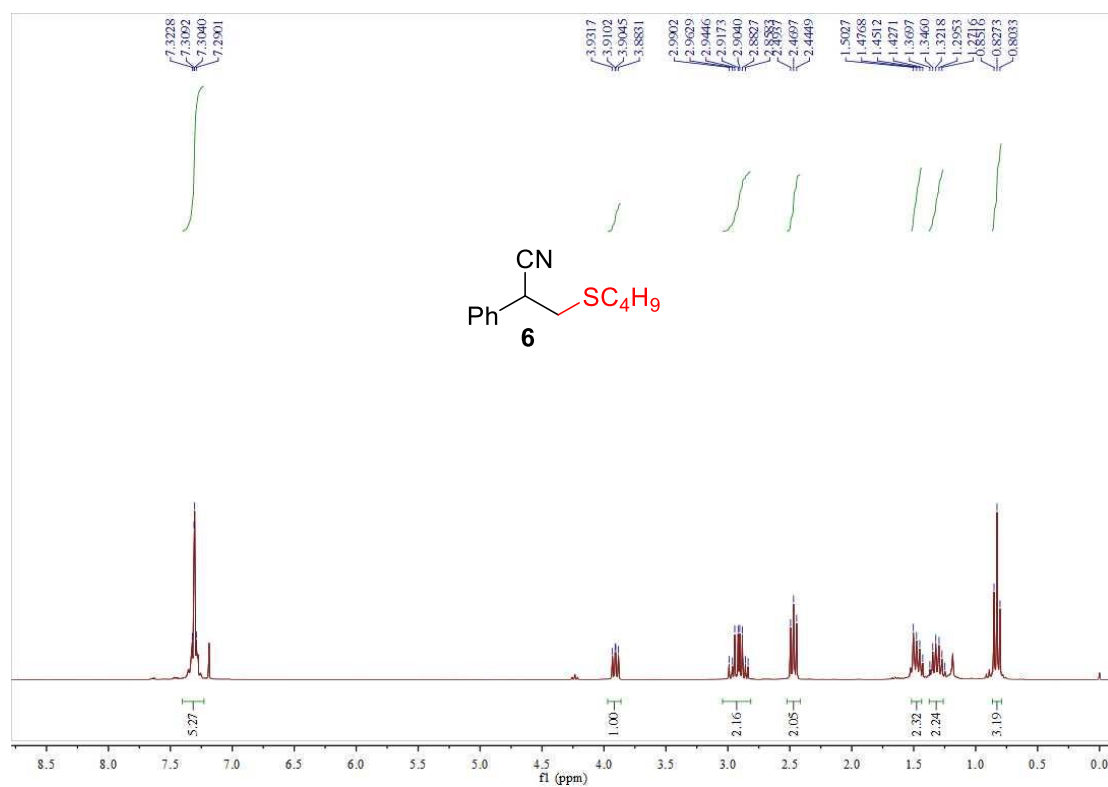
m/z : 368.0671 (100.0%), 370.0642 (32.0%), 369.0705 (19.5%), 370.0629 (9.0%), 371.0676 (6.2%), 372.0600 (2.9%), 370.0739 (1.8%), 371.0663 (1.8%), 369.0665 (1.6%)

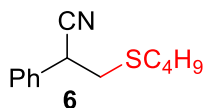
Elemental Analysis: C, 58.60; H, 5.74; Cl, 9.61; O, 8.67; S, 17.38

Sample Name	20161215-L9-55-3	Position	P1-68	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	Inj Position		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	20161215-L9-55-3.d	ACQ Method	0103.m	Comment		Acquired Time	12/15/2016 11:06:55 AM



HRMS (ESI, m/z) calcd for $C_{18}H_{21}ClO_2S_2$ $[M+Na]^+$ 391.0564, found 391.0562.





Chemical Formula: $C_{13}H_{17}NS$

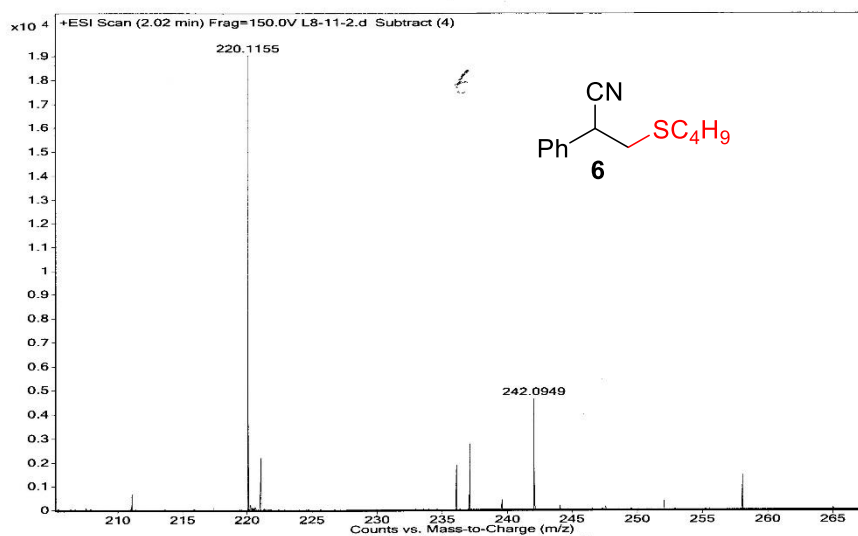
Exact Mass: 219.1082

Molecular Weight: 219.3460

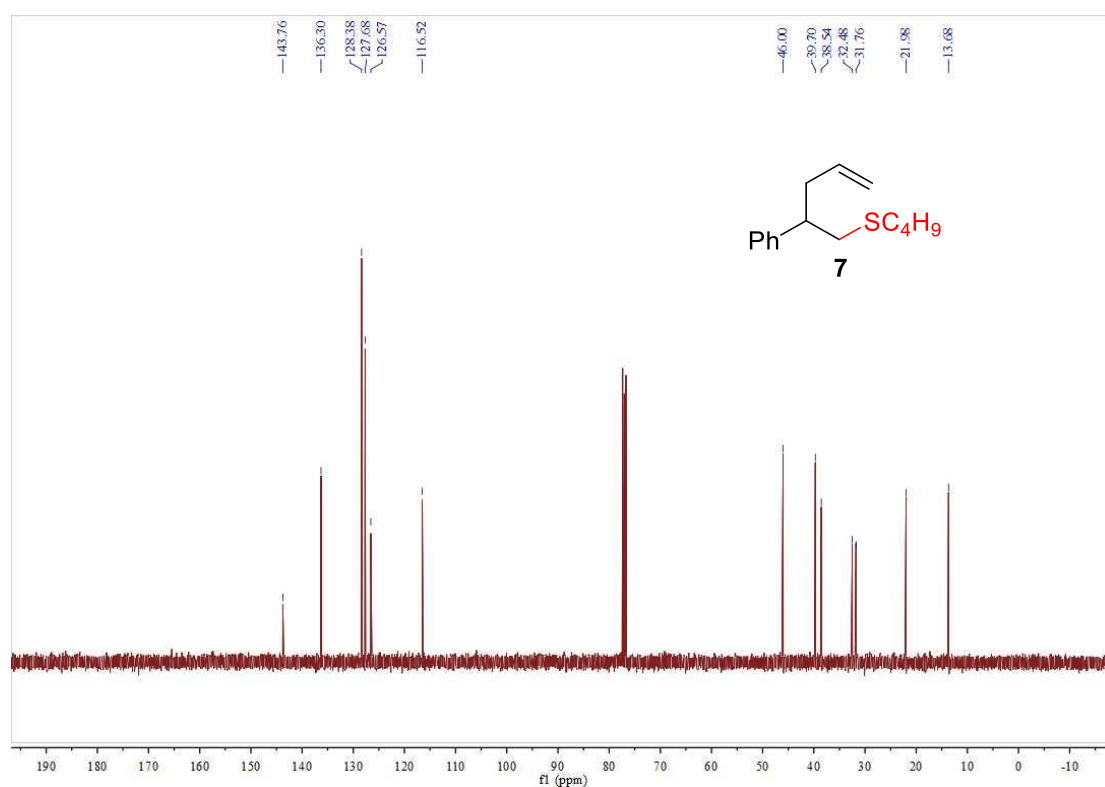
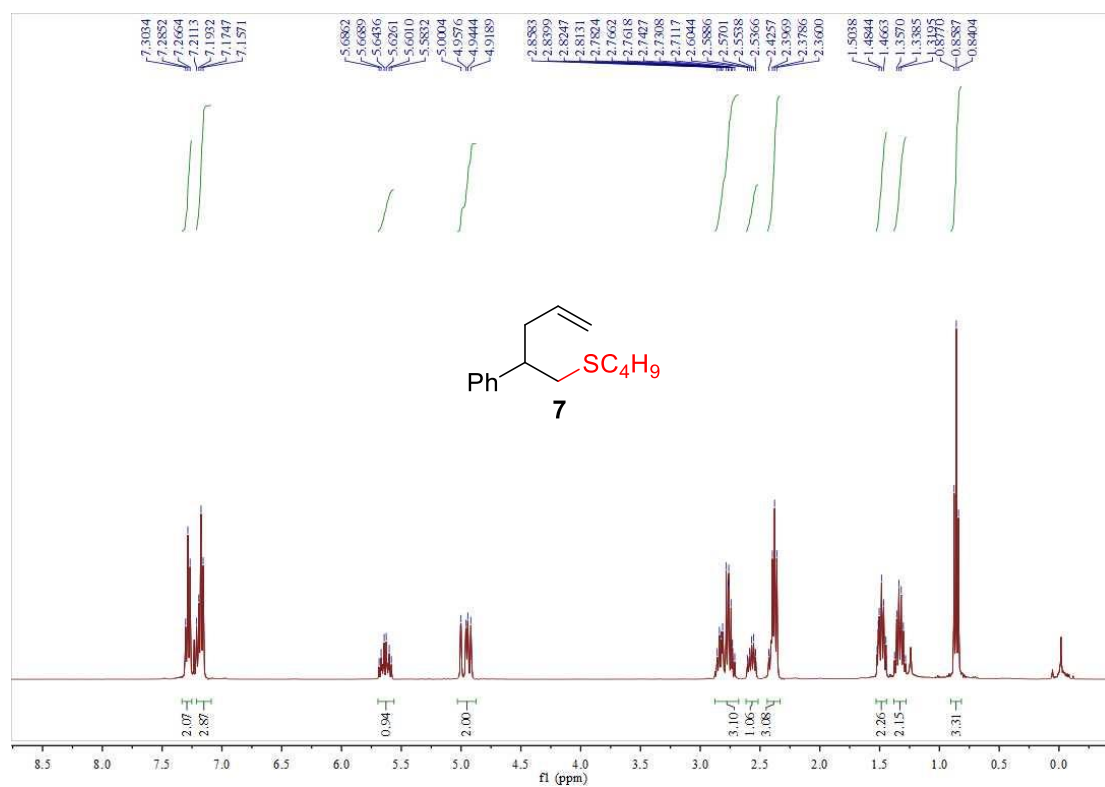
m/z : 219.1082 (100.0%), 220.1115 (14.1%), 221.1040 (4.5%)

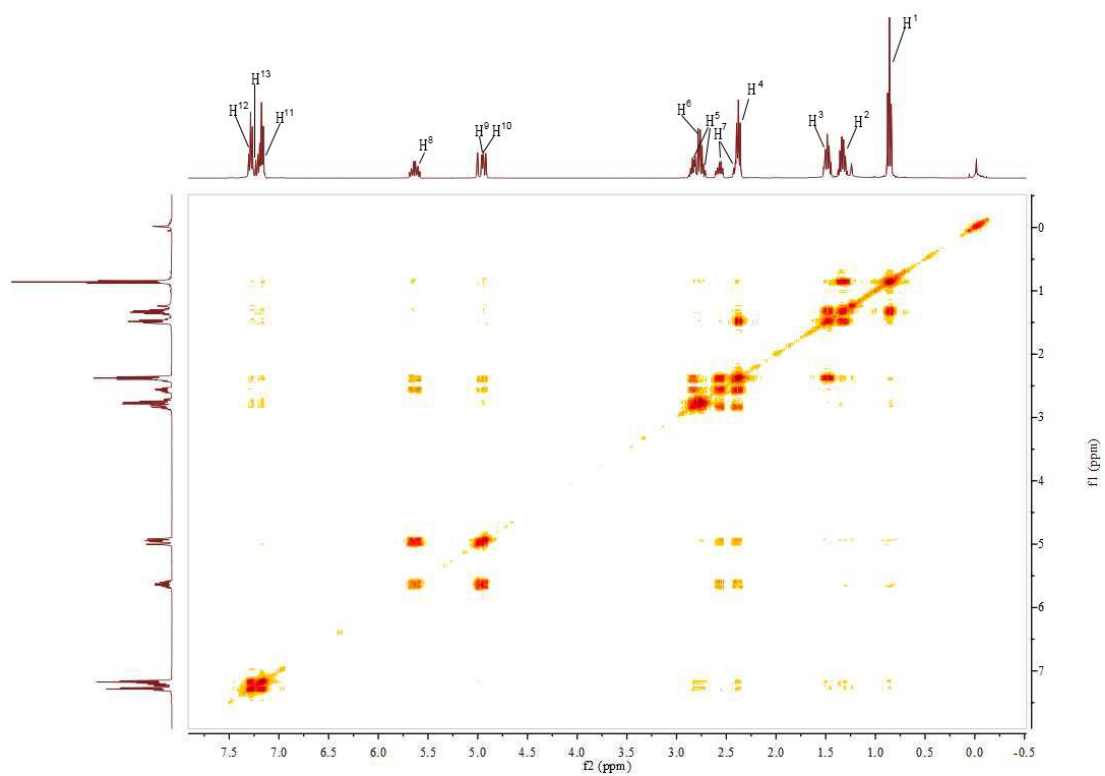
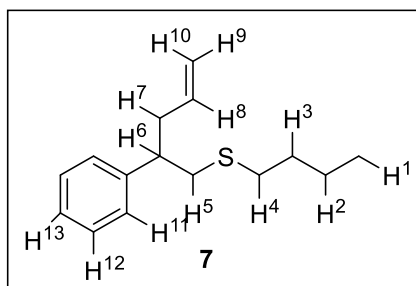
Elemental Analysis: C, 71.19; H, 7.81; N, 6.39; S, 14.62

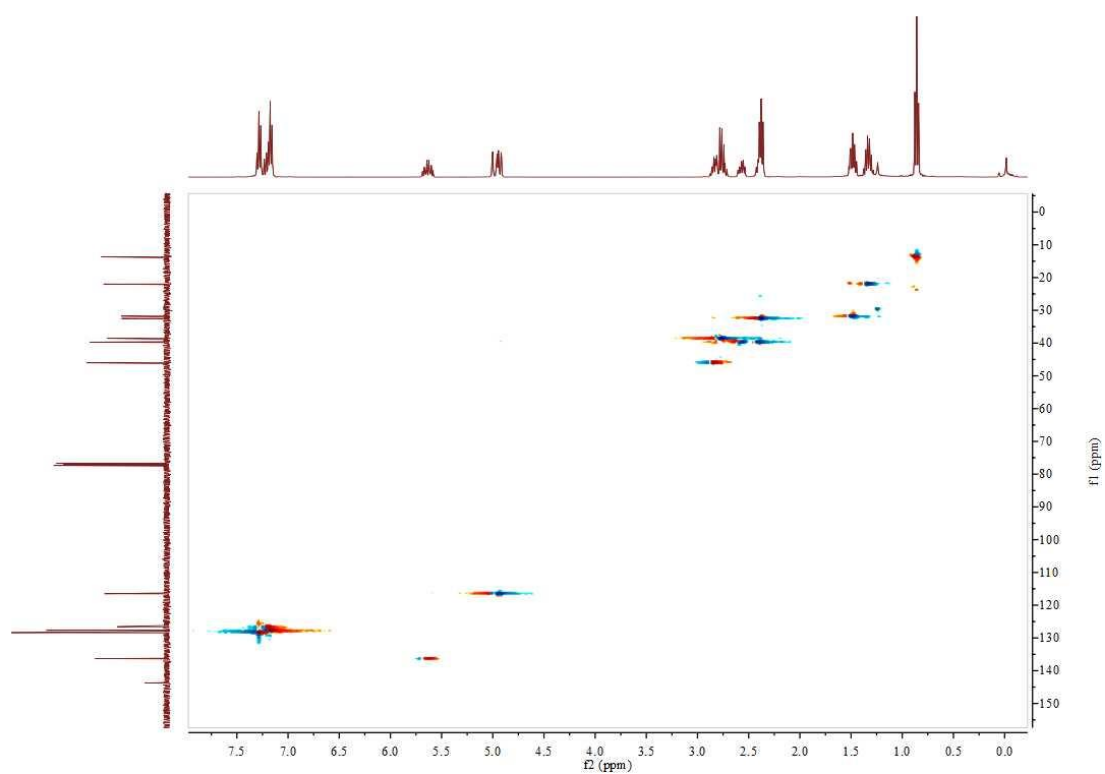
Sample Name	Position	Instrument Name	User Name
L8-11-2	P1-E7	Instrument 1	IRM Calibration Status
Inj Vol	InjPosition	SampleType	Acquired Time
Data Filename	ACQ Method	Comment	Success
L8-11-2.d	0103.m		5/10/2016 12:35:33 PM

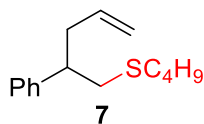


HRMS (ESI, m/z) calcd for $C_{13}H_{17}NS$ $[M+H]^+$ 220.1154, found 220.1155.









Chemical Formula: C₁₅H₂₂S

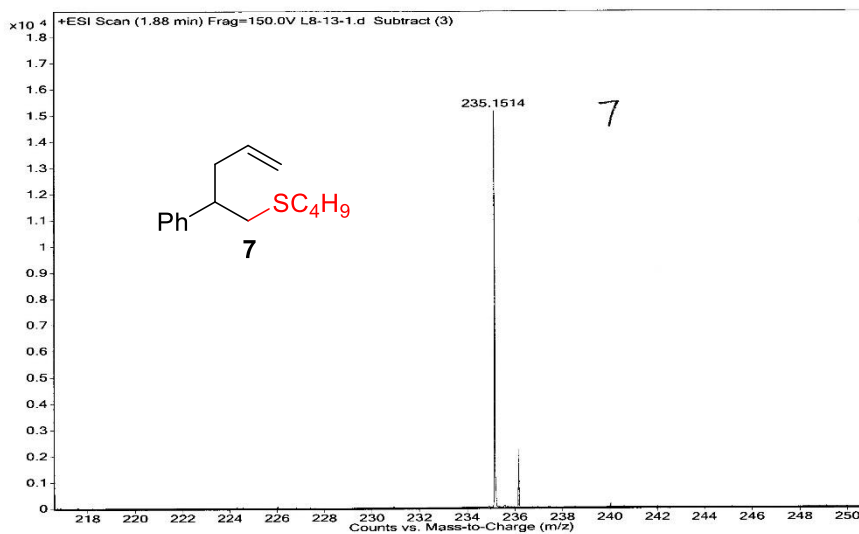
Exact Mass: 234.1442

Molecular Weight: 234.4010

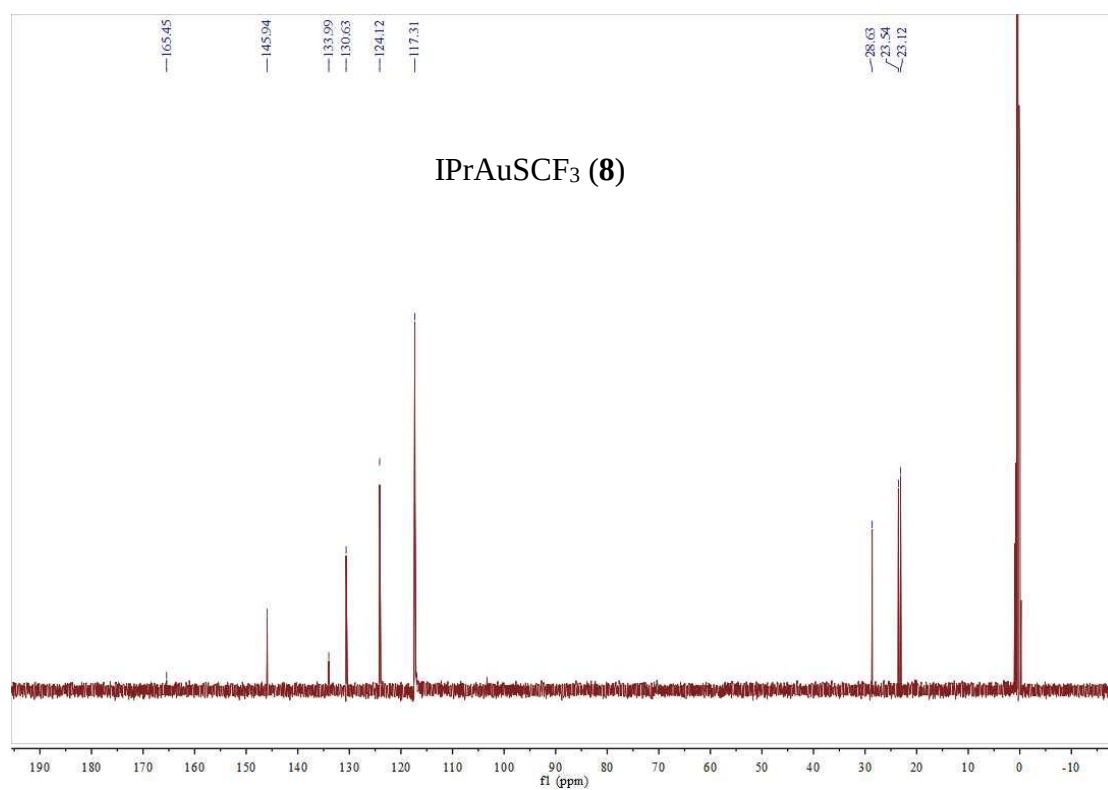
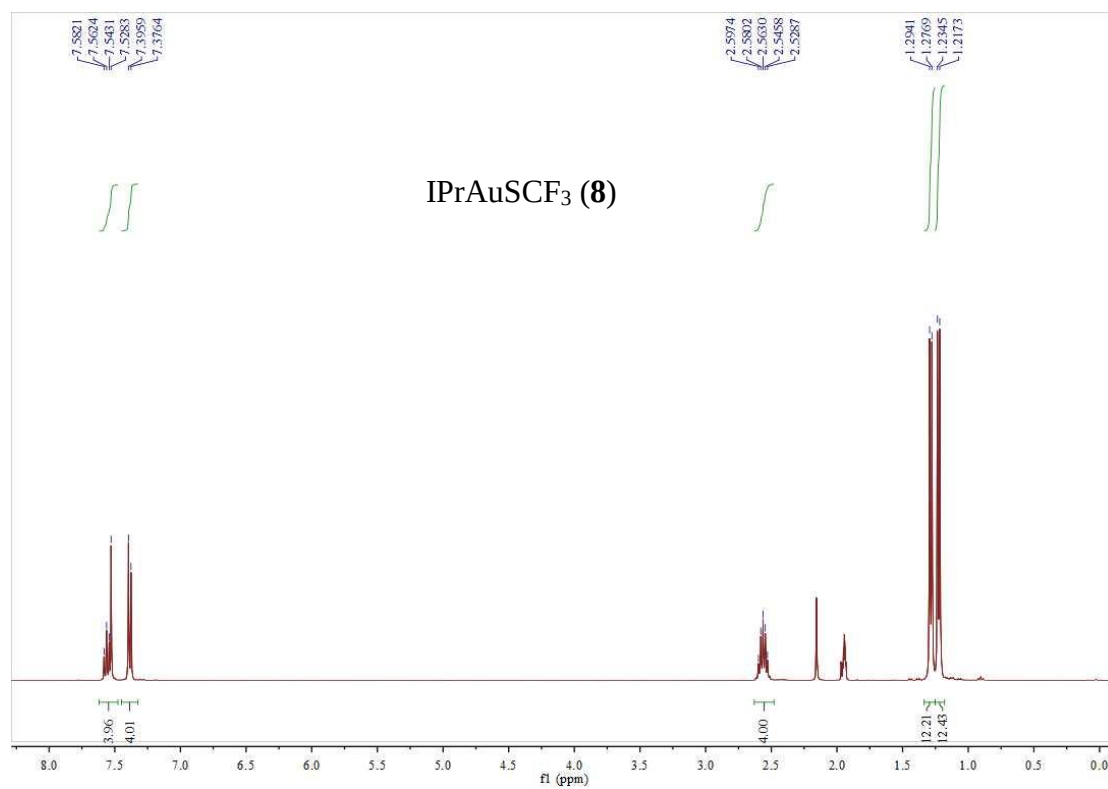
m/z: 234.1442 (100.0%), 235.1476 (16.2%), 236.1400 (4.5%), 236.1509 (1.2%)

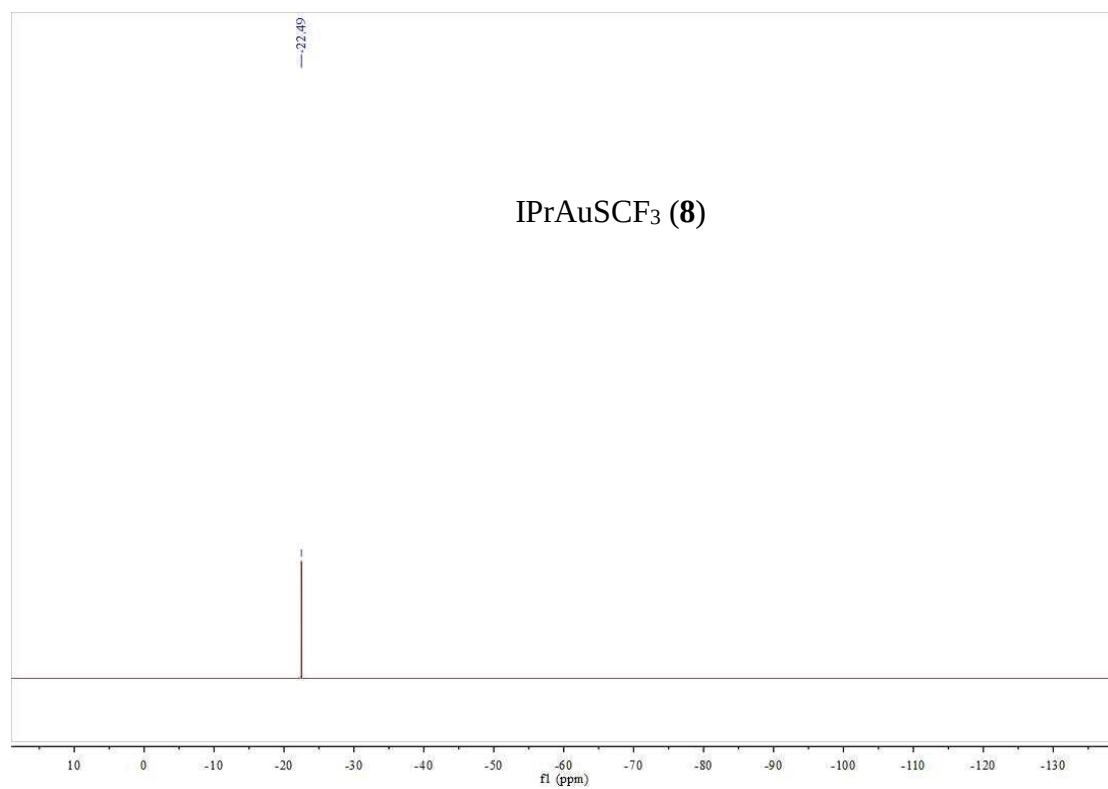
Elemental Analysis: C, 76.86; H, 9.46; S, 13.68

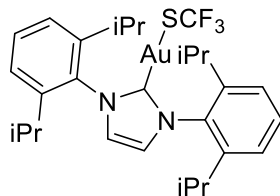
Sample Name	L8-13-1	Position	P1-F7	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	L8-13-1.d	ACQ Method	0103.m	Comment		Acquired Time	5/10/2016 12:38:32 PM



HRMS (ESI, m/z) calcd for C₁₅H₂₂S [M+H]⁺ 235.1515, found 235.1514.







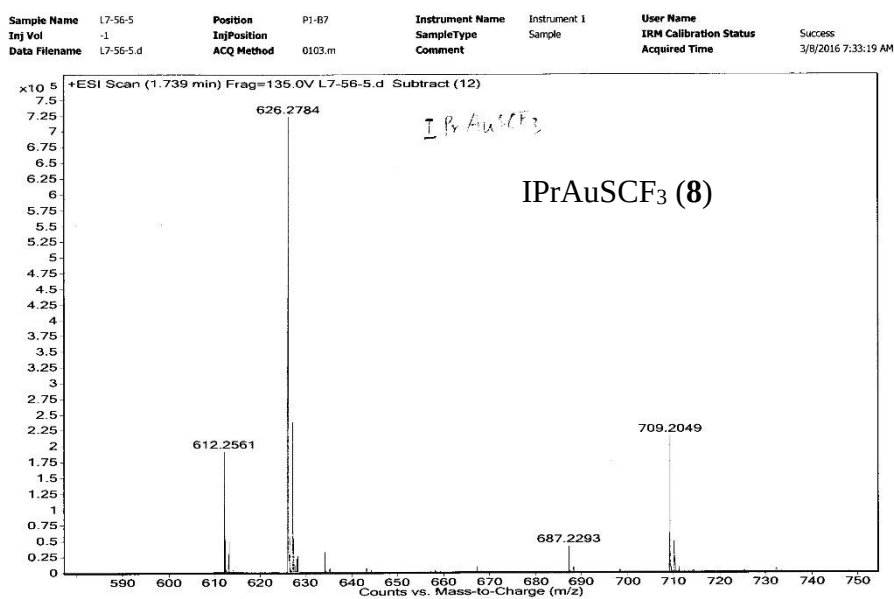
Chemical Formula: $C_{28}H_{36}AuF_3N_2S$

Exact Mass: 686.2217

Molecular Weight: 686.6318

m/z: 686.2217 (100.0%), 687.2250 (30.3%), 688.2175 (4.5%), 688.2284 (3.0%),
688.2284 (1.4%), 689.2208 (1.4%)

Elemental Analysis: C, 48.98; H, 5.28; Au, 28.69; F, 8.30; N, 4.08; S, 4.67



HRMS (ESI, m/z) calcd for $C_{28}H_{36}AuF_3N_2S$ $[M+H]^+$ 687.2290, found 687.2293.

