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Supporting Information

Radical-Mediated Vicinal Addition of Alkoxysulfonyl/Fluorosulfonyl and Trifluoromethyl Groups to Aryl Alkyl Alkynes

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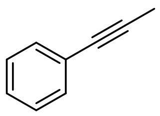
I. General considerations

Reagents. Unless otherwise indicated, all reactions were carried out in screw-cap test tube under an argon atmosphere with dry solvents. THF was dried and purified by distillation from sodium/benzophenone. CH_3CN, MeOH, and CH_2Cl_2 were distilled from CaH_2. Acetone was dried and distilled from anhydrous K_2CO_3. bpyCu$(CF_3)_3$ was purchased from Shanghai Kecui Industrial Co., Ltd. and used as received. All other reagents were purchased from commercial sources and used as received.

Analytical methods. All new compounds were characterized by ^{1}H NMR, ^{13}C NMR, ^{19}F NMR (where applicable), and HRMS. NMR spectra were record on a Bruker Advance 300, 400, 500, or 600 MHz spectrometer in $CDCl_3$. All ^{1}H NMR spectra are reported in ppm downfield from tetramethylsilane (0 ppm). All ^{13}C NMR spectra are reported in ppm relative to residual $CHCl_3$ (77.0 ppm). All ^{19}F NMR spectra are reported in ppm relative to a $CFCl_3$ external standard (0 ppm). Coupling constants are reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and brs (broad singlet). Reactions were monitored by thin-layer chromatography (TLC) carried out on commercial silica gel plates (GF254) under UV light. Flash chromatography was performed on silica gel 60 (200-300 mesh). High resolution mass spectra (HRMS) were obtained on an Agilent 6540 Ultra-High-Definition (UHD) Accurate-Mass Quadrupole Time-of-Flight (Q-TOF) spectrometer using the ESI technique and an Agilent 7250&JEOL-JMS-T100LP AccuTOF spectrometer using the EI technique.

II. Synthesis and characterization of substrates

1. Commercially-available alkynes



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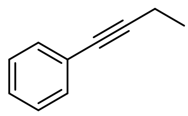

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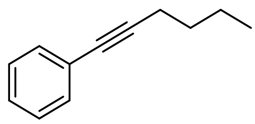

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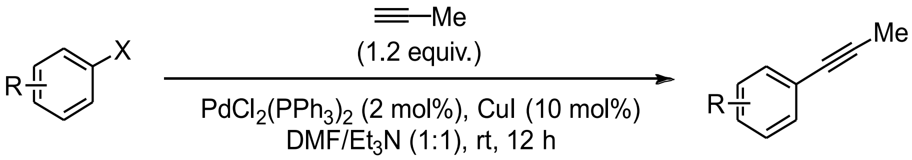
2. Synthesis and characterization of alkynes

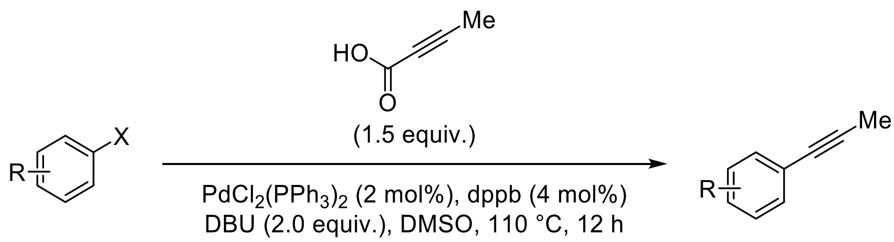
2.1 Procedures and characterization of alkyne substrates

2.1.1 General procedure A



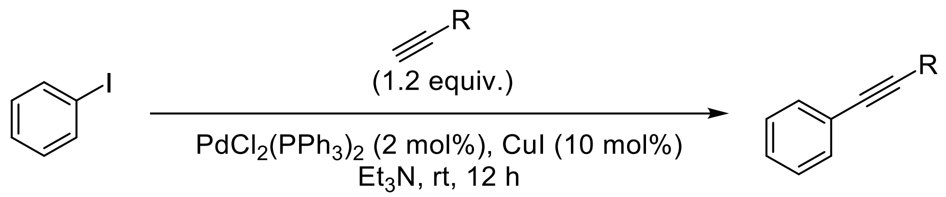
An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with aryl halide (5.0 mmol, 1.0 equiv., if it is a solid), $PdCl_2(PPh_3)_2$ (70.2 mg, 2 mol%), and CuI (95.2 mg, 10 mol%), was evacuated and backfilled with argon. The aryl halide (5.0 mmol, 1.0 equiv., if it is a liquid), Et_3N (6 mL), and propyne (1.0 M in DMF, 6 mL, 6.0 mmol) were added through the septum via syringe at room temperature. The reaction was stirred at room temperature for 12 h. Saturated aqueous NH_4Cl (15 mL) and EtOAc (20 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 15 mL). The combined organic layers were washed with water (3 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The crude material was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

2.1.2 General procedure B



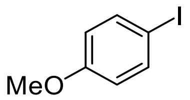
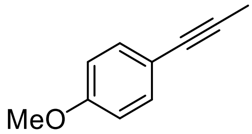
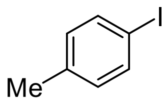
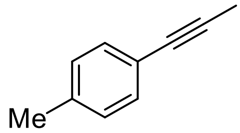
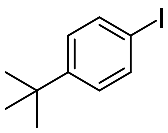
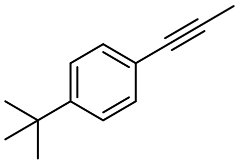
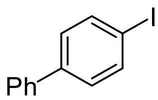
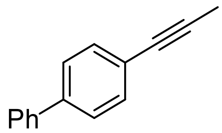
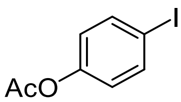
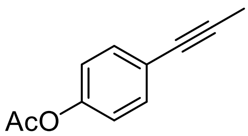
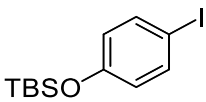
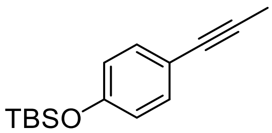
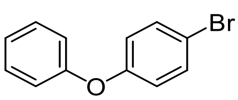
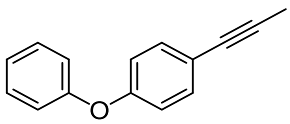
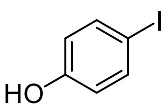
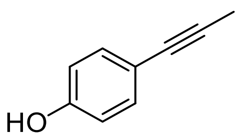
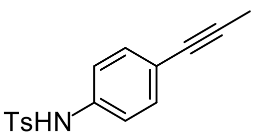
An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with aryl halide (5.0 mmol, 1.0 equiv., if it is a solid), $PdCl_2(PPh_3)_2$ (70.2 mg, 2 mol%), 1,4-bis(diphenyl-phosphino)butane (dppb, 85.3 mg, 4 mol%), and but-2-ynoic acid (0.63 g, 7.5 mmol), was evacuated and backfilled with argon. The aryl halide (5.0 mmol, 1.0 equiv., if it is a liquid), DMSO (10 mL), and DBU (1.49 mL, 10.0 mmol) were added through the septum via syringe at room temperature. The reaction was stirred at 110 °C for 12 h. Saturated aqueous NH_4Cl (15 mL) and EtOAc (20 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 15 mL). The combined organic layers were washed with water (3 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The crude material was purified flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

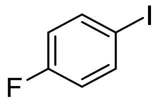
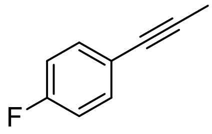
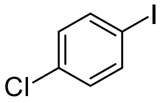
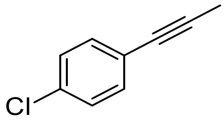
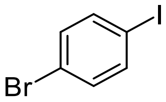
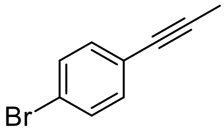
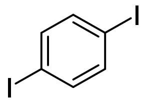
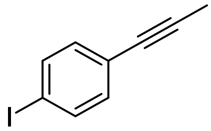
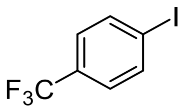
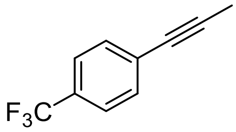
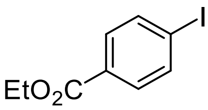
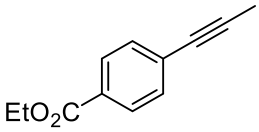
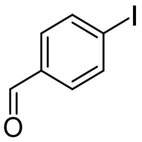
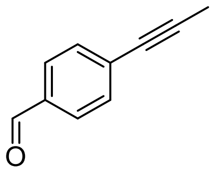
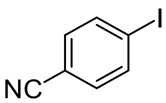
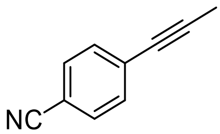
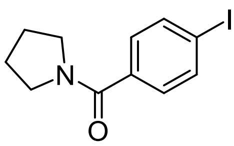
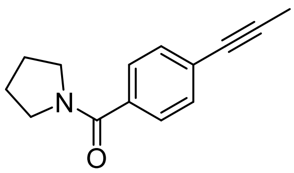
2.1.3 General procedure C



An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with $PdCl_2(PPh_3)_2$ (70.2 mg, 2 mol%) and CuI (95.2 mg, 10 mol%), was evacuated and backfilled with argon. Iodobenzene (0.56 mL, 5.0 mmol, 1.0 equiv.), substituted alkyne (6.0 mmol), and Et_3N (10 mL) were added through the septum via syringe at room temperature. The reaction was stirred at room temperature for 12 h. Saturated aqueous NH_4Cl (15 mL) and EtOAc (20 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 15 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The crude material was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

Table S1. Synthesis of Starting Alkyl Arylalkynes

Aryl halide or alkyne	Alkyne product	General procedure	Analytical reference
	 **1a**	A	*J. Am. Chem. Soc.* **2018**, *140*, 6006.
	 **1c**	A	*J. Am. Chem. Soc.* **2018**, *140*, 6006.
	 **1d**	A	*Org. Lett.* **2018**, *20*, 1576.
	 **1e**	A	*J. Am. Chem. Soc.* **2010**, *132*, 4101.
	 **1f**	A	*Chem. Commun.* **2019**, *55*, 9547.
	 **1g**	A	See details in below
	 **1h**	B	*Org. Biomol. Chem.* **2012**, *10*, 7483.
	 **1i**	A	*Org. Lett.* **2018**, *20*, 1693.
	 **1j**	A	*Org. Lett.* **2017**, *19*, 1962.

Aryl halide or alkyne	Alkyne product	General procedure	Analytical reference
	 **1k**	A	*J. Am. Chem. Soc.* **2018,** *140,* 7267.
	 **1l**	A	*J. Am. Chem. Soc.* **2018**, *140*, 6006.
	 **1m**	A	*J. Am. Chem. Soc.* **2018**, *140*, 6006.
	 **1n**	A	See details in below
	 **1o**	A	*Org. Lett.* **2018**, *20*, 1576.
	 **1p**	A	*Angew. Chem. Int. Ed.* **2016**, *55*, 5824.
	 **1q**	A	*J. Am. Chem. Soc.* **2004**, *126*, 329.
	 **1r**	A	*J. Am. Chem. Soc.* **2004**, *126*, 329.
	 **1t**	A	See details in below

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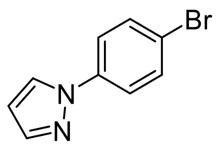
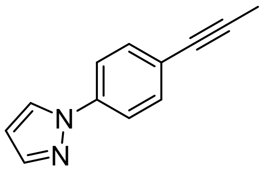
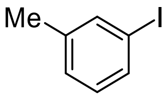
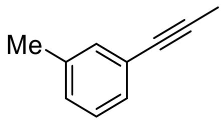
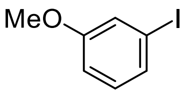
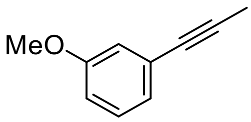
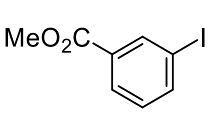
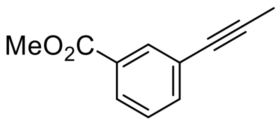
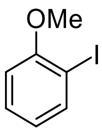
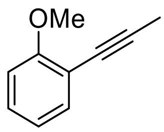
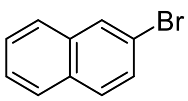
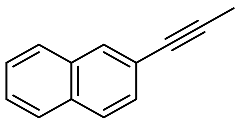
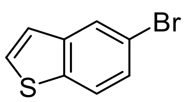
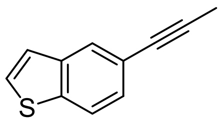
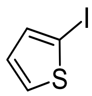
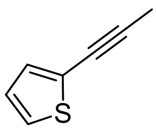
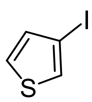
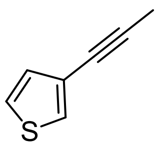
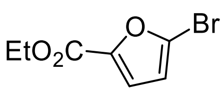
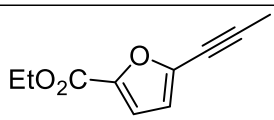
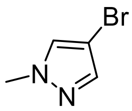
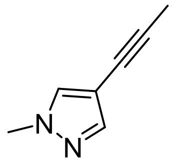
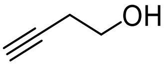
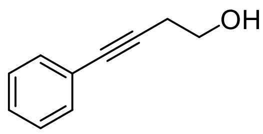
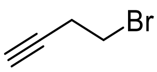
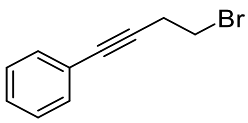
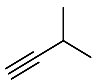
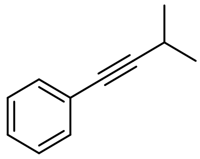
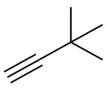
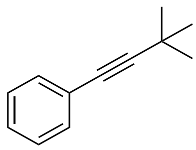
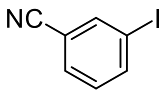
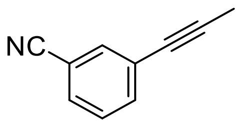
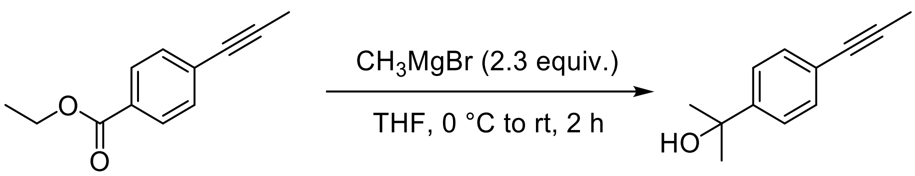
	 **1u**	B	See details in below
	 **1w**	A	*Catal. Commun.* **2020**, *133*, 105835.
	 **1x**	A	*Catal. Commun.* **2020**, *133*, 105835.
	 **1y**	A	See details in below
	 **1aa**	A	*Catal. Commun.* **2020**, *133*, 105835.
	 **1ab**	B	*J. Am. Chem. Soc.* **2018**, *140*, 6006.
	 **1ac**	B	See details in below
	 **1ad**	A	*J. Am. Chem. Soc.* **2004**, *126*, 329.
	 **1ae**	A	*Org. Biomol. Chem.* **2017**, *15*, 5756.
	 **1af**	B	See details in below

Aryl halide or alkyne	Alkyne product	General procedure	Analytical reference
	 **1ag**	B	See details in below
	 **1ai**	C	*J. Am. Chem. Soc.* **2020**, *142*, 7328.
	 **1aj**	C	*J. Am. Chem. Soc.* **2020**, *142,* 7328.
	 **1ak**	C	*J. Org. Chem.* **2012**, *77*, 7092.
	 **1al**	C	*Angew. Chem. Int. Ed.* **2020**, *59*, 14404.
	 **1aw**	A	*Tetrahedron* **2010**, *66*, 8654.

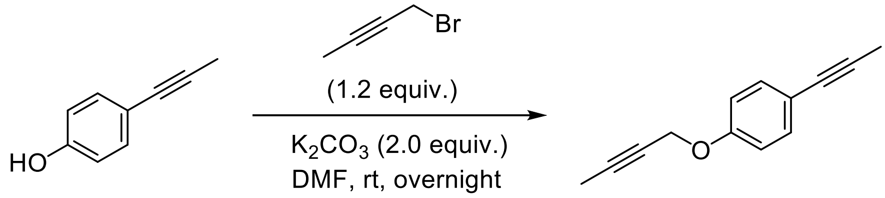
2.2 Procedures and characterization of other alkyne substrates

2.2.1 Synthesis of 2-(4-(Prop-1-yn-1-yl)phenyl)propan-2-ol (1s).



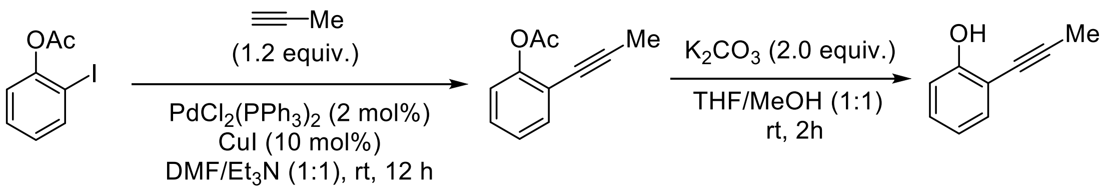
To a solution of ethyl 4-(prop-1-yn-1-yl)benzoate (0.51 g, 2.7 mmol, 1.0 equiv.) in THF (8 mL) was added dropwise CH_3MgBr (2 M in THF, 3.1 mL, 6.2 mmol) at 0 °C. The reaction mixture was stirred at room temperature for 2 h and quenched with saturated aqueous NH_4Cl (15 mL). The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 15 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The crude material was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford the title product (0.35 g, 75% yield).

2.2.2 Synthesis of 1-(But-2-yn-1-yloxy)-4-(prop-1-yn-1-yl)benzene (1v).



To a solution of 4-(prop-1-yn-1-yl)phenol (0.26 g, 2.0 mmol, 1.0 equiv.) in DMF (3 mL) was added K_2CO_3 (0.55 g, 4.0 mmol) and 1-bromobut-2-yne (0.32 g, 2.4 mmol) at room temperature. The reaction was stirred at room temperature overnight. Water (10 mL) and EtOAc (15 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 15 mL). The combined organic layers were washed with water (2 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (petroleum ether) to afford the desired product (0.34 g, 91% yield).

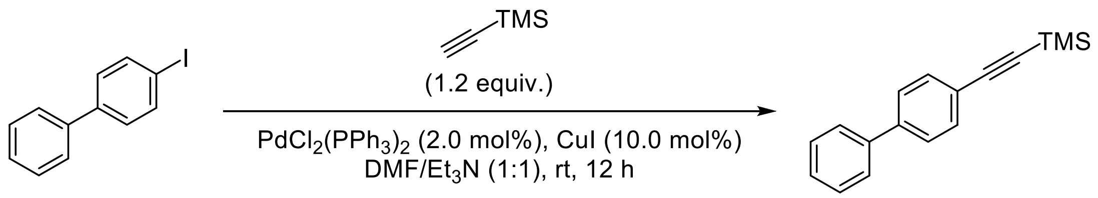
2.2.3 Synthesis of 2-(Prop-1-yn-1-yl)phenol (1z).



2-(Prop-1-yn-1-yl)phenyl Acetate： Following the general procedure A with 2-iodophenyl acetate (1.31 g, 5.0 mmol, 1.0 equiv.), the crude product was purified by flash chromatography on silica gel (petroleum ether) to afford the title product as colorless liquid (0.73 g, 84% yield).

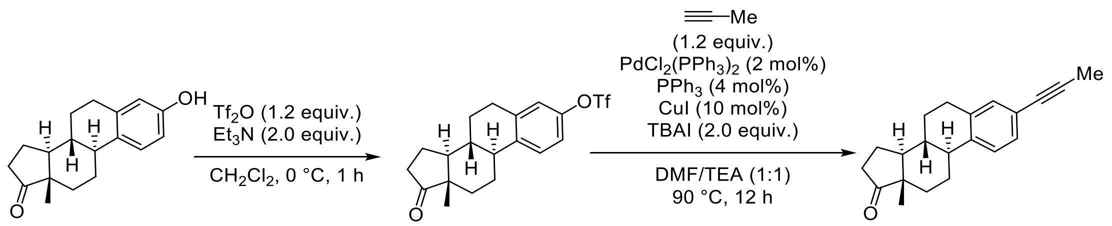
2-(Prop-1-yn-1-yl)phenol (1z): To a solution of 2-(prop-1-yn-1-yl)phenyl acetate (0.35 g, 2.0 mmol, 1.0 equiv.) in THF (2.5 mL) and MeOH (2.5 mL) was added K_2CO_3 (0.55 g, 4.0 mmol) at room temperature. The reaction mixture was stirred at room temperature for 3 h. Water (10 mL) and EtOAc (15 mL) was added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 15 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The crude material was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford the title product (0.26 g, 98% yield). The ^{1}H NMR spectral data are identical to those previously reported.[1]

2.2.4 Synthesis of ([1,1'-Biphenyl]-4-ylethynyl)trimethylsilane (1am).



An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with 4-iodo-1,1'-biphenyl (1.40 g, 5.0 mmol, 1.0 equiv.), $PdCl_2(PPh_3)_2$ (70.2 mg, 2 mol%), and CuI (95.2 mg, 10 mol%), was evacuated and backfilled with argon. Ethynyltrimethylsilane (0.85 mL, 6.0 mmol), Et_3N (5 mL), and DMF (5 mL) were added through the septum via syringe at room temperature. The reaction was stirred at room temperature for 12 h. Saturated aqueous NH_4Cl (10 mL) and EtOAc (15 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 15 mL). The combined organic layers were washed with water (2 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (petroleum ether) to afford the desired product (1.03 g, 82% yield). The ^{1}H NMR spectral data are identical to those previously reported.[2]

2.2.5 Synthesis of (8*R*,9*S*,13*S*,14*S*)-13-Methyl-3-(prop-1-yn-1-yl)-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[a]phenanthren-17-one (1ar).

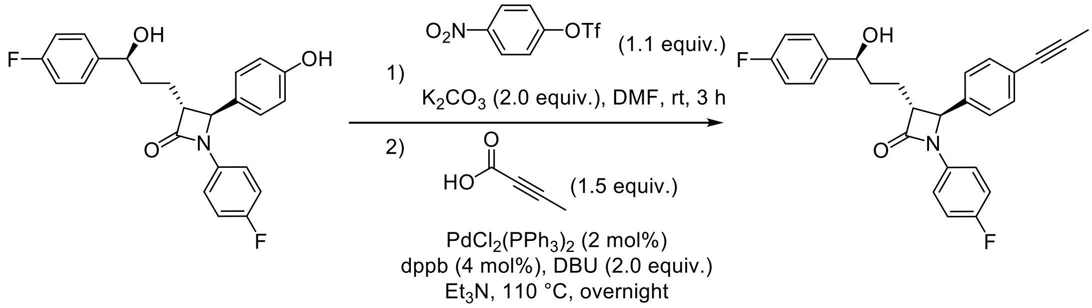


To a solution of estrone (1.35 g, 5.0 mmol, 1.0 equiv.) and Et_3N (1.39 mL, 10.0 mmol) in CH_2Cl_2 (25 mL) was added dropwise trifluoromethanesulfonic anhydride (1.01 mL, 6.0 mmol) under argon atmosphere at 0 °C. The reaction mixture was stirred at 0 °C for 1 h and quenched with saturated aqueous $NaHCO_3$ (20 mL). The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford estronyl triflate (1.88 g, 93% yield).

An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with estronyl triflate (1.61 g, 4.0 mmol, 1.0 equiv.), PPh_3 (42.0 mg, 4 mol%), $PdCl_2(PPh_3)_2$ (56.1 mg, 2 mol%), CuI (76.2 mg, 10 mol%), and tetrabutylammonium iodide (2.95 g, 8.0 mmol), was evacuated and backfilled with argon. Propyne (1.0 M in DMF, 4.8 mL, 4.8 mmol) and Et_3N (4.0 mL) were added through the septum via syringe at room temperature. The reaction was stirred at 90 °C for 12 h. Saturated aqueous NH_4Cl (10 mL) and EtOAc (15 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 15 mL). The combined organic layers were washed with water (2 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford the title product (0.64 g, 54% yield). The ^{1}H NMR spectral data are identical to those previously reported.[3]

2.2.6 Synthesis of (3*R*,4*R*)-1-(4-Fluorophenyl)-3-((*S*)-3-(4-fluorophenyl)-3-hydroxypropyl)-4-(

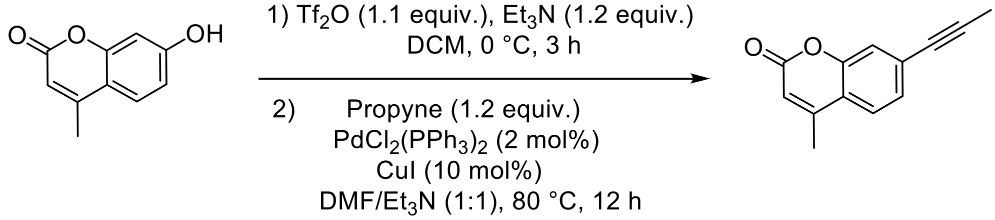
4-(Prop-1-yn-1-yl)phenyl)azetidin-2-one (1as)



To a mixture of ezetimibe (0.82 g, 2.0 mmol, 1.0 equiv.) and K_2CO_3 (0.55 g, 4.0 mmol) in DMF (10 mL) was added 4-nitrophenyl trifluoromethanesulfonate (0.60 g, 2.2 mmol) at room temperature. The reaction mixture was stirred at room temperature for 3 h. Saturated aqueous $NaHCO_3$ (10 mL) and EtOAc (15 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with water (2 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford ezetimibe triflate (0.96 g, 89% yield). The ^{1}H NMR spectral data are identical to those previously reported.[4]

An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with ezetimibe triflate (541.5 mg, 1.0 mmol, 1.0 equiv.), $PdCl_2(PPh_3)_2$ (14.0 mg, 2 mol%), 1,4-bis(diphenyl-phosphino)butane (dppb, 17.1 mg, 4 mol%), and but-2-ynoic acid (126.1 mg, 1.5 mmol), was evacuated and backfilled with argon. DMSO (5 mL) was added through the septum via syringe at room temperature. The reaction mixture was stirred at 110 °C for 12 h. Saturated aqueous NH_4Cl (10 mL) and EtOAc (15 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 15 mL). The combined organic layers were washed with water (2 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford the title product (0.36 g, 84% yield).

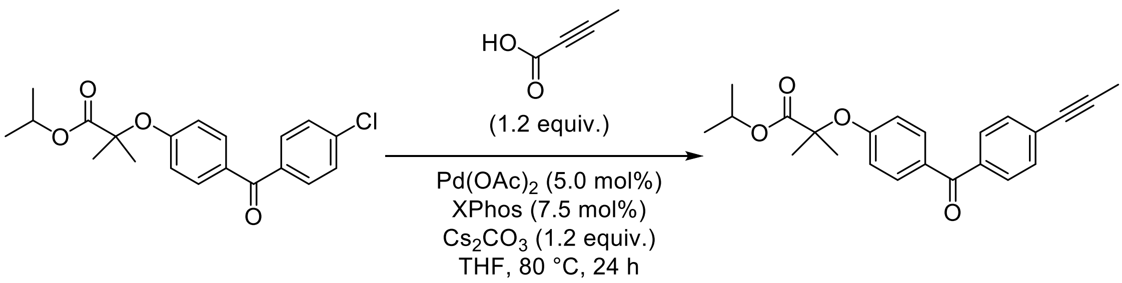
2.2.7 Synthesis of 4-Methyl-7-(prop-1-yn-1-yl)-2*H*-chromen-2-one (1at)



To a solution of 4-methylumbelliferone (0.88 g, 5.0 mmol, 1.0 equiv.) and Et_3N (0.83 mL, 6.0 mmol) in CH_2Cl_2 (20 mL) was added dropwise trifluoromethanesulfonic anhydride (0.93 mL, 5.5 mmol) under argon atmosphere at 0 °C. The reaction mixture was stirred at 0 °C for 3 h and quenched with saturated aqueous $NaHCO_3$ (10 mL). The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford 4-methylumbelliferone triflate (1.27 g, 83% yield).

An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with 4-methylumbelliferone triflate (0.61 g, 2.0 mmol, 1.0 equiv.), $PdCl_2(PPh_3)_2$ (28.1 mg, 2 mol%), and CuI (38.1 mg, 10 mol%), was evacuated and backfilled with argon. Propyne (1.0 M in DMF, 2.4 mL, 2.4 mmol) and Et_3N (2.0 mL) were added through the septum via syringe at room temperature. The reaction was stirred at 80 °C for 12 h. Saturated aqueous NH_4Cl (10 mL) and EtOAc (20 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 20 mL). The combined organic layers were washed with water (2 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford the title product (0.31g, 78% yield). The ^{1}H NMR spectral data are identical to those previously reported.[5]

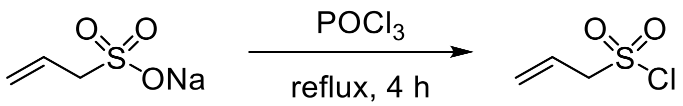
2.2.8 Synthesis of Isopropyl 2-Methyl-2-(4-(4-(prop-1-yn-1-yl)benzoyl)phenoxy)propanoate (1au)



An oven-dried round bottom flask, which was equipped with a magnetic stir bar and charged with fenofibrate (1.80 g, 5.0 mmol, 1.0 equiv.), $Pd(OAc)_2$ (56.1 mg, 5 mol%), XPhos (178.9 mg, 7.5 mol%), Cs_2CO_3 (1.95 g, 6.0 mmol), and but-2-ynoic acid (0.50 g, 6.0 mmol), was evacuated and backfilled with argon. THF (20 mL) was added through the septum via syringe at room temperature. The reaction was stirred at 80 °C for 24 h and saturated aqueous NH_4Cl (10 mL) was added. The two layers were separated and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford the title product (1.02 g, 56% yield).

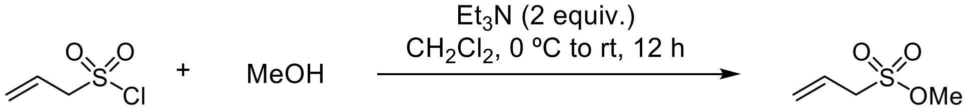
3. Synthesis and characterization of allylsulfonates and allylsulfonyl fluoride

3.1 Synthesis of Allylsulfonyl Chloride



A mixture of sodium allylsulfonate (50.0 g, 0.35 mol) and phosphoryl chloride (100 mL) was refluxed for 4 h. The reaction mixture was cooled to room temperature and filtered through a short pad of silica gel. The filtrate was concentrated and purified by distillation to afford allylsulfonyl chloride as colorless liquid (40.2 g, 82% yield). The ^{1}H NMR spectral data are identical to those previously reported.[6]

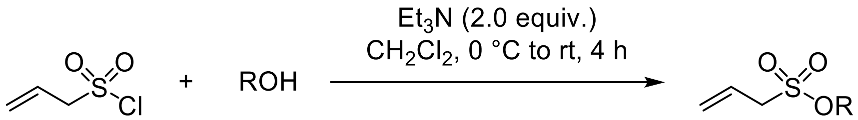
3.2 Synthesis of Methyl Prop-2-ene-1-sulfonate (2a)



(1.5 equiv.) (1 equiv.) **2a**

To a solution of MeOH (4.0 mL, 0.1 mol, 1.0 equiv.) and Et_3N (27.8 mL, 0.2 mol) in dry CH_2Cl_2 (200 mL) was added allylsulfonyl chloride (21.1 g, 0.15 mol) at 0 °C. The reaction was stirred at room temperature for 12 h and water (50 mL) was added. The two layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 100 mL). The combined organic layers were washed with saturated aqueous $NaHCO_3$ (2 × 40 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product (7.1 g, 52% yield).

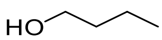
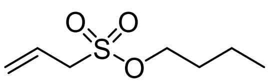
3.3 General procedure D: synthesis of alkyl allylsulfonates

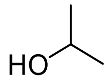
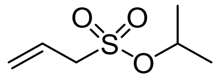
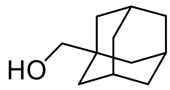
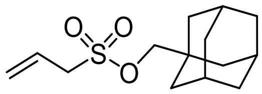
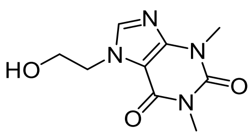
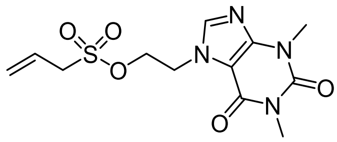


(1.5 equiv.) (1.0 equiv.)

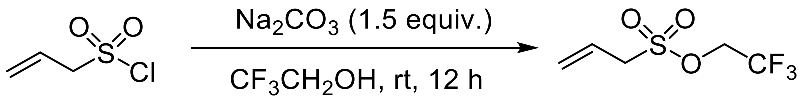
To a solution of alcohol (5.0 mmol, 1.0 equiv.) and Et_3N (1.39 mL, 10.0 mmol) in dry CH_2Cl_2 (10 mL) was added allylsulfonyl chloride (1.05 g, 7.5 mmol) at 0 °C. The reaction was stirred at room temperature for 4 h and water (10 mL) was added. The two layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with saturated aqueous $NaHCO_3$ (2 × 5 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

Table S2. Synthesis of Alkyl Allylsulfonates

Alcohol	Allylsulfonate	General procedure	Analytical reference
	 **2b**	D	See details in below

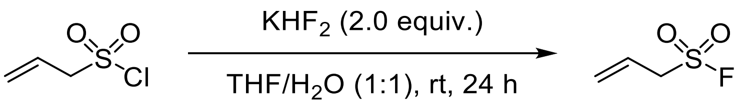
	 **2c**	D	*Chem. Eur. J.* **2010**, *16*, 5969.
	 **2e**	D	See details in below
	 **2f**	D	See details in below

3.4 Synthesis of 2,2,2-Trifluoroethyl Prop-2-ene-1-sulfonate (2d)



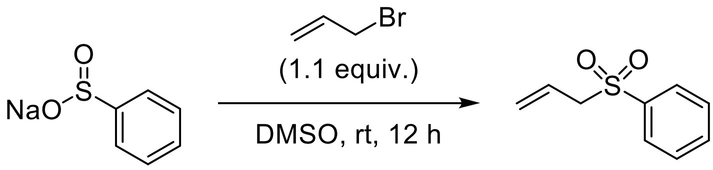
To a mixture of Na_2CO_3 (0.78 g, 7.5 mmol) in CF_3CH_2OH (3 mL) was added allylsulfonyl chloride (0.70 g, 5.0 mmol, 1.0 equiv.) at room temperature. The reaction was stirred at room temperature 12 h. Water (10 mL) and EtOAc (15 mL) were added. The two layers were separated and the aqueous layers were extracted with EtOAc (2 × 10 mL). The organic layers were washed with saturated aqueous $NaHCO_3$ (2 × 5 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford the title product (0.46 g, 45% yield).

3.5 Synthesis of Allylsulfonyl Fluoride (4)



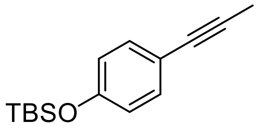
To a solution of KHF_2 (15.6 g, 0.2 mol) in MeCN (75 mL) and H_2O (75 mL) was added dropwise allylsulfonyl chloride (14.1 g, 0.1 mol, 1.0 equiv.) at room temperature. The reaction was stirred at room temperature for 24 h and CH_2Cl_2 (75 mL) was added. The two layers were separated and the aqueous layer was extracted with CH_2Cl_2 (2 × 100 mL). The combined organic layers were washed with saturated aqueous $NaHCO_3$ (3 × 30 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by distillation to afford allylsulfonyl fluoride **4** as colorless liquid (9.8 g, 79% yield).

3.6 Synthesis of (Allylsulfonyl)benzene



To a solution of sodium benzenesulfinate (1.64 g, 10.0 mmol, 1 equiv.) in DMSO (18 mL) was added allyl bromide (0.95 mL, 11.0 mmol) at room temperature. The reaction mixture was stirred at room temperature for 12 h. Water (10 mL) and EtOAc (20 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 20 mL). The organic layers were washed with water (3 × 10 mL) and brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford the title product (1.50 g, 82% yield). The ^1H NMR spectral data are identical to those previously reported.[7]

4. Characterization of substrates



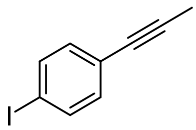
***tert*-Butyldimethyl(4-(prop-1-yn-1-yl)phenoxy)silane (1g)**

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (petroleum ether) to afford **1g** as colorless oil (1.14 g, 92% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (d, 2H, *J* = 8.7 Hz), 6.76 (d, 2H, *J* = 8.7 Hz), 2.04 (s, 3H), 0.99 (s, 9H), 0.20 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 155.2, 132.7, 120.0, 116.8, 84.2, 79.4, 25.6, 18.2, 4.3, -4.5.

HRMS (ESI) calcd for $C_{15}H_{23}OSi^+$ $[M+H]^+$ 247.1513, found 247.1511.



1-Iodo-4-(prop-1-yn-1-yl)benzene (1n)

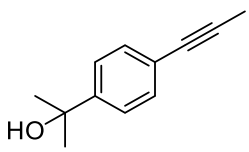
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (petroleum ether) to afford **1n** as a white solid (0.80 g, 66% yield).

m.p. 36.7–37.8 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61 (d, 2H, *J* = 8.5 Hz), 7.11 (d, 2H, *J* = 8.5 Hz), 2.03 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 137.3, 133.1, 123.5, 93.1, 87.4, 78.9, 4.4.

HRMS (EI) calcd for $C_9H_7I^+$ $[M]^+$ 241.9587, found 241.9586.



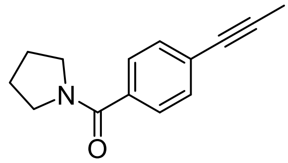
2-(4-(Prop-1-yn-1-yl)phenyl)propan-2-ol (1s)

m.p. 64.0–65.2 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (d, 2H, *J* = 8.7 Hz), 7.36 (d, 2H, *J* = 8.7 Hz), 2.05 (s, 3H), 1.71 (s, 1H), 1.57 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 148.4, 131.2, 124.3, 122.2, 85.5, 79.5, 72.3, 31.5, 4.3.

HRMS (ESI) calcd for $C_{12}H_{14}NaO^+$ $[M+Na]^+$ 197.0937, found 197.0934.



(4-(Prop-1-yn-1-yl)phenyl)(pyrrolidin-1-yl)methanone (1t)

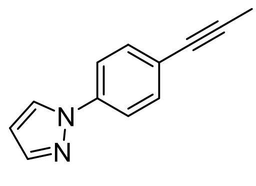
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **1t** as a white solid (0.91 g, 85% yield).

m.p. 139.2–140.8 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, 2H, *J* = 8.5 Hz), 7.40 (d, 2H, *J* = 8.5 Hz), 3.64 (t, 2H, *J* = 6.7 Hz), 3.42 (t, 2H, *J* = 6.7 Hz), 2.06 (s, 3H), 2.00-1.83 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 168.9, 135.8, 131.1, 126.9, 125.5, 87.4, 79.1, 49.4, 46.1, 26.2, 24.2, 4.2.

HRMS (ESI) calcd for $C_{14}H_{16}NO^+$ $[M+H]^+$ 214.1226, found 214.1231.



1-(4-(Prop-1-yn-1-yl)phenyl)-1H-pyrazole (1u)

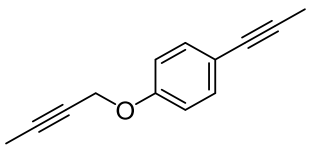
Following the general procedure B, the crude product was purified by flash chromatography on silica gel (4:1 petroleum ether/EtOAc) to afford **1u** as a white solid (0.75 g, 82% yield).

m.p. 80.2–81.6 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (d, 1H, *J* = 2.5 Hz), 7.72 (d, 1H, *J* = 1.5 Hz), 7.62 (d, 2H, *J* = 8.7 Hz), 7.46 (d, 2H, *J* = 8.7 Hz), 6.46 (dd, 1H, *J* = 2.5, 1.5 Hz), 2.06 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 141.1, 139.0, 132.5, 126.5, 122.0, 118.6, 107.7, 86.6, 78.9, 4.3.

HRMS (ESI) calcd for $C_{12}H_{11}N_2^+$ $[M+H]^+$ 183.0917, found 183.0917.



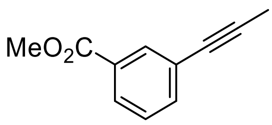
1-(But-2-yn-1-yloxy)-4-(prop-1-yn-1-yl)benzene (1v)

m.p. 49.1–51.2 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (d, 2H, *J* = 8.9 Hz), 6.87 (d, 2H, *J* = 8.9 Hz), 4.63 (q, 2H, *J* = 2.3 Hz), 2.03 (s, 3H), 1.86 (t, 3H, *J* = 2.3 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 157.1, 132.6, 116.7, 114.6, 84.2, 83.9, 79.3, 73.7, 56.3, 4.2, 3.6.

HRMS (ESI) calcd for $C_{13}H_{13}O^+$ $[M+H]^+$ 185.0961, found 185.0963.



Methyl 3-(Prop-1-yn-1-yl)benzoate (1y)

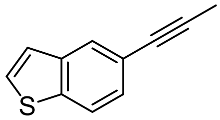
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **1y** as a white solid (0.72 g, 83% yield).

m.p. 27.9–30.1 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, 1H, *J* = 1.4, 1.4 Hz), 7.93 (ddd, 1H, *J* = 7.8, 1.4, 1.4 Hz), 7.56 (ddd, 1H, *J* = 7.7, 1.4, 1.4 Hz), 7.36 (dd, 1H, *J* = 7.8, 7.7 Hz), 3.91 (s, 3H), 2.06 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 135.6, 132.5, 130.2, 128.4, 128.2, 124.4, 86.9, 78.7, 52.1, 4.2.

HRMS (ESI) calcd for $C_{11}H_{11}O_2^+$ [M+H]$^+$ 175.0754, found 175.0755.



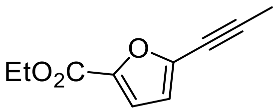
5-(Prop-1-yn-1-yl)benzo[b]thiophene (1ac)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **1ac** as colorless liquid (0.72 g, 84% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (dd, 1H, *J* = 1.5, 0.6 Hz), 7.75 (d, 1H, *J* = 8.4 Hz), 7.40 (d, 1H, *J* = 5.6 Hz), 7.34 (dd, 1H, *J* = 8.4, 1.5 Hz), 7.24 (dd, 1H, *J* = 5.6, 0.6 Hz), 2.06 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 139.4, 138.8, 127.3, 127.0, 126.5, 123.4, 122.1, 119.8, 85.2, 79.9, 4.2.

HRMS (EI) calcd for $C_{11}H_7S^+$ [M]$^+$ 172.0341, found 171.0336.



Ethyl 5-(Prop-1-yn-1-yl)furan-2-carboxylate (1af)

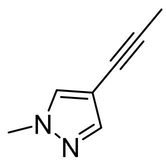
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford **1af** as a white solid (0.56 g, 63% yield).

m.p. 31.8–32.6 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.12 (d, 1H, *J* = 3.5 Hz), 6.51 (d, 1H, *J* = 3.5 Hz), 4.36 (q, 2H, *J* = 7.1 Hz), 2.09 (s, 3H), 1.37 (t, 3H, *J* = 7.1 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 158.0, 143.8, 140.5, 118.4, 115.0, 92.6, 69.6, 60.9, 14.2, 4.4.

HRMS (ESI) calcd for $C_{10}H_{10}NaO_3^+$ [M+Na]$^+$ 201.0522, found 201.0524.



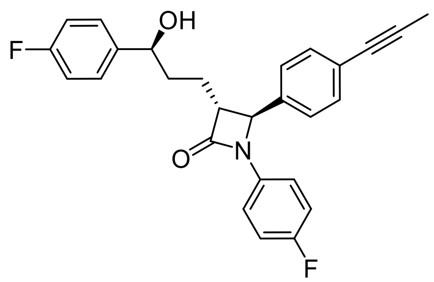
Methyl-4-(prop-1-yn-1-yl)-1H-pyrazole (1ag)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **1ag** as colorless liquid (0.44 g, 73% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.40 (s, 1H), 3.85 (s, 3H), 2.00 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 141.4, 131.9, 103.6, 85.7, 70.3, 38.7, 4.0.

HRMS (ESI) calcd for $C_7H_9N_2^+$ $[M+H]^+$ 121.0760, found 121.0762.



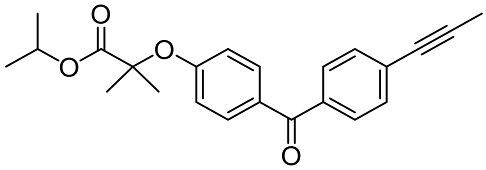
(3*R*,4*S*)-1-(4-Fluorophenyl)-3-((*S*)-3-(4-fluorophenyl)-3-hydroxypropyl)-4-(4-(prop-1-yn-1-yl)phenyl)azetidin-2-one (1as)

m.p. 56.7–58.2 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (d, 2H, *J* = 8.3 Hz), 7.33-7.16 (m, 6H), 7.07-6.88 (m, 4H), 4.76-4.68 (m, 1H), 4.60 (d, 1H, *J* = 2.4 Hz), 3.13-3.03 (m, 1H), 2.21 (brd, 1H, *J* = 3.2 Hz), 2.05 (s, 3H), 2.06-1.82 (m, 4H).

^{13}C NMR (101 MHz, acetone-d_6) δ 167.8, 162.6 (d, *J* = 242.4 Hz), 159.9 (d, *J* = 240.6 Hz), 142.8 (d, *J* = 2.9 Hz), 138.8, 135.3 (d, *J* = 2.6 Hz), 132.8, 128.4 (d, *J* = 7.9 Hz), 127.1, 125.0, 119.1 (d, *J* = 7.9 Hz), 116.4 (d, *J* = 22.8 Hz), 115.5 (d, *J* = 21.3 Hz), 87.3, 79.9, 72.9, 61.3, 61.1, 37.6, 25.8, 4.0.

HRMS (ESI) calcd for $C_{27}H_{23}F_2KNO_2^+$ $[M+K]^+$ 470.1328, found 470.1318.

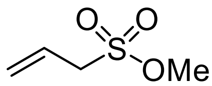


Isopropyl 2-Methyl-2-(4-(4-(prop-1-yn-1-yl)benzoyl)phenoxy)propanoate (1au)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (d, 2H, *J* = 8.8 Hz), 7.68 (d, 2H, *J* = 8.2 Hz), 7.47 (d, 2H, *J* = 8.2 Hz), 6.86 (d, 2H, *J* = 8.8 Hz), 5.09 (hept, 1H, *J* = 6.3 Hz), 2.09 (s, 3H), 1.66 (s, 6H), 1.20 (d, 6H, *J* = 6.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.5, 172.9, 159.4, 136.6, 131.8, 131.1, 130.3, 129.5, 127.9, 117.1, 89.0, 79.23, 79.20, 69.1, 25.2, 21.4, 4.3.

HRMS (ESI) calcd for $C_{23}H_{25}O_4^+$ $[M+H]^+$ 365.1747, found 365.1739.

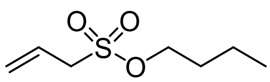


Methyl Prop-2-ene-1-sulfonate (2a)

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.91 (ddt, 1H, *J* = 17.2, 9.8, 7.2 Hz), 5.55-5.49 (m, 1H), 5.48-5.43 (m, 1H), 3.92 (s, 3H), 3.86 (d, 2H, *J* = 7.2 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 124.4, 124.2, 56.2, 54.0.

HRMS (ESI) calcd for $C_3H_5O_3S^-$ $[M-CH_3]^-$ 120.9965, found 120.9964.



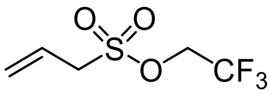
Butyl Prop-2-ene-1-sulfonate (2b)

Following the general procedure D, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **2b** as colorless liquid (0.64 g, 73% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.91 (ddt, 1H, *J* = 17.4, 10.3, 7.2 Hz), 5.51-5.42 (m, 2H), 4.25 (t, 2H, *J* = 6.5 Hz), 3.83 (d, 2H, *J* = 7.2 Hz), 1.78-1.67 (m, 2H), 1.50-1.38 (m, 2H), 0.95 (t, 3H, *J* = 7.4 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 124.5, 124.2, 70.5, 54.6, 31.0, 18.5, 13.3.

HRMS (ESI) calcd for $C_7H_{15}O_3S^+$ $[M+H]^+$ 179.0736, found 179.0738.



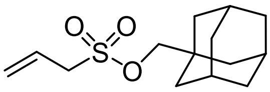
2,2,2-Trifluoroethyl Prop-2-ene-1-sulfonate (2d)

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.90 (ddt, 1H, J = 17.3, 10.2, 7.2 Hz), 5.60-5.47 (m, 2H), 4.52 (q, 2H, J = 7.9 Hz), 3.96 (d, 2H, J = 7.2 Hz).

^{13}C NMR (75 MHz, $CDCl_3$) δ 125.7, 123.2, 121.8 (q, J = 275.8 Hz), 64.6 (q, J = 38.5 Hz), 55.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -74.0 (t, J = 7.9 Hz).

HRMS (EI) calcd for $C_5H_7F_3O_3S^+$ $[M]^+$ 204.0063, found 204.0053.



((3*r*,5*r*,7*r*)-Adamantan-1-yl)methyl prop-2-ene-1-sulfonate (2e)

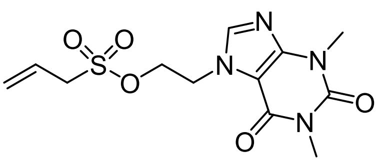
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **2d** as a white solid (0.78 g, 57% yield).

m.p. 30.2–31.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.91 (ddt, 1H, J = 17.5, 10.3, 7.2 Hz), 5.50-5.41 (m, 2H), 3.83 (d, 2H, J = 7.2Hz), 3.79 (s, 2H), 2.06-1.97 (m, 3H), 1.80-1.58 (m, 6H), 1.59-1.53 (m, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 124.5, 124.3, 79.9, 54.4, 38.6, 36.6, 33.5, 27.7.

HRMS (ESI) calcd for $C_{14}H_{22}NaO_3S^+$ $[M+Na]^+$ 293.1182, found 293.1180.



2-(1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7H-purin-7-yl)ethylprop-2-en e-1-sulfonate (2f)

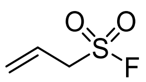
Following the general procedure D, the crude product was purified by flash chromatography on silica gel (1:2 petroleum ether/EtOAc) to afford **2f** as a white solid (0.67 g, 41% yield).

m.p. 131.0–132.1 °C.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (s, 1H), 5.81 (ddt, 1H, *J* = 17.3, 10.1, 7.2 Hz), 5.49-5.35 (m, 2H), 4.62 (s, 4H), 3.81 (d, 2H, *J* = 7.2 Hz), 3.61 (s, 3H), 3.42 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 155.2, 151.4, 149.1, 142.1, 124.9, 123.7, 106.2, 68.1, 54.9, 46.5, 29.7, 27.9.

HRMS (ESI) calcd for $C_{12}H_{16}N_4NaO_5S^+$ $[M+Na]^+$ 351.0734, found 351.0733.



Prop-2-ene-1-sulfonyl fluoride (4)

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.92 (ddt, 1H, *J* = 17.3, 10.2, 7.2 Hz), 5.65-5.55 (m, 2H), 4.13-4.04 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 126.6, 122.0, 54.8 (d, *J* = 18.1 Hz).

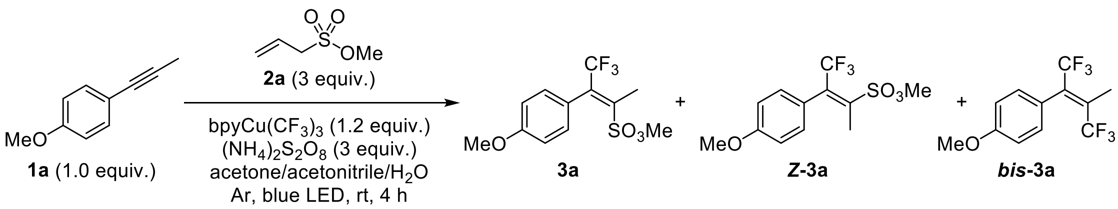
^{19}F NMR (282 MHz, $CDCl_3$) δ 52.0.

HRMS (ESI) calcd for $C_3H_6FO_2S^+$ $[M+H]^+$ 125.0067, found 125.0059.

III. Screening of reaction conditions

Standard conditions: To a screw-cap test tube, which was equipped with a stir bar and charged with bpyCu(CF_3)$_3$ (102.4 mg, 0.24 mmol, 1.2 equiv.) and $(NH_4)_2S_2O_8$ (136.8 mg, 0.60 mmol, 3.0 equiv.), was evacuated and backfilled with argon. 1-Methoxy-4-(prop-1-yn-1-yl)benzene **1a** (29.2 mg, 0.20 mmol, 1.0 equiv.), methyl prop-2-ene-1-sulfonate **2a** (81.6 mg, 0.60 mmol, 3.0 equiv.), acetone (2 mL), CH_3CN (2 mL), and H_2O (80 μL) were added through septum via syringe. The reaction mixture was stirred at room temperature under blue LEDs (λ_{max} = 460 nm) irradiation for 4 h. (Trifluoromethoxy)benzene was added as an internal standard and the yields were determined by ^{19}F NMR spectroscopy.

Table S3. Screening of Reaction Conditions



Entry	Conditions	^{19}F NMR yield (%)			Ratio of 3a/Z-3a
		3a	*Z*-3a	*bis*-3a	
1	Standard conditions	77	6	15	13 : 1
2	acetone (4 mL) as solvent	55	6	26	9 : 1
3	acetone/H_2O (2 mL/2 mL) as solvent	7	ND	5	-
4	acetone/H_2O (3.2 mL/0.8 mL) as solvent	52	5	20	10: 1
5	acetone/H_2O (4 mL/80 uL) as solvent	68	5	23	14 : 1
6	CH_3CN (4 mL) as solvent	57	12	17	5 : 1
7	CH_3CN/H_2O (4 mL/80 uL) as solvent	69	6	10	12 : 1
8	THF/H_2O (4 mL/80 uL) as solvent	ND	ND	trace	-
9	CH_2Cl_2/H_2O (4 mL/80 uL) as solvent	43	5	19	9 : 1
10	EtOAc/H_2O (4 mL/80 uL) as solvent	29	ND	30	-
11	acetone/CH_3CN (2 mL/2 mL) as solvent	64	8	22	8 : 1
12	$Na_2S_2O_8$ instead of $(NH_4)_2S_2O_8$	52	5	16	10 : 1
13	$K_2S_2O_8$ instead of $(NH_4)_2S_2O_8$	46	4	20	11 : 1
14	without $(NH_4)_2S_2O_8$	4	ND	24	-
15	365 nm instead of blue LED	64	5	13	13 : 1
16	254 nm instead of blue LED	40	4	10	10 : 1
17	performed in dark	ND	ND	ND	-
18	2 equiv. of **2a** used instead	66	7	26	9 : 1
19	AcOH (4 equiv.)	61	7	24	9 : 1
20	TFA (4 equiv.)	63	5	12	13 : 1
21	CF_3SO_3H (4 equiv.)	18	ND	trace	-
22	KF (4 equiv.)	50	4	22	13 : 1
23	NaOAc (4 equiv.)	33	trace	22	-
24	Cs_2CO_3 (4 equiv.)	31	trace	30	-
25	K_3PO_4 (4 equiv.)	ND	ND	26	-
26	pyridine (4 equiv.)	4	ND	7	-
27	Et_3N (4 equiv.)	28	trace	26	-
28	$FeCl_3$ (4 equiv.)	9	ND	4	-
29	$AlCl_3$ (4 equiv.)	10	trace	5	-

IV. Synthesis and characterization of products

4.1 General procedures for the synthesis of products

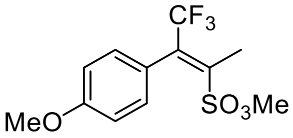
General procedure A: To a screw-cap test tube, which was equipped with a stir bar and charged with alkyne (0.20 mmol, 1.0 equiv., if it is a solid), bpyCu(CF_3)$_3$ (102.4 mg, 0.24 mmol, 1.2 equiv.), and $(NH_4)_2S_2O_8$ (136.8 mg, 0.60 mmol, 3.0 equiv.), was evacuated and backfilled with argon. Alkyne (0.20 mmol, 1.0 equiv., if it is liquid), alkyl allylsulfonate (0.60 mmol, 3 equiv.), acetone (2 mL), CH_3CN (2 mL), and H_2O (80 μL) were added through septum via syringe. The reaction mixture was stirred at room temperature under blue LEDs (λ_{max} = 460 nm) irradiation for 4 h. The solvent was removed on rotovap and the crude product was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

General procedure B: To a screw-cap test tube, which was equipped with a stir bar and charged with alkyne (0.20 mmol, 1.0 equiv., if it is a solid), bpyCu(CF_3)$_3$ (128.0 mg, 0.30 mmol, 1.5 equiv.), and $(NH_4)_2S_2O_8$ (136.8 mg, 0.60 mmol, 3.0 equiv.), was evacuated and backfilled with argon. Alkyne (0.20 mmol, 1.0 equiv., if it is liquid), alkyl allylsulfonate (0.60 mmol, 3 equiv.), acetone (2 mL), CH_3CN (2 mL), and H_2O (80 μL) were added through septum via syringe. The reaction mixture was stirred at room temperature under blue LEDs (λ_{max} = 460 nm) irradiation for 8 h. The solvent was removed on rotovap and the crude product was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

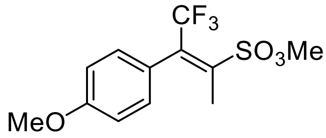
General procedure C: To a screw-cap test tube, which was equipped with a stir bar and charged with alkyne (0.20 mmol, 1.0 equiv., if it is a solid), bpyCu(CF_3)$_3$ (128.0 mg, 0.30 mmol, 1.5 equiv.), and $(NH_4)_2S_2O_8$ (136.8 mg, 0.60 mmol, 3.0 equiv.), was evacuated and backfilled with argon. Alkyne (0.20 mmol, 1.0 equiv., if it is liquid), allylsulfonyl fluoride (74.5 mg, 0.60 mmol, 3 equiv.), acetone (2 mL), CH_3CN (2 mL), and H_2O (80 μL) were added through septum via syringe. The reaction mixture was stirred at room temperature under 365 nm (5 W) irradiation for 4 h. The solvent was removed on rotovap and the crude product was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

General procedure D: To a screw-cap test tube, which was equipped with a stir bar and charged with alkyne (0.20 mmol, 1.0 equiv., if it is a solid), bpyCu$(CF_3)_3$ (128.0 mg, 0.30 mmol, 1.5 equiv.), and $(NH_4)_2S_2O_8$ (136.8 mg, 0.60 mmol, 3.0 equiv.), was evacuated and backfilled with argon. Alkyne (0.20 mmol, 1.0 equiv., if it is liquid), allylsulfonyl fluoride (99.3 mg, 0.80 mmol, 4 equiv.), acetone (2 mL), CH_3CN (2 mL), and H_2O (80 μL) were added through septum via syringe. The reaction mixture was stirred at room temperature under 365 nm (5 W) irradiation for 8 h. The solvent was removed on rotovap and the crude product was purified by flash chromatography on silica gel (petroleum ether/EtOAc) to afford the title product.

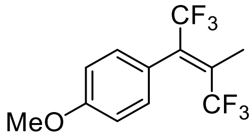
4.2 Characterization of products



3a



***Z*-3a**



***bis*-3a**

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (petroleum ether to 60:1 petroleum ether/EtOAc) to sequentially afford ***bis*-3a (**colorless liquid, 5.2 mg, 9% yield**)**, **3a** (white solid, 45.1 mg, 73% yield), and ***Z*-3a (**colorless liquid, 1.3 mg, 2% yield).

Methyl (*E*)-4,4,4-Trifluoro-3-(4-methoxyphenyl)but-2-ene-2-sulfonate (3a)

m.p. 82.3–84.2 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.17 (d, 2H, *J* = 8.8 Hz), 6.92 (d, 2H, *J* = 8.8 Hz), 3.83 (s, 3H), 3.66 (s, 3H), 2.44 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 142.3 (q, *J* = 2.4 Hz), 139.1 (q, *J* = 31.3 Hz), 130.4, 123.3 (q, *J* = 1.2 Hz), 122.4 (q, *J* = 278.7 Hz), 113.6, 56.1, 55.2, 16.8 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.1 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_4S^+$ $[M+Na]^+$ 333.0379, found 333.0378.

Methyl (*Z*)-4,4,4-Trifluoro-3-(4-methoxyphenyl)but-2-ene-2-sulfonate (*Z*-3a)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.11 (d, 2H, *J* = 8.6 Hz), 6.97 (d, 2H, *J* = 8.6 Hz), 3.98 (s, 3H), 3.85 (s, 3H), 2.01 (q, 3H, *J* = 2.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 141.5 (q, *J* = 2.6 Hz), 138.5 (q, *J* = 34.5 Hz), 129.6, 125.1 (q, *J* = 2.1 Hz), 120.8 (q, *J* = 276.0 Hz), 114.4, 56.6, 55.3, 19.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -56.4 (q, *J* = 2.1 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_4S^+$ $[M+Na]^+$ 333.0379, found 333.0377.

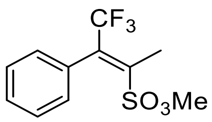
(*E*)-1-(1,1,1,4,4,4-Hexafluoro-3-methylbut-2-en-2-yl)-4-methoxybenzene (*bis*-3a)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.08 (d, 2H, *J* = 8.9 Hz), 6.89 (d, 2 H, *J* = 8.9 Hz), 3.82 (s, 3H), 2.18 (q, 3H, *J* = 2.5 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 136.0 (qq, *J* = 31.3, 3.2 Hz), 134.4 (qq, *J* = 29.2, 2.6 Hz), 130.2 (q, *J* = 1.8 Hz), 124.2 (q, *J* = 1.5 Hz), 123.0 (q, *J* = 276.6 Hz), 122.8 (q, *J* = 276.6 Hz), 113.5, 55.2, 14.3 (qq, *J* = 5.4, 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.0 (m), -61.2 (m).

HRMS (EI) calcd for $C_{12}H_{10}F_6O^+$ $[M]^+$ 284.0630, found 284.0626.



Methyl (*E*)-4,4,4-Trifluoro-3-(p-tolyl)but-2-ene-2-sulfonate (3b)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3b** as a white solid (41.5 mg, 74% yield).

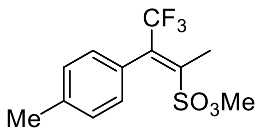
m.p. 66.1–67.8 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46-7.37 (m, 3H), 7.26-7.21 (m, 2H), 3.65 (s, 3H), 2.46 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4 (q, *J* = 2.4 Hz), 139.2 (q, *J* = 31.3 Hz), 131.4 (q, *J* = 1.2 Hz), 129.4, 128.8, 128.1, 122.3 (q, *J* = 278.7 Hz), 56.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{11}H_{11}F_3NaO_3S^+$ $[M+Na]^+$ 303.0273, found 303.0273.



Methyl (*E*)-4,4,4-Trifluoro-3-(p-tolyl)but-2-ene-2-sulfonate (3c)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3c** as a white solid (38.1mg, 65% yield).

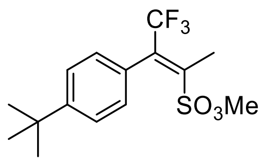
m.p. 64.2–66.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.22 (d, 2H, *J* = 8.1 Hz), 7.12 (d, 2H, *J* = 8.1 Hz), 3.66 (s, 3H), 2.44 (q, 3H, *J* = 2.4 Hz), 2.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.2 (q, *J* = 2.4 Hz), 139.5, 139.4 (q, *J* = 31.2 Hz), 128.8, 128.7, 128.4 (q, *J* = 1.2 Hz), 122.4 (q, *J* = 278.7 Hz), 56.1, 21.4, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.9 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_3S^+$ $[M+Na]^+$ 317.0430, found 317.0429.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-(tert-butyl)phenyl)but-2-ene-2-sulfonate (3d)

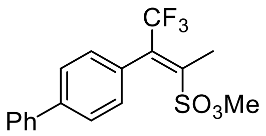
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3d** as colorless oil (43.1mg, 64% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (d, 2H, *J* = 8.4 Hz), 7.16 (d, 2H, *J* = 8.4 Hz), 3.61 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.5, 142.2 (q, *J* = 2.4 Hz), 139.3 (q, *J* = 31.3 Hz), 128.6, 128.3 (q, *J* = 1.2 Hz), 125.0, 122.4 (q, *J* = 278.7 Hz), 56.1, 34.7, 31.2, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.9 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{15}H_{19}F_3NaO_3S^+$ $[M+Na]^+$ 359.0899, found 359.0900.



Methyl (*E*)-4,4,4-Trifluoro-3-([1,1'-biphenyl]-4-yl)but-2-ene-2-sulfonate (3e)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3e** as a white solid (51.9 mg, 73% yield).

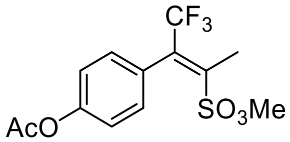
m.p. 110.1–111.8 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67-7.59 (m, 4H), 7.50-7.34 (m, 3H), 7.31 (d, 2H, *J* = 8.2 Hz), 3.68 (s, 3H), 2.48 (q, 3H, *J* = 2.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (q, *J* = 2.2 Hz), 142.2, 140.0, 139.0 (q, *J* = 31.2 Hz), 130.2, 129.3, 128.8, 127.8, 127.1, 126.7, 122.4 (q, *J* = 278.7 Hz), 56.1, 16.8 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.7 (q, *J* = 2.3 Hz).

HRMS (ESI) calcd for $C_{17}H_{15}F_3NaO_3S^+$ $[M+Na]^+$ 379.0586, found 379.0579.



(*E*)-4-(1,1,1-Trifluoro-3-(methoxysulfonyl)but-2-en-2-yl)phenyl acetate (3f)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **3f** as a white solid (48.5 mg, 72% yield).

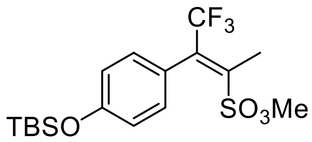
m.p. 63.4–65.0 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26 (d, 2H, *J* = 8.6 Hz), 7.16 (d, 2H, *J* = 8.6 Hz), 3.63 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz), 2.31 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 151.5, 143.2 (q, *J* = 2.3 Hz), 138.2 (q, *J* = 31.5 Hz), 130.2, 128.7 (q, *J* = 1.2 Hz), 122.2 (q, *J* = 278.7 Hz), 121.4, 56.1, 21.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.7 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{13}H_{13}F_3NaO_5S^+$ [M+Na]$^+$ 361.0328, found 361.0324.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-((tert-butyldimethylsilyl)oxy)phenyl)but-2-ene-2-sulfonate (3g)

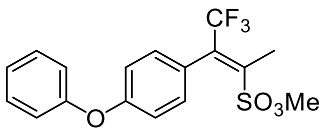
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3g** as colorless oil (49.1 mg, 60% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.10 (d, 2H, *J* = 8.5 Hz), 6.85 (d, 2H, *J* = 8.5 Hz), 3.62 (s, 3H), 2.43 (q, 3H, *J* = 2.4 Hz), 0.98 (s, 9H), 0.21 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8, 142.3 (q, *J* = 2.4 Hz), 139.0 (q, *J* = 31.3 Hz), 130.4, 123.9 (q, *J* = 1.2 Hz), 122.4 (q, *J* = 278.7 Hz), 119.7, 56.0, 25.6, 18.2, 16.7 (q, *J* = 2.8 Hz), -4.4.

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.0 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{17}H_{25}F_3NaO_4SSi^+$ [M+Na]$^+$ 433.1087, found 433.1081.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-phenoxyphenyl)but-2-ene-2-sulfonate (3h)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3h** as a white solid (48.3 mg, 65% yield).

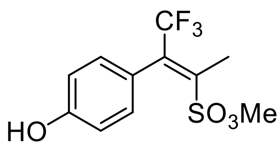
m.p. 70.0–71.6 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (t, 2H, *J* = 7.9 Hz), 7.18 (d, 2H, *J* = 8.5 Hz), 7.16 (t, 1H, *J* = 7.9 Hz), 7.06 (d, 2H, *J* = 7.9 Hz), 7.00 (d, 2H, *J* = 8.5 Hz), 3.70 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 156.1, 142.7 (q, *J* = 2.3 Hz), 138.8 (q, *J* = 31.3 Hz), 130.5, 129.9, 125.5 (q, *J* = 1.1 Hz), 124.0, 122.4 (q, *J* = 278.7 Hz), 119.7, 117.6, 56.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.0 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{17}H_{15}F_3NaO_4S^+$ $[M+Na]^+$ 395.0535, found 395.0530.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-hydroxyphenyl)but-2-ene-2-sulfonate (3i)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **3i** as a white solid (39.8 mg, 67% yield).

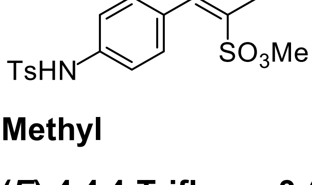
m.p. 134.8–136.2 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.12 (d, 2H, *J* = 8.7 Hz), 6.85 (d, 2H, *J* = 8.7 Hz), 5.20 (s, 1H), 3.67 (s, 3H), 2.44 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, CD_3OD) δ 159.8, 143.6 (q, *J* = 2.3 Hz), 140.4 (q, *J* = 31.1 Hz), 131.7, 124.1 (q, *J* = 277.8 Hz), 123.5, 115.9, 57.4, 17.0 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.1 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{11}H_{11}F_3NaO_4S^+$ $[M+Na]^+$ 319.0222, found 319.0219.



Methyl

(*E*)-4,4,4-Trifluoro-3-(4-((4-methylphenyl)sulfonamido)phenyl)but-2-ene-2-sulfonate (3j)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (3:1 petroleum ether/EtOAc) to afford **3j** as a white solid (57.4 mg, 64% yield).

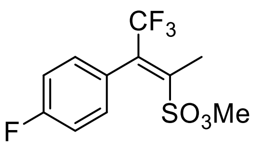
m.p. 120.5–122.4 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, 2H, *J* = 8.3 Hz), 7.23 (d, 2H, *J* = 8.3 Hz), 7.14-7.06 (m, 4H), 6.56 (brs, 1H), 3.61 (s, 3H), 2.42 (q, 3H, *J* = 2.4 Hz), 2.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.1, 143.0 (q, *J* = 2.3 Hz), 138.3 (q, *J* = 31.5 Hz), 137.9, 135.8, 130.0, 129.7, 128.0 (q, *J* = 1.2 Hz), 127.2, 122.2 (q, *J* = 278.7 Hz), 120.6, 56.1, 21.5, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.9 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{18}H_{18}F_3NNaO_5S_2^+$ $[M+Na]^+$ 472.0471, found 472.0468.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-fluorophenyl)but-2-ene-2-sulfonate (3k)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3k** as a white solid (37.8 mg, 63% yield).

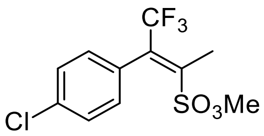
m.p. 65.3–66.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26-7.19 (m, 2H), 7.15-7.07 (m, 2H), 3.69 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.3 (d, *J* = 249.8 Hz), 143.2 (q, *J* = 2.3 Hz), 138.3 (q, *J* = 31.5 Hz), 130.9 (d, *J* = 8.6 Hz), 127.2 (m), 122.2 (q, *J* = 278.7 Hz), 115.4 (d, *J* = 22.0 Hz), 56.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.9 (q, *J* = 2.4 Hz), -110.9 (tt, *J* = 8.2, 5.2 Hz).

HRMS (ESI) calcd for $C_{11}H_{10}F_4NaO_3S^+$ $[M+Na]^+$ 321.0179, found 321.0179.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-chlorophenyl)but-2-ene-2-sulfonate (3l)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3l** as a white solid (47.7 mg, 76% yield).

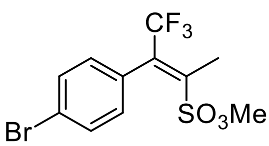
m.p. 68.3–69.9 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (d, 2H, *J* = 8.4 Hz), 7.17 (d, 2H, *J* = 8.4 Hz), 3.70 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2 (q, *J* = 2.4 Hz), 138.1 (q, *J* = 31.5 Hz), 135.8, 130.2, 129.7 (q, *J* = 1.1 Hz), 128.5, 122.2 (q, *J* = 278.7 Hz), 56.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{11}H_{10}ClF_3NaO_3S^+$ $[M+Na]^+$ 336.9883, found 336.9886.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-bromophenyl)but-2-ene-2-sulfonate (3m)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3m** as a white solid (51.5 mg, 72% yield).

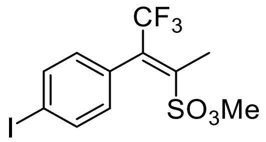
m.p. 83.7–85.2 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, 2H, *J* = 8.4 Hz), 7.11 (d, 2H, *J* = 8.4 Hz), 3.70 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1 (q, *J* = 2.3 Hz), 138.1 (q, *J* = 31.5 Hz), 131.4, 130.5, 130.2 (q, *J* = 1.1 Hz), 124.0, 122.1 (q, *J* = 278.7 Hz), 56.2, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (EI) calcd for $C_{11}H_{10}BrF_3O_3S^+$ $[M]^+$ 357.9481, found 357.9500.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-iodophenyl)but-2-ene-2-sulfonate (3n)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3n** as a white solid (54.7 mg, 67% yield).

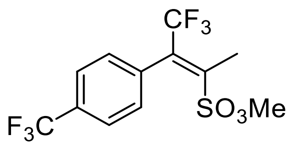
m.p. 106.5–108.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, 2H, *J* = 8.4 Hz), 6.98 (d, 2H, *J* = 8.4 Hz), 3.70 (s, 3H), 2.44 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1 (q, *J* = 2.3 Hz), 138.2 (q, *J* = 31.5 Hz), 137.3, 130.9 (q, *J* = 1.3 Hz), 130.5, 122.0 (q, *J* = 278.7 Hz), 95.8, 56.2, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{11}H_{10}F_3INaO_3S^+$ $[M+Na]^+$ 428.9240, found 428.9242.



Methyl

(*E*)-4,4,4-Trifluoro-3-(4-trifluoromethylphenyl)but-2-ene-2-sulfonate (3o)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3o** as a white solid (40.6 mg, 58% yield).

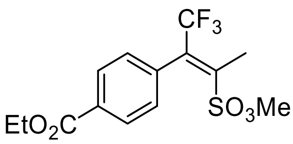
m.p. 61.7–63.0 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (d, 2H, *J* = 8.2 Hz), 7.37 (d, 2H, *J* = 8.2 Hz), 3.72 (s, 3H), 2.48 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5 (q, *J* = 2.4 Hz), 137.9 (q, *J* = 31.8 Hz), 135.1 (m), 131.5 (q, *J* = 32.8 Hz), 129.4, 125.2 (q, *J* = 3.8 Hz), 123.7 (q, *J* = 272.5 Hz), 122.1 (q, *J* = 278.7 Hz), 56.2, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.6 (q, *J* = 2.4 Hz), -62.9.

HRMS (ESI) calcd for $C_{12}H_{10}F_6NaO_3S^+$ $[M+Na]^+$ 371.0147, found 371.0138.



Ethyl (*E*)-4-(1,1,1-Trifluoro-3-(methoxysulfonyl)but-2-en-2-yl)benzoate (3p)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (25:1 petroleum ether/EtOAc) to afford **3p** as a white solid (44.4 mg, 63% yield).

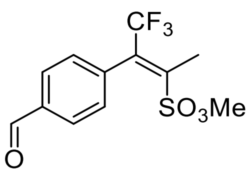
m.p. 79.2–80.6 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (d, 2H, *J* = 8.3 Hz), 7.32 (d, 2H, *J* = 8.3 Hz), 4.39 (q, 2H, *J* = 7.2 Hz), 3.69 (s, 3H), 2.47 (q, 3H, *J* = 2.4 Hz), 1.40 (t, 3H, *J* = 7.2 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 143.1 (q, *J* = 2.4 Hz), 138.4 (q, *J* = 31.2 Hz), 135.9 (q, *J* = 1.2 Hz), 131.4, 129.3, 128.9, 122.1 (q, *J* = 278.7 Hz), 61.2, 56.1, 16.7 (q, *J* = 2.8 Hz), 14.3.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.6 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{14}H_{15}F_3NaO_5S^+$ $[M+Na]^+$ 375.0484, found 375.0481.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-formylphenyl)but-2-ene-2-sulfonate (3q)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (25:1 petroleum ether/EtOAc) to afford **3q** as a white solid (32.6 mg, 53% yield).

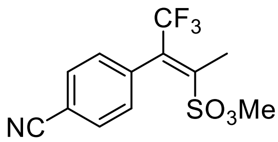
m.p. 94.5–95.9 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.06 (s, 1H), 7.94 (d, 2H, *J* = 8.2 Hz), 7.42 (d, 2H, *J* = 8.2 Hz), 3.73 (s, 3H), 2.48 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.4, 143.4 (q, *J* = 2.3 Hz), 138.0 (q, *J* = 31.2 Hz), 137.4 (q, *J* = 1.2 Hz), 136.7, 129.6, 129.3, 122.0 (q, *J* = 278.7 Hz), 56.2, 16.6 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.5 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{12}F_3O_4S^+$ $[M+H]^+$ 309.0403, found 309.0402.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-cyanophenyl)but-2-ene-2-sulfonate (3r)

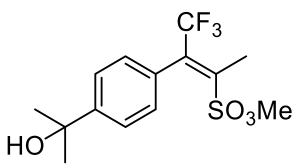
Following the general procedure B, the crude product was purified by flash chromatography on silica gel (25:1 petroleum ether/EtOAc) to afford **3r** as colorless oil (31.6 mg, 52% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71 (d, 2H, *J* = 8.4 Hz), 7.36 (d, 2H, *J* = 8.4 Hz), 3.75 (s, 3H), 2.48 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9 (q, *J* = 2.4 Hz), 137.3 (q, *J* = 32.1 Hz), 136.1 (q, *J* = 1.1 Hz), 131.9, 129.7, 121.9 (q, *J* = 278.7 Hz), 118.0, 113.5, 56.3, 16.6 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.5 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{11}F_3NO_3S^+$ $[M+H]^+$ 306.0406, found 306.0407.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-(2-hydroxypropan-2-yl)phenyl)but-2-ene-2-sulfonate (3s)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford **3s** as a white solid (50.8 mg, 75% yield).

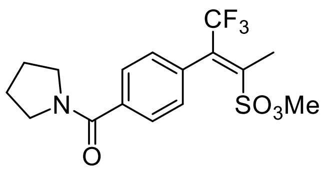
m.p. 78.0–79.5 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (d, 2H, *J* = 8.4 Hz), 7.21 (d, 2H, *J* = 8.4 Hz), 3.65 (s, 3H), 2.45 (q, 3H, *J* = 2.4 Hz), 1.77 (brs, 1H), 1.60 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.5, 142.4 (q, *J* = 2.3 Hz), 139.2 (q, *J* = 31.2 Hz), 129.7 (q, *J* = 1.2 Hz), 128.7, 124.2, 122.3 (q, *J* = 278.7 Hz), 72.4, 56.1, 31.6, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{14}H_{17}F_3NaO_4S^+$ $[M+Na]^+$ 361.0692, found 361.0689.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-(pyrrolidine-1-carbonyl)phenyl)but-2-ene-2- sulfonate (3t)

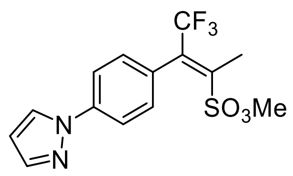
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (3:1 petroleum ether/EtOAc) to afford **3t** as colorless oil (53.3 mg, 71% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 (d, 2H, *J* = 8.2 Hz), 7.27 (d, 2H, *J* = 8.2 Hz), 3.68 (s, 3H), 3.65 (t, 2H, *J* = 6.8 Hz), 3.43 (t, 2H, *J* = 6.8 Hz), 2.46 (q, 3H, *J* = 2.5 Hz), 2.01-1.92 (m, 2H), 1.92-1.83 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 142.9 (q, *J* = 2.4 Hz), 138.5 (q, *J* = 31.5 Hz), 138.1, 132.8 (q, *J* = 1.2 Hz), 128.8, 126.9, 122.1 (q, *J* = 278.7 Hz), 56.2, 49.6, 46.2, 26.4, 24.4, 16.6 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.6 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{16}H_{19}F_3NO_4S^+$ $[M+H]^+$ 378.0981, found 378.0975.



Methyl

(*E*)-4,4,4-Trifluoro-3-(4-(1H-pyrazol-1-yl)phenyl)but-2-ene-2-sulfonate (3u)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (25:1 petroleum ether/EtOAc) to afford **3u** as a white solid (48.3 mg, 70% yield).

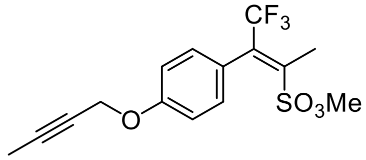
m.p. 101.5–103.7 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (dd, 1H, *J* = 2.5, 0.5 Hz), 7.77 (d, 2H, *J* = 8.7 Hz), 7.74 (dd, 1H, *J* = 1.9, 0.5 Hz), 7.34 (d, 2H, *J* = 8.7 Hz), 6.49 (dd, 1H, *J* = 2.5, 1.9 Hz), 3.70 (s, 3H), 2.47 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1 (q, *J* = 2.4 Hz), 141.5, 140.8, 138.3 (q, *J* = 31.6 Hz), 130.2, 129.1 (q, *J* = 1.2 Hz), 126.7, 122.2 (q, *J* = 278.7 Hz), 118.4, 108.1, 56.2, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{14}H_{13}F_3N_2NaO_3S^+$ $[M+Na]^+$ 369.0491, found 369.0487.



Methyl

(*E*)-4,4,4-Trifluoro-3-(4-(but-2-yn-1-yloxy)phenyl)but-2-ene-2-sulfonate (3v)

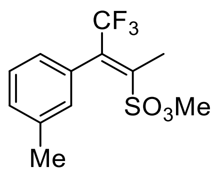
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3v** as colorless oil (36.8 mg, 53% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.17 (d, 2H, *J* = 8.7 Hz), 6.98 (d, 2H, *J* = 8.7 Hz), 4.67 (q, 2H, *J* = 2.4 Hz), 3.65 (s, 3H), 2.44 (q, 3H, *J* = 2.5 Hz), 1.87 (t, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 142.4 (q, *J* = 2.4 Hz), 138.9 (q, *J* = 31.3 Hz), 130.3, 123.8 (q, *J* = 1.2 Hz), 122.4 (q, *J* = 278.7 Hz), 114.4, 84.1, 73.6, 56.5, 56.1, 16.7 (q, *J* = 2.8 Hz), 3.6.

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.0 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{15}H_{15}F_3NaO_4S^+$ $[M+Na]^+$ 371.0535, found 371.0531.



Methyl (*E*)-4,4,4-Trifluoro-3-(m-tolyl)but-2-ene-2-sulfonate (3w)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3w** as a white solid (38.2 mg, 65% yield).

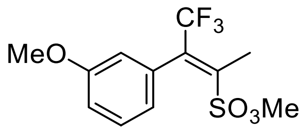
m.p. 58.3–59.6 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33-7.21 (m, 2H), 7.06-7.00 (m, 2H), 3.65 (s, 3H), 2.44 (q, 3H, *J* = 2.4 Hz), 2.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1 (q, *J* = 2.4 Hz), 139.4 (q, *J* = 31.2 Hz), 137.8, 131.3 (q, *J* = 1.2 Hz), 130.2, 129.3, 127.9, 125.9, 122.4 (q, *J* = 278.7 Hz), 56.0, 21.4, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_3S^+$ $[M+Na]^+$ 317.0430, found 317.0428.



Methyl (*E*)-4,4,4-Trifluoro-3-(3-methoxyphenyl)but-2-ene-2-sulfonate (3x)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3x** as a white solid (42.9 mg, 69% yield).

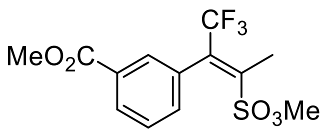
m.p. 50.2–51.4 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (dd, 1H, *J* = 8.4, 7.6 Hz), 6.96 (ddd, 1H, *J* = 8.4, 2.5, 0.8 Hz), 6.82 (d, 1H, *J* = 7.6 Hz), 6.79-6.75 (m, 1H), 3.82 (s, 3H), 3.67 (s, 3H), 2.45 (q, 3H, *J* = 2.5 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 142.4 (q, *J* = 2.2 Hz), 138.9 (q, *J* = 31.5 Hz), 132.5 (q, *J* = 1.2 Hz), 129.2, 122.3 (q, *J* = 278.7 Hz), 121.1, 114.80, 114.78, 56.1, 55.3, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_4S^+$ $[M+Na]^+$ 333.0379, found 333.0378.



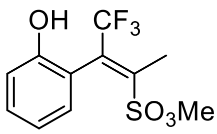
Methyl (*E*)-3-(1,1,1-Trifluoro-3-(methoxysulfonyl)but-2-en-2-yl)benzoate (3y)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **3y** as a white solid (47.1 mg, 70% yield).

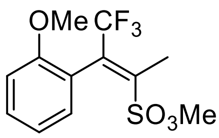
m.p. 52.2–53.4 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 (d, 1H, *J* = 7.5 Hz), 7.92 (s, 1H), 7.50 (dd, 1H, *J* = 7.9, 7.5 Hz), 7.43 (d, 1H, *J* = 7.9 Hz), 3.92 (s, 3H), 3.69 (s, 3H), 2.47 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 143.3 (q, *J* = 2.4 Hz), 138.3 (q, *J* = 31.5 Hz), 133.3, 131.7 (q, *J* = 1.2 Hz), 130.5, 130.2, 129.9, 128.3, 122.2 (q, *J* = 278.7 Hz), 56.1, 52.3, 16.7 (q, *J* = 2.8 Hz).
^{19}F NMR (282 MHz, $CDCl_3$) δ -58.7 (q, *J* = 2.4 Hz).
HRMS (ESI) calcd for $C_{13}H_{13}F_3NaO_5S^+$ $[M+Na]^+$ 361.0328, found 361.0326.



Methyl (*E*)-4,4,4-Trifluoro-3-(2-hydroxyphenyl)but-2-ene-2-sulfonate (3z)
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **3z** as colorless oil (40.5 mg, 68% yield).
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (ddd, 1H, *J* = 8.2, 8.0, 1.6 Hz), 7.11 (dd, 1H, *J* = 7.6, 1.6 Hz), 6.98 (ddd, 1H, *J* = 8.0, 7.6, 0.8 Hz), 6.81 (dd, 1H, *J* = 8.2, 0.8 Hz), 5.17 (brs, 1H), 3.73 (s, 3H), 2.46 (q, 3H, *J* = 2.3 Hz).
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 142.9 (q, *J* = 2.4 Hz), 137.2 (q, *J* = 32.7 Hz), 131.1, 130.5, 122.2 (q, *J* = 278.7 Hz), 120.5, 119.2 (q, *J* = 2.3 Hz), 115.5, 56.7, 16.6 (q, *J* = 2.5 Hz).
^{19}F NMR (282 MHz, $CDCl_3$) δ -59.9 (q, *J* = 2.3 Hz).
HRMS (ESI) calcd for $C_{11}H_{11}F_3NaO_4S^+$ $[M+Na]^+$ 319.0222, found 319.0220.



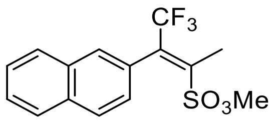
Methyl (*E*)-4,4,4-Trifluoro-3-(2-methoxyphenyl)but-2-ene-2-sulfonate (3aa)
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3aa** as colorless oil (26.5 mg, 43% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (ddd, 1H, *J* = 8.3, 7.5, 1.7 Hz), 7.13 (dd, 1H, *J* = 7.5, 1.7 Hz), 6.99 (ddd, 1H, *J* = 8.3, 7.5, 0.9 Hz), 6.93 (dd, 1H, *J* = 8.3, 0.9 Hz), 3.83 (s, 3H), 3.69 (s, 3H), 2.44 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.9, 142.2 (q, *J* = 2.4 Hz), 137.6 (q, *J* = 32.1 Hz), 131.1, 130.5, 122.1 (q, *J* = 278.7 Hz), 120.9 (q, *J* = 1.1 Hz), 120.3, 110.4, 56.4, 55.6, 16.5 (q, *J* = 2.5 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -60.2 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_4S^+$ $[M+Na]^+$ 333.0379, found 333.0378.



Methyl (*E*)-4,4,4-Trifluoro-3-(naphthalen-2-yl)but-2-ene-2-sulfonate (3ab)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3ab** as a white solid (35.6 mg, 54% yield).

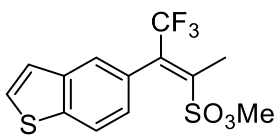
m.p. 90.2–91.7 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92-7.83 (m, 3H), 7.74 (d, 1H, *J* = 1.4 Hz), 7.58-7.49 (m, 2H), 7.31 (dd, 1H, *J* = 8.6, 1.4 Hz), 3.62 (s, 3H), 2.51 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.8 (q, *J* = 2.4 Hz), 139.2 (q, *J* = 31.5 Hz), 133.3, 132.5, 128.80 (q, *J* = 1.2 Hz), 128.76, 128.3, 127.8, 127.1, 126.7, 125.8, 122.5 (q, *J* = 278.7 Hz), 56.1, 16.8 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.6 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{15}H_{13}F_3NaO_3S^+$ $[M+Na]^+$ 353.0430, found 353.0429.



Methyl (*E*)-4,4,4-Trifluoro-3-(benzo[b]thiophen-5-yl)but-2-ene-2-sulfonate (3ac)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (25:1 petroleum ether/EtOAc) to afford **3ac** as a white solid (38.9 mg, 58% yield).

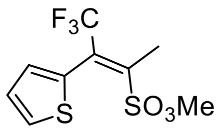
m.p. 101.2–102.9 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (d, 1H, *J* = 8.4 Hz), 7.71 (d, 1H, *J* = 1.1 Hz), 7.51 (d, 1H, *J* = 5.4 Hz), 7.36 (d, 1H, *J* = 5.4 Hz), 7.19 (dd, 1H, *J* = 8.4, 1.1 Hz), 3.64 (s, 3H), 2.49 (q, 3H, *J* = 2.4 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7 (q, *J* = 2.4 Hz), 140.7, 139.2 (q, *J* = 31.5 Hz), 139.1, 127.6, 127.3 (q, *J* = 1.2 Hz), 124.4, 124.2, 123.9, 122.4 (q, *J* = 278.7 Hz), 122.2, 56.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.7 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{13}H_{11}F_3NaO_3S_2^+$ $[M+Na]^+$ 358.9994, found 358.9993.



Methyl (*Z*)-4,4,4-Trifluoro-3-(thiophen-2-yl)but-2-ene-2-sulfonate (3ad)

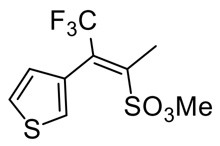
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3ad** as a colorless oil (30.2 mg, 53% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (dd, 1H, *J* = 5.0, 1.2 Hz), 7.12 (dd, 1H, *J* = 3.7, 1.2 Hz), 7.07 (dd, 1H, *J* = 5.0, 3.7 Hz), 3.74 (s, 3H), 2.46 (q, 3H, *J* = 2.5 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.7 (q, *J* = 2.1 Hz), 132.5 (q, *J* = 32.7 Hz), 131.3, 129.8 (q, *J* = 1.2 Hz), 129.1, 126.8, 121.7 (q, *J* = 278.7 Hz), 56.5, 17.2 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.8 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_9H_9F_3NaO_3S_2^+$ $[M+Na]^+$ 308.9837, found 308.9837.



Methyl (*E*)-4,4,4-Trifluoro-3-(thiophen-3-yl)but-2-ene-2-sulfonate (3ae)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (60:1 petroleum ether/EtOAc) to afford **3ae** as a white solid (33.7 mg, 59% yield).

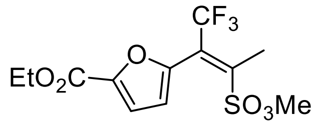
m.p. 53.1–54.3 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40-7.36 (m, 2H), 7.04-7.00 (m, 1H), 3.68 (s, 3H), 2.44 (q, 3H, *J* = 2.5 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4 (q, *J* = 2.4 Hz), 134.5 (q, *J* = 32.1 Hz), 130.0 (q, *J* = 1.2 Hz), 127.9, 127.4, 125.6, 122.1 (q, *J* = 278.7 Hz), 56.2, 16.9 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.6 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_9H_9F_3NaO_3S_2^+$ $[M+Na]^+$ 308.9837, found 308.9838.



Ethyl (*E*)-5-(1,1,1-Trifluoro-3-(methoxysulfonyl)but-2-en-2-yl)furan-2-carboxylate (3af)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford **3af** as a white solid (48.8 mg, 71% yield).

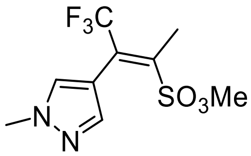
m.p. 36.9–38.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 (d, 1H, *J* = 3.6 Hz), 6.66 (d, 1H, *J* = 3.6 Hz), 4.36 (q, 2H, *J* = 7.2 Hz), 3.90 (s, 3H), 2.47 (q, 3H, *J* = 2.4 Hz), 1.37 (t, 3H, *J* = 7.2 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 148.2 (q, *J* = 2.0 Hz), 146.0, 144.7 (q, *J* = 1.5 Hz), 127.9 (q, *J* = 34.1 Hz), 121.4 (q, *J* = 278.7 Hz), 118.5, 115.6, 61.3, 57.5, 16.9 (q, *J* = 2.5 Hz), 14.2.

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.7 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_6S^+$ $[M+Na]^+$ 365.0277, found 365.0273.



Methyl (*E*)-4,4,4-Trifluoro-3-(1-methyl-1H-pyrazol-4-yl)but-2-ene-2-sulfonate (3ag)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (3:1 petroleum ether/EtOAc) to afford **3ag** as a white solid (35.2 mg, 62% yield).

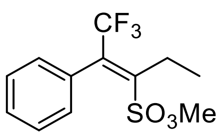
m.p. 173.1 ºC (dec.)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.50 (s, 1H), 3.93 (s, 3H), 3.70 (s, 3H), 2.41 (q, 3H, *J* = 2.6 Hz); (300 MHz, CD_3OD) δ 8.32 (s, 2H), 4.14 (s, 6H), 2.40 (q, 3H, *J* = 2.7 Hz).

^{13}C NMR (101 MHz, CD_3OD) δ 157.7 (q, *J* = 2.4 Hz), 139.2, 124.3 (q, *J* = 276.1 Hz), 118.8 (q, *J* = 32.2 Hz), 115.6 (q, *J* = 1.8 Hz), 37.1, 17.9 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -60.1 (q, *J* = 2.6 Hz).

HRMS (ESI) calcd for $C_9H_{12}F_3N_2O_3S^+$ $[M+H]^+$ 285.0515, found 285.0512.



Methyl (*E*)-1,1,1-Trifluoro-2-phenylpent-2-ene-3-sulfonate (3ah)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3ah** as a white solid (40.8 mg, 69% yield).

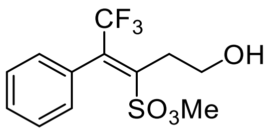
m.p. 60.1–62.0 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45-7.37 (m, 3H), 7.29-7.22 (m, 2H), 3.56 (s, 3H), 2.85 (qq, 2H, *J* = 7.3, 1.7 Hz), 1.37 (t, 3H, *J* = 7.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.0 (q, *J* = 2.5 Hz), 138.7 (q, *J* = 31.2 Hz), 131.6 (q, *J* = 1.2 Hz), 129.4, 128.9, 128.0, 122.5 (q, *J* = 278.7 Hz), 55.7, 24.5 (q, *J* = 2.6 Hz), 14.2.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.2.

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_3S^+$ $[M+Na]^+$ 317.0430, found 317.0428.



Methyl (*E*)-1,1,1-Trifluoro-5-hydroxy-2-phenylpent-2-ene-3-sulfonate (3ai)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (10:1 petroleum ether/EtOAc) to afford **3ai** as a white solid (43.4 mg, 70% yield).

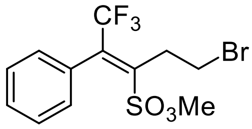
m.p. 67.2–70.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47-7.38 (m, 3H), 7.30-7.24 (m, 2H), 4.01 (dt, 2H, *J* = 6.7, 6.3 Hz), 3.57 (s, 3H), 3.13 (tq, 2H, *J* = 6.7, 1.7 Hz), 1.89 (t, 1H, *J* = 6.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2 (q, *J* = 2.2 Hz), 140.9 (q, *J* = 31.3 Hz), 131.4 (q, *J* = 1.2 Hz), 129.5, 128.9, 128.0, 122.3 (q, *J* = 278.7 Hz), 61.4 (q, *J* = 1.5 Hz), 56.0, 33.9 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.3.

HRMS (ESI) calcd for $C_{12}H_{13}F_3NaO_4S^+$ $[M+Na]^+$ 333.0379, found 333.0377.



Methyl (*E*)-5-Bromo-1,1,1-trifluoro-2-phenylpent-2-ene-3-sulfonate (3aj)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **3aj** as a white solid (47.6 mg, 64% yield).

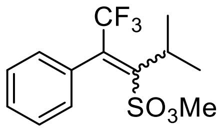
m.p. 69.1–70.8 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) (major *E*-isomer) δ 7.47-7.39 (m, 3H), 7.29-7.22 (m, 2H), 3.66 (t, 2H, *J* = 8.0 Hz), 3.58 (s, 3H), 3.36 (tq, 2H, *J* = 8.0, 1.3 Hz); (minor *Z*-isomer) δ 7.52-7.45 (m, 3H), 7.29-7.22 (m, 2H), 4.04 (s, 3H), 3.45 (t, 2H, *J* = 7.5 Hz), 2.87 (tq, 2H, *J* = 7.9, 1.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) (major *E*-isomer) δ 144.0 (q, *J* = 2.2 Hz), 141.6 (q, *J* = 31.6 Hz), 131.0 (q, *J* = 1.1 Hz), 129.75, 128.7, 128.1, 122.1 (q, *J* = 278.7 Hz), 56.1, 33.9 (q, *J* = 2.6 Hz), 28.0 (q, *J* = 1.8 Hz); (minor *Z*-isomer) δ 129.79, 129.1, 128.0, 56.8, 35.9, (some carbon peaks were missed due to the small amount.).

^{19}F NMR (282 MHz, $CDCl_3$) δ -56.9 (minor *Z*-isomer), -58.3 (major *E*-isomer).

HRMS (ESI) calcd for $C_{12}H_{12}BrF_3NaO_3S^+$ $[M+Na]^+$ 394.9535, found 394.9535.



Methyl 1,1,1-Trifluoro-4-methyl-2-phenylpent-2-ene-3-sulfonate (3ak)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3ak** as a 1:1 *E*/*Z* mixture as colorless oil (37.8 mg, 61% yield).

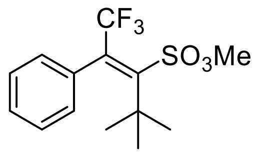
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47-7.43 (m, 0.5 × 3H), 7.42-7.38 (m, 0.5 × 3H), 7.26-7.23 (m, 0.5 × 2H), 7.20-7.16 (m, 0.5 × 2H), 3.99 (s, 0.5 × 3H), 3.51 (hept, 0.5 × 1H, *J* = 8.7 Hz), 3.47 (s, 0.5 × 3H), 2.74 (hept, 0.5 × 1H, *J* = 8.7 Hz), 1.47

(d, 0.5 × 6H, *J* = 8.7 Hz), 1.21 (d, 0.5 × 6H, *J* = 8.7 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.5 (q, *J* = 2.2 Hz), 151.0 (q, *J* = 2.6 Hz), 138.3 (q, *J* = 31.0 Hz), 138.0 (q, *J* = 33.8 Hz), 133.5 (q, *J* = 1.9 Hz), 131.9 (q, *J* = 1.4 Hz), 129.3, 129.2, 129.0, 128.9, 127.9 (two peaks overlay), 122.5 (q, *J* = 278.7 Hz), 120.9 (q, *J* = 276.2 Hz), 55.9, 55.1, 33.7, 31.5 (q, *J* = 2.8 Hz), 20.4, 19.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -57.2, -57.4.

HRMS (ESI) calcd for $C_{13}H_{15}F_3NaO_3S^+$ $[M+Na]^+$ 331.0586, found 331.0585.



Methyl (*Z*)-1,1,1-Trifluoro-4,4-dimethyl-2-phenylpent-2-ene-3-sulfonate (3al)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **3al** as a white solid (16.8 mg, 26% yield).

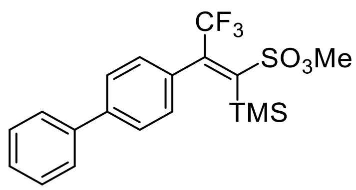
m.p. 63.8–64.5 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50-7.35 (m, 3H), 7.28-7.22 (m, 2H), 3.99 (s, 3H), 1.15 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.6 (q, *J* = 2.3 Hz), 138.7 (q, *J* = 32.3 Hz), 133.3 (q, *J* = 1.8 Hz), 131.3 129.9, 127.9, 121.2 (q, *J* = 277.2 Hz), 56.2, 40.3, 31.8.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.9.

HRMS (ESI) calcd for $C_{14}H_{21}F_3NO_3S^+$ $[M+NH_4]^+$ 340.1189, found 340.1193.



Methyl (*Z*)-3,3,3-Trifluoro-2-([1,1'-biphenyl]-4-yl)-1-(trimethylsilyl)prop-1-ene-1-Sulfonate (3am)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3am** as a white solid (48.7 mg, 59% yield).

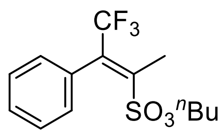
m.p. 78.1–79.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69-7.60 (m, 4H), 7.52-7.37 (m, 3H), 7.34 (d, 2H, *J* = 8.4 Hz), 3.98 (s, 3H), -0.01 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2 (q, *J* = 1.8 Hz), 148.9 (q, *J* = 32.9 Hz), 143.3, 139.6, 132.3 (q, *J* = 1.5 Hz), 131.3, 129.0, 128.1, 127.1, 126.9, 120.4 (q, *J* = 279.6 Hz), 55.7, 0.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.2.

HRMS (ESI) calcd for $C_{19}H_{21}F_3NaO_3SSi^+$ $[M+Na]^+$ 437.0825, found 437.0811.



Butyl (*E*)-4,4,4-Trifluoro-3-phenylbut-2-ene-2-sulfonate (3an)

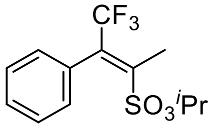
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3an** the title compound as colorless oil (40.8 mg, 63% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44-7.36 (m, 3H), 7.27-7.20 (m, 2H), 3.97 (t, 2H, *J* = 6.6 Hz), 2.45 (q, 3H, *J* = 2.5 Hz), 1.63-1.52 (m, 2H), 1.40-1.26 (m, 2H), 0.90 (t, 3H, *J* = 6.6 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0 (q, *J* = 2.5 Hz), 138.7 (q, *J* = 31.3 Hz), 131.5, 129.3, 128.9, 128.0, 122.4 (q, *J* = 278.7 Hz), 70.8, 30.9, 18.6, 16.6 (q, *J* = 2.8 Hz), 13.4.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{14}H_{17}F_3NaO_3S^+$ $[M+Na]^+$ 345.0743, found 345.0741.



Isopropyl (*E*)-4,4,4-Trifluoro-3-phenylbut-2-ene-2-sulfonate (3ao)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3ao** as a white solid (39.5 mg, 64% yield).

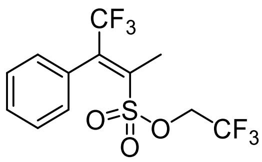
m.p. 37.1–38.3 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44-7.36 (m, 3H), 7.25-7.20 (m, 2H), 4.76 (hept, 1H, *J* = 6.3 Hz), 2.45 (q, 3H, *J* = 2.5 Hz), 1.31 (d, 6H, *J* = 6.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7 (q, *J* = 2.5 Hz), 138.2 (q, *J* = 31.2 Hz), 131.6 (q, *J* = 1.2 Hz), 129.2, 129.0, 128.0, 122.5 (q, *J* = 278.7 Hz), 78.2, 22.8, 16.6 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{13}H_{15}F_3NaO_3S^+$ $[M+Na]^+$ 331.0586, found 331.0586.



2,2,2-Trifluoroethyl (*E*)-4,4,4-Trifluoro-3-phenylbut-2-ene-2-sulfonate (3ap)

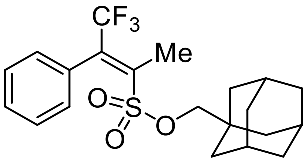
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3ap** as colorless oil (42.3 mg, 61% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48-7.39 (m, 3H), 7.25-7.20 (m, 2H), 4.20 (q, 2H, *J* = 7.9 Hz), 2.49 (q, 3H, *J* = 2.5 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.5 (q, *J* = 2.2 Hz), 140.3 (q, *J* = 31.5 Hz), 131.0, 129.7, 128.8, 128.3, 122.2 (q, *J* = 278.7 Hz), 121.7 (q, *J* = 278.7 Hz), 64.4 (q, *J* = 38.4 Hz), 16.5 (q, *J* = 2.5 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.1 (q, *J* = 2.4 Hz), -73.8 (t, *J* = 7.9 Hz).

HRMS (ESI) calcd for $C_{12}H_{10}F_6NaO_3S^+$ $[M+Na]^+$ 371.0147, found 371.0141.



((3r,5r,7r)-Adamantan-1-yl)methyl (*E*)-4,4,4-Trifluoro-3-phenylbut-2-ene-1-Sulfonate (3aq)

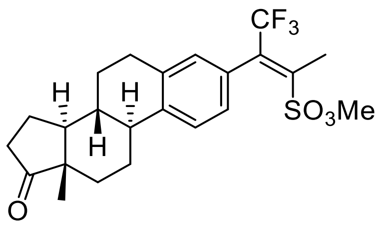
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **3aq** as colorless oil (54.8 mg, 66% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44-7.36 (m, 3H), 7.25-7.20 (m, 2H), 3.54 (s, 2H), 2.44 (q, 3H, *J* = 2.5 Hz), 2.02-1.94 (m, 3H), 1.77-1.66 (m, 3H), 1.66-1.57 (m, 3H), 1.50-1.44 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.9 (q, *J* = 2.5 Hz), 138.7 (q, *J* = 31.3 Hz), 131.5 (q, *J* = 1.2 Hz), 129.3, 128.9, 128.0, 122.5 (q, *J* = 278.7 Hz), 80.1, 38.6, 36.6, 33.4, 27.7, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -55.7 (q, *J* = 2.1 Hz, minor *Z*-isomer), -58.8 (q, *J* = 2.5 Hz, major *E*-isomer).

HRMS (ESI) calcd for $C_{21}H_{25}F_3NaO_3S^+$ $[M+Na]^+$ 437.1369, found 437.1362.



Methyl

(*E*)-4,4,4-Trifluoro-3-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)but-2-ene-2-sulfonate (3ar)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **3ar** as a white solid (59.5 mg, 65% yield).

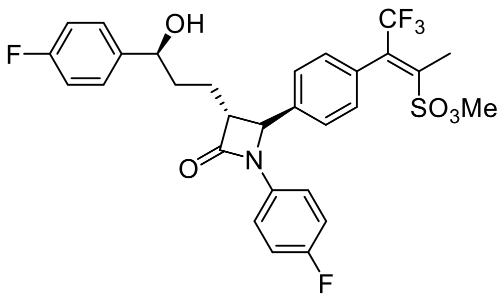
m.p. 162.0–163.8 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 (d, 1H, *J* = 8.1 Hz), 7.00 (d, 1H, *J* = 8.1 Hz), 6.96 (s, 1H), 3.69 (s, 3H), 2.98-2.88 (m, 2H), 2.58-2.25 (m, 3H), 2.44 (q, 3H, *J* = 2.4 Hz), 2.24-1.92 (m, 4H), 1.74-1.39 (m, 6H), 0.92 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 220.6, 141.9, 141.1, 139.4 (q, *J* = 31.3 Hz), 136.3, 129.3, 128.7, 126.1, 124.9, 122.4 (q, *J* = 278.7 Hz), 56.1, 50.5, 47.9, 44.3, 37.7, 35.8, 31.5, 29.1, 26.3, 25.4, 21.5, 16.7 (q, *J* = 2.7 Hz), 13.8.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8.

HRMS (ESI) calcd for $C_{23}H_{27}F_3NaO_4S^+$ $[M+Na]^+$ 479.1474, found 479.1474.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-((2*R*,3*R*)-1-(4-fluorophenyl)-3-((*S*)-3-(4-fluorophenyl)-3-hydroxypropyl)-4-oxoazetidin-2-yl)phenyl)but-2-ene-2-sulfonate (3as)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (3:1 petroleum ether/EtOAc) to afford **3as** as a brown solid (68.9 mg, 58% yield).

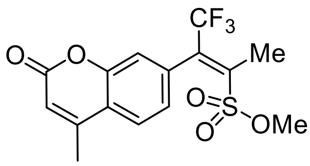
m.p. 136.5–138.0 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.19 (m, 8 H), 7.02 (t, 2H, *J* = 8.7 Hz), 6.94 (t, 2H, *J* = 8.7 Hz), 4.75-4.68 (m, 1H), 4.65 (d, 1H, *J* = 2.1 Hz), 3.65 (s, 3H), 3.20-3.11 (m, 1H), 2.45 (q, 3H, *J* = 2.5 Hz), 2.21 (d, 1H, *J* = 3.4 Hz), 2.09-1.86 (m, 4H).

^{13}C NMR (101 MHz, acetone-*d*$_6$) δ 167.8, 162.6 (d, *J* = 242.3 Hz), 159.0 (d, *J* = 241.8 Hz), 144.2 (q, *J* = 2.5 Hz), 142.9 (d, *J* = 3.0 Hz), 140.7, 138.8 (q, *J* = 31.2 Hz), 135.4 (d, *J* = 2.7 Hz), 132.6 (q, *J* = 1.1 Hz), 130.7, 128.5 (d, *J* = 8.0 Hz), 126.8, 123.5 (q, *J* = 277.8 Hz), 119.2 (d, *J* = 8.0 Hz), 116.4 (d, *J* = 23.0 Hz), 115.5 (d, *J* = 21.4 Hz), 72.7, 61.2, 61.1, 57.7, 37.6, 25.7, 16.9 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.8 (q, *J* = 2.5 Hz), -114.8 (m), -117.8 (m).

HRMS (ESI) calcd for $C_{29}H_{26}F_5NNaO_5S^+$ [M+Na]$^+$ 618.1344, found 618.1341.



Methyl (*E*)-4,4,4-Trifluoro-3-(4-methyl-2-oxo-2H-chromen-7-yl)but-2-ene-2-sulfonate (3at)

Following the general procedure B, the crude product was purified by flash chromatography on silica gel (25:1 petroleum ether/EtOAc) to afford **3at** as a white solid (53.7 mg, 74% yield).

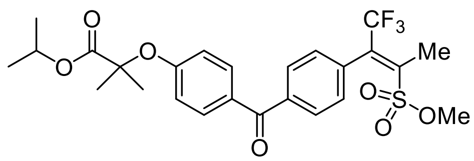
m.p. 142.7–143.8 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, 1H, *J* = 8.1 Hz), 7.22-7.17 (m, 2H), 6.36 (d, 1H, *J* = 1.6 Hz), 3.77 (s, 3H), 2.49 (q, 3H, *J* = 2.5 Hz), 2.46 (d, 3H, *J* = 1.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 152.8, 151.8, 143.6 (q, *J* = 2.1 Hz), 137.4 (q, *J* = 31.9 Hz), 134.8, 124.9, 124.5, 122.0 (q, *J* = 278.5 Hz), 120.6, 117.4, 116.1, 56.4, 18.5, 16.7 (q, *J* = 2.5 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.6 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{15}H_{14}F_3O_5S^+$ [M+H]$^+$ 363.0509, found 363.0502.



Isopropyl (*E*)-2-Methyl-2-(4-(4-(1,1,1-trifluoro-3-(methoxysulfonyl)but-2-en-2-yl) benzoyl)phenoxy)propanoate (3au)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **3au** as a white solid (66.5 mg, 63% yield).

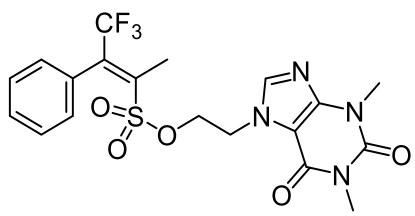
m.p. 60.2–61.7 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, 2H, *J* = 8.5 Hz), 7.76 (d, 2H, *J* = 8.8 Hz), 7.35 (d, 2H, *J* = 8.5 Hz), 6.87 (d, 2H, *J* = 8.8 Hz), 5.09 (hept, 1H, *J* = 6.2 Hz), 3.72 (s, 3H), 2.48 (q, 3H, *J* = 2.4 Hz), 1.67 (s, 6H), 1.20 (d, 6H, *J* = 6.2 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.5, 173.0, 159.7, 134.0 (q, *J* = 2.2 Hz), 138.7, 138.3 (q, *J* = 31.6 Hz), 134.9 (q, *J* = 1.1 Hz), 132.0, 130.0, 129.4, 128.8, 122.1 (q, *J* = 278.9 Hz), 117.1, 79.3, 69.3, 56.2, 25.3, 21.5, 16.6 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.5 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{25}H_{28}F_3O_7S^+$ $[M+H]^+$ 529.1502, found 529.1498.



2-(1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7H-purin-7-yl)ethyl (*E*)-4,4,4-Trifluoro-3-phenylbut-2-ene-2-sulfonate (3av)

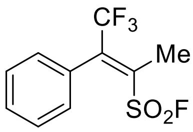
Following the general procedure A, the crude product was purified by flash chromatography on silica gel (20:1 CH_2Cl_2/MeOH) to afford **3av** as colorless liquid (55.7 mg, 59% yield).

^{1}H NMR (300 MHz, $CDCl_3$) (major *E*-isomer) δ 7.50 (s, 1H), 7.43-7.36 (m 3H), 7.21-7.15 (m, 2H), 4.44 (t, 2H, *J* = 4.6 Hz), 4.32 (t, 2H, *J* = 4.6 Hz), 3.60 (s, 3H), 3.41 (s, 3H), 2.31 (q, 3H, J = 2.5 Hz); (minor Z-isomer) 7.68 (s, 1H), 7.47-7.39 (m, 3H), 7.15-7.11 (m, 2H), 4.71 (t, 2H, J = 4.4 Hz), 4.67 (t, 2H, J = 4.4 Hz), 3.60 (s, 3H), 3.42 (s, 3H), 1.88 (q, 3H, J = 2.0 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) (major E-isomer) δ 155.2, 151.5, 149.2, 142.11, 142.2 (q, J = 2.4 Hz), 139.6 (q, J = 31.5 Hz), 131.1 (q, J = 1.1 Hz), 129.46, 128.7, 128.1, 122.1 (q, J = 278.7 Hz), 106.2, 68.2, 46.3, 29.8, 27.91, 16.4 (q, J = 2.7 Hz); (minor Z-isomer) δ 155.3, 151.4, 149.3, 142.2, 142.13 (q, J = 2.1 Hz), 129.52, 129.0, 127.8, 106.3, 68.6, 46.4, 27.94, 19.6 (some carbon peaks were missed due to the low amount.).

^{19}F NMR (282 MHz, $CDCl_3$) δ -56.1 (q, J = 2.0 Hz, minor Z-isomer), -59.0 (q, J = 2.5 Hz, major E-isomer).

HRMS (ESI) calcd for $C_{19}H_{19}F_3N_4NaO_5S^+$ $[M+Na]^+$ 495.0920, found 495.0920.



(E)-4,4,4-Trifluoro-3-phenylbut-2-ene-2-sulfonyl Fluoride (5a)

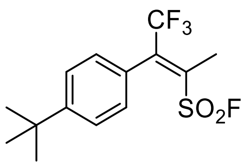
Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5a** as colorless liquid (32.5 mg, 61% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52-7.40 (m, 3H), 7.28-7.22 (m, 2H), 2.55 (q, 3H, J = 2.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0 (qd, J = 32.1, 2.6 Hz), 141.3 (dq, J = 23.8, 2.3 Hz), 130.3 (q, J = 1.1 Hz), 130.1, 128.7, 128.5, 121.9 (qd, J = 278.5, 4.7 Hz), 16.6 (q, J = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 57.9, -59.3.

HRMS (EI) calcd for $C_{10}H_8F_4O_2S^+$ $[M]^+$ 268.0181, found 268.0187.



(*E*)-3-(4-(*tert*-Butyl)phenyl)-4,4,4-trifluorobut-2-ene-2-sulfonyl Fluoride (5b)

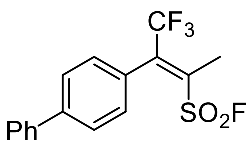
Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5b** as colorless liquid (37.8 mg, 58% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (d, 2H, *J* = 8.5 Hz), 7.16 (d, 2H, *J* = 8.5 Hz), 2.53 (q, 3H, *J* = 2.4 Hz), 1.33 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 142.2 (qd, *J* = 32.2, 2.7 Hz), 141.0 (dq, *J* = 23.7, 2.2 Hz), 128.5, 127.3 (q, *J* = 1.1 Hz), 125.4, 122.0 (qd, *J* = 278.3, 4.6 Hz), 34.8, 31.1, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 57.6, -59.4.

HRMS (EI) calcd for $C_{14}H_{16}F_4O_2S^+$ $[M]^+$ 324.0802, found 324.0796.



(*E*)-3-([1,1'-Biphenyl]-4-yl)-4,4,4-trifluorobut-2-ene-2-sulfonyl Fluoride (5c)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5c** as a white solid (44.3 mg, 64% yield).

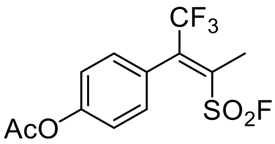
m.p. 145.1–146.6 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70-7.58 (m, 4H), 7.50-7.35 (m, 3H), 7.32 (d, 2H, *J* = 8.1 Hz), 2.57 (q, 3H, *J* = 2.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1, 141.9 (qd, *J* = 32.4, 2.5 Hz), 141.4 (dq, *J* = 24.0, 2.2 Hz), 139.9, 129.3, 129.1 (q, *J* = 1.1 Hz), 128.9, 128.0, 127.2, 127.1, 122.0 (qd, *J* = 278.6, 4.7 Hz), 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 57.9, -59.3.

HRMS (EI) calcd for $C_{16}H_{12}F_4O_2S^+$ $[M]^+$ 344.0489, found 344.0491.



(*E*)-4-(1,1,1-Trifluoro-3-(fluorosulfonyl)but-2-en-2-yl)phenyl Acetate (5d)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5d** as a white solid (39.2 mg, 60% yield).

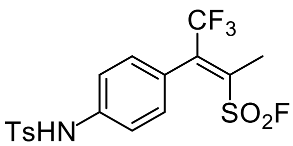
m.p. 60.1–60.9 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27 (d, 2H, *J* = 8.8 Hz), 7.20 (d, 2H, *J* = 8.8 Hz), 2.54 (q, 3H, *J* = 2.2 Hz), 2.31 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 152.1, 141.8 (dq, *J* = 24.1, 2.2 Hz), 141.2 (qd, *J* = 32.4, 2.5 Hz), 130.1, 127.5 (q, *J* = 1.1 Hz), 121.8 (qd, *J* = 278.8, 4.6 Hz), 121.7, 21.1, 16.7 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 57.9, -59.3 (q, *J* = 2.2 Hz).

HRMS (ESI) calcd for $C_{12}H_{11}F_4O_4S^+$ $[M+H]^+$ 327.0309, found 327.0306.



(*E*)-4,4,4-Trifluoro-3-(4-((4-methylphenyl)sulfonamido)phenyl)but-2-ene-2-sulfonyl Fluoride (5e)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (20:1 petroleum ether/EtOAc) to afford **5e** as a white solid (48.3 mg, 55% yield).

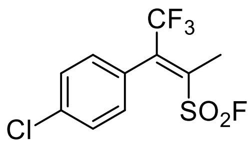
m.p. 105.7–107.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61 (d, 2H, *J* = 8.3 Hz), 7.23 (d, 2H, *J* = 8.3 Hz), 7.12 (s, 4H), 6.62 (brs, 1H), 2.52 (q, 3H, *J* = 2.1 Hz), 2.38 (s, 3H).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 144.3, 141.6 (dq, *J* = 23.8, 2.2 Hz), 141.2 (qd, *J* = 32.6, 2.5 Hz), 138.7, 135.5, 129.9, 129.7, 127.1, 126.6 (q, *J* = 1.1 Hz), 121.7 (qd, *J* = 278.5, 4.8 Hz), 120.6, 21.5, 16.6 (q, *J* = 2.8 Hz).

^{19}**F NMR** (282 MHz, $CDCl_3$) δ 57.9, -59.4.

HRMS (ESI) calcd for $C_{17}H_{16}F_4NO_4S_2^+$ $[M+H]^+$ 438.0451, found 438.0447.



(*E*)-3-(4-Chlorophenyl)-4,4,4-trifluorobut-2-ene-2-sulfonyl Fluoride (5f)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (petroleum ether) to afford **5f** as a white solid (34.5 mg, 57% yield).

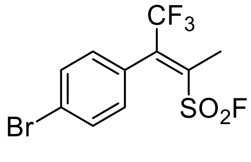
m.p. 35.7–36.5 ºC.

^{1}**H NMR** (300 MHz, $CDCl_3$) δ 7.42 (d, 2H, *J* = 8.5 Hz), 7.18 (d, 2H, *J* = 8.5 Hz), 2.55 (q, 3H, *J* = 2.3 Hz).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 142.0 (dq, *J* = 24.1, 2.3 Hz), 140.9 (qd, *J* = 32.5, 2.5 Hz), 136.6, 130.1, 128.9, 128.6 (q, *J* = 1.4 Hz), 121.7 (qd, *J* = 278.9, 4.7 Hz), 16.6 (q, *J* = 2.8 Hz).

^{19}**F NMR** (282 MHz, $CDCl_3$) δ 58.0, -59.4.

HRMS (EI) calcd for $C_{10}H_7ClF_4O_2S^+$ $[M]^+$ 301.9786, found 301.9787.



(*E*)-3-(4-Bromophenyl)-4,4,4-Trifluorobut-2-ene-2-sulfonyl Fluoride (5g)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (petroleum ether) to afford **5g** as a white solid (42.3 mg, 61% yield).

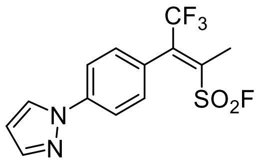
m.p. 39.1–40.3 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, 2H, *J* = 8.5 Hz), 7.12 (d, 2H, *J* = 8.5 Hz), 2.54 (q, 3H, *J* = 2.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9 (dq, *J* = 24.1, 2.4 Hz), 140.9 (qd, *J* = 32.7, 2.6 Hz), 131.9, 130.3, 129.1 (q, *J* = 1.1 Hz), 124.9, 121.6 (qd, *J* = 278.5, 4.4 Hz), 16.7 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 58.0, -59.3.

HRMS (EI) calcd for $C_{10}H_7BrF_4O_2S^+$ $[M]^+$ 345.9286, found 345.9289.



(*E*)-3-(4-(1*H*-Pyrazol-1-yl)phenyl)-4,4,4-trifluorobut-2-ene-2-sulfonyl Fluoride (5h)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5h** as a white solid (36.0 mg, 54% yield).

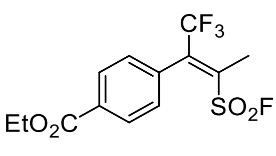
m.p. 70.2–71.4 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, 1H, *J* = 2.5 Hz), 7.80 (d, 2H, *J* = 8.7 Hz), 7.75 (d, 1H, *J* = 1.4 Hz), 7.34 (d, 2H, *J* = 8.7 Hz), 6.50 (dd, 1H, *J* = 2.5, 1.4 Hz), 2.57 (q, 3H, *J* = 2.2 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8 (dq, *J* = 24.0, 2.5 Hz), 141.7, 141.3, 141.2 (qd, *J* = 32.1, 2.6 Hz), 130.1, 127.9 (q, *J* = 1.4 Hz), 126.7, 121.8 (qd, *J* = 279.4, 4.5 Hz), 118.7, 108.2, 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 58.0, -59.3.

HRMS (ESI) calcd for $C_{13}H_{11}F_4N_2O_2S^+$ $[M+H]^+$ 335.0472, found 335.0461.



Ethyl (*E*)-4-(1,1,1-Trifluoro-3-(fluorosulfonyl)but-2-en-2-yl)benzoate (5i)

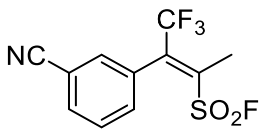
Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5i** as colorless oil (36.8 mg, 54% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (d, 2H, *J* = 8.4 Hz), 7.33 (d, 2H, *J* = 8.4 Hz), 4.40 (q, 2H, *J* = 7.1 Hz), 2.57 (q, 3H, *J* = 2.3 Hz), 1.40 (t, 3 H, *J* = 7.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 141.8 (dq, *J* = 24.6, 2.5 Hz), 141.2 (qd, *J* = 32.5, 2.5 Hz), 134.6 (q, *J* = 1.1 Hz), 132.1, 129.6, 128.8, 121.7 (qd, *J* = 278.8, 4.5 Hz), 61.3, 16.7 (q, *J* = 2.7 Hz), 14.3.

^{19}F NMR (282 MHz, $CDCl_3$) δ 58.3, -59.1.

HRMS (ESI) calcd for $C_{13}H_{13}F_4O_4S^+$ $[M+H]^+$ 341.0465, found 341.0459.



(*E*)-3-(3-Cyanophenyl)-4,4,4-trifluorobut-2-ene-2-sulfonyl Fluoride (5j)

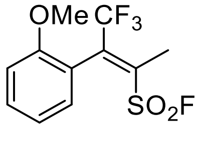
Following the general procedure D, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5j** as colorless liquid (29.8 mg, 51% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, 1H, *J* = 7.8 Hz), 7.59 (t, 1H, *J* = 7.8 Hz), 7.56 (s, 1H), 7.49 (d, 1 H, *J* = 7.8 Hz), 2.58 (q, 3H, *J* = 2.7 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ142.9 (dq, *J* = 24.7, 2.2 Hz), 139.5 (qd, *J* = 32.9, 2.5 Hz), 133.6, 133.0, 132.1, 131.6 (q, *J* = 1.1 Hz), 129.5, 121.4 (qd, *J* = 279.3, 4.4 Hz), 117.6, 113.2, 16.6 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 58.4, -59.1.

HRMS (EI) calcd for $C_{11}H_7F_4NO_2S^+$ $[M]^+$ 293.0128, found 293.0128.



(*E*)-4,4,4-Trifluoro-3-(2-methoxyphenyl)but-2-ene-2-sulfonyl Fluoride (5k)

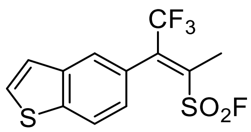
Following the general procedure D, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5k** as colorless liquid (26.2 mg, 44% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 (ddd, 1H, *J* = 8.4, 7.5, 1.8 Hz), 7.12 (dd, 1H, *J* = 7.8, 1.8 Hz), 7.00 (ddd, 1H, *J* = 7.8, 7.5, 1.0 Hz), 6.94 (dd, 1H, *J* = 8.4, 1.0 Hz), 3.84 (s, 3H), 2.53 (q, 3H, *J* = 2.1 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 141.2 (dq, *J* = 24.1, 2.5 Hz), 140.3 (qd, *J* = 33.3, 2.7 Hz), 131.9, 129.9, 121.7 (qd, *J* = 279.5, 4.5 Hz), 120.4, 119.8 (q, *J* = 1.1 Hz), 110.8, 55.7, 16.5 (q, *J* = 2.6 Hz).

^{19}F NMR (282 MHz, CDCl3) δ 56.8, -60.5.

HRMS (ESI) calcd for $C_{11}H_{10}F_4NaO_3S^+$ $[M+Na]^+$ 321.0179, found 321.0175.



(*E*)-3-(Benzo[*b*]thiophen-5-yl)-4,4,4-trifluorobut-2-ene-2-sulfonyl Fluoride (5l)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5l** as a white solid (34.6 mg, 53% yield).

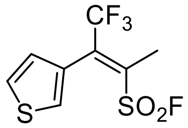
m.p. 68.1–69.7 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, 1H, *J* = 8.3 Hz), 7.74 (d,1H, *J* = 1.1 Hz), 7.56 (d, 1H, *J* = 5.4 Hz), 7.40 (d, 1H, *J* = 5.4 Hz), 7.22 (dd, 1H, *J* = 8.3, 1.1 Hz), 2.61 (q, 3H, *J* = 2.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ142.1 (qd, *J* = 32.1, 2.6 Hz), 141.6 (dq, *J* = 23.6, 2.2 Hz), 141.4, 139.3, 128.0, 126.3 (q, *J* = 1.1 Hz), 124.1, 123.9, 122.7, 120.0 (qd, *J* = 278.5, 4.7 Hz), 16.7 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 57.7, -59.3.

HRMS (ESI) calcd for $C_{12}H_8F_4NaO_2S_2^+$ $[M+Na]^+$ 346.9794, found 346.9789.



(*E*)-4,4,4-T

rifluoro-3-(thiophen-3-yl)but-2-ene-2-sulfonyl Fluoride (5m)

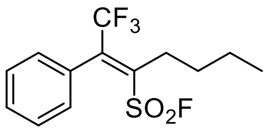
Following the general procedure C, the crude product was purified by flash chromatography on silica gel (petroleum ether) to afford **5m** as colorless liquid (26.8 mg, 49% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45-7.40 (m, 2H), 7.06-7.01 (m, 1H), 2.53 (qd, 3H, *J* = 2.4, 1.2 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1 (dq, *J* = 24.2, 2.3 Hz), 137.4 (qd, *J* = 33.1, 2.6 Hz), 129.0 (q, *J* = 1.2 Hz), 128.2, 127.6, 126.5, 121.6 (qd, *J* = 278.6, 4.7 Hz), 16.8 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 56.7, -60.1.

HRMS (EI) calcd for $C_8H_6F_4O_2S_2^+$ $[M]^+$ 273.9740, found 273.9742.



(*E*)-1,1,1-Trifluoro-2-phenylhept-2-ene-3-sulfonyl Fluoride (5n)

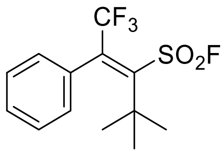
Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5n** as colorless liquid (34.3 mg, 55% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52-7.39 (m, 3H), 7.28-7.22 (m, 2H), 2.90-2.80 (m, 2H), 1.82-1.69 (m, 2H), 1.49 (tq, 2H, *J* = 7.3, 7.3 Hz), 0.99 (t, 3H, *J* = 7.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ146.8 (dq, *J* = 19.0, 2.3 Hz), 141.7 (qd, *J* = 32.2, 1.4 Hz), 130.5 (q, *J* = 1.1 Hz), 130.0, 128.8, 128.4, 122.2 (qd, *J* = 279.1, 4.4 Hz), 31.5, 30.8 (q, *J* = 2.2 Hz), 22.7, 13.5.

^{19}F NMR (282 MHz, $CDCl_3$) δ 62.5, -58.7.

HRMS (EI) calcd for $C_{13}H_{14}F_4O_2S^+$ [M]$^+$ 310.0645, found 310.0648.



(*Z*)-1,1,1-Trifluoro-4,4-dimethyl-2-phenylpent-2-ene-3-sulfonyl Fluoride (5o)

Following the general procedure C, the crude product was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **5o** as a white solid (19.9 mg, 32% yield).

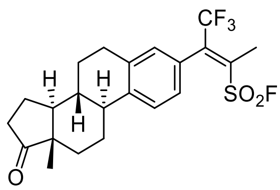
m.p. 76.8–77.9 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54-7.39 (m, 3H), 7.32-7.25 (m, 2H), 1.17 (d, 9H, *J* = 0.6 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ152.9 (dq, *J* = 14.1, 2.1 Hz), 141.5 (q, *J* = 33.2 Hz), 132.2 (q, *J* = 3.2 Hz), 131.1, 130.5, 128.3, 121.0 (q, *J* = 277.7 Hz), 40.6, 31.8 (d, *J* = 2.5 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 69.4 (q, *J* = 19.8 Hz), -59.3 (d, *J* = 19.8 Hz).

HRMS (ESI) calcd for $C_{13}H_{15}F_4O_2S^+$ [M+H]$^+$ 311.0723, found 311.0733.



(*E*)-4,4,4-Trifluoro-3-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)but-2-ene-2-sulfonyl Fluoride (5p)

Following the general procedure D, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **5p** as a white solid (54.4 mg, 61% yield).

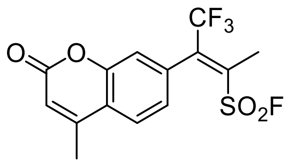
m.p. 45.8-47.0 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (d, 1H, *J* = 8.2 Hz), 7.01 (d,1H, *J* = 8.2 Hz), 6.96 (s, 1H), 3.00-2.86 (m, 2H), 2.58-2.25 (m, 3H), 2.53 (q, 3H, *J* = 2.4 Hz), 2.24-1.98 (m, 4H), 1.74-1.41 (m, 6H), 0.93 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 220.7, 142.2 (qd, *J* = 35.2, 2.5 Hz), 142.0, 140.8 (dq, *J* = 24.9, 2.6 Hz), 136.8, 129.1, 127.6, 126.0, 125.4, 121.9 (qd, *J* = 279.0, 4.7 Hz), 50.5, 47.9, 44.3, 37.7, 35.8, 31.5, 29.1, 26.2, 25.4, 21.5, 16.6 (q, *J* = 2.6 Hz), 13.8.

^{19}F NMR (282 MHz, $CDCl_3$) δ 57.6, -59.4.

HRMS (ESI) calcd for $C_{22}H_{25}F_4O_3S^+$ $[M+H]^+$ 445.1455, found 445.1453.



(*E*)-4,4,4-Trifluoro-3-(4-methyl-2-oxo-2H-chromen-7-yl)but-2-ene-2-sulfonyl Fluoride (5q)

Following the general procedure D, the crude product was purified by flash chromatography on silica gel (20:1 petroleum ether/EtOAc) to afford **5q** as a white solid (46.9 mg, 67% yield).

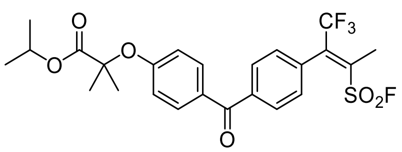
m.p. 141.6-143.2 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (d, 1H, *J* = 8.2 Hz), 7.24 (d, 1H, *J* = 1.5 Hz), 7.18 (dd, 1H, *J* = 8.2, 1.5 Hz), 6.38 (q, 1H, *J* = 1.2 Hz), 2.59 (q, 3H, *J* = 2.4 Hz), 2.47 (d, 3H, *J* = 1.2 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 153.0, 151.6, 142.4 (dq, *J* = 24.5, 2.5 Hz), 140.1 (qd, *J* = 32.8, 2.6 Hz), 133.4 (q, *J* = 1.4 Hz), 124.9, 124.5, 121.5 (qd, *J* = 279.3, 4.4 Hz), 121.3, 117.5, 116.5, 18.5, 16.7 (q, *J* = 2.5 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 58.4, -59.0.

HRMS (ESI) calcd for $C_{14}H_{11}F_4O_4S^+$ $[M+H]^+$ 351.0309, found 351.0299.



Isopropyl (*E*)-2-Methyl-2-(4-(4-(1,1,1-trifluoro-3-(fluorosulfonyl)but-2-en-2-yl)benzoyl)phenoxy)propanoate (5r)

Following the general procedure D, the crude product was purified by flash chromatography on silica gel (30:1 petroleum ether/EtOAc) to afford **5r** as a white solid (53.5 mg, 52% yield).

m.p. 60.1-61.4 ºC.

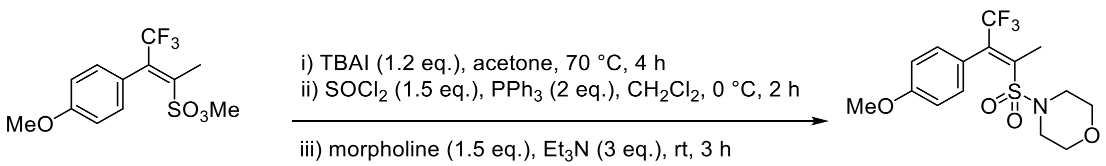
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, 2H, *J* = 8.3 Hz), 7.76 (d, 2H, *J* = 8.9 Hz), 7.36 (d, 2H, *J* = 8.3 Hz), 6.88 (d, 2H, *J* = 8.9 Hz), 5.09 (hept, 1H, *J* = 6.3 Hz), 2.58 (q, 3H, *J* = 2.3 Hz), 1.67 (s, 6H), 1.20 (d, 6H, *J* = 6.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.4, 173.0, 159.9, 141.8 (dq, *J* = 24.2, 2.4 Hz), 141.2 (qd, *J* = 32.8, 2.6 Hz), 139.5, 133.6, 132.1, 129.9, 129.6, 128.7, 121.7 (qd, *J* = 279.3, 4.1 Hz), 117.2, 79.4, 69.3, 25.3, 21.5, 16.7 (q, *J* = 2.5 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ 58.2, -59.0.

HRMS (ESI) calcd for $C_{24}H_{25}F_4O_6S^+$ $[M+H]^+$ 517.1302, found 517.1295.

Synthesis of (*E*)-4-((4,4,4-Trifluoro-3-(4-methoxyphenyl)but-2-en-2-yl)sulfonyl)morpholine (6)



A mixture of **3a** (62.1 mg, 0.2 mmol, 1.0 equiv.) and TBAI (88.7 mg, 0.24 mmol) in acetone (1 mL) was heated to reflux for 4 h. The solvent was evaporated to afford crude sulfonic acid. Then PPh_3 (104.9 mg, 0.4 mmol), anhydrous CH_2Cl_2 (1 mL), and $SOCl_2$ (21.8 μL, 0.3 mmol) was added at 0 ºC. The mixture was stirred at this temperature for 2 h. To the mixture were added Et_3N (83.0 μL, 0.6 mmol) and morpholine (26.1 μL). The reaction mixture was stirred at room temperature for 3 h. EtOAc (10 mL) and water (8 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 8 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (3:1 petroleum ether/EtOAc) to afford **6** (49.9 mg, 68% yield) as a pale-yellow solid.

m.p. 135.4–137.0 ºC.

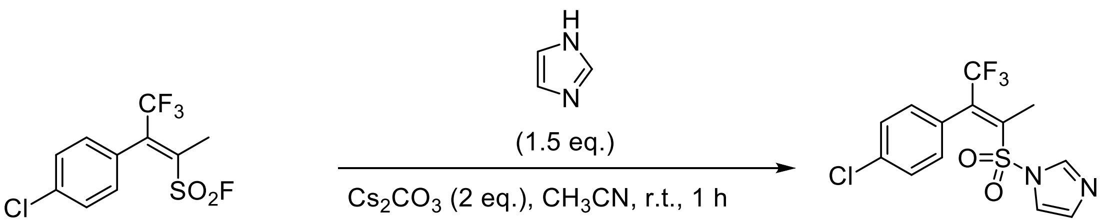
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.14 (d, 2H, *J* = 8.7 Hz), 6.92 (d, 2H, *J* = 8.7 Hz), 3.82 (s, 3H), 3.65-3.57 (m, 4H), 3.08-2.99 (m, 4H), 2.36 (q, 3H, *J* = 2.5 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 144.9 (q, *J* = 2.2 Hz), 137.1 (q, *J* = 30.8 Hz), 130.5, 123.8 (q, *J* = 1.1 Hz), 122.7 (q, *J* = 278.9 Hz), 113.4, 66.6, 55.1, 45.3, 16.9 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.6 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{15}H_{19}F_3NO_4S^+$ $[M+H]^+$ 366.0981, found 366.0982.

Synthesis of (*E*)-1-((3-(4-Chlorophenyl)-4,4,4-trifluorobut-2-en-2-yl)sulfonyl)-1*H*-imidazole (7)



A mixture of **5f** (60.4 mg, 0.2 mmol, 1.0 equiv.), imidazole (20.4 mg, 0.3 mmol), and Cs_2CO_3 (130.3 mg, 0.4 mmol) in CH_3CN (1 mL) was stirred at room temperature for 1 h. EtOAc (10 mL) and water (8 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 8 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **7** (33.5 mg, 48% yield) as a white solid.

m.p. 64.3–66.5 ºC.

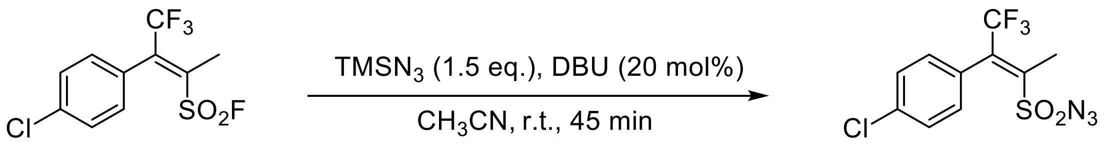
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60-7.58 (m, 1H), 7.42 (d, 2H, *J* = 8.6 Hz), 7.14-7.12 (m, 1H), 7.09 (d, 2H, *J* = 8.6 Hz), 7.06 (dd, 1H, *J* = 1.5, 1.4 Hz), 2.34 (q, 3H, *J* = 2.3 Hz).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1 (q, *J* = 2.2 Hz), 139.8 (q, *J* = 32.2 Hz), 137.1, 136.4, 131.5, 130.1, 128.8, 128.3 (*J* = 1.2 Hz), 121.7 (q, *J* = 279.1 Hz), 117.5, 16.1 (q, *J* = 2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.2 (d, *J* = 2.3 Hz).

HRMS (ESI) calcd for $C_{13}H_{11}ClF_3N_2O_2S^+$ $[M+H]^+$ 351.0176, found 351.0174.

Synthesis of (*E*)-3-(4-Chlorophenyl)-4,4,4-trifluorobut-2-ene-2-sulfonyl azide (8)



A mixture of **5f** (60.4 mg, 0.2 mmol, 1.0 equiv.), $TMSN_3$ (40 μL, 0.3 mmol), and DBU (6.0 μL, 0.04 mmol) in CH_3CN (1 mL) was stirred at room temperature for 45 min. EtOAc (10 mL) and water (8 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 8 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (100:1 petroleum ether/EtOAc) to afford **8** (46.0 mg, 71% yield) as a white solid.

m.p. 61.5–62.7 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (d, 2H, *J* = 8.5 Hz), 7.19 (d, 2H, *J* = 8.5 Hz), 2.51 (q, 3H, *J* = 2.4 Hz).

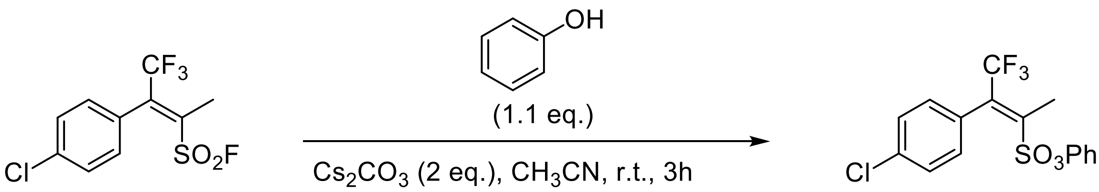
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0 (q, *J* = 2.2 Hz), 138.7 (q, *J* = 32.2 Hz), 136.3, 130.3, 128.9 (q, *J* = 1.4 Hz), 128.8, 122.0 (q, *J* = 279.1 Hz), 16.8 (q, *J* =

2.8 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.1 (q, *J* = 2.4 Hz).

HRMS (ESI) calcd for $C_{10}H_8ClF_3NO_2S^+$ $[M-N_2+H]^+$ 297.9911, found 297.9907.

Synthesis of Phenyl (*E*)-3-(4-chlorophenyl)-4,4,4-trifluorobut-2-ene-2-sulfonate (9)



A mixture of **3f** (60.4 mg, 0.2 mmol, 1.0 equiv.), phenol (20.7 mg, 0.22 mmol), and Cs_2CO_3 (130.3 mg, 0.4 mmol) in CH_3CN (1 mL) was stirred at room temperature for 3 h. EtOAc (10 mL) and water (8 mL) were added. The two layers were separated and the aqueous layer was extracted with EtOAc (2 × 8 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by flash chromatography on silica gel (5:1 petroleum ether/EtOAc) to afford **9** (62.5 mg, 83% yield) as a white solid.

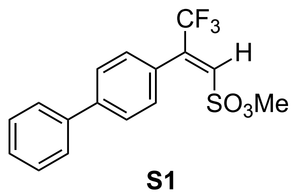
m.p. 82.4–84.1 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47-7.34 (m, 3H), 7.23 (d, 2H, *J* = 8.6 Hz), 7.12-7.05 (m, 2H), 6.73 (d, 2H, *J* = 8.6 Hz), 2.59 (q, 3H, *J* = 2.5 Hz).

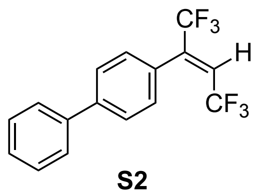
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.7, 142.2 (q, *J* = 2.2 Hz), 139.8 (q, *J* = 31.7 Hz), 135.5, 130.0, 129.8, 129.4 (q, *J* = 1.1 Hz), 128.2, 127.7, 122.2, 122.0 (q, *J* = 279.0 Hz), 17.0 (q, *J* = 2.9 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -59.1 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{16}H_{12}ClF_3NaO_3S^+$ $[M+Na]^+$ 399.0040, found 399.0038.



S1



S2

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (100:1 to 50:1 petroleum ether/EtOAc) to afford **S1** (25.5 mg, 37%) and **S2** (24.5 mg, 39% yield) as white solids.

Methyl (*E*)-3,3,3-Trifluoro-2-([1,1'-biphenyl]-4-yl)prop-1-ene-1-sulfonate (S1)

m.p. 117.9–119.3 ºC.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, 2H, J = 8.5 Hz), 7.62 (d, 2H, J = 6.9 Hz), 7.51-7.35 (m, 4H), 3.39 (t, 1H, J = 7.2 Hz), 7.07 (q, 1H, J = 1.3 Hz), 3.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 143.3 (q, J = 32.0 Hz), 139.8, 129.3, 129.2 (q, J = 5.4 Hz), 128.9, 128.0, 127.2, 127.1, 126.7, 121.6 (q, J = 276.6 Hz), 56.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -67.2.

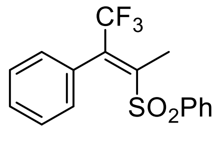
HRMS (ESI) calcd for $C_{16}H_{13}F_3NaO_3S^+$ [M+Na]$^+$ 365.0430, found 365.0423.

(*E*)-4-(1,1,1,4,4,4-Hexafluoro-3-methylbut-2-en-2-yl)-1,1'-biphenyl (S2)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, 2H, J = 8.3 Hz), 7.61 (d, 2H, J = 8.0 Hz), 7.46 (t, 2H, J = 7.5 Hz), 7.42-7.34 (m, 3H), 6.52 (qq, 1H, J = 7.3, 1.4 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -57.9 (dq, J = 7.3, 1.4 Hz), -68.1.

The ^{1}H NMR and ^{19}F NMR spectral data correspond well to those previously reported.[15a]



(*E*)-(1,1,1-Trifluoro-3-(phenylsulfonyl)but-2-en-2-yl)benzene (S3)

Following the general procedure A, the crude product was purified by flash chromatography on silica gel (80:1 petroleum ether/EtOAc) to afford **S3** as a white solid (20.4 mg, 31% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (tt, 1H, *J* = 7.2, 1.6 Hz), 7.41-7.27 (m, 5 H), 7.20 (dd, 2H, *J* = 7.8, 7.2 Hz), 6.94 (d, 2H, *J* = 7.8 Hz), 2.50 (q, 3H, *J* = 2.5 Hz).

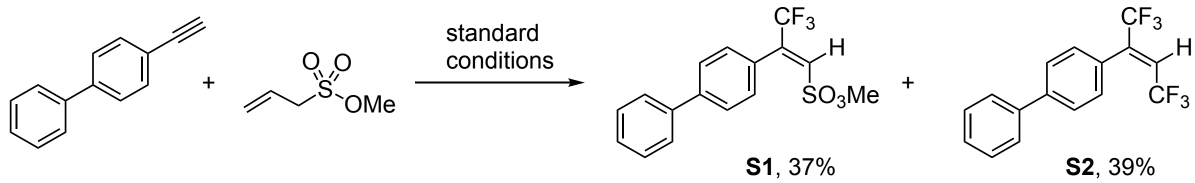
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3 (q, *J* = 2.3 Hz), 139.5, 138.4 (q, *J* = 31.5 Hz), 133.3, 130.6 (q, *J* = 1.3 Hz), 129.8, 128.9, 128.8, 127.8, 127.6, 122.4 (q, *J* = 278.2 Hz), 15.9 (q, *J* = 2.7 Hz).

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.9 (q, *J* = 2.5 Hz).

HRMS (ESI) calcd for $C_{16}H_{13}F_3NaO_2S^+$ $[M+Na]^+$ 349.0481, found 349.0480.

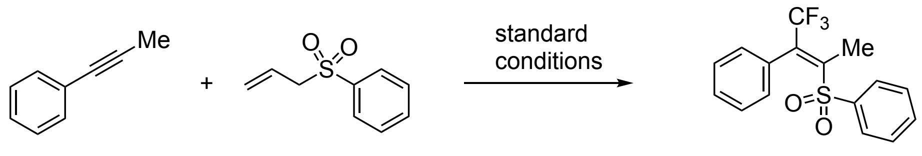
V. Additional substrates explored

(1)



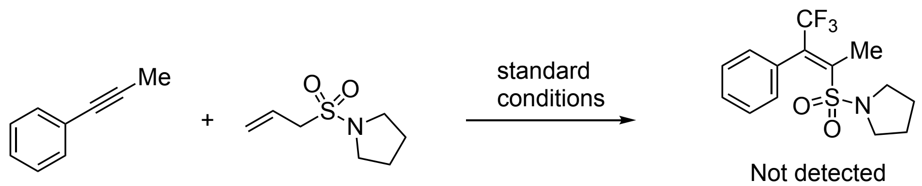
S1, 37% **S2**, 39%

(2)



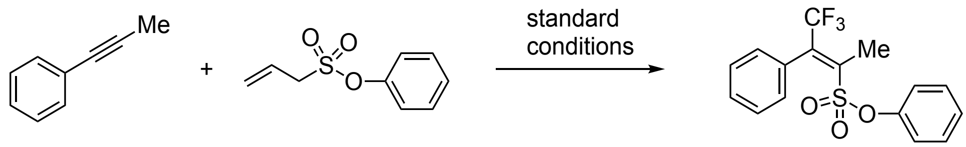
S3, 31%

(3)



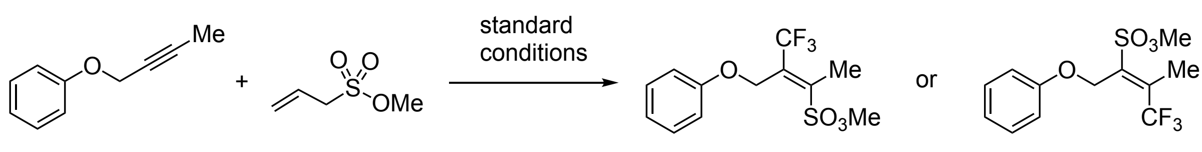
Not detected

(4)



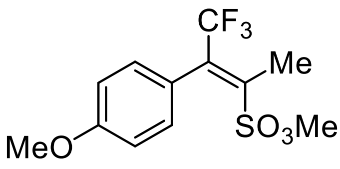
Not detected

(5)



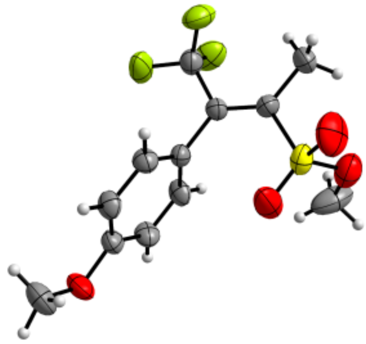
Not detected

VI. Single Crystal X-Ray Data

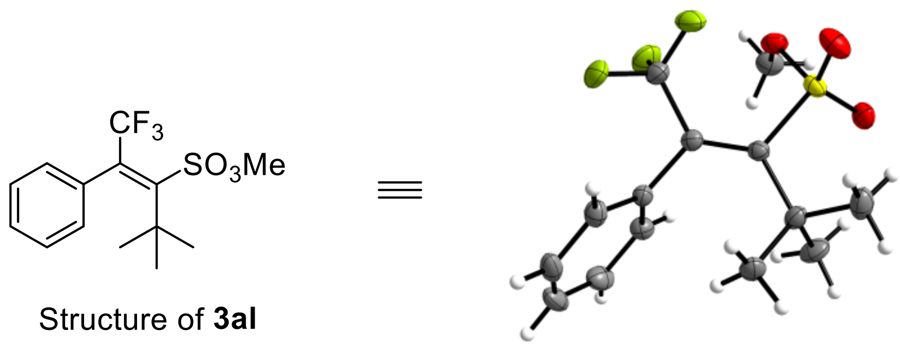


Structure of **3a**

≡

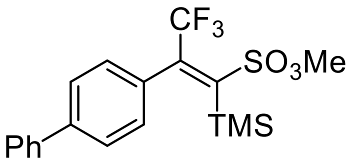


CDCC	**2083910**
Identification code	**3a**
Empirical formula	$C_{12}H_{13}F_3O_4S$
Formula weight	310.28
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.086(2)
b/Å	5.508(2)
c/Å	12.766(3)
α/°	90
β/°	108.14(3)
γ/°	90
Volume/Å^3	674.0(3)
Z	2
ρ_{calc}g/cm^3	1.529
μ/mm^{-1}	0.286
F (000)	320.0
Crystal size/mm^3	0.13 × 0.12 × 0.10
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.25 to 55.036
Index ranges	-13 ≤ h ≤ 13, -4 ≤ k ≤ 7, -16 ≤ l ≤ 15
Reflections collected	5559
Independent reflections	2333 [R_{int} = 0.0450, R_{sigma} = 0.0529]
Data/restraints/parameters	2333/1/185
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0576, wR_2 = 0.1507
Final R indexes [all data]	R_1 = 0.0709, wR_2 = 0.1614
Largest diff. peak/hole / e Å^{-3}	0.81/-0.27



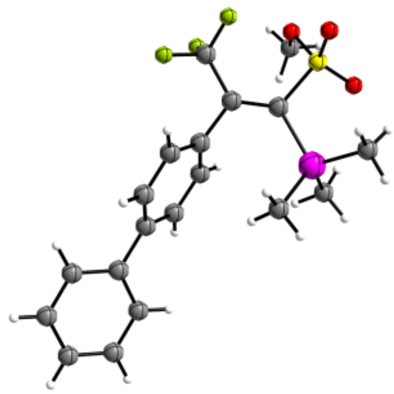
Structure of **3al**

CDCC	**2083911**
Identification code	**3al**
Empirical formula	$C_{14}H_{17}F_3O_3S$
Formula weight	322.33
Temperature/K	170.00(10) K
Crystal system	monoclinic
Space group	P 1 21/c 1
a/Å	6.8048(3)
b/Å	12.4774(5)
c/Å	17.3856(6)
α/°	90
β/°	93.185(3)
γ/°	90
Volume/Å^3	1473.87(10)
Z	4
Density (calculated)	1.453 Mg/m^3
Absorption coefficient	0.259 mm^{-1}
F (000)	672
Crystal size/mm^3	0.38 × 0.32 × 0.26
2Θ range for data collection/°	3.265 to 27.484
Index ranges	-8<=h<=8, -16<=k<=16, -22<=l<=22
Reflections collected	25409
Independent reflections	3377 [R(int) = 0.0533]
Data/restraints/parameters	3377/0/194
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R1 = 0.0347, wR2 = 0.0899
Final R indexes [all data]	R1 = 0.0401, wR2 = 0.0935
Largest diff. peak/hole / e Å^{-3}	0.337 and -0.486 e Å^{-3}

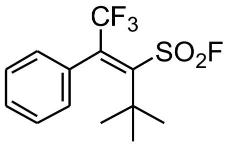


Structure of **3am**

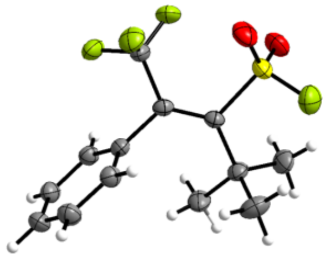
$\equiv$



CDCC	**2083912**
Identification code	**3am**
Empirical formula	$C_{19}H_{21}F_3O_3SSi$
Formula weight	414.51
Temperature/K	193.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.4060(3)
b/Å	15.9894(6)
c/Å	34.9562(12)
α/°	90
β/°	94.362(3)
γ/°	90
Volume/$Å^3$	4127.4(3)
Z	8
ρ_{calc}g/cm^3	1.334
μ/mm^{-1}	1.519
F (000)	1728.0
Crystal size/mm^3	0.05 × 0.01 × 0.01
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	6.526 to 110.184
Index ranges	-9 ≤ h ≤ 8, -19 ≤ k ≤ 19, -40 ≤ l ≤ 42
Reflections collected	46817
Independent reflections	7828 [R_{int} = 0.0959, R_{sigma} = 0.0793]
Data/restraints/parameters	7828/0/495
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0718, wR_2 = 0.1544
Final R indexes [all data]	R_1 = 0.1485, wR_2 = 0.1955
Largest diff. peak/hole / e $Å^{-3}$	0.27/-0.54



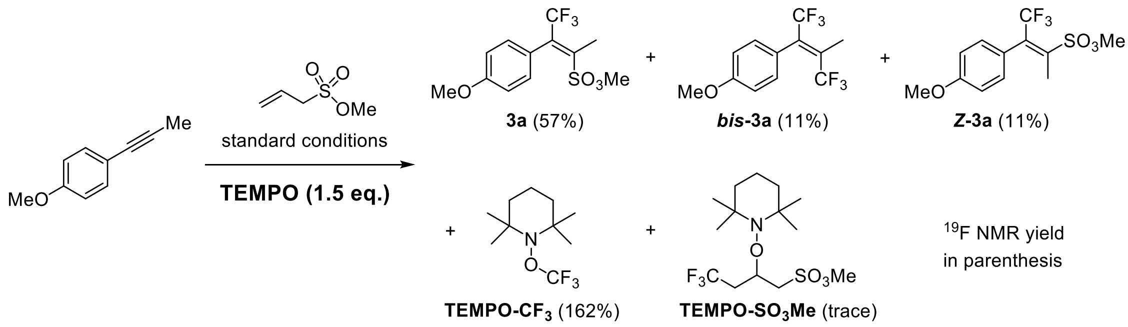
Structure of **5o**

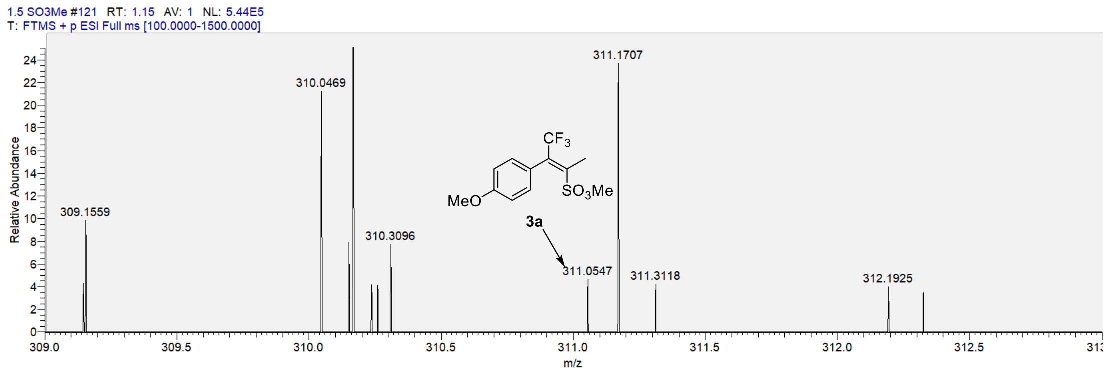


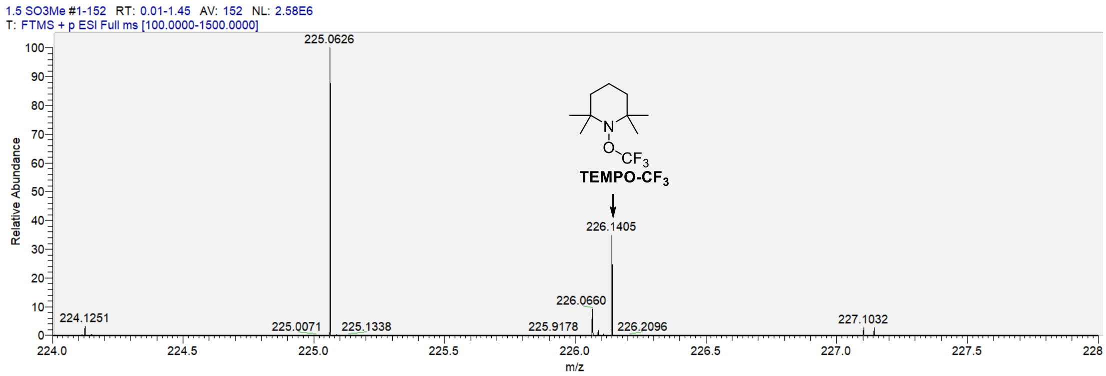
CDCC	**2083913**
Identification code	**5o**
Empirical formula	$C_{13}H_{14}F_4O_2S$
Formula weight	310.30
Temperature/K	273.15
Crystal system	monoclinic
Space group	Pc
a/Å	11.1315(7)
b/Å	8.3917(5)
c/Å	15.5384(10)
α/°	90
β/°	109.425(3)
γ/°	90
Volume/Å^3	1368.85(15)
Z	4
ρ_{calc}g/cm^3	1.506
μ/mm^{-1}	2.556
F (000)	640.0
Crystal size/mm^3	0.11× 0.10 × 0.09
Radiation	MoKα (λ = 1.54178)
2Θ range for data collection/°	4.25 to 55.036
Index ranges	-13 ≤ h ≤ 12, -9 ≤ k ≤ 10, -16 ≤ l ≤ 18
Reflections collected	8209
Independent reflections	3662 [R_{int} = 0.0193, R_{sigma} = 0.0321]
Data/restraints/parameters	3662/3/367
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0246, wR_2 = 0.0623
Final R indexes [all data]	R_1 = 0.0249, wR_2 = 0.0625
Largest diff. peak/hole / e Å^{-3}	0.21/-0.24

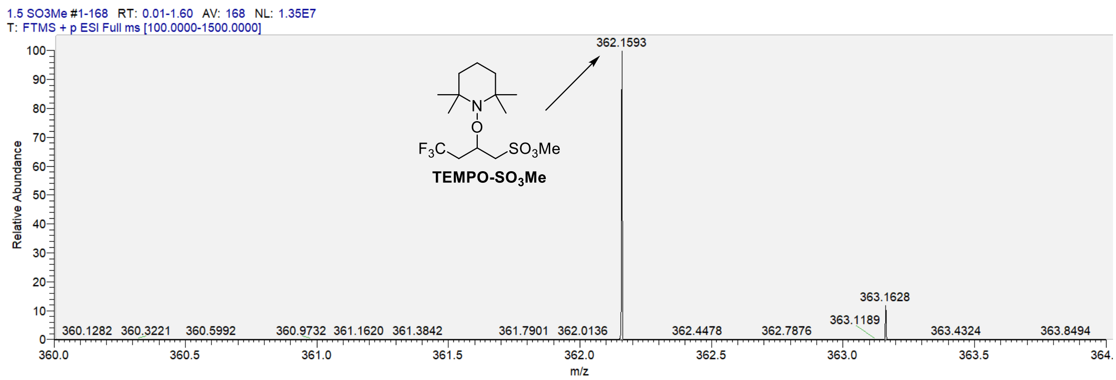
VII. Mechanistic studies

(1) Standard reaction in the presence of 1.5 equiv. of TEMPO

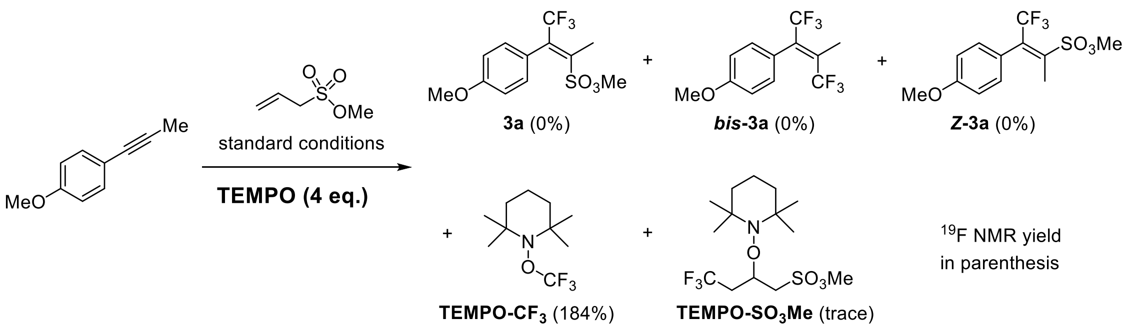


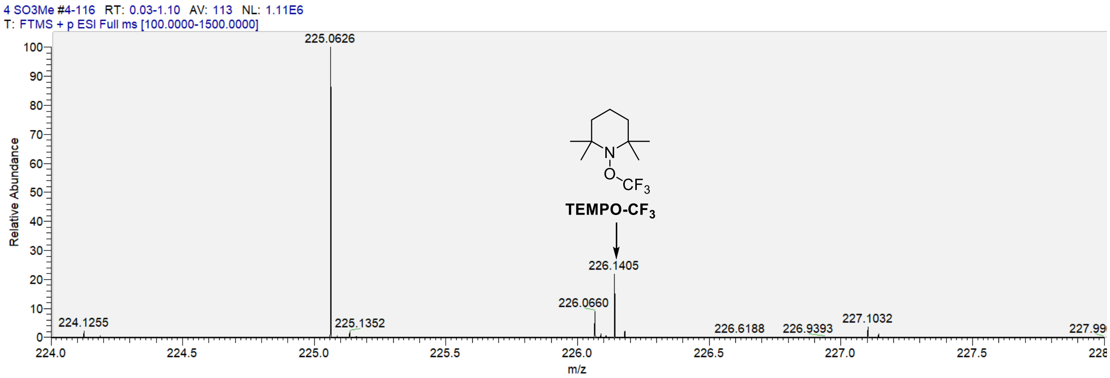


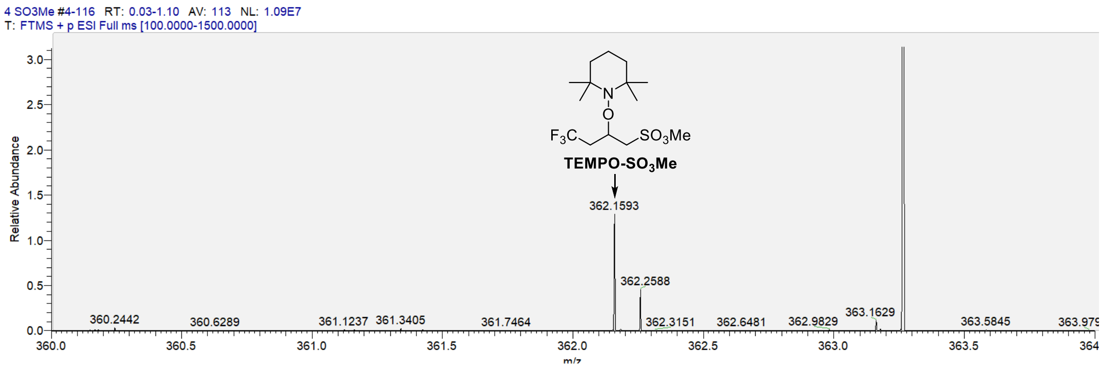




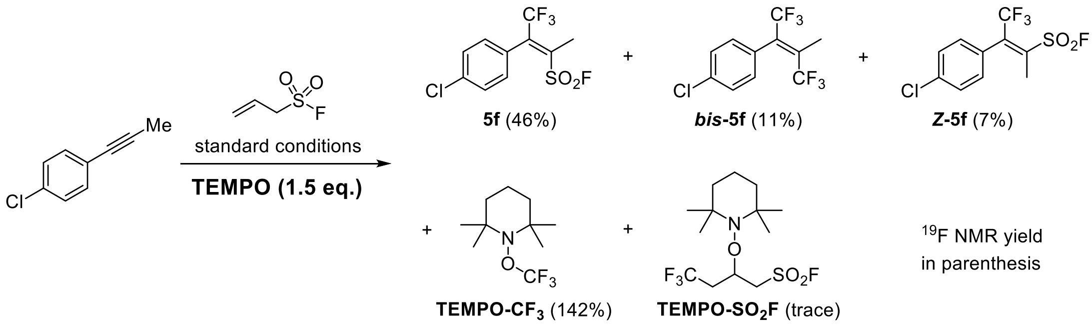
(2) Standard reaction in the presence of 4 equiv. of TEMPO

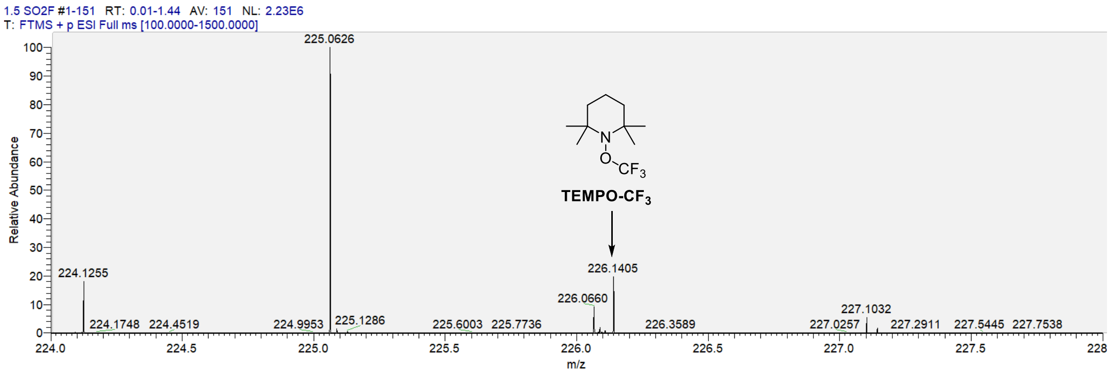


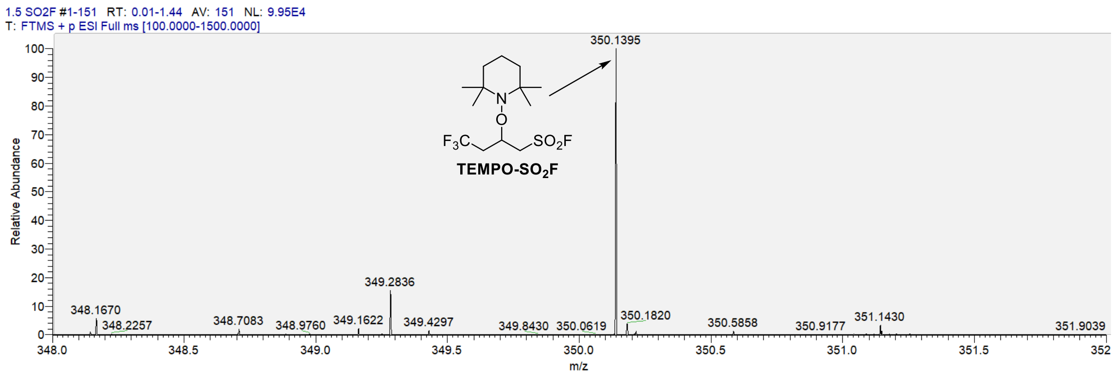




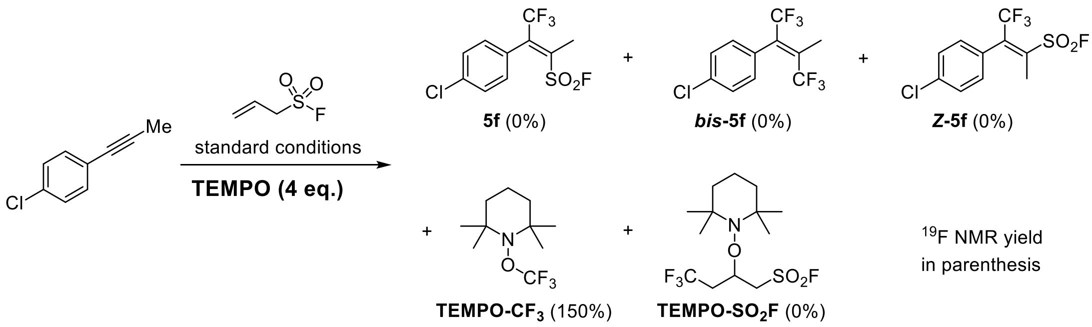
(3) Standard reaction in the presence of 1.5 equiv. of TEMPO

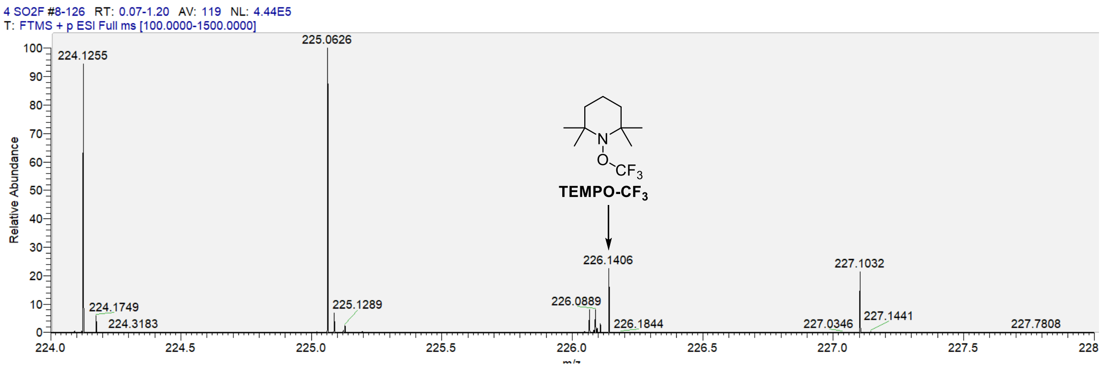






(4) Standard reaction in the presence of 4 equiv. of TEMPO





VIII. Computational studies

8.1 Computational details

All calculations were carried out by using the Gaussian 09 suite of computational programs.[8] The obtained transition states were fully optimized at the DFT level using the M06-L functional,[9] which has been found reliable in completing the thermo-chemistry calculations of transition-metal-containing systems.[10] The standard 6-311G** basis set[11] was applied for all atoms except the Cu atom, in which LANL2DZ ECP was used.[12] Frequencies were analytically computed at the same level of theory to get the thermodynamic corrections and to confirm whether the structures are the corresponding transition states (only one imaginary frequency). Electronic energies were obtained from single-point calculations on the M06-L/LANL2DZ(Cu)-6-311G** geometries using M06-L functional with the def2-TZVPP basis set for all atoms.[13] The obtained Gibbs free energies in the gas phase were reported herein. All energies were reported in kcal/mol. Visualization was completed using VMD (Visual Molecular Dynamics)[14] and CLYview software.[15]

Previous studies demonstrated that a trifluoromethyl radical and bpyCu$(CF_3)_2$ species were generated when bpyCu$(CF_3)_3$ was exposed to light.[16] Moreover, the binding of sulfate to the copper species were found to lower the overall activation energy and accelerate the reaction rate. In view that hydrogen sulfate could be generated under our reaction conditions, we use bpyCu$(CF_3)(OSO_3H)$ and trifluoro-methyl radical, together with prop-1-yn-1-ylbenzene **1b** and methyl prop-2-ene-1-sulfonate **2a**, as the starting point in this calculation (Figure S1). The computational results are reported herein.

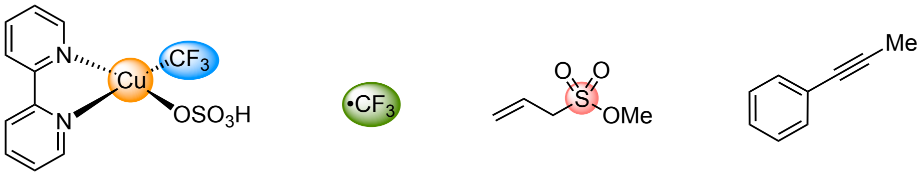


Figure S1. Model catalysts and substrates.

8.2. Computational results and discussion

8.2.1 The potential energy surface leading to the major product

As shown in Figure S2, the alkoxysulfonyltrifluoromethylation process proceeded facilely through the addition of trifluoromethyl radical into the unsaturated double or triple bond. The activation energy of **TS1**, which corresponded to the addition of CF_3• into allyl sulfonate, was calculated to be 9.2 kcal/mol. This was 0.8 kcal/mol lower than the energy of **TSA** that was formed from the addition of CF_3• to alkynyl carbon. This disparity might originate from the steric effect of the methyl group on the alkyne and allow for the former process more feasible herein. Importantly, the resulting intermediates after the addition steps, **INT1** and **INTA**, were far more stable than the corresponding transition states **TS1** and **TSA** by > 30 kcal/mol. Such high backward energy rendered the addition processes irreversible.

Along the pathway of product formation, a secondary alkyl radical species **INT1** could be obtained *via* **TS1**. This transition state adopted a planar structure to accommodate the unpaired electron. Subsequently, sulfonyl radical **INT2** could be readily accessed *via* β-fragmentation by passing the energy barrier of **TS2** in 12.2 kcal/mol. Free sulfonyl radical **INT2**, together with 4,4,4-trifluoromethyl-1-butene, was found to be more stable than **INT1** by 3.0 kcal/mol. The addition of sulfonyl radical **INT2** onto the carbon atom adjacent to methyl in alkyne required activation energy of 12.5 kcal/mol relative to **INT2**. Then, a linear allenyl radical intermediate **INT3** was obtained, which would recombine with the copper(II) species to form intermediate **INT4$_{E}$**. This intermediate was 37.9 kcal/mol more stabilized than the starting point. Eventually, the reductive elimination proceeded through **TS4$_{E}$** in energetic barrier of 12.3 kcal/mol to afford the Cu(I) species **INT5$_{E}$** coordinated to the double bond in product.

In conclusion, the formation of the product could be achieved *via* the sequential generation of sulfonyl radical, addition of sulfonyl radical into the triple bond, and the reductive elimination. Among these, the preference of the S-addition product was mainly determined by the energy difference between **TS1** and **TSA**, which would irreversibly lead to the corresponding product. The following steps could facilely proceed, because the activation energy barriers of the following transition states were all less than 13 kcal/mol.

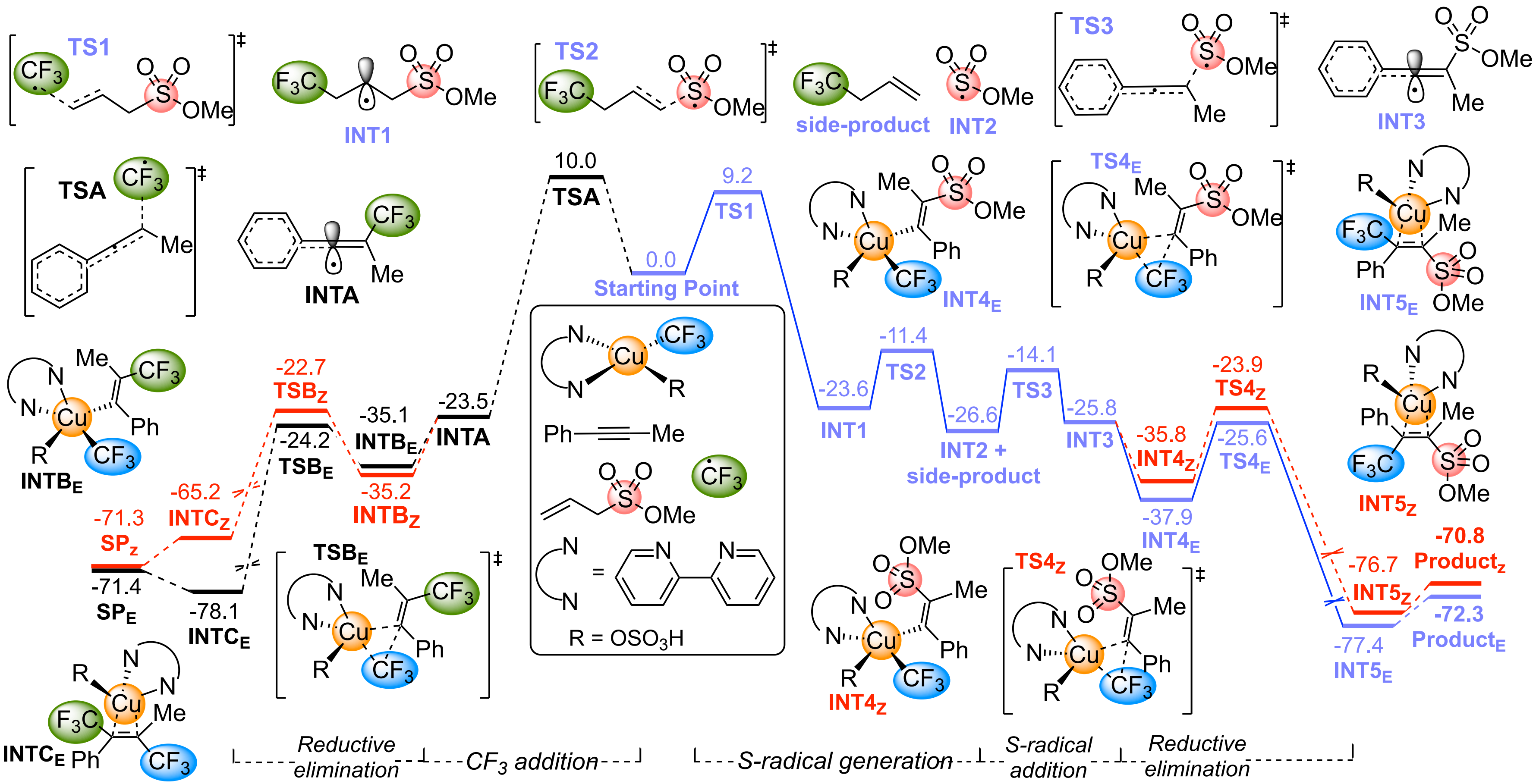


Figure S2. The potential energy surface leading to the products.

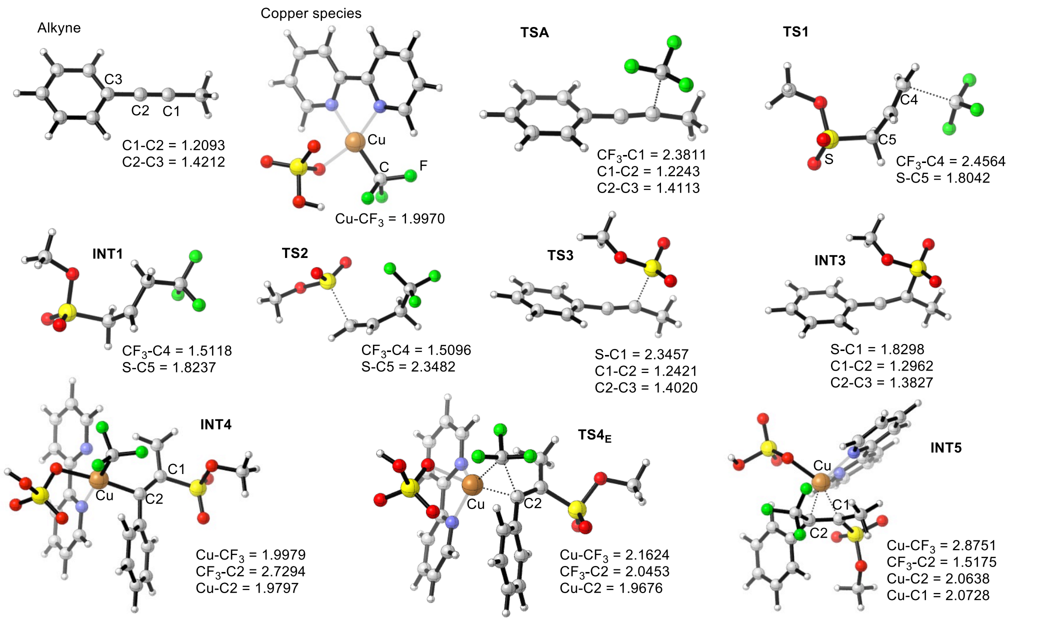


Figure S3. The optimized geometric structures of selected intermediates and transition states. Bond lengths are shown in angstroms (Å).

8.2.2 Other competing reaction pathways

Theoretically, both *sp*-hybridized carbons on the alkynyl substrate were prone to be attacked by a radical species (**Figure S4**). Besides **TSA** and **TS3**, the transition states **TS1'** and **TS3'** were depicted by the addition of CF_3• and $MeOSO_2$• into the alkynyl carbon adjacent to the phenyl group, respectively. The latter cases were calculated to be more energy-demanding with 15.0 kcal/mol for **TS1'** and -12.4 kcal/mol for **TS3'**, respectively.

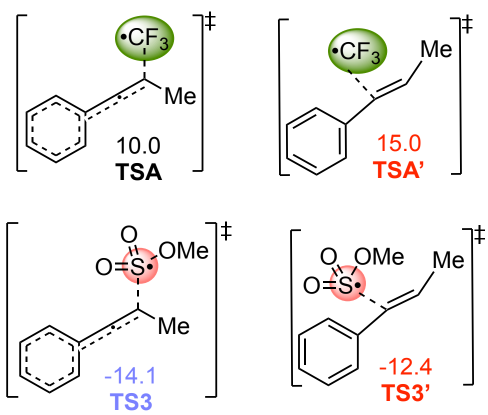


Figure S4. Comparison of the radical addition steps.

Furthermore, the transition states of reductive elimination steps, which corresponded to the formation of *E*/*Z* isomers in this difunctionalization process, were shown in **Figure S5**. No matter the reactions were triggered by CF_3 radical or sulfonyl radical, the transition states leading to the formation of *E*-isomers were uniformly favored by approximately 1.5 kcal/mol. This was consistent with the experimental observation.

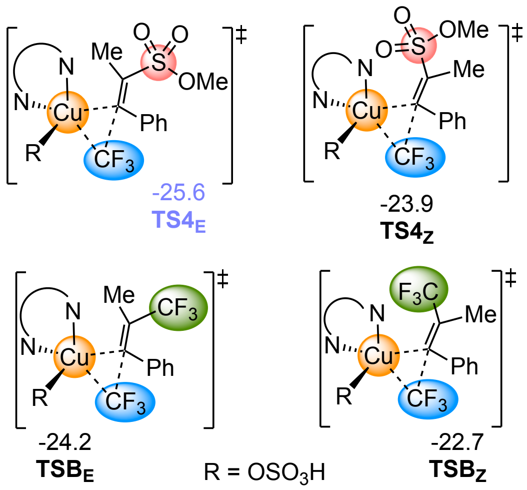


Figure S5. Comparison of the reductive elimination steps.

8.3. Cartesian coordinates

Alkyne

C	0.749193	1.207135	-0.000558
C	0.032248	-0.000210	-0.000987
C	0.749490	-1.207353	-0.000553
C	2.136429	-1.202745	0.000396
C	2.835822	0.000179	0.000904
C	2.136098	1.202932	0.000394
H	0.201512	2.143618	-0.000834
H	0.202021	-2.143965	-0.000825
H	2.675699	-2.144732	0.000821
H	3.920863	0.000338	0.001751
H	2.675091	2.145079	0.000817
C	-1.388897	-0.000232	-0.001295

C	-2.598164	0.000415	-0.000915
C	-4.043428	0.000215	0.001224
H	-4.440892	-0.424369	0.927931
H	-4.443056	1.013570	-0.094173
H	-4.443982	-0.591554	-0.827149

CF_3 radical

C	0.000000	0.000000	0.335151
F	0.000000	1.256101	-0.074478
F	1.087815	-0.628050	-0.074478

Sulfonate

C	-3.287458	-0.365804	0.257941
H	-3.232097	-1.365186	0.679921
H	-4.201581	0.189128	0.433979
C	-2.284177	0.151336	-0.441410
H	-2.352376	1.158769	-0.845610
C	-1.013989	-0.575876	-0.709578
H	-1.033294	-1.606909	-0.352740
H	-0.735206	-0.561050	-1.766434
S	0.358341	0.230062	0.136781
O	0.292230	-0.008985	1.562325
O	0.516825	1.577207	-0.370080
O	1.521824	-0.724376	-0.512408
C	2.853199	-0.409999	-0.078057
H	3.500935	-1.117513	-0.591184
H	3.120648	0.610355	-0.362293
H	2.947036	-0.537289	1.003791

TS1

C	1.132310	1.122751	0.501153
H	1.138094	1.493178	-0.520117
H	1.626304	1.738076	1.244217
C	0.365458	0.078683	0.855991
H	0.290449	-0.221317	1.897578
C	-0.376692	-0.745930	-0.128296
H	-0.128640	-0.508500	-1.164850
H	-0.235682	-1.820729	0.022616
S	-2.163924	-0.540059	0.008021
O	-2.563107	-0.537321	1.400903
O	-2.821806	-1.409748	-0.941885
O	-2.201528	0.997674	-0.549660
C	-3.410610	1.713907	-0.259896
H	-3.259260	2.711179	-0.666283
H	-4.268096	1.244017	-0.748782
H	-3.576537	1.767660	0.818262
C	3.274535	0.078547	-0.094070
F	3.853234	-0.375713	1.005296
F	2.928053	-0.933002	-0.880991
F	4.087343	0.902581	-0.739321

INT1

C	1.414553	0.552464	0.459545
H	0.975444	1.222329	-0.285697
H	1.574070	1.133482	1.372331
C	0.543892	-0.624127	0.706885
H	0.576826	-1.119067	1.671149
C	-0.397214	-1.118103	-0.306046
H	-0.141994	-0.828379	-1.328217
H	-0.544850	-2.201119	-0.273031

S	-2.083143	-0.475599	-0.040215
O	-2.473082	-0.666708	1.341109
O	-2.956125	-0.893156	-1.115510
O	-1.679010	1.103790	-0.252166
C	-2.735069	2.029662	0.047334
H	-2.312973	3.017560	-0.121837
H	-3.586399	1.873807	-0.620047
H	-3.049350	1.930642	1.089127
C	2.780434	0.147753	-0.046711
F	3.417713	-0.648681	0.829225
F	2.691122	-0.532077	-1.208322
F	3.565129	1.214427	-0.266885

TSA

C	-1.298391	0.553304	-0.132812
C	-1.833249	-0.239380	-1.165590
C	-2.086766	0.801084	1.006094
C	-3.111291	-0.763188	-1.057419
C	-3.364463	0.273247	1.102916
C	-3.882770	-0.509207	0.074087
H	-1.226265	-0.438936	-2.042102
H	-1.679015	1.409611	1.805924
H	-3.509409	-1.376126	-1.859369
H	-3.960947	0.471824	1.987284
H	-4.883191	-0.920925	0.154496
C	0.005291	1.082962	-0.240639
C	1.193946	1.368821	-0.305569
C	2.224324	-0.718611	0.195229
F	3.121286	-0.999028	-0.751497
F	2.836998	-0.651988	1.375369

F	1.292184	-1.658200	0.222512
C	2.435248	2.105153	-0.486338
H	3.050973	2.073738	0.416875
H	3.031049	1.685390	-1.300727
H	2.231303	3.153250	-0.719586

INTA

C	-1.298772	0.040594	0.172608
C	-2.036328	1.220634	-0.144314
C	-2.017898	-1.187634	0.279892
C	-3.401116	1.161501	-0.333566
C	-3.382537	-1.217748	0.085436
C	-4.087779	-0.050694	-0.221766
H	-1.503412	2.160961	-0.234321
H	-1.470129	-2.093679	0.514533
H	-3.944959	2.069753	-0.573024
H	-3.911919	-2.161403	0.171820
H	-5.161200	-0.085661	-0.372798
C	0.058382	0.077577	0.355285
C	1.327521	0.120612	0.645255
C	2.354410	-0.078058	-0.438051
F	3.158704	1.002100	-0.547637
F	3.162918	-1.122763	-0.153159
F	1.819863	-0.303239	-1.641726
C	1.905724	0.358339	2.014648
H	2.523344	-0.490347	2.321115
H	2.547537	1.243632	2.010887
H	1.117731	0.501117	2.751931

TSA’

C	-0.916785	0.484406	-0.116949
C	-1.865875	1.342332	0.460639
C	-1.347145	-0.744728	-0.632972
C	-3.202847	0.978483	0.516702
C	-2.687478	-1.100496	-0.576495
C	-3.619936	-0.243896	-0.001636
H	-1.535721	2.294122	0.863156
H	-0.627427	-1.415732	-1.087311
H	-3.923205	1.652676	0.968702
H	-3.004714	-2.054587	-0.984662
H	-4.666278	-0.527273	0.043339
C	0.455500	0.911941	-0.183131
C	1.344371	1.760836	-0.273472
C	1.625199	-1.020182	0.187288
F	1.044390	-1.780150	1.110146
F	1.778799	-1.727408	-0.935208
F	2.823502	-0.636131	0.621397
C	2.578083	2.502904	-0.353916
H	2.673414	3.210443	0.474806
H	3.442013	1.830028	-0.316290
H	2.643168	3.073911	-1.285095

TS2

C	-1.857975	0.930356	-0.732457
H	-2.611090	1.670974	-1.030039
H	-1.474544	0.465403	-1.644726
C	-0.765147	1.558018	0.057339
H	-0.989407	1.822764	1.087905
C	0.522514	1.672696	-0.404879
H	0.723344	1.592031	-1.470419

H	1.244295	2.249216	0.165574
S	1.562000	-0.410634	-0.099882
O	1.072803	-1.278559	-1.156606
O	1.561301	-0.815706	1.301203
O	3.127184	-0.057020	-0.550651
C	3.969348	0.445489	0.489466
H	4.946779	0.581654	0.029639
H	3.612609	1.409997	0.866019
H	4.035922	-0.261625	1.318081
C	-2.585994	-0.128252	0.060136
F	-1.746921	-1.074097	0.506700
F	-3.196906	0.402110	1.139475
F	-3.530251	-0.730217	-0.678743

Side-product

C	0.445703	0.286203	-0.791061
H	0.596685	1.368092	-0.825405
H	0.236778	-0.049409	-1.813053
C	1.642680	-0.408332	-0.229444
H	1.574329	-1.491916	-0.153498
C	2.744045	0.215601	0.168709
H	2.838658	1.296385	0.110154
H	3.594038	-0.326526	0.566912
C	-0.806632	0.028863	0.006466
F	-1.125342	-1.281275	0.027469
F	-0.680513	0.425167	1.283835
F	-1.860285	0.686036	-0.512763

INT2

S	0.579816	0.059769	-0.265679

O	0.397425	1.442938	0.187213
O	1.654576	-0.791607	0.229495
O	-0.811297	-0.791804	0.073674
C	-2.028328	-0.037275	0.038315
H	-2.806370	-0.746651	0.315069
H	-1.995517	0.790914	0.748010
H	-2.230841	0.346869	-0.965152

TS3

C	1.466237	0.779304	0.026551
C	1.952372	0.285014	1.255390
C	2.277325	0.665327	-1.122830
C	3.201020	-0.307638	1.321808
C	3.525879	0.074134	-1.040343
C	3.992843	-0.414712	0.179014
H	1.321519	0.355537	2.134518
H	1.905072	1.044131	-2.068935
H	3.561420	-0.694091	2.269171
H	4.141668	-0.008673	-1.929833
H	4.971860	-0.878615	0.238411
C	0.187037	1.347119	-0.055995
C	-1.030585	1.588639	-0.098582
C	-2.166834	2.505137	-0.182248
H	-2.807161	2.255194	-1.032410
H	-2.781265	2.446650	0.719991
H	-1.817443	3.532740	-0.300598
S	-2.157641	-0.454883	0.138314
O	-2.884784	-0.815292	-1.081439
O	-2.805956	-0.490763	1.442198
O	-0.866927	-1.485180	0.301630

C	-0.271858	-1.915591	-0.926338
H	0.693098	-2.341599	-0.650362
H	-0.896129	-2.664978	-1.417710
H	-0.109678	-1.078694	-1.612950

TS3'

C	-1.188853	0.528357	-0.214170
C	-2.123429	1.248450	0.546251
C	-1.597777	-0.640552	-0.866648
C	-3.436153	0.812575	0.640137
C	-2.915051	-1.066964	-0.768549
C	-3.837285	-0.346221	-0.017931
H	-1.803194	2.150944	1.057284
H	-0.884768	-1.208811	-1.453070
H	-4.148478	1.379184	1.231146
H	-3.221092	-1.971786	-1.283050
H	-4.864938	-0.686416	0.056378
C	0.164249	1.033694	-0.301673
C	0.883300	2.059843	-0.281338
C	2.046581	2.906874	-0.302353
H	2.061599	3.544453	-1.190952
H	2.089869	3.554265	0.578142
H	2.951175	2.285428	-0.310851
S	1.606236	-0.734850	-0.354316
O	2.899804	-0.171340	0.023412
O	1.489267	-1.631260	-1.495800
O	1.033679	-1.642286	0.917121
C	1.187315	-1.039523	2.202657
H	0.774627	-1.755217	2.911591
H	2.240357	-0.853361	2.425231

H	0.625690	-0.101188	2.271037

INT3

C	1.428385	0.649638	-0.116800
C	2.029362	0.594980	1.169867
C	2.199871	0.240141	-1.237888
C	3.326664	0.145027	1.314456
C	3.495963	-0.205891	-1.069549
C	4.070081	-0.256320	0.202307
H	1.443971	0.894552	2.031992
H	1.753680	0.285902	-2.226292
H	3.768241	0.099096	2.304750
H	4.071098	-0.516699	-1.935628
H	5.089384	-0.606237	0.325861
C	0.132346	1.107155	-0.267871
C	-1.162296	1.170782	-0.262518
C	-2.061752	2.323679	-0.580428
H	-2.722575	2.075994	-1.415508
H	-2.692830	2.566065	0.278772
H	-1.473688	3.201512	-0.844379
S	-2.116748	-0.313671	0.220821
O	-2.873811	-0.768663	-0.929946
O	-2.752822	-0.047654	1.488235
O	-0.938277	-1.384699	0.548775
C	-0.446517	-2.154926	-0.558871
H	0.424772	-2.683139	-0.174011
H	-1.203110	-2.862740	-0.900394
H	-0.144330	-1.513022	-1.391040

CuS

Cu	-0.390360	-0.368312	-0.529671
N	0.924849	1.228414	-0.680604
C	0.570585	2.464498	-1.037723
H	-0.463767	2.581243	-1.346577
C	1.458125	3.530958	-0.987295
H	1.130103	4.520669	-1.280200
C	2.751412	3.296995	-0.542927
H	3.470258	4.107029	-0.483021
C	3.116748	2.013542	-0.161642
H	4.118515	1.817669	0.200551
C	2.174174	0.991261	-0.239796
N	1.405971	-1.259148	0.041346
C	2.442567	-0.402139	0.162296
C	3.672738	-0.831994	0.655397
H	4.498340	-0.137016	0.746960
C	3.828620	-2.155473	1.038161
H	4.779301	-2.501397	1.428984
C	2.753149	-3.023622	0.919020
H	2.828022	-4.063752	1.211839
C	1.557864	-2.532577	0.412389
H	0.685396	-3.164050	0.292995
C	-1.671522	-1.881217	-0.769742
F	-1.157768	-3.150166	-0.826694
F	-2.570367	-1.920918	0.277170
F	-2.417301	-1.742675	-1.884115
O	-1.974770	0.941292	-0.564116
S	-2.087845	1.312940	0.910309
O	-2.229674	2.728025	1.135750
O	-1.016454	0.594325	1.624596
O	-3.502034	0.673565	1.375502

H	-3.470333	-0.266439	1.138875

INT4$_E$

Cu	0.482468	0.183517	-0.517239
N	1.455588	2.072432	0.482767
C	1.577219	3.298030	-0.022722
H	0.919464	3.538979	-0.853332
C	2.487663	4.233490	0.450475
H	2.545407	5.216949	-0.000354
C	3.316946	3.865309	1.500433
H	4.048072	4.559374	1.900639
C	3.210500	2.586268	2.022819
H	3.871394	2.273997	2.821147
C	2.266986	1.706122	1.486604
N	1.358133	-0.515883	1.233448
C	2.142863	0.309825	1.956251
C	2.830288	-0.162639	3.073848
H	3.434923	0.510681	3.666867
C	2.742086	-1.501111	3.421899
H	3.279288	-1.875980	4.286314
C	1.974495	-2.348945	2.639736
H	1.897758	-3.408671	2.848531
C	1.299650	-1.812846	1.553655
H	0.719555	-2.441363	0.889483
C	-0.263448	0.665370	-2.306976
F	0.155312	-0.257920	-3.179979
F	-1.571134	0.855512	-2.534281
F	0.351161	1.835395	-2.613943
C	-1.390834	-0.093791	0.060025
C	-2.154105	0.971255	0.283726

C	-1.574224	-1.514718	0.263450
C	-1.891320	-2.023929	1.535547
C	-1.323129	-2.412654	-0.786199
C	-1.999862	-3.390231	1.733643
C	-1.434487	-3.778848	-0.579744
C	-1.773411	-4.271230	0.677890
H	-2.055076	-1.334607	2.356820
H	-1.010980	-2.031081	-1.752124
H	-2.258765	-3.771352	2.715893
H	-1.231905	-4.460629	-1.398105
H	-1.848269	-5.341668	0.839199
O	2.328160	0.151416	-1.357006
S	2.806565	-1.282270	-1.490228
O	3.233674	-1.418744	-3.061093
O	1.684080	-2.204545	-1.362253
O	4.000354	-1.521798	-0.698100
H	4.087839	-0.981360	-3.161778
C	-1.811209	2.407855	0.066582
H	-2.598410	2.914004	-0.495720
H	-1.686953	2.934397	1.016972
H	-0.884624	2.478306	-0.497658
S	-3.863305	0.785840	0.804289
O	-4.118300	1.746558	1.862248
O	-4.290046	-0.588042	0.960659
O	-4.512943	1.360345	-0.590535
C	-5.930313	1.173220	-0.704663
H	-6.458988	1.705708	0.090854
H	-6.199243	1.595414	-1.670245
H	-6.182286	0.110740	-0.677151

TS4$_E$

Cu	0.593315	0.115089	-0.516052
N	1.494126	2.101192	0.089448
C	1.667625	3.160412	-0.700027
H	1.052955	3.191179	-1.596181
C	2.575848	4.173993	-0.428556
H	2.678382	5.012250	-1.107117
C	3.345323	4.071260	0.722144
H	4.072685	4.835604	0.973356
C	3.188975	2.961748	1.537393
H	3.810058	2.843854	2.416394
C	2.255422	1.982998	1.189998
N	1.421382	-0.261427	1.371743
C	2.108391	0.731408	1.965569
C	2.690992	0.550875	3.219913
H	3.213484	1.365062	3.706021
C	2.594854	-0.684322	3.842613
H	3.044574	-0.839068	4.817466
C	1.934533	-1.717489	3.193950
H	1.864143	-2.708054	3.626264
C	1.361260	-1.460683	1.956653
H	0.862999	-2.237544	1.387640
C	-0.683142	0.039364	-2.259868
F	0.122850	-0.826854	-2.883226
F	-1.915383	-0.219858	-2.719489
F	-0.372494	1.286139	-2.676848
C	-1.354557	-0.093868	-0.332503
C	-2.151011	0.968431	-0.104357
C	-1.496293	-1.461478	0.160229
C	-1.805190	-1.641208	1.521605

C	-1.258395	-2.592584	-0.631283
C	-1.936052	-2.912612	2.053339
C	-1.381469	-3.862828	-0.088596
C	-1.727723	-4.029470	1.248480
H	-1.931822	-0.770353	2.158533
H	-0.960502	-2.485595	-1.665516
H	-2.190352	-3.031132	3.101285
H	-1.191165	-4.727420	-0.714481
H	-1.818603	-5.026602	1.666503
O	2.441098	-0.029335	-1.438646
S	2.877299	-1.466051	-1.303754
O	3.164032	-1.959438	-2.842572
O	1.745582	-2.301323	-0.898465
O	4.128918	-1.603478	-0.578927
H	4.031002	-1.614742	-3.087171
C	-1.883566	2.394319	-0.455564
H	-2.436514	2.700927	-1.347369
H	-2.196512	3.049594	0.361505
H	-0.820516	2.542123	-0.619361
S	-3.747000	0.729826	0.679618
O	-3.708899	1.270738	2.026579
O	-4.312164	-0.581247	0.443247
O	-4.548306	1.796483	-0.280355
C	-5.976863	1.681445	-0.217713
H	-6.338828	1.875198	0.795707
H	-6.356177	2.444368	-0.893856
H	-6.299376	0.691728	-0.547589

INT5$_E$

Cu	0.442646	-0.417364	-0.269676

N	2.411742	-0.011910	-1.025209
C	2.837583	-0.337484	-2.245707
H	2.141834	-0.912492	-2.851032
C	4.089693	0.019419	-2.724677
H	4.396741	-0.269854	-3.722421
C	4.926009	0.750577	-1.890153
H	5.909973	1.058736	-2.226966
C	4.496209	1.070911	-0.611907
H	5.144379	1.623503	0.056608
C	3.227332	0.663367	-0.196507
N	1.488656	0.375267	1.418379
C	2.708491	0.885133	1.170531
C	3.438076	1.539744	2.160386
H	4.414987	1.954689	1.946187
C	2.896820	1.651072	3.432456
H	3.447709	2.159518	4.216506
C	1.651540	1.095326	3.687685
H	1.199916	1.146019	4.670773
C	0.980771	0.465943	2.648174
H	0.006817	0.013661	2.792695
C	-1.597794	-0.968159	-2.218927
F	-2.163514	-2.116297	-1.856592
F	-2.393216	-0.402964	-3.159384
F	-0.436165	-1.272815	-2.840257
C	-1.431854	-0.027154	-1.039986
C	-0.621291	1.105924	-1.188430
C	-2.554639	-0.114029	-0.057925
C	-2.524328	-0.972731	1.038074
C	-3.683463	0.675797	-0.291269
C	-3.600702	-1.012962	1.914358

C	-4.761948	0.623591	0.583360
C	-4.718506	-0.215017	1.692221
H	-1.651454	-1.589172	1.221949
H	-3.708461	1.330889	-1.157619
H	-3.560857	-1.675185	2.772588
H	-5.636863	1.238679	0.396893
H	-5.558068	-0.250805	2.378849
O	0.512101	-2.399472	-0.312504
S	0.519030	-3.232625	0.951877
O	-0.937325	-4.005864	0.885116
O	0.372300	-2.412070	2.144456
O	1.547414	-4.250576	0.912799
H	-0.911418	-4.596653	0.122846
C	0.003703	1.611430	-2.457908
H	-0.670083	2.345323	-2.914491
H	0.950023	2.113468	-2.257599
H	0.168813	0.815255	-3.178193
S	-0.684799	2.411832	0.053101
O	0.570559	3.130619	-0.030006
O	-1.175699	1.958541	1.336974
O	-1.846237	3.330097	-0.652748
C	-2.760601	3.992038	0.236806
H	-2.245100	4.750268	0.830949
H	-3.491020	4.469005	-0.413910
H	-3.250532	3.269971	0.893613

INT4$_Z$

Cu	-0.092783	-0.116532	-0.535821
N	2.171186	-0.510493	-0.322480
C	3.127266	-0.366819	-1.237103

H	2.837475	0.149101	-2.144204
C	4.425006	-0.830032	-1.051921
H	5.167446	-0.692556	-1.829115
C	4.734647	-1.467143	0.141382
H	5.734629	-1.844264	0.327417
C	3.740747	-1.625539	1.094728
H	3.961804	-2.134517	2.024500
C	2.459094	-1.138658	0.825722
N	0.123943	-0.865467	1.367740
C	1.335634	-1.304634	1.769497
C	1.485744	-1.924633	3.009838
H	2.459286	-2.271551	3.330032
C	0.381643	-2.119016	3.823392
H	0.492159	-2.609577	4.784384
C	-0.861827	-1.697526	3.379682
H	-1.760354	-1.851844	3.963758
C	-0.943651	-1.077926	2.142636
H	-1.896563	-0.765646	1.734144
C	-0.428568	0.454514	-2.417774
F	-1.392110	-0.345583	-2.903806
F	-0.761055	1.707953	-2.730941
F	0.706155	0.158003	-3.062766
C	-1.059105	1.523355	0.007808
C	-0.464331	2.707909	0.185631
C	-2.446234	1.250380	0.367903
C	-2.911656	1.634588	1.641184
C	-3.326602	0.580815	-0.492752
C	-4.219701	1.382069	2.023260
C	-4.637477	0.341596	-0.108712
C	-5.089232	0.738256	1.145598

H	-2.223060	2.115236	2.329791
H	-2.973695	0.226176	-1.450835
H	-4.561105	1.682543	3.008575
H	-5.303285	-0.180227	-0.787129
H	-6.111643	0.533901	1.446036
O	0.159491	-2.037569	-1.260214
S	-0.983675	-2.908276	-0.820691
O	-1.388229	-3.602727	-2.248977
O	-2.119150	-2.084579	-0.391993
O	-0.596480	-3.986933	0.074610
H	-1.850311	-4.421414	-2.032971
C	-1.111424	3.996602	0.601160
H	-0.835370	4.276505	1.622783
H	-0.784991	4.813621	-0.045638
H	-2.195808	3.908754	0.544997
S	1.282472	2.874622	-0.093002
O	1.679578	4.255586	0.096855
O	1.715414	2.168357	-1.283322
O	1.777077	2.020866	1.230790
C	3.188901	2.079475	1.468349
H	3.509415	3.108564	1.650007
H	3.360300	1.475588	2.358222
H	3.745942	1.658064	0.624879

TS4$_{Z}$

Cu	0.004920	0.099683	0.413285
N	2.169992	0.426841	0.698685
C	2.945285	-0.038014	1.678663
H	2.456074	-0.668741	2.409604
C	4.302872	0.242678	1.767307

H	4.887022	-0.155524	2.588310
C	4.878739	1.031696	0.781452
H	5.938297	1.263699	0.802823
C	4.075933	1.527987	-0.233492
H	4.508089	2.147943	-1.008905
C	2.712539	1.221676	-0.238088
N	0.507816	1.331821	-1.206811
C	1.781526	1.773959	-1.245619
C	2.173252	2.757606	-2.153820
H	3.192116	3.122446	-2.160568
C	1.240008	3.301380	-3.022093
H	1.532583	4.075826	-3.722846
C	-0.072405	2.862953	-2.952894
H	-0.846601	3.282962	-3.582908
C	-0.394267	1.884617	-2.023553
H	-1.417285	1.557387	-1.881369
C	-0.863366	-1.207498	1.904962
F	-1.848200	-0.414284	2.307461
F	-1.228689	-2.473580	2.152151
F	0.200194	-0.968040	2.689285
C	-1.093068	-1.468661	-0.115752
C	-0.461656	-2.497092	-0.722023
C	-2.457942	-1.095223	-0.523514
C	-2.620886	-0.635339	-1.839075
C	-3.594306	-1.237590	0.279765
C	-3.870806	-0.280252	-2.321281
C	-4.844132	-0.887174	-0.209570
C	-4.988083	-0.393126	-1.501187
H	-1.747620	-0.570287	-2.481399
H	-3.508902	-1.630650	1.283459

H	-3.972962	0.082180	-3.339035
H	-5.714389	-1.000963	0.427882
H	-5.967437	-0.108084	-1.870384
O	-0.137102	1.834021	1.672433
S	-1.299537	2.614151	1.164354
O	-2.115664	2.895592	2.564951
O	-2.171634	1.768270	0.328819
O	-0.973424	3.916078	0.598803
H	-2.768643	3.577068	2.366989
C	-1.030753	-3.380672	-1.787184
H	-0.615314	-3.135123	-2.770451
H	-0.772470	-4.423181	-1.589477
H	-2.113409	-3.275119	-1.836468
S	1.234100	-2.874077	-0.357728
O	1.555346	-4.207151	-0.824012
O	1.589253	-2.481803	0.990889
O	1.892932	-1.793842	-1.412205
C	3.321222	-1.869784	-1.520481
H	3.631471	-2.856095	-1.874956
H	3.598038	-1.109710	-2.248993
H	3.795345	-1.649592	-0.558339

INT5$_Z$

Cu	0.003177	-0.080173	-0.221748
N	1.958442	0.606125	-0.618651
C	2.279209	1.276883	-1.725716
H	1.445585	1.634899	-2.320746
C	3.594858	1.519789	-2.096490
H	3.810376	2.063090	-3.008479
C	4.609454	1.043690	-1.277312

H	5.650518	1.206885	-1.534665
C	4.277663	0.333752	-0.133294
H	5.056149	-0.079988	0.495496
C	2.933834	0.117197	0.165464
N	1.188613	-1.041657	1.318096
C	2.491279	-0.708702	1.309003
C	3.361484	-1.170103	2.295862
H	4.404239	-0.877476	2.292354
C	2.878677	-2.018228	3.281028
H	3.543097	-2.390870	4.053236
C	1.542755	-2.394749	3.254986
H	1.131897	-3.078048	3.988054
C	0.735340	-1.876609	2.252480
H	-0.313302	-2.152932	2.176217
C	-2.179075	1.188724	-1.582529
F	-3.032567	0.405168	-2.246700
F	-2.740484	2.415137	-1.506458
F	-1.077220	1.296651	-2.342085
C	-1.916359	0.627143	-0.190263
C	-1.131914	1.264902	0.787173
C	-2.931153	-0.375399	0.269790
C	-2.681952	-1.747013	0.245657
C	-4.154210	0.098935	0.752059
C	-3.646507	-2.633313	0.714953
C	-5.116188	-0.792385	1.209836
C	-4.861876	-2.160662	1.196589
H	-1.742349	-2.126412	-0.144786
H	-4.346032	1.168875	0.767287
H	-3.439991	-3.698346	0.693156
H	-6.063857	-0.416332	1.581132

H	-5.612737	-2.855570	1.558145
O	-0.029141	-1.443167	-1.697410
S	0.788943	-2.675410	-1.426771
O	0.586408	-3.420519	-2.873240
O	0.192841	-3.536419	-0.406843
O	2.213757	-2.401569	-1.271499
H	1.029921	-4.274369	-2.802731
C	-1.282702	0.944748	2.251870
H	-0.338318	1.064770	2.781422
H	-2.014689	1.620930	2.705694
H	-1.639884	-0.075421	2.386994
S	-0.418394	2.904161	0.567634
O	-1.274313	3.848906	1.253274
O	0.033861	3.163941	-0.780746
O	0.908931	2.637510	1.502276
C	2.032762	3.478907	1.215528
H	1.798852	4.528195	1.414358
H	2.817895	3.145295	1.891730
H	2.353720	3.359459	0.177553

$INTB_E$

Cu	0.227261	0.215916	-0.517686
N	1.573499	1.828618	0.597918
C	2.032057	2.979027	0.109520
H	1.433191	3.438922	-0.672103
C	3.209543	3.578158	0.537887
H	3.537361	4.513380	0.100120
C	3.950572	2.935735	1.519177
H	4.885453	3.356000	1.873838
C	3.488490	1.732259	2.028077

H	4.072304	1.196946	2.766084
C	2.290170	1.203469	1.544164
N	0.823755	-0.692765	1.257140
C	1.777144	-0.102629	2.006890
C	2.275990	-0.730554	3.147865
H	3.012435	-0.230953	3.763757
C	1.825888	-1.995627	3.489180
H	2.212604	-2.492623	4.372256
C	0.891770	-2.616904	2.675364
H	0.533204	-3.618591	2.876943
C	0.418691	-1.928385	1.569095
H	-0.280817	-2.388213	0.882413
C	-0.265739	0.883838	-2.328193
F	0.019662	-0.095265	-3.194852
F	-1.478548	1.352247	-2.653162
F	0.605591	1.897835	-2.542683
C	-1.684035	0.374936	-0.075942
C	-2.227512	1.569433	0.159832
C	-2.208684	-0.970961	0.069098
C	-2.781415	-1.388934	1.284043
C	-2.060849	-1.905578	-0.967030
C	-3.227211	-2.692451	1.436350
C	-2.507147	-3.208875	-0.805919
C	-3.090907	-3.606841	0.393599
H	-2.873739	-0.677919	2.098385
H	-1.562064	-1.611275	-1.884037
H	-3.676175	-2.999977	2.375274
H	-2.377979	-3.920748	-1.613700
H	-3.429025	-4.630038	0.520662
O	2.085596	-0.193316	-1.229886

S	2.264188	-1.684242	-1.356045
O	2.838277	-1.771154	-2.885910
O	0.961989	-2.357254	-1.326570
O	3.293296	-2.227049	-0.484787
H	3.269412	-2.630157	-2.969871
C	-1.533963	2.881815	-0.005242
H	-2.079696	3.524619	-0.699716
H	-1.462884	3.418304	0.947497
H	-0.528649	2.729834	-0.385475
C	-3.655758	1.696458	0.630087
F	-3.717790	1.730510	1.987862
F	-4.466668	0.711287	0.228008
F	-4.208815	2.850460	0.206125

TSB$_E$

Cu	-0.279245	-0.160715	-0.456070
N	-1.713345	-1.824397	0.161416
C	-2.105573	-2.849307	-0.594002
H	-1.431604	-3.134384	-1.397518
C	-3.301834	-3.526931	-0.403615
H	-3.572347	-4.350872	-1.052871
C	-4.134065	-3.106852	0.624133
H	-5.083786	-3.598130	0.805886
C	-3.744638	-2.029932	1.404386
H	-4.399674	-1.662837	2.184227
C	-2.525190	-1.401160	1.144782
N	-1.074237	0.505296	1.362304
C	-2.096827	-0.195397	1.887701
C	-2.743829	0.238529	3.044812
H	-3.544188	-0.346997	3.478801

C	-2.356894	1.431018	3.636015
H	-2.856203	1.781915	4.532714
C	-1.339741	2.172557	3.053586
H	-1.027088	3.126672	3.459562
C	-0.726124	1.670418	1.915323
H	0.049418	2.224339	1.399383
C	0.950814	-0.545435	-2.170921
F	0.421091	0.469629	-2.862702
F	2.204415	-0.680601	-2.633174
F	0.299254	-1.678277	-2.516542
C	1.658179	-0.418182	-0.246512
C	2.159484	-1.620368	0.101182
C	2.153932	0.914069	0.106148
C	2.467044	1.164380	1.454830
C	2.271231	1.964274	-0.813363
C	2.932173	2.406133	1.855970
C	2.728680	3.207709	-0.402808
C	3.066563	3.434200	0.926976
H	2.335228	0.371699	2.183869
H	1.994720	1.819670	-1.848648
H	3.178750	2.574635	2.899198
H	2.809835	4.008900	-1.128965
H	3.419607	4.410826	1.241065
O	-2.039443	0.412630	-1.425846
S	-2.080297	1.907069	-1.356801
O	-2.316563	2.273113	-2.941160
O	-0.758968	2.437348	-0.982852
O	-3.213287	2.452862	-0.626630
H	-2.621089	3.187917	-2.967351
C	1.510960	-2.938141	-0.175066

H	2.005637	-3.466131	-0.996530
H	1.582797	-3.583904	0.705195
H	0.461106	-2.812236	-0.414108
C	3.485481	-1.766210	0.801098
F	3.332341	-1.886179	2.145979
F	4.350325	-0.769968	0.588695
F	4.099456	-2.900114	0.399177

INTC$_E$

Cu	-0.143975	-0.445242	-0.256790
N	-2.024557	-1.280121	-0.017798
C	-2.426946	-2.334209	-0.730187
H	-1.660727	-2.826131	-1.323841
C	-3.738700	-2.781310	-0.738486
H	-4.019845	-3.637605	-1.339100
C	-4.667865	-2.094081	0.031715
H	-5.706498	-2.405849	0.052938
C	-4.257579	-0.989973	0.760720
H	-4.976768	-0.427276	1.341668
C	-2.922282	-0.591306	0.710493
N	-1.138432	0.944519	1.134783
C	-2.418984	0.622784	1.387587
C	-3.222656	1.421258	2.199085
H	-4.248505	1.145238	2.407624
C	-2.697530	2.591187	2.726277
H	-3.311489	3.231274	3.350727
C	-1.385826	2.934695	2.433533
H	-0.942533	3.849562	2.807122
C	-0.643275	2.075209	1.636051
H	0.387664	2.299005	1.377371

C	2.128492	-1.406591	-1.702890
F	2.528675	-0.478126	-2.564197
F	3.108717	-2.341348	-1.632636
F	1.054676	-2.021613	-2.250760
C	1.858266	-0.831847	-0.322497
C	1.253677	-1.658268	0.638050
C	2.690385	0.368196	-0.007082
C	2.323186	1.640466	-0.450086
C	3.883942	0.200042	0.699122
C	3.127507	2.734627	-0.156151
C	4.690126	1.296363	0.978952
C	4.310200	2.566344	0.557668
H	1.402480	1.773997	-1.010688
H	4.174294	-0.792362	1.031491
H	2.823950	3.720457	-0.493312
H	5.614750	1.157258	1.529375
H	4.937828	3.422705	0.782091
O	-0.433877	0.519682	-2.001769
S	-1.365892	1.697466	-1.989291
O	-1.478643	1.935218	-3.609882
O	-0.761164	2.900035	-1.422419
O	-2.701565	1.366456	-1.502354
H	-1.945349	2.771250	-3.727330
C	0.947730	-3.123281	0.456218
H	1.737569	-3.714847	0.932265
H	0.007510	-3.388035	0.942347
H	0.896583	-3.421208	-0.585426
C	1.289407	-1.301084	2.106668
F	1.405663	0.001986	2.380506
F	2.321932	-1.927452	2.719442

F	0.166327	-1.729237	2.723666

INTB$_Z$

Cu	0.031768	0.034177	-0.501967
N	2.299242	0.054669	-0.034087
C	3.301302	0.510909	-0.780527
H	3.016745	1.036112	-1.685050
C	4.637881	0.341414	-0.441856
H	5.417160	0.729705	-1.086805
C	4.938119	-0.329537	0.734755
H	5.967376	-0.476422	1.043975
C	3.899830	-0.821727	1.509667
H	4.118058	-1.358561	2.424048
C	2.583461	-0.622378	1.087496
N	0.200120	-0.930237	1.312608
C	1.426044	-1.174092	1.821888
C	1.571106	-1.958329	2.966433
H	2.555255	-2.153696	3.370946
C	0.453850	-2.510194	3.571384
H	0.563126	-3.129769	4.454903
C	-0.795351	-2.276847	3.017810
H	-1.696087	-2.709211	3.435004
C	-0.874835	-1.483241	1.884437
H	-1.820336	-1.307411	1.386992
C	-0.273575	0.817169	-2.308705
F	-1.034654	-0.050655	-2.993410
F	-0.804555	2.032054	-2.495103
F	0.945995	0.826007	-2.877800
C	-1.084905	1.498711	0.199620
C	-0.621968	2.712353	0.515190

C	-2.422021	0.988947	0.477057
C	-2.949796	1.097496	1.778286
C	-3.181049	0.328440	-0.499207
C	-4.207532	0.595994	2.076920
C	-4.440131	-0.167949	-0.195503
C	-4.958827	-0.036240	1.088796
H	-2.348518	1.564360	2.552870
H	-2.768326	0.179321	-1.488659
H	-4.599210	0.689155	3.084815
H	-5.008914	-0.681355	-0.962848
H	-5.938627	-0.438335	1.324641
O	0.675286	-1.673268	-1.416728
S	-0.342253	-2.771568	-1.268389
O	-0.455678	-3.275918	-2.822719
O	-1.643176	-2.213110	-0.886475
O	0.125451	-3.909124	-0.493142
H	-0.771457	-4.186762	-2.790817
C	-1.464959	3.819961	1.084935
H	-1.148042	4.084108	2.099961
H	-1.361122	4.723446	0.479233
H	-2.516099	3.541599	1.114560
C	0.822964	3.069495	0.336401
F	1.347395	2.632982	-0.824551
F	1.592448	2.553230	1.328788
F	1.022880	4.400368	0.367045

TSB$_Z$

Cu	0.045315	-0.075701	-0.452508
N	2.245998	-0.410134	-0.616918
C	3.089918	0.118663	-1.501867

H	2.635676	0.668384	-2.318459
C	4.469183	-0.000899	-1.400012
H	5.111763	0.447073	-2.148464
C	4.990885	-0.691201	-0.314866
H	6.063067	-0.785839	-0.180332
C	4.119492	-1.270234	0.594099
H	4.507629	-1.818751	1.443270
C	2.743826	-1.130205	0.401899
N	0.455763	-1.471425	1.069216
C	1.748607	-1.799116	1.266877
C	2.109696	-2.782932	2.187914
H	3.150219	-3.047177	2.326879
C	1.123523	-3.453234	2.894515
H	1.392114	-4.227464	3.605253
C	-0.205317	-3.140703	2.651230
H	-1.012703	-3.663700	3.148902
C	-0.494187	-2.146059	1.727686
H	-1.514301	-1.885486	1.465178
C	-0.642812	1.532179	-1.702630
F	-1.727003	0.937538	-2.186913
F	-0.863268	2.857625	-1.748852
F	0.374753	1.305467	-2.560106
C	-0.706744	1.552556	0.383501
C	0.094189	2.435549	1.010119
C	-2.063848	1.230167	0.850924
C	-2.189081	0.562390	2.077867
C	-3.227950	1.596397	0.166645
C	-3.436961	0.242695	2.591101
C	-4.474167	1.275673	0.684510
C	-4.585893	0.588717	1.888367

H	-1.288229	0.304522	2.627157
H	-3.161876	2.137586	-0.767888
H	-3.511759	-0.278404	3.540313
H	-5.366721	1.563440	0.139354
H	-5.563883	0.330084	2.280021
O	-0.228242	-1.551275	-1.918942
S	-1.501171	-2.253988	-1.583289
O	-2.307316	-2.134681	-3.011206
O	-2.267524	-1.475610	-0.592707
O	-1.374514	-3.675086	-1.299546
H	-2.992499	-2.812819	-2.991181
C	-0.301996	3.195567	2.241078
H	0.342931	2.932699	3.086743
H	-0.180075	4.269609	2.077490
H	-1.333414	2.997077	2.521697
C	1.506258	2.701047	0.591487
F	1.742562	2.470633	-0.707904
F	2.378039	1.928971	1.293291
F	1.865517	3.976469	0.829359

$INTC_Z$

Cu	-1.140966	0.044955	-0.914309
N	-0.146622	-1.739100	-1.182970
C	1.148931	-1.851690	-1.508107
H	1.603435	-0.976569	-1.956285
C	1.889461	-3.003958	-1.284776
H	2.939870	-3.027652	-1.549900
C	1.251937	-4.101931	-0.720267
H	1.795378	-5.019898	-0.524576
C	-0.095920	-4.004534	-0.403467

H	-0.612189	-4.842109	0.050650
C	-0.772792	-2.809174	-0.641490
N	-2.586063	-1.316819	-0.232232
C	-2.186790	-2.602414	-0.267418
C	-3.053281	-3.645031	0.058152
H	-2.726662	-4.676569	-0.004606
C	-4.350823	-3.342794	0.447640
H	-5.042096	-4.138295	0.704584
C	-4.748874	-2.012743	0.499191
H	-5.750396	-1.736316	0.807062
C	-3.836142	-1.027200	0.143162
H	-4.075021	0.033500	0.168887
C	2.162052	1.770748	-0.447229
F	1.456877	2.885941	-0.228783
F	3.427591	2.169111	-0.663523
F	1.704074	1.244462	-1.602977
C	2.063753	0.787750	0.709111
C	3.068003	-0.075230	0.989526
C	0.800171	0.764062	1.485281
C	0.209277	-0.486539	1.741749
C	0.146111	1.907839	1.962975
C	-0.986439	-0.589530	2.437221
C	-1.058781	1.800974	2.643696
C	-1.631514	0.558697	2.881526
H	0.696238	-1.384286	1.374061
H	0.563900	2.888862	1.794083
H	-1.428022	-1.567801	2.605268
H	-1.567430	2.704915	2.957290
H	-2.586943	0.488576	3.390527
O	-1.191292	1.940466	-1.231384

S	-2.353691	2.757384	-0.709365
O	-1.614807	3.874217	0.256707
O	-3.170876	2.005156	0.233964
O	-3.010044	3.501371	-1.765186
H	-1.184926	4.502428	-0.336411
C	3.151483	-0.871350	2.256577
H	2.950400	-1.935083	2.099275
H	4.170220	-0.809360	2.651693
H	2.461682	-0.496899	3.009769
C	4.254679	-0.329704	0.088462
F	3.973172	-0.245699	-1.223840
F	4.699883	-1.598000	0.278968
F	5.295906	0.474738	0.345481

Product$_E$

C	2.191406	-1.144598	0.235939
F	3.160198	-0.223237	0.206376
F	2.262122	-1.753425	1.438189
F	2.503134	-2.070646	-0.691845
C	0.820173	-0.538806	0.002657
C	-0.231993	-1.367532	-0.089135
C	0.759618	0.939643	-0.035904
C	1.315870	1.655611	-1.097356
C	0.146066	1.629072	1.010790
C	1.223071	3.038696	-1.128486
C	0.066679	3.016087	0.982649
C	0.596202	3.722188	-0.090551
H	1.796645	1.121779	-1.910896
H	-0.271940	1.068291	1.840789
H	1.638915	3.586614	-1.967522

H	-0.410742	3.544947	1.801437
H	0.526194	4.804544	-0.118191
C	-0.249801	-2.846845	0.086666
H	-0.960564	-3.114857	0.874383
H	-0.597736	-3.341361	-0.822487
H	0.727659	-3.237274	0.356249
S	-1.860071	-0.710298	-0.511614
O	-2.648694	-1.826046	-0.982471
O	-1.784761	0.510597	-1.282409
O	-2.348331	-0.342333	1.010190
C	-3.216074	0.796542	1.130849
H	-4.173089	0.613010	0.636493
H	-3.373488	0.919944	2.200638
H	-2.742838	1.686829	0.709254

Product$_Z$

C	0.015508	1.571367	-0.311600
F	0.924811	2.435879	0.181720
F	-0.032668	1.775313	-1.634530
F	-1.162117	1.934327	0.216270
C	0.414082	0.148036	0.013723
C	-0.433440	-0.887195	0.147423
C	1.881245	-0.082532	0.089994
C	2.661006	0.405879	1.141098
C	2.492821	-0.824677	-0.924303
C	4.024148	0.143639	1.179527
C	3.858882	-1.073544	-0.889812
C	4.626685	-0.592975	0.164472
H	2.195478	0.984047	1.931850
H	1.886882	-1.198519	-1.744823

H	4.619003	0.518807	2.005843
H	4.322558	-1.644177	-1.687624
H	5.693037	-0.790781	0.195940
C	-0.025994	-2.260519	0.569371
H	-0.686567	-2.618295	1.363751
H	-0.122954	-2.976866	-0.250315
H	1.001299	-2.270051	0.930114
S	-2.193243	-0.812127	-0.258237
O	-2.635084	-2.182588	-0.385338
O	-2.459291	0.138869	-1.313374
O	-2.749666	-0.229539	1.158857
C	-3.877425	0.658086	1.082714
H	-4.768452	0.125166	0.742280
H	-4.025829	1.012330	2.100470
H	-3.665592	1.495385	0.416366

SP_E

C	1.037142	0.005662	-0.000199
C	1.696227	-0.239874	-1.204619
C	1.696310	-0.238911	1.204397
C	2.987342	-0.750703	-1.203084
C	2.987438	-0.749772	1.203174
C	3.634767	-1.008853	0.000115
H	1.187251	-0.038742	-2.142318
H	1.187415	-0.036949	2.141976
H	3.488654	-0.947841	-2.145048
H	3.488806	-0.946167	2.145284
H	4.643545	-1.408519	0.000242
C	-0.342549	0.569514	-0.000277
C	-1.487147	-0.131004	-0.000043

C	-1.503821	-1.639902	0.000188
F	-0.320835	-2.250784	0.000275
F	-2.177849	-2.085340	1.084214
F	-2.177793	-2.085533	-1.083984
C	-0.307383	2.077381	-0.000178
F	-1.504284	2.681427	-0.001272
F	0.353077	2.530047	1.083703
F	0.355236	2.530329	-1.082519
C	-2.891755	0.413342	-0.000076
H	-3.085462	1.029674	0.878108
H	-3.085706	1.028979	-0.878677
H	-3.611883	-0.403034	0.000308

SP_Z

C	-1.451244	-0.160848	-0.008836
C	-2.048414	-0.984515	0.948461
C	-2.255825	0.445633	-0.977337
C	-3.418472	-1.212614	0.927994
C	-3.623860	0.209477	-1.001351
C	-4.208766	-0.620581	-0.050439
H	-1.429710	-1.440439	1.716027
H	-1.802783	1.100396	-1.715643
H	-3.868975	-1.852486	1.679724
H	-4.235815	0.678048	-1.765095
H	-5.278581	-0.800403	-0.069221
C	0.012103	0.087793	0.016703
C	0.911769	-0.900467	-0.145390
C	0.383949	1.545362	0.202970
C	2.410651	-0.674903	-0.095534
F	-0.618037	2.226433	0.786236

F	1.464500	1.725842	0.971234
F	0.617804	2.147140	-0.982469
F	2.846709	-0.550774	1.170500
F	2.814717	0.401145	-0.783141
F	3.070601	-1.727868	-0.620897
C	0.535088	-2.327837	-0.381661
H	0.915415	-2.968043	0.421180
H	-0.541296	-2.459894	-0.449945
H	0.993231	-2.693455	-1.30368

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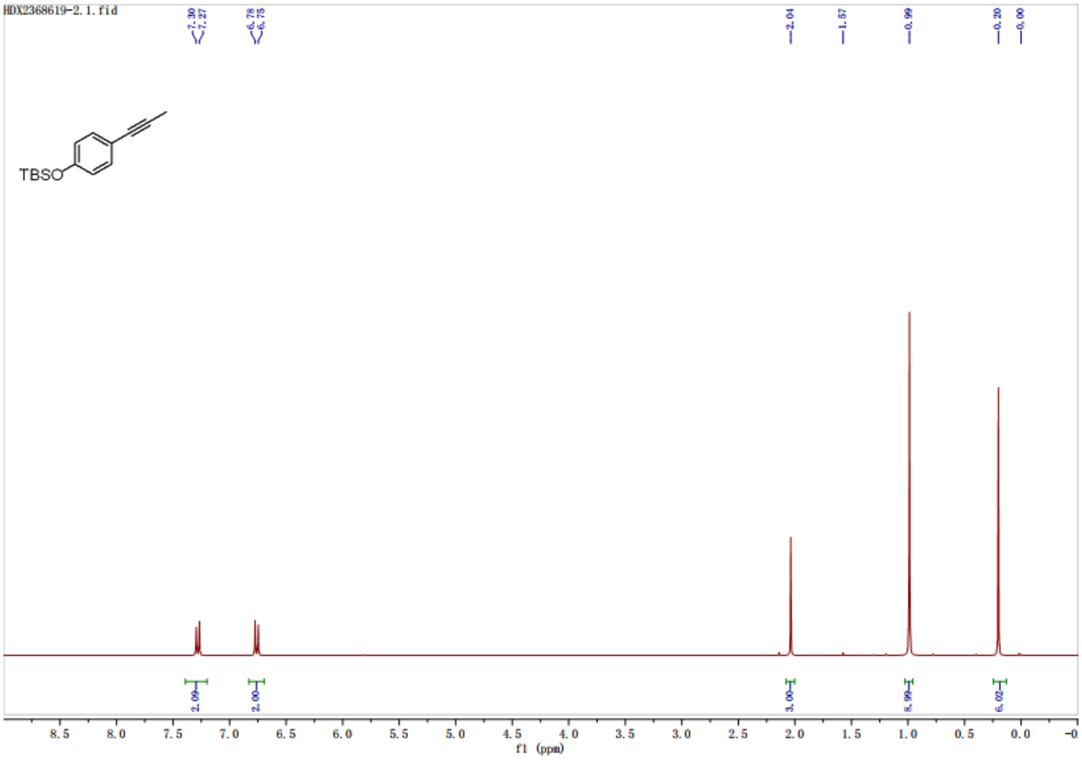
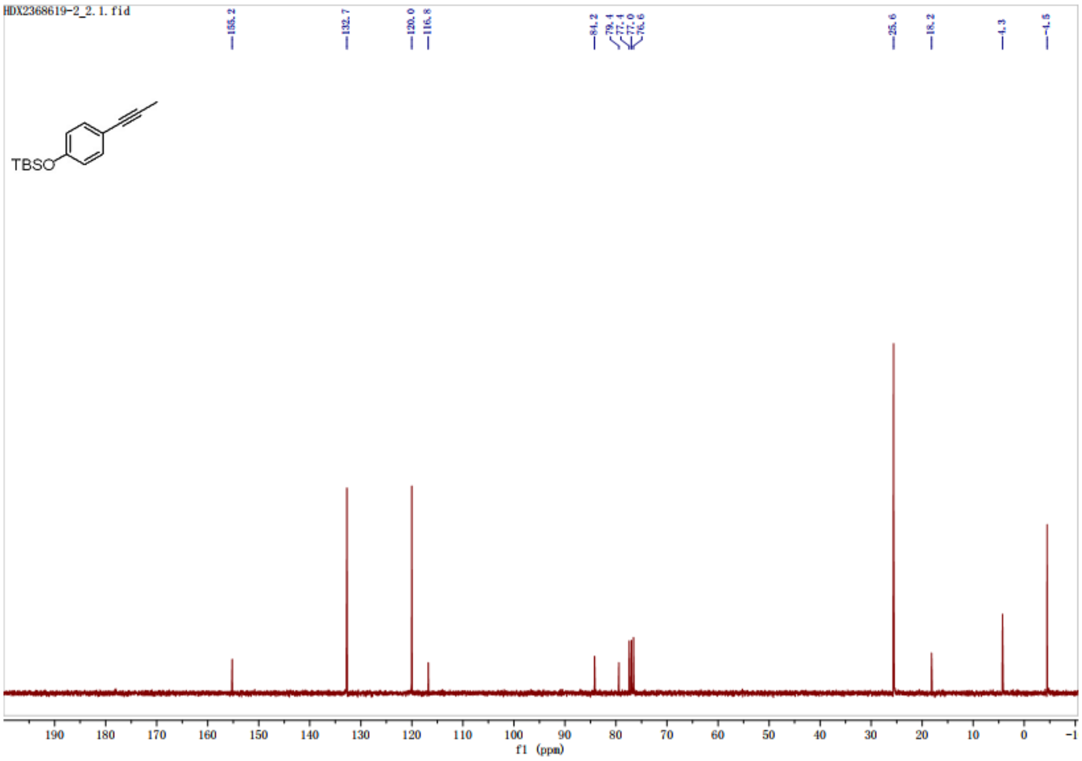
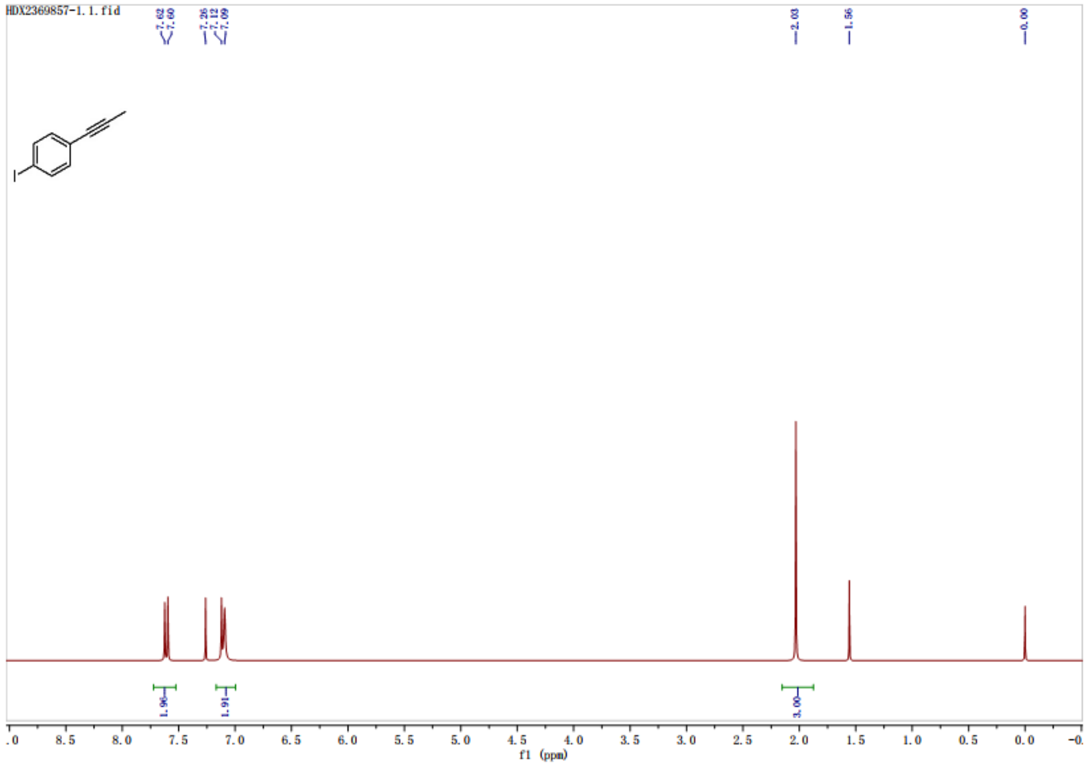
IX. Copies of NMR spectra







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7.26
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1.56
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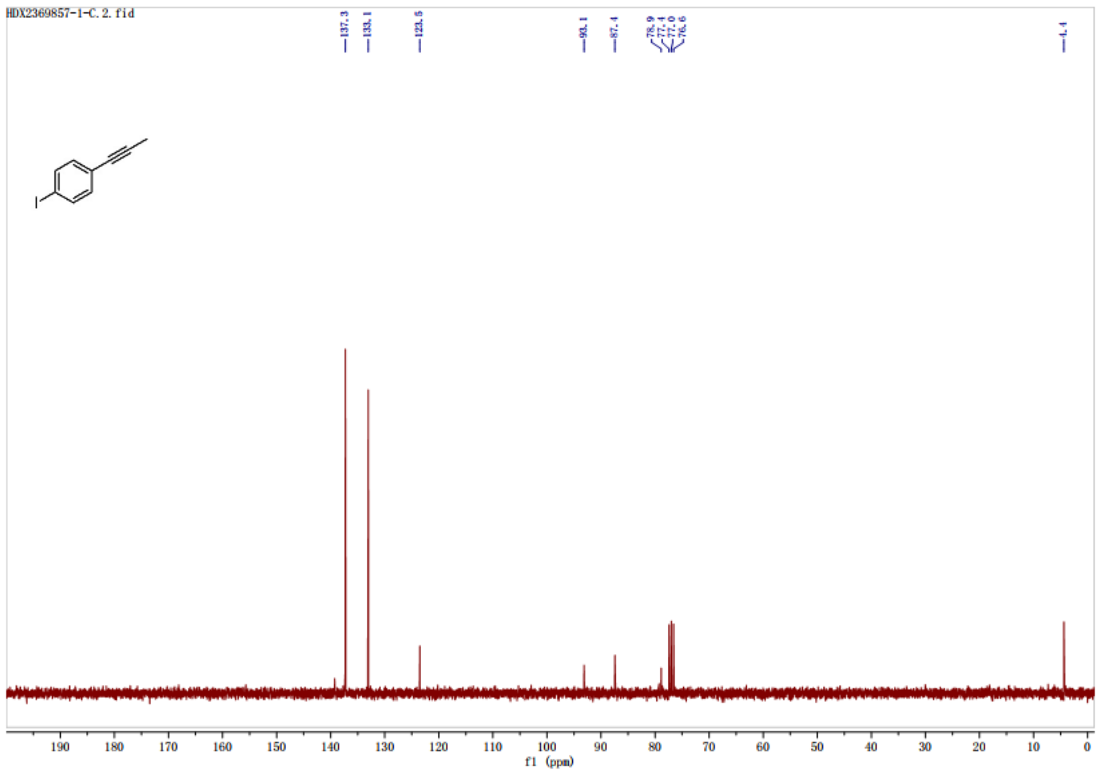
1.91
3.00
f1 (ppm)



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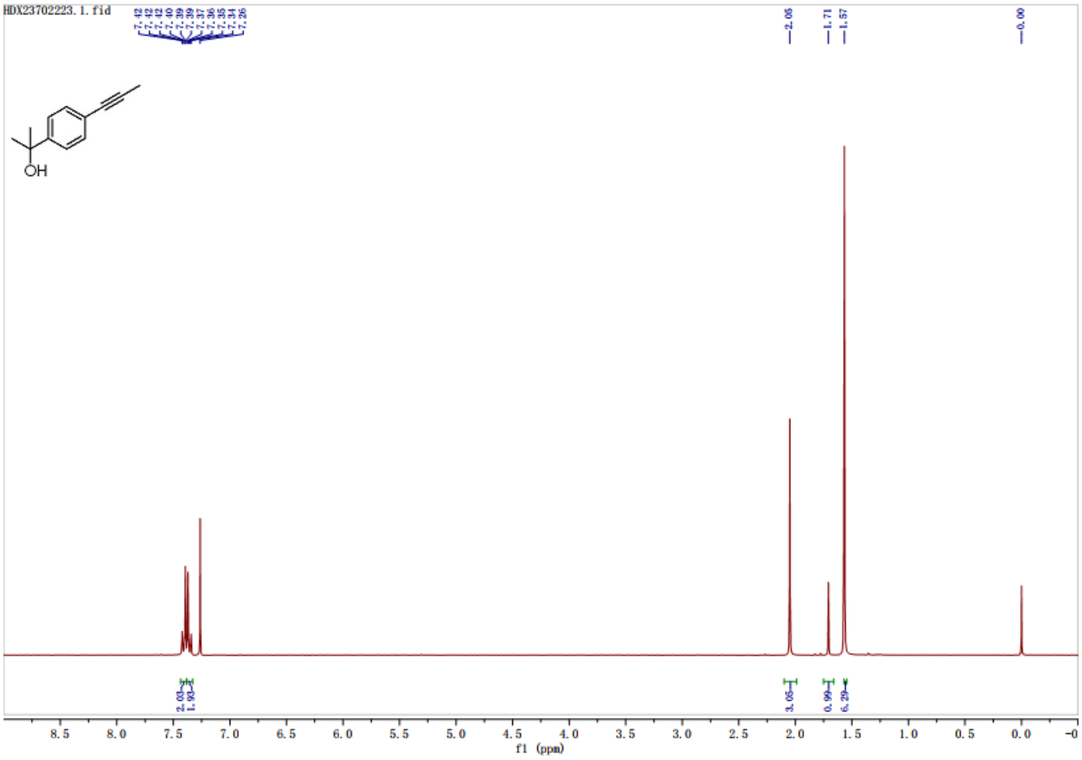
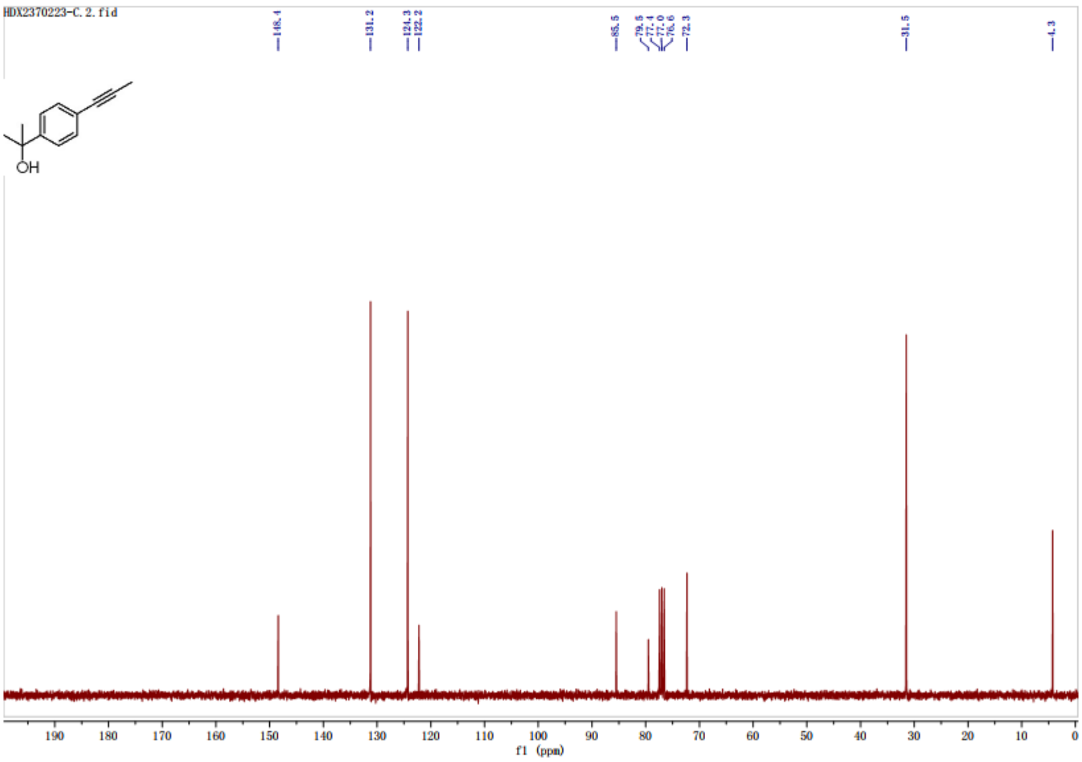
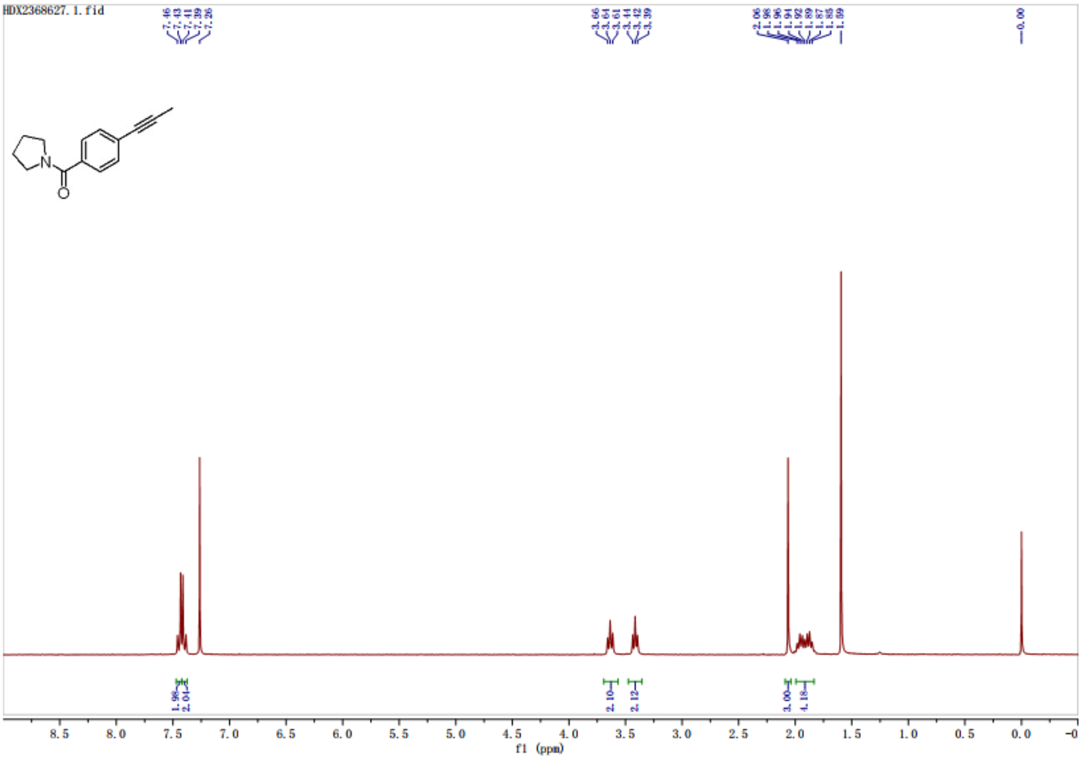
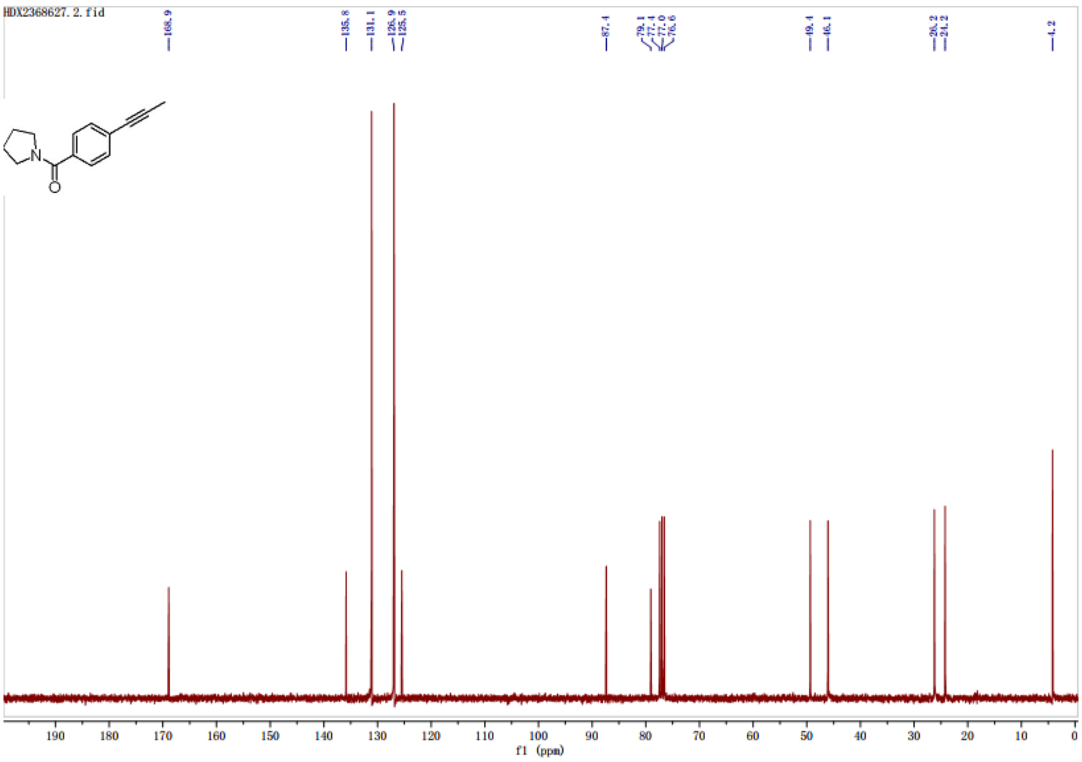
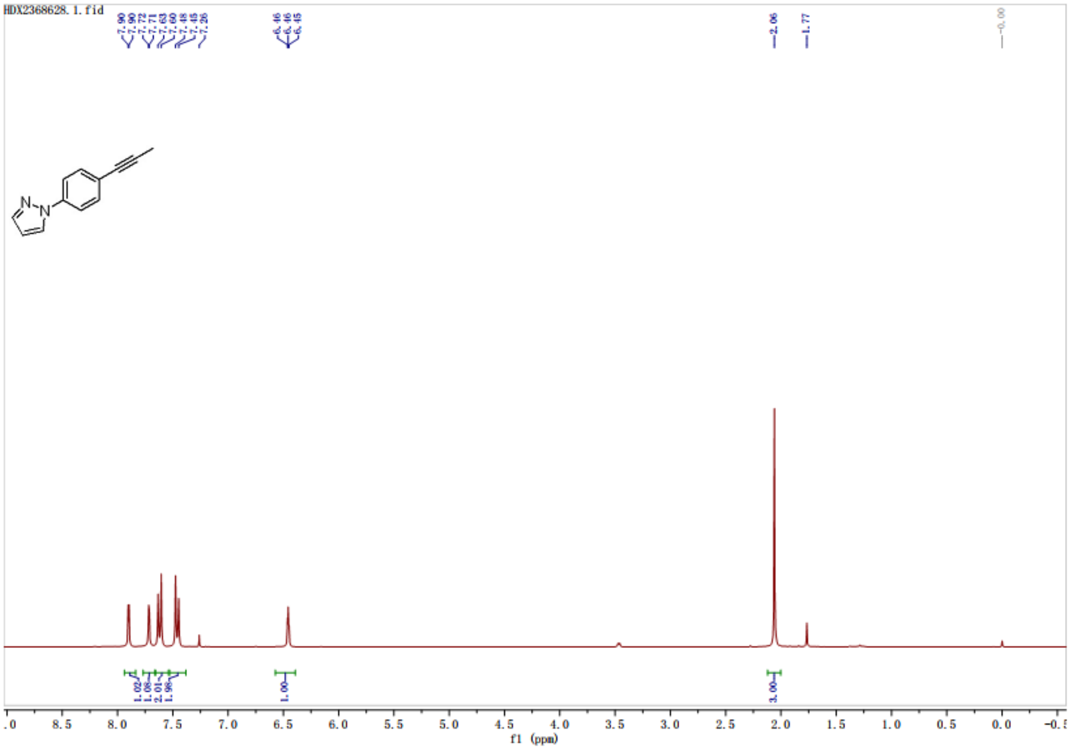
123.5
93.1
87.4
78.9
77.4
77.0
76.6
4.4
I
f1 (ppm)

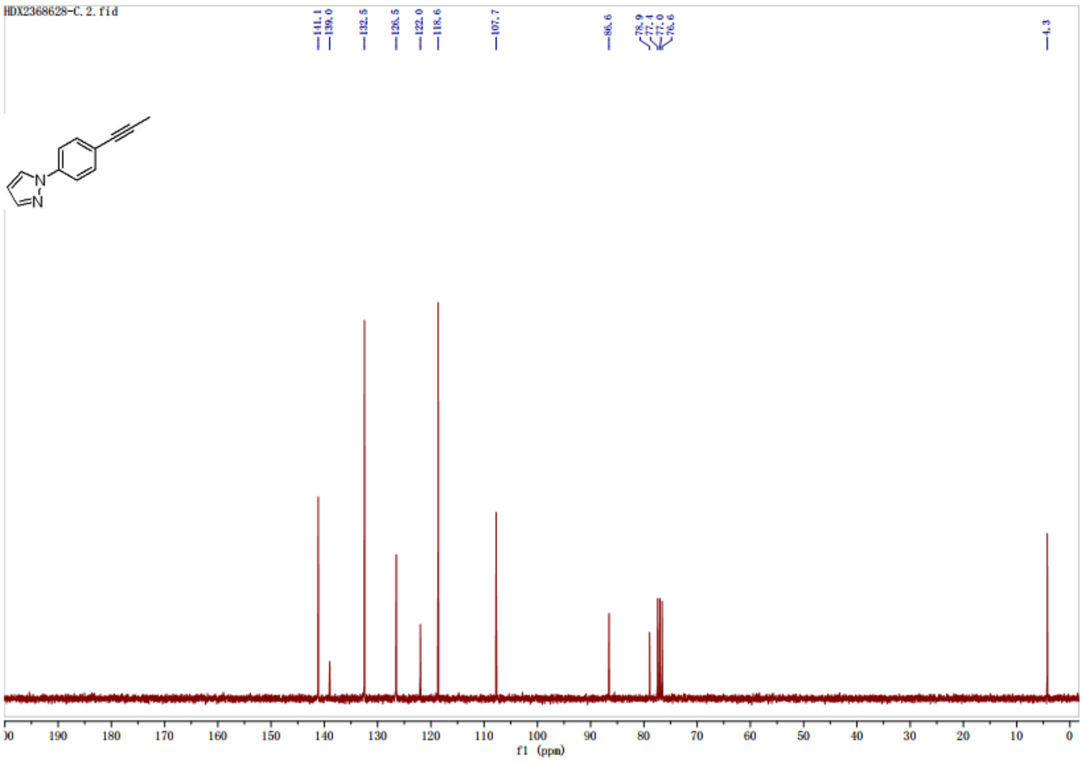

HDX23702223.1.fid
7.42
7.42
7.42
7.40
7.39
7.39
7.37
7.36
7.35
7.34
7.26
2.05
1.71
1.57
0.00
OH
2.03
1.93
3.05
0.99
6.29
f1 (ppm)

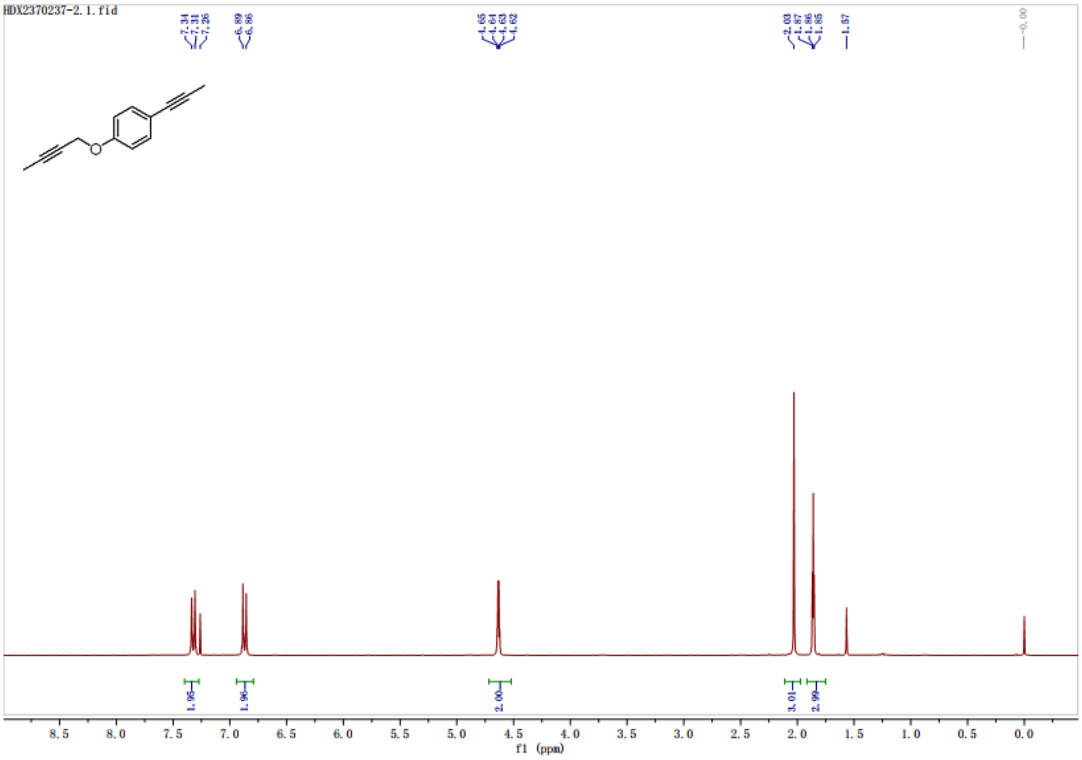

HDX2370223-C.2.fid
148.4
131.2
124.3
122.2
85.5
79.5
77.4
77.0
76.6
72.3
31.5
4.3
OH
f1 (ppm)

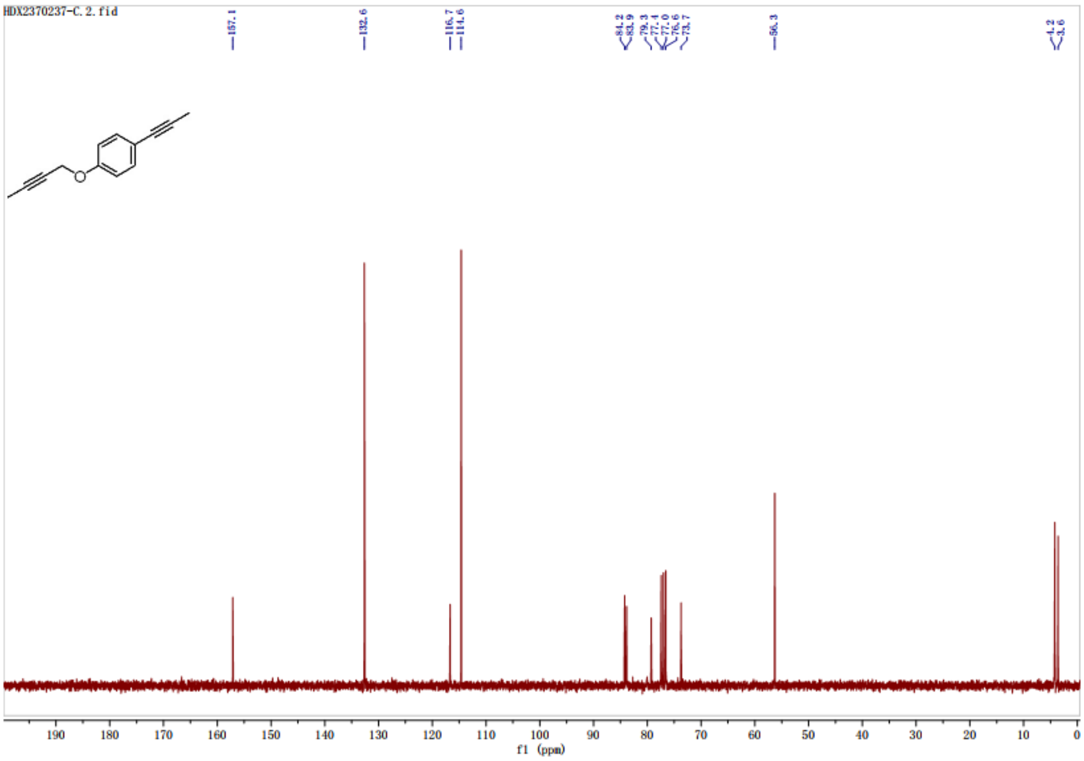


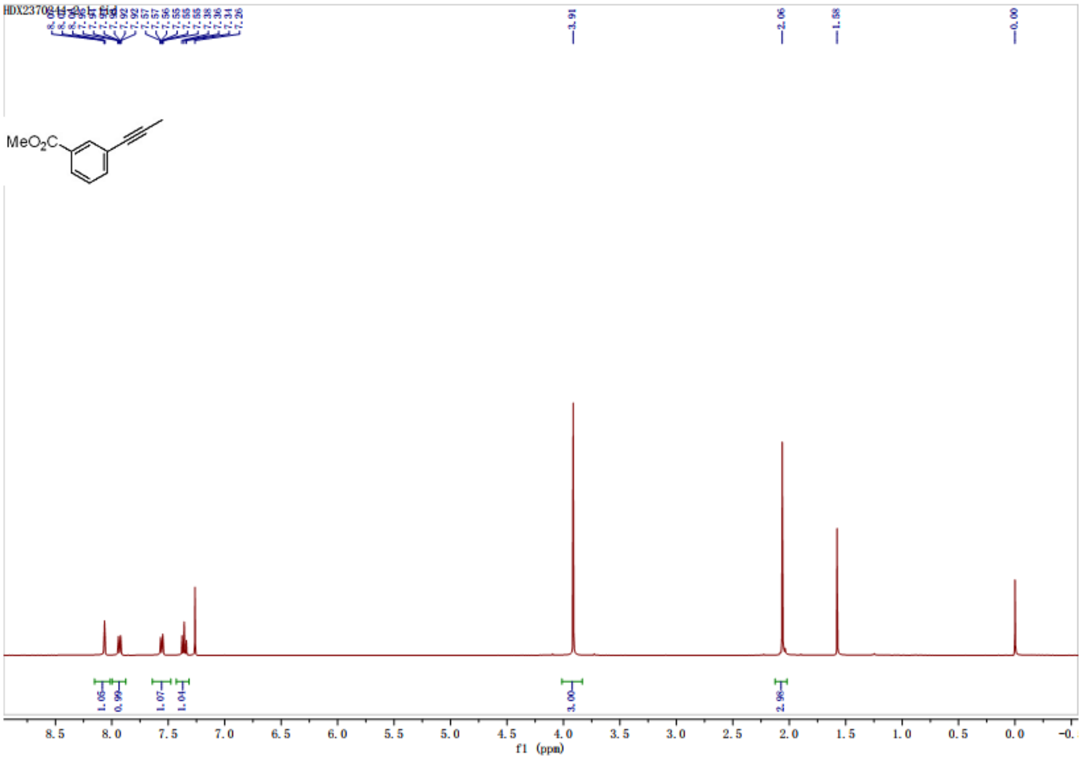


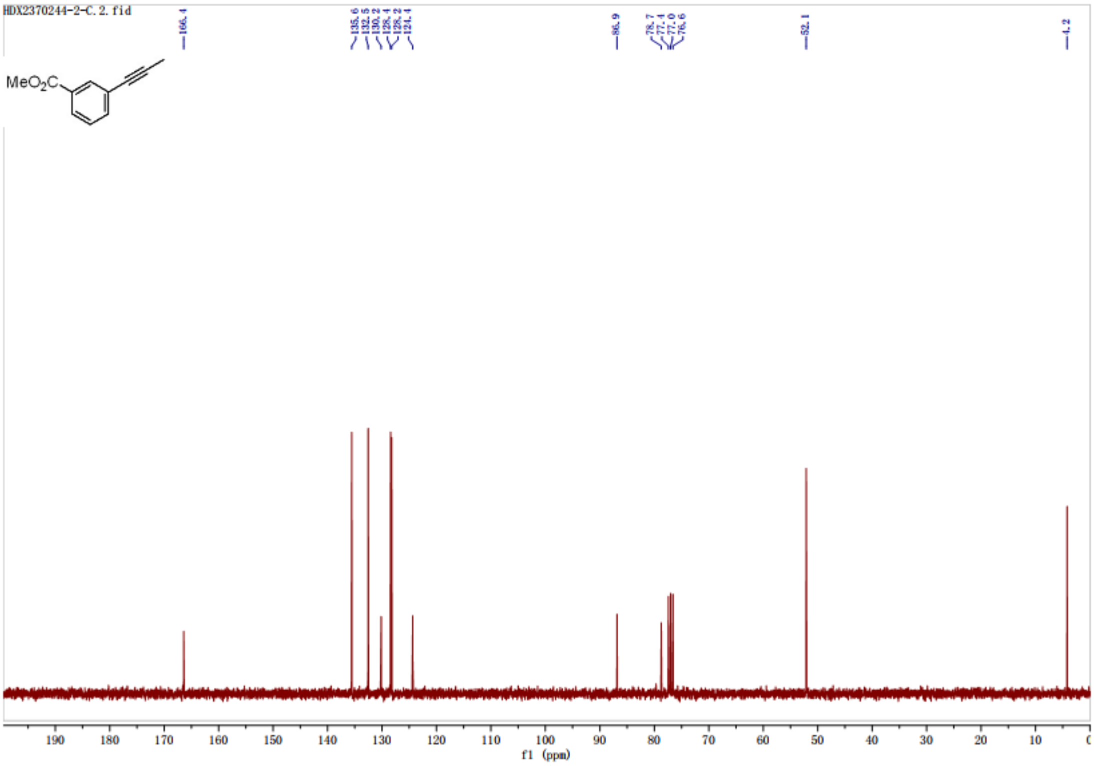

HDX2368628.1.fid
7.90
7.90
7.72
7.71
7.63
7.60
7.48
7.45
7.26
6.46
6.46
6.45
2.06
1.77
0.00
1.02
1.08
2.01
1.98
1.00
3.00
f1 (ppm)

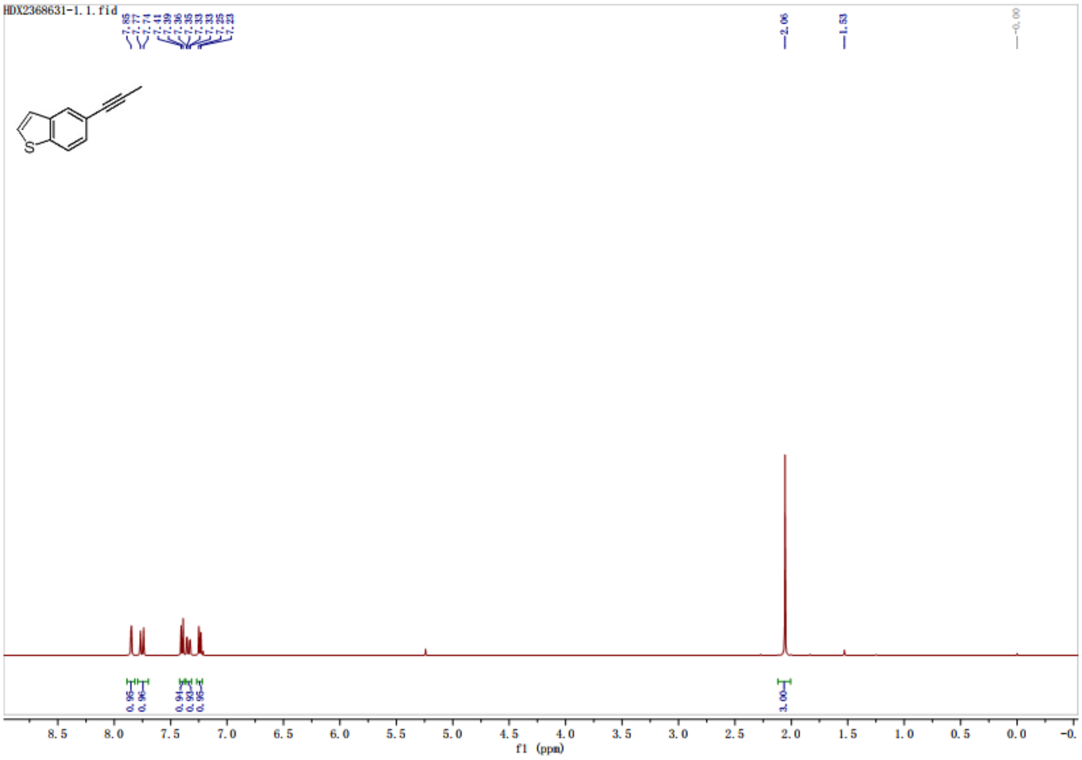

HDX2368628-C.2.fid
141.1
139.0
132.5
126.5
122.0
118.6
107.7
86.6
78.9
77.4
77.0
76.6
4.3
f1 (ppm)


HDX2370237-2.1.fid
7.34
7.31
7.26
6.89
6.86
4.65
4.64
4.63
4.62
2.03
1.87
1.86
1.85
1.57
0.00
1.95
1.96
2.00
3.01
2.99
f1 (ppm)

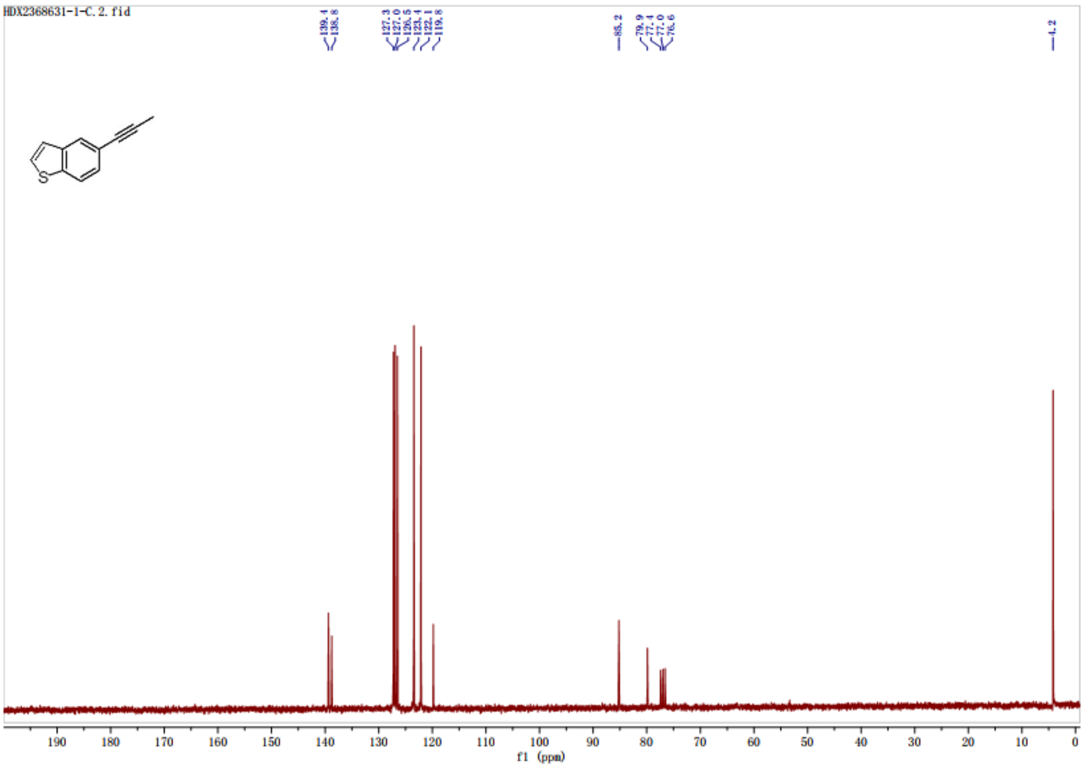

HDX2370237-C.2.fid
157.1
132.6
116.7
114.6
84.2
83.9
79.3
77.4
77.0
76.6
73.7
56.3
4.2
3.6
f1 (ppm)



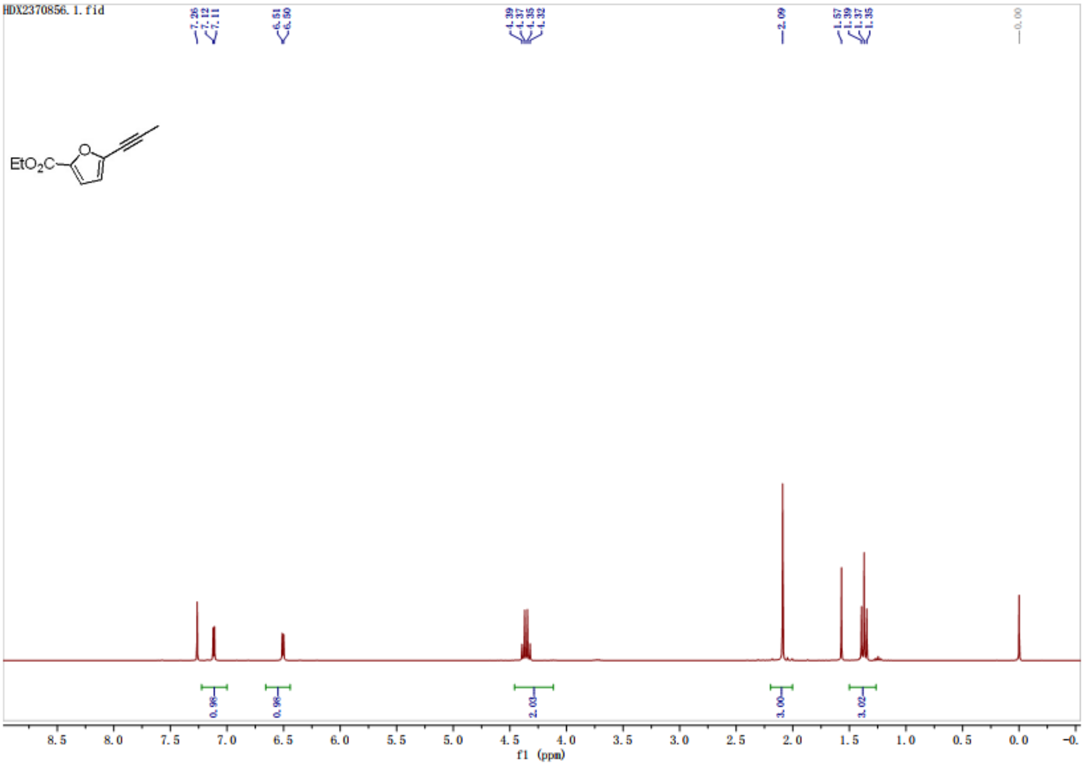


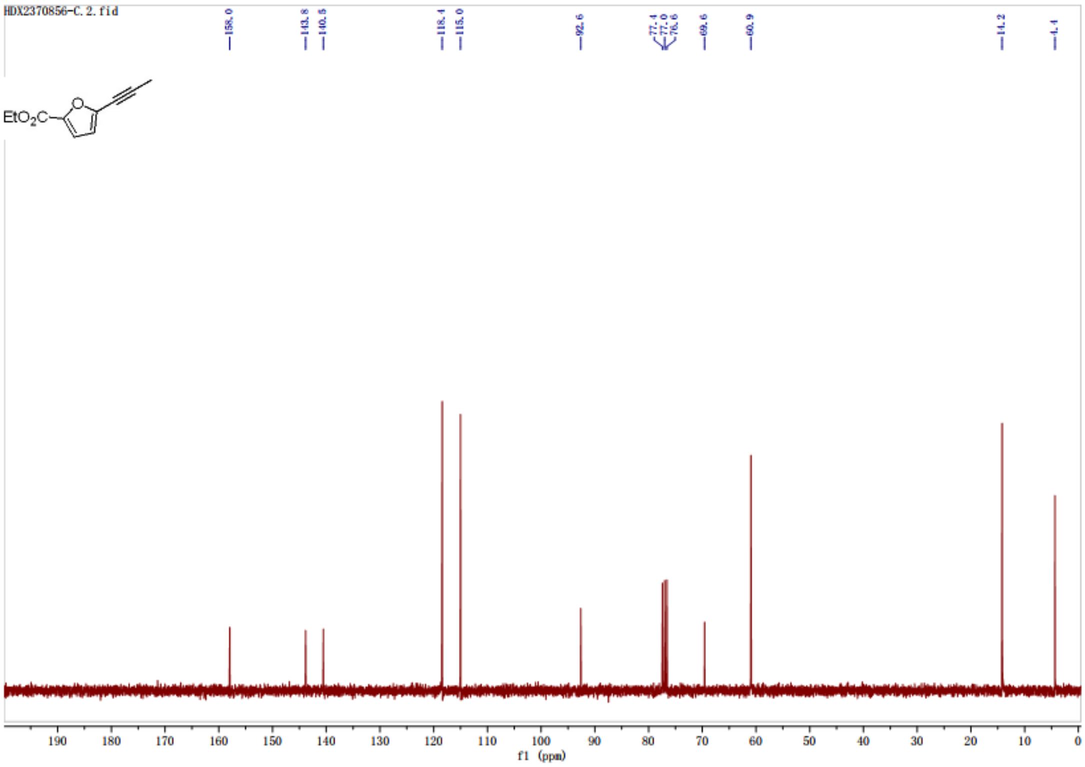


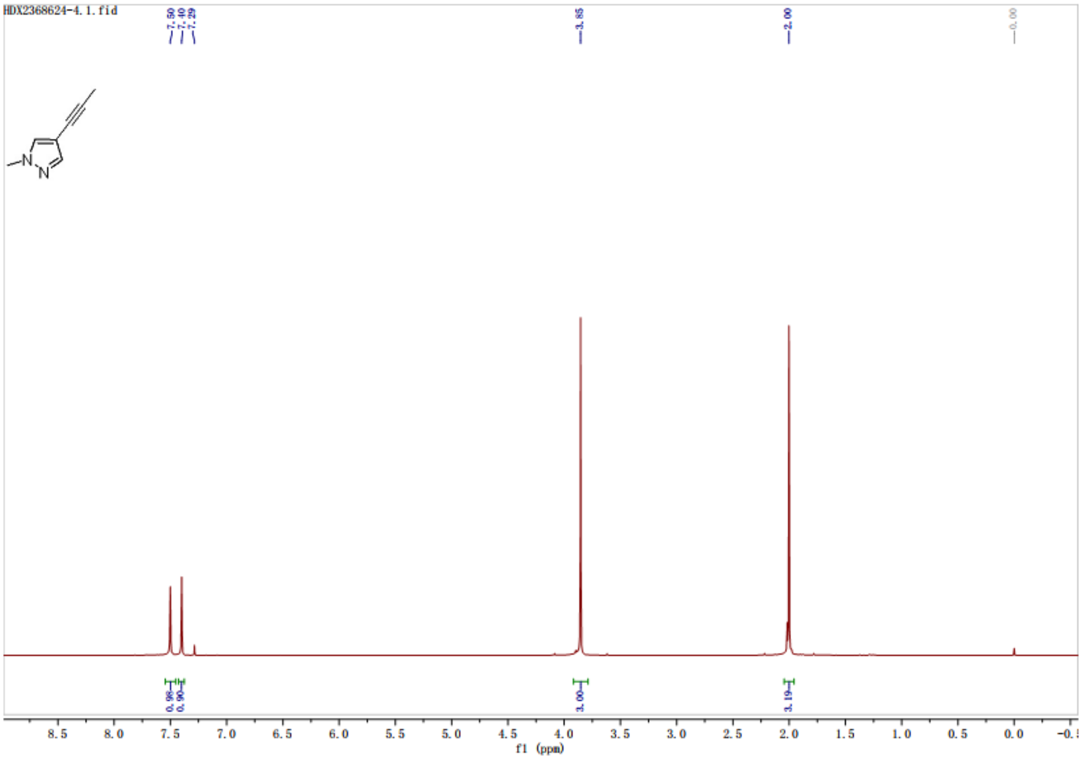
HDX2368631-1.1.fid
f1 (ppm)

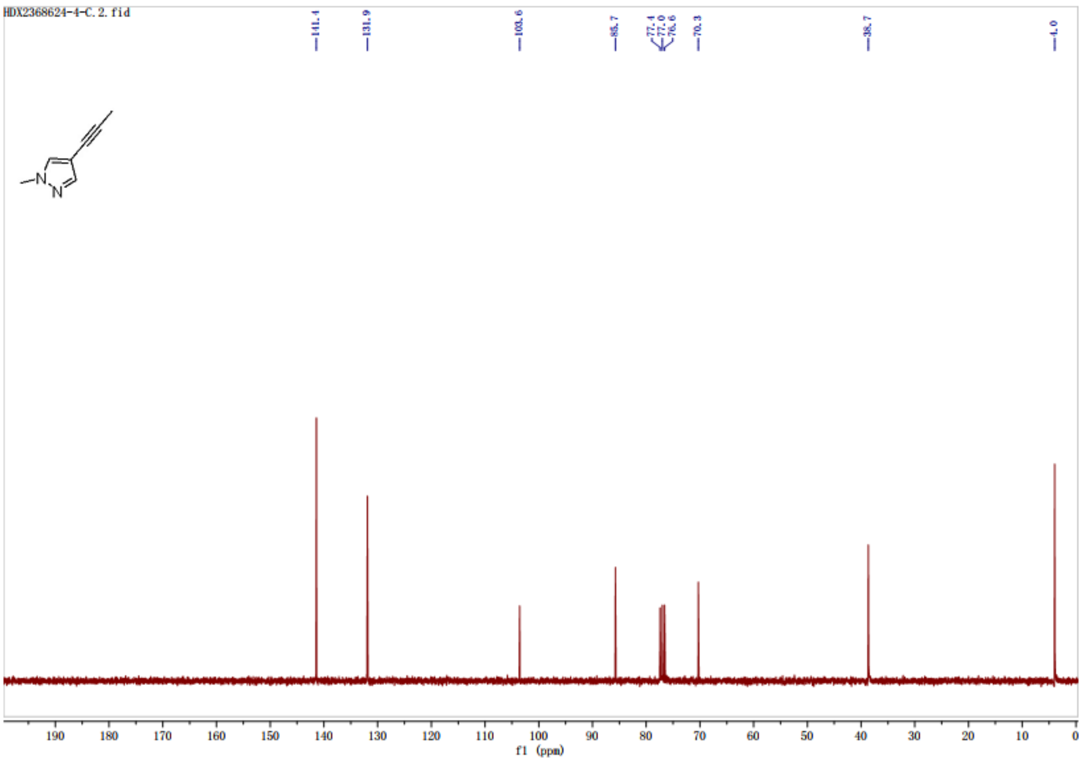


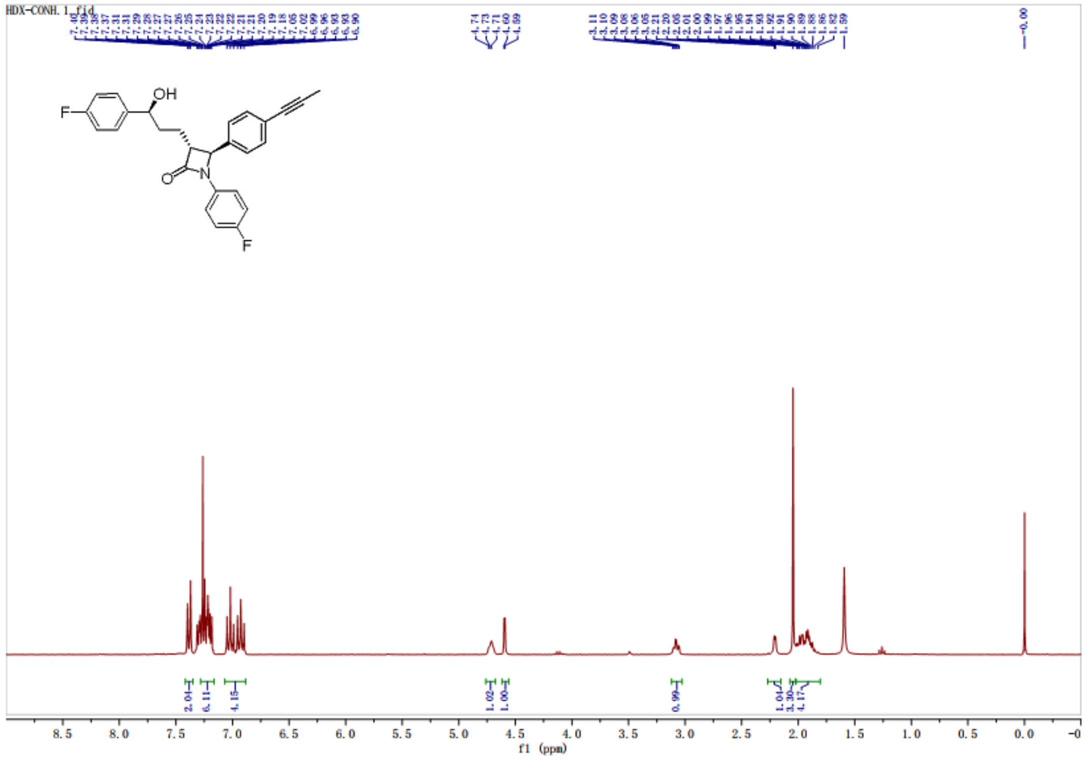
HDX2368631-1-C.2.fid
f1 (ppm)

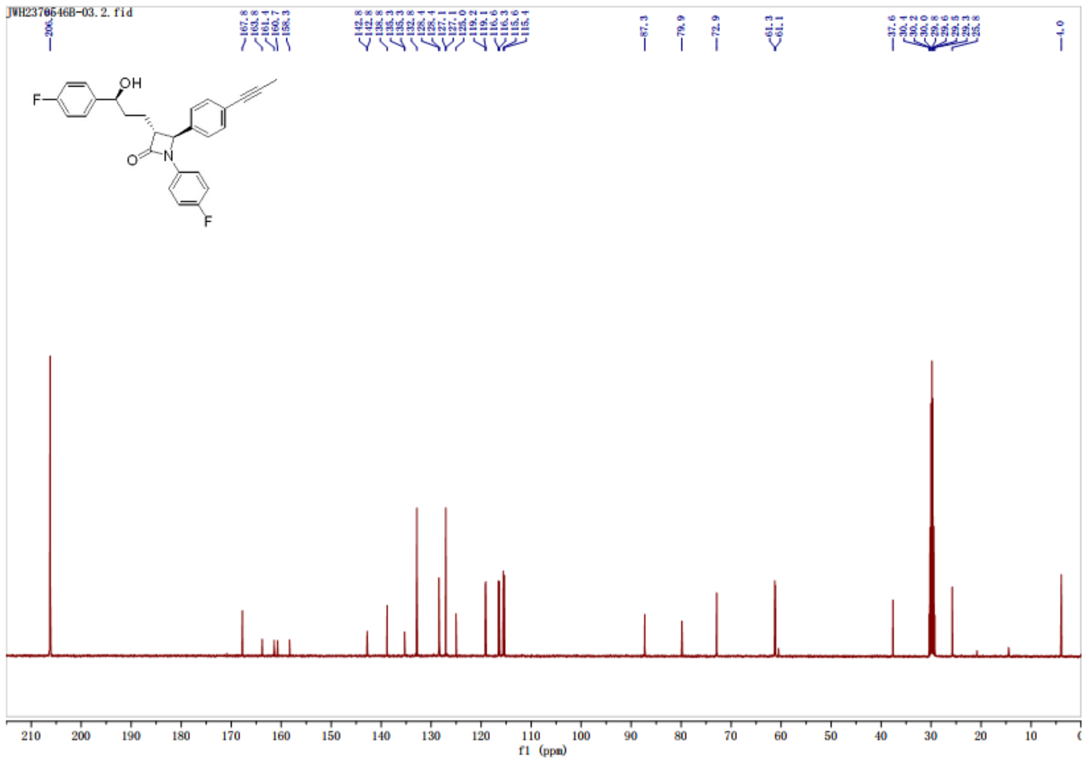

HDX2370856.1.fid
7.26
7.12
7.11
6.51
6.50
4.39
4.37
4.35
4.32
2.09
1.57
1.39
1.37
1.35
0.00
EtO2C
O
0.98
0.98
2.03
3.00
3.02
f1 (ppm)

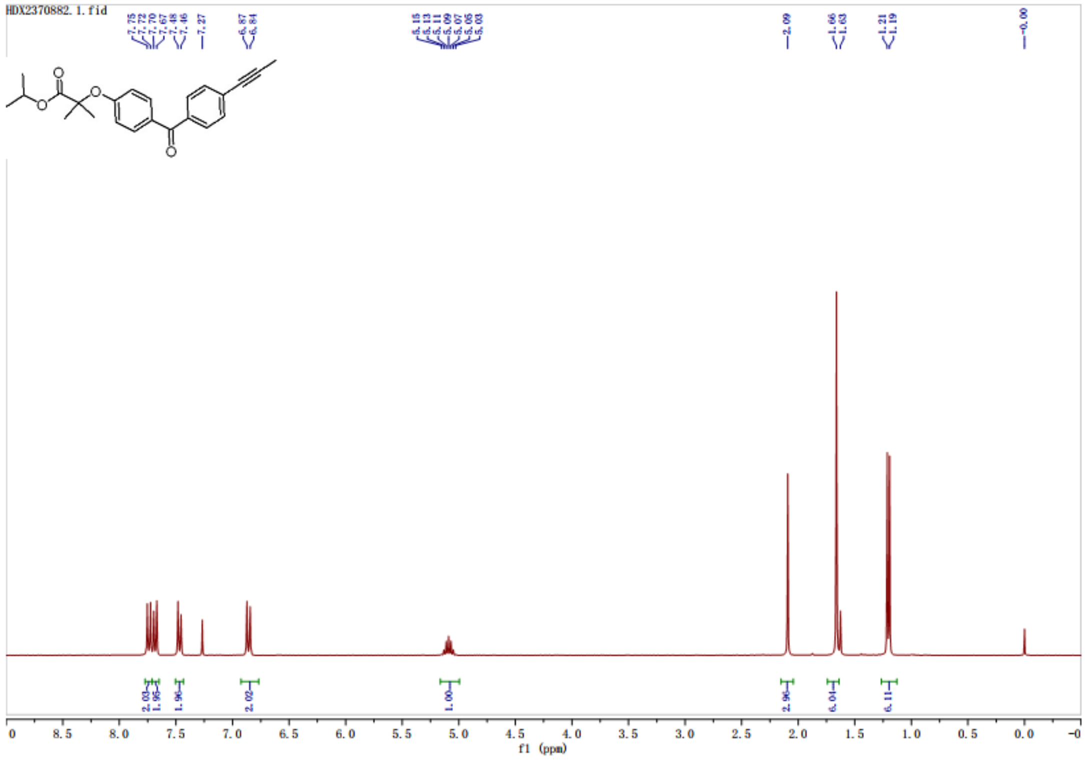

HDX2370856-C.2.fid
158.0
143.8
140.5
118.4
115.0
92.6
77.4
77.0
76.6
69.6
60.9
14.2
4.4
EtO2C
O
f1 (ppm)

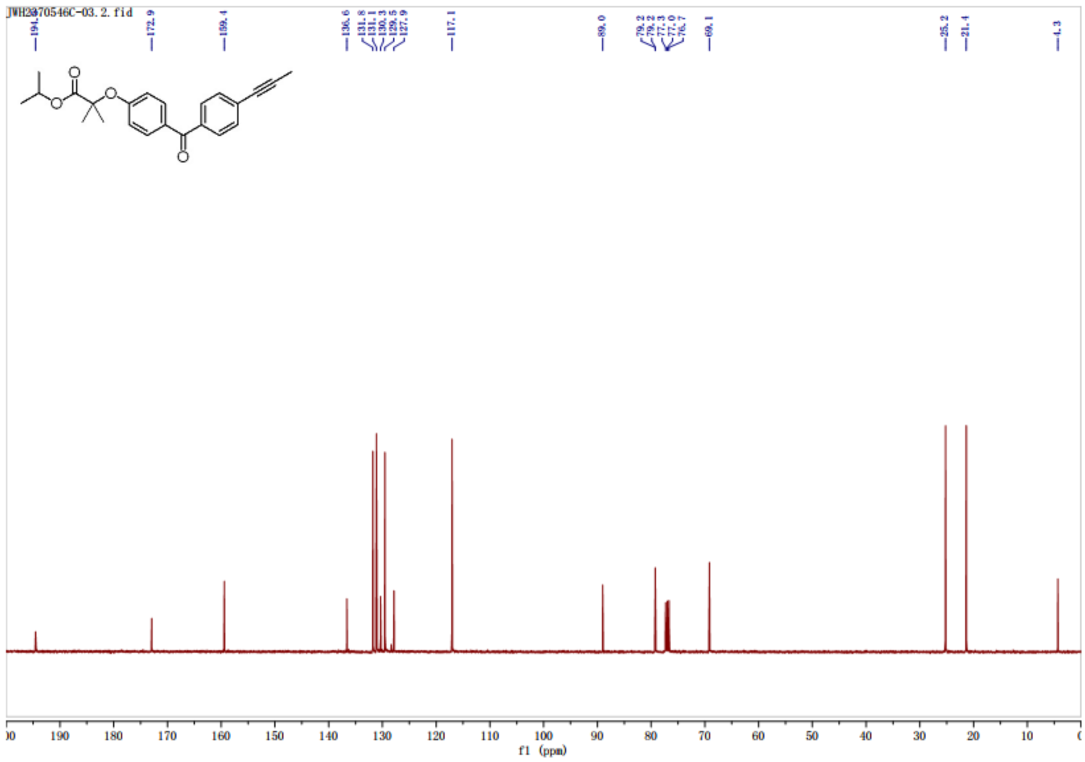

HDX2368624-4.1.fid
7.50
7.40
7.29
3.85
2.00
0.00
N
N
0.98
0.90
3.00
3.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

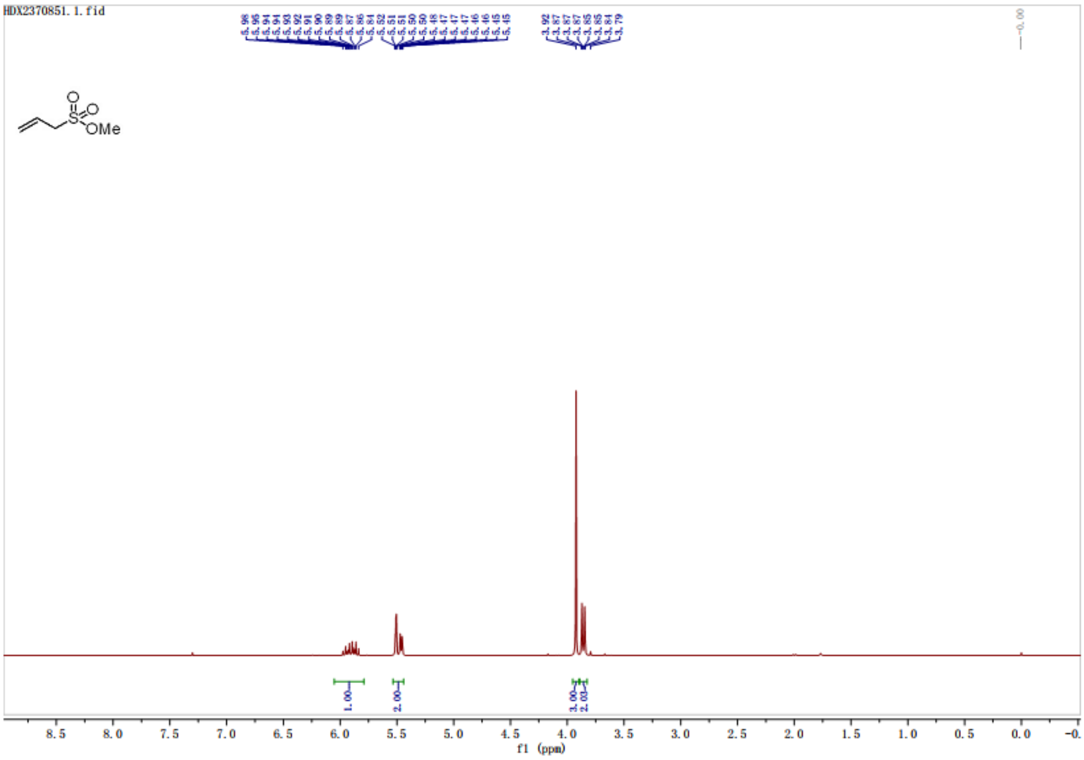

HDX2368624-4-C.2.fid
141.4
131.9
103.6
85.7
77.4
77.0
76.6
70.3
38.7
4.0
N
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

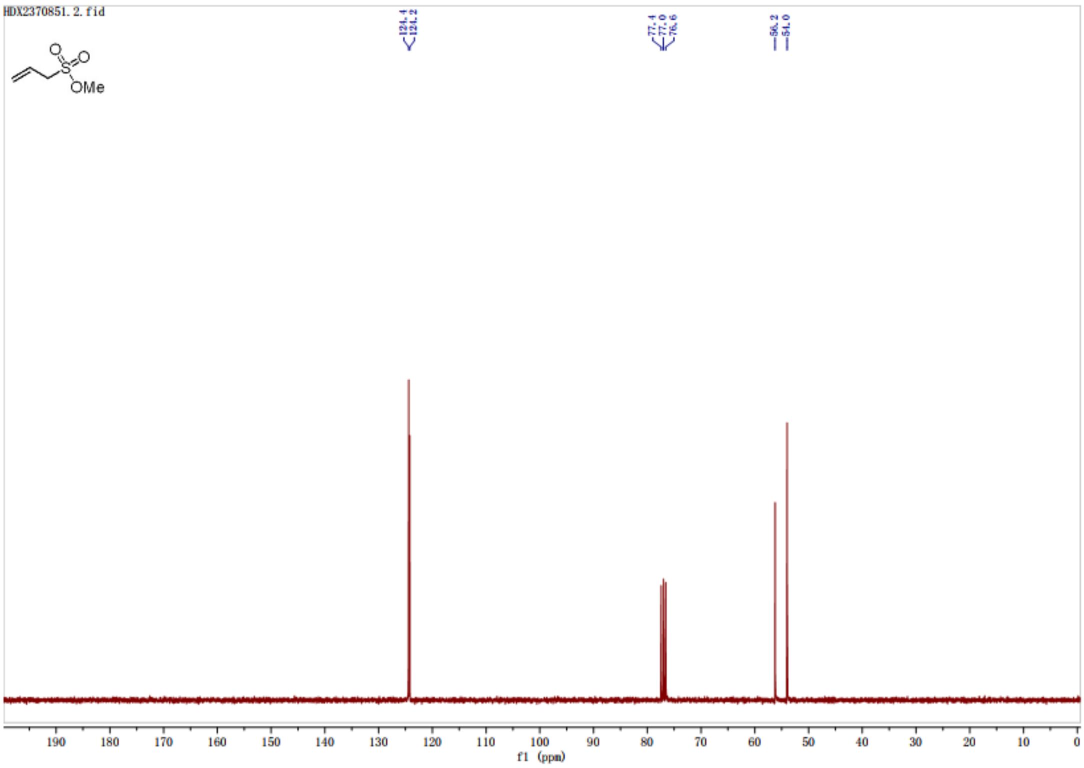


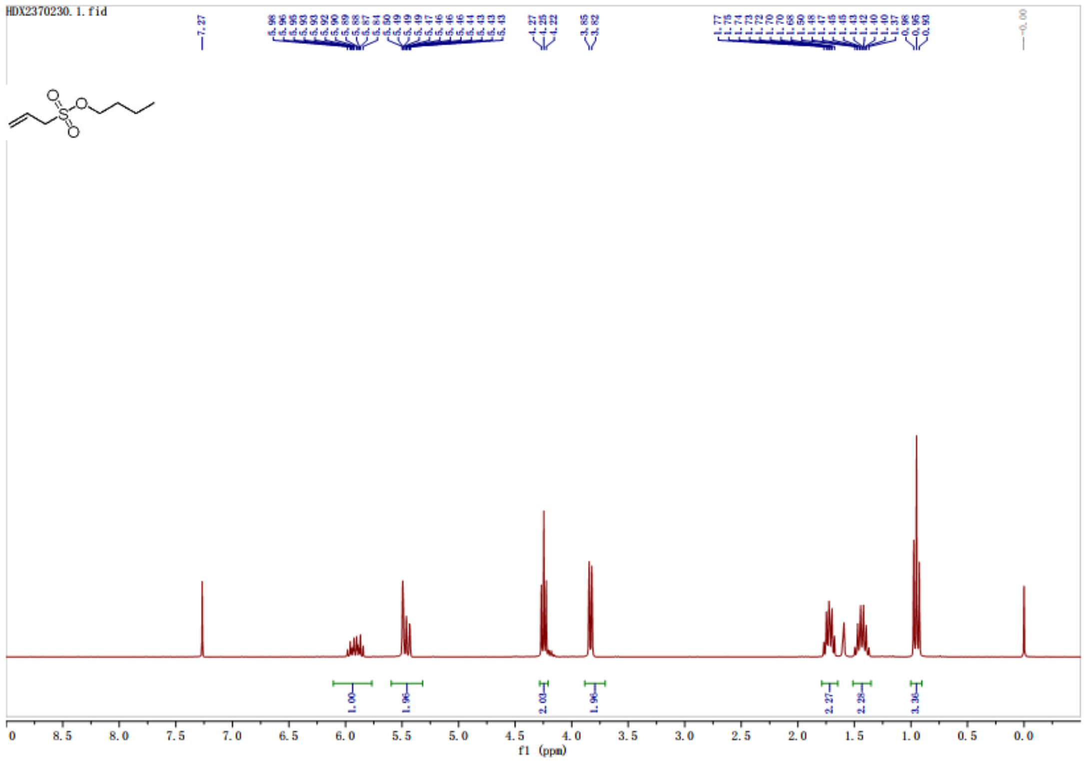


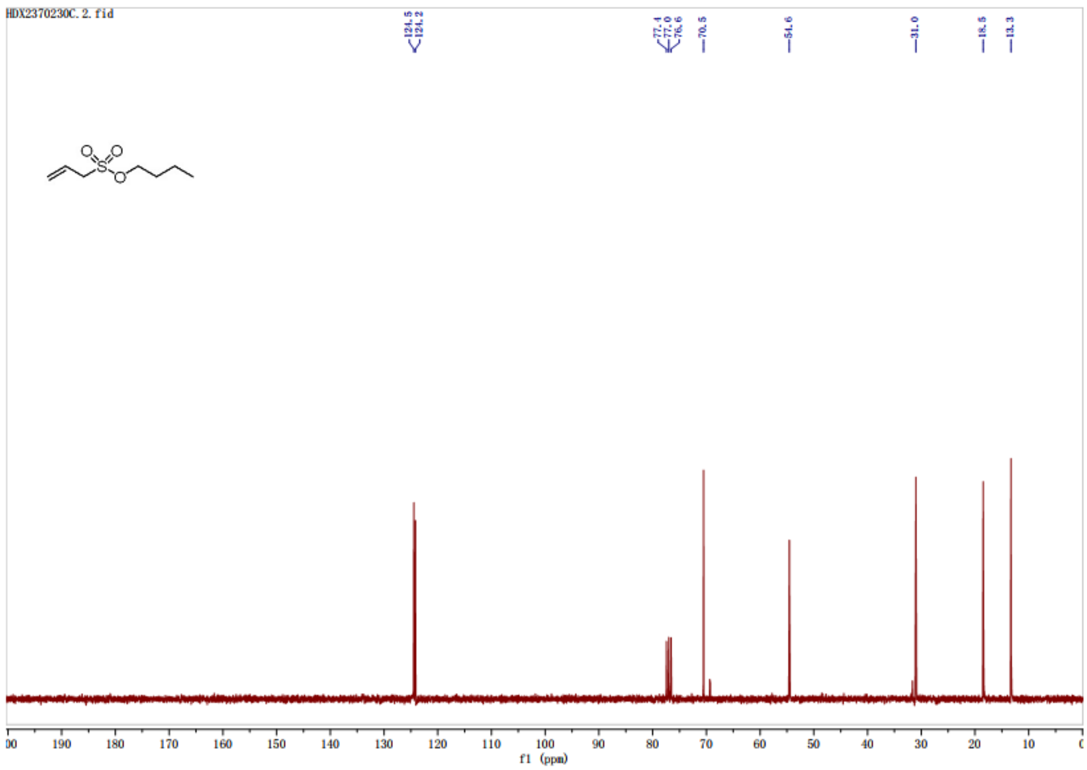

HDX2370882.1.fid
7.75
7.72
7.70
7.67
7.48
7.46
7.27
6.87
6.84
5.15
5.13
5.11
5.09
5.07
5.05
5.03
2.09
1.66
1.63
1.21
1.19
0.00
2.03
1.95
1.96
2.02
1.00
2.96
6.04
6.11
f1 (ppm)

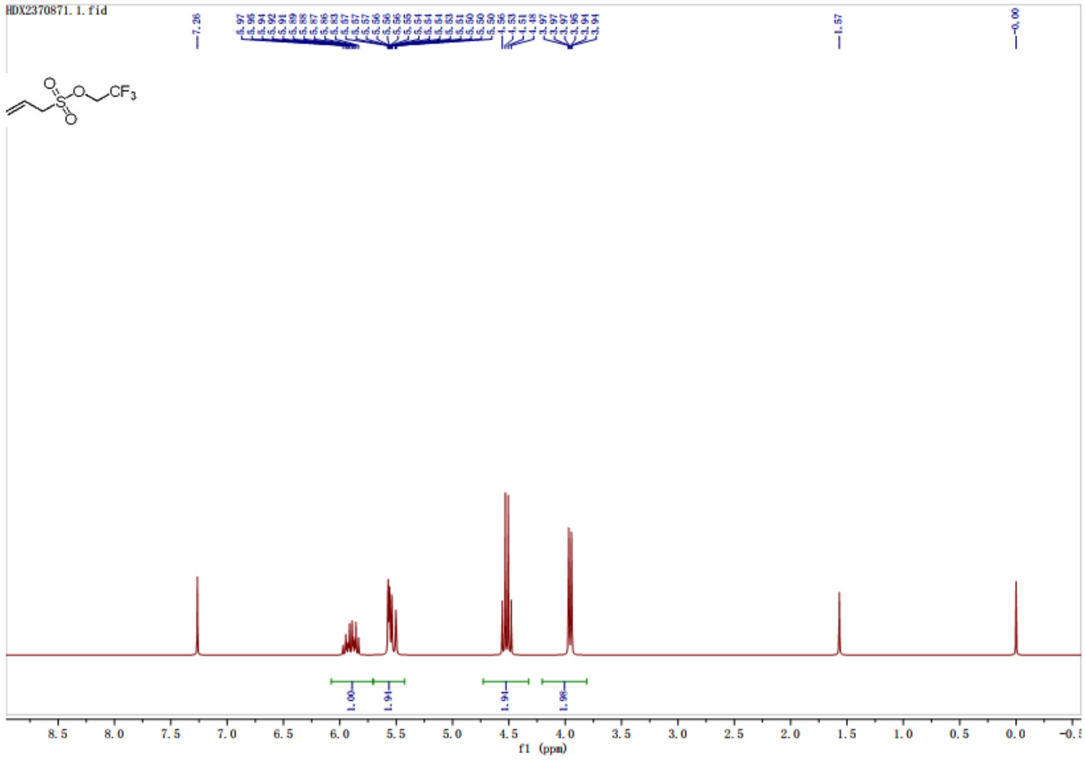

JWH2070546C-03.2.fid
194.
172.9
159.4
136.6
131.8
131.1
130.3
129.5
127.9
117.1
89.0
79.2
79.2
77.3
77.0
76.7
69.1
25.2
21.4
4.3
f1 (ppm)

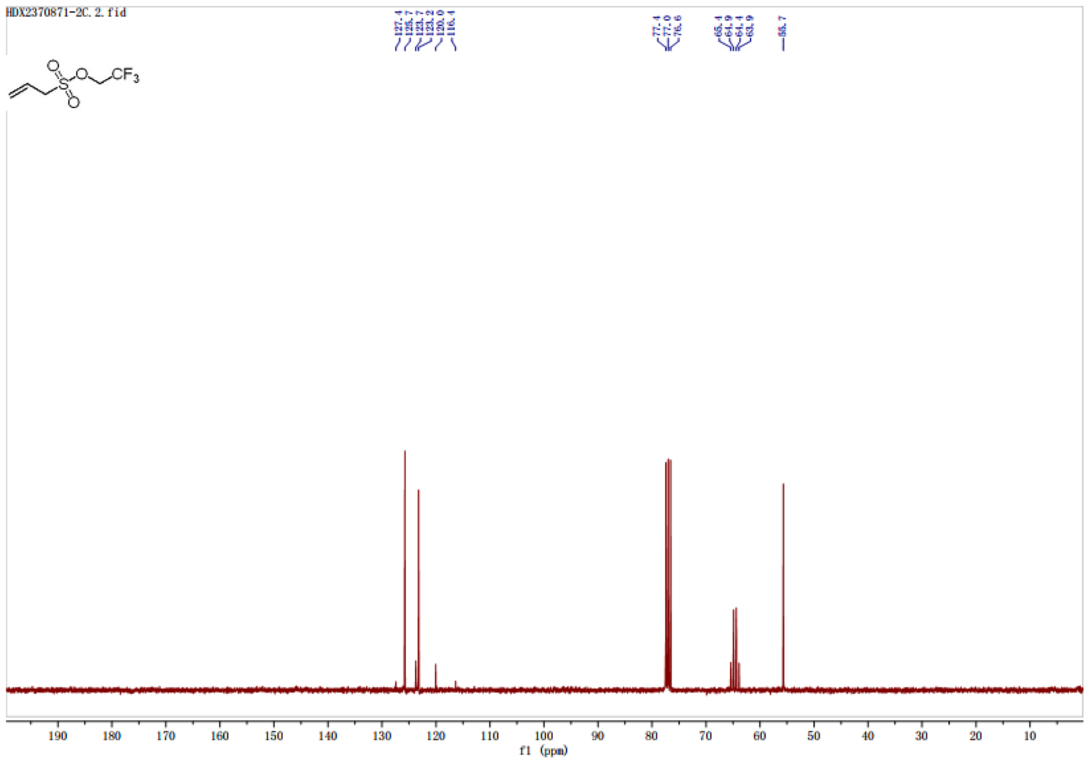

HDX2370851.1.fid
OMe
f1 (ppm)

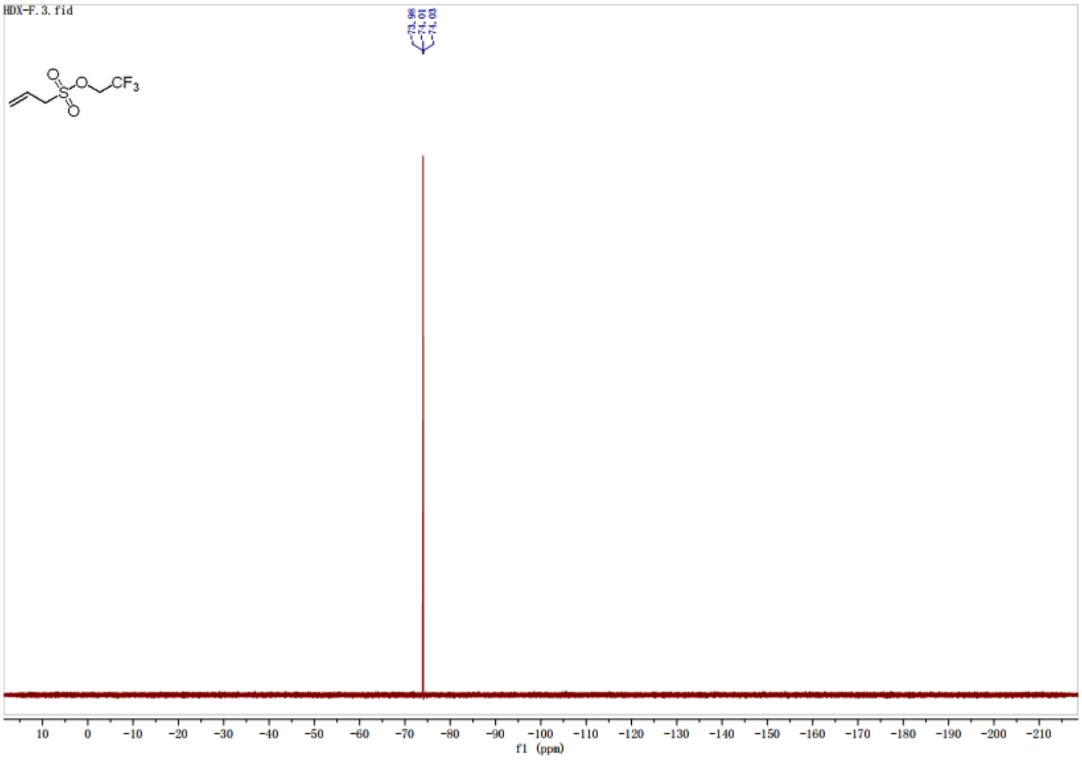

HDX2370851.2.fid
124.4
124.2
77.4
77.0
76.6
56.2
54.0
OMe
f1 (ppm)


HDX2370230.1.fid
f1 (ppm)


HDX2370230C.2.fid
f1 (ppm)






HDX-F.3.fid
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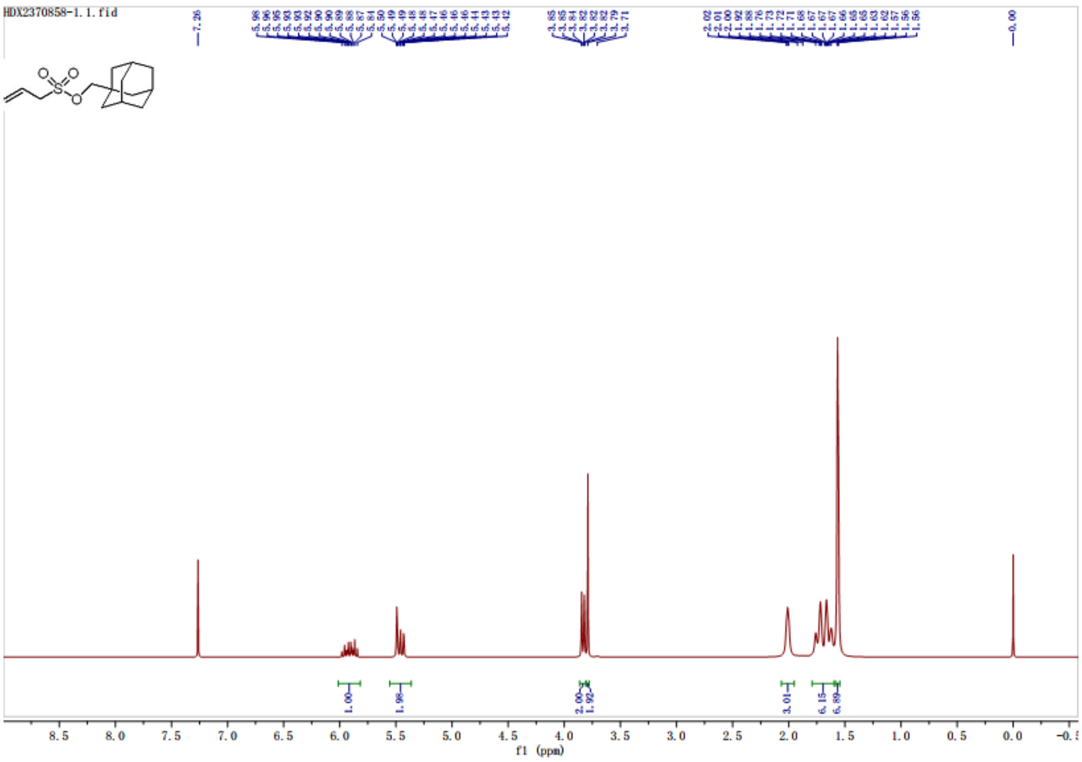
-74.01
-74.03
CF3
f1 (ppm)


HDX2370858-1.1.fid
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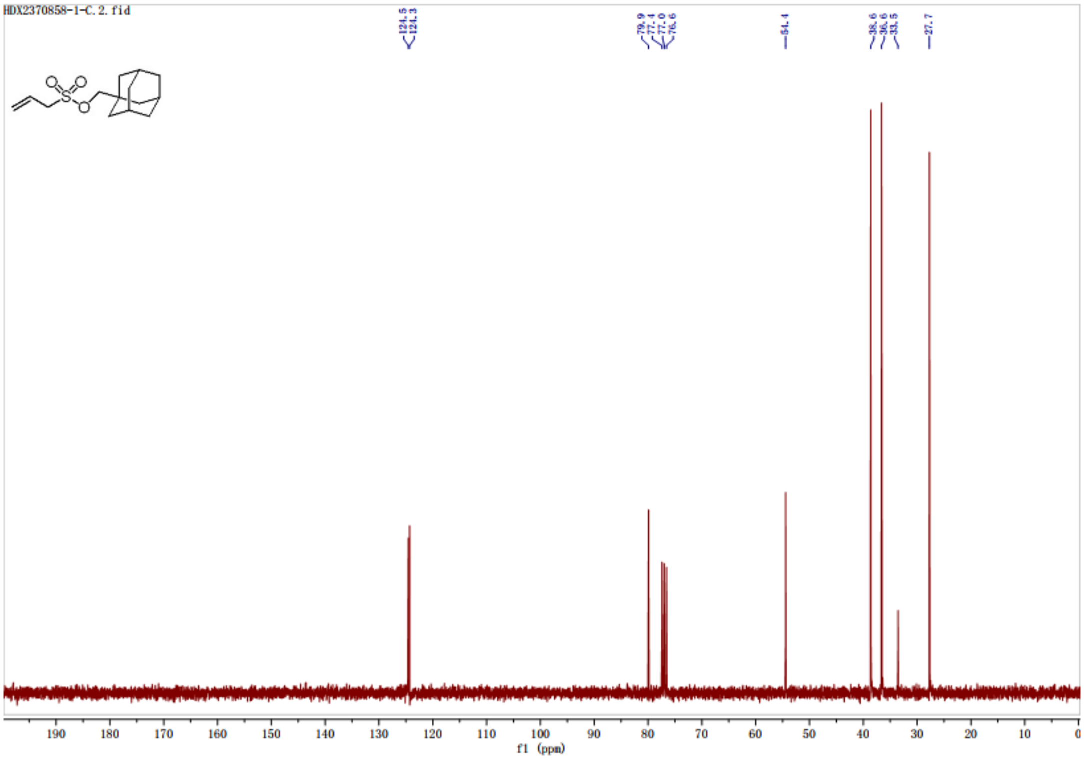
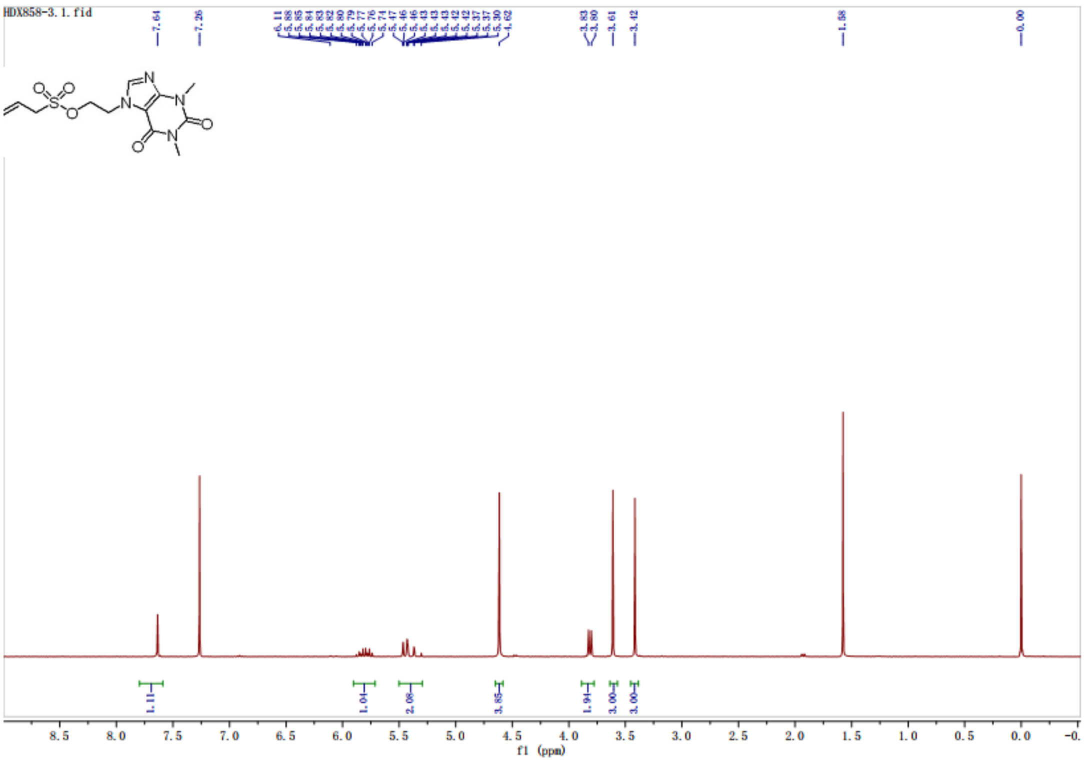
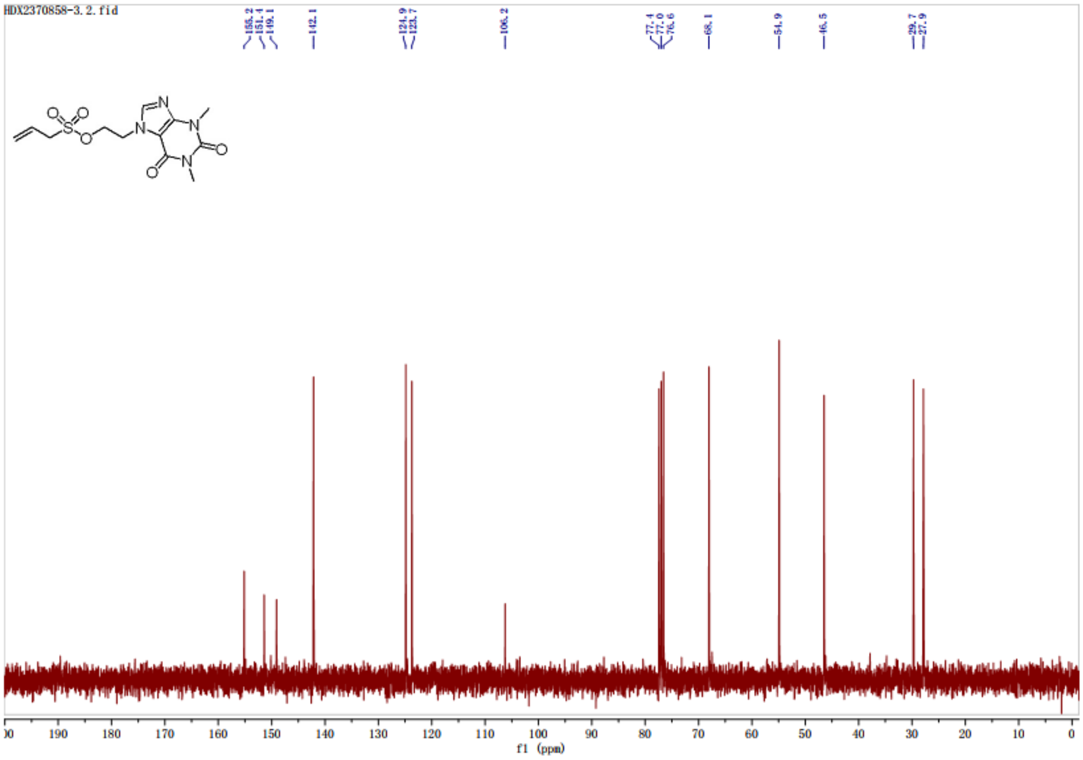
-0.00
1.00
1.98
2.00
1.92
3.01
6.15
6.89
f1 (ppm)

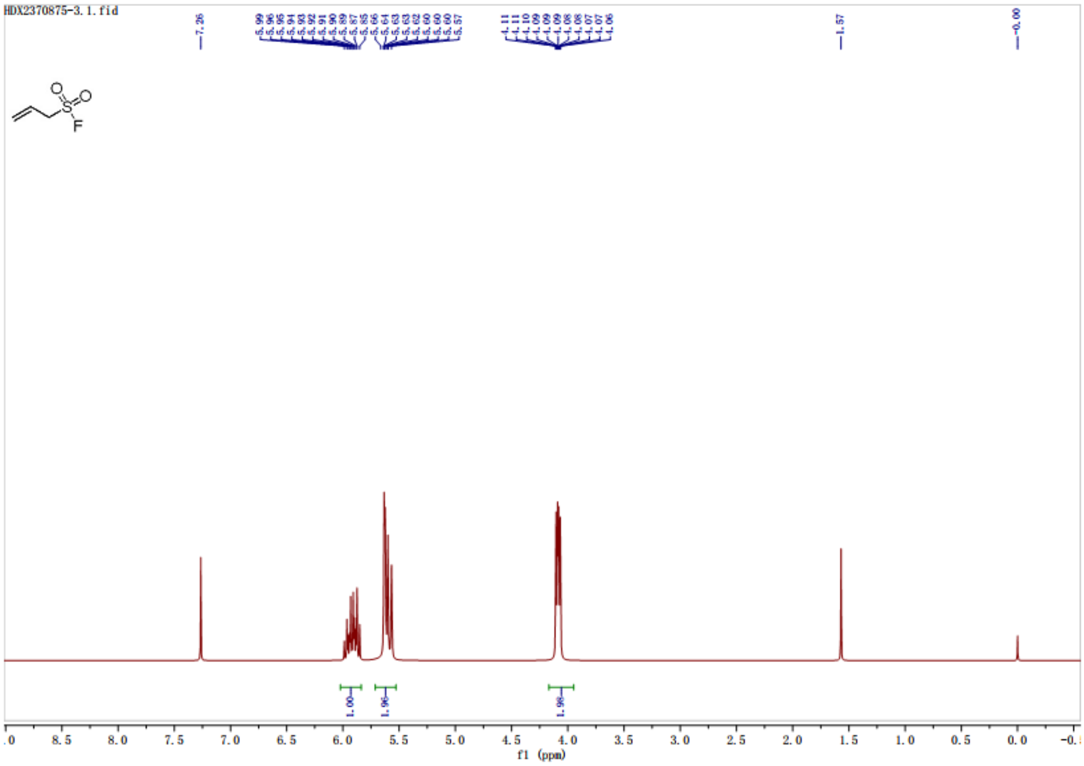


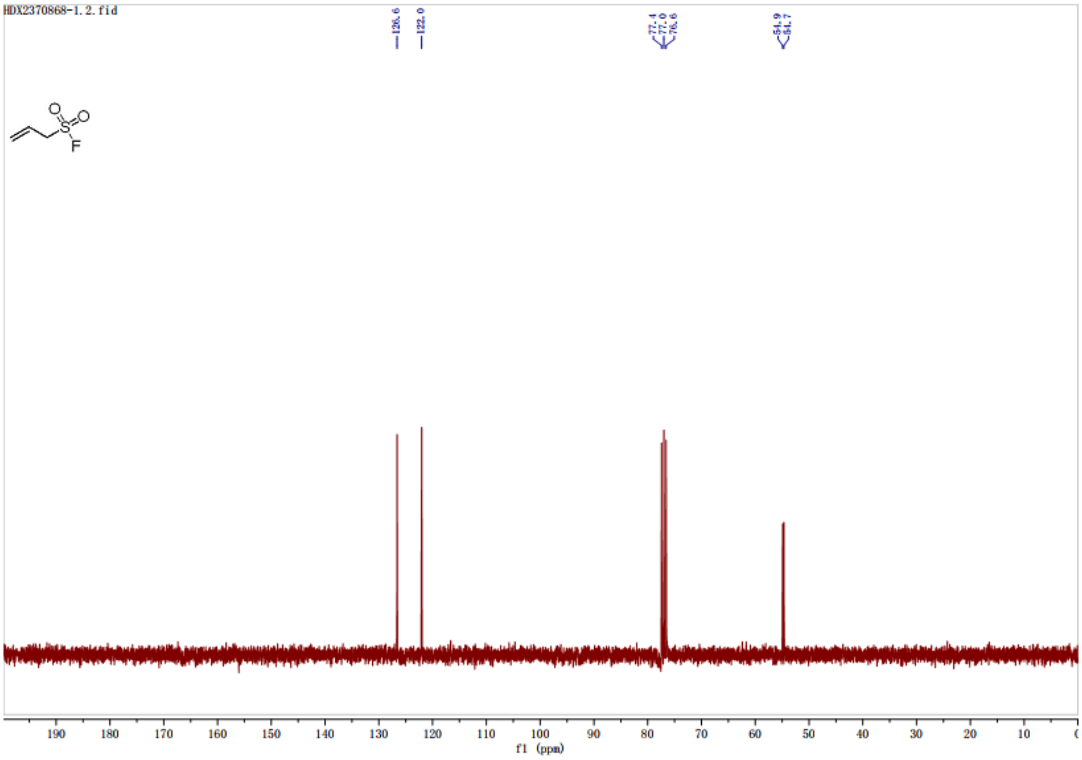
HDX2370858-1-C.2.fid
124.5
124.3
79.9
77.4
77.0
76.6
54.4
38.6
36.6
33.5
27.7
f1 (ppm)



HDX858-3.1.fid
7.64
7.26
4.62
3.83
3.80
3.61
3.42
1.58
0.00
1.11
1.04
2.08
3.85
1.94
3.00
3.00
f1 (ppm)






HDX2370868-1.2.fid
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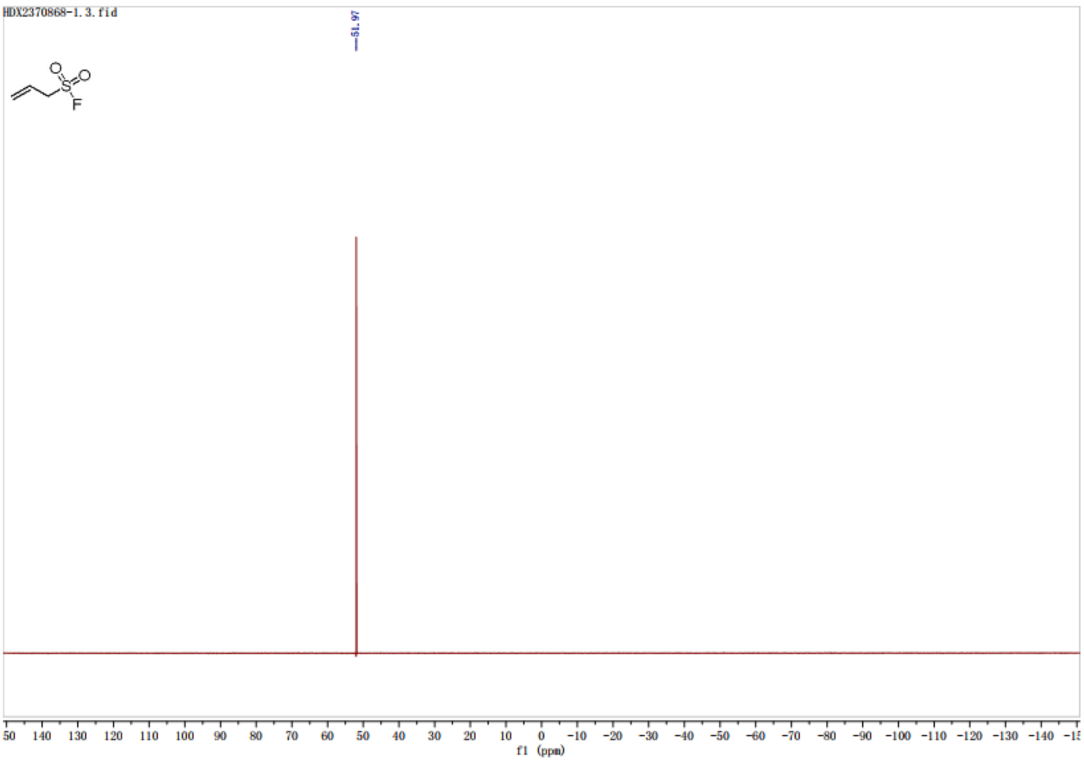
122.0
77.4
77.0
76.6
54.9
54.7
f1 (ppm)


HDX2370868-1.3.fid
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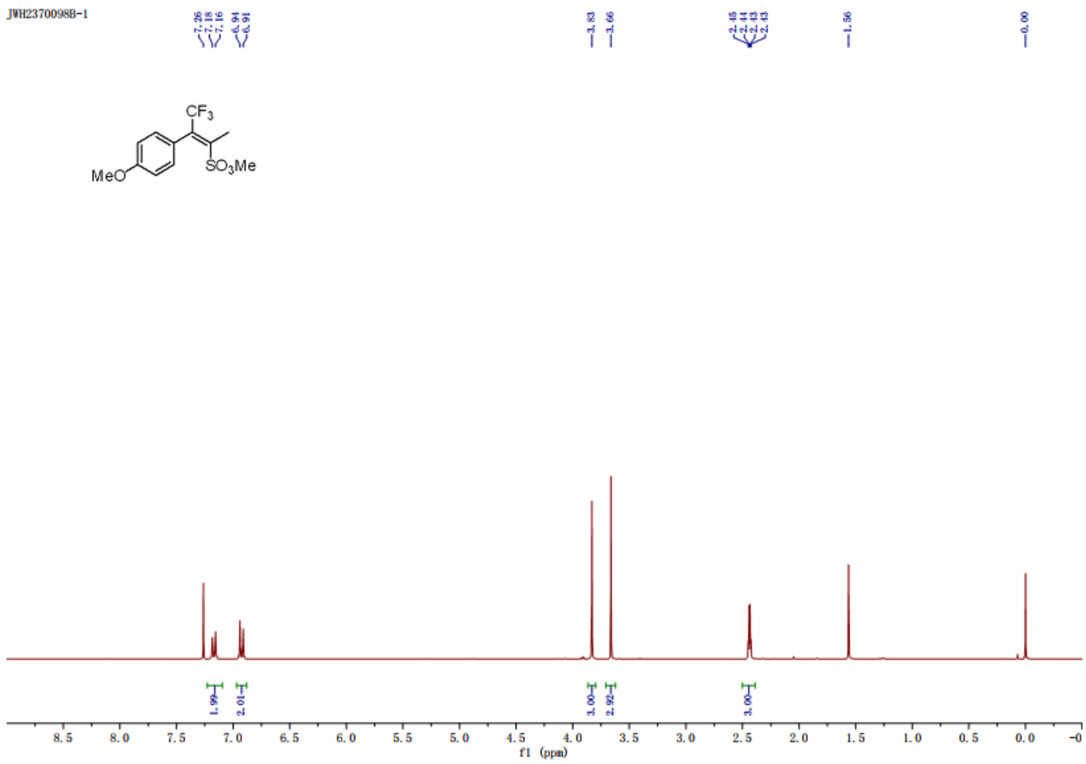
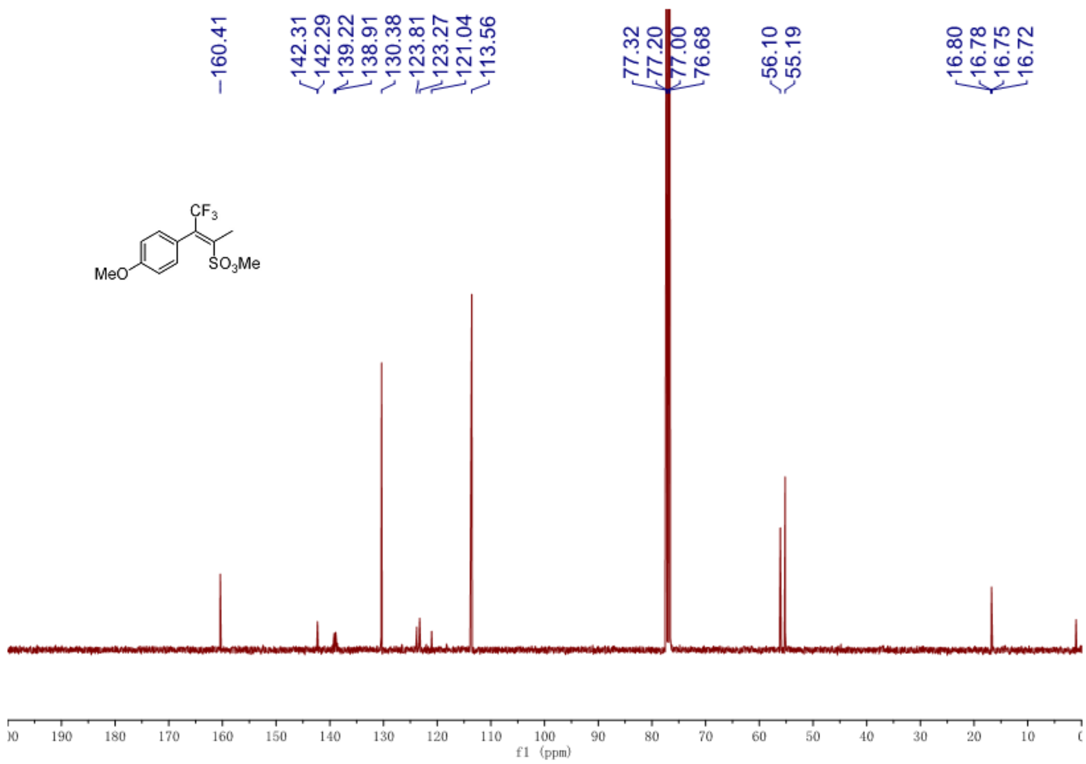
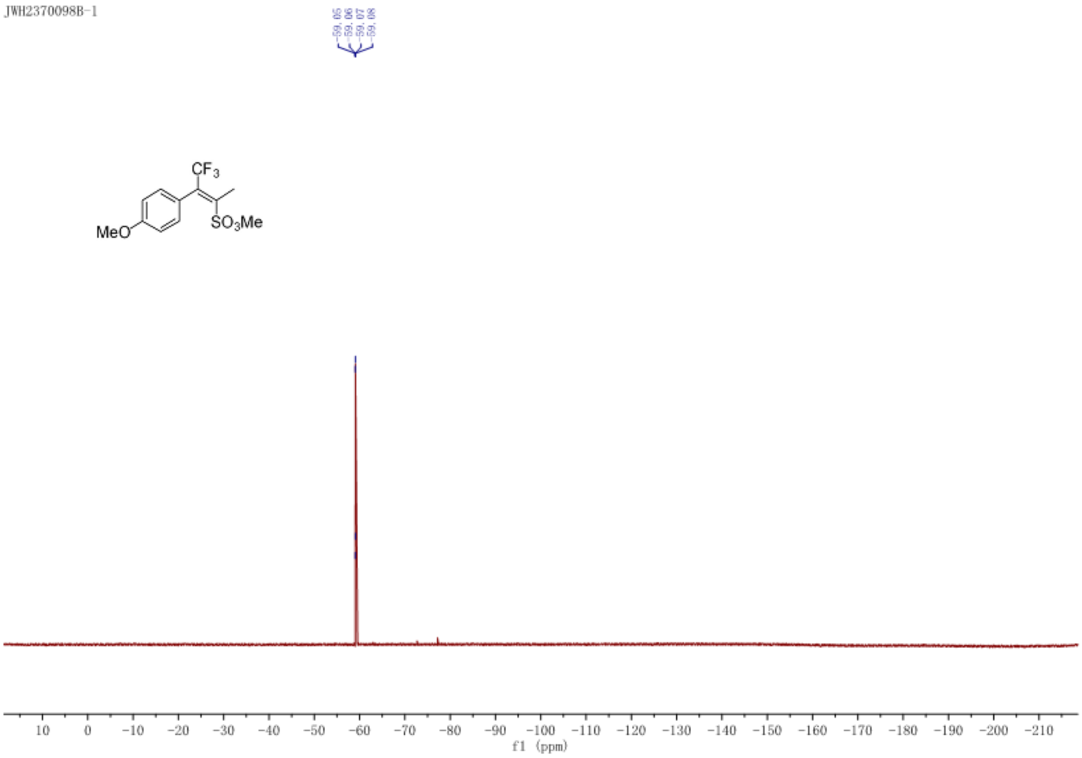
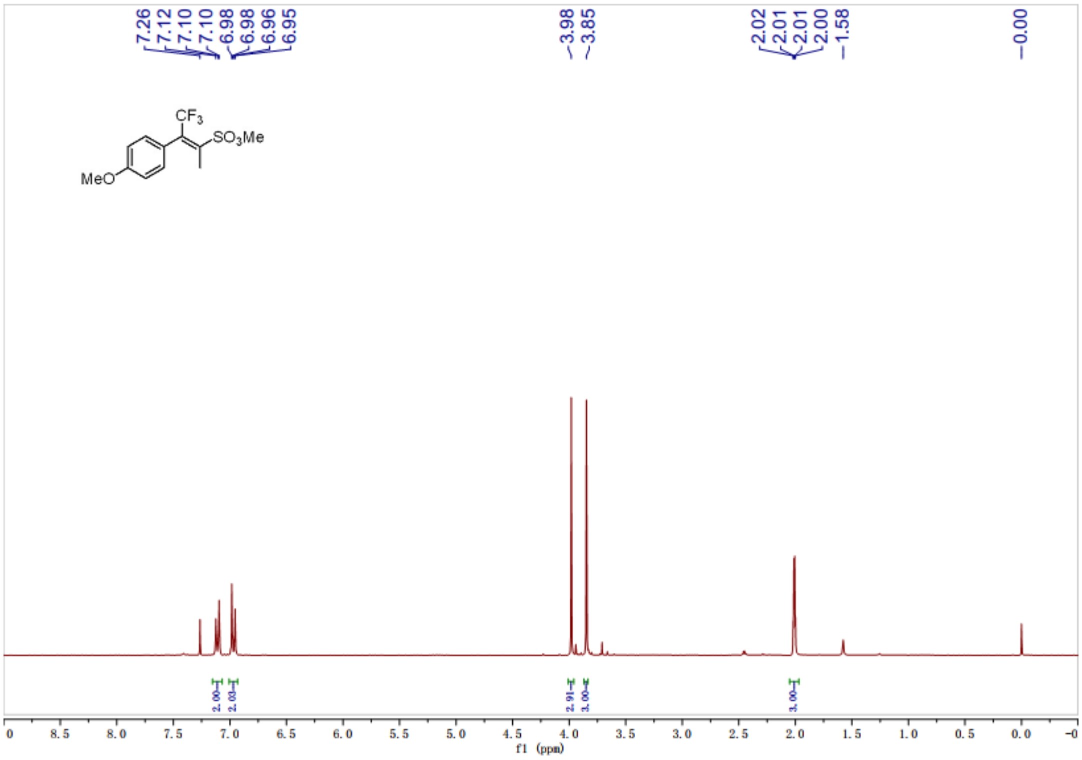
f1 (ppm)

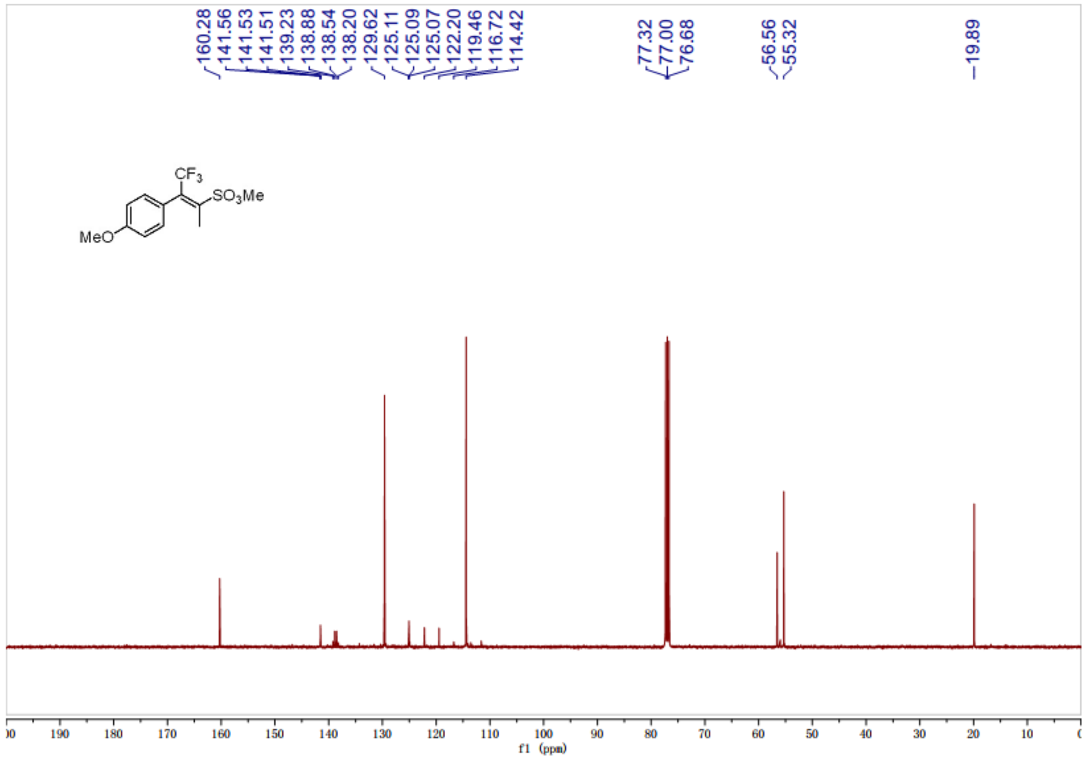




JWH2370098B-1






160.28
141.56
141.53
141.51
139.23
138.88
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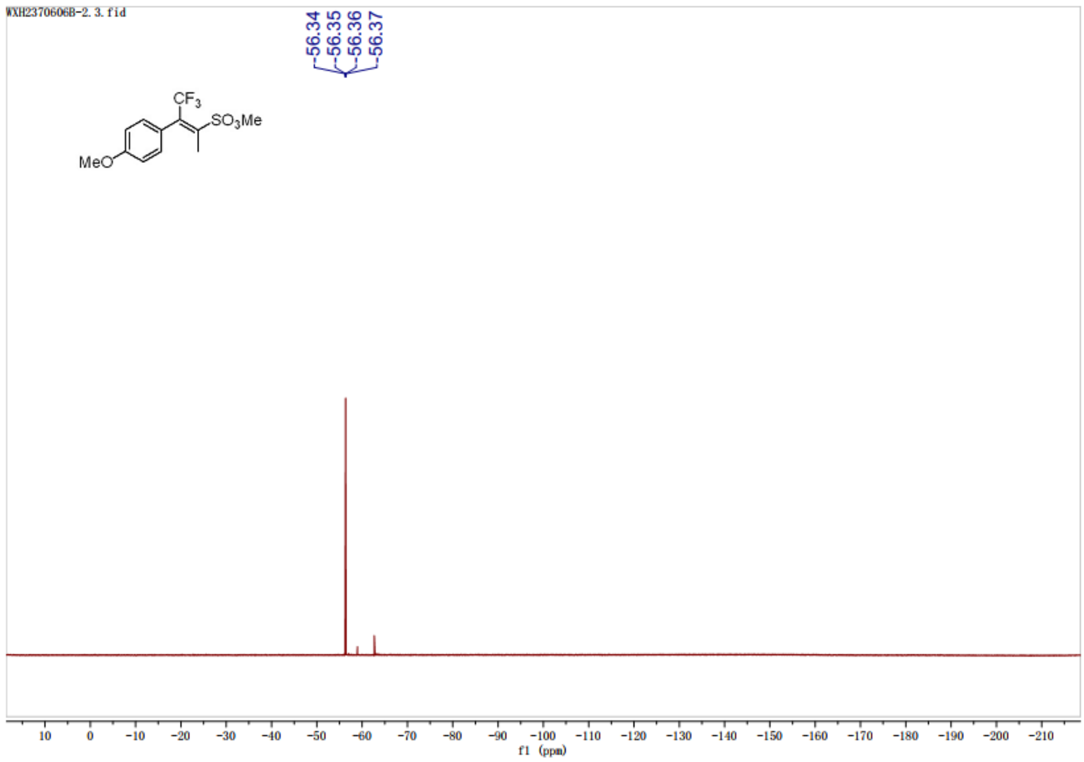
138.20
129.62
125.11
125.09
125.07
122.20
119.46
116.72
114.42
77.32
77.00
76.68
56.56
55.32
19.89
CF_3
SO_3Me
MeO
f1 (ppm)


WXH2370606B-2.3.fid
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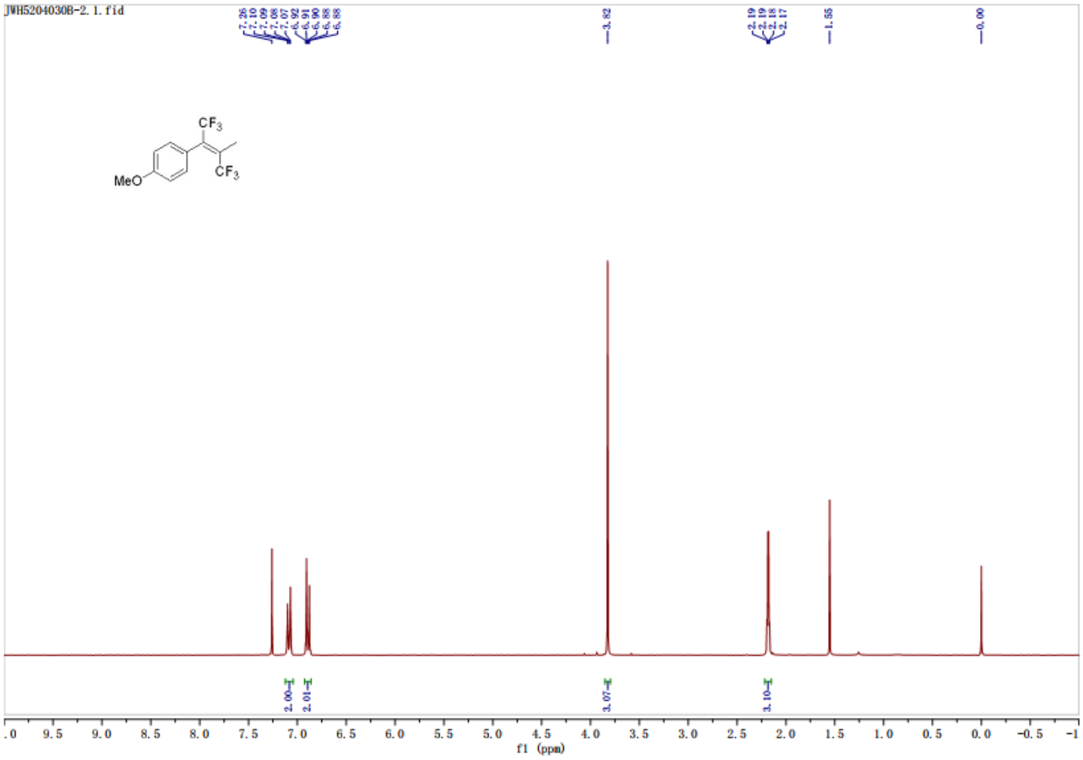
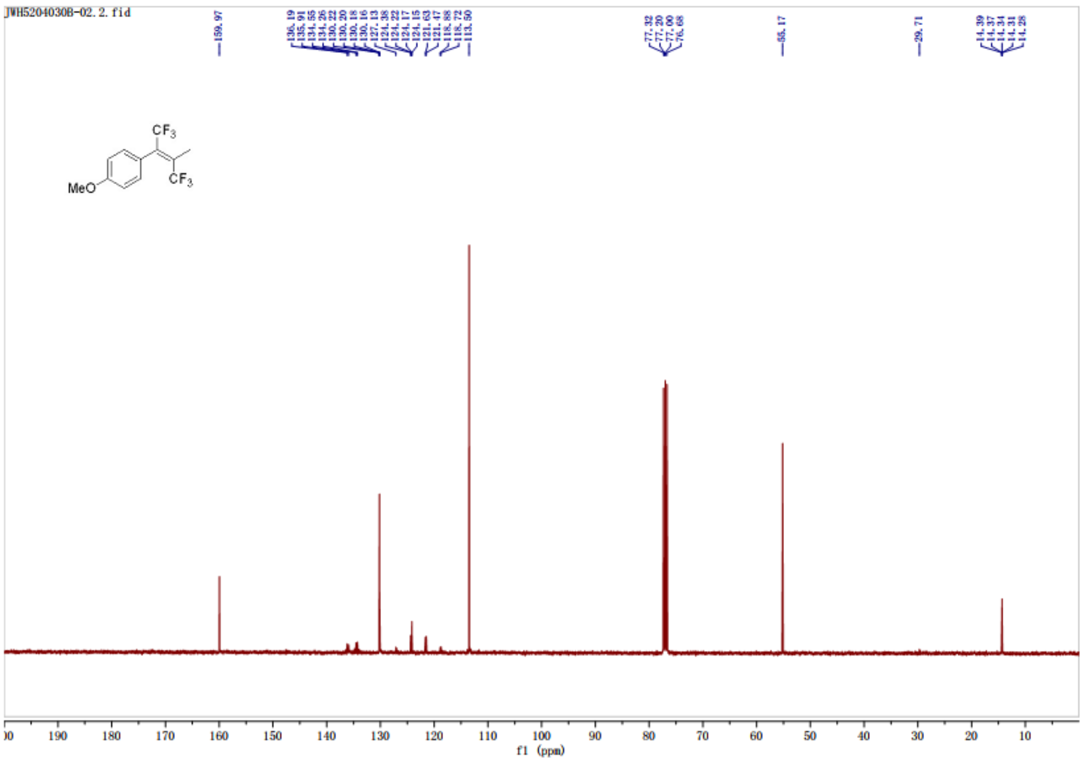
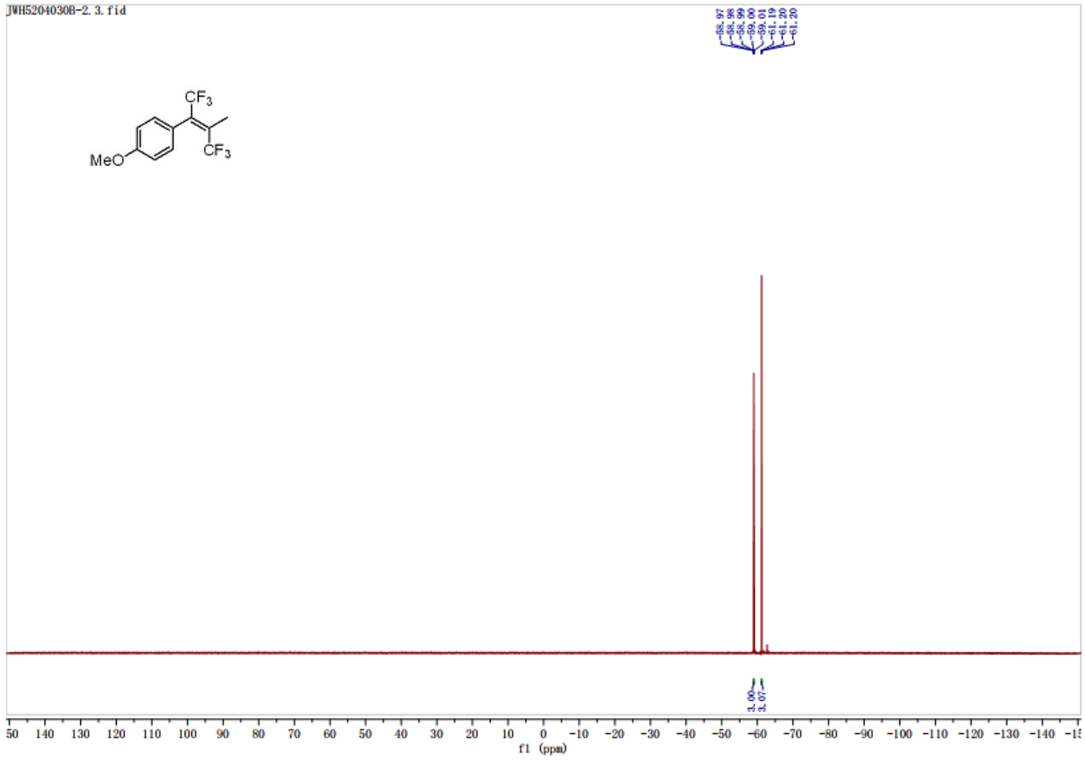
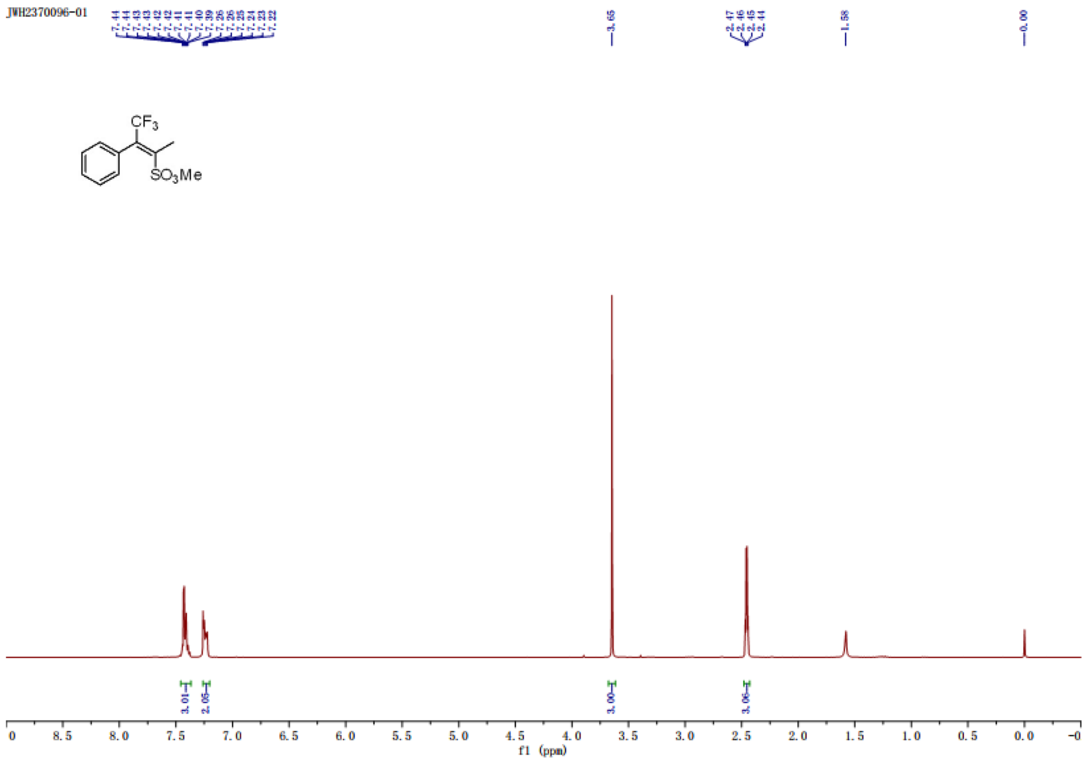
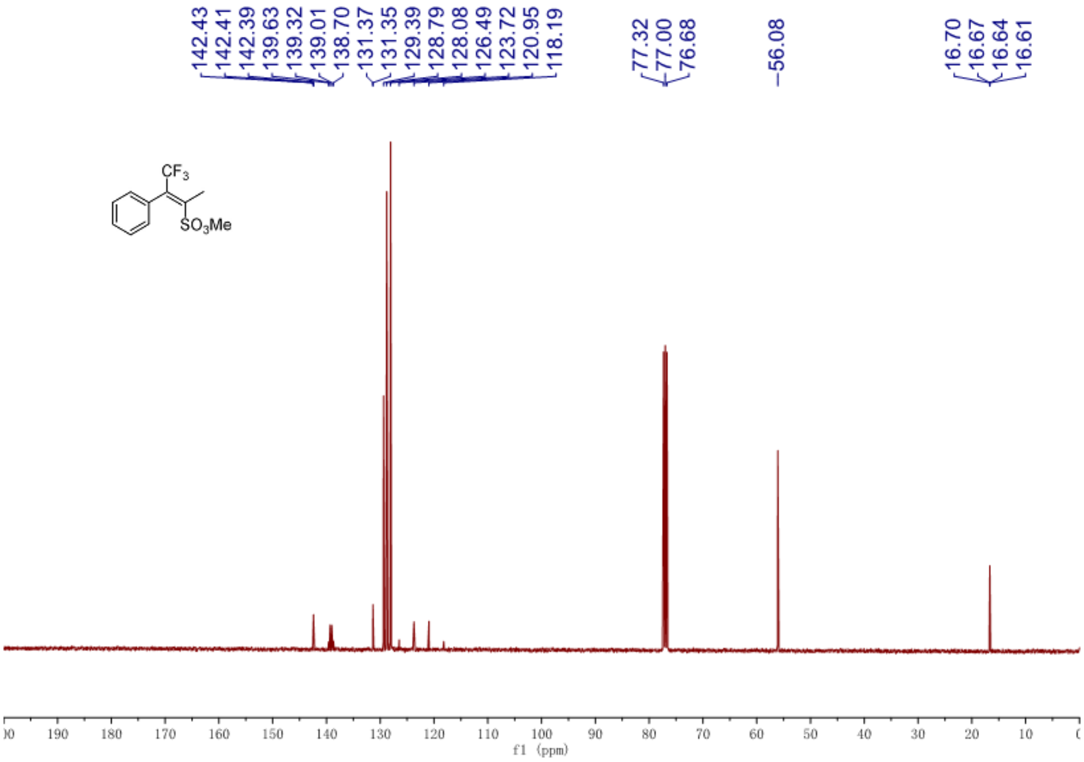
-56.36
-56.37
CF_3
SO_3Me
MeO
f1 (ppm)







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142.41
142.39
139.63
139.32
139.01
138.70
131.37
131.35
129.39
128.79
128.08
126.49
123.72
120.95
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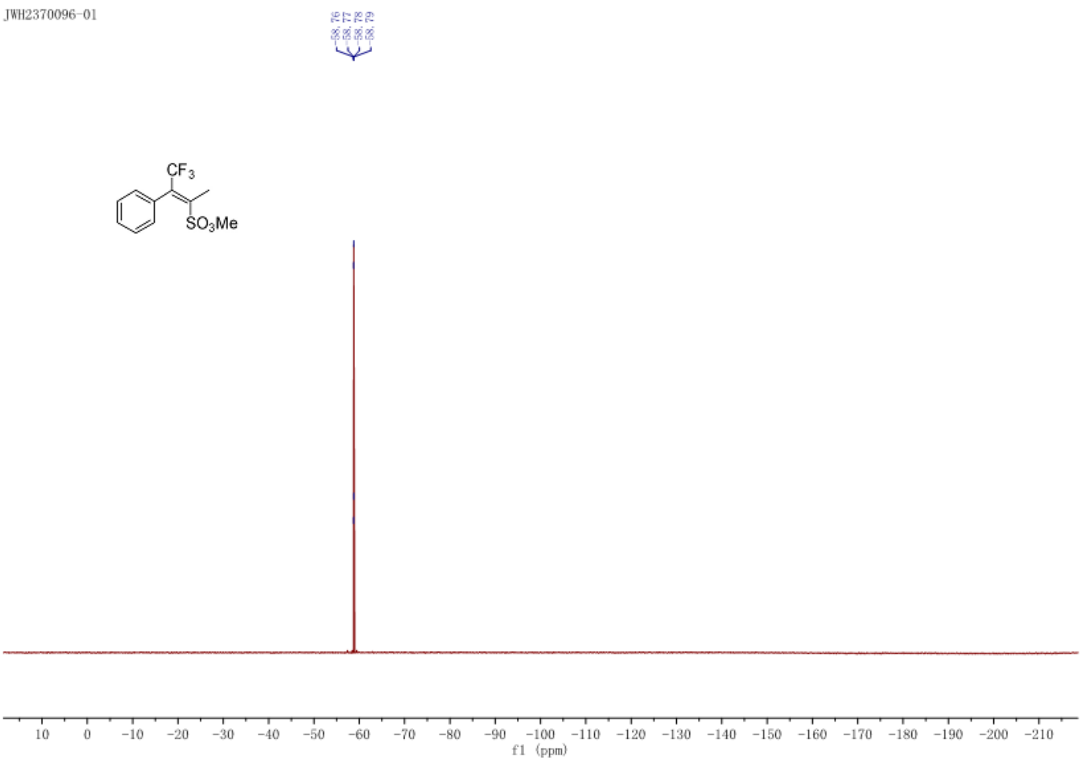
CF3
SO3Me
f1 (ppm)


JWH2370096-01
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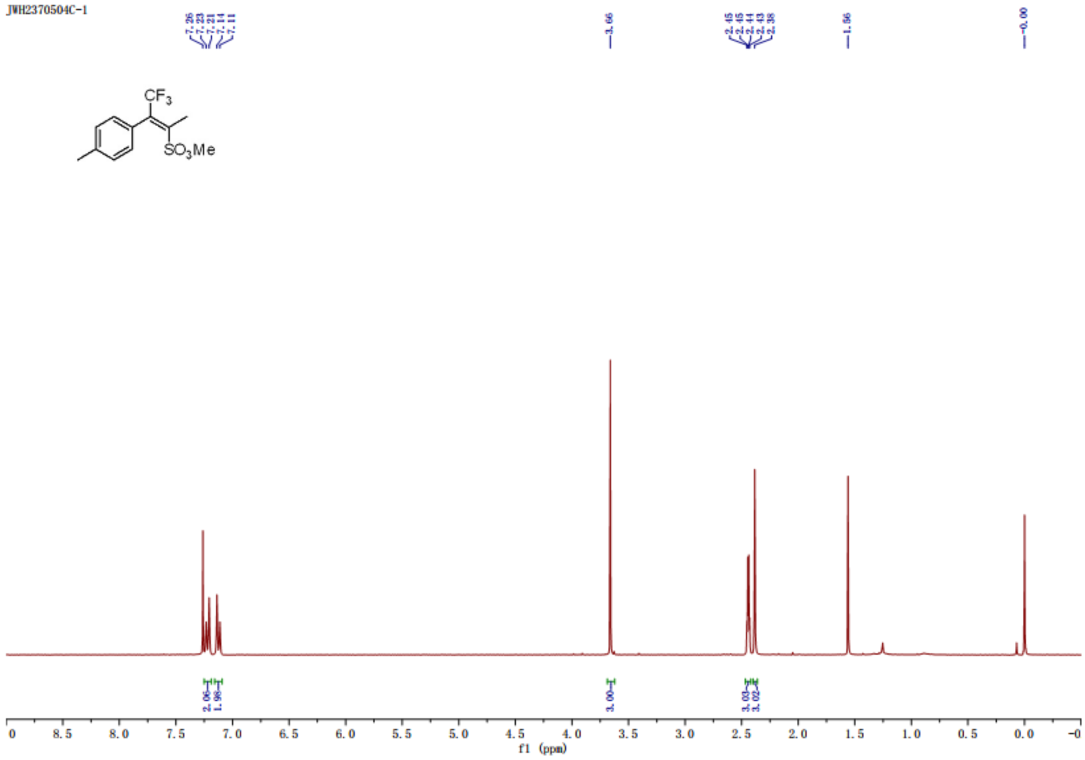
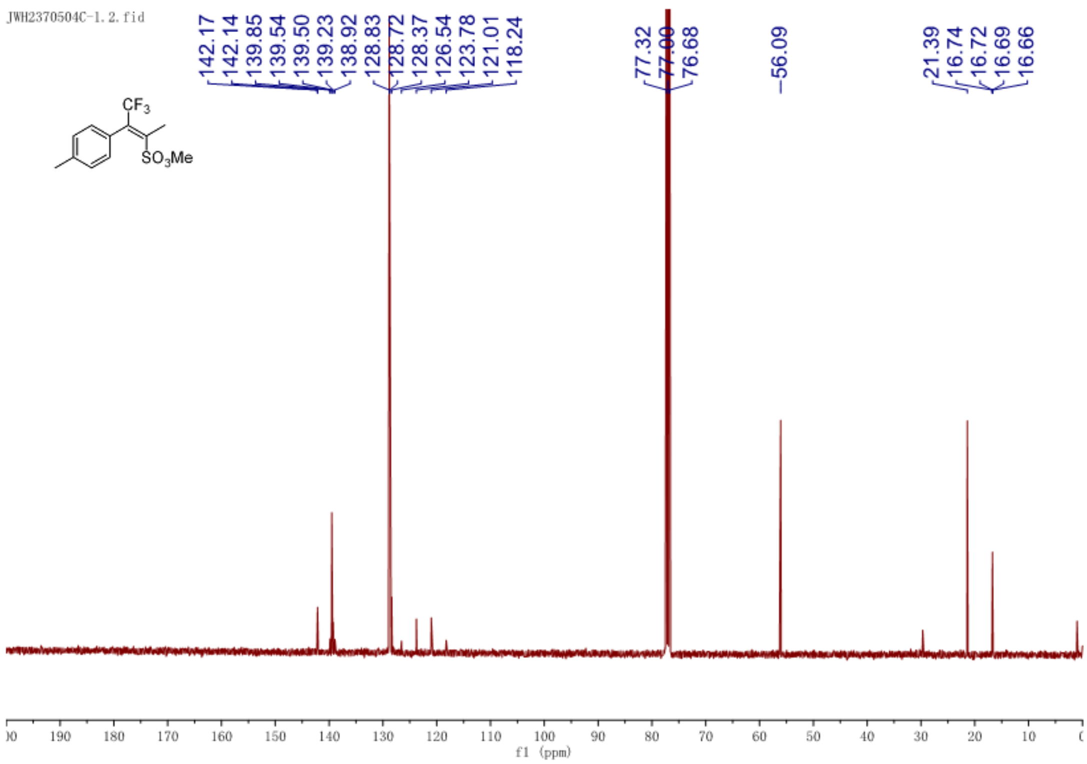
-58.77
-58.78
-58.79
CF3
SO3Me
f1 (ppm)



JWH2370504C-1
7.26
7.23
7.21
7.14
7.11
3.66
2.45
2.45
2.44
2.43
2.38
1.56
0.00
2.06
1.98
3.00
3.03
3.02
f1 (ppm)



JWH2370504C-1.2.fid
142.17
142.14
139.85
139.54
139.50
139.23
138.92
128.83
128.72
128.37
126.54
123.78
121.01
118.24
77.32
77.00
76.68
56.09
21.39
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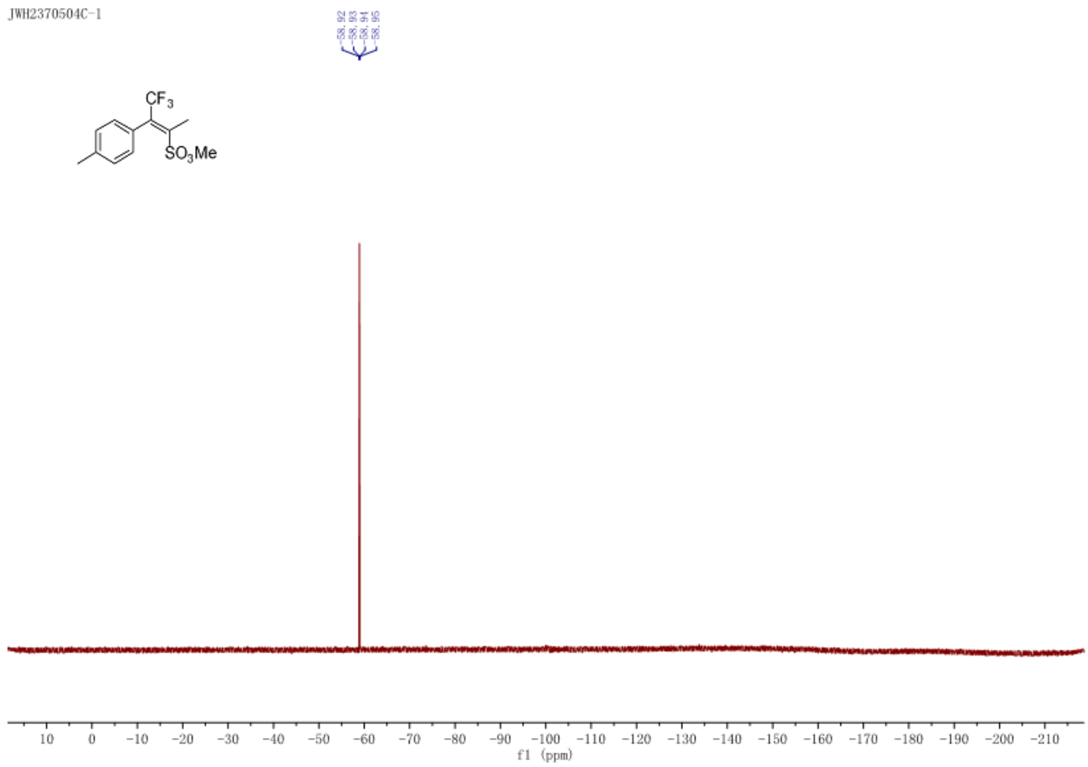
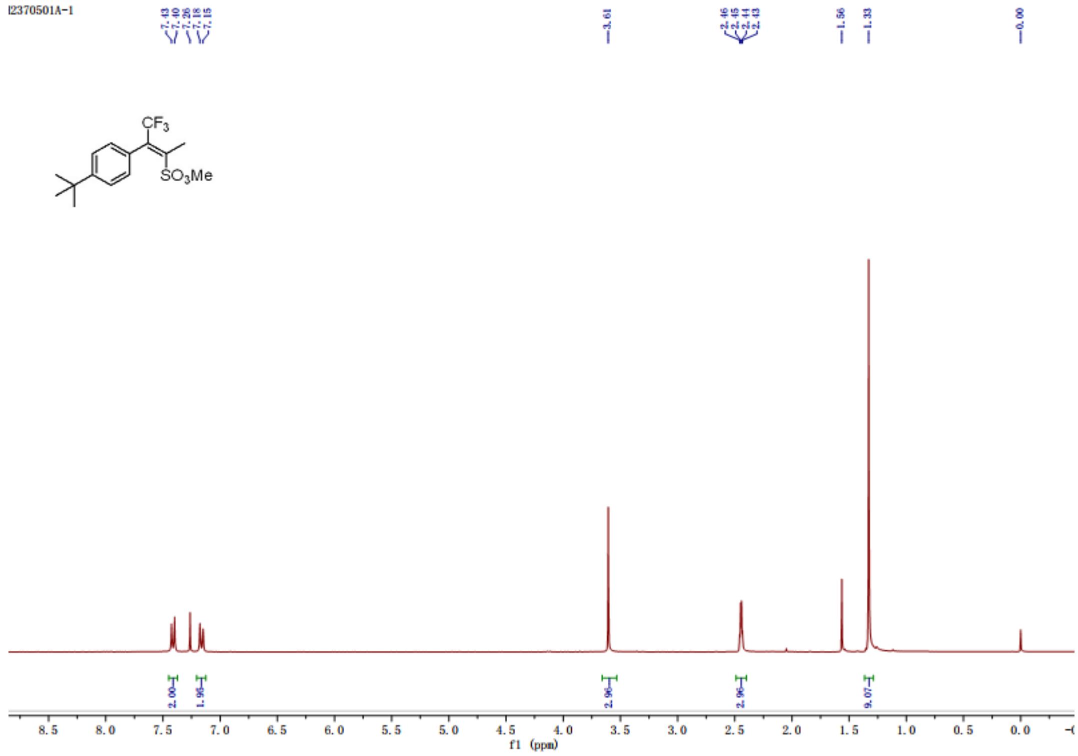
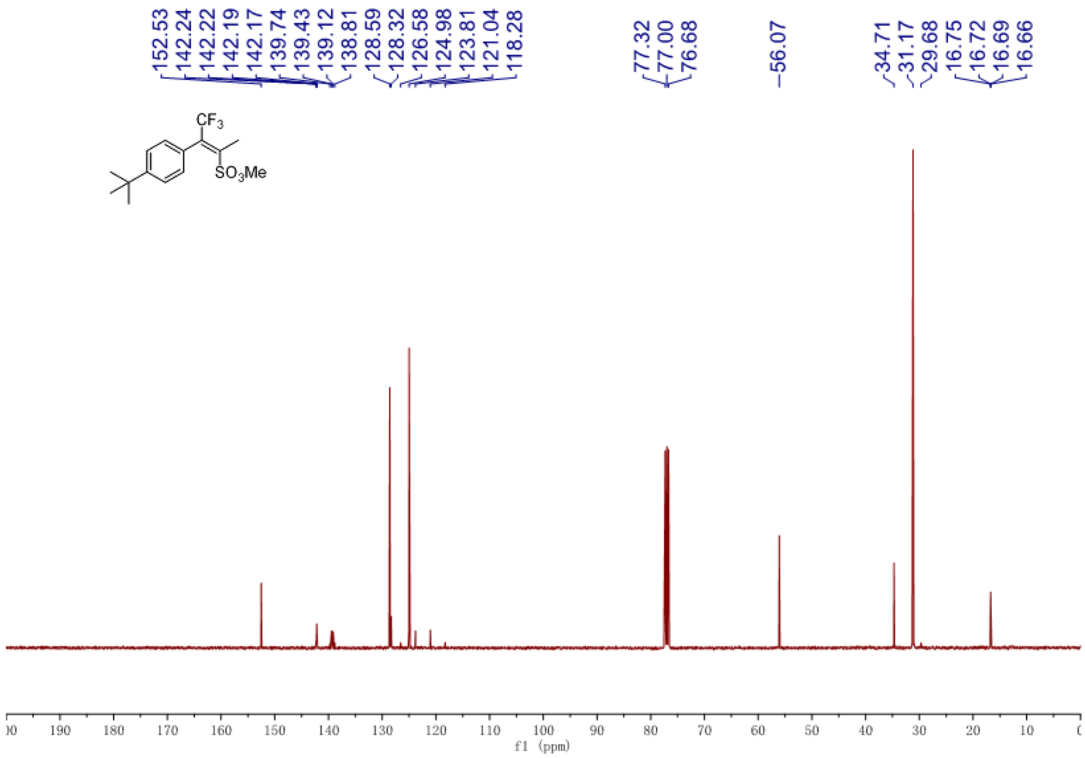
16.69
16.66
f1 (ppm)


JWH2370504C-1
-58.92
-58.93
-58.94
-58.95
f1 (ppm)


I2370501A-1
f1 (ppm)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139.43
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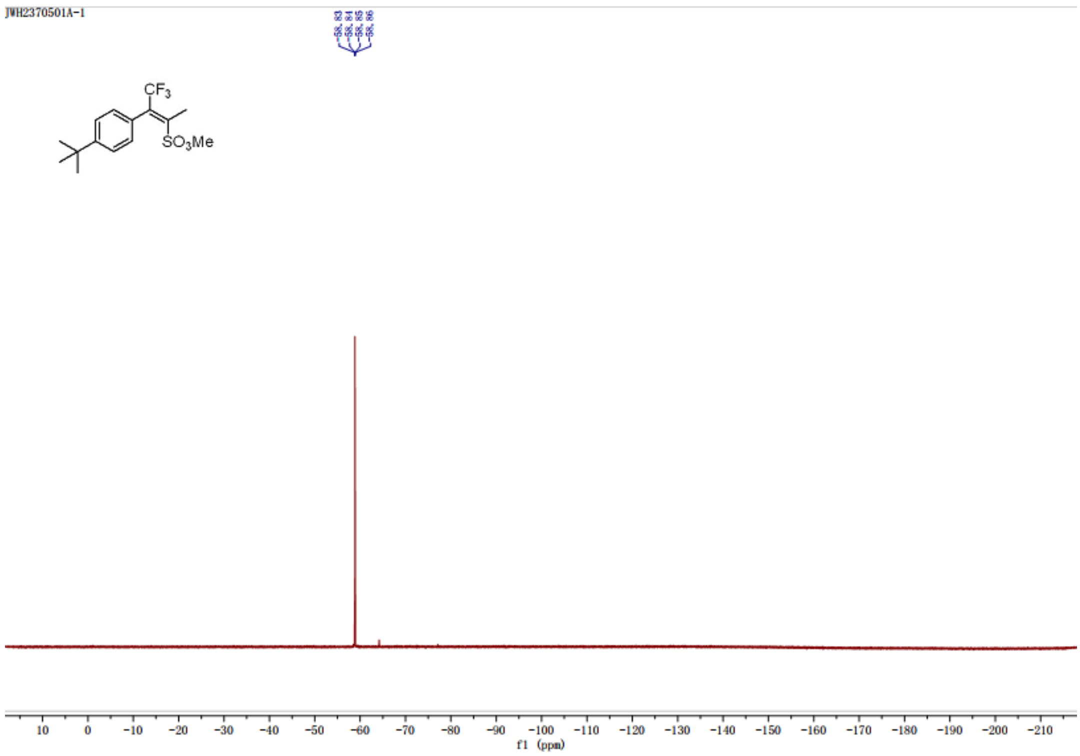
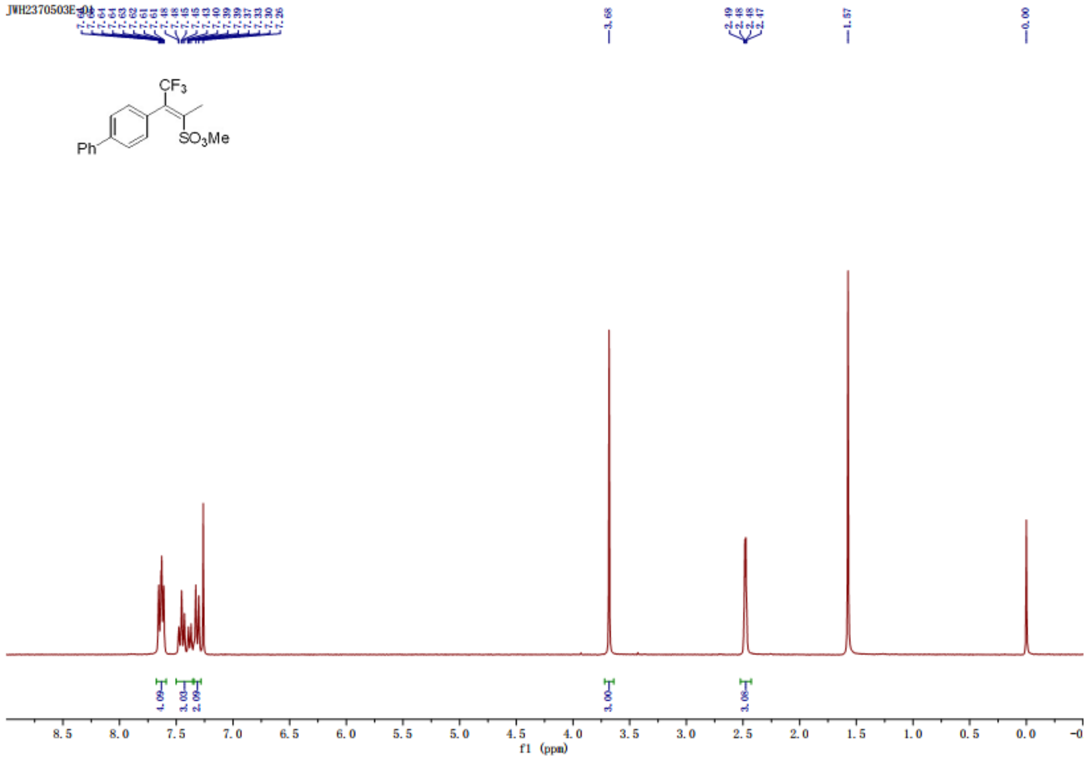
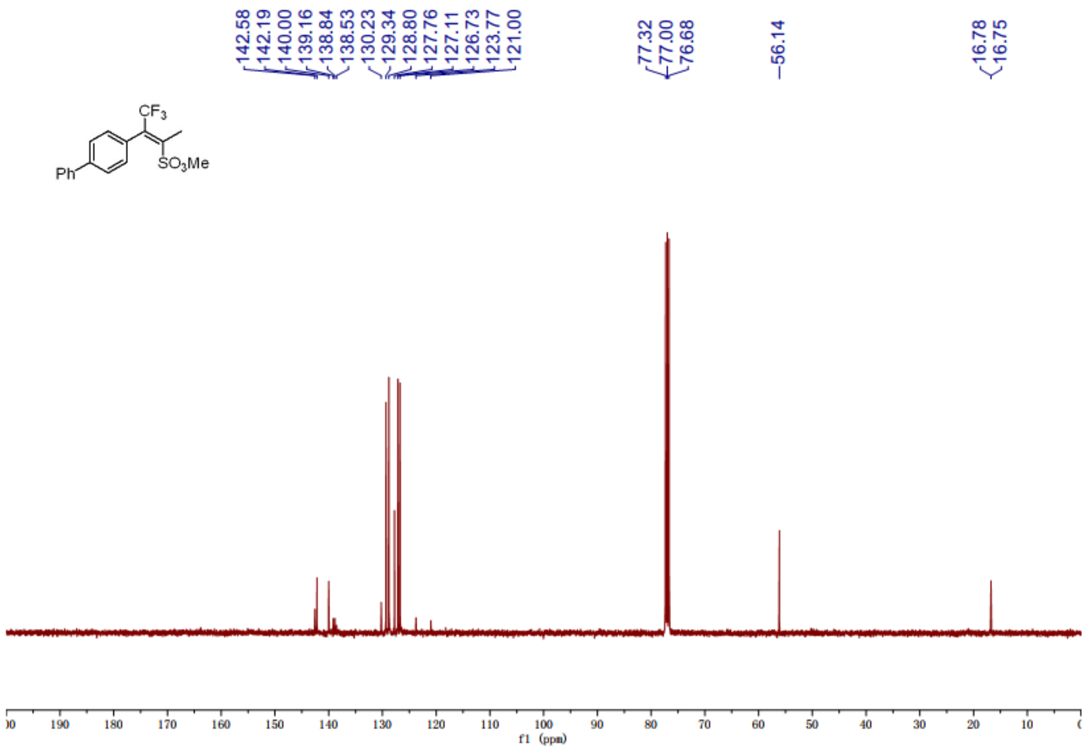
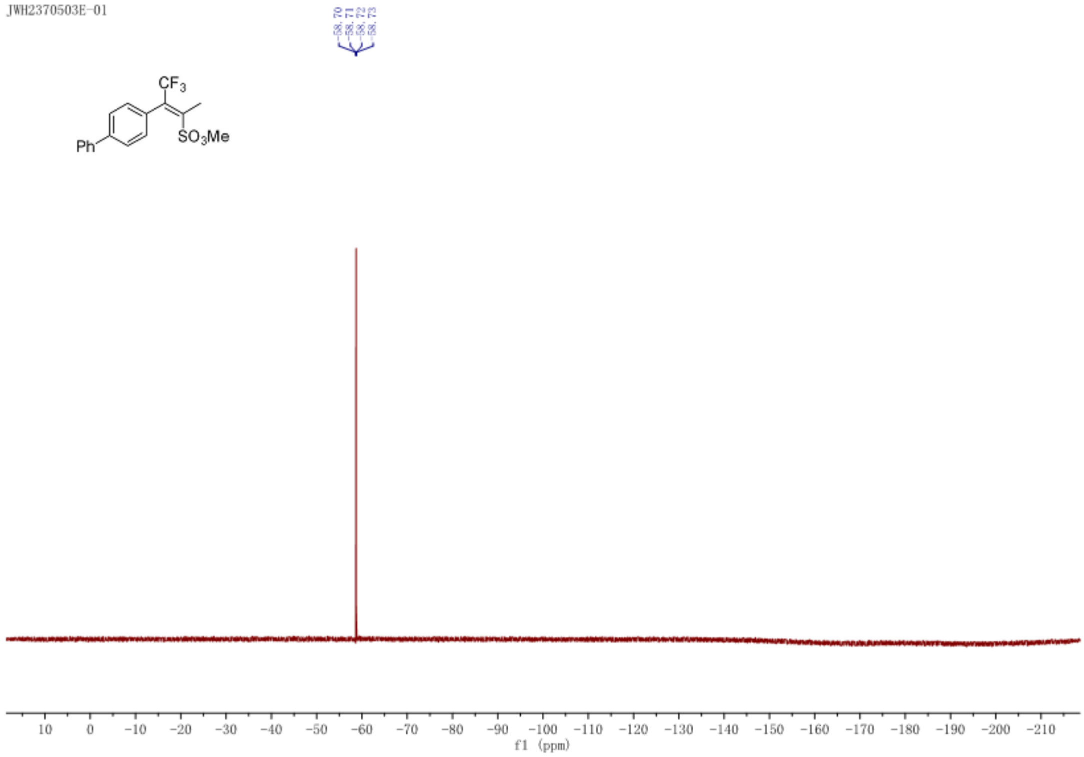
126.58
124.98
123.81
121.04
118.28
77.32
77.00
76.68
56.07
34.71
31.17
29.68
16.75
16.72
16.69
16.66
CF3
SO3Me
f1 (ppm)


JWH2370501A-1
CF3
SO3Me
f1 (ppm)

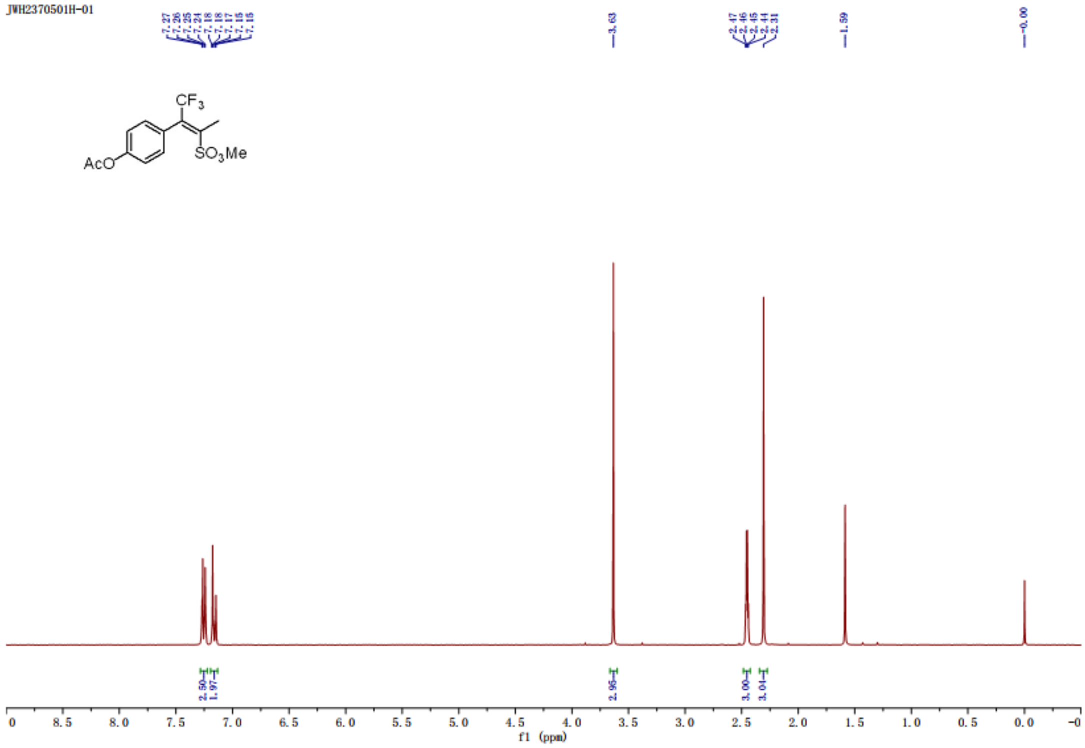


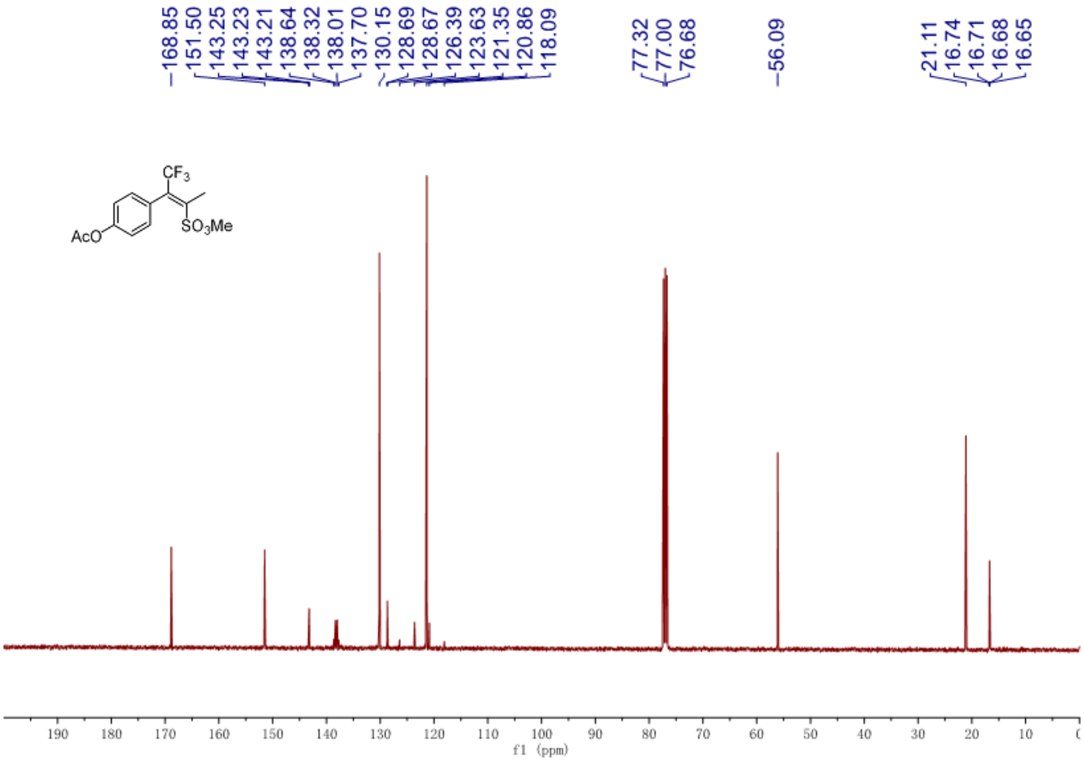


JWH2370503E-01



JWH2370501H-01

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143.23
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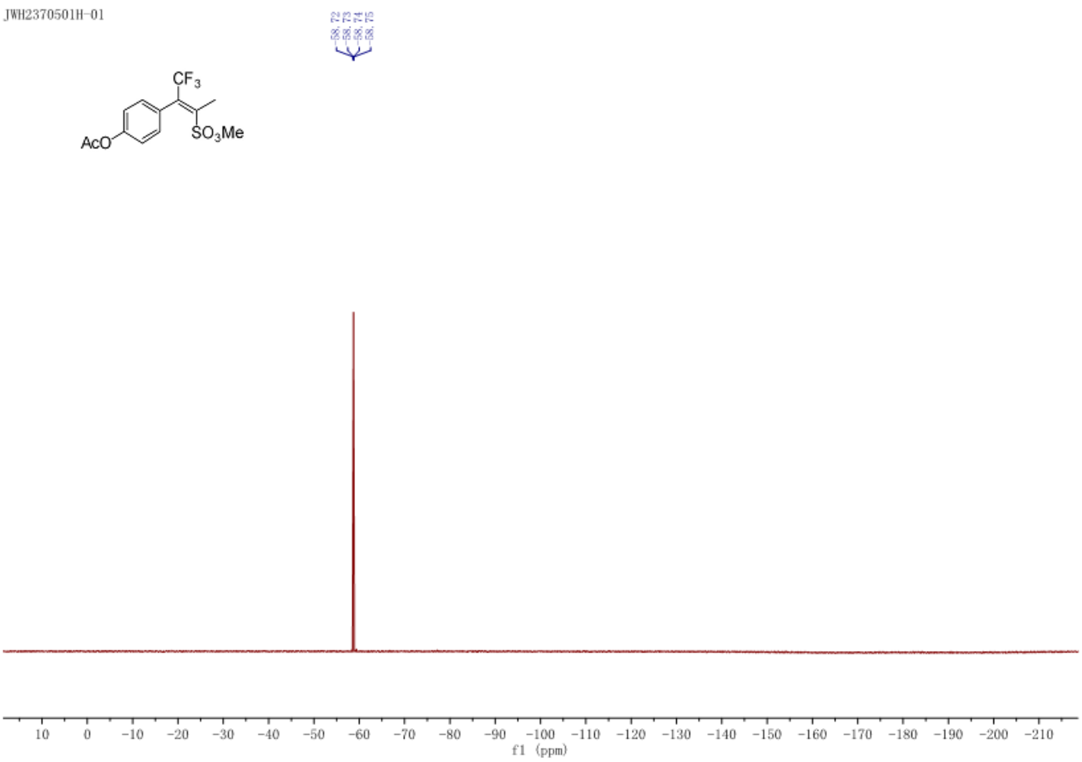
138.64
138.32
138.01
137.70
130.15
128.69
128.67
126.39
123.63
121.35
120.86
118.09
77.32
77.00
76.68
56.09
21.11
16.74
16.71
16.68
16.65
CF3
AcO
SO3Me
f1 (ppm)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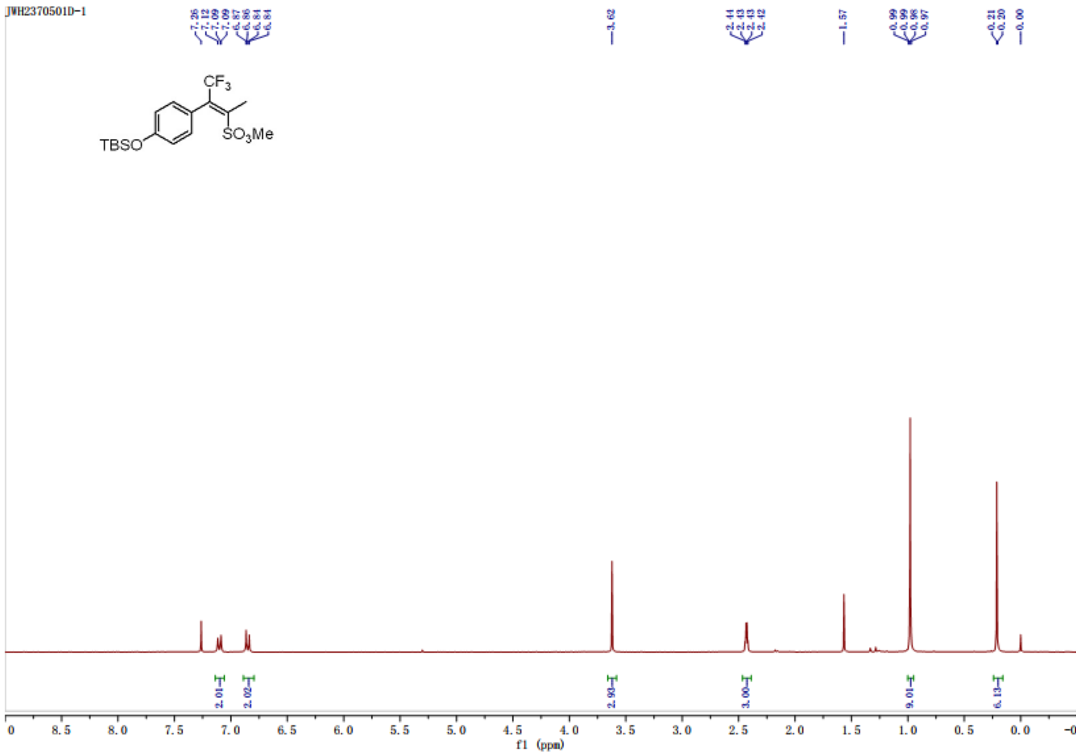
AcO
SO3Me
f1 (ppm)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7.09
6.87
6.86
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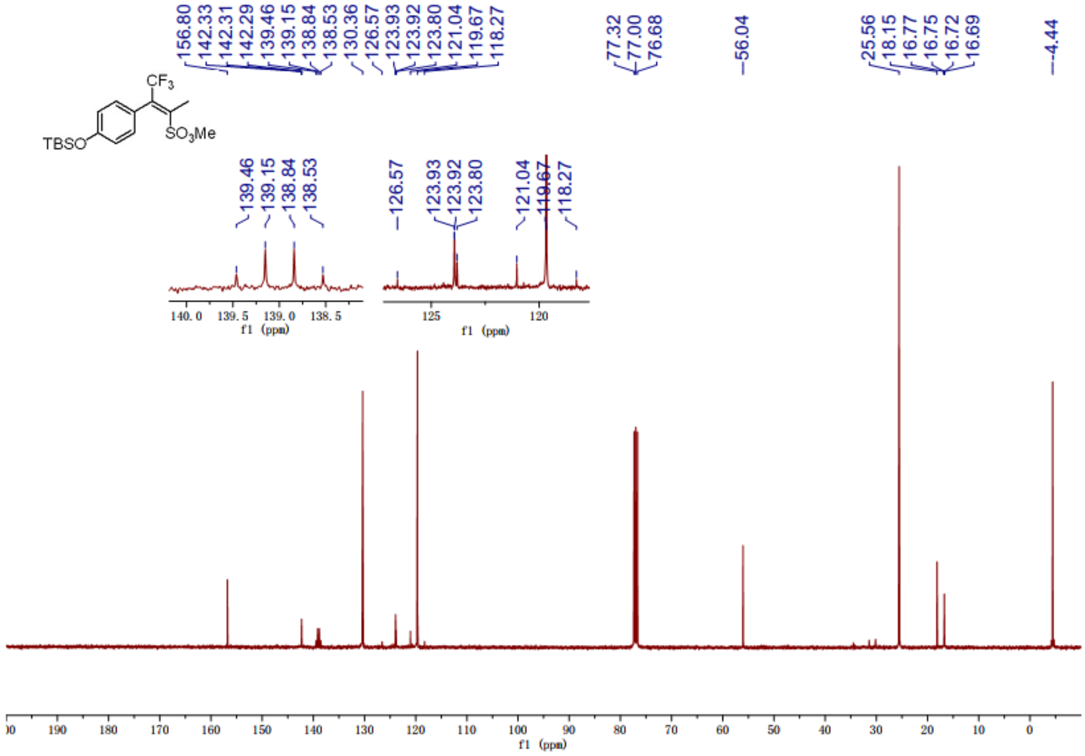
6.84
3.62
2.44
2.43
2.43
2.42
1.57
0.99
0.99
0.98
0.97
0.21
0.20
0.00
CF3
TBSO
SO3Me
2.01
2.02
2.93
3.00
9.01
6.13
f1 (ppm)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142.31
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138.53
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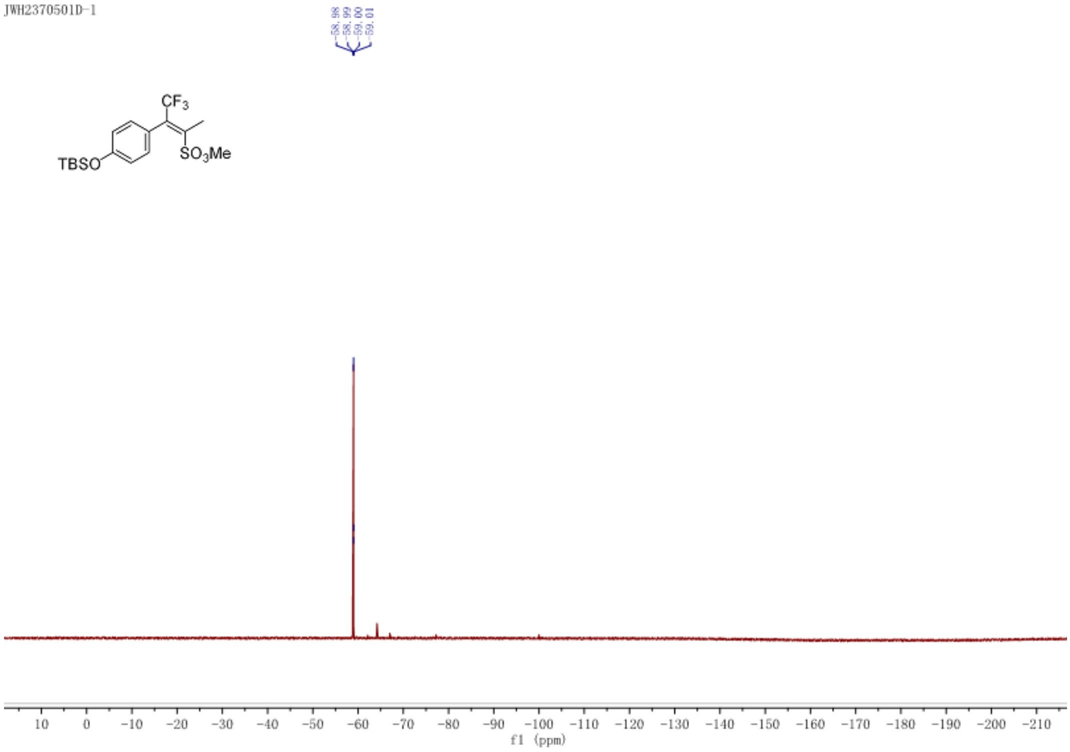
126.57
123.93
123.92
123.80
121.04
119.67
118.27
77.32
77.00
76.68
56.04
25.56
18.15
16.77
16.75
16.72
16.69
-4.44
CF3
TBSO
SO3Me
f1 (ppm)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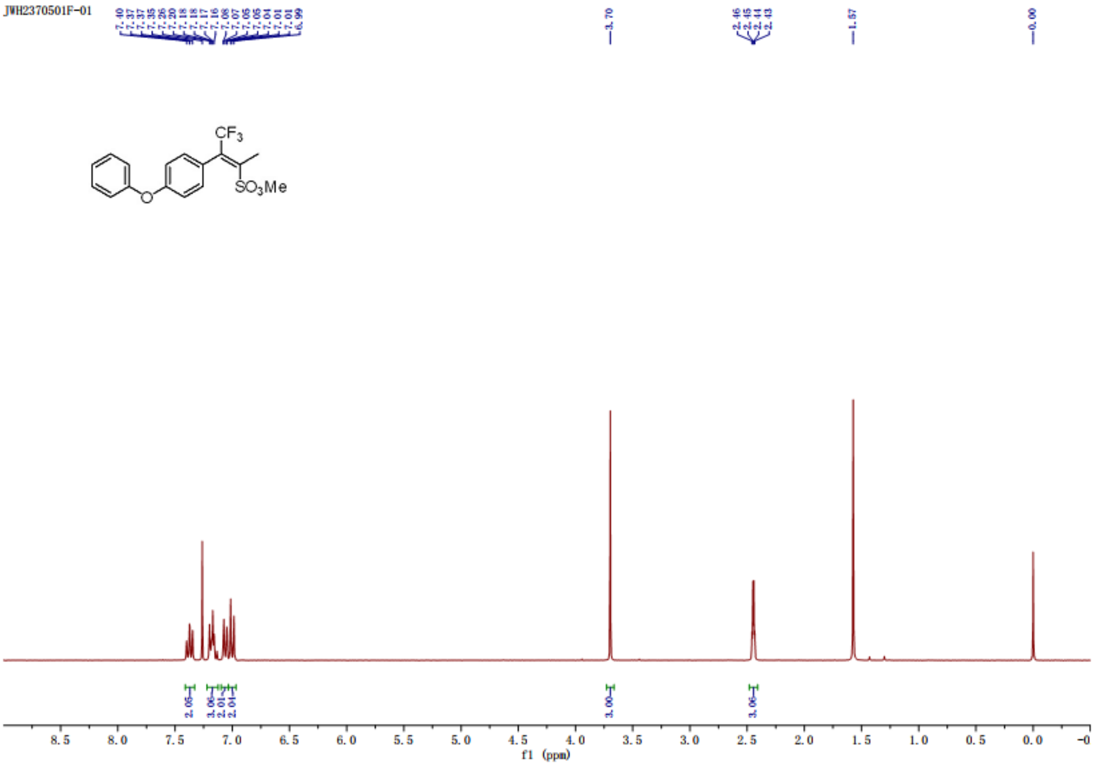
CF3
TBSO
SO3Me
f1 (ppm)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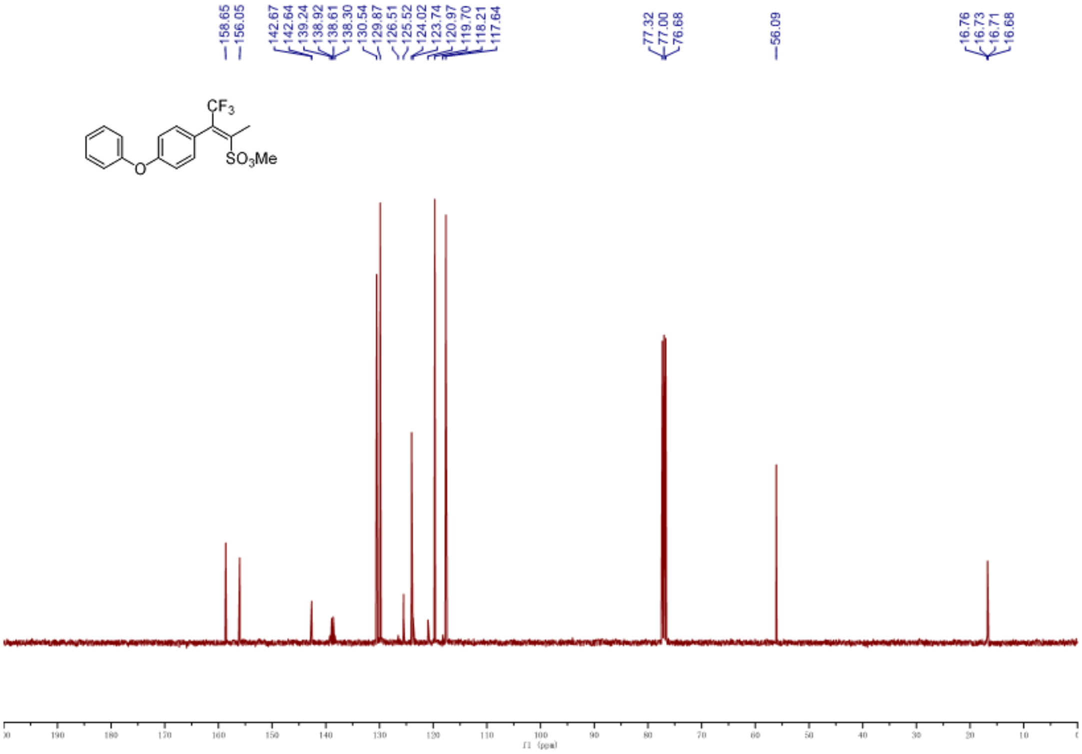
7.37
7.35
7.26
7.20
7.18
7.17
7.16
7.08
7.07
7.05
7.05
7.04
7.01
7.01
6.99
3.70
2.46
2.45
2.44
2.43
1.57
0.00
CF3
SO3Me
O
2.05
1.06
2.01
2.04
3.00
3.06
f1 (ppm)



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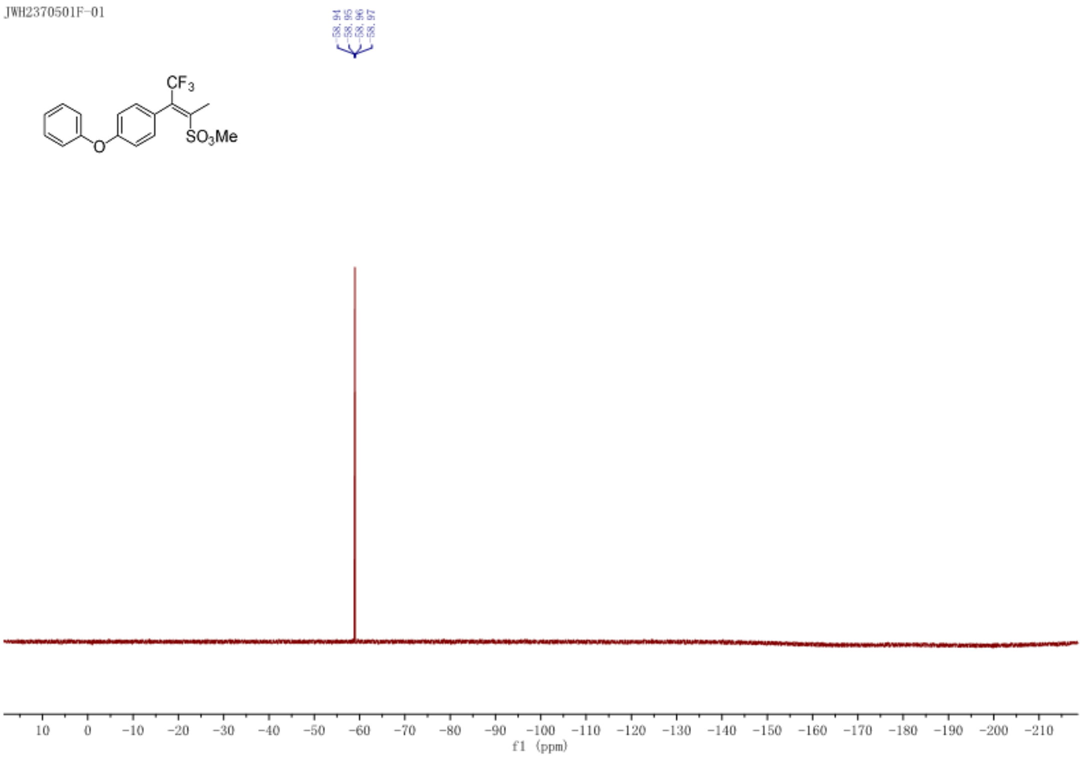

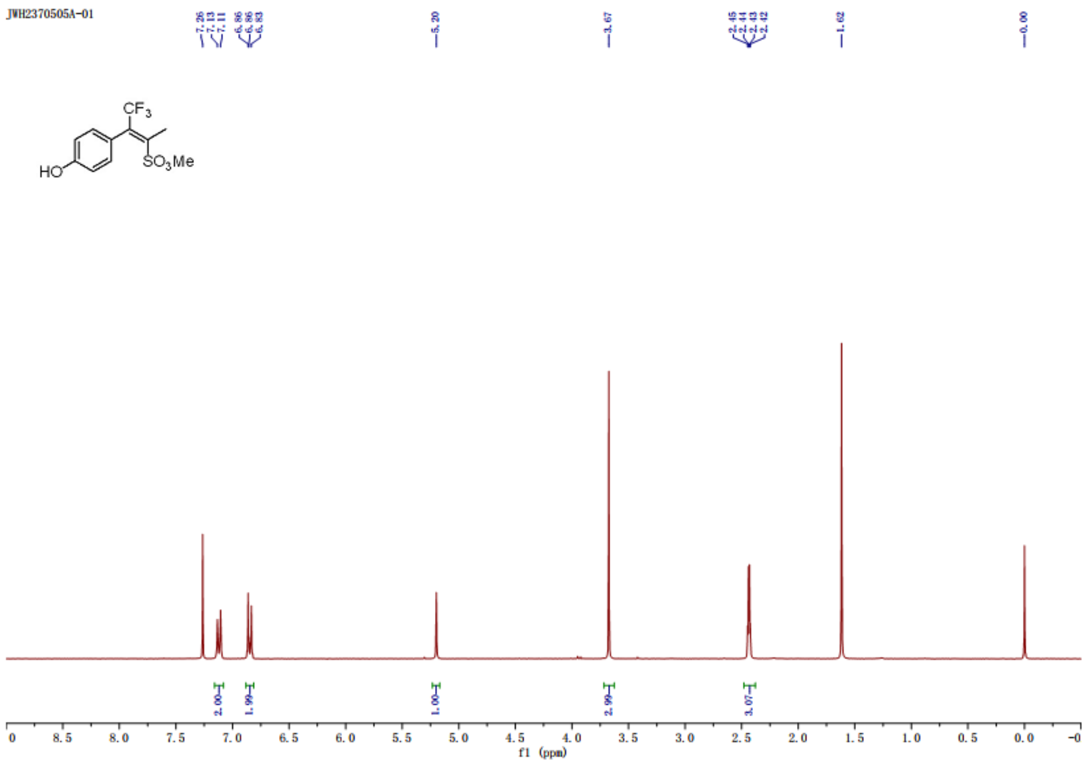
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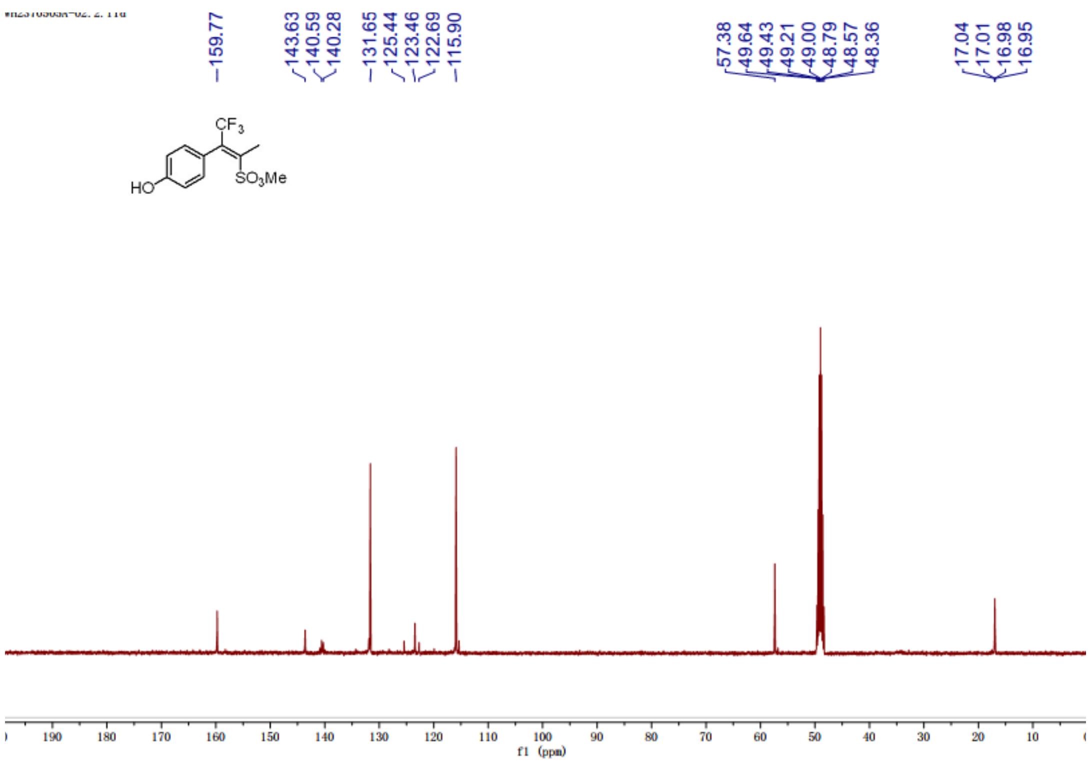
7.13
7.11
6.86
6.86
6.83
5.20
3.67
2.45
2.44
2.43
2.42
1.62
0.00
CF3
HO
SO3Me
2.00
1.99
1.00
2.99
3.07
f1 (ppm)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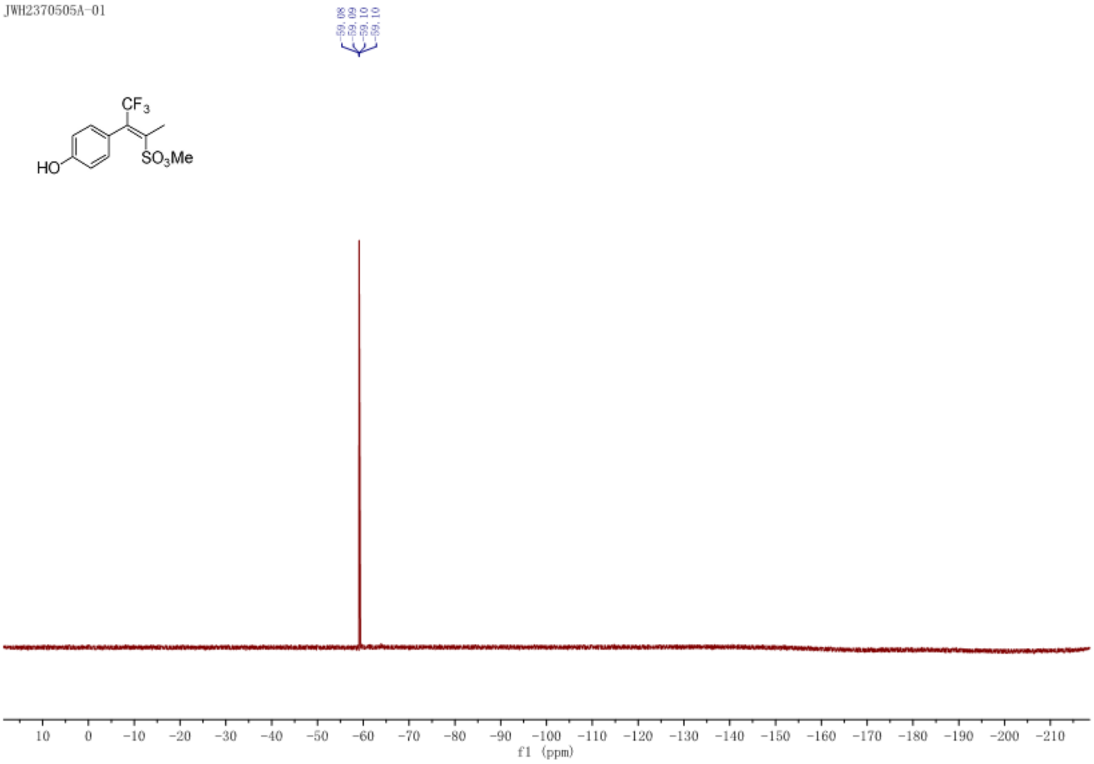
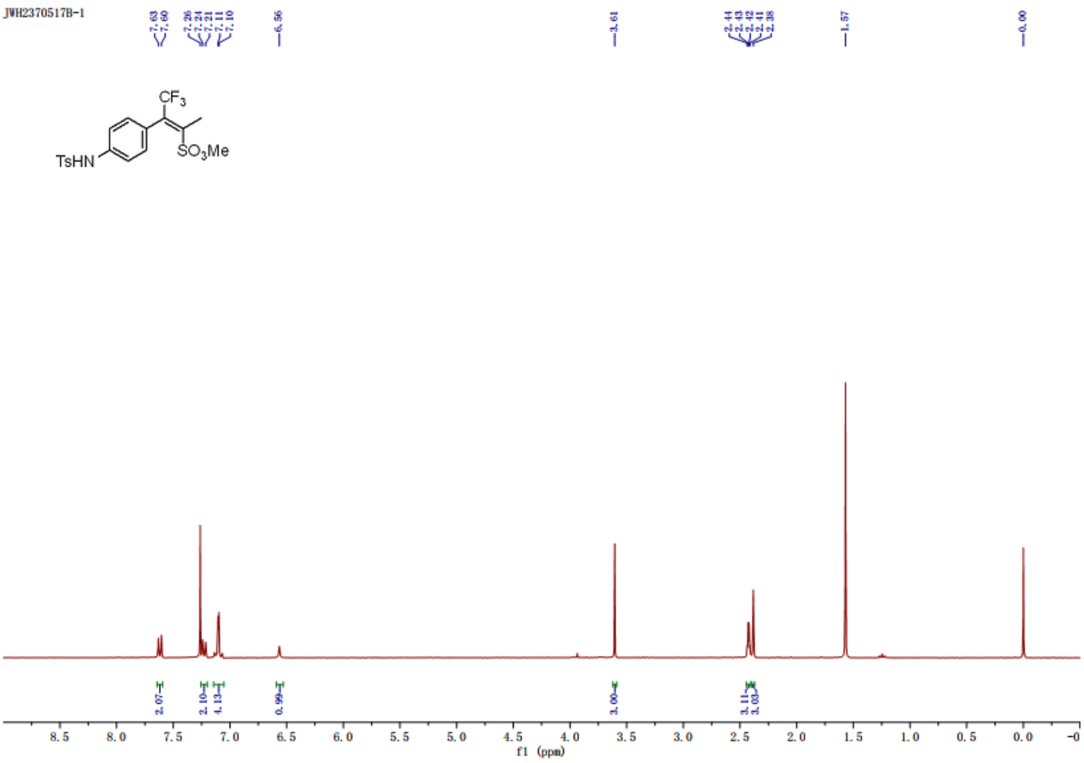
122.69
115.90
57.38
49.64
49.43
49.21
49.00
48.79
48.57
48.36
17.04
17.01
16.98
16.95
CF3
HO
SO3Me
f1 (ppm)



JWH2370505A-01
-59.08
-59.09
-59.10
-59.10
CF3
HO
SO3Me
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)



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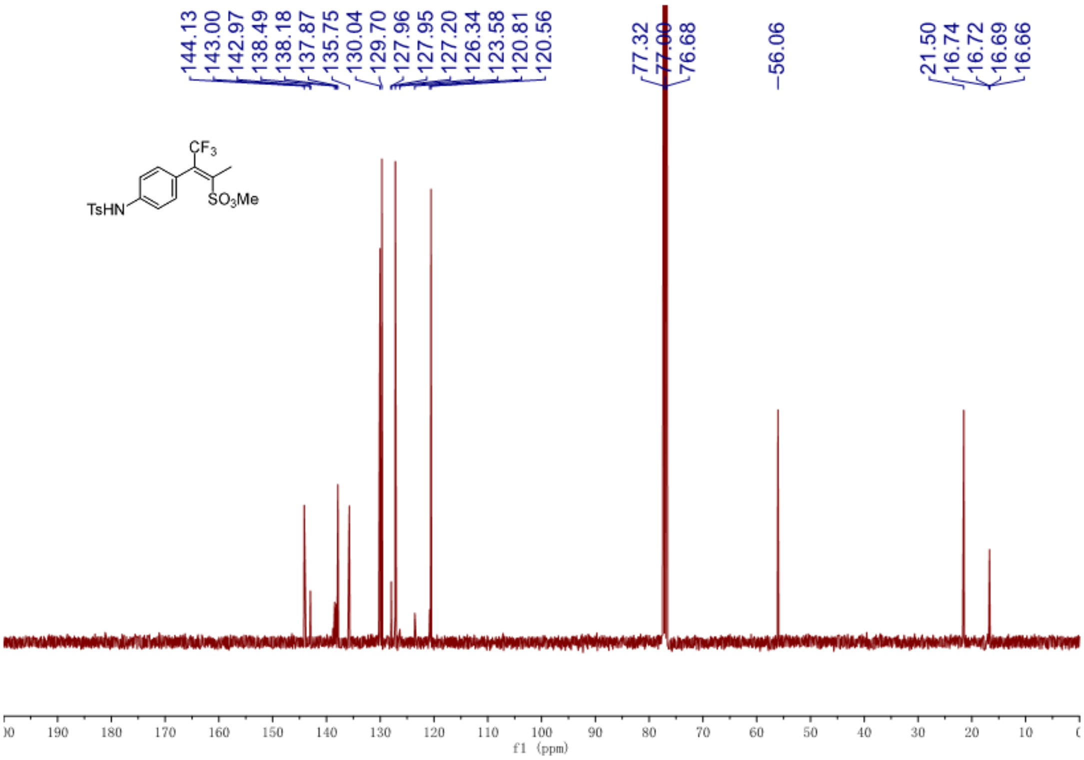
7.60
7.26
7.24
7.21
7.11
7.10
6.56
3.61
2.44
2.43
2.42
2.41
2.38
1.57
0.00
CF3
TsHN
SO3Me
2.07
2.10
4.13
0.99
3.00
3.11
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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143.00
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138.18
137.87
135.75
130.04
129.70
127.96
127.95
127.20
126.34
123.58
120.81
120.56
77.32
77.00
76.68
56.06
21.50
16.74
16.72
16.69
16.66
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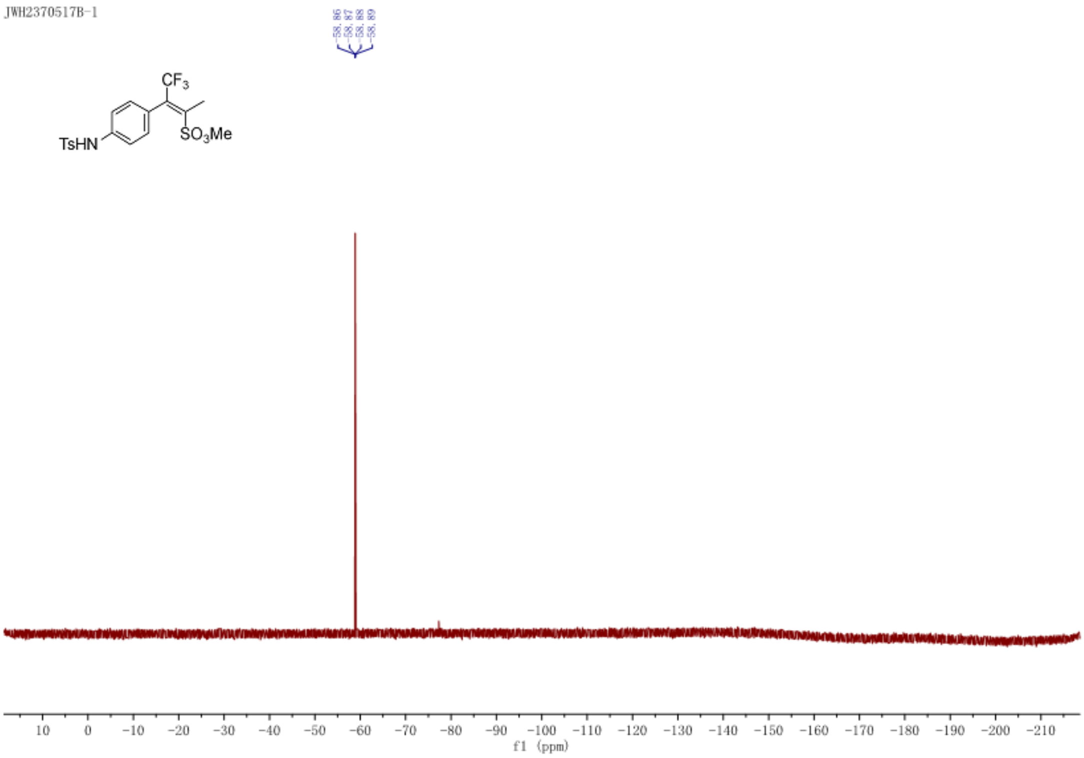
TsHN
SO3Me
f1 (ppm)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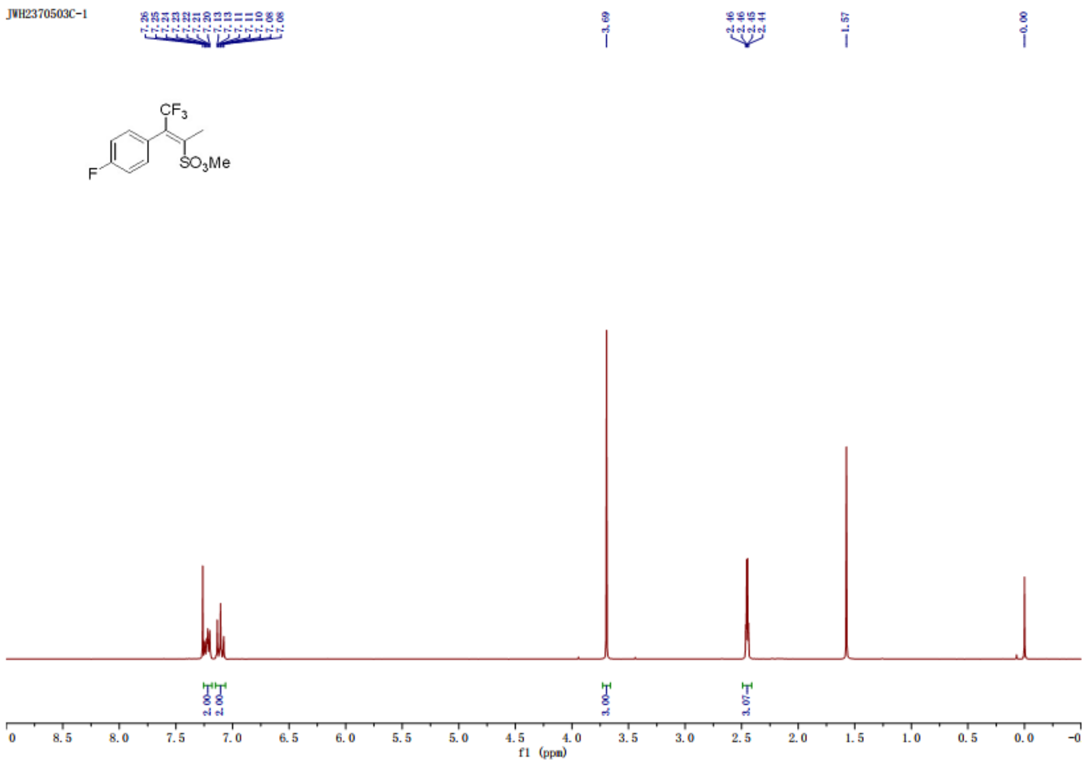
CF3
TsHN
SO3Me
f1 (ppm)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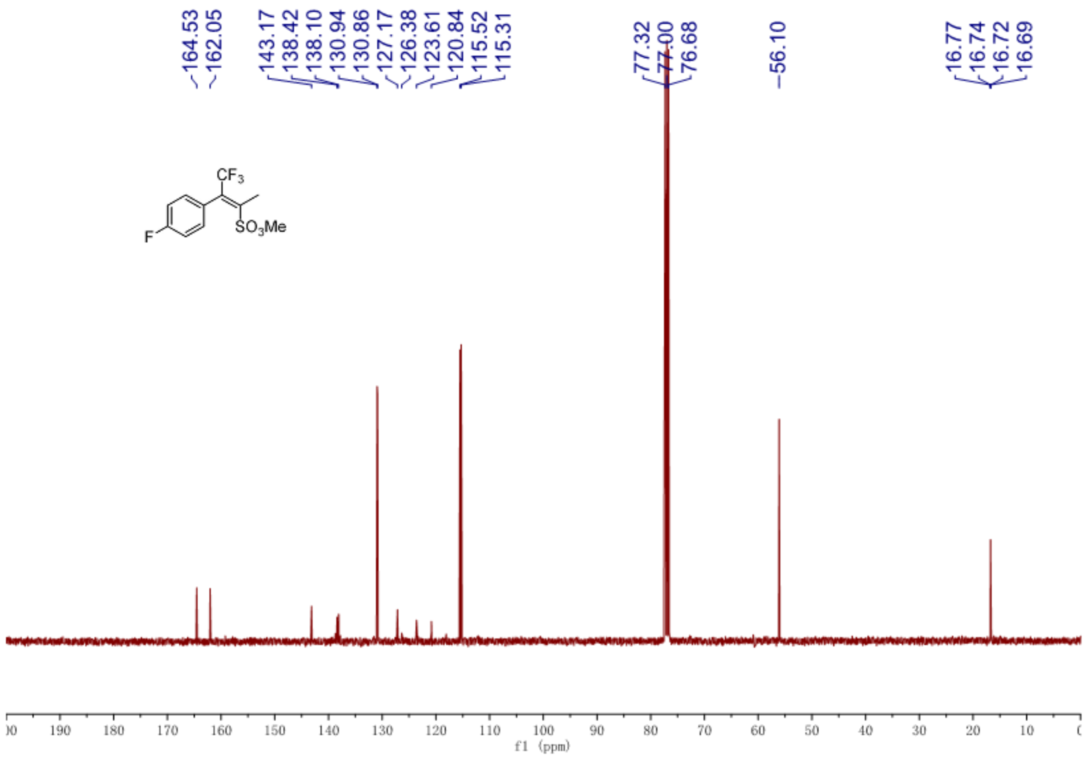
1.57
0.00
f1 (ppm)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162.05
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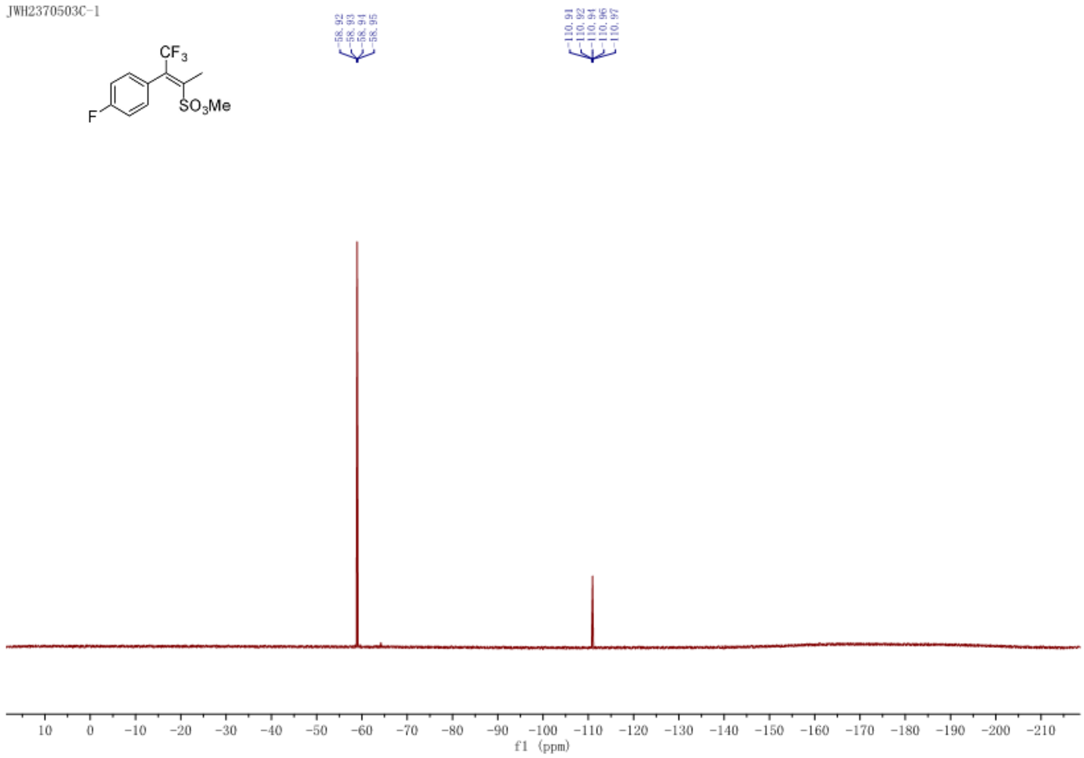
138.10
130.94
130.86
127.17
126.38
123.61
120.84
115.52
115.31
77.32
77.00
76.68
56.10
16.77
16.74
16.72
16.69
f1 (ppm)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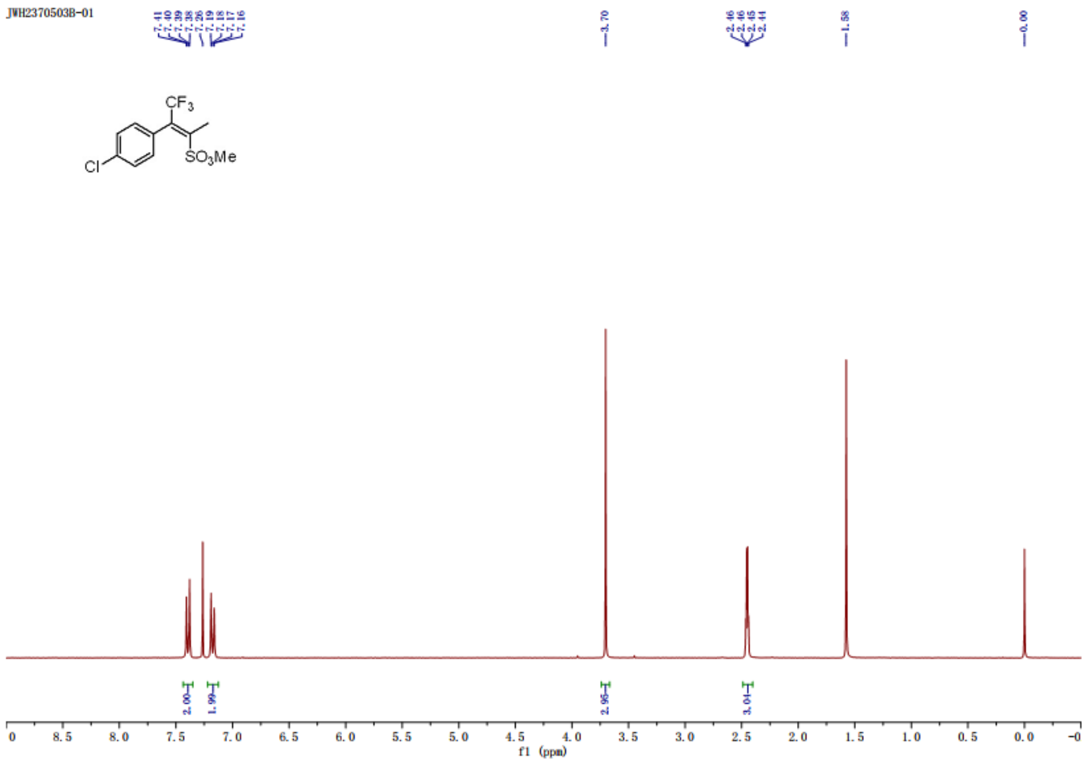
CF3
SO3Me
F
f1 (ppm)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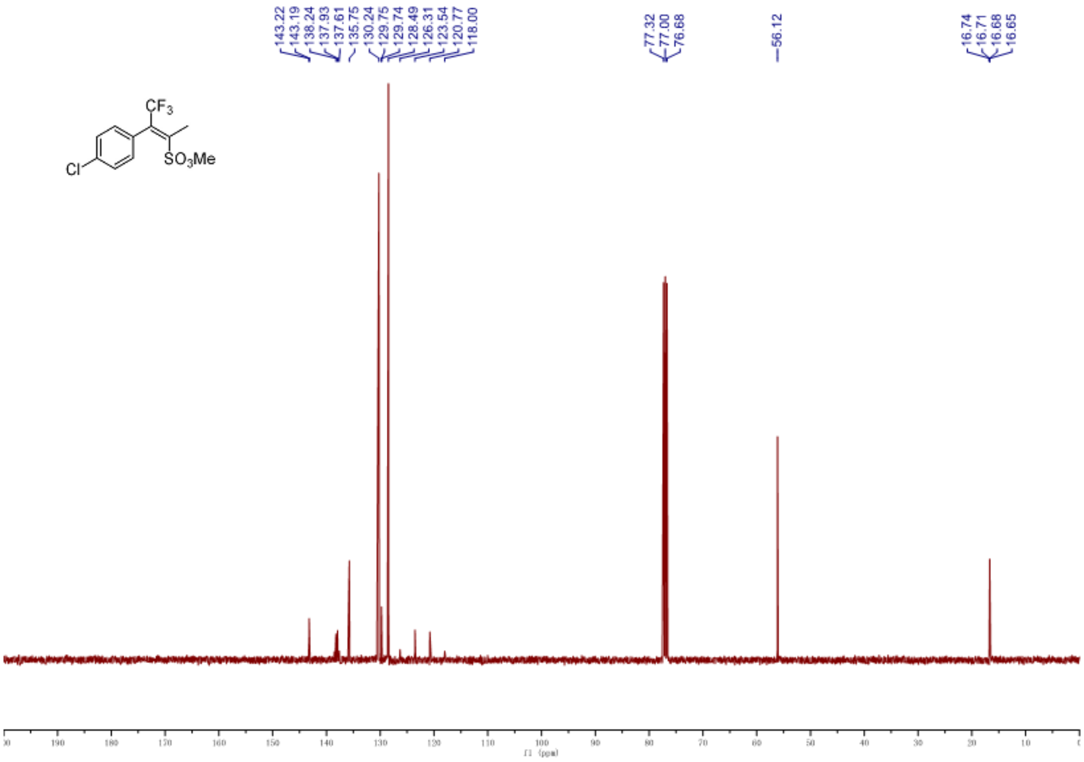
CF3
SO3Me
Cl
f1 (ppm)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130.24
129.75
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128.49
126.31
123.54
120.77
118.00
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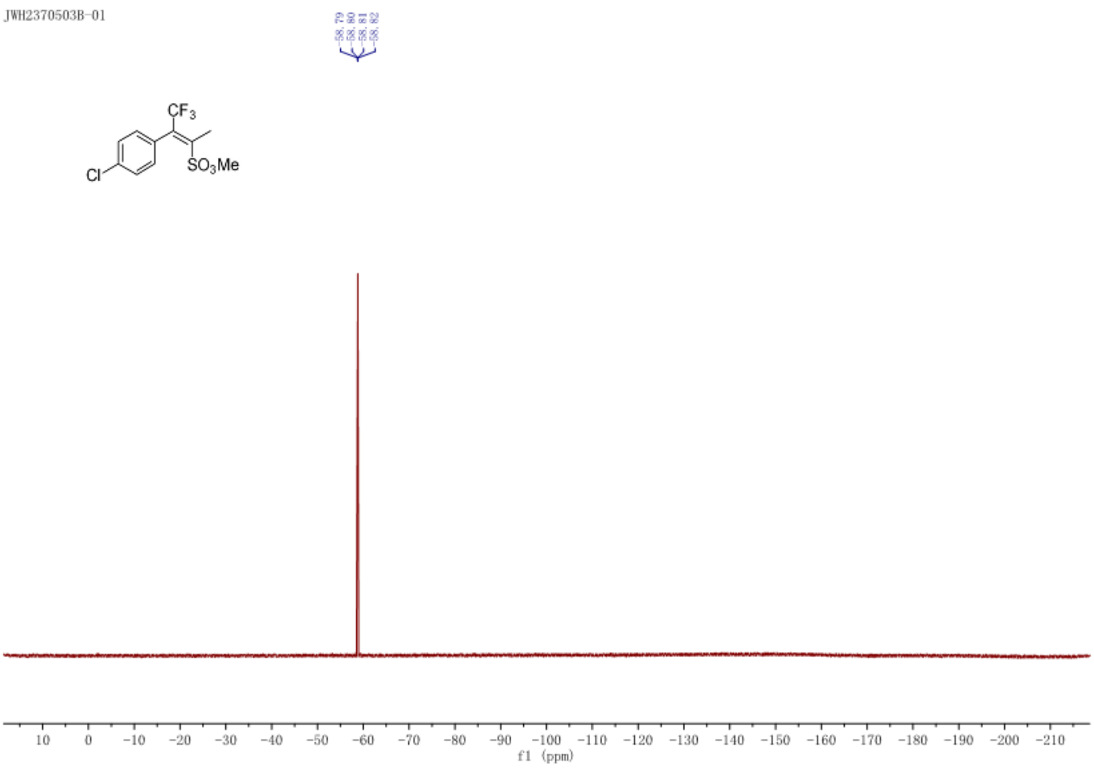
77.00
76.68
56.12
16.74
16.71
16.68
16.65
CF3
Cl
SO3Me
f1 (ppm)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Cl
SO3Me
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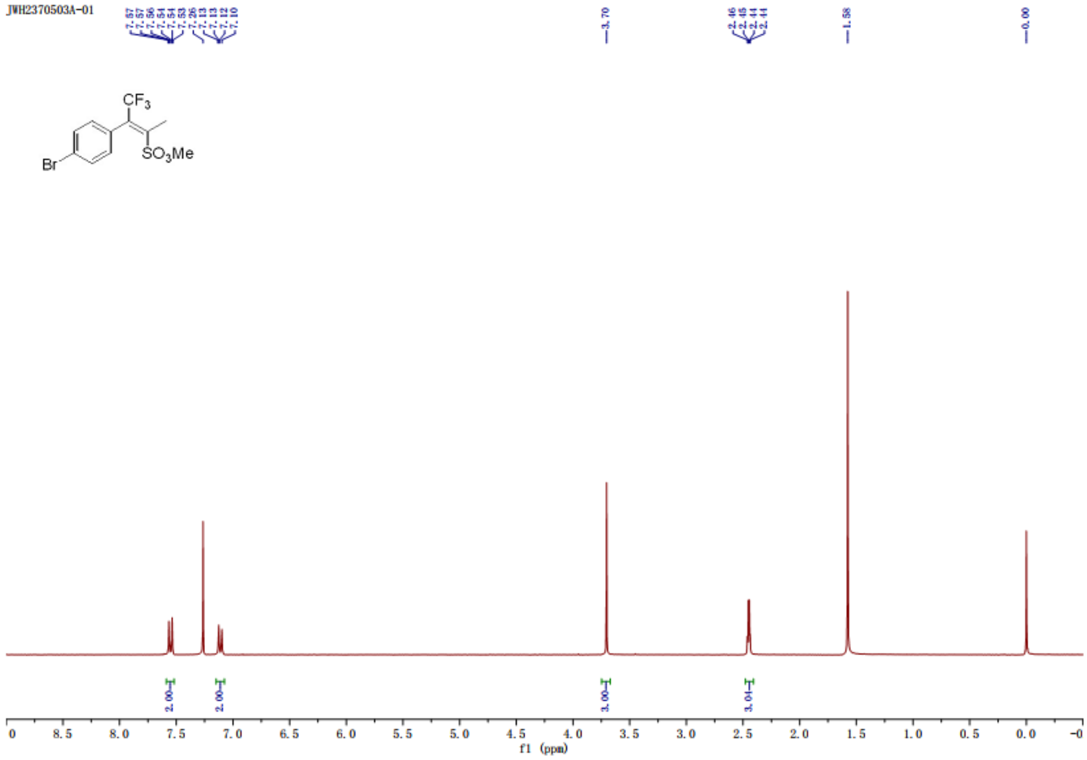
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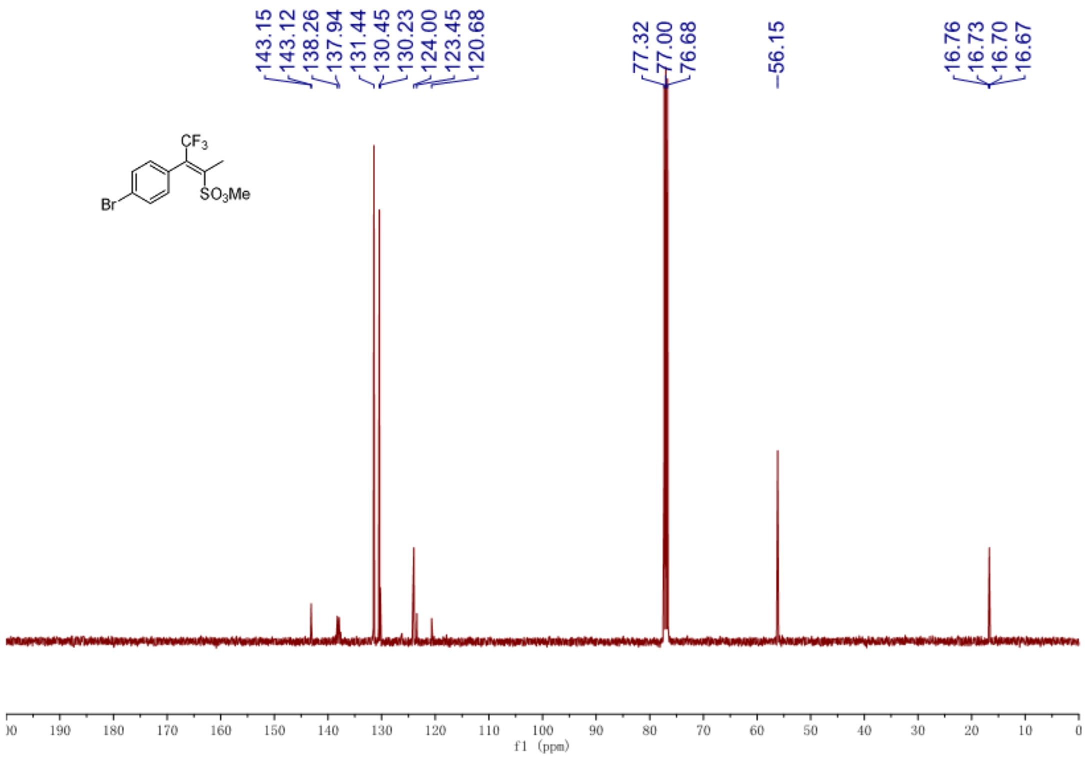
7.54
7.54
7.53
7.26
7.13
7.13
7.12
7.10
3.70
2.46
2.45
2.44
2.44
1.58
0.00
CF3
Br
SO3Me
2.00
2.00
3.00
3.04
f1 (ppm)


143.15
143.12
138.26
137.94
131.44
130.45
130.23
124.00
123.45
120.68
77.32
77.00
76.68
56.15
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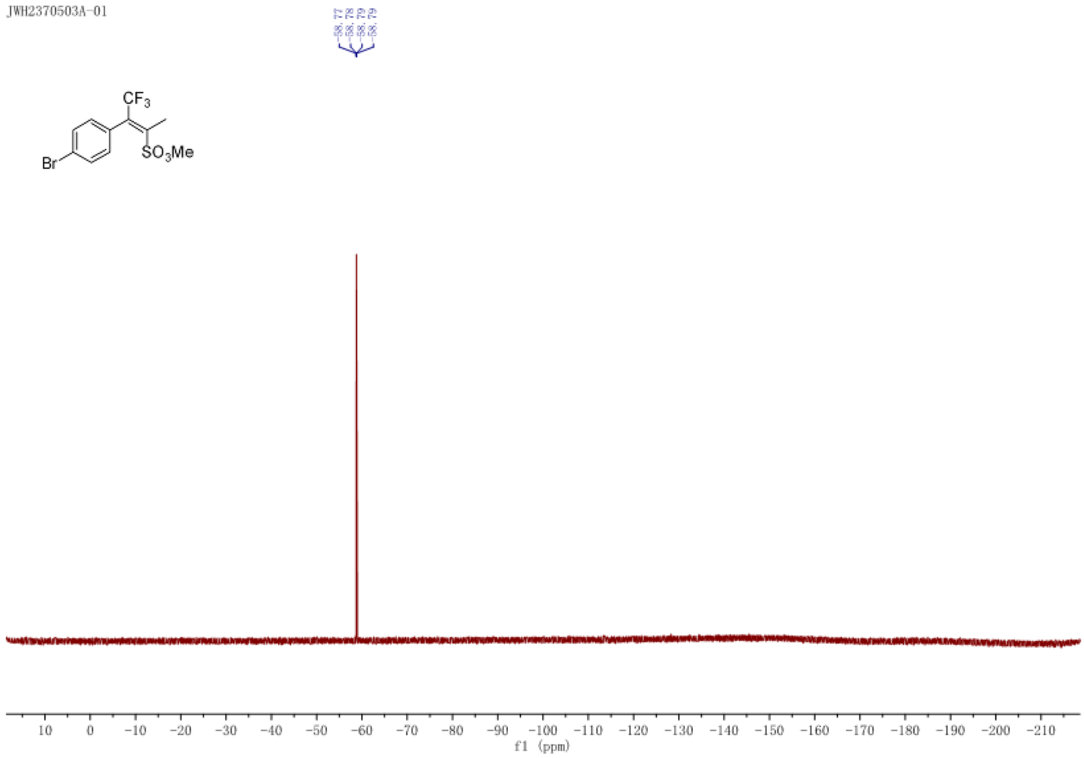
16.73
16.70
16.67
CF3
Br
SO3Me
f1 (ppm)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-58.79
-58.79
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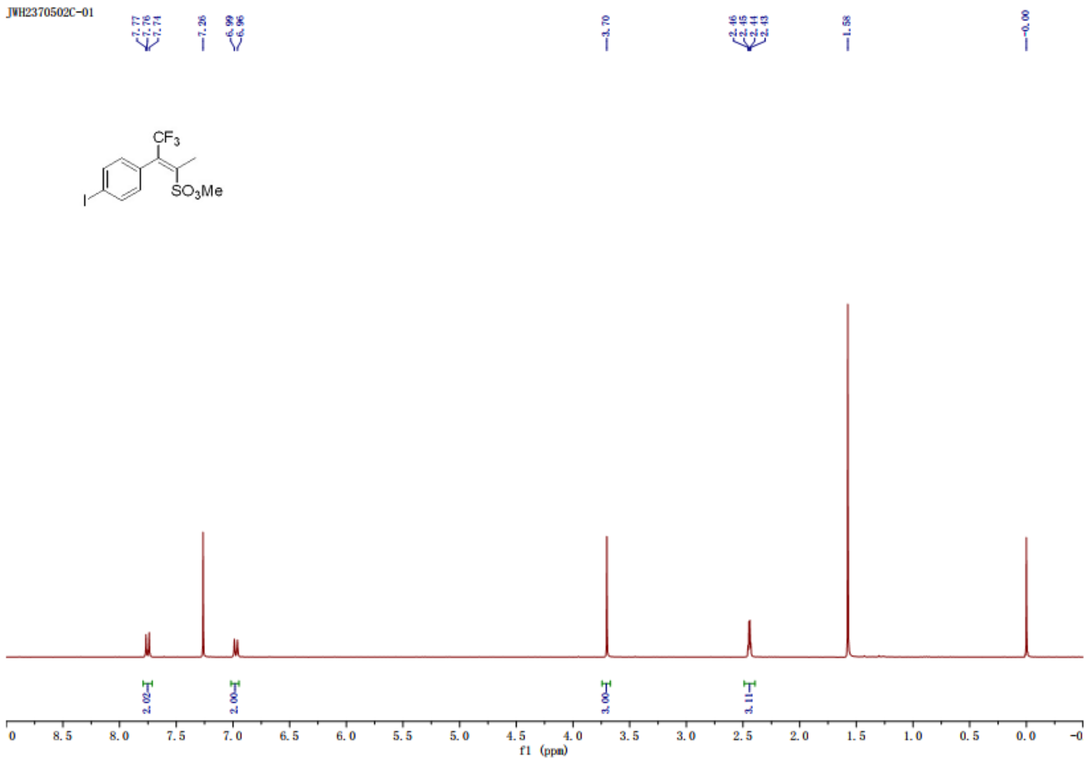
Br
SO3Me
f1 (ppm)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2.45
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1.58
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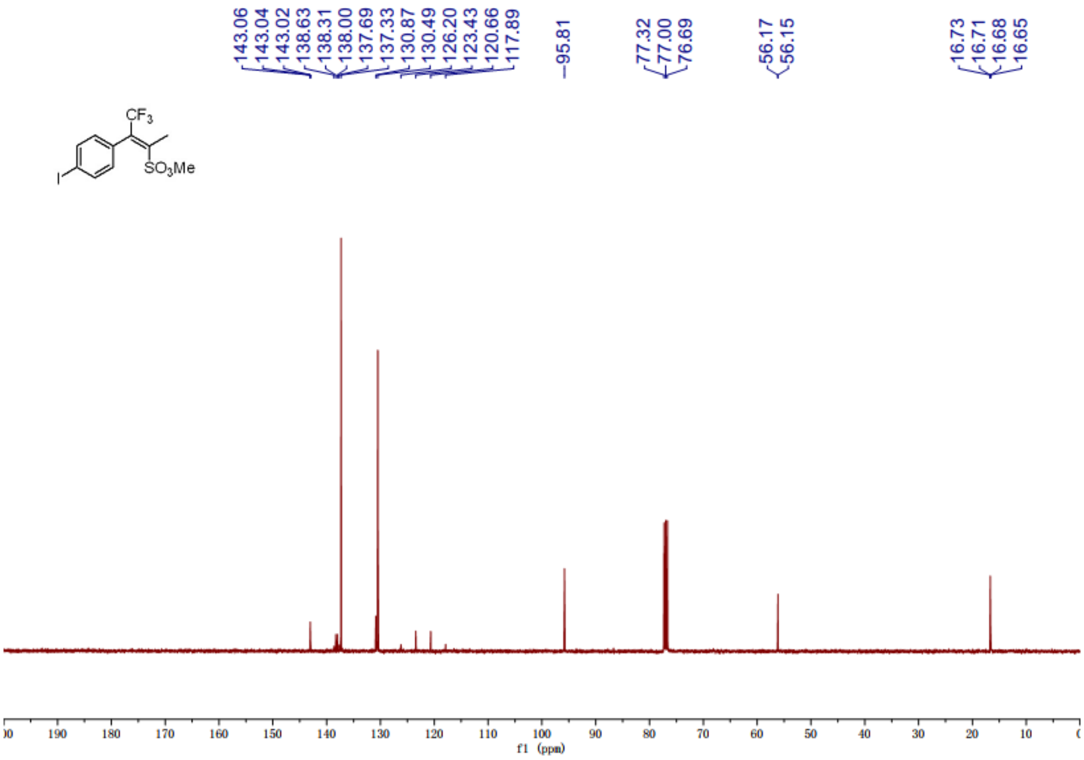
I
SO3Me
2.02
2.00
3.00
3.11
f1 (ppm)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138.31
138.00
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137.33
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130.49
126.20
123.43
120.66
117.89
95.81
77.32
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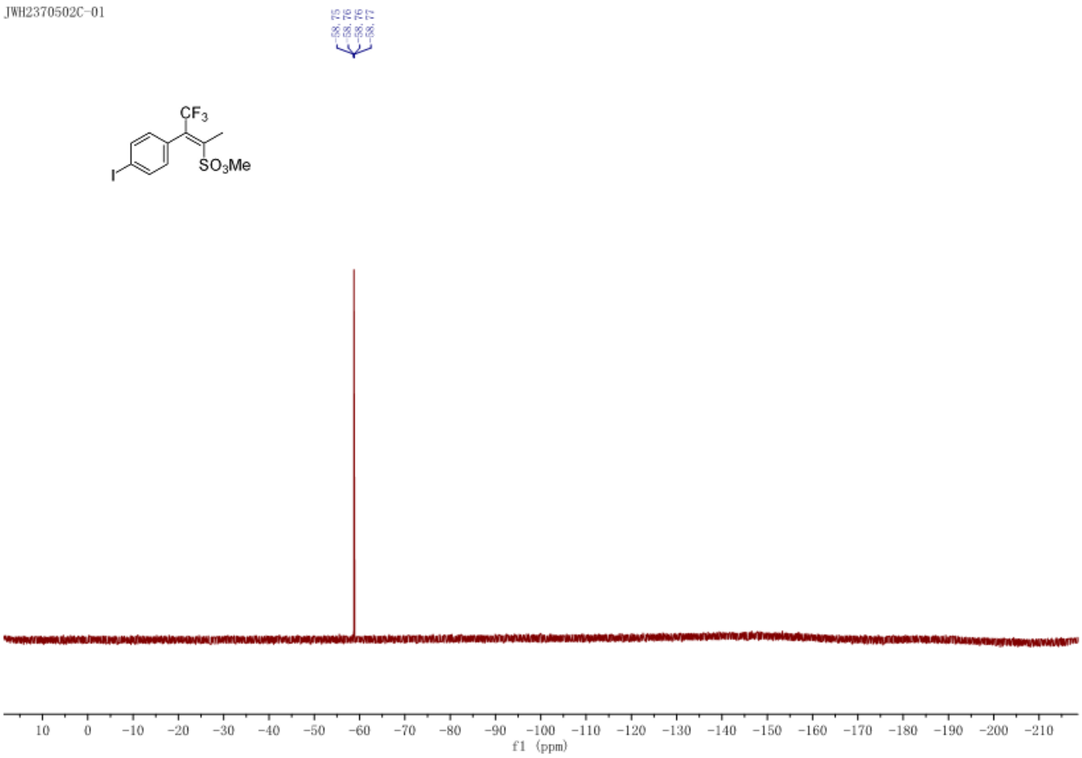
56.17
56.15
16.73
16.71
16.68
16.65
CF3
I
SO3Me
f1 (ppm)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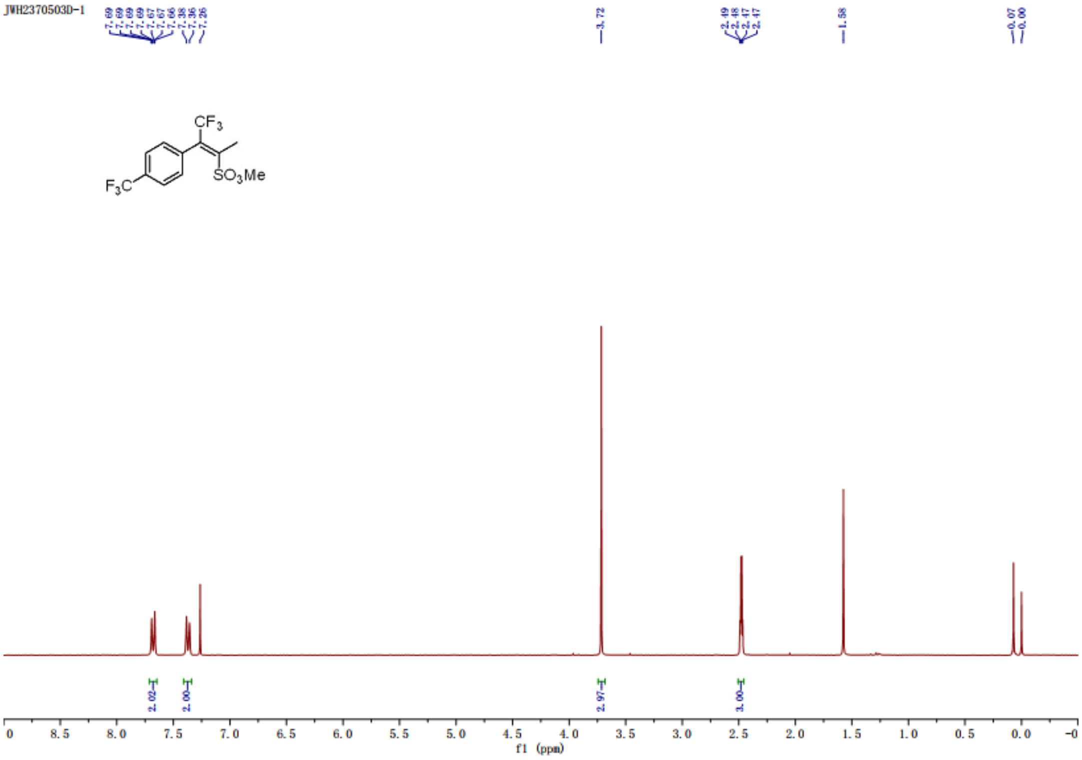
I
SO3Me
f1 (ppm)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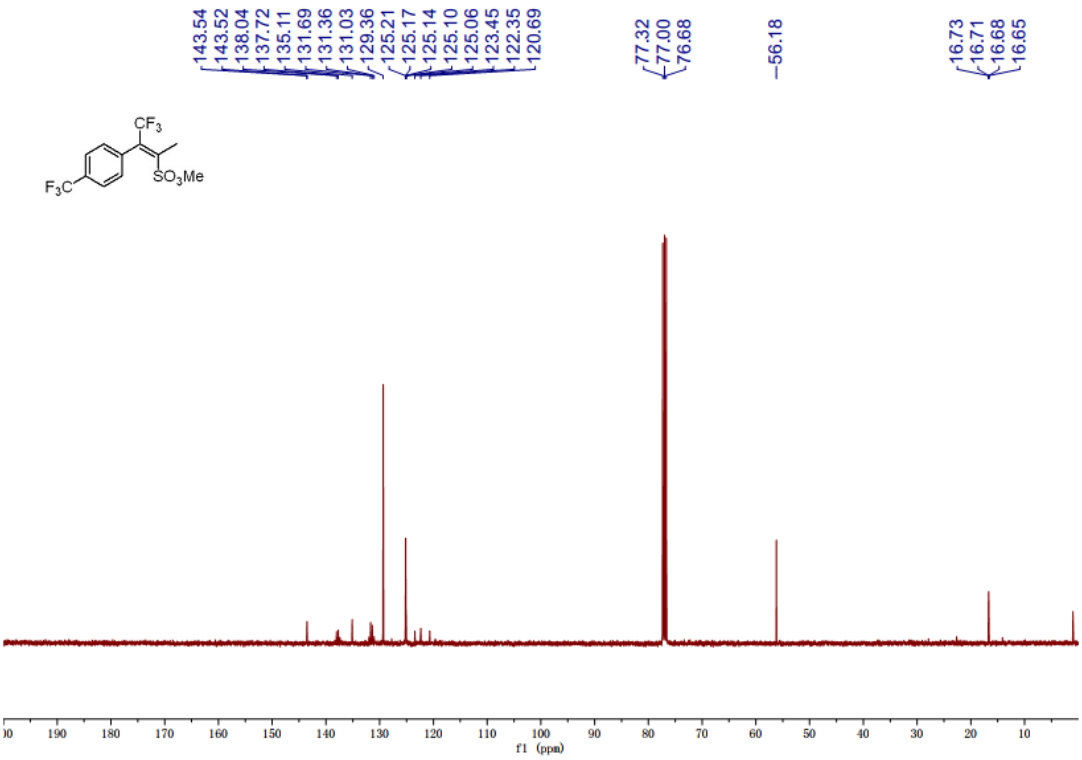
7.69
7.69
7.69
7.67
7.66
7.38
7.36
7.26
3.72
2.49
2.48
2.47
2.47
1.58
0.07
0.00
CF3
F3C
SO3Me
2.02
2.00
2.97
3.00
f1 (ppm)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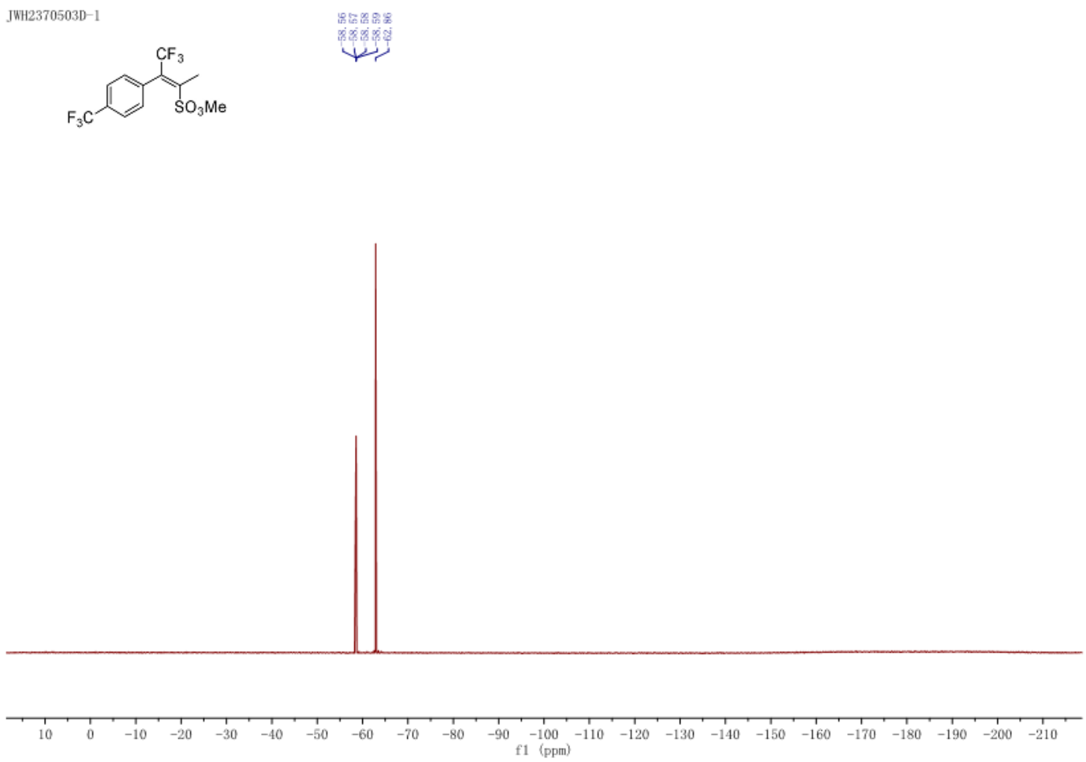
137.72
135.11
131.69
131.36
131.03
129.36
125.21
125.17
125.14
125.10
125.06
123.45
122.35
120.69
77.32
77.00
76.68
56.18
16.73
16.71
16.68
16.65
CF3
F3C
SO3Me
f1 (ppm)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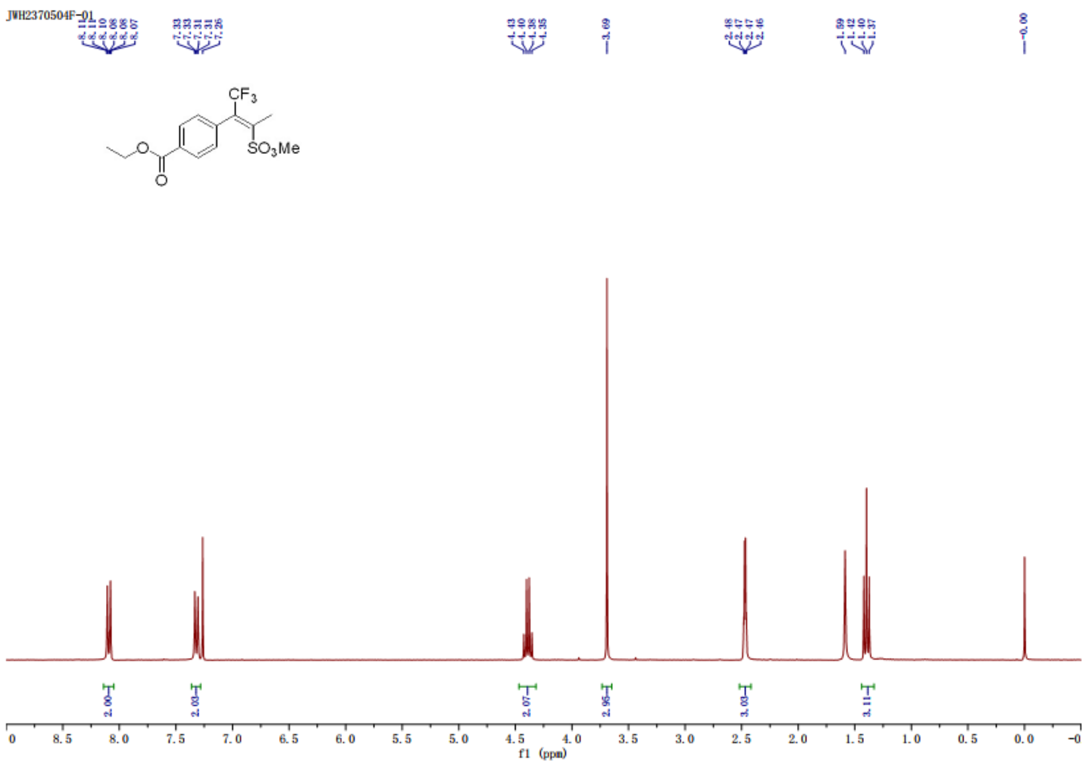
F3C
SO3Me
f1 (ppm)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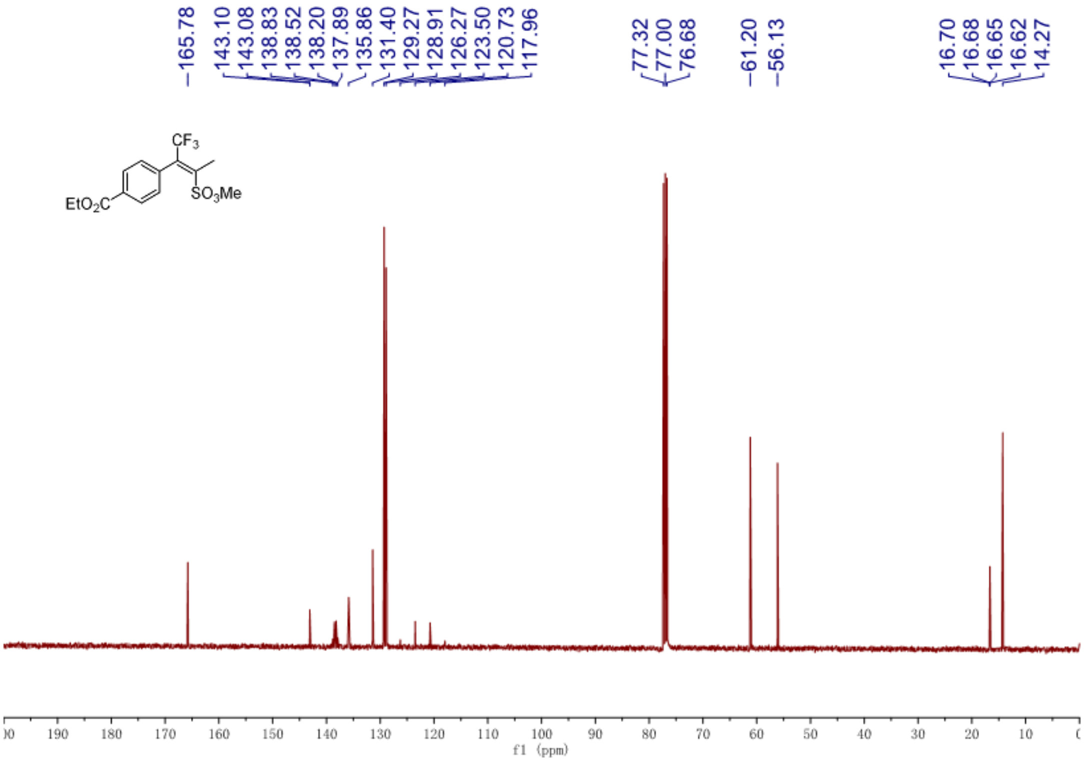
CF3
SO3Me
f1 (ppm)



165.78
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138.20
137.89
135.86
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129.27
128.91
126.27
123.50
120.73
117.96
77.32
77.00
76.68
61.20
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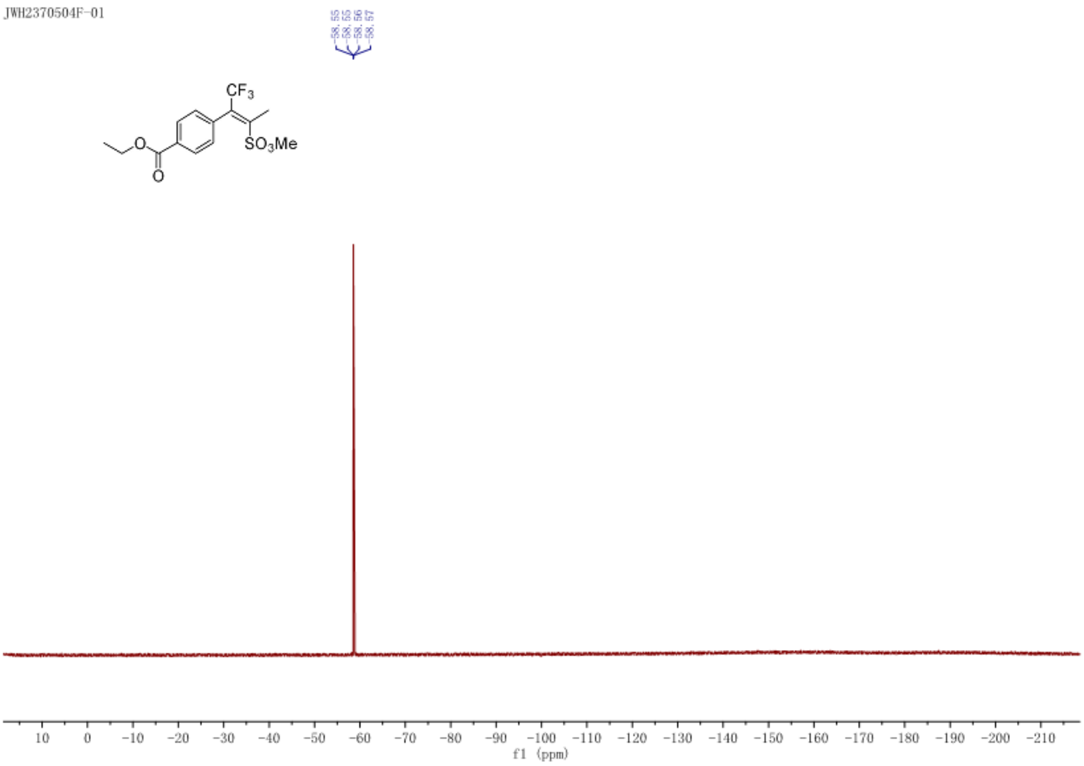
16.65
16.62
14.27
EtO2C
CF3
SO3Me
f1 (ppm)



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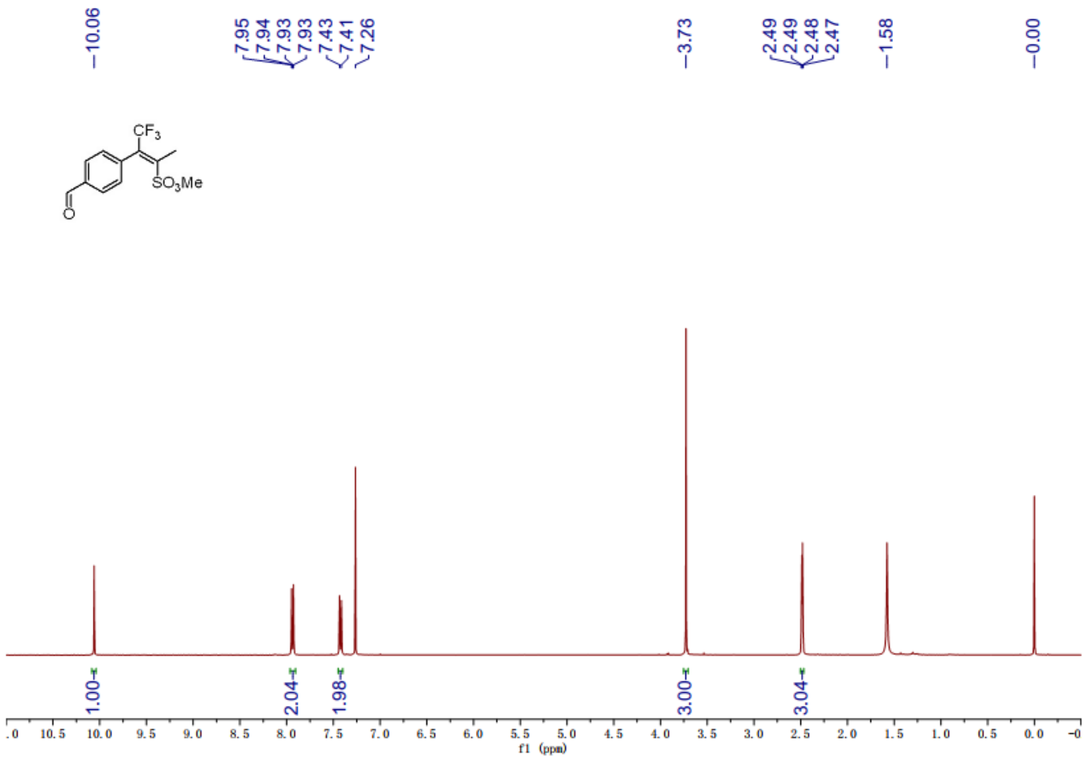
-58.57
CF3
SO3Me
O
O
f1 (ppm)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7.93
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7.43
7.41
7.26
3.73
2.49
2.49
2.48
2.47
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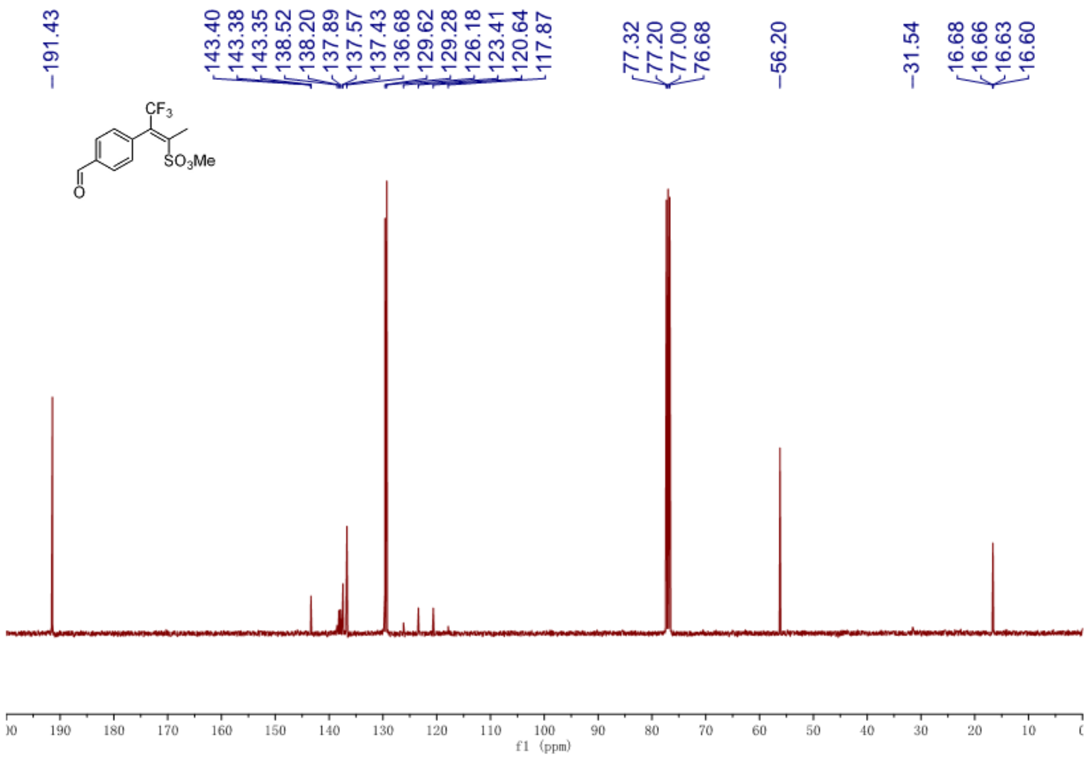
0.00
CF3
SO3Me
O
1.00
2.04
1.98
3.00
3.04
f1 (ppm)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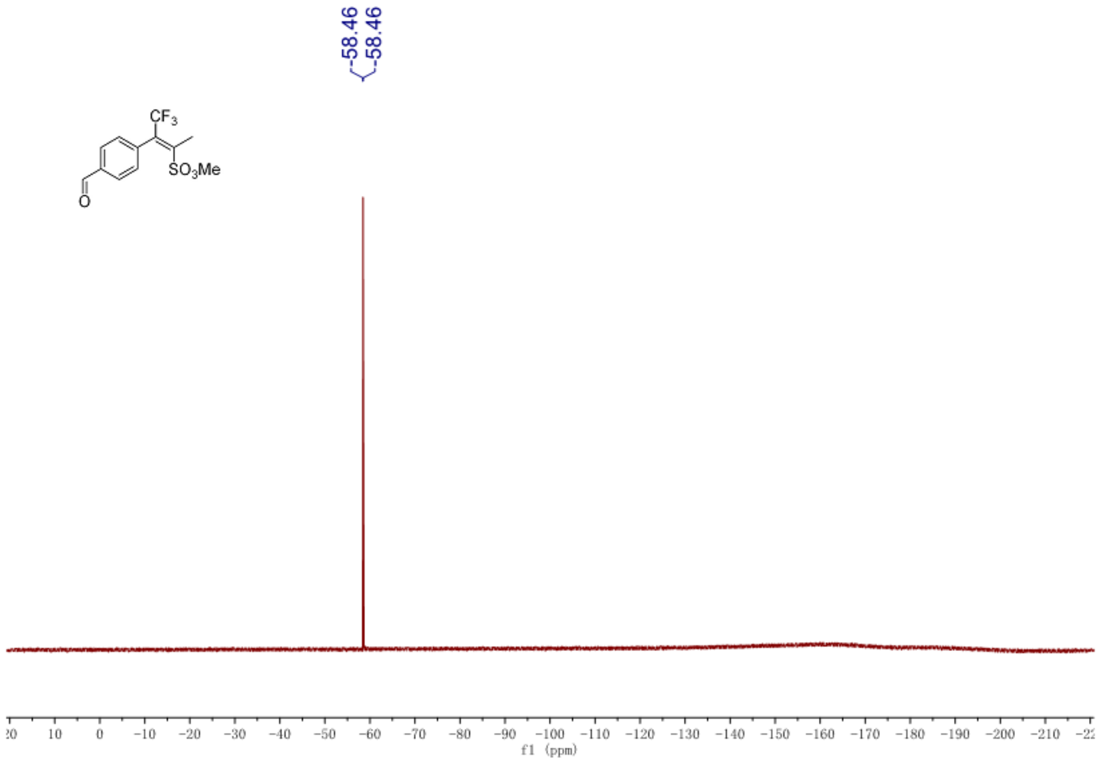
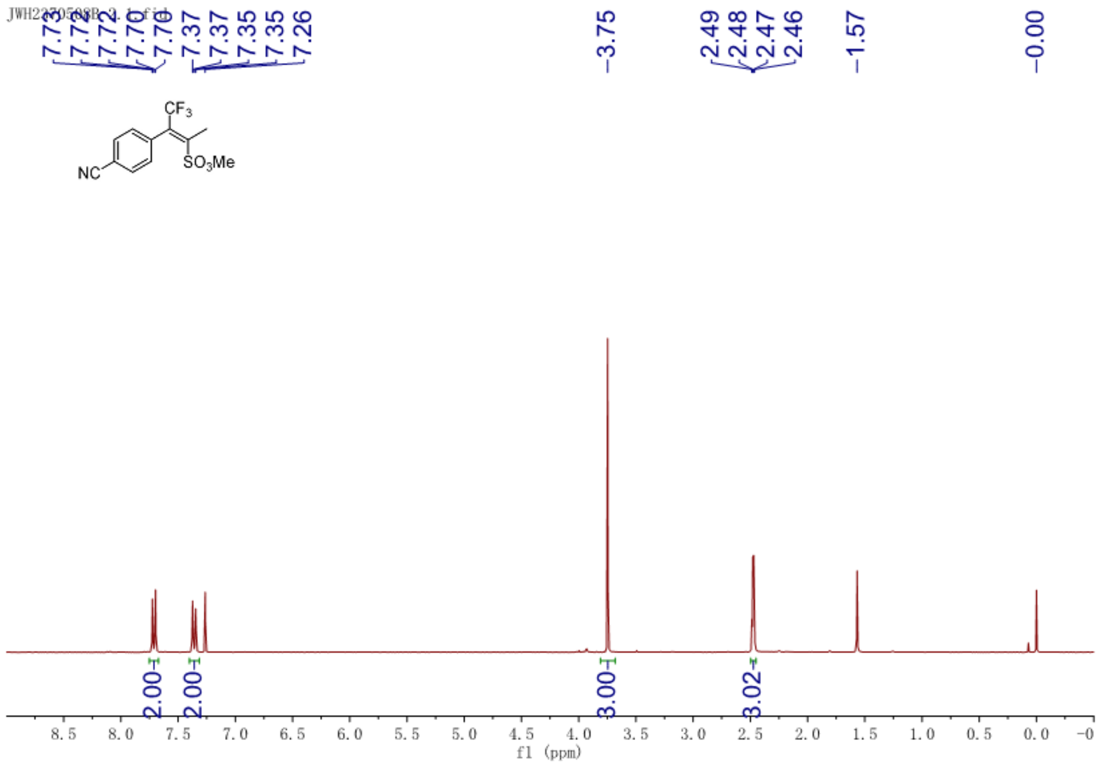
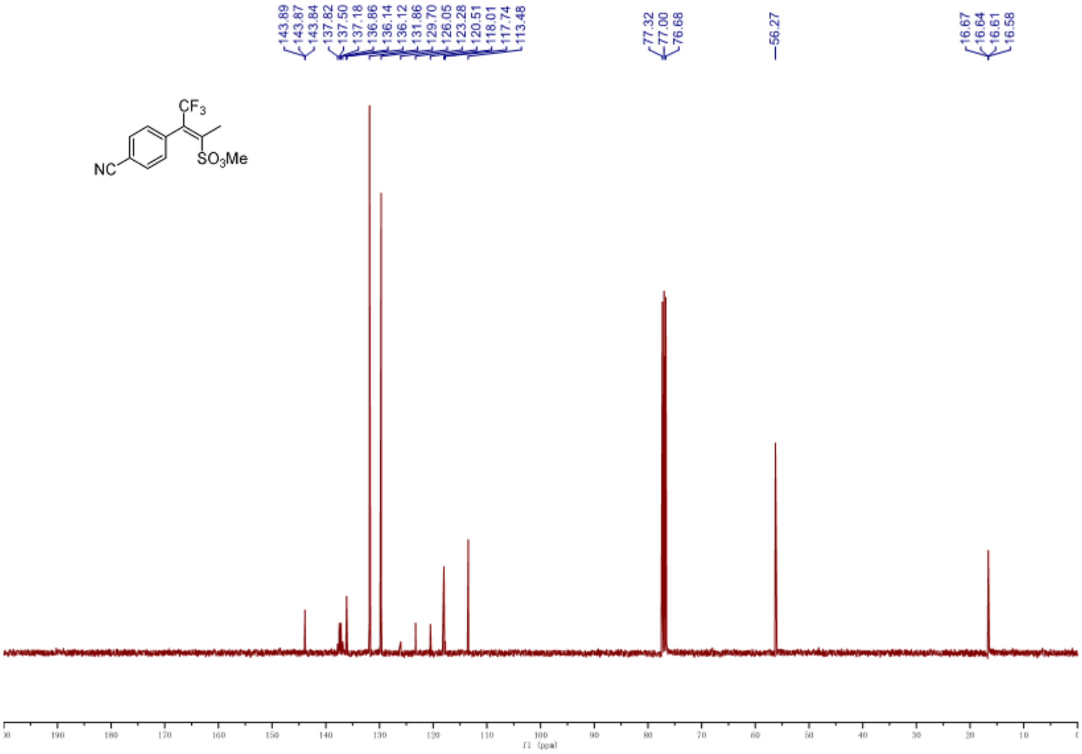
137.57
137.43
136.68
129.62
129.28
126.18
123.41
120.64
117.87
77.32
77.20
77.00
76.68
56.20
31.54
16.68
16.66
16.63
16.60
CF3
SO3Me
O
f1 (ppm)



-58.46
-58.46
CF3
SO3Me
O
f1 (ppm)



7.73
7.72
7.72
7.70
7.70
7.37
7.37
7.35
7.35
7.26
3.75
2.49
2.48
2.47
2.46
1.57
0.00
CF3
NC
SO3Me
2.00
2.00
3.00
3.02
f1 (ppm)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129.70
126.05
123.28
120.51
118.01
117.74
113.48
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76.68
56.27
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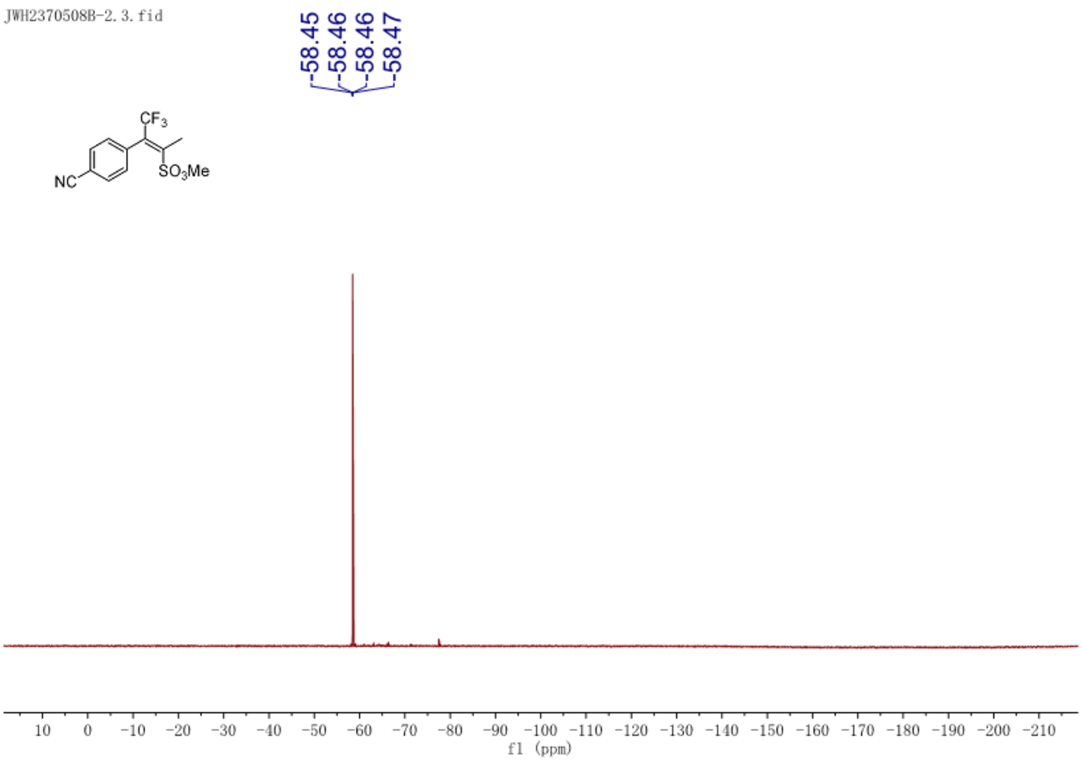
16.64
16.61
16.58
CF3
NC
SO3Me
f1 (ppm)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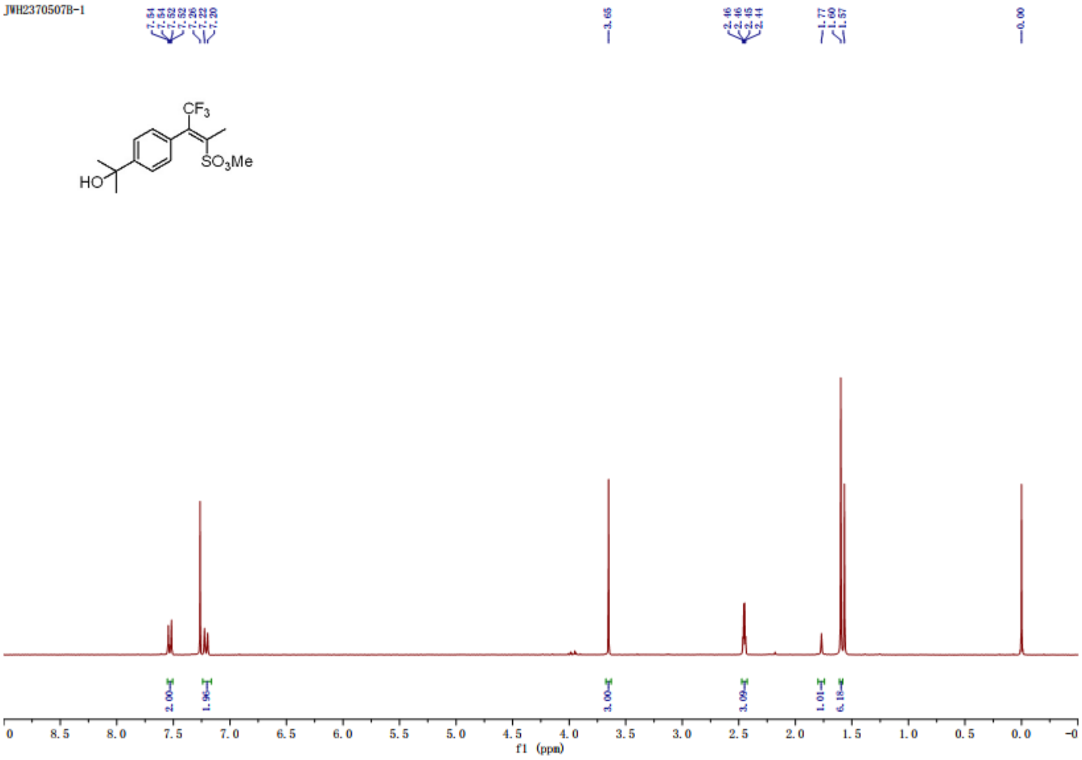
-58.46
-58.46
-58.47
CF3
NC
SO3Me
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)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7.26
7.22
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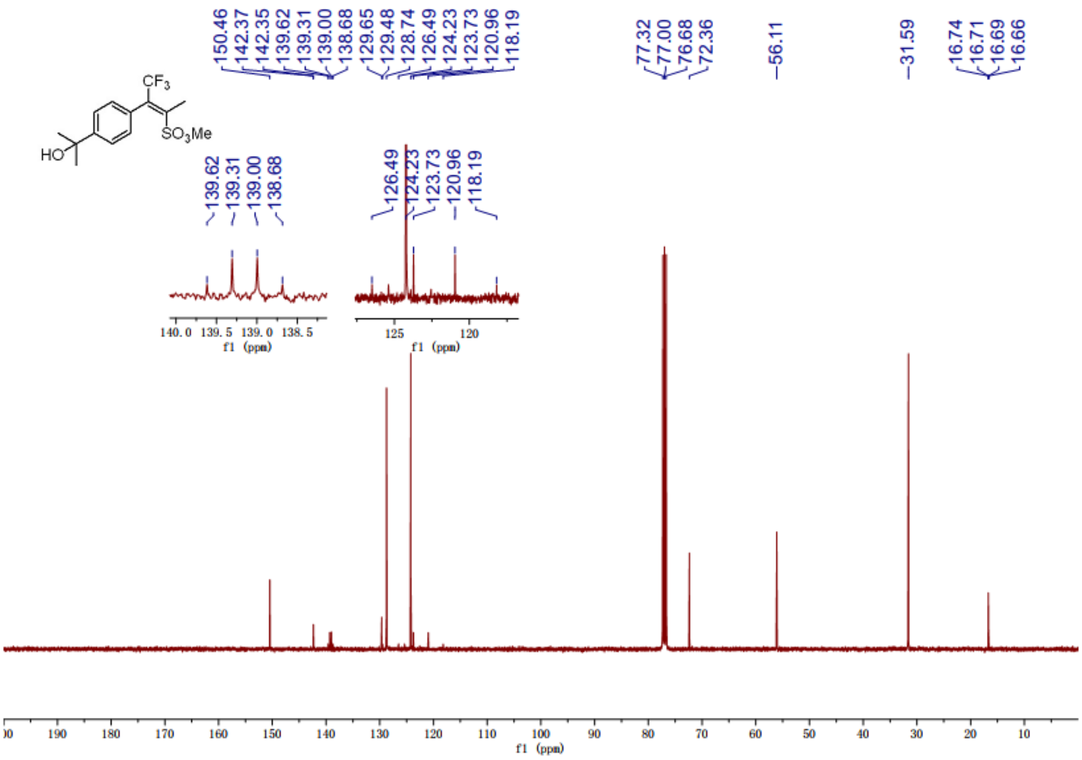
2.46
2.46
2.45
2.44
1.77
1.60
1.57
0.00
CF3
SO3Me
HO
2.00
1.96
3.00
3.09
1.01
6.18
f1 (ppm)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142.37
142.35
139.62
139.31
139.00
138.68
129.65
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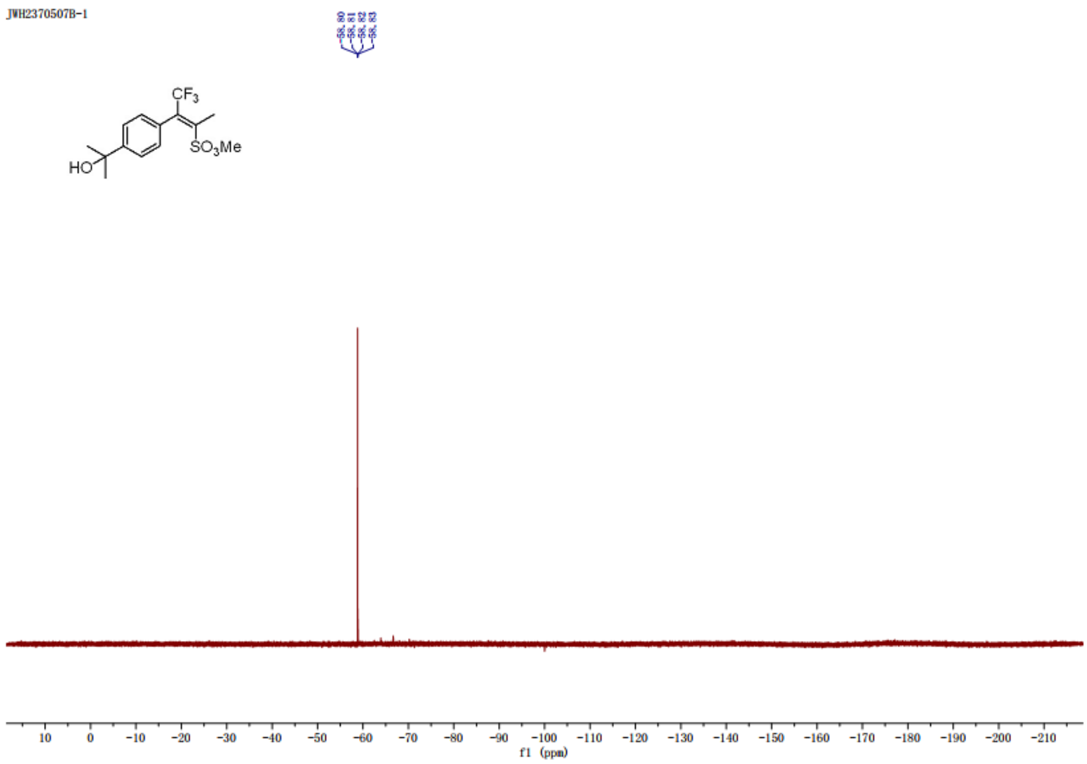
128.74
126.49
124.23
123.73
120.96
118.19
77.32
77.00
76.68
72.36
56.11
31.59
16.74
16.71
16.69
16.66
CF3
SO3Me
HO
f1 (ppm)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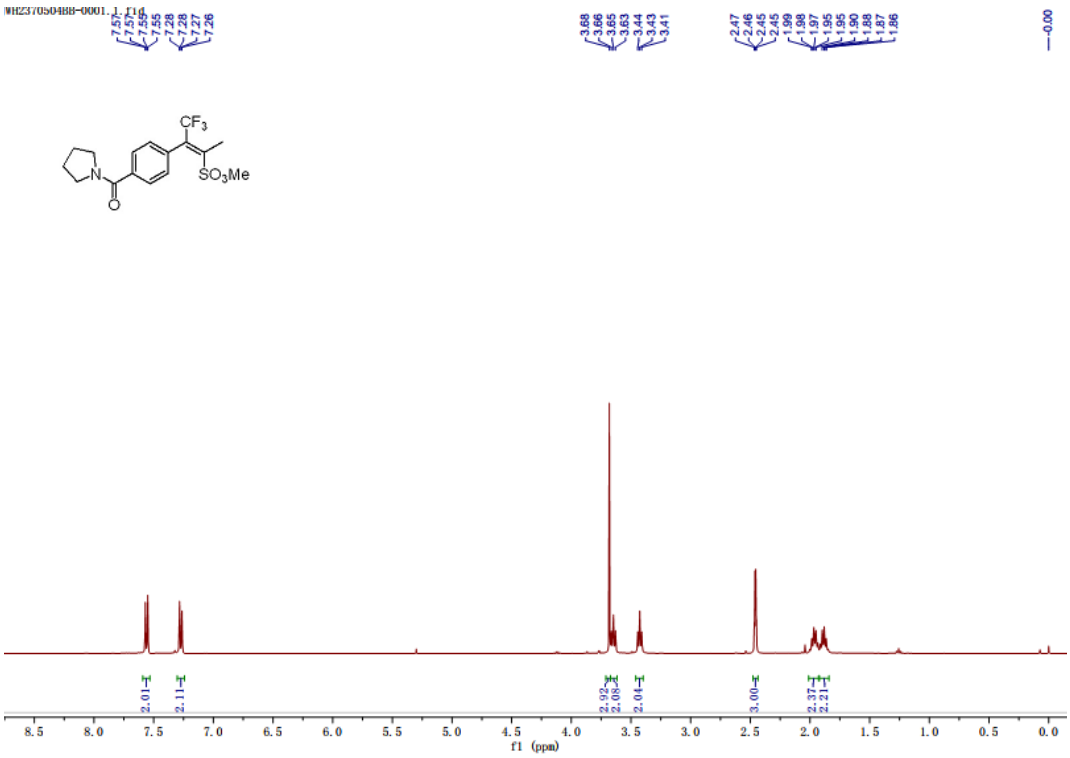
-58.82
-58.83
CF3
SO3Me
HO
f1 (ppm)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7.55
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7.27
7.26
3.68
3.66
3.65
3.63
3.44
3.43
3.41
2.47
2.46
2.45
2.45
1.99
1.98
1.97
1.95
1.95
1.90
1.88
1.87
1.86
0.00
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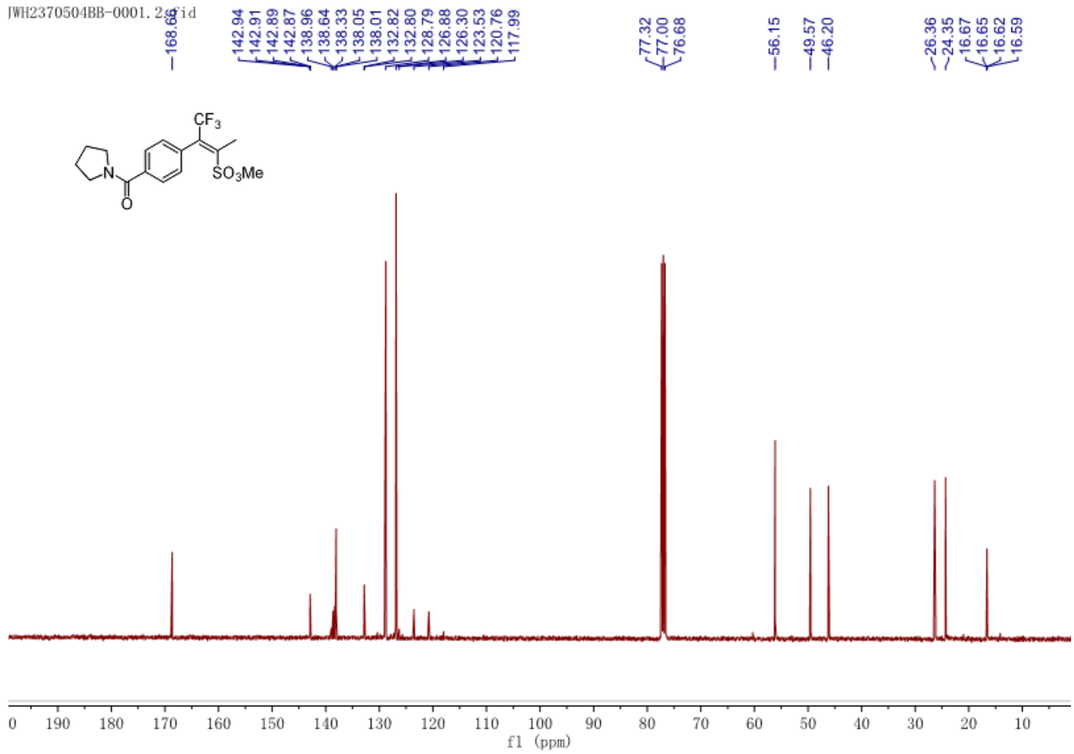
O
SO3Me
2.01
2.11
2.92
2.08
2.04
3.00
2.37
2.21
f1 (ppm)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132.82
132.80
128.79
126.88
126.30
123.53
120.76
117.99
77.32
77.00
76.68
56.15
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24.35
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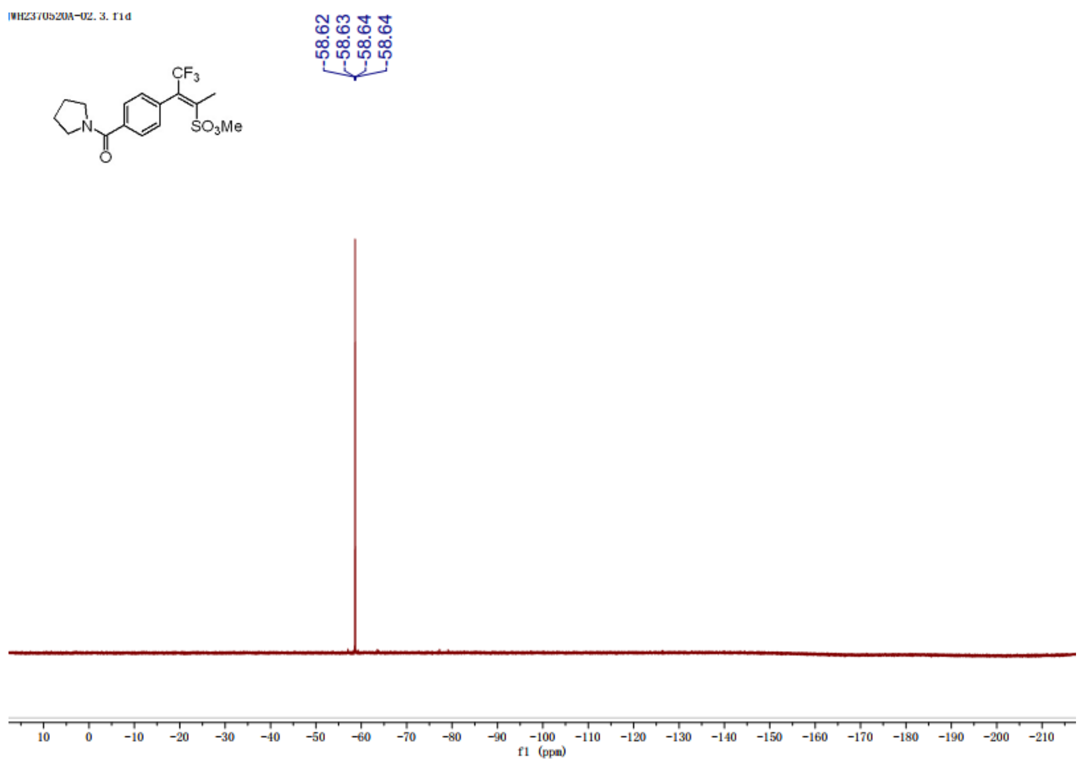
O
SO3Me
f1 (ppm)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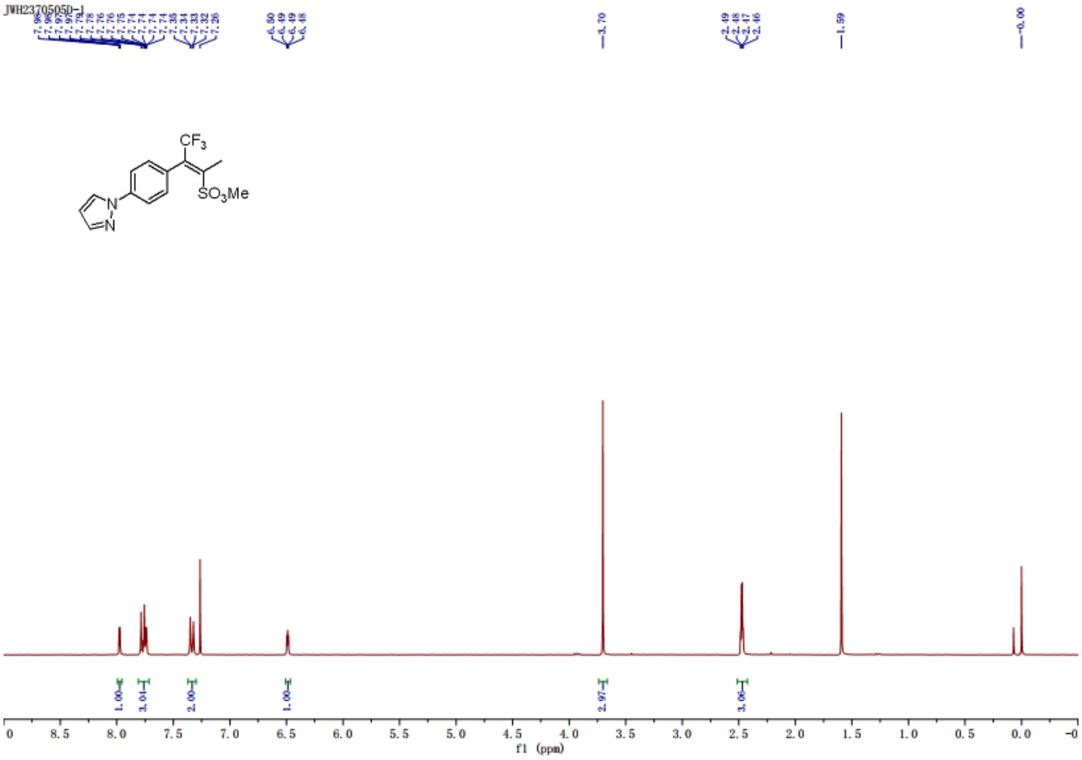
O
SO3Me
f1 (ppm)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N
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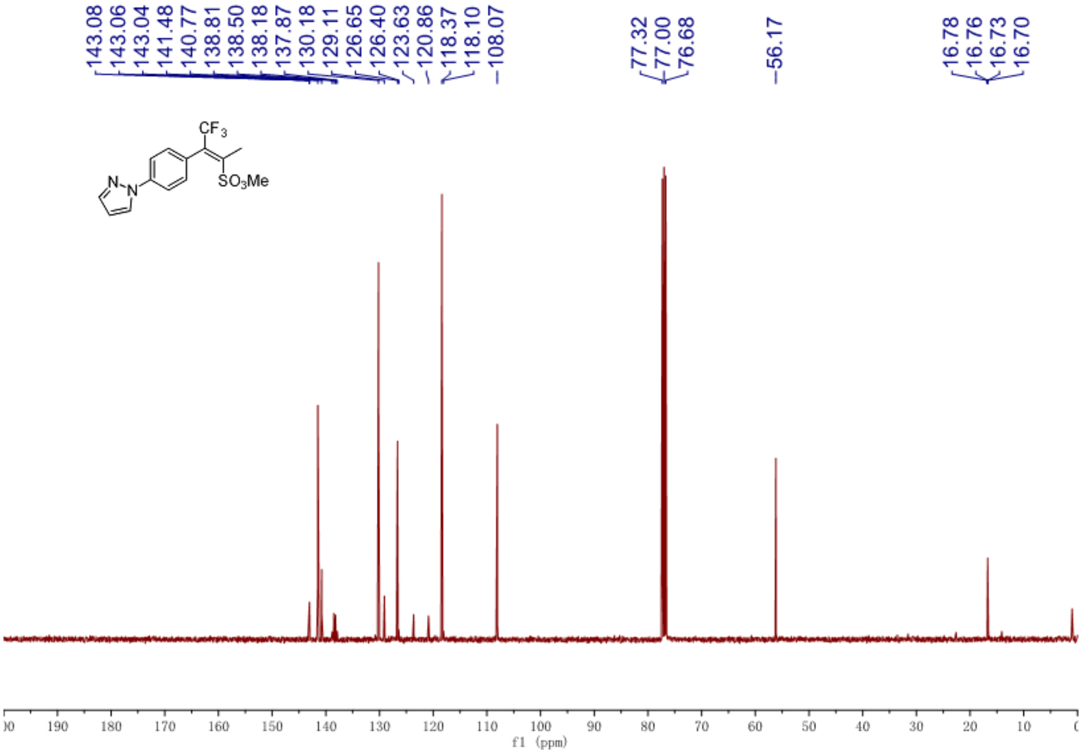
0.00
1.00
3.04
2.00
1.00
2.97
3.06
f1 (ppm)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143.04
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140.77
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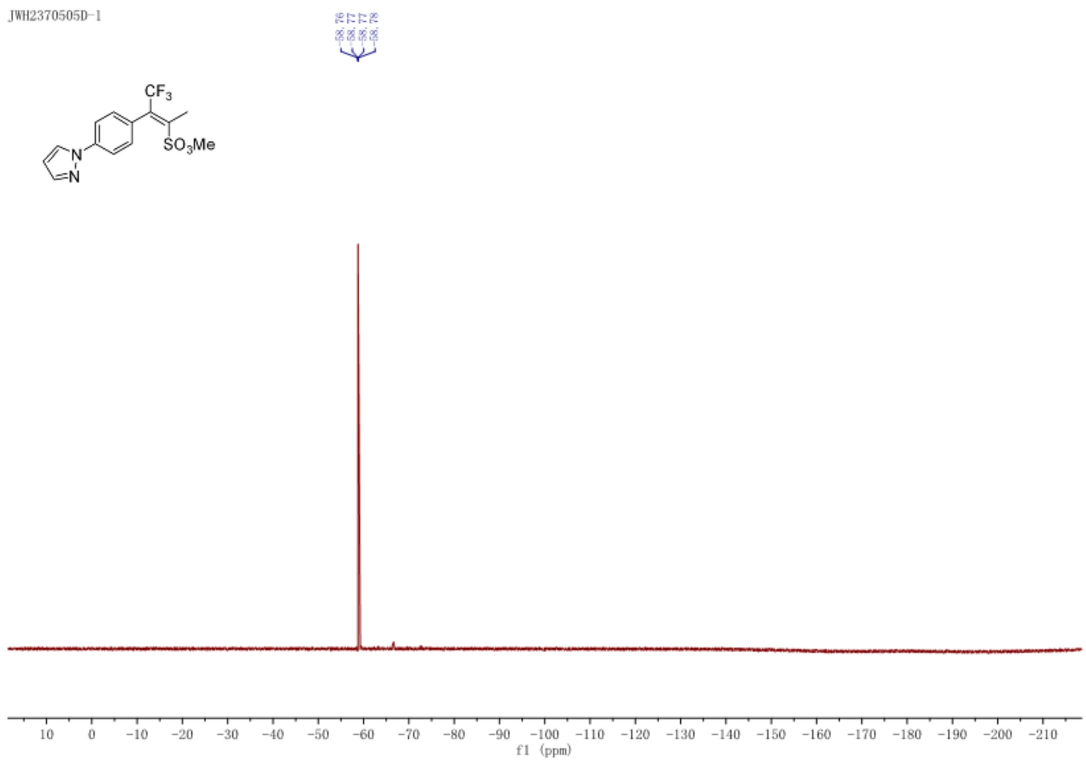
138.50
138.18
137.87
130.18
129.11
126.65
126.40
123.63
120.86
118.37
118.10
108.07
77.32
77.00
76.68
56.17
16.78
16.76
16.73
16.70
CF3
SO3Me
N
N
f1 (ppm)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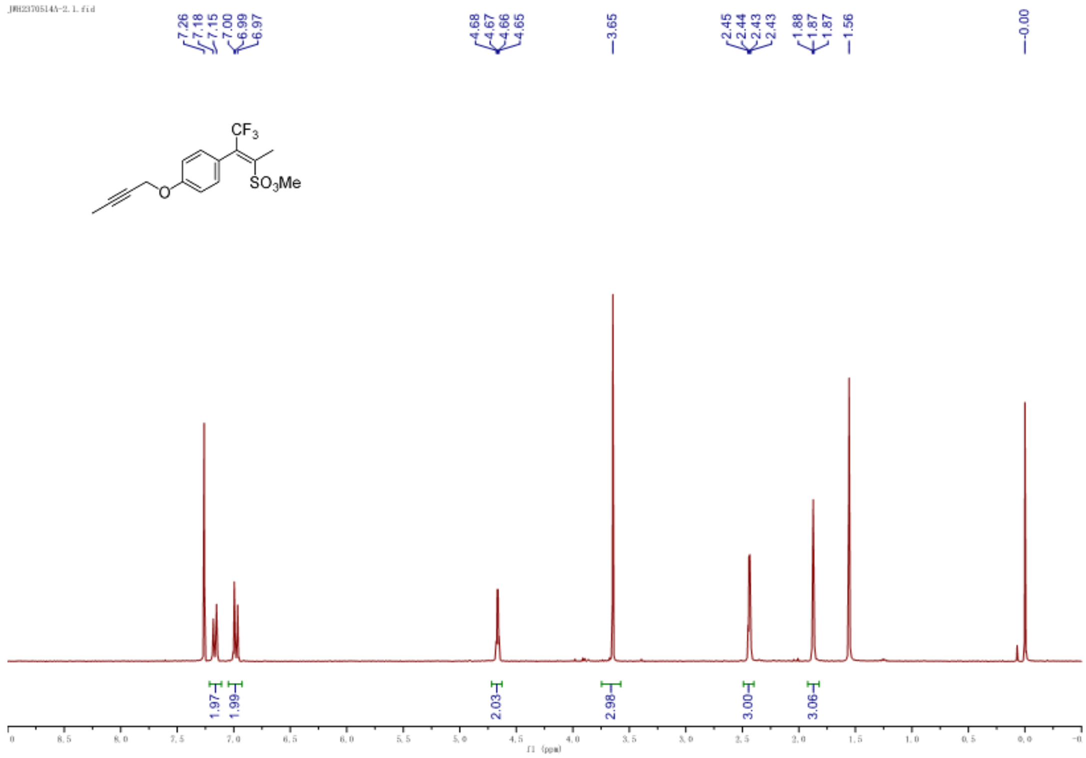
-58.78
CF_3
SO_3Me
f1 (ppm)


7.26
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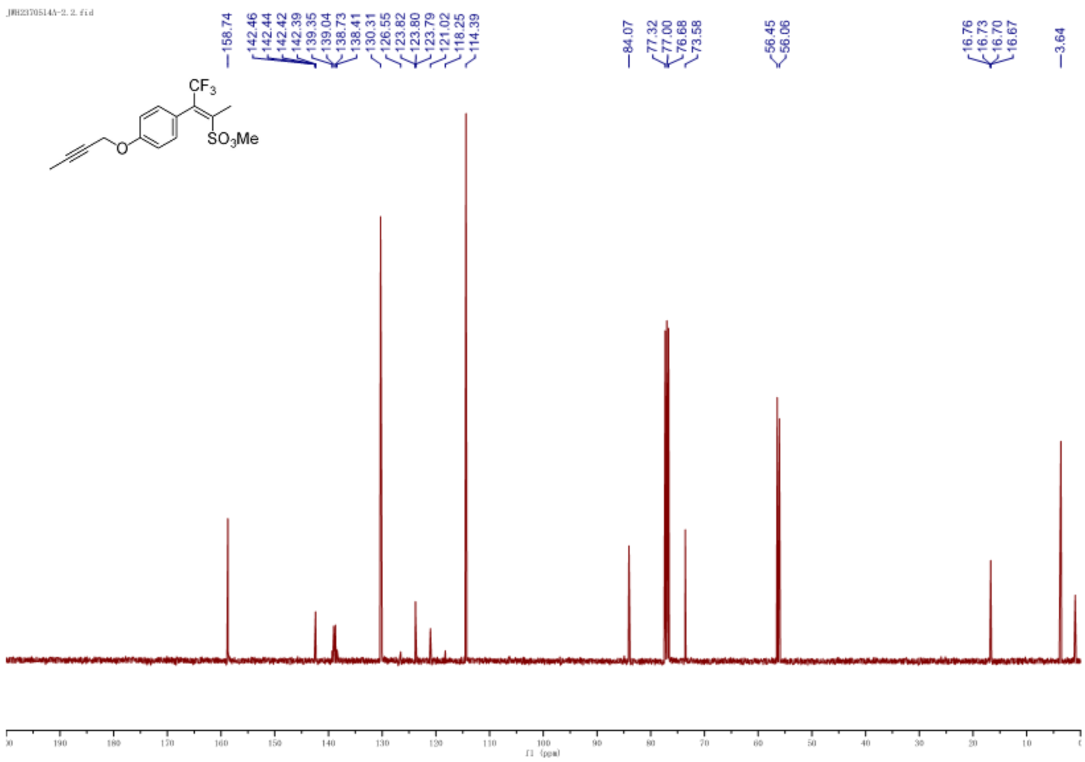
6.97
4.68
4.67
4.66
4.65
3.65
2.45
2.44
2.43
2.43
1.88
1.87
1.87
1.56
-0.00
CF_3
SO_3Me
1.97
1.99
2.03
2.98
3.00
3.06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138.73
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121.02
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77.00
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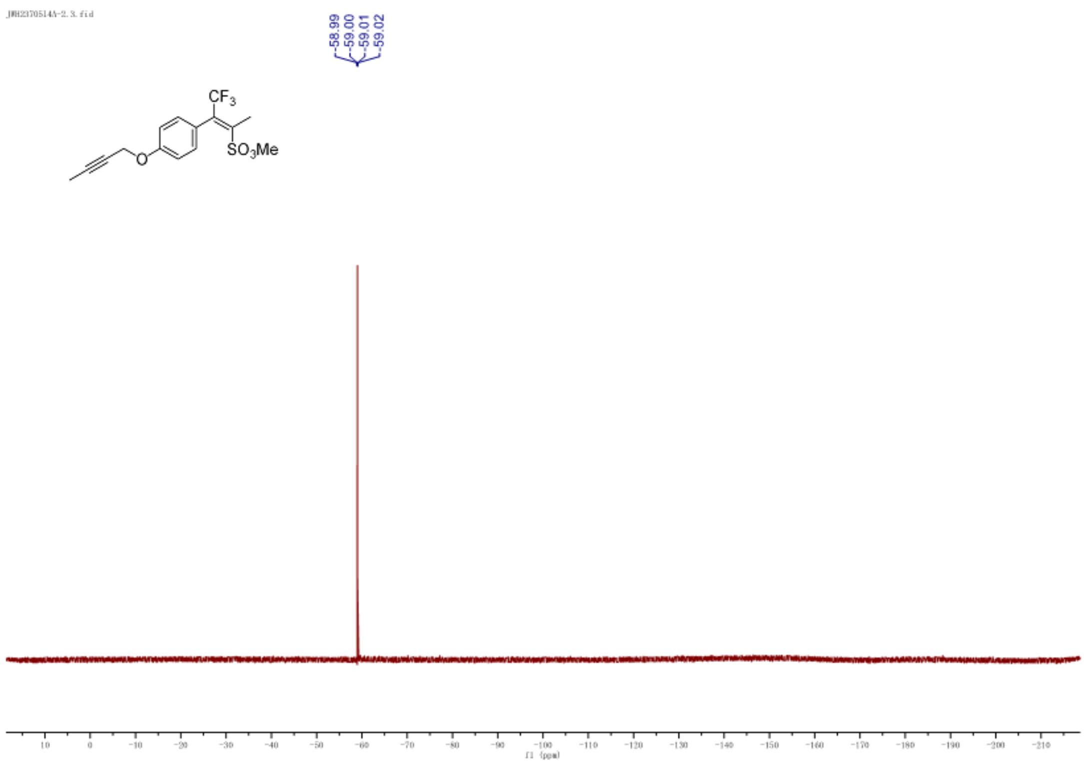
SO3Me
O
f1 (ppm)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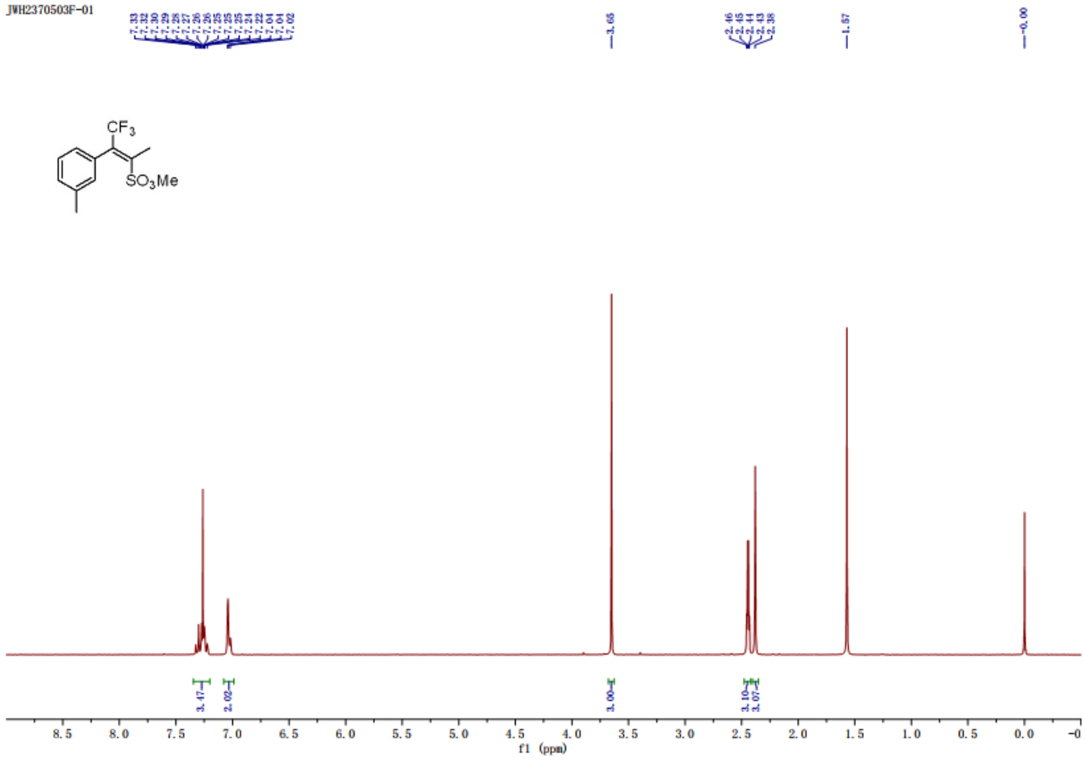
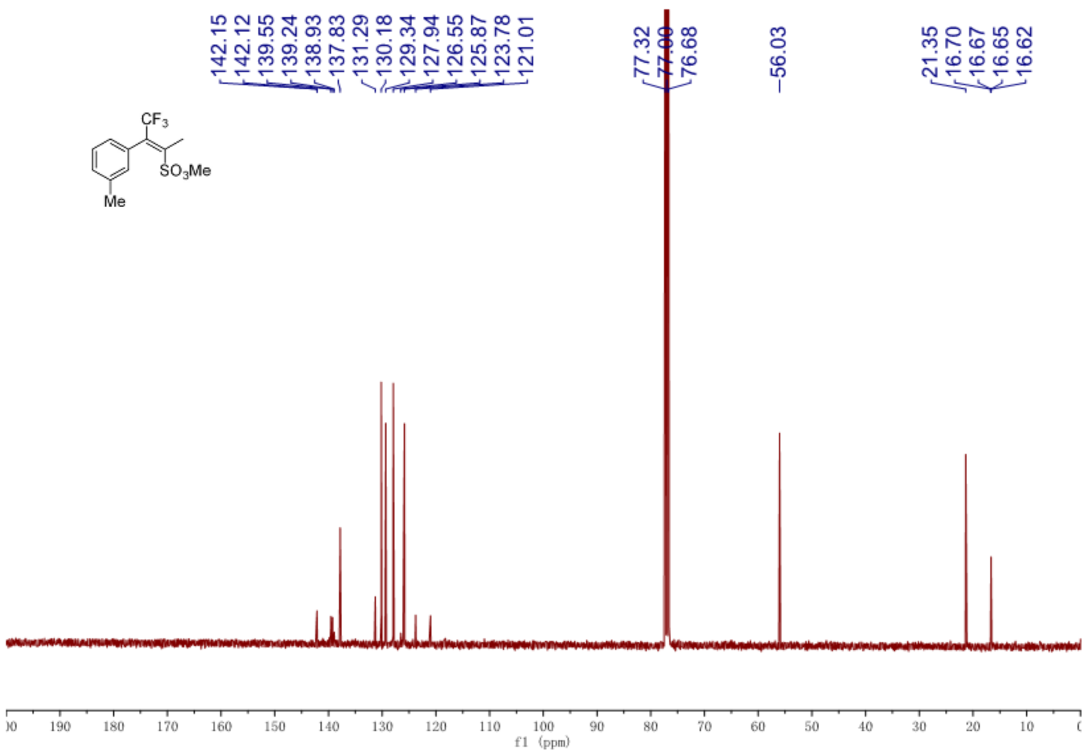
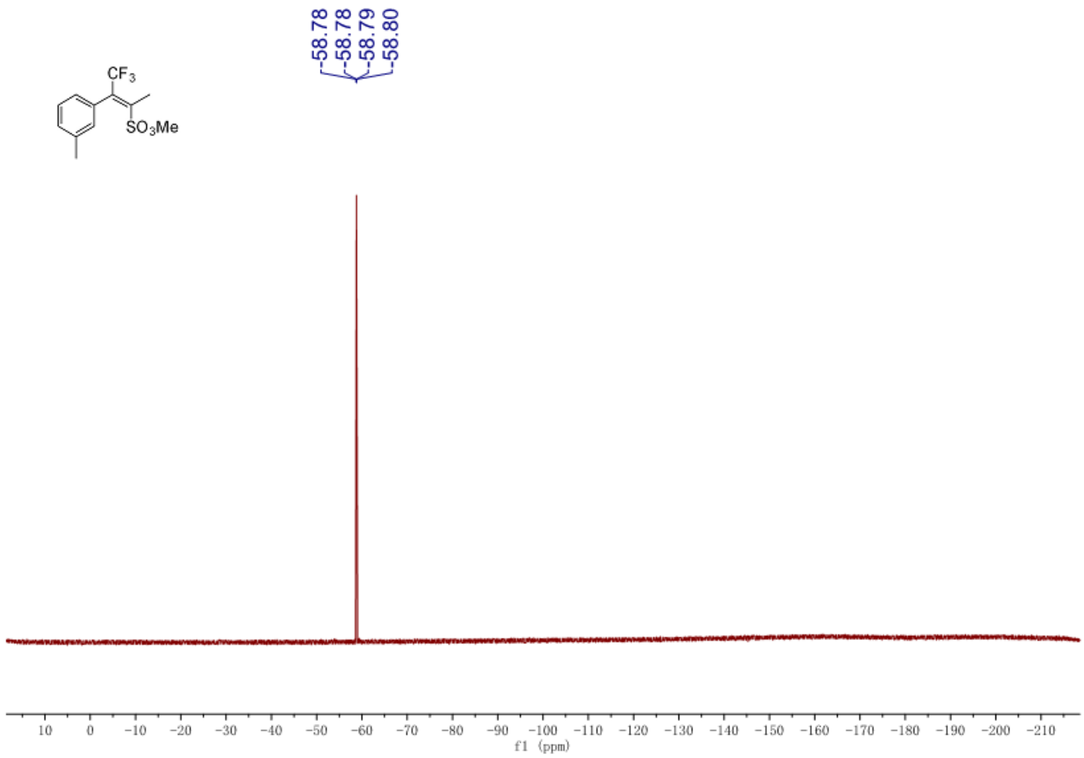
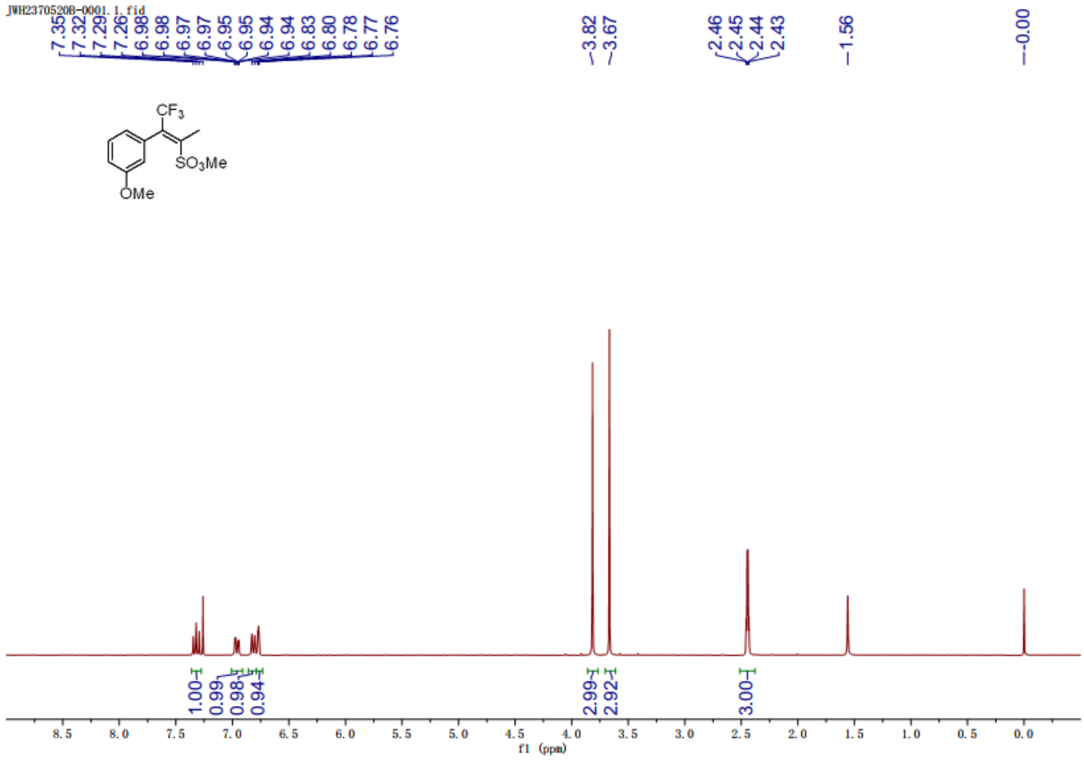
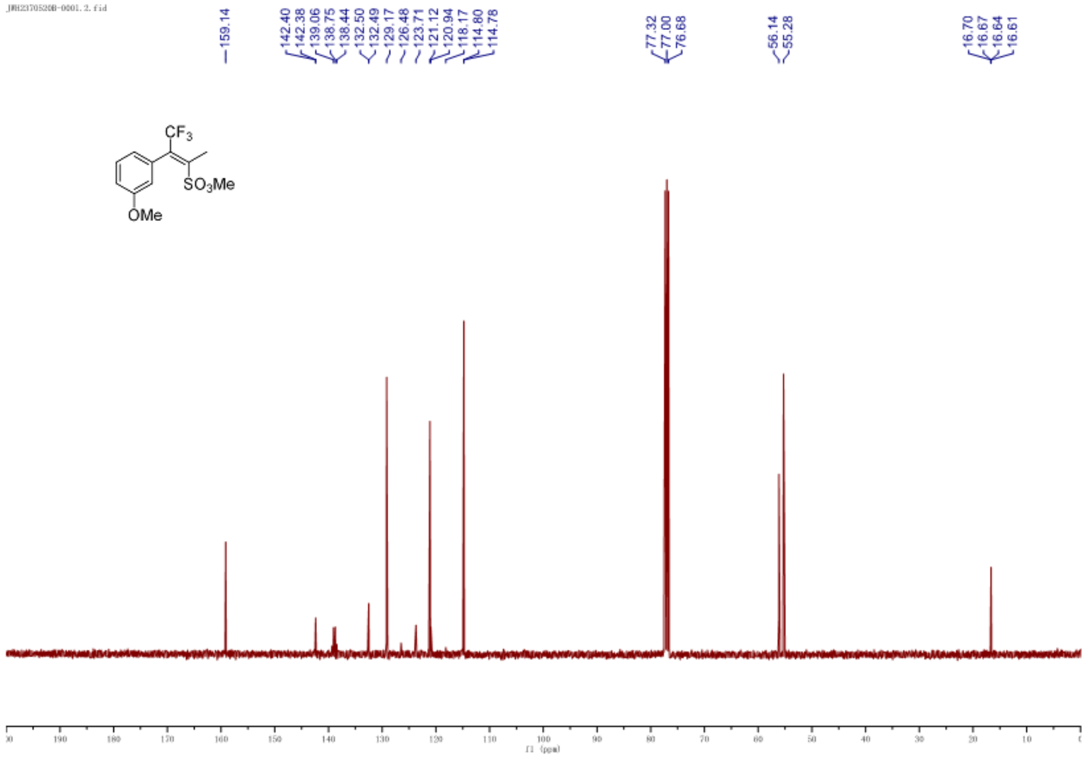
-59.01
-59.02
CF3
SO3Me
O
f1 (ppm)







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132.49
129.17
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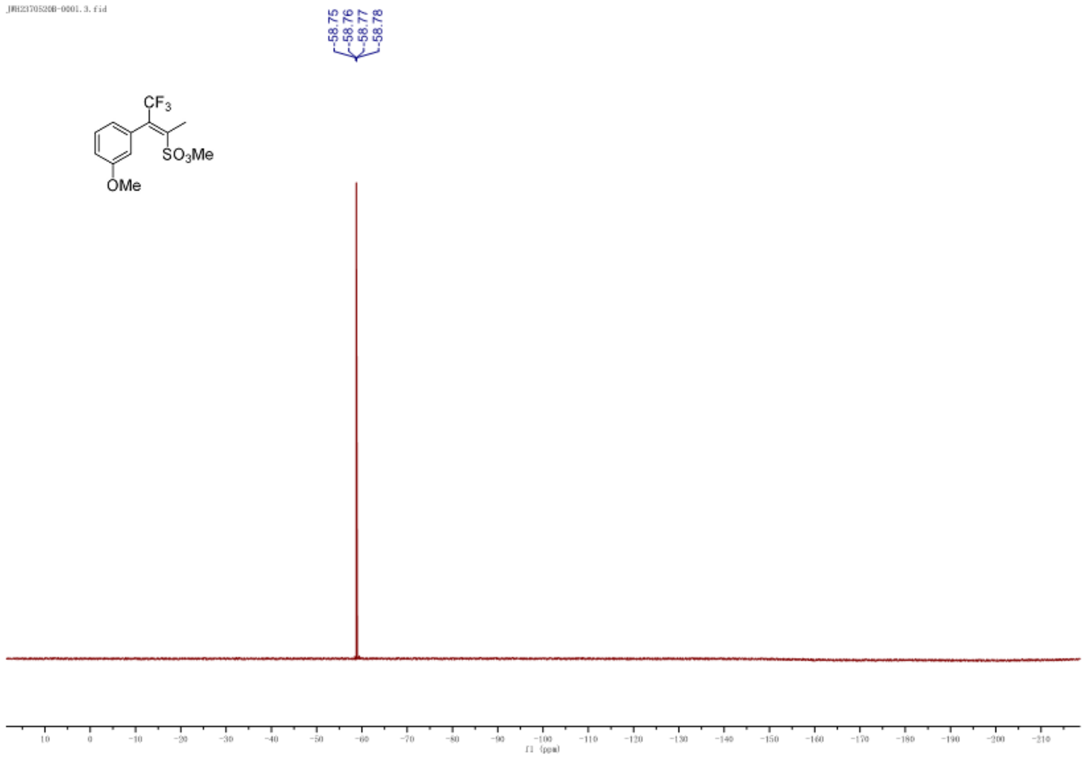
118.17
114.80
114.78
77.32
77.00
76.68
56.14
55.28
16.70
16.67
16.64
16.61
CF3
SO3Me
OMe
f1 (ppm)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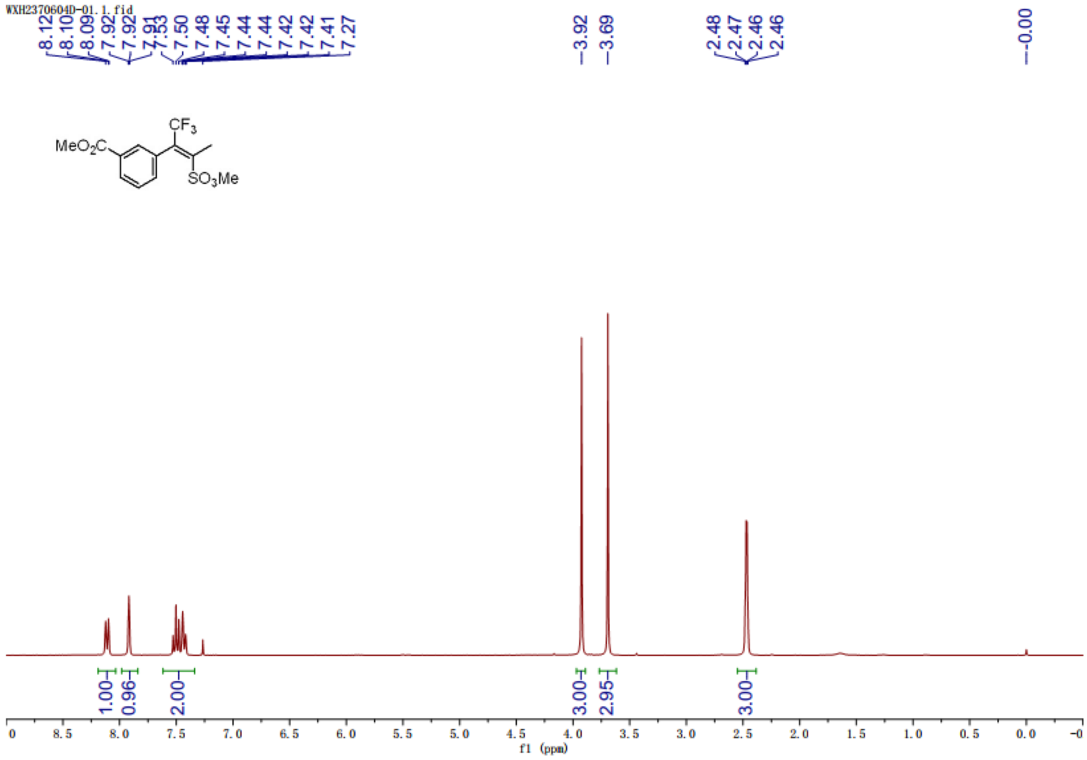
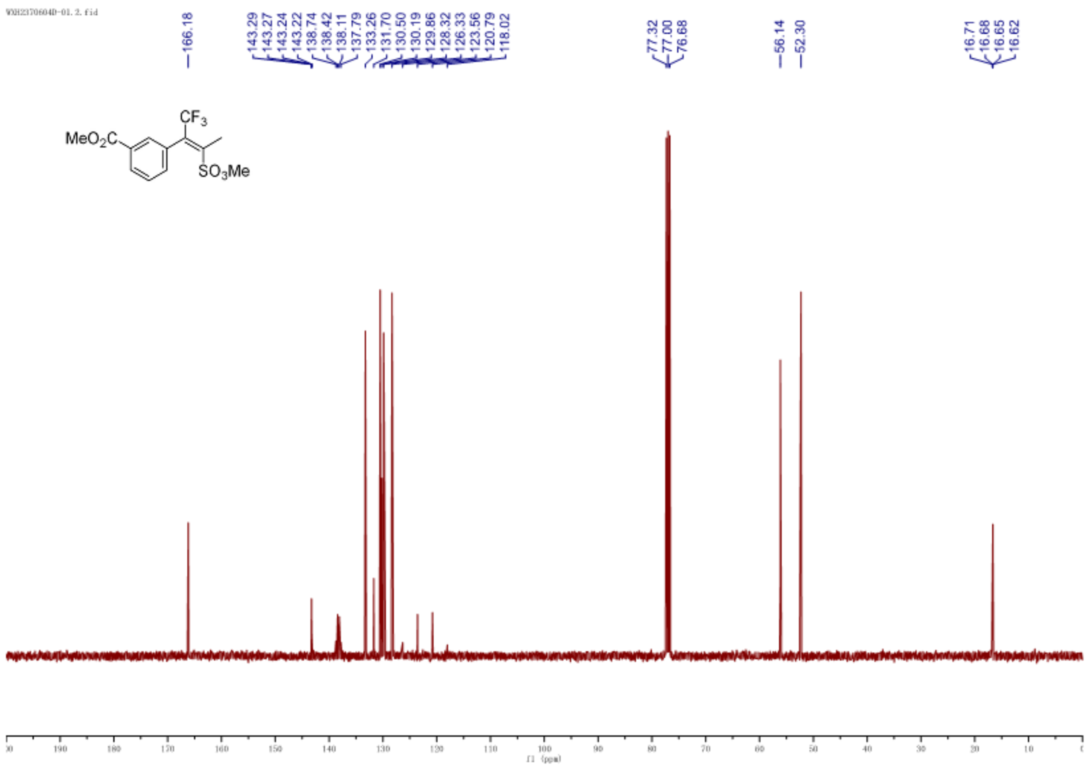
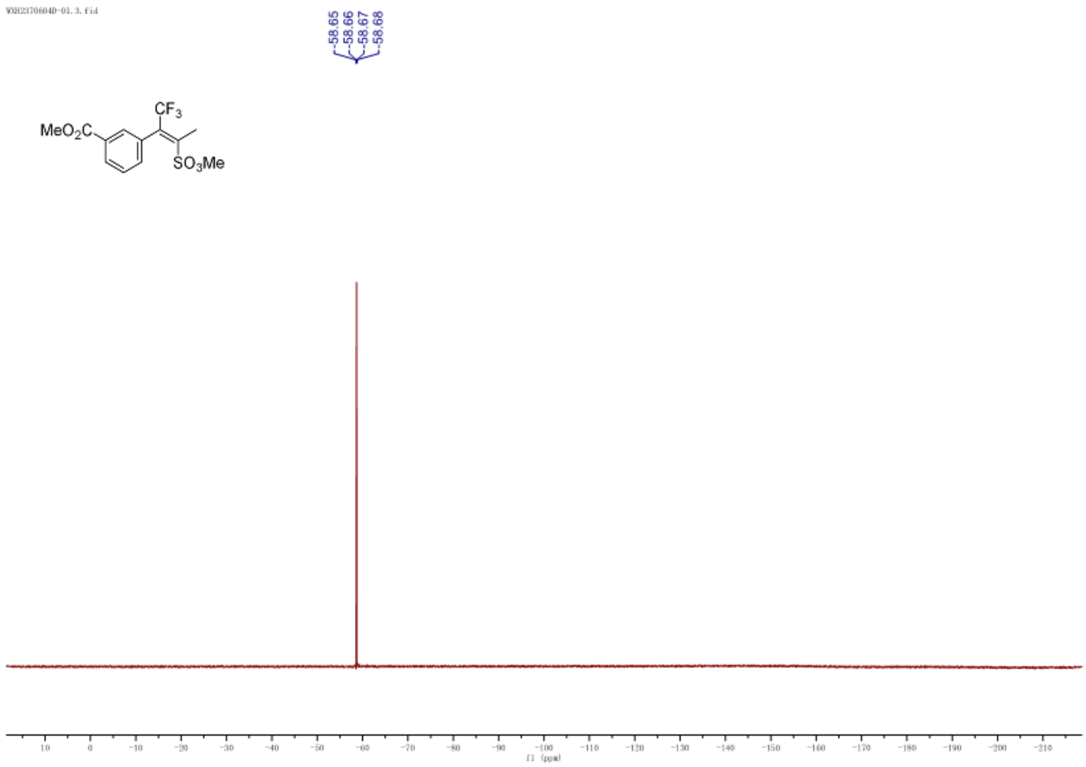
-58.77
-58.78
CF3
SO3Me
OMe
f1 (ppm)



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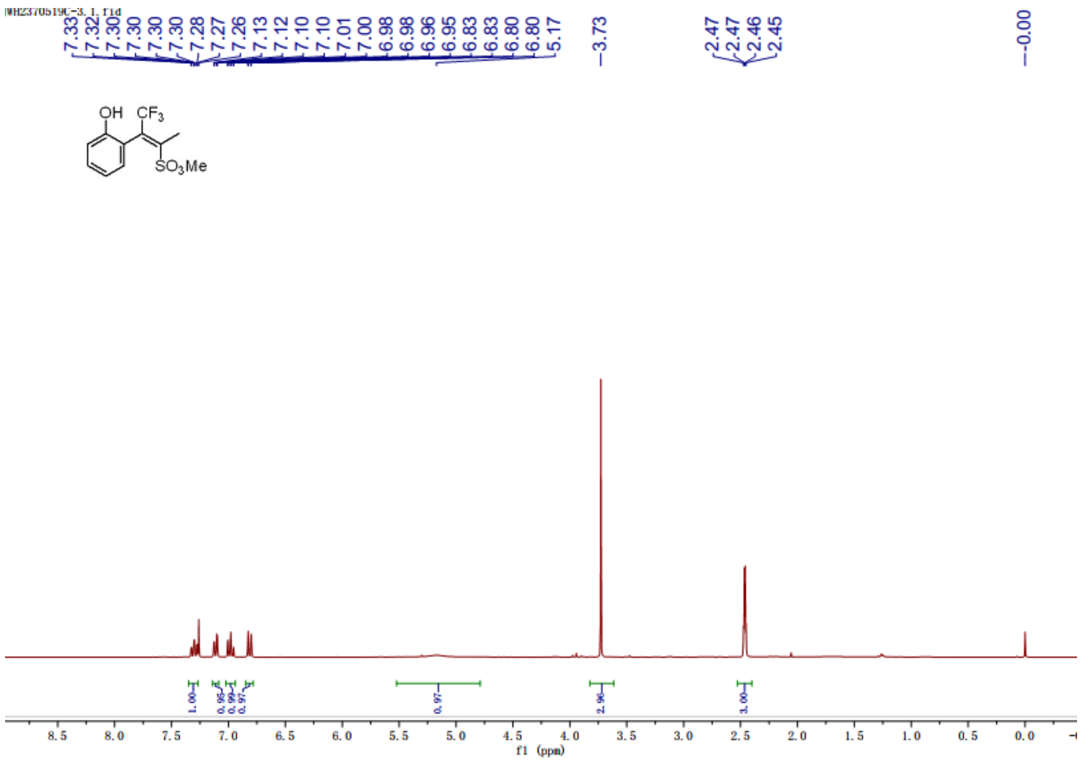
MeO2C
CF3
SO3Me
f1 (ppm)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7.27
7.26
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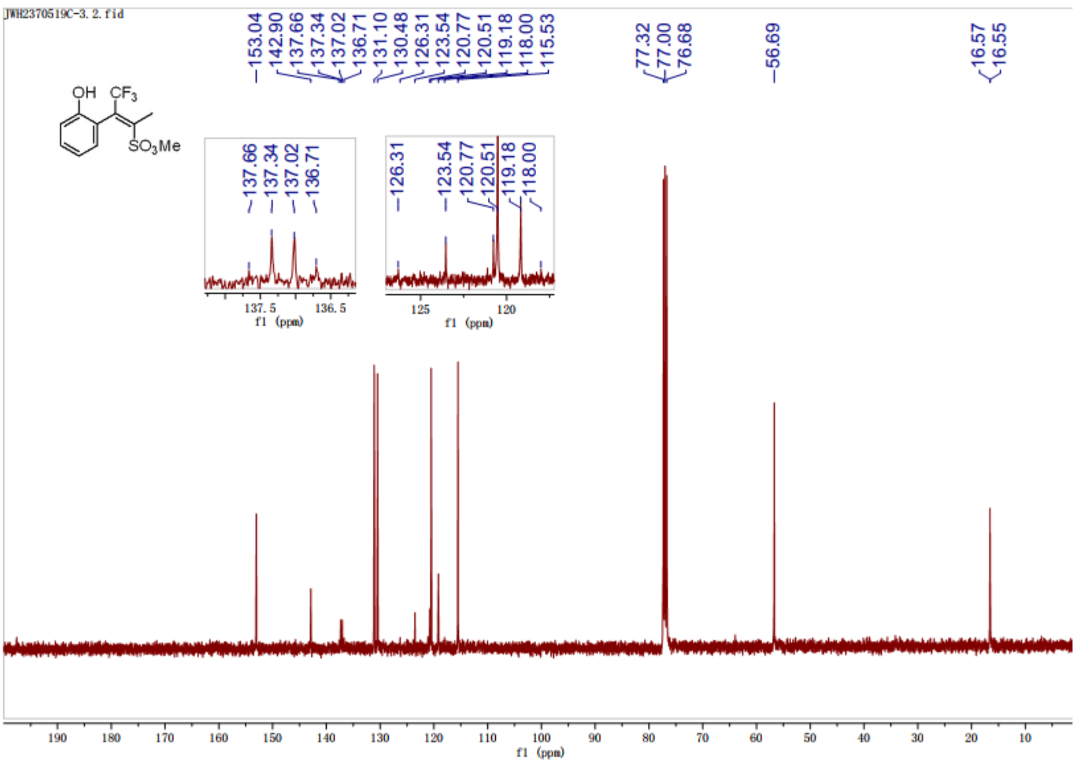
7.10
7.01
7.00
6.98
6.98
6.96
6.95
6.83
6.83
6.80
6.80
5.17
3.73
2.47
2.47
2.46
2.45
-0.00
OH
CF3
SO3Me
1.00
0.95
0.99
0.97
0.97
2.96
3.00
f1 (ppm)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137.02
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131.10
130.48
126.31
123.54
120.77
120.51
119.18
118.00
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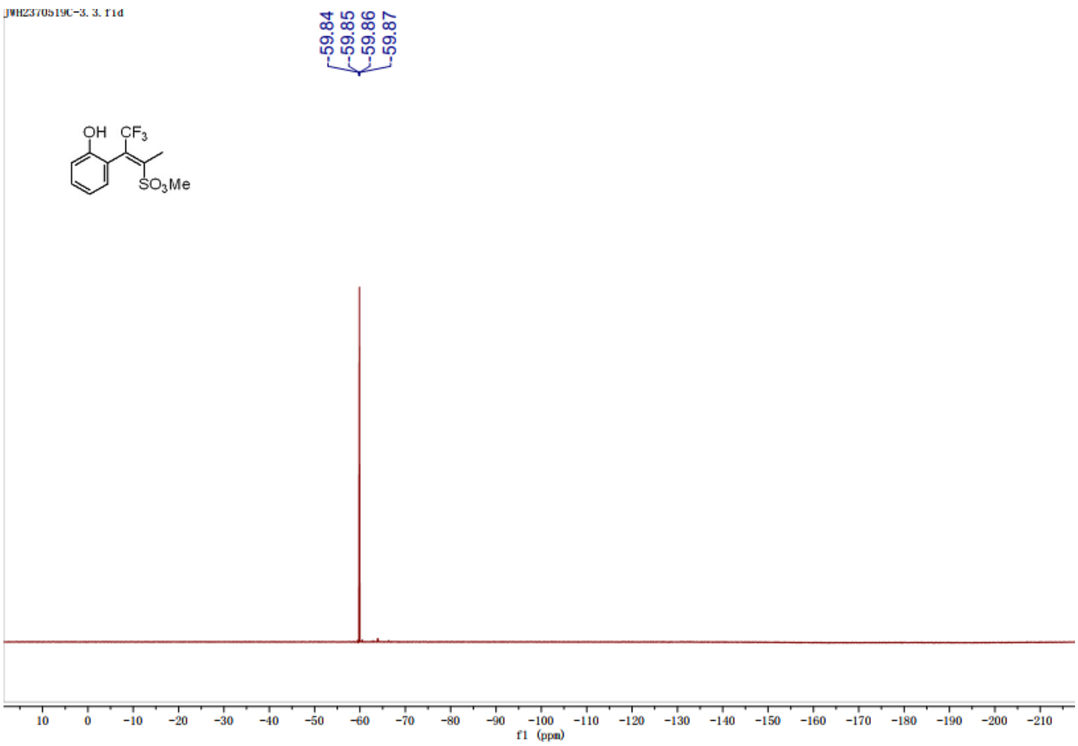
77.32
77.00
76.68
56.69
16.57
16.55
OH
CF3
SO3Me
f1 (ppm)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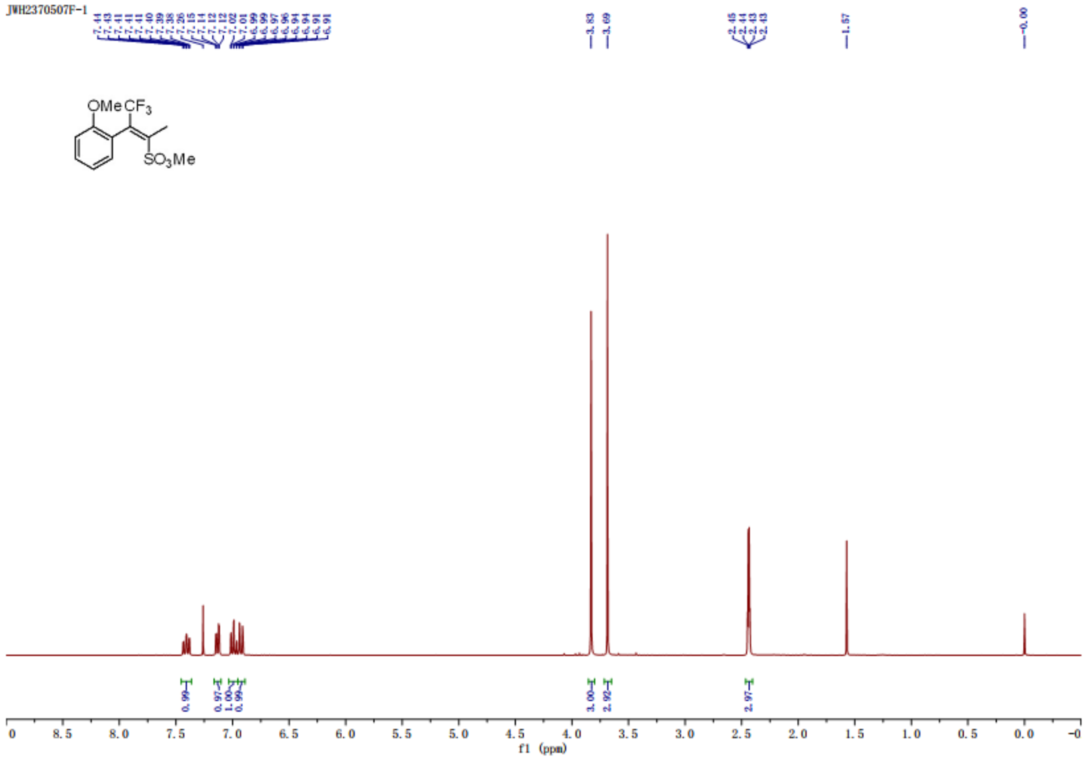
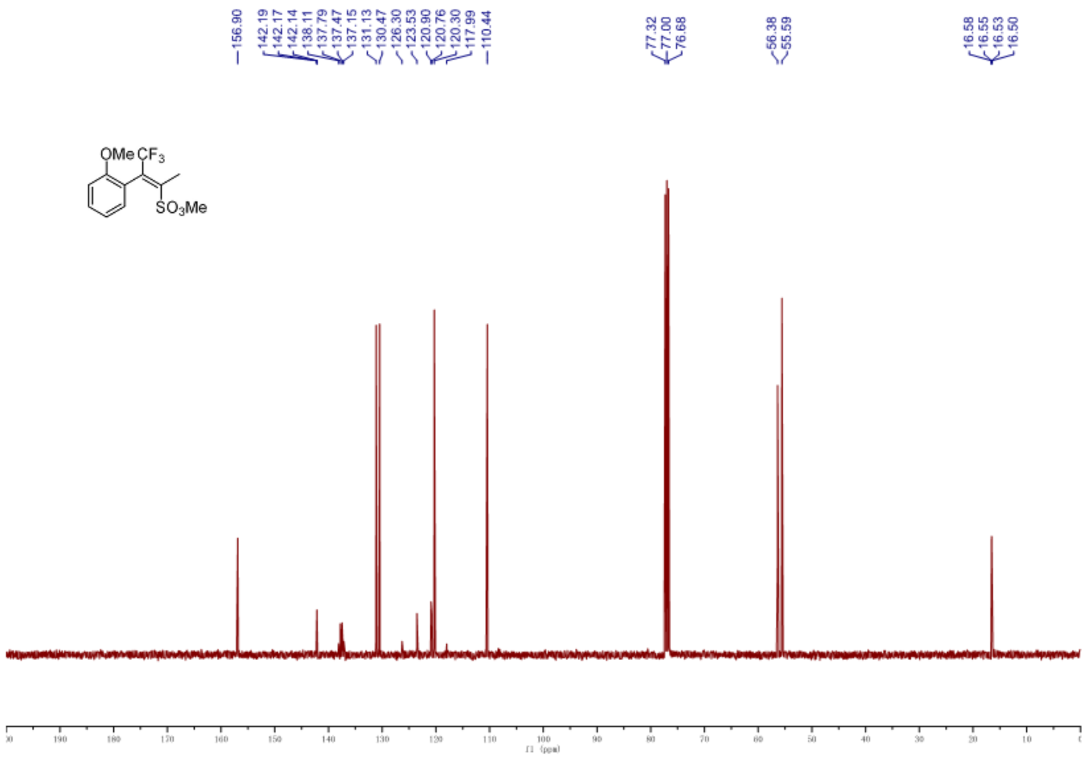
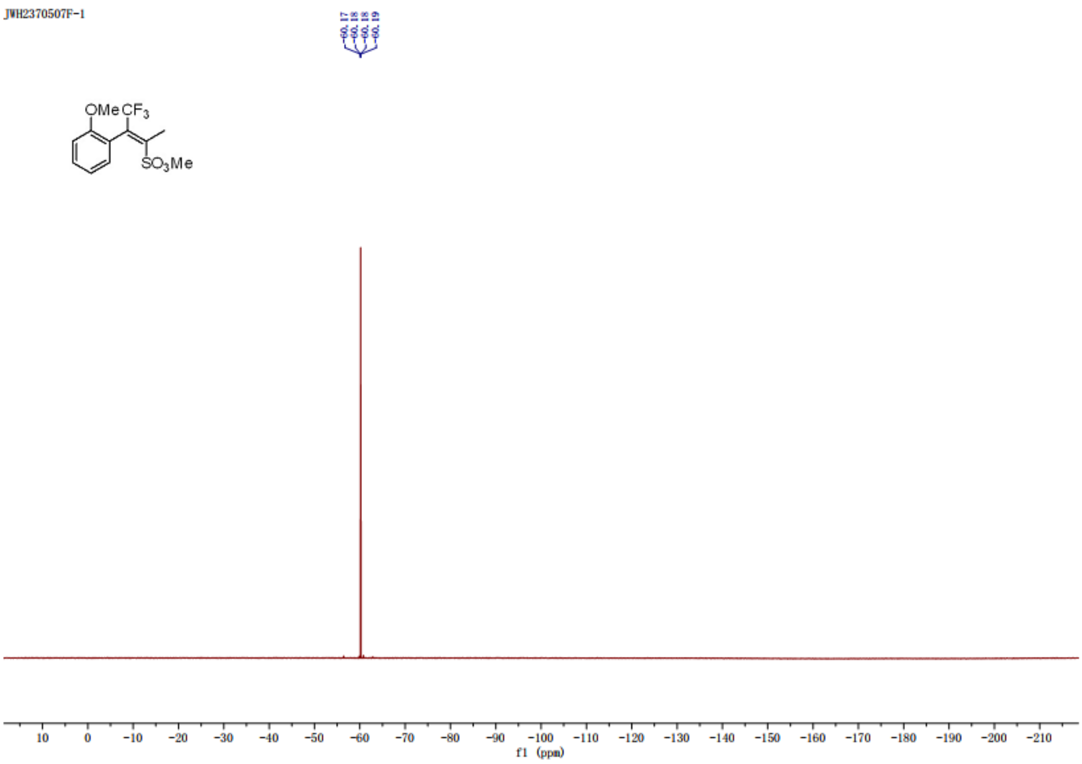
CF3
SO3Me
f1 (ppm)



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-60.18
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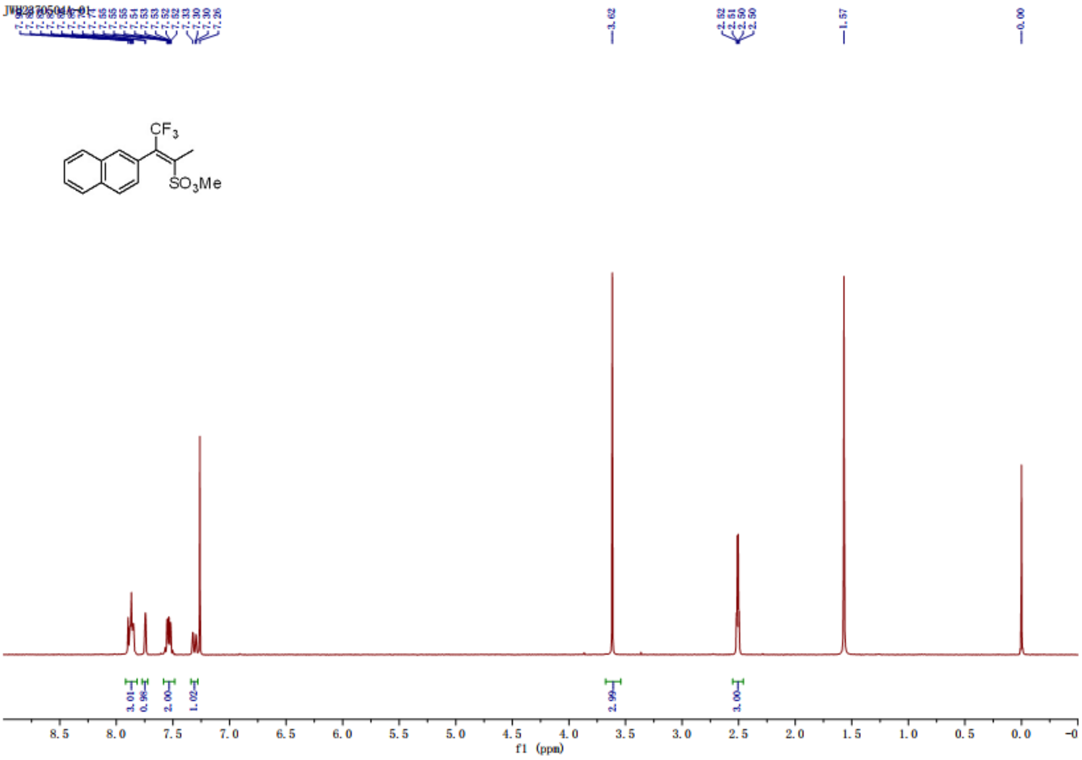
OMe
CF_3
SO_3Me
f1 (ppm)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1.02
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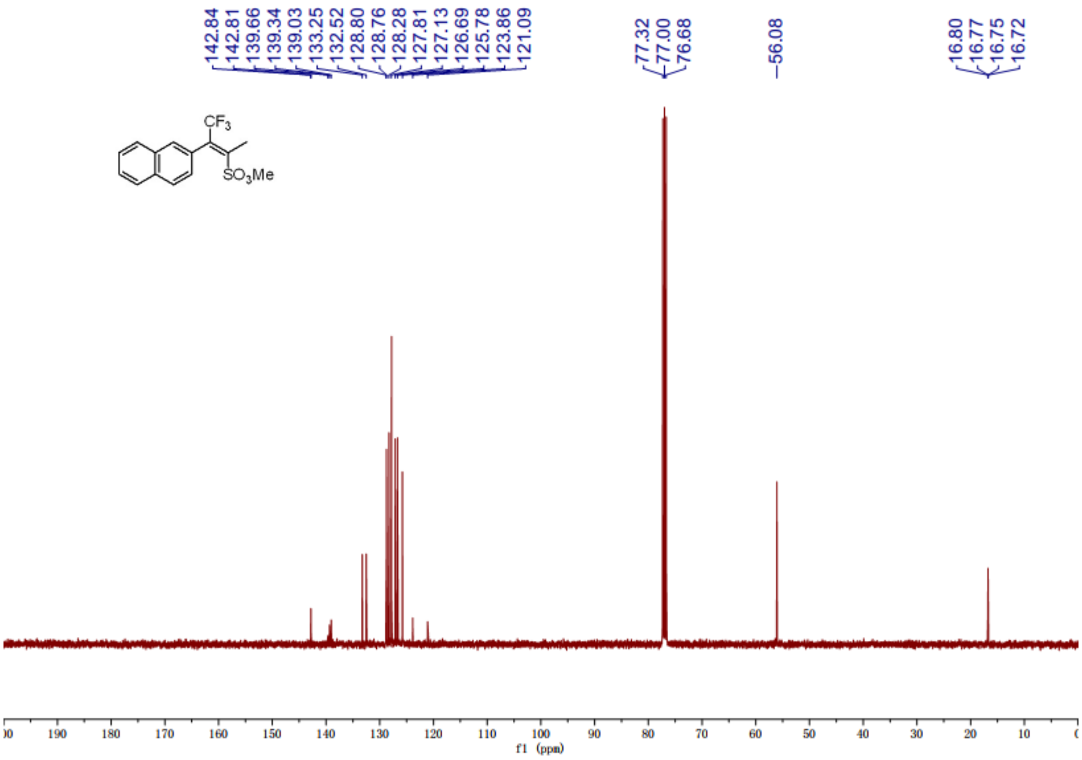
3.00
f1 (ppm)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126.69
125.78
123.86
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16.77
16.75
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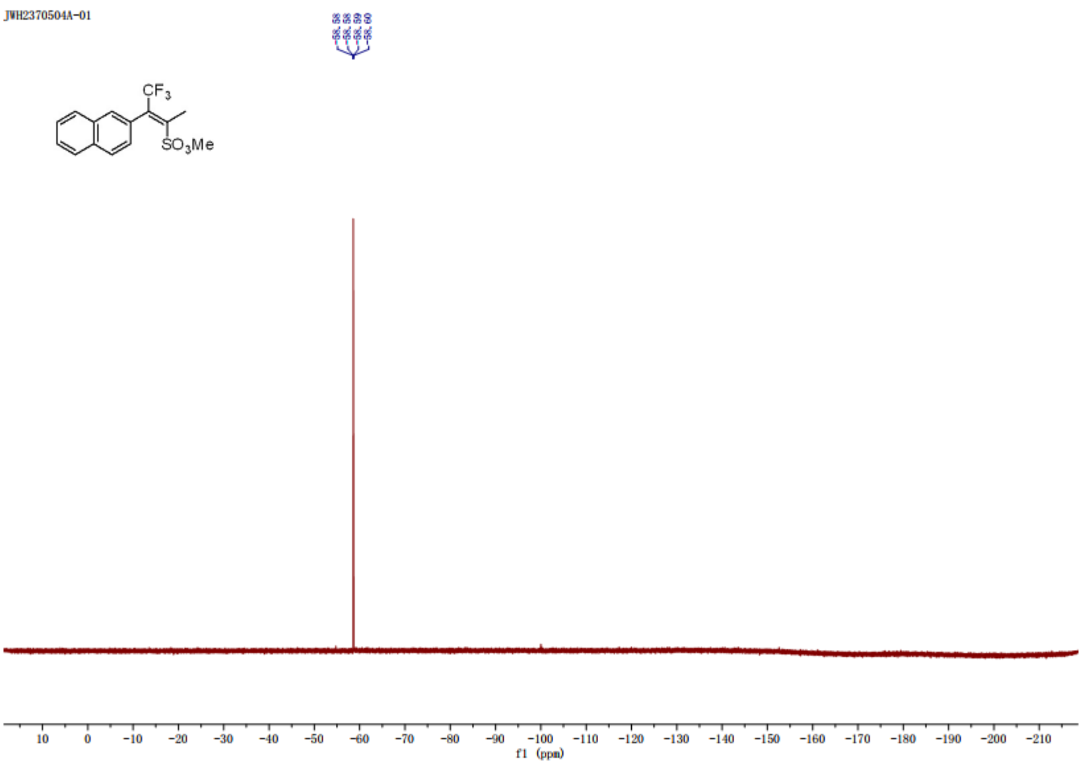
SO3Me
f1 (ppm)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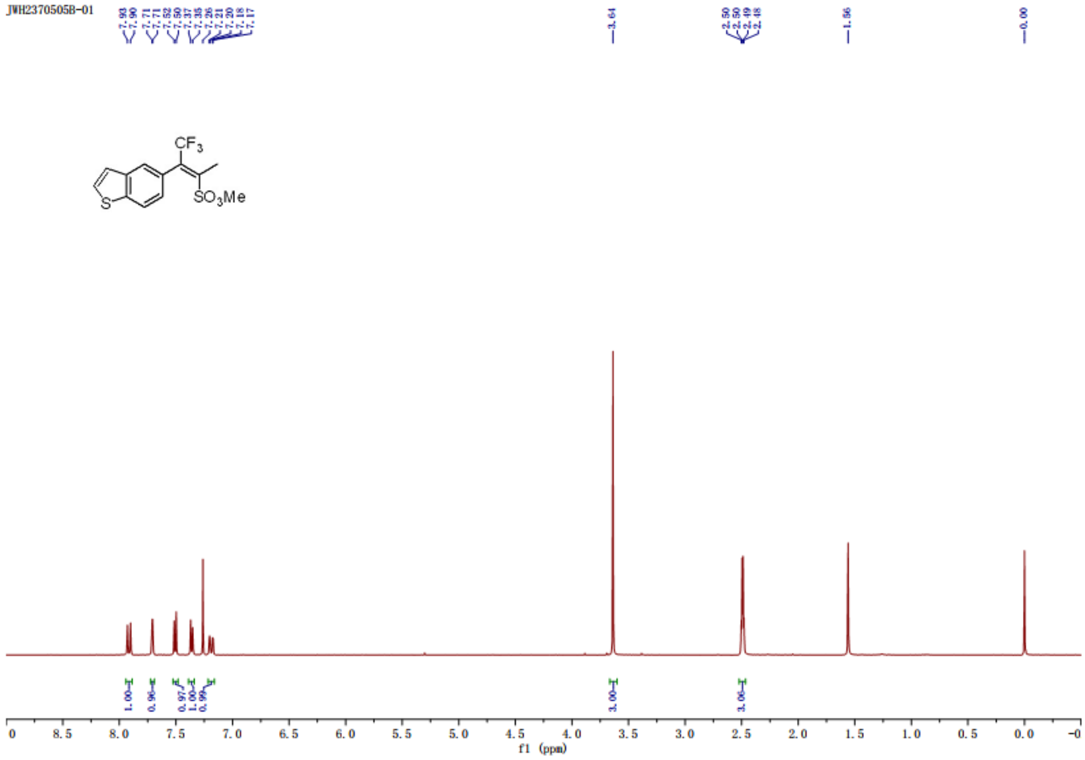
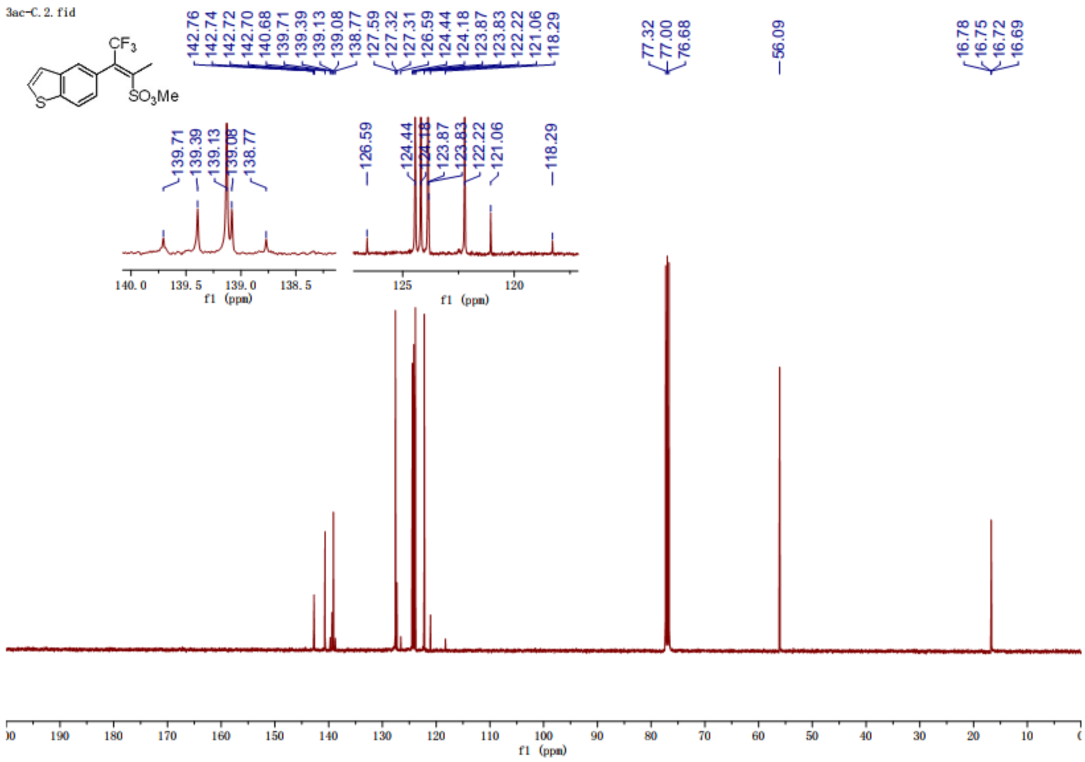
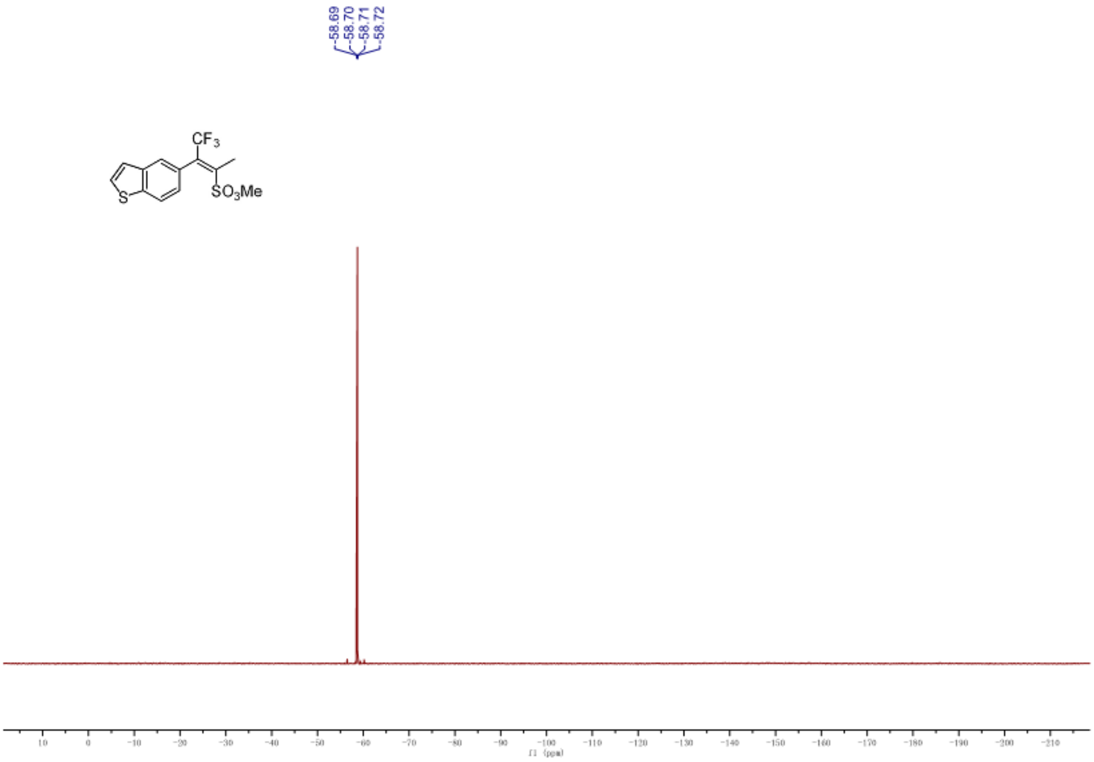
SO3Me
f1 (ppm)



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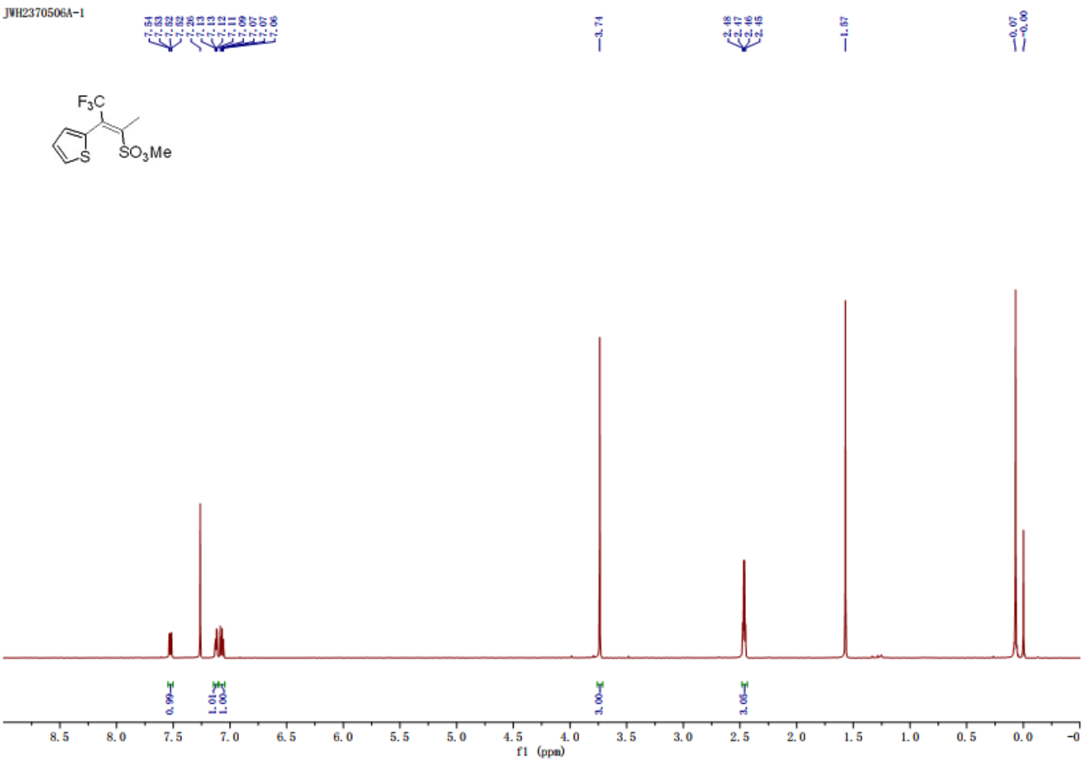
CF3
S
SO3Me
f1 (ppm)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7.12
7.11
7.09
7.07
7.06
3.74
2.48
2.47
2.46
2.45
1.57
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F3C
S
SO3Me
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1.00
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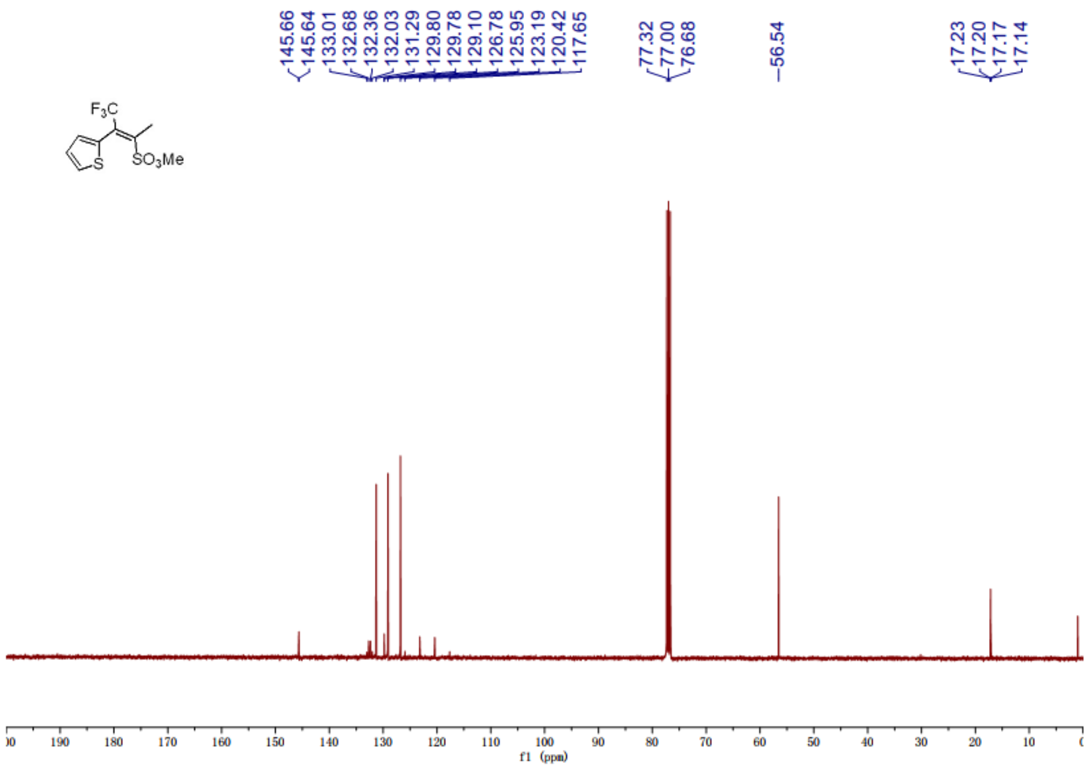
3.05
f1 (ppm)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123.19
120.42
117.65
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56.54
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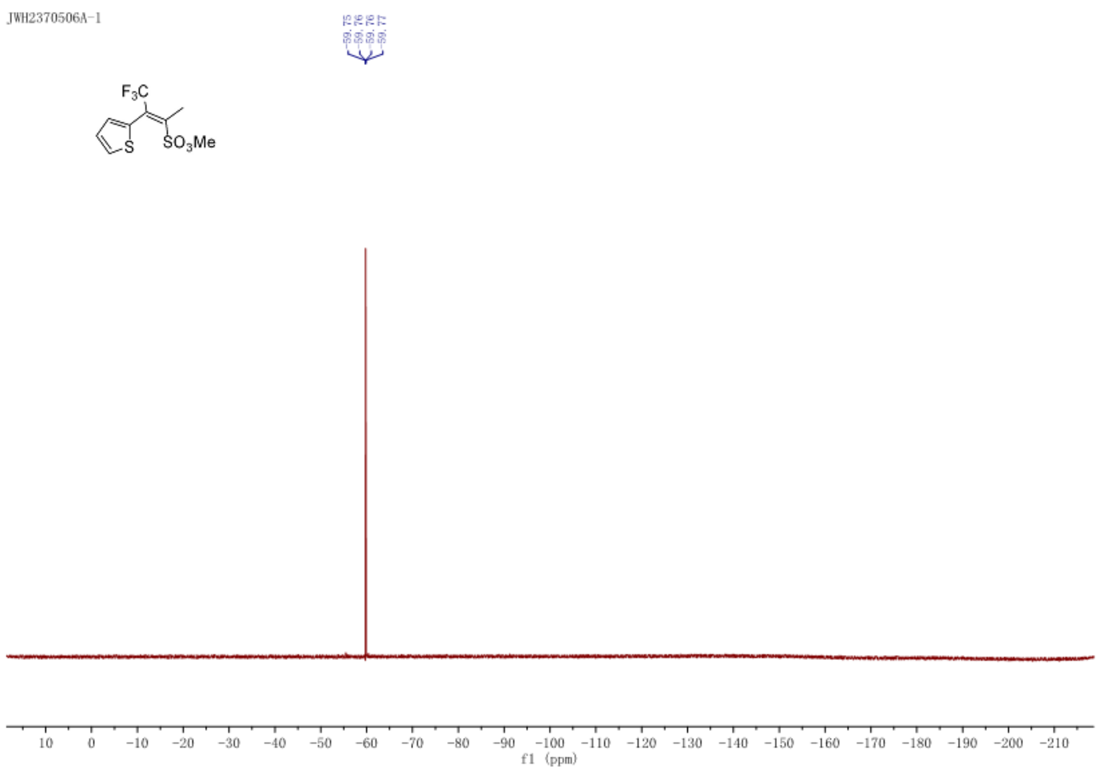
17.17
17.14
F3C
S
SO3Me
f1 (ppm)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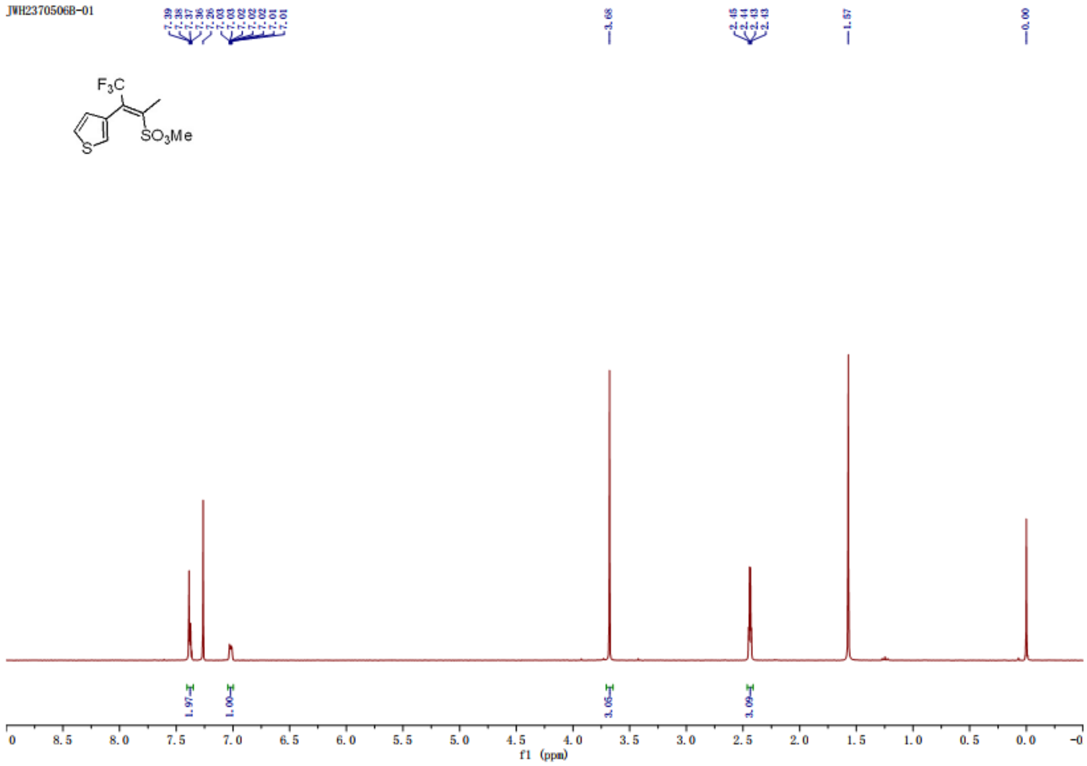
SO3Me
f1 (ppm)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S
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7.02
7.02
7.01
7.01
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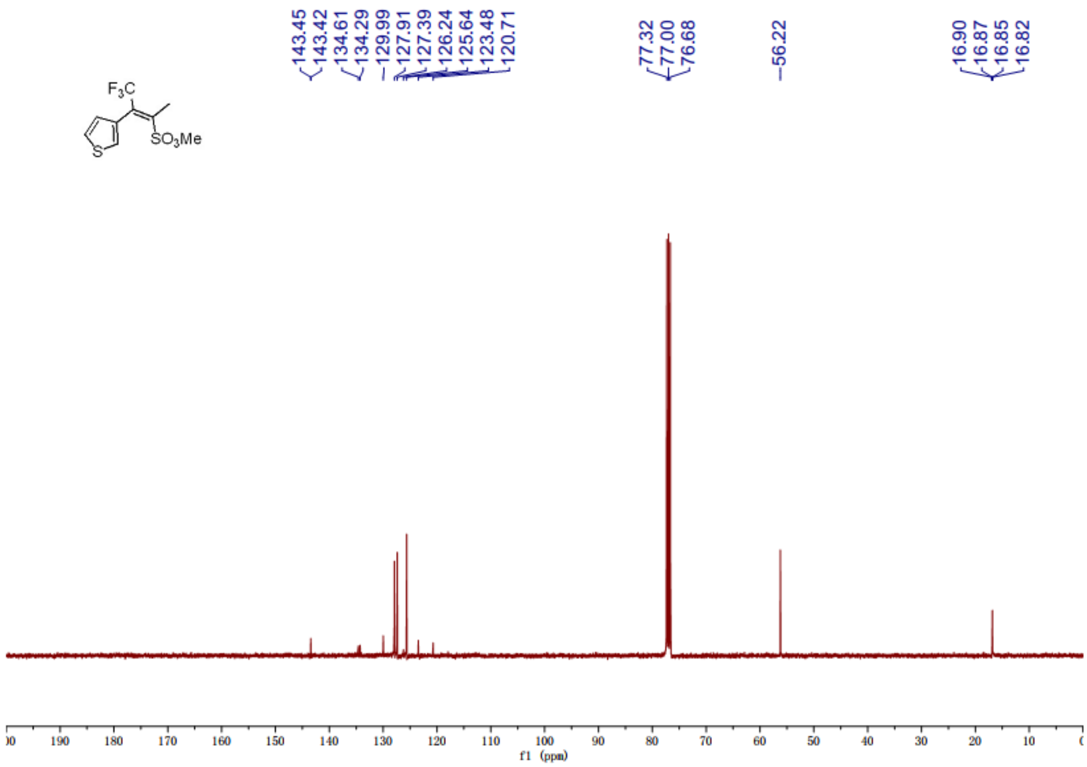
3.09
f1 (ppm)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S
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126.24
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77.00
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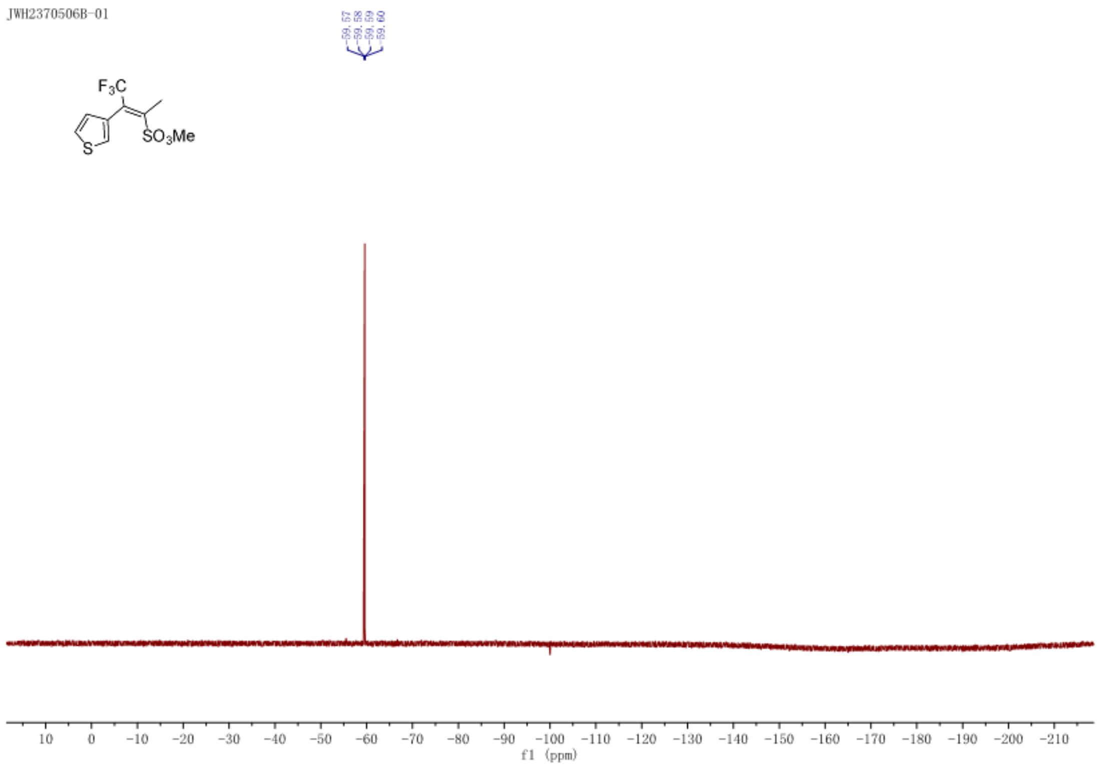
16.82
f1 (ppm)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SO_3Me
S
-59.57
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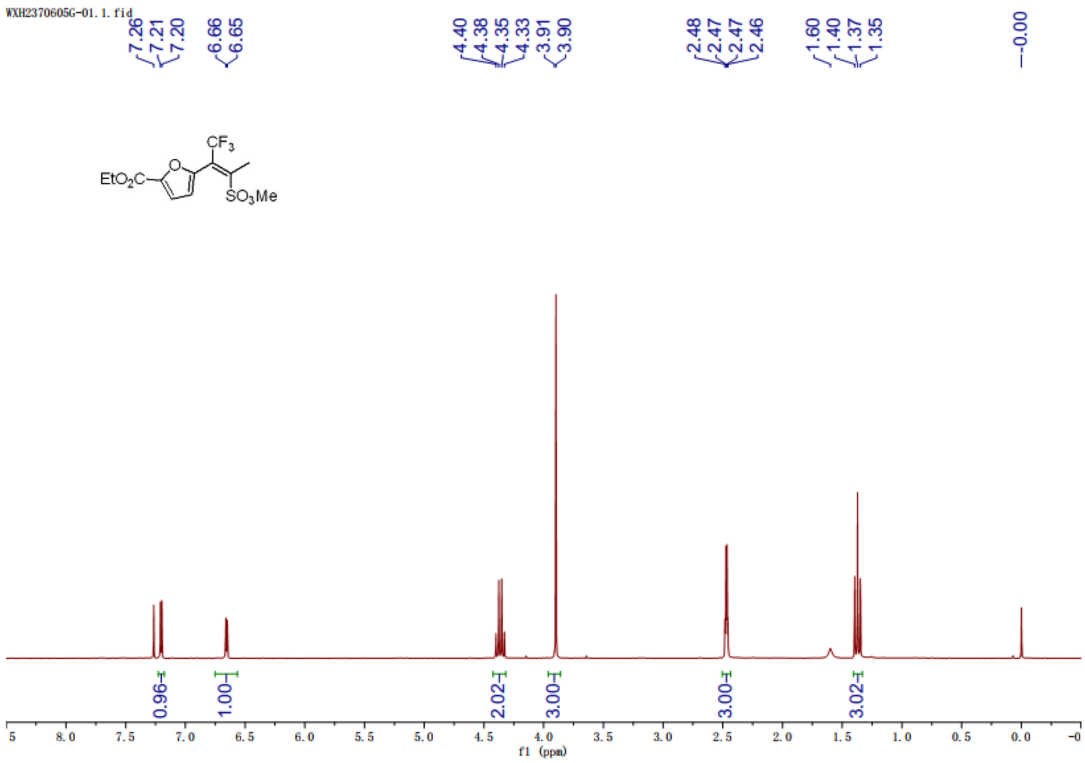
-59.59
-59.60
f1 (ppm)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6.65
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4.38
4.35
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3.90
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2.47
2.47
2.46
1.60
1.40
1.37
1.35
-0.00
EtO_2C
O
CF_3
SO_3Me
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1.00
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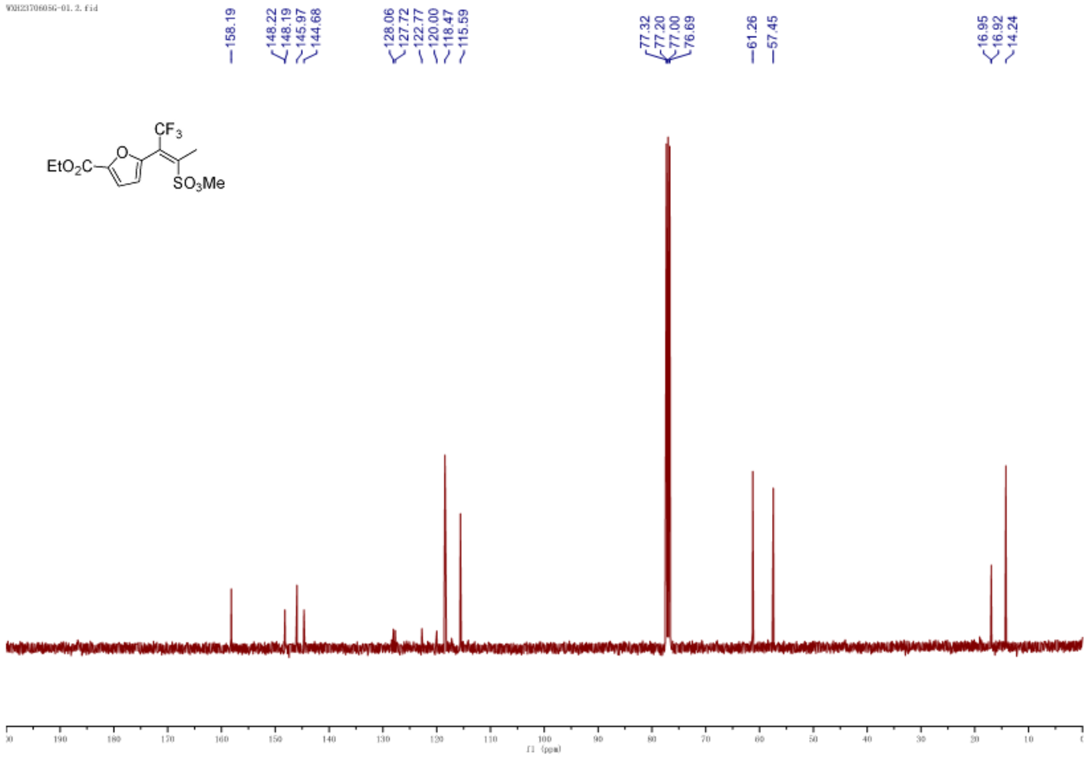
3.00
3.00
3.02
f1 (ppm)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127.72
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120.00
118.47
115.59
77.32
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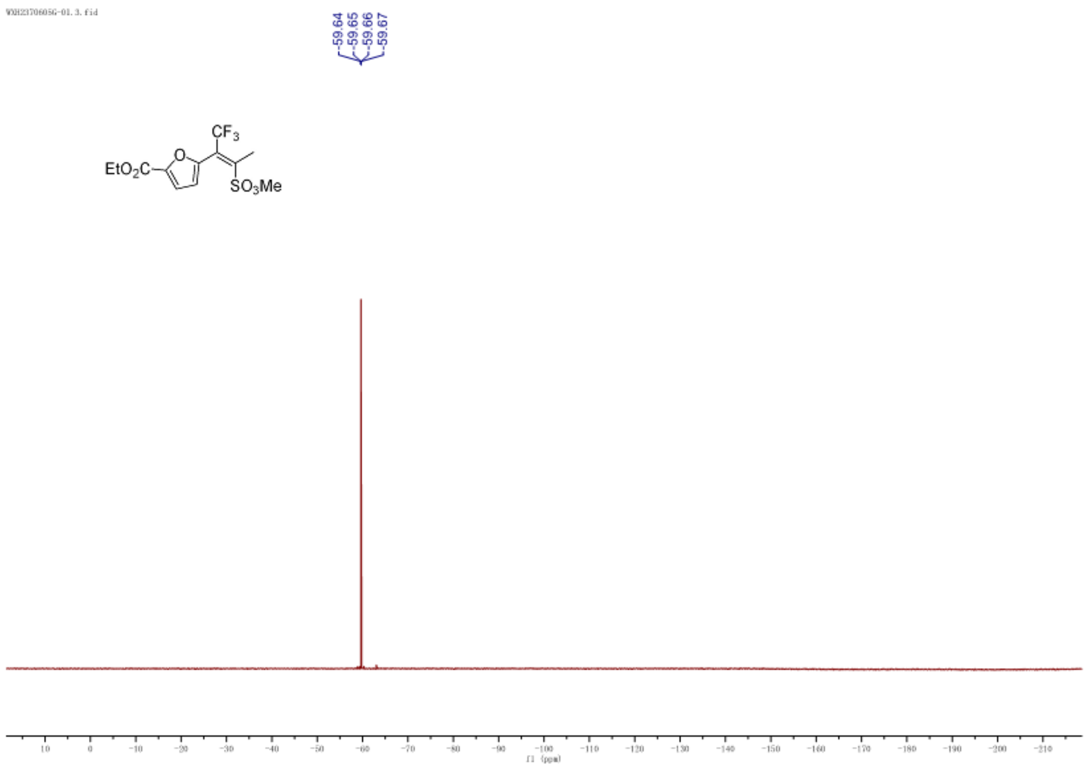
SO3Me
f1 (ppm)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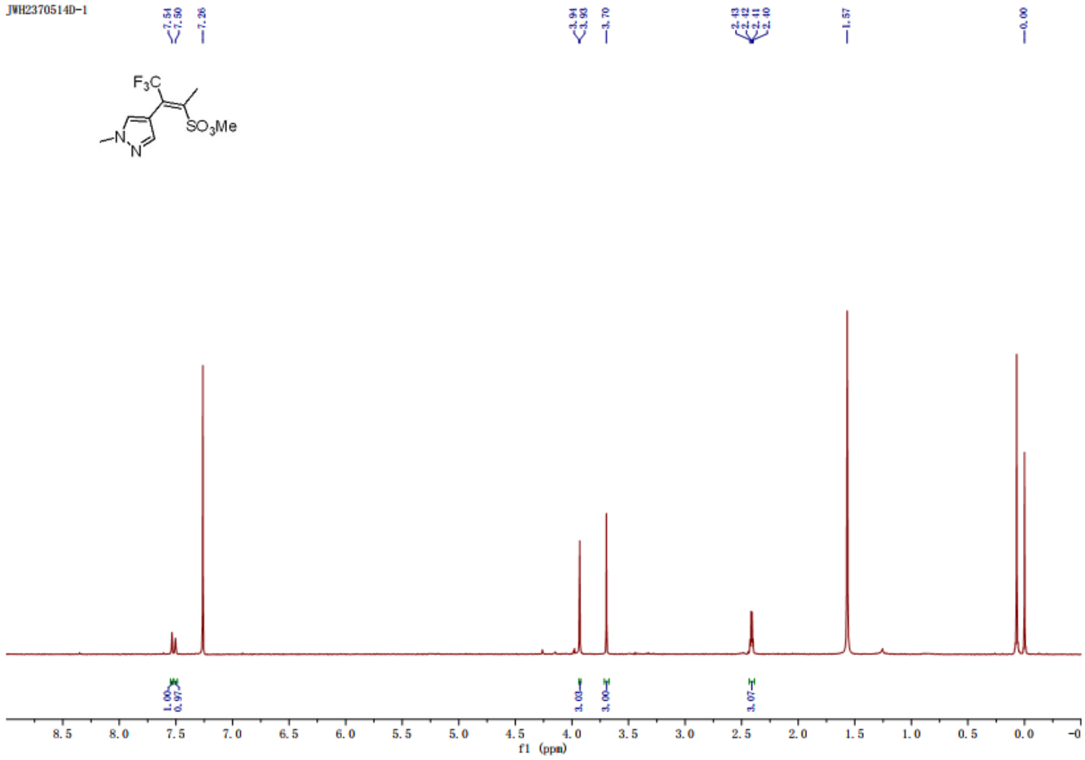

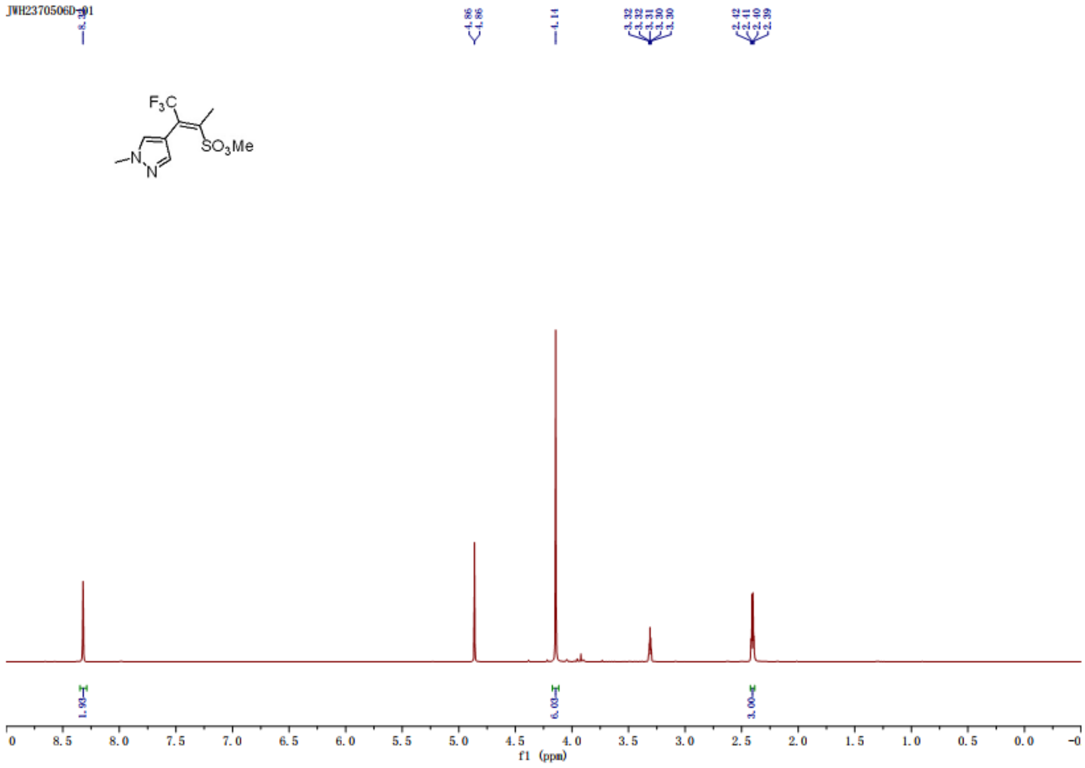

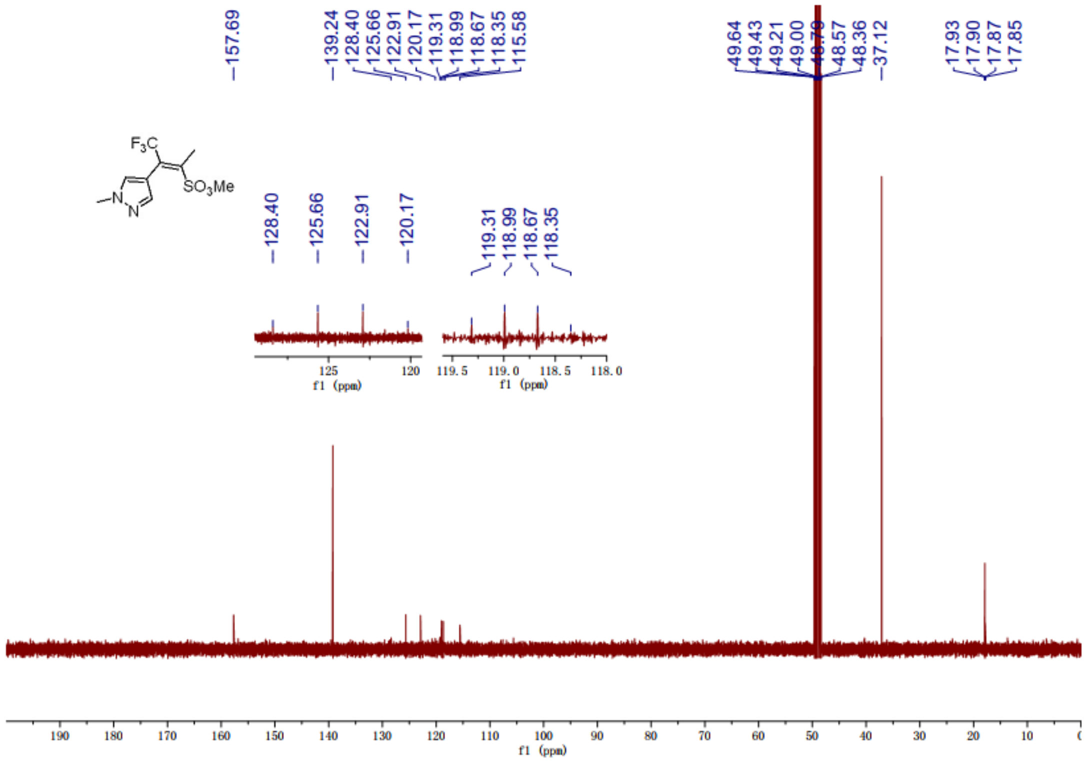
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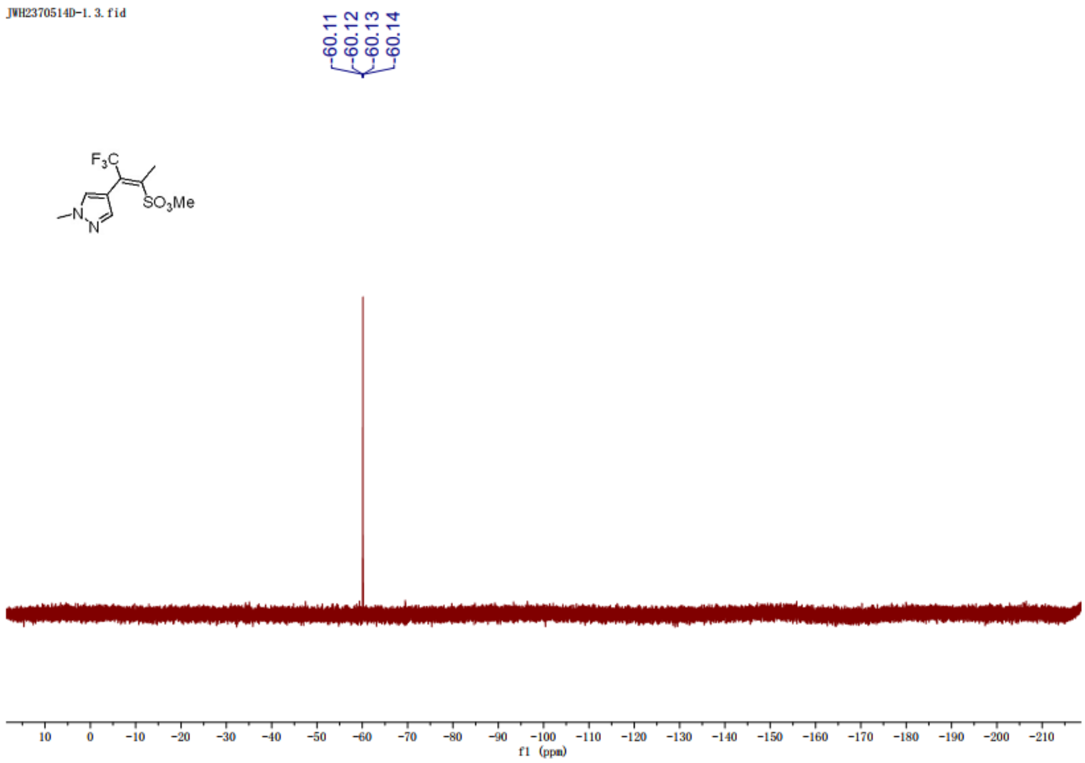
120.17
119.31
118.99
118.67
118.35
115.58
49.64
49.43
49.21
49.00
48.57
48.36
37.12
17.93
17.90
17.87
17.85
F3C
SO3Me
N
f1 (ppm)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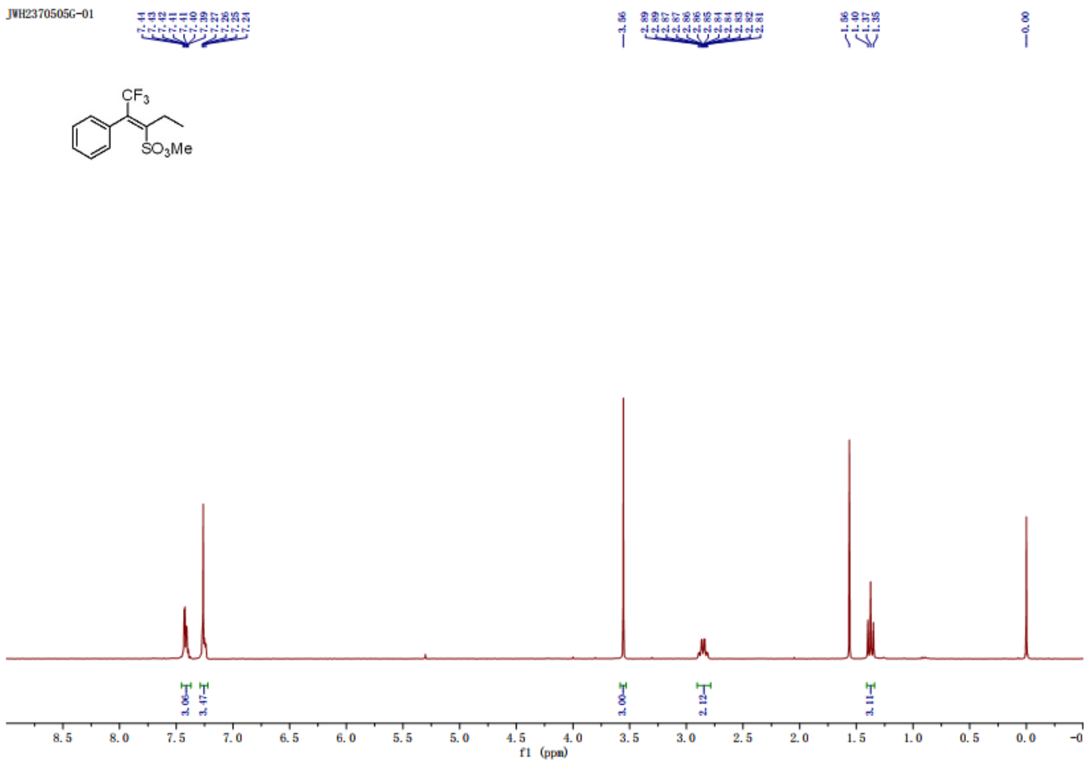
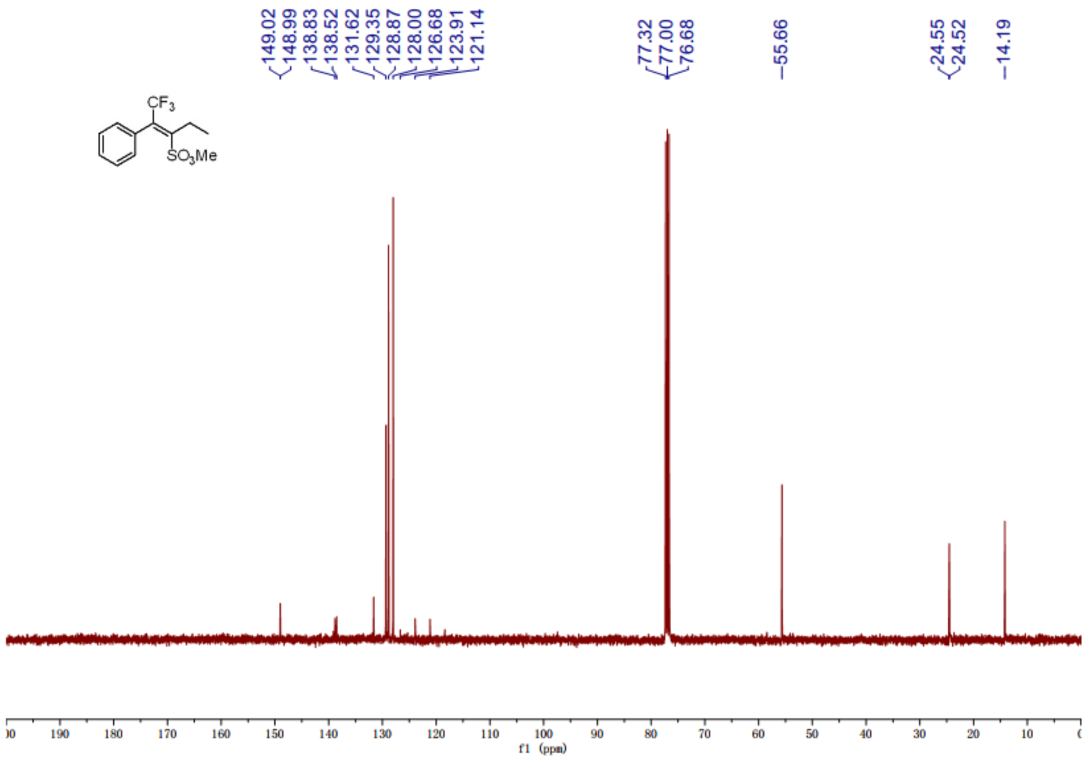
F3C
SO3Me
N
f1 (ppm)


JWH2370505G-01
CF3
SO3Me
f1 (ppm)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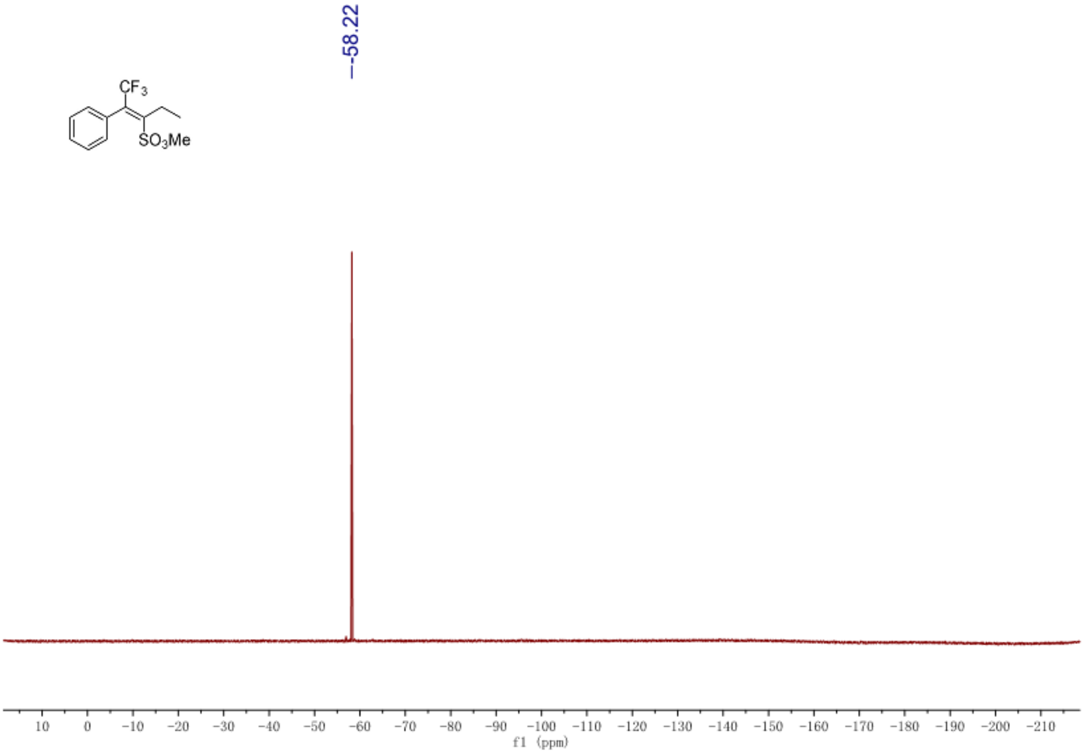
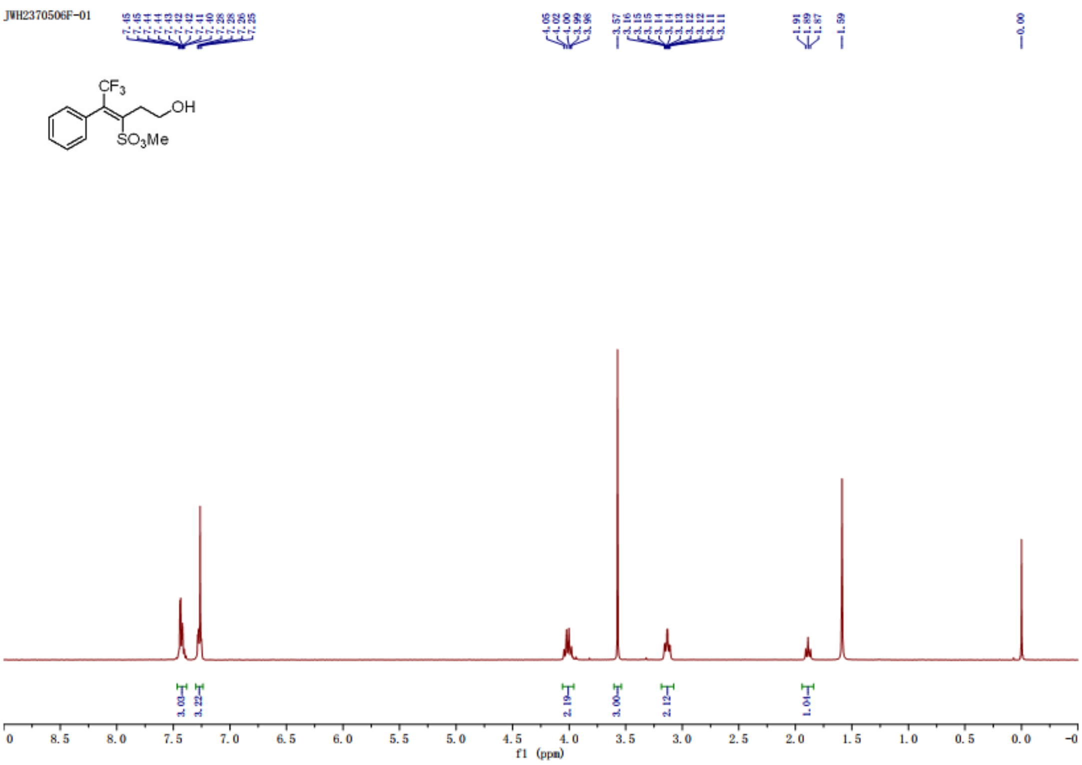
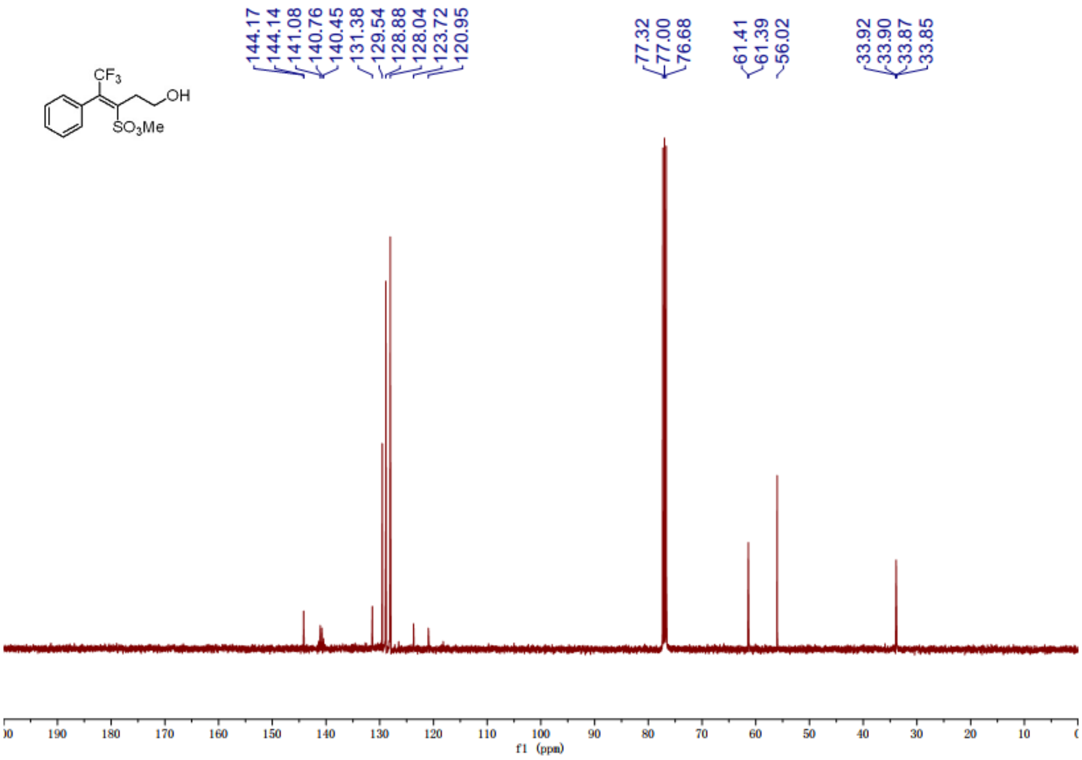
129.35
128.87
128.00
126.68
123.91
121.14
77.32
77.00
76.68
55.66
24.55
24.52
14.19
CF3
SO3Me
f1 (ppm)



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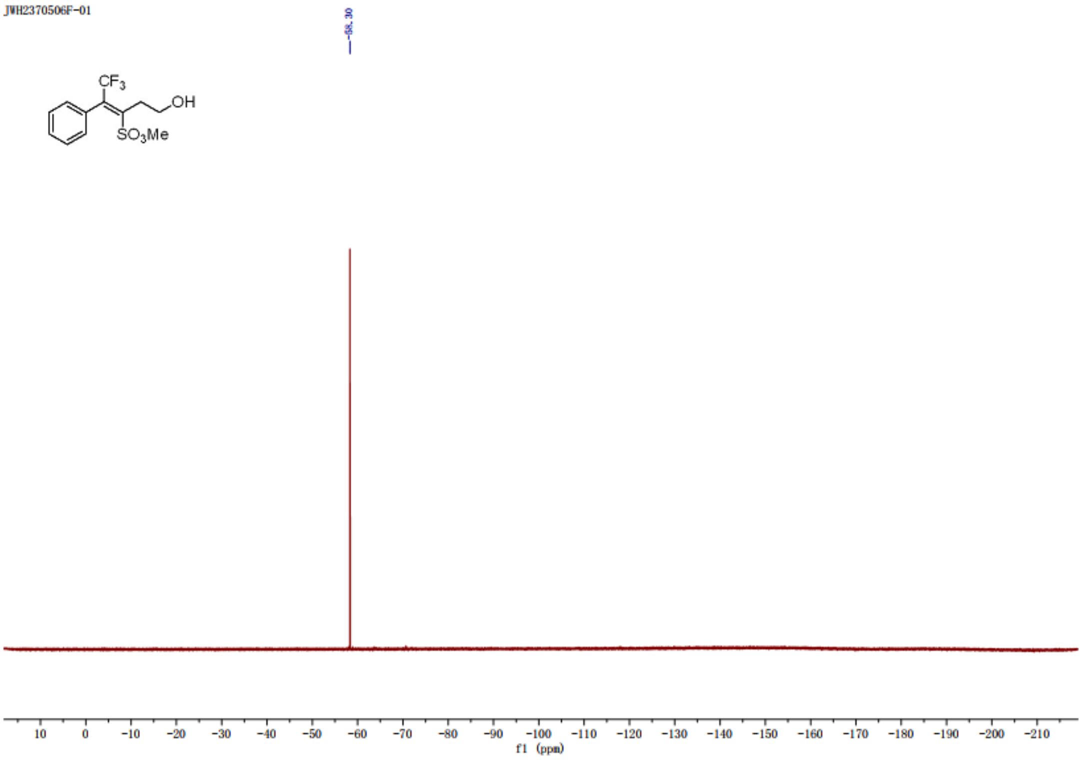
144.14
141.08
140.76
140.45
131.38
129.54
128.88
128.04
123.72
120.95
77.32
77.00
76.68
61.41
61.39
56.02
33.92
33.90
33.87
33.85
CF3
OH
SO3Me
f1 (ppm)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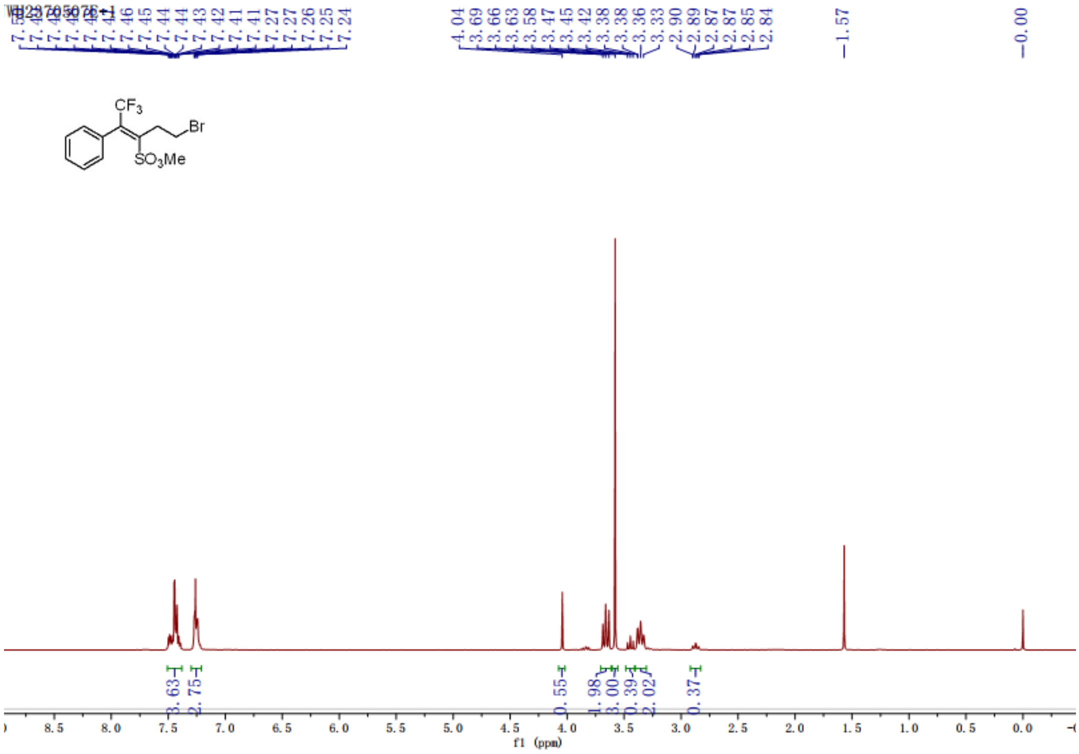
SO3Me
f1 (ppm)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7.45
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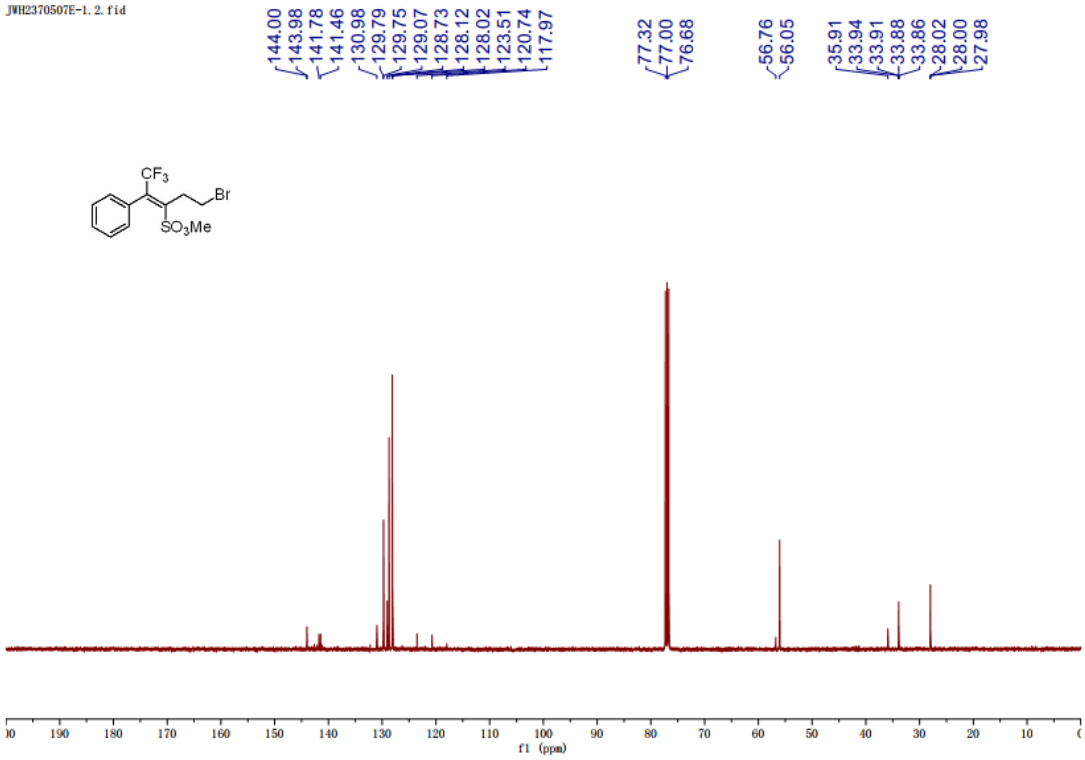
7.44
7.43
7.42
7.41
7.41
7.27
7.26
7.25
7.24
4.04
3.69
3.66
3.63
3.58
3.47
3.45
3.42
3.38
3.38
3.36
3.33
2.90
2.89
2.87
2.87
2.85
2.84
1.57
0.00
CF3
Br
SO3Me
3.63
2.75
0.55
1.98
3.00
0.39
2.02
0.37
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.75
129.07
128.73
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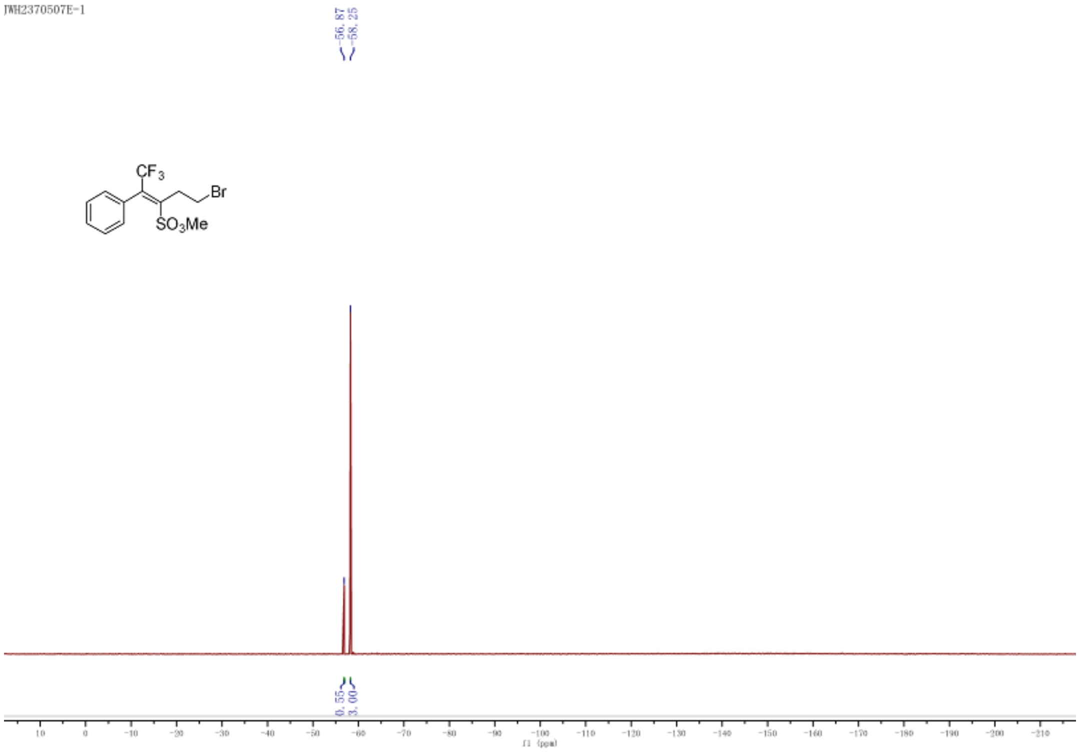
128.02
123.51
120.74
117.97
77.32
77.00
76.68
56.76
56.05
35.91
33.94
33.91
33.88
33.86
28.02
28.00
27.98
CF3
Br
SO3Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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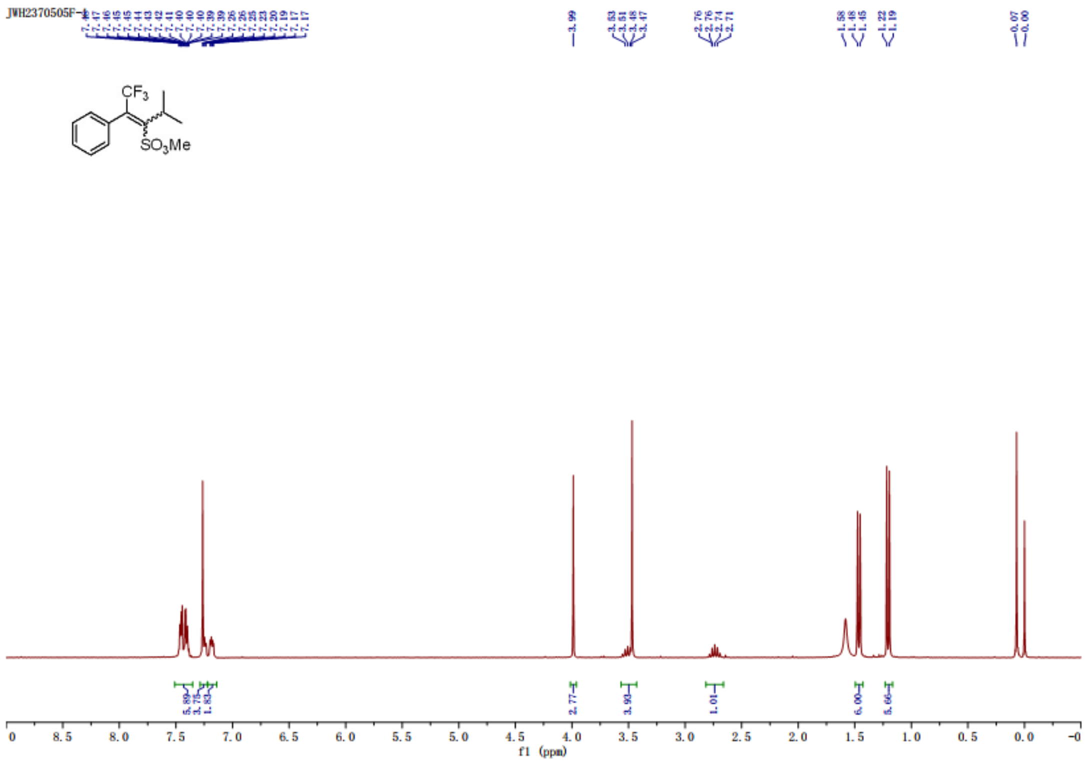
CF3
Br
SO3Me
0.55
3.00
f1 (ppm)


JWH2370505F-1
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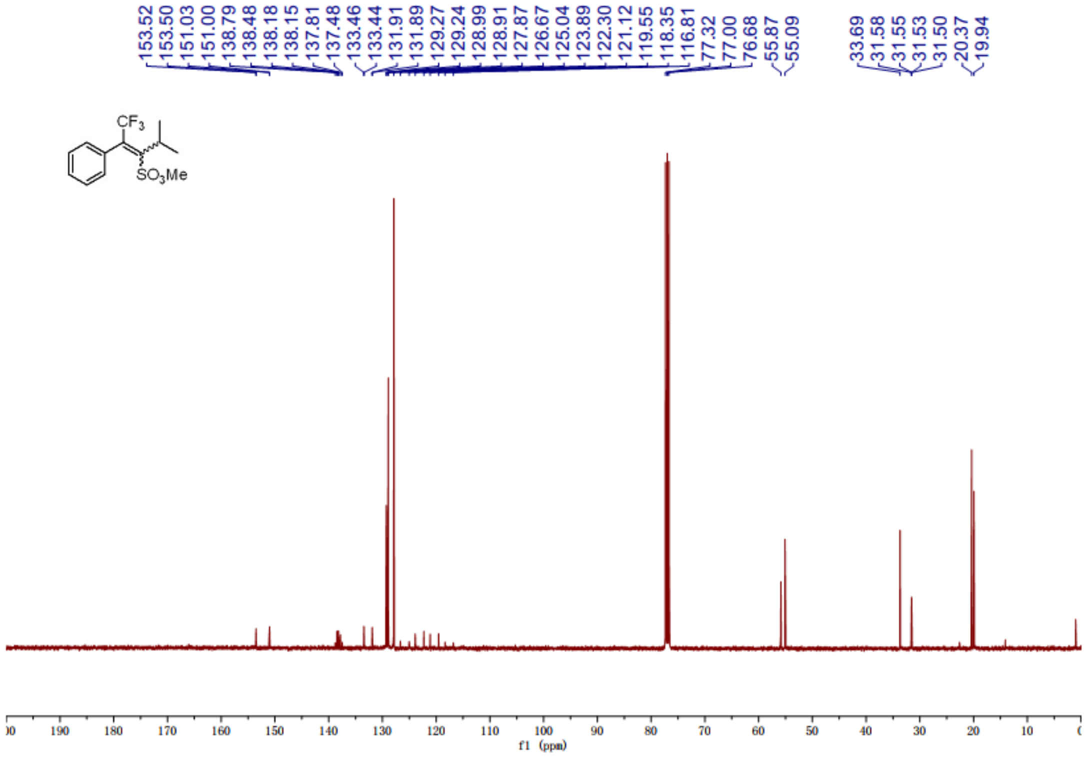
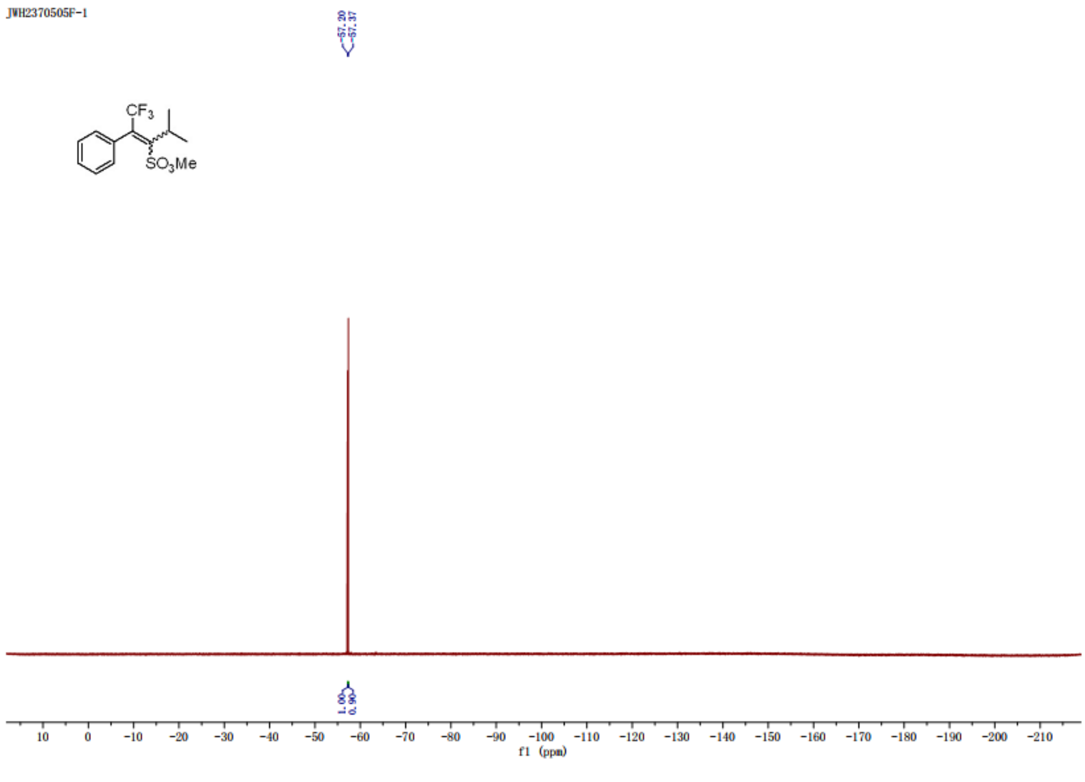
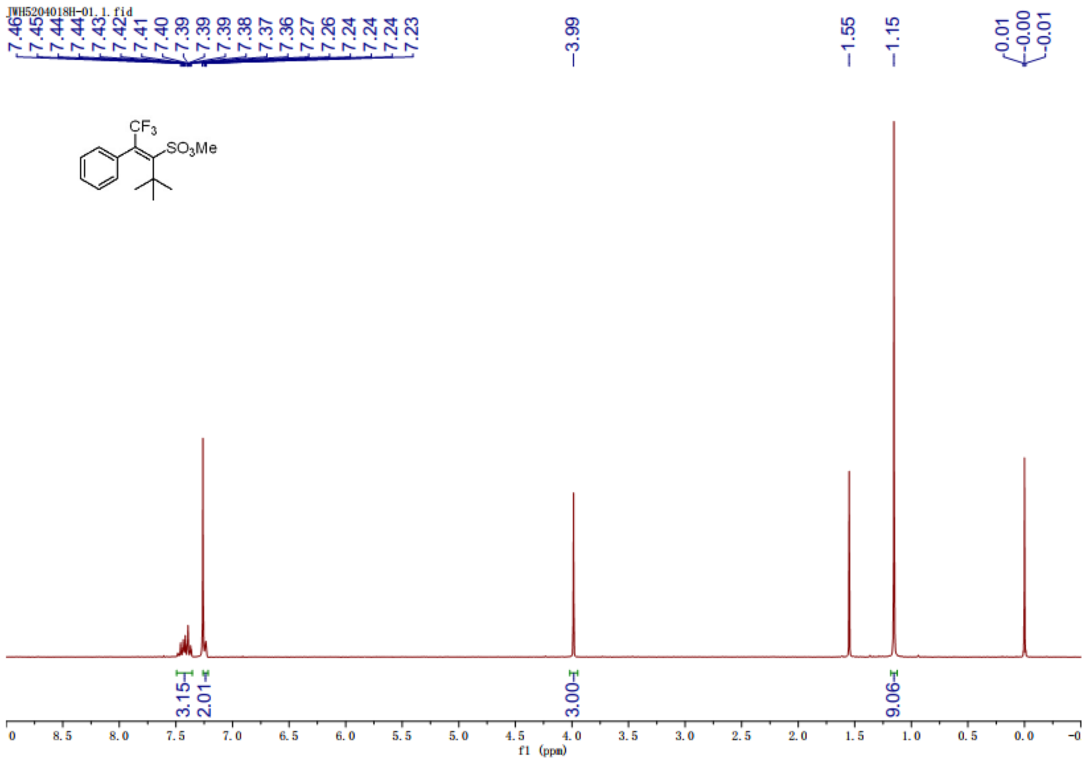
3.53
3.51
3.48
3.47
2.76
2.76
2.74
2.71
1.58
1.48
1.45
1.22
1.19
0.07
0.00
CF3
SO3Me
5.89
1.75
1.83
2.77
3.93
1.01
6.00
5.66
f1 (ppm)



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7.44
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7.41
7.40
7.39
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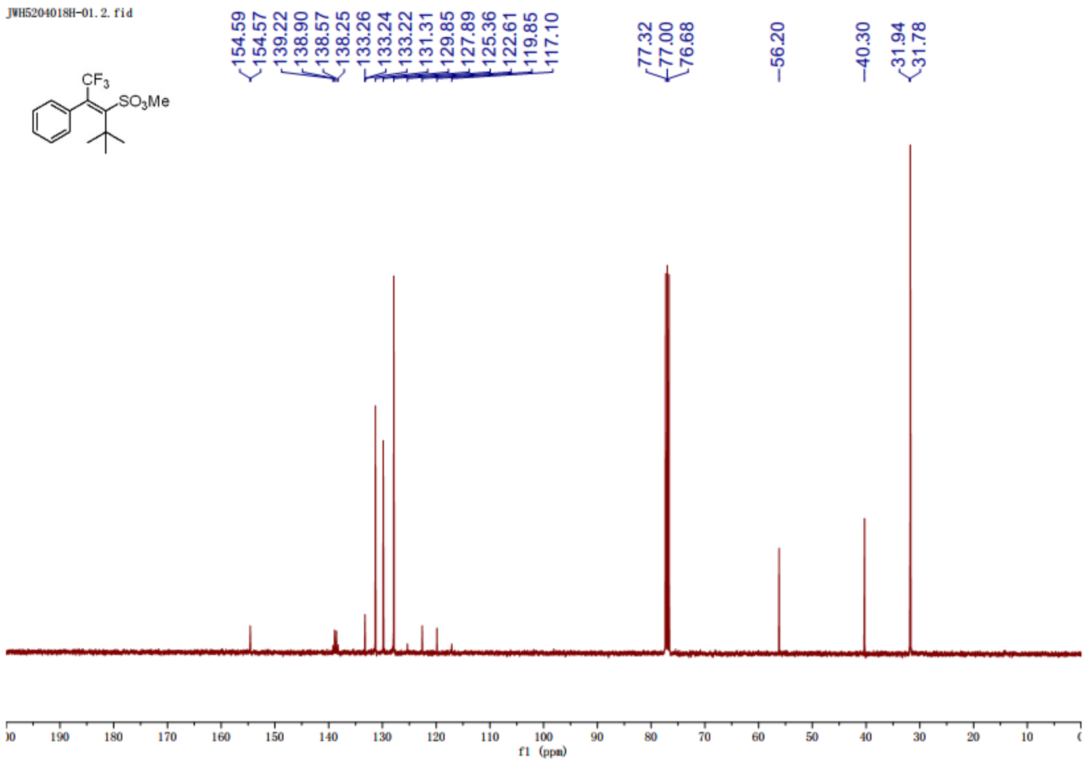
7.38
7.37
7.36
7.27
7.26
7.24
7.24
7.24
7.23
3.99
1.55
1.15
0.01
-0.00
-0.01
CF3
SO3Me
3.15
2.01
3.00
9.06
f1 (ppm)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139.22
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133.26
133.24
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131.31
129.85
127.89
125.36
122.61
119.85
117.10
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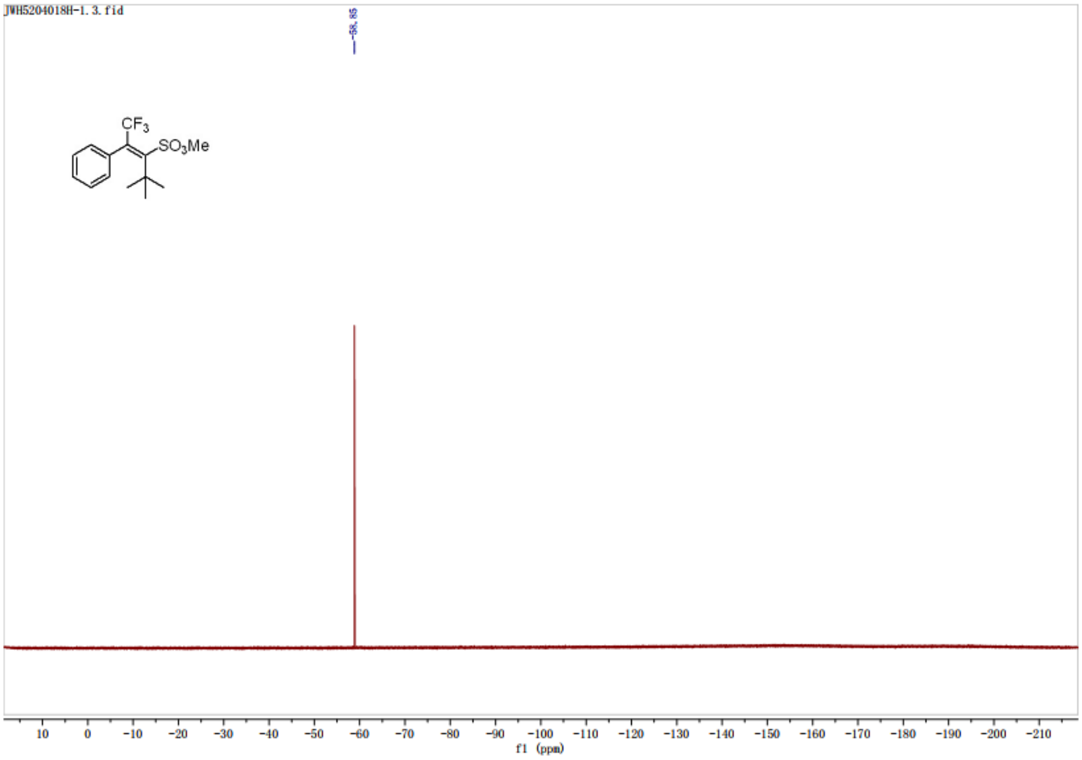
77.00
76.68
56.20
40.30
31.94
31.78
CF3
SO3Me
f1 (ppm)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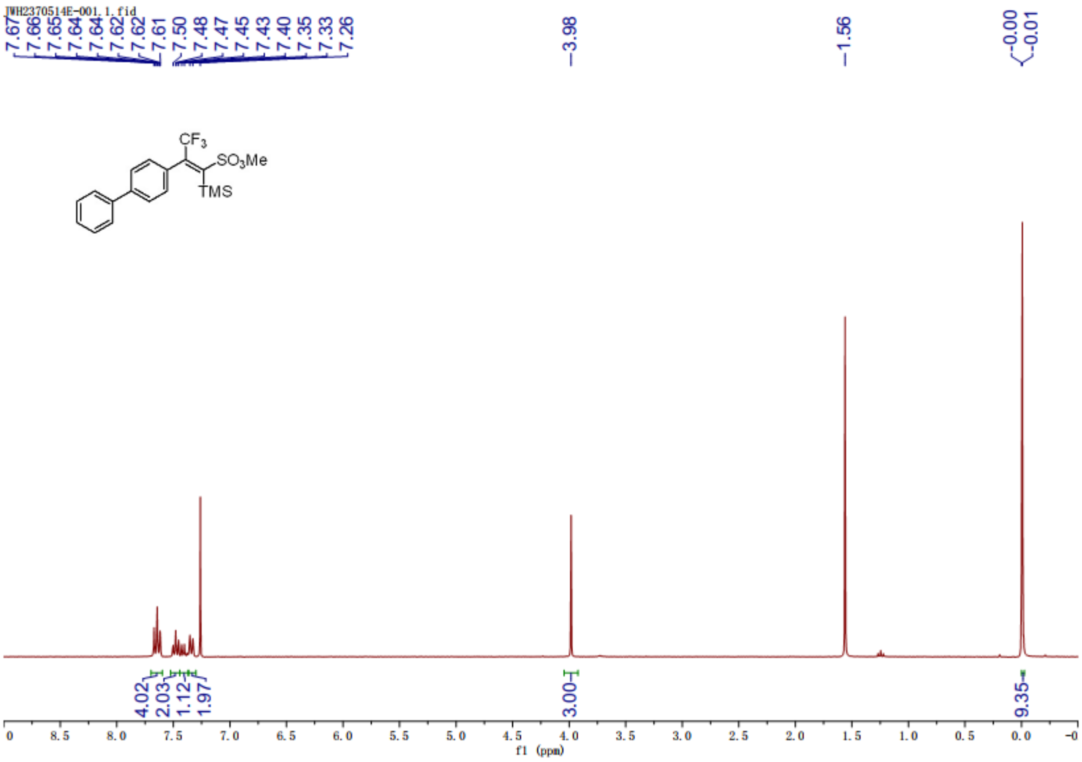
SO3Me
f1 (ppm)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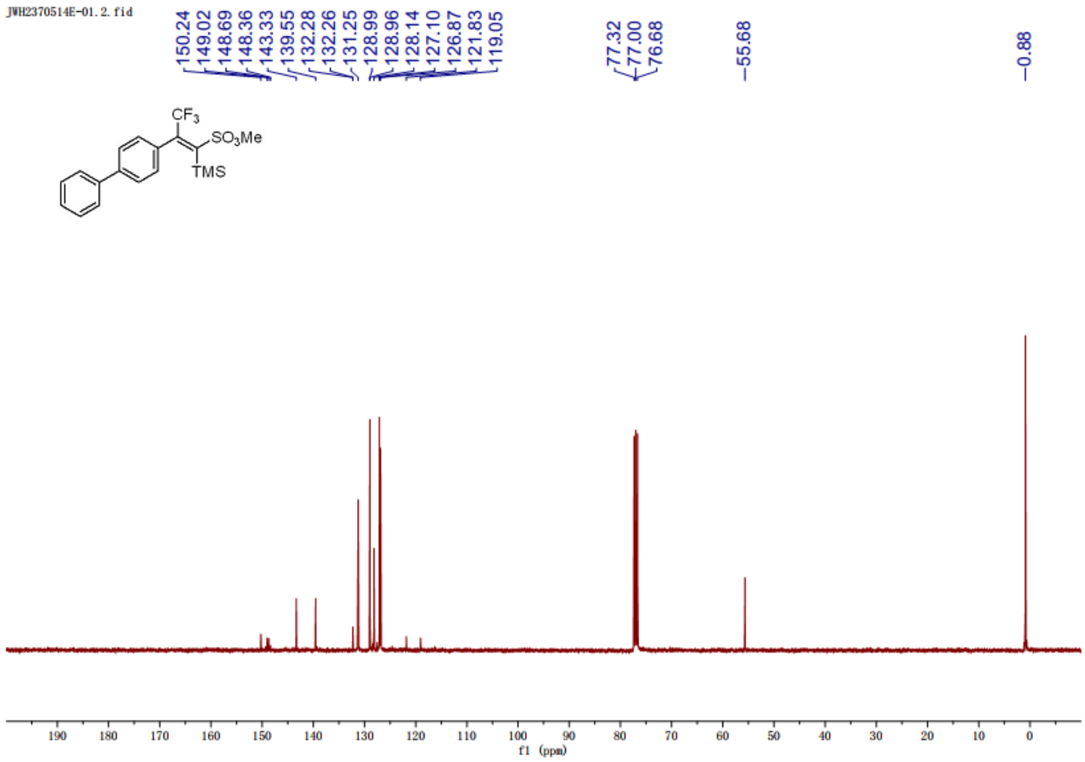
7.66
7.65
7.64
7.64
7.62
7.62
7.61
7.50
7.48
7.47
7.45
7.43
7.40
7.35
7.33
7.26
3.98
1.56
-0.00
-0.01
CF3
SO3Me
TMS
4.02
2.03
1.12
1.97
3.00
9.35
f1 (ppm)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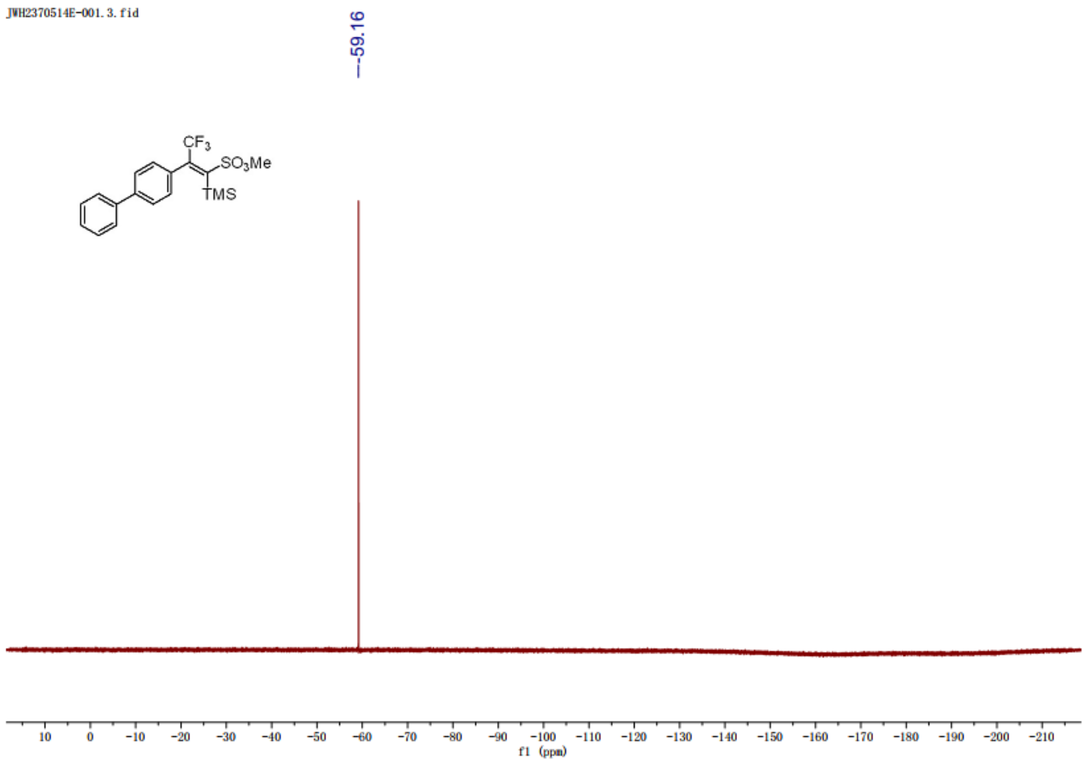
148.69
148.36
143.33
139.55
132.28
132.26
131.25
128.99
128.96
128.14
127.10
126.87
121.83
119.05
77.32
77.00
76.68
55.68
0.88
CF3
SO3Me
TMS
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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CF3
SO3Me
TMS
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0
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-30
-40
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-60
-70
-80
-90
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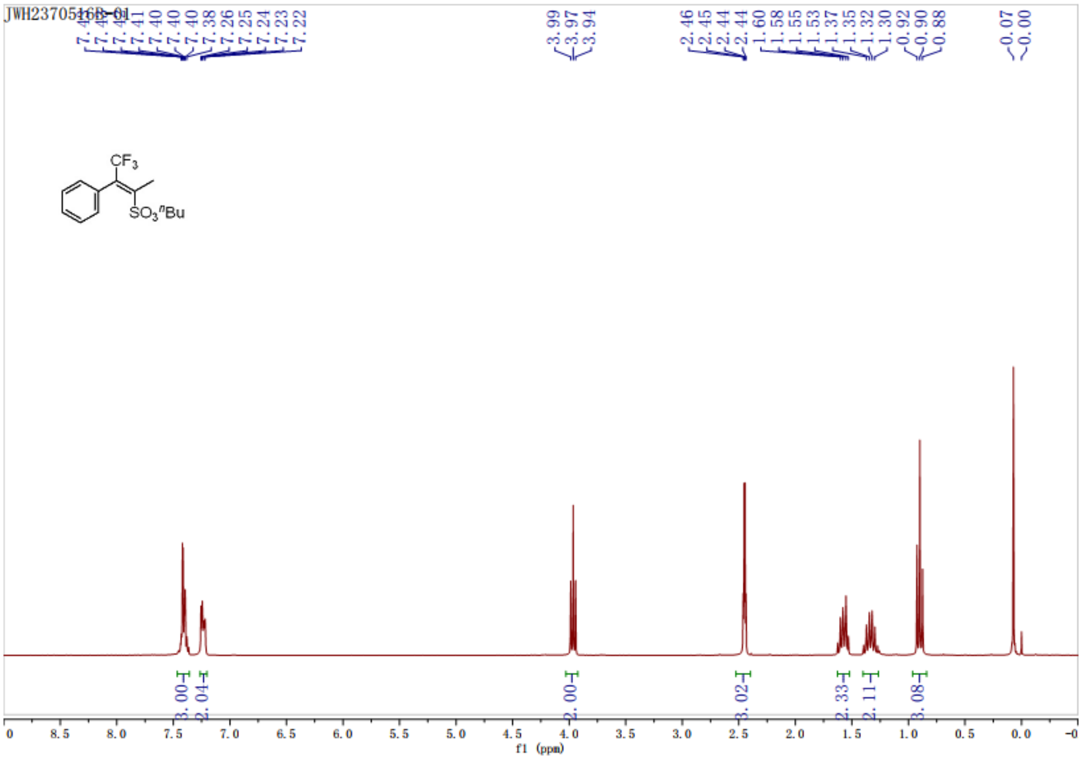
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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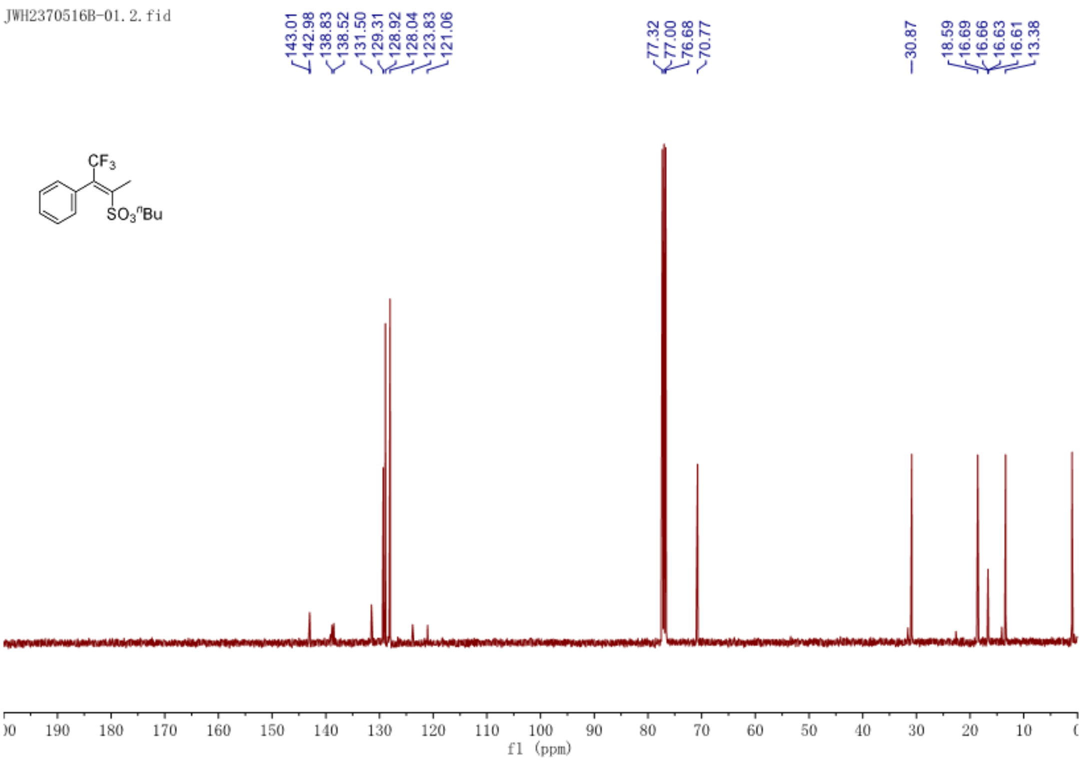
7.38
7.26
7.25
7.24
7.23
7.22
3.99
3.97
3.94
2.46
2.45
2.44
2.44
1.60
1.58
1.55
1.53
1.37
1.35
1.32
1.30
0.92
0.90
0.88
0.07
0.00
CF3
SO3nBu
3.00
2.04
2.00
3.02
2.33
2.11
3.08
f1 (ppm)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128.04
123.83
121.06
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77.00
76.68
70.77
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16.63
16.61
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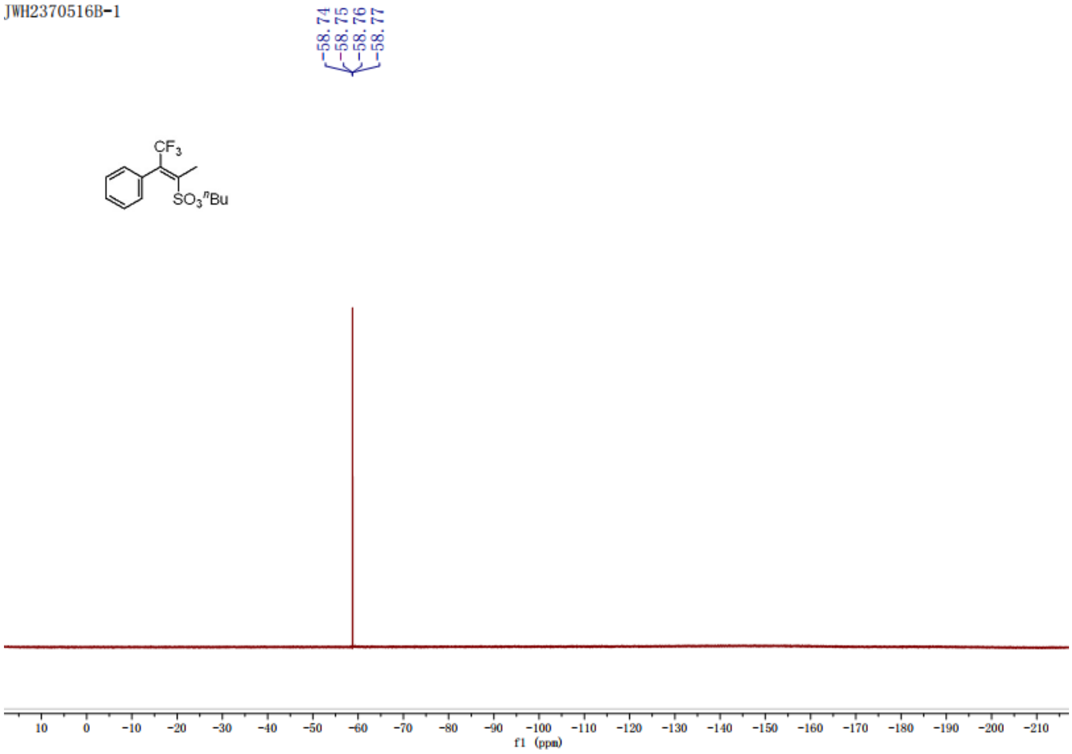
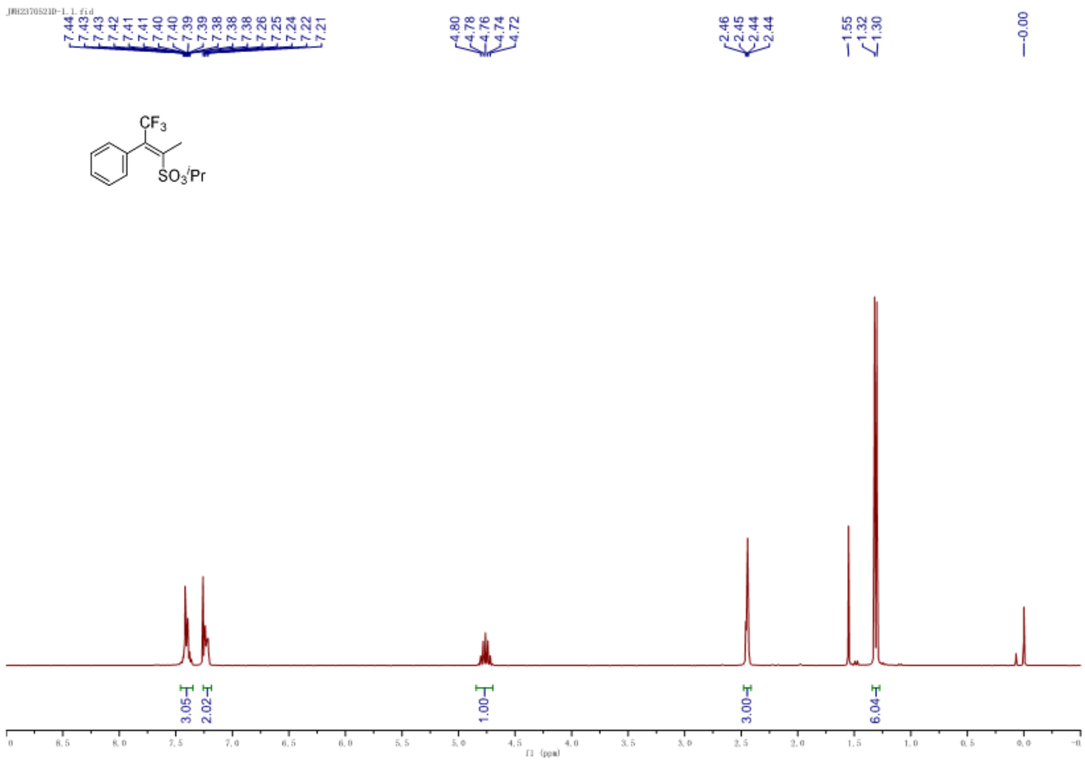
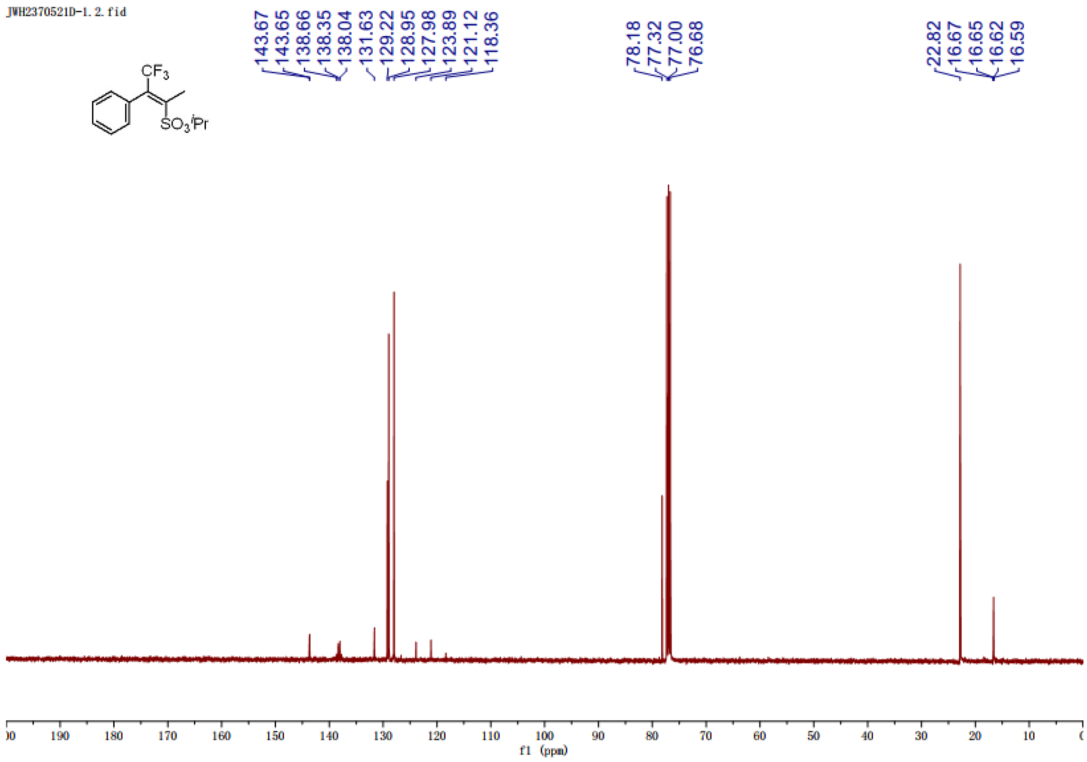
CF3
SO3nBu
f1 (ppm)

JWH2370516B-1



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129.22
128.95
127.98
123.89
121.12
118.36
78.18
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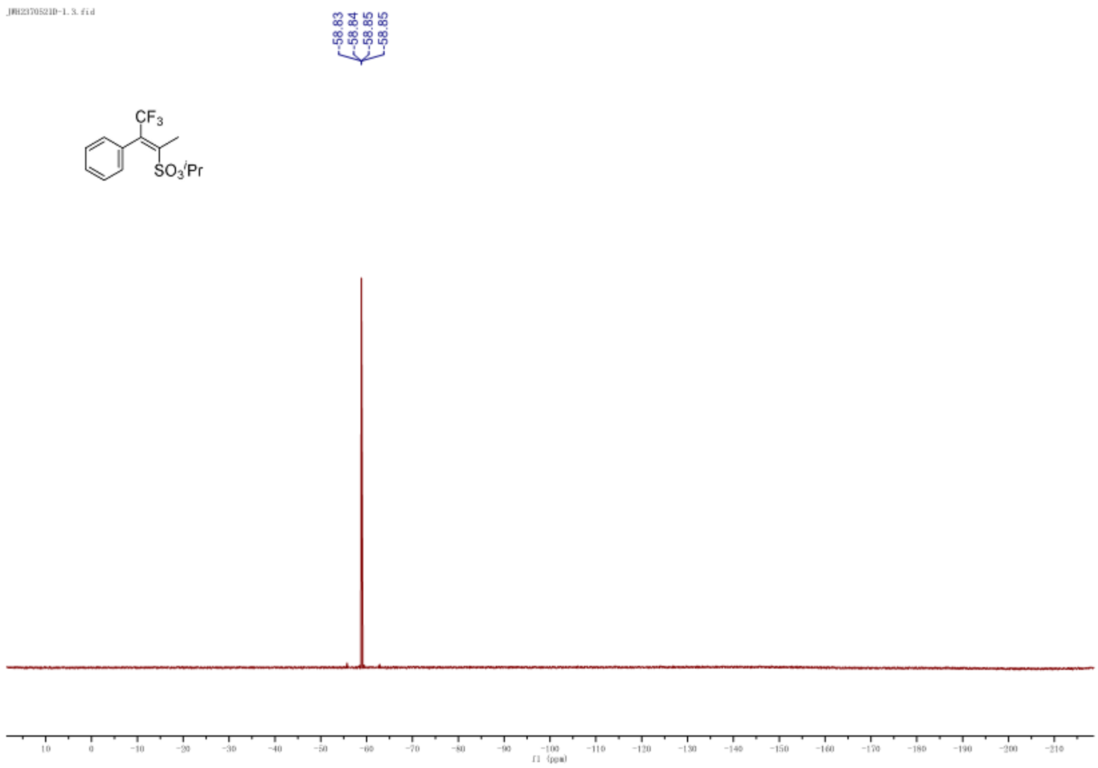
76.68
22.82
16.67
16.65
16.62
16.59
CF3
SO3iPr
f1 (ppm)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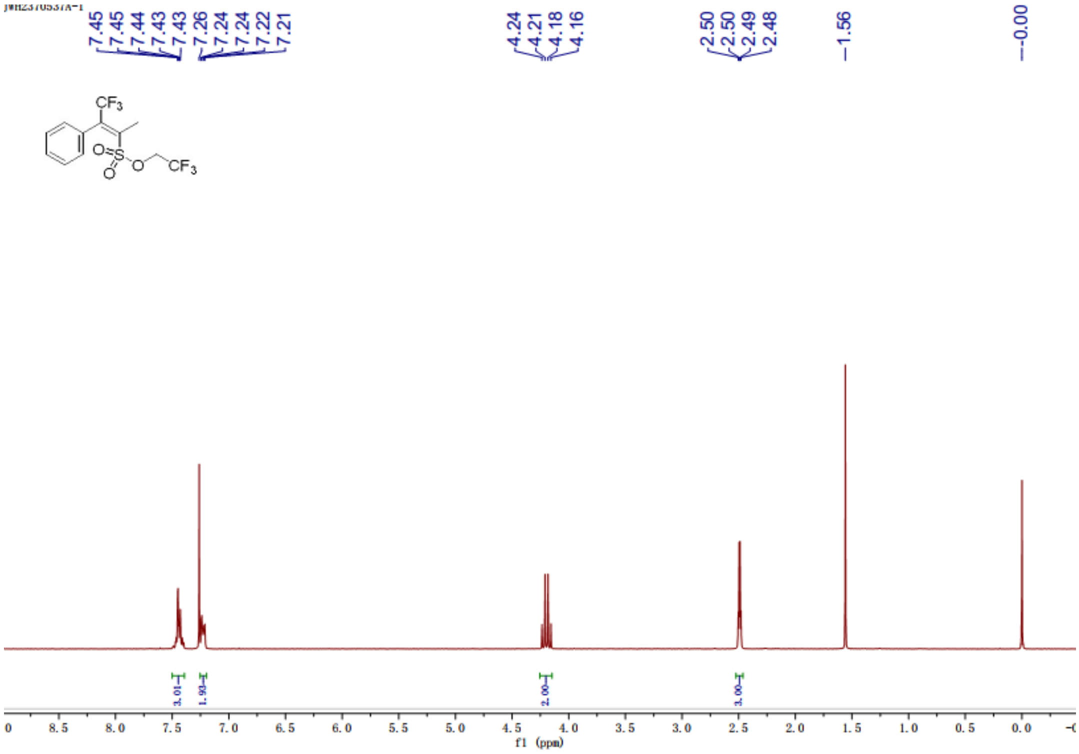
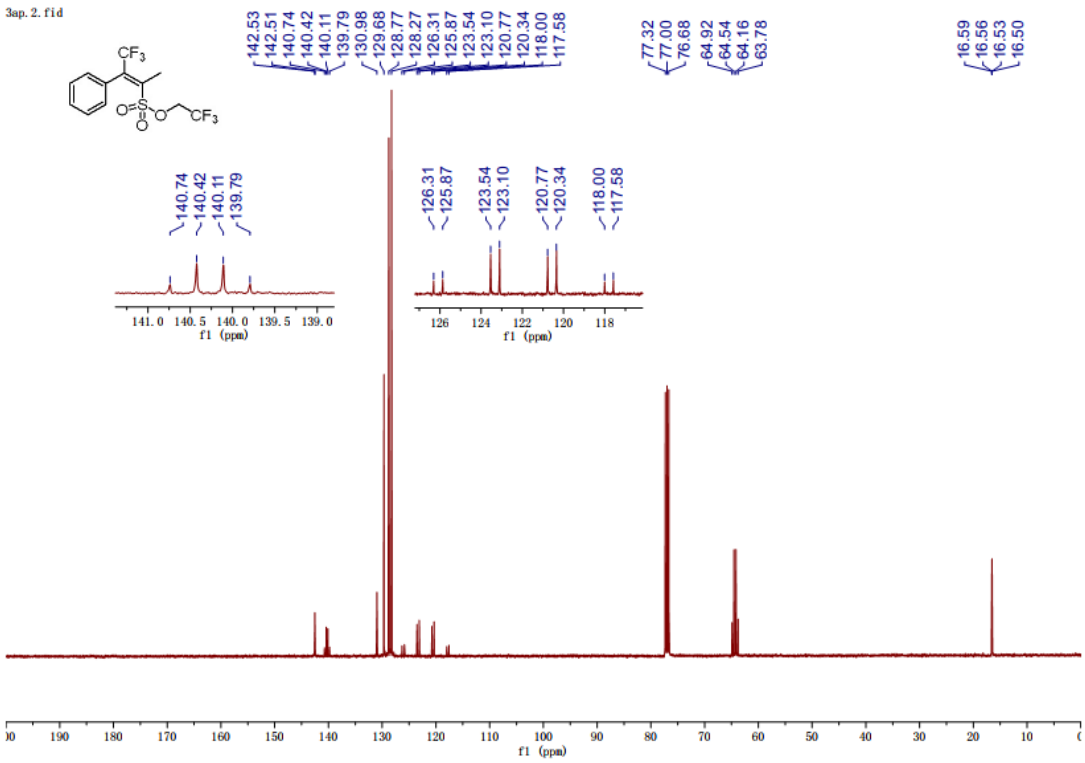
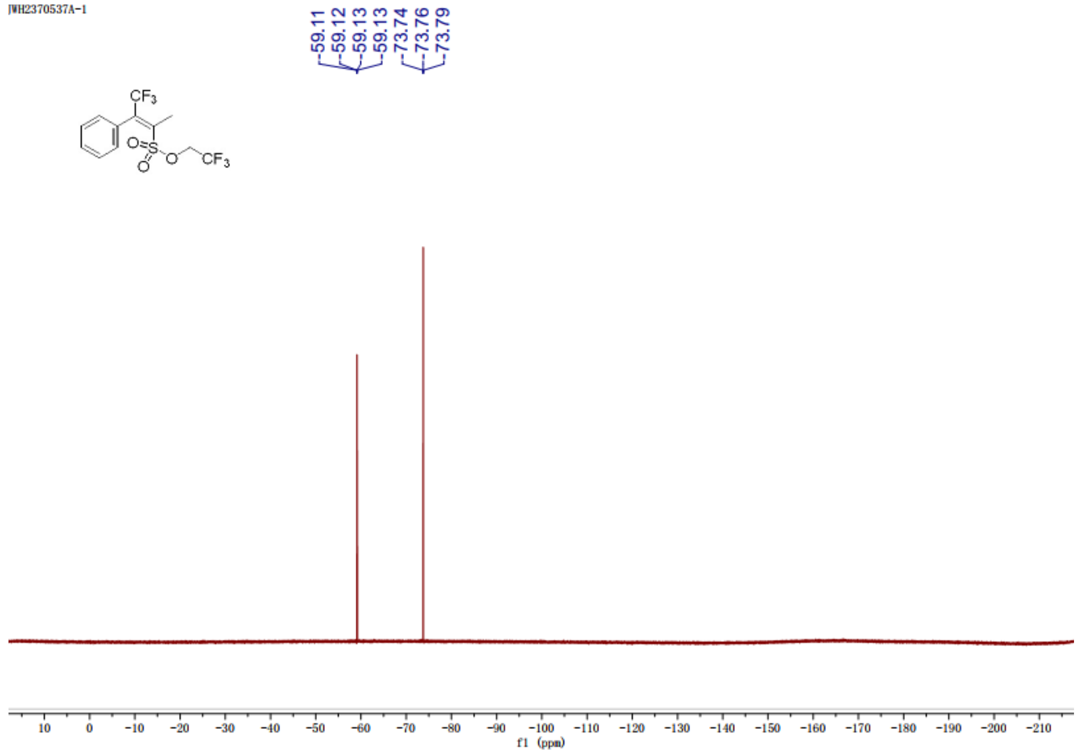
-58.85
CF3
SO3iPr
f1 (ppm)



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-73.74
-73.76
-73.79
CF3
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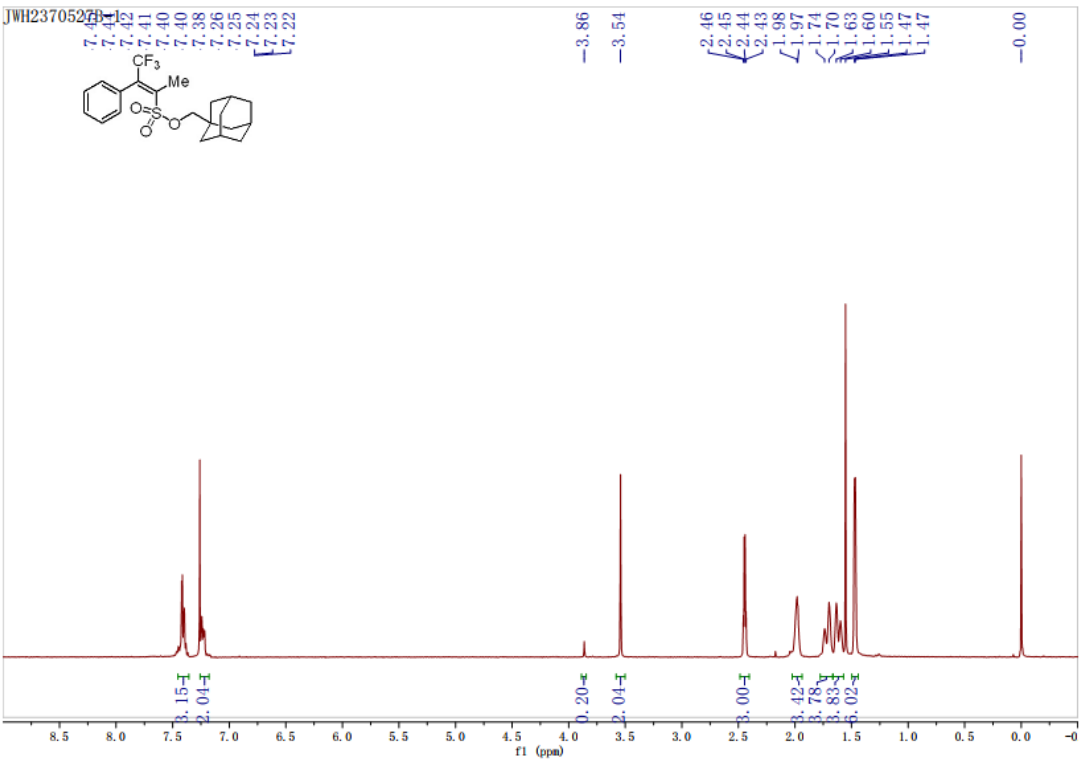
O
O
CF3
f1 (ppm)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Me
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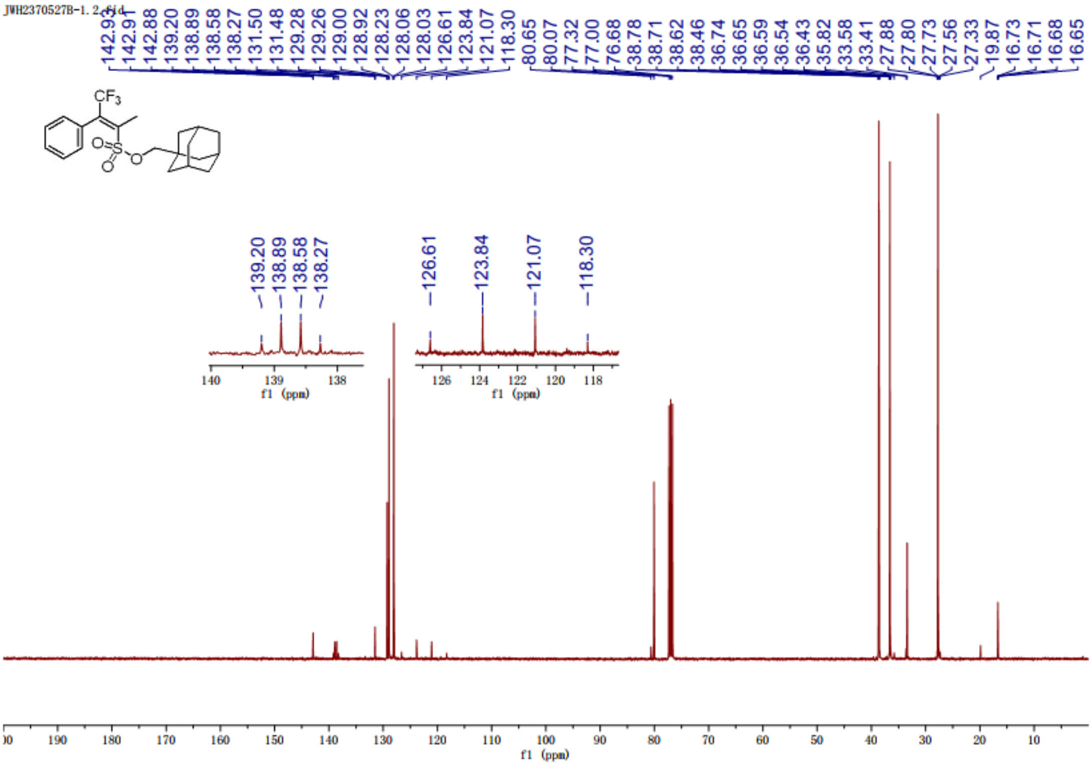
S
O
O
f1 (ppm)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129.00
128.92
128.23
128.06
128.03
126.61
123.84
121.07
118.30
80.65
80.07
77.32
77.00
76.68
38.78
38.71
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35.82
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33.41
27.88
27.80
27.73
27.56
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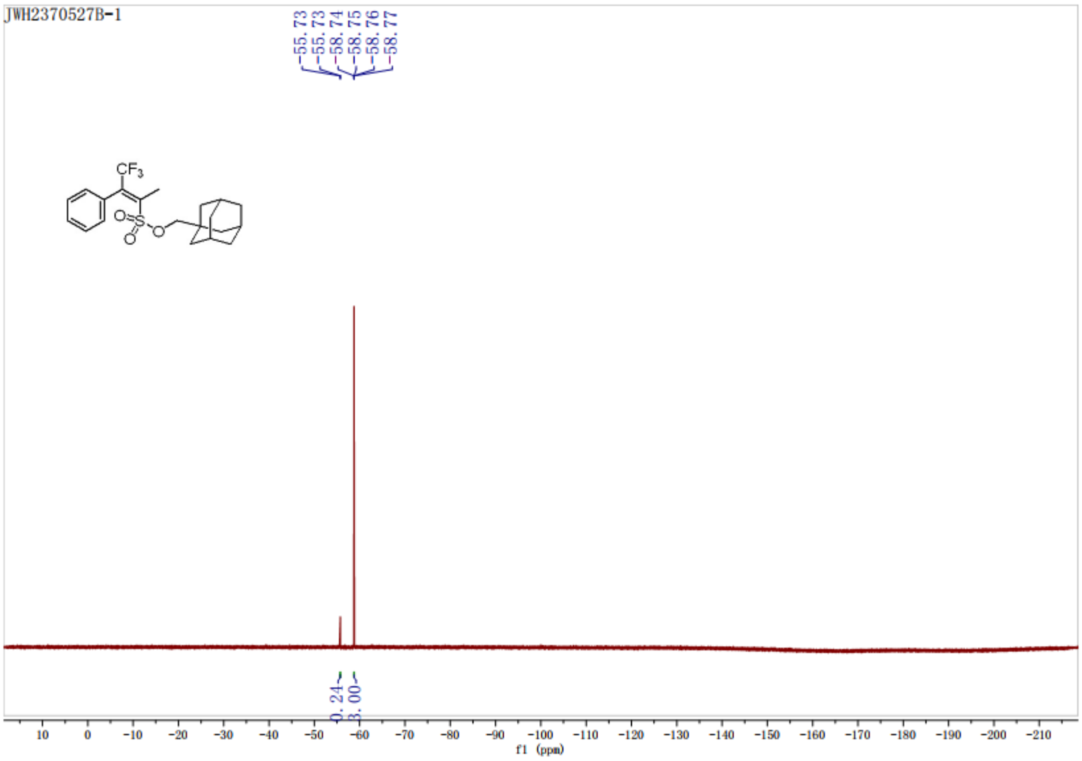
19.87
16.73
16.71
16.68
16.65
CF_3
O
S
O
O
f1 (ppm)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-55.73
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-58.76
-58.77
CF_3
O
S
O
O
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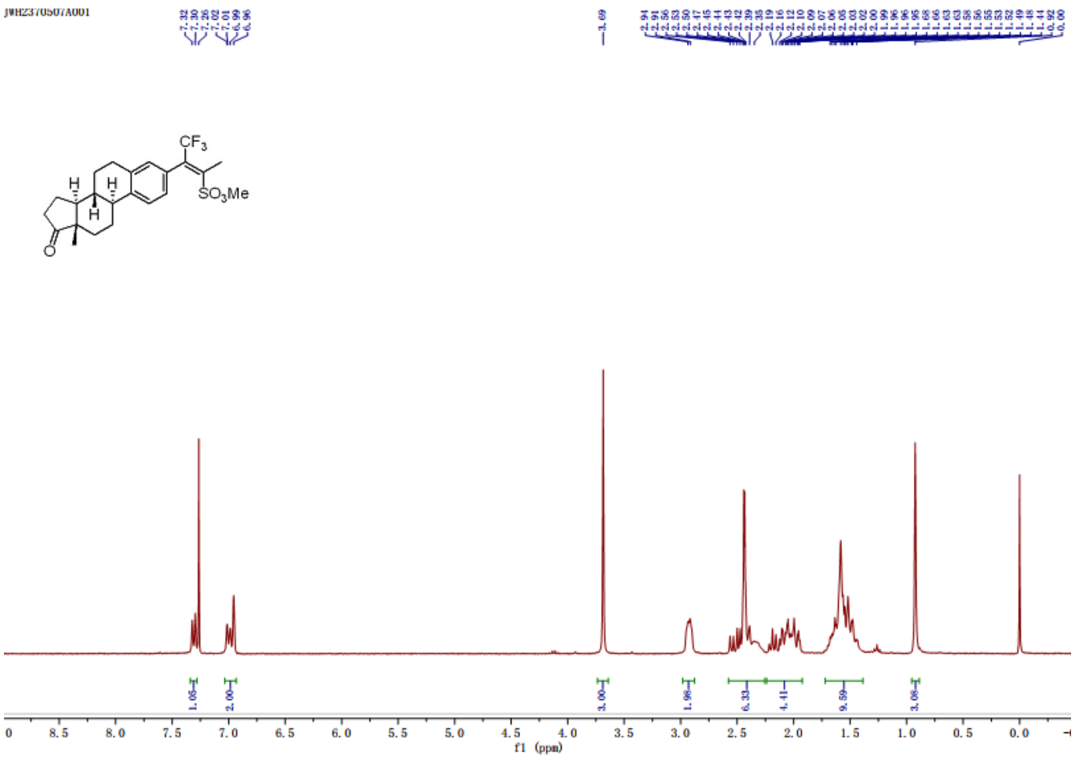
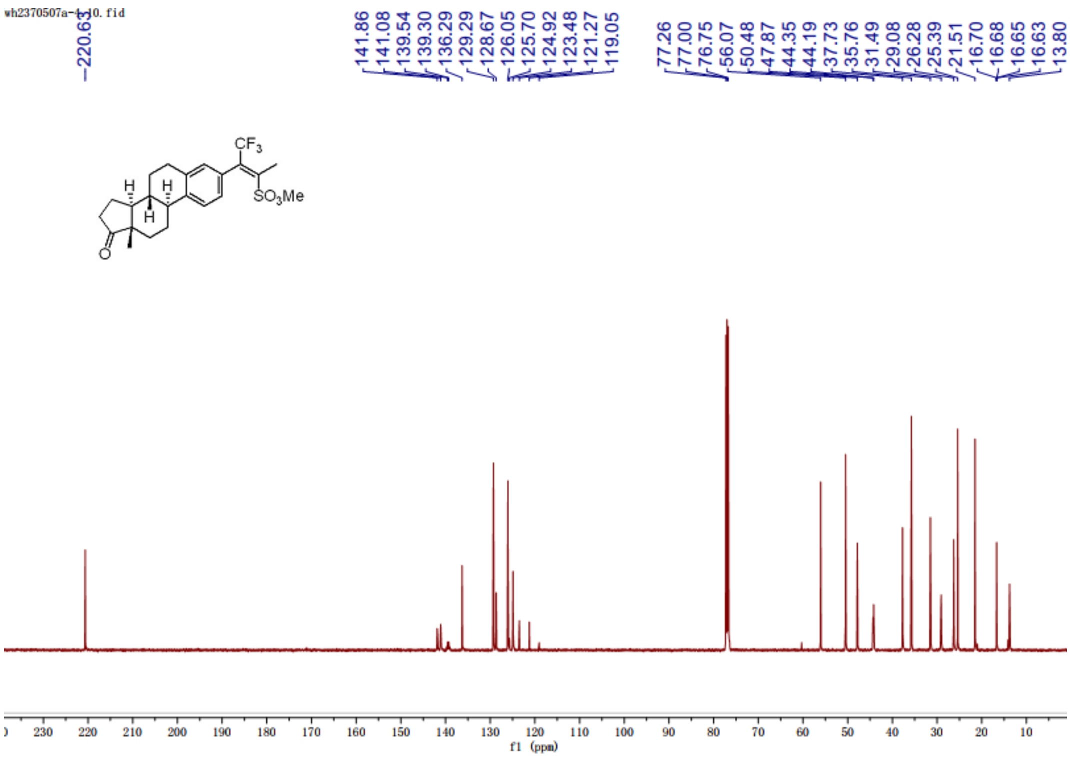
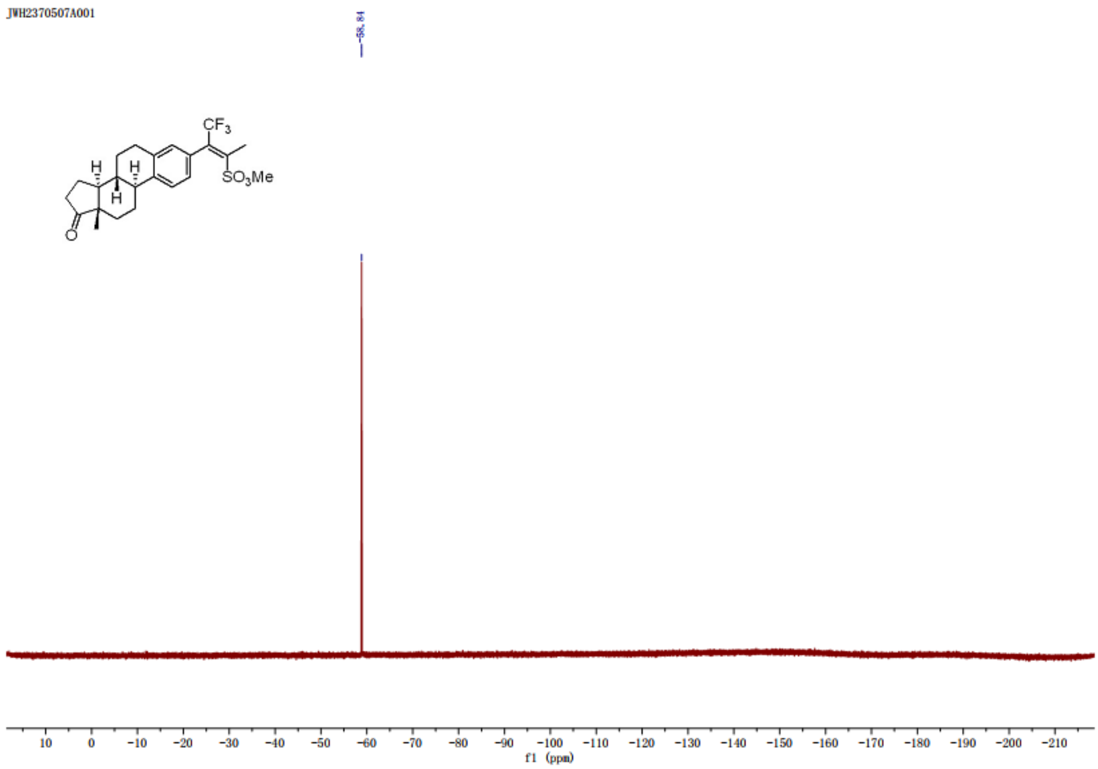
3.00
f1 (ppm)






JWH2370507A001
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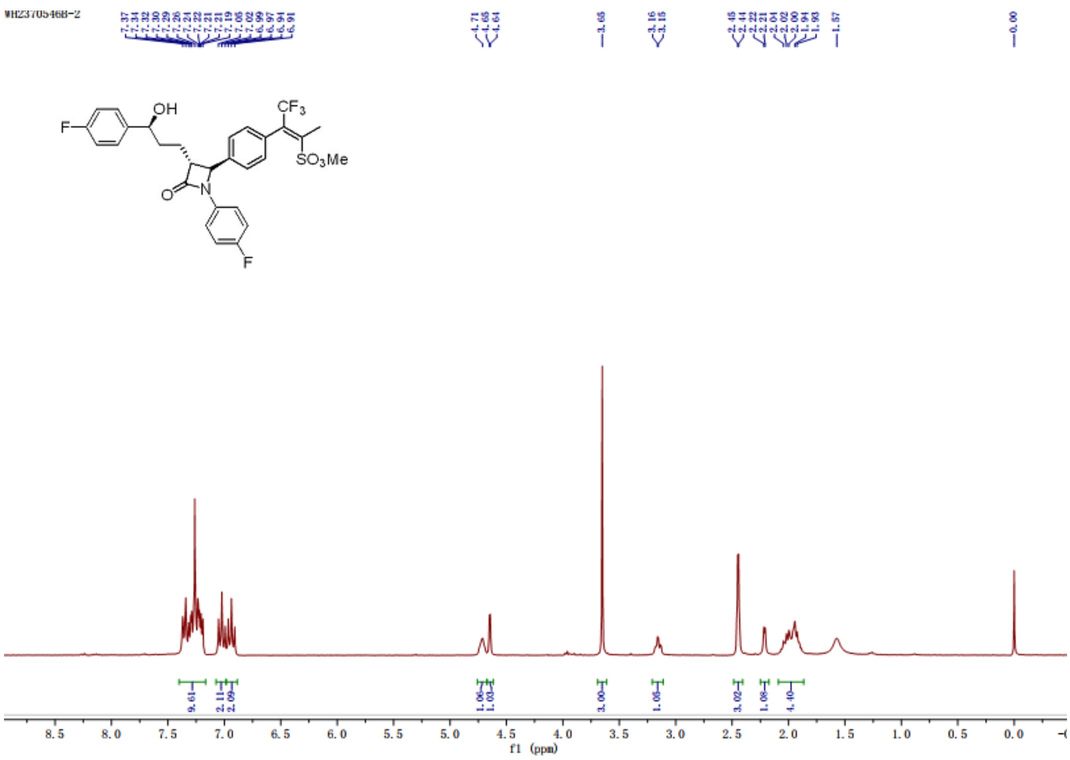
CF3
SO3Me
H
H
H
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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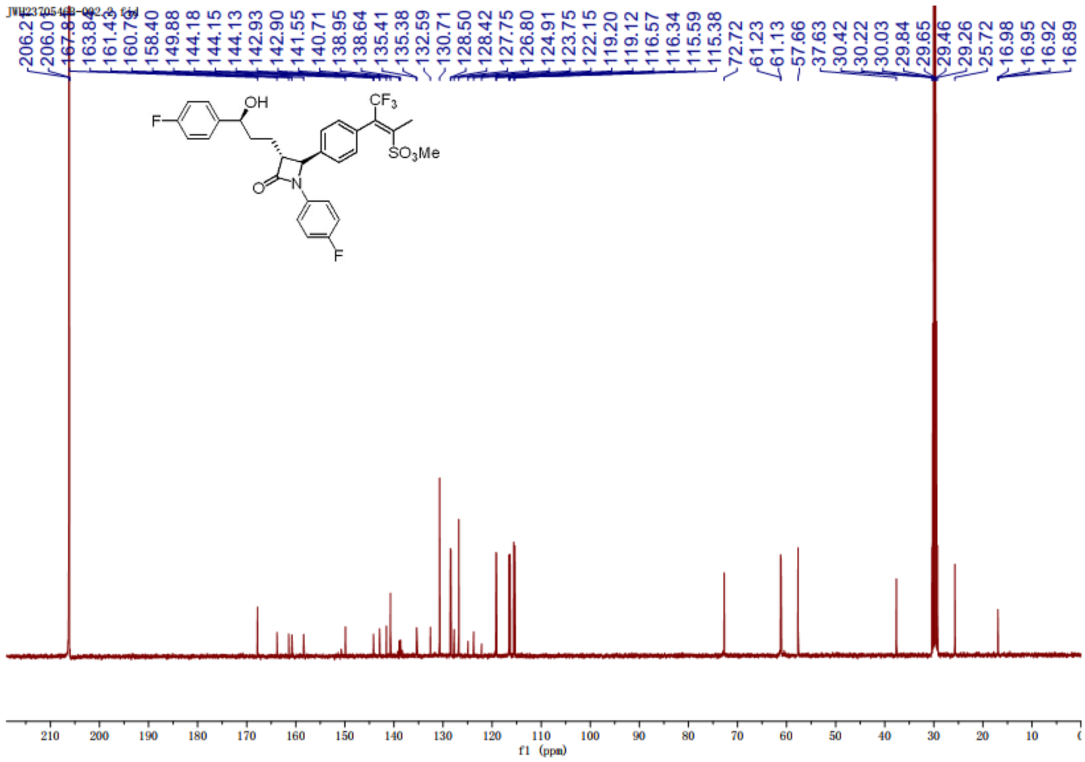
4.71 4.65 4.64
3.65
3.16 3.15
2.45 2.44 2.22 2.21 2.04 2.02 2.00 1.94 1.93
1.57
0.00
F
OH
CF3
SO3Me
O
N
F
9.61 2.11 2.09
1.06 1.03
3.00
1.05
3.02 1.08 4.40
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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142.93
142.90
141.55
140.71
138.95
138.64
135.41
135.38
132.59
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128.50
128.42
127.75
126.80
124.91
123.75
122.15
119.20
119.12
116.57
116.34
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115.38
72.72
61.23
61.13
57.66
37.63
30.42
30.22
30.03
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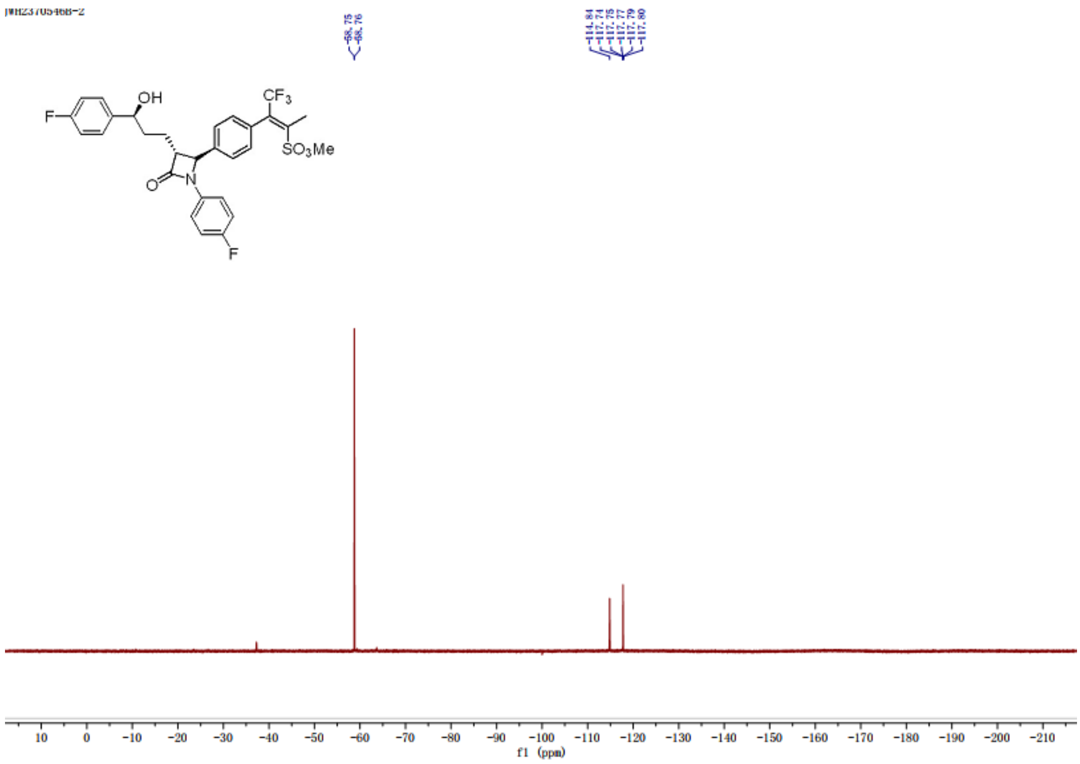
O
N
F
f1 (ppm)


JWH2370546B-2
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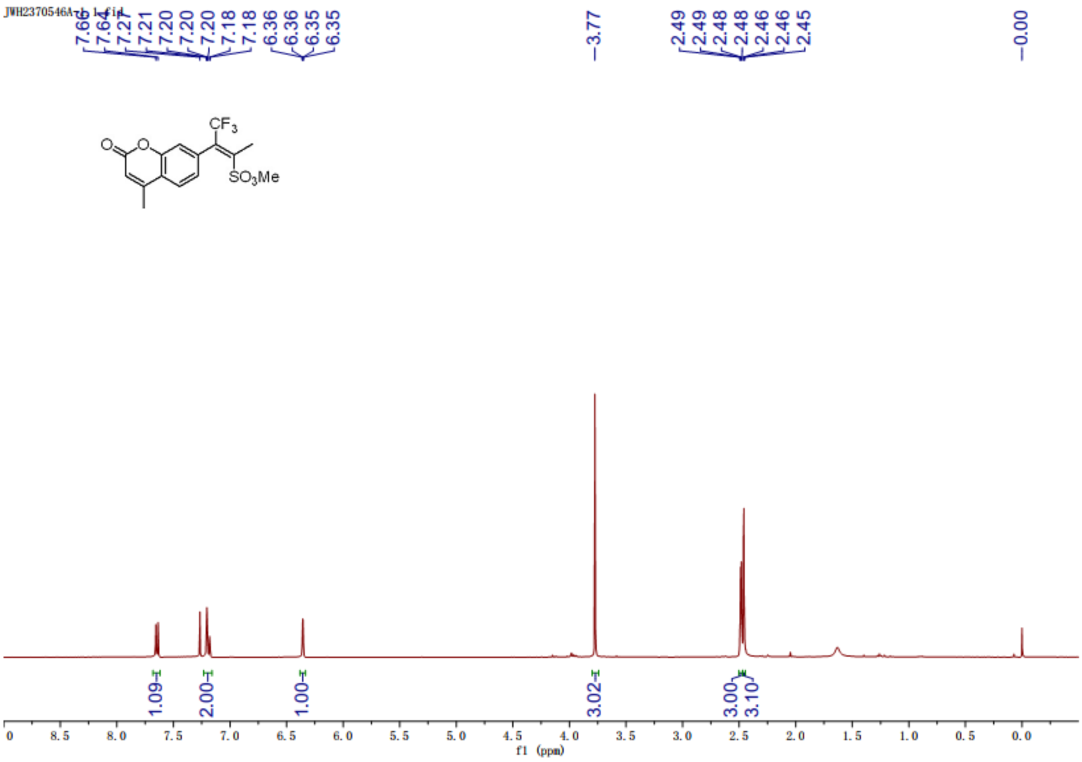
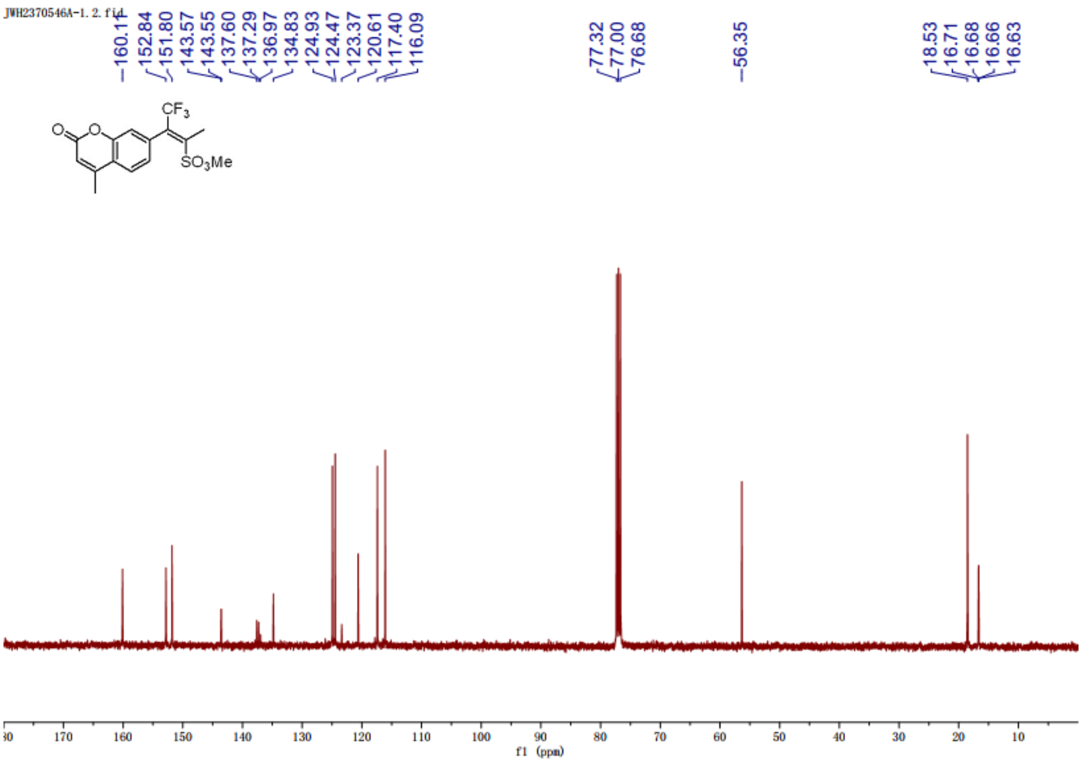
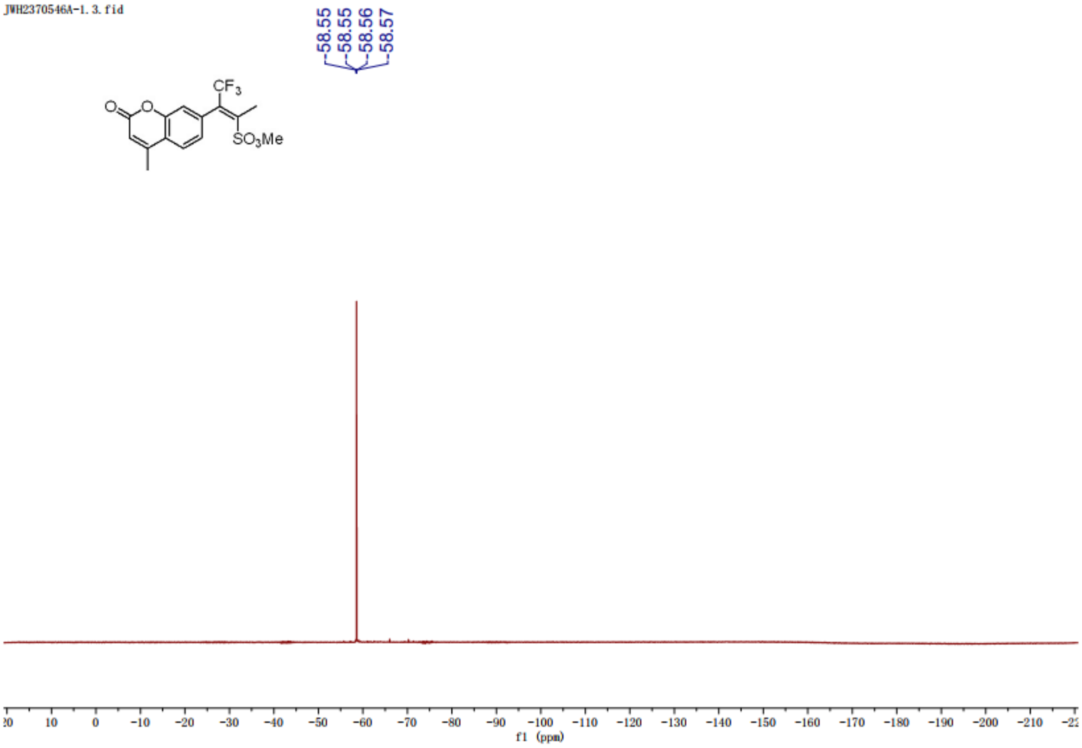
SO3Me
O
N
F
f1 (ppm)



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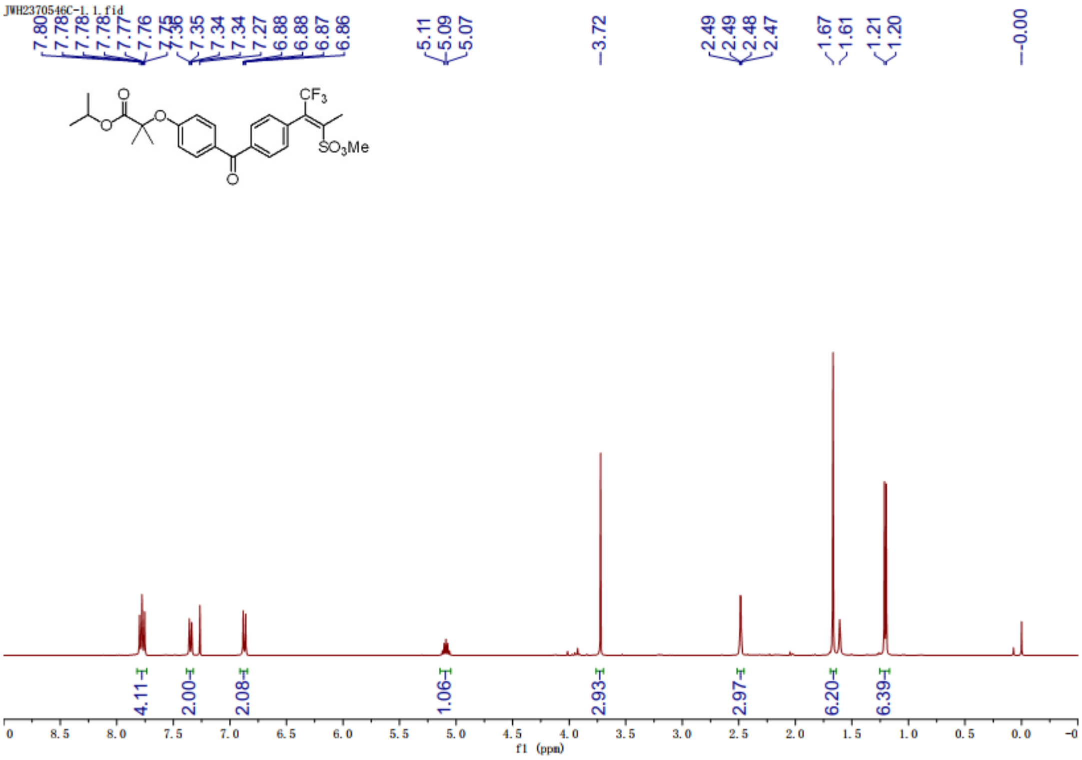
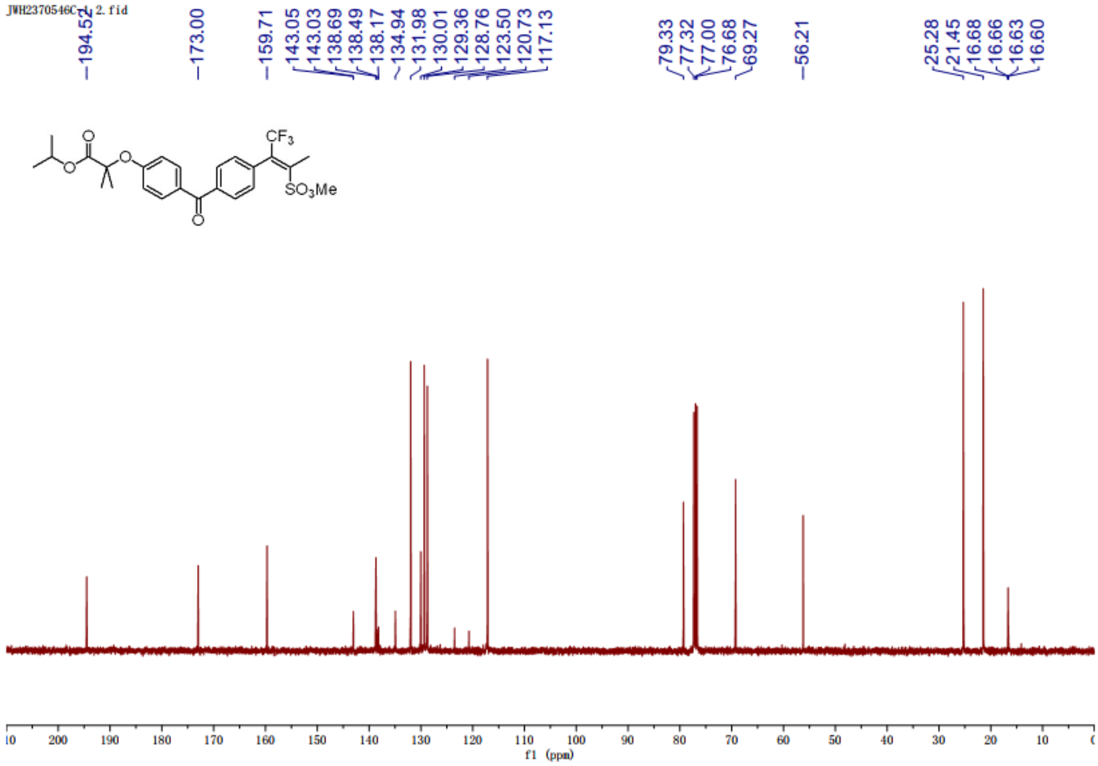
-58.55
-58.56
-58.57
CF3
SO3Me
f1 (ppm)


JWH2370546C-1.1.fid
7.80 7.78 7.78 7.78 7.77 7.76 7.75 7.35 7.35 7.34 7.34 7.27 6.88 6.88 6.87 6.86
5.11 5.09 5.07
3.72
2.49 2.49 2.48 2.47
1.67 1.61
1.21 1.20
0.00
CF3
SO3Me
4.11
2.00
2.08
1.06
2.93
2.97
6.20
6.39
f1 (ppm)


JWH2370546C-1.2.fid
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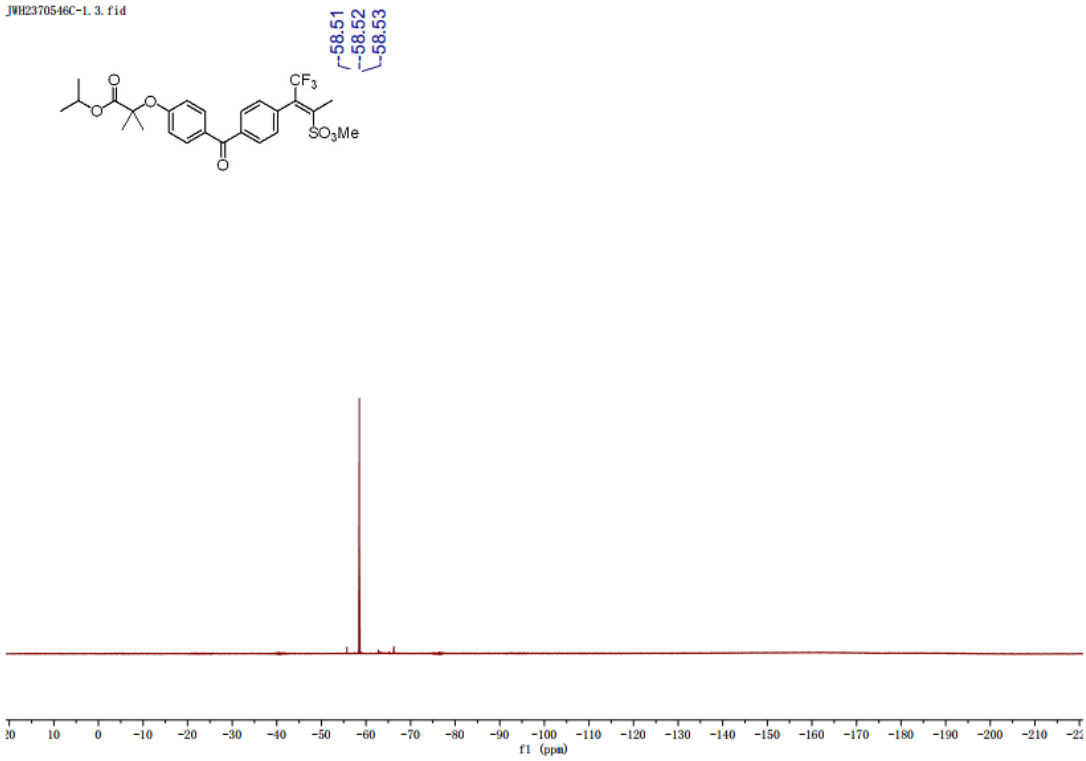
173.00
159.71
143.05
143.03
138.69
138.49
138.17
134.94
131.98
130.01
129.36
128.76
123.50
120.73
117.13
79.33
77.32
77.00
76.68
69.27
56.21
25.28
21.45
16.68
16.66
16.63
16.60
CF3
SO3Me
f1 (ppm)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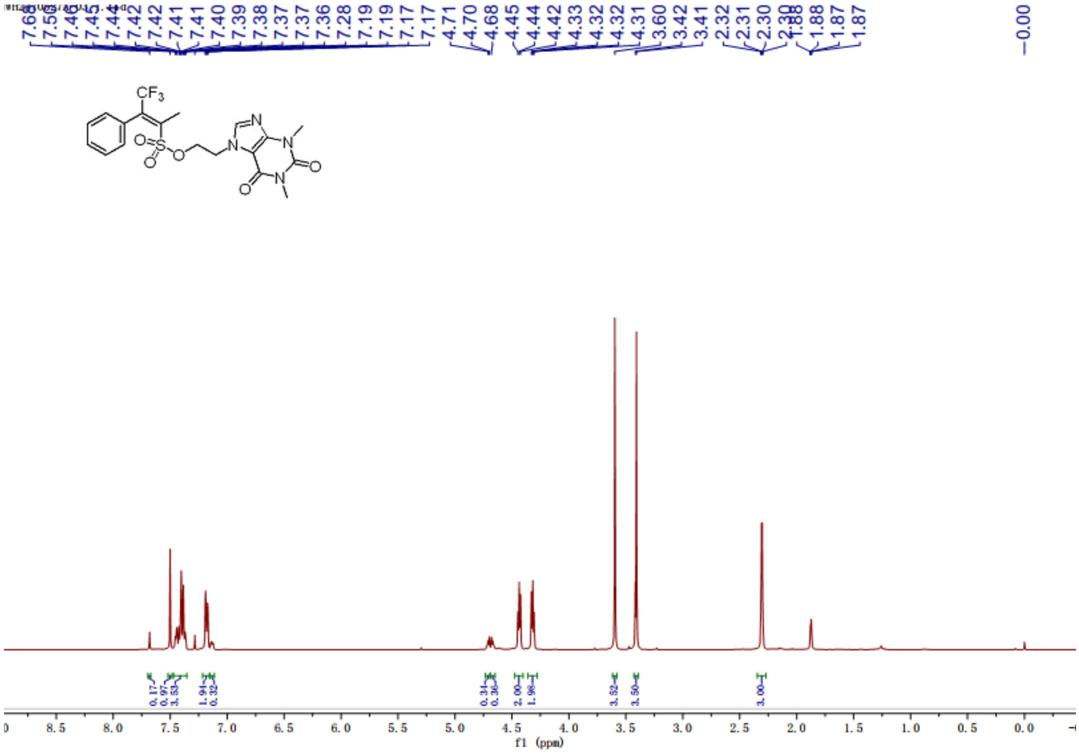
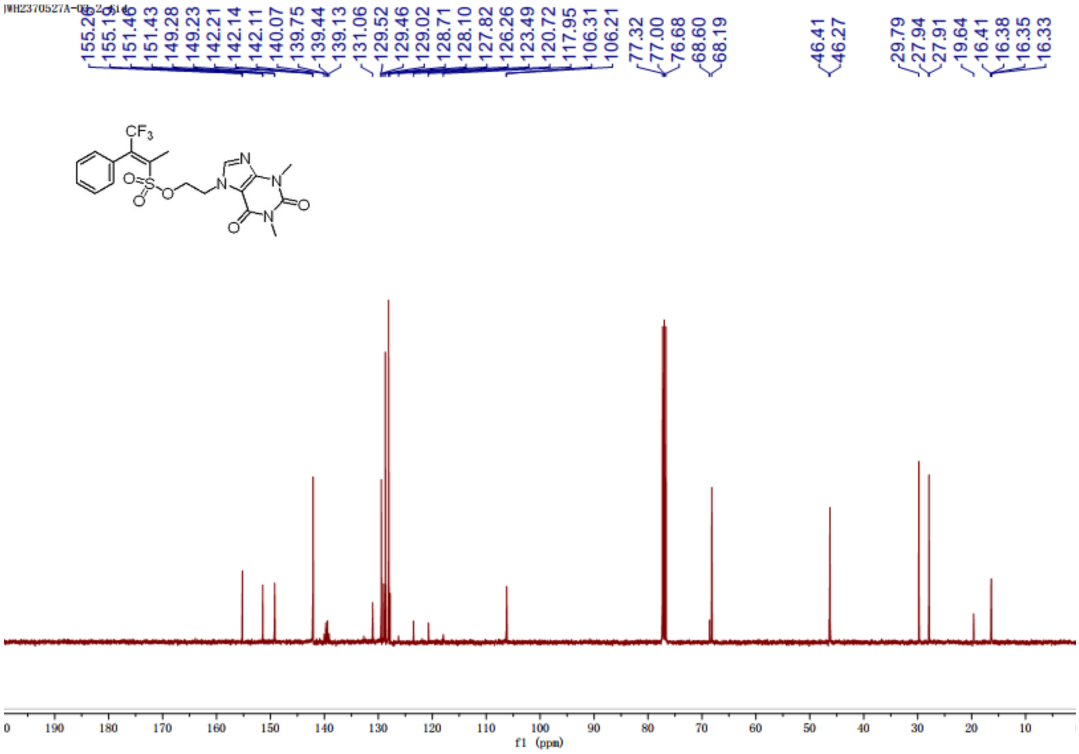
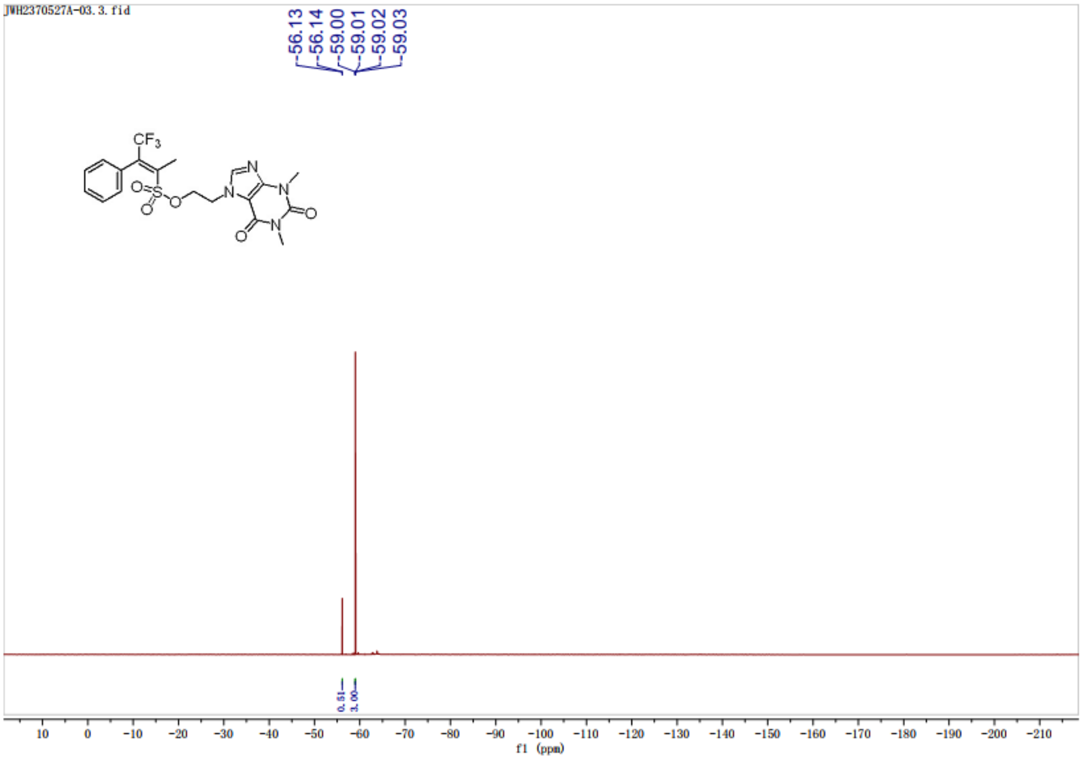
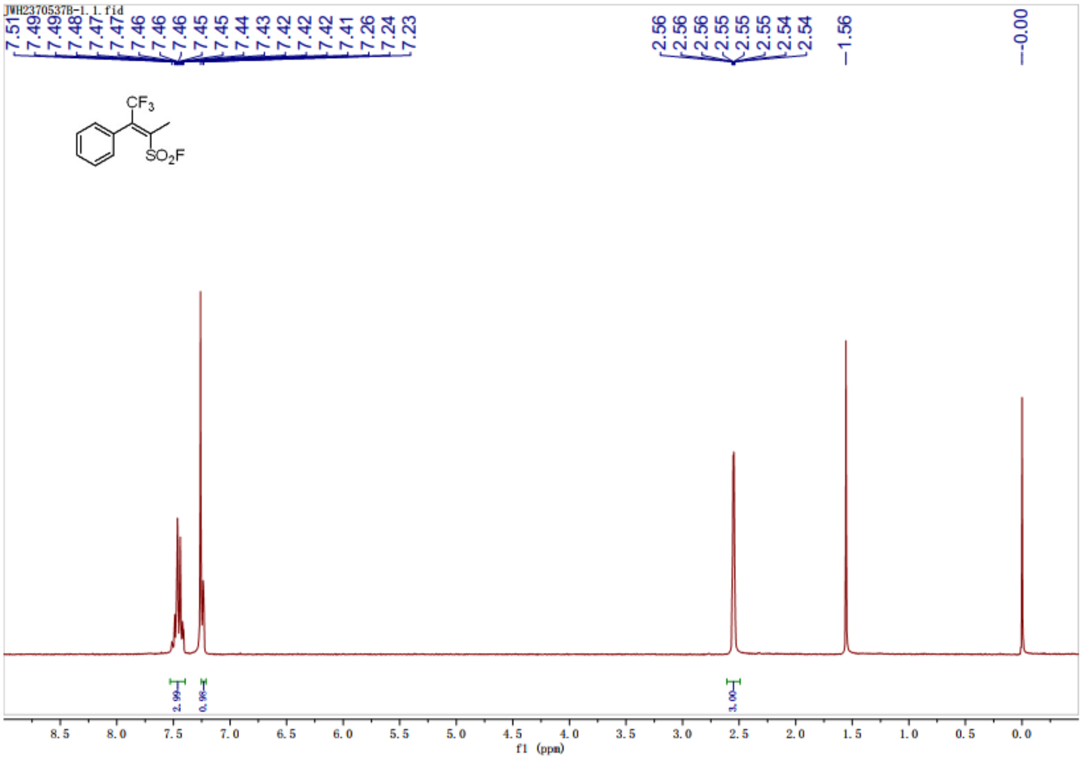
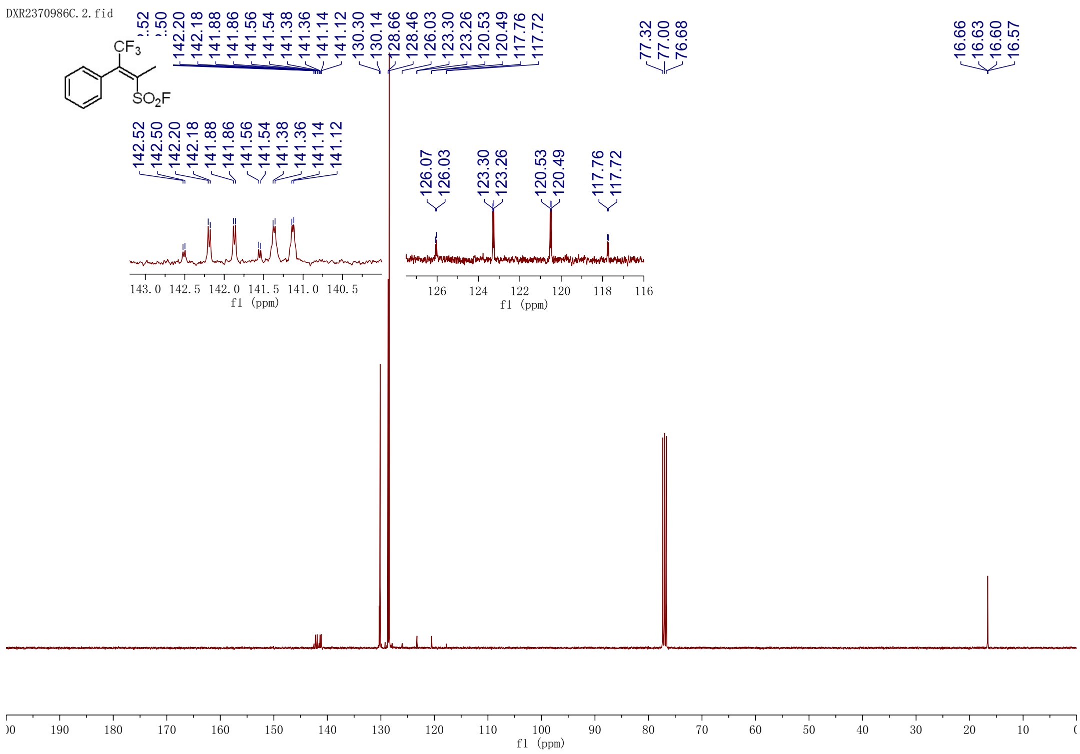
-58.53
CF3
SO3Me
f1 (ppm)

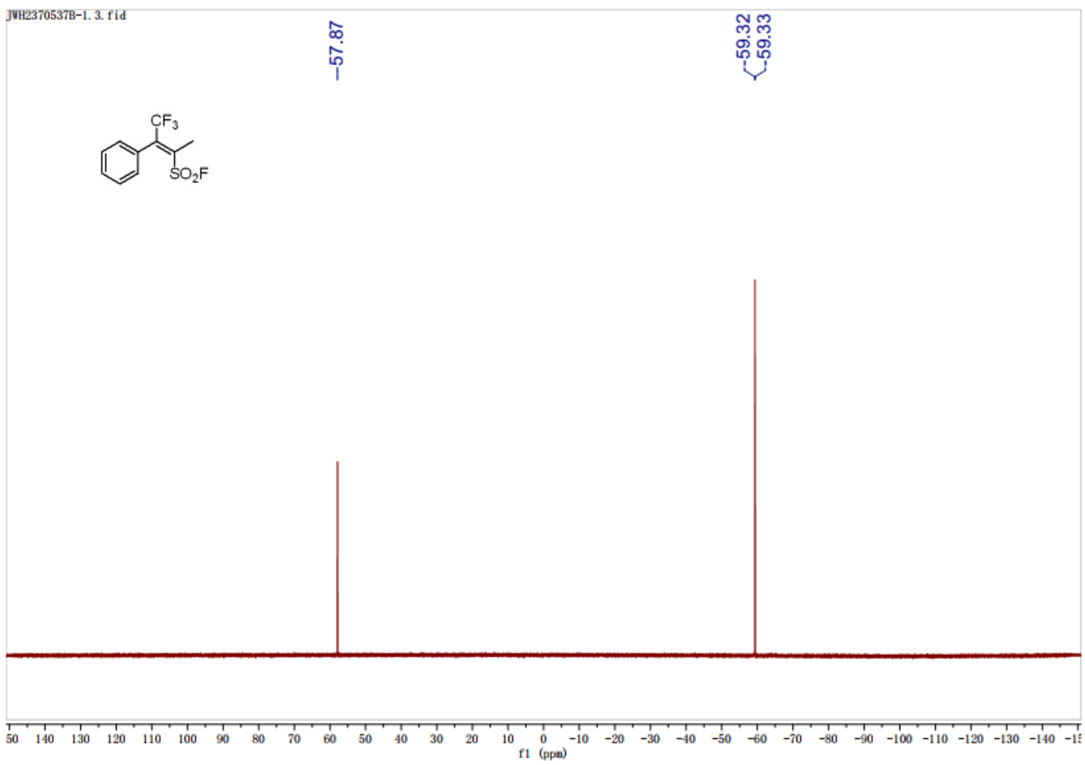









DXR2370986C.2.fid
CF3
SO2F
f1 (ppm)


JWH2370537B-1.3.fid
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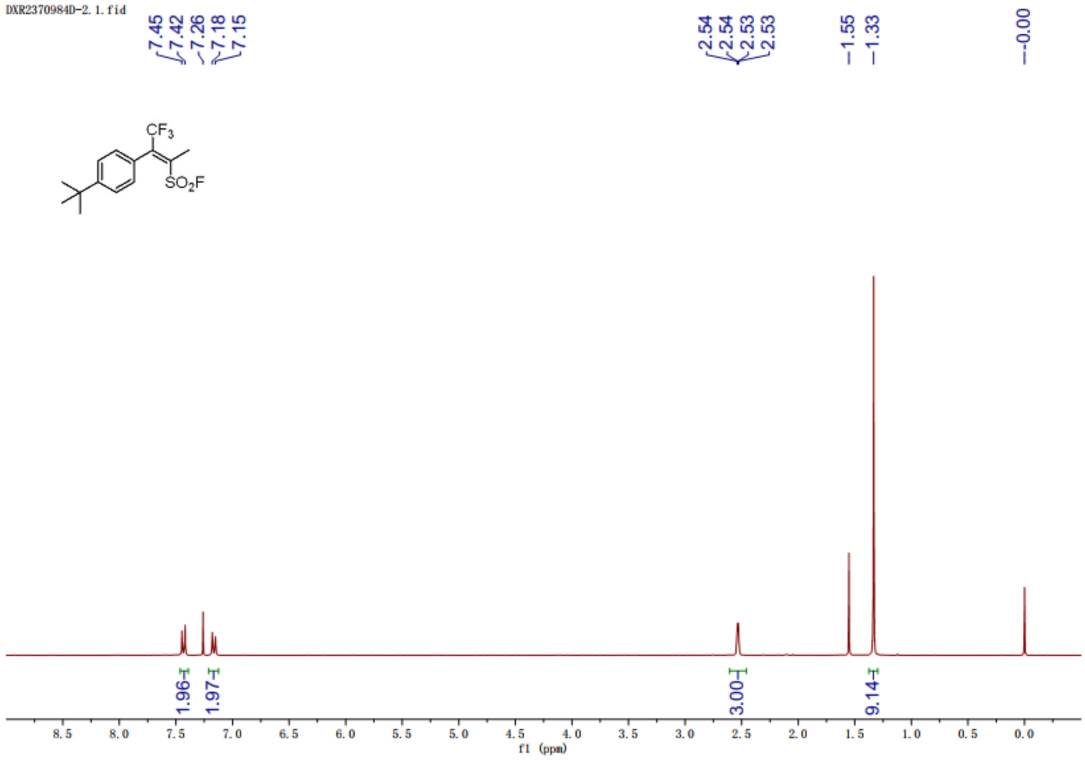
-59.33
CF3
SO2F
f1 (ppm)


DXR2370984D-2.1.fid
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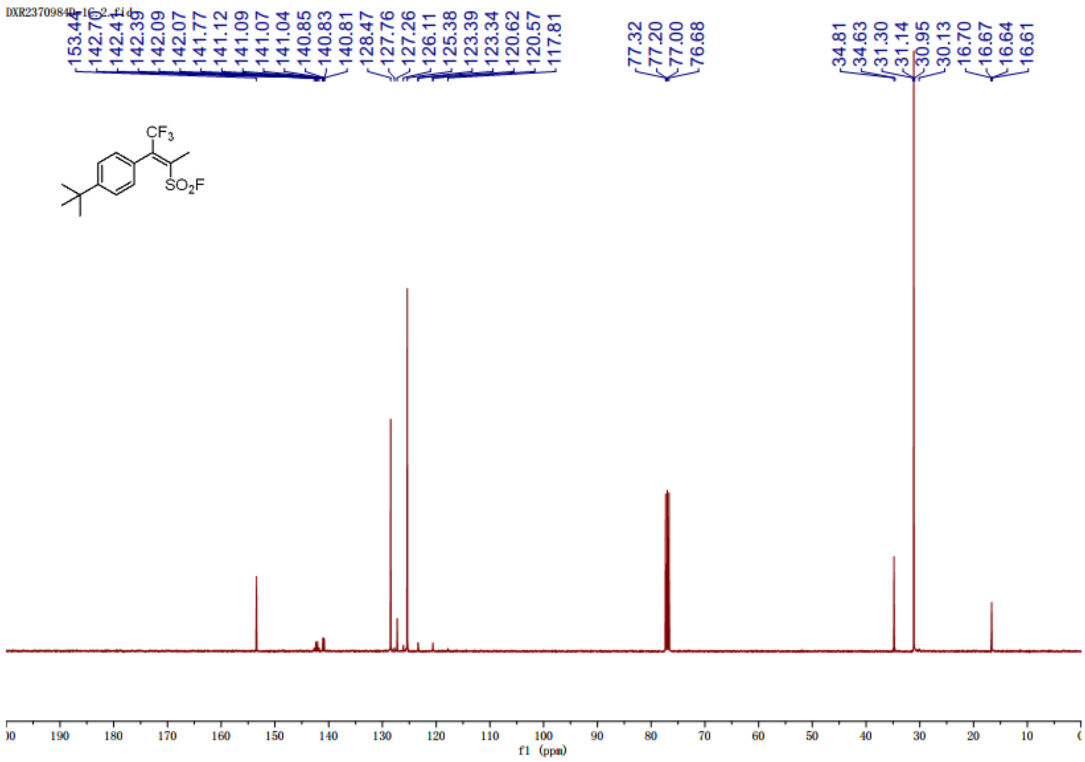
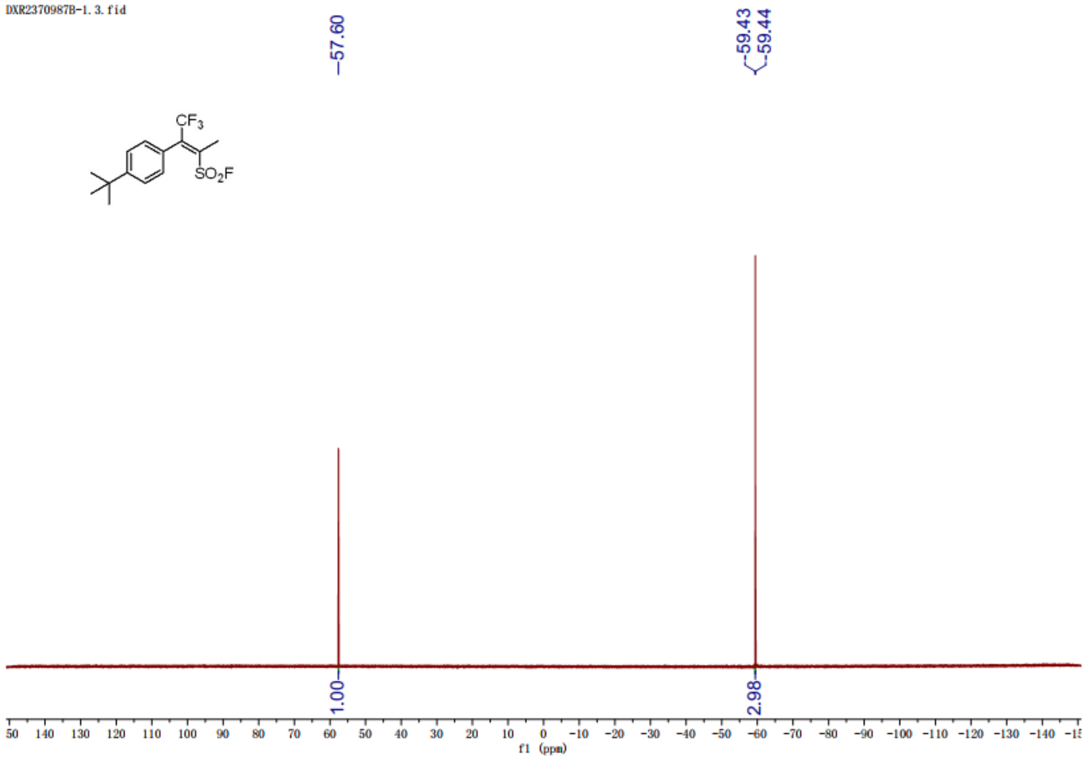
7.42
7.26
7.18
7.15
2.54
2.54
2.53
2.53
1.55
1.33
0.00
CF3
SO2F
1.96
1.97
3.00
9.14
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


153.44
142.70
142.41
142.39
142.09
142.07
141.77
141.12
141.09
141.07
141.04
140.85
140.83
140.81
128.47
127.76
127.26
126.11
125.38
123.39
123.34
120.62
120.57
117.81
77.32
77.20
77.00
76.68
34.81
34.63
31.30
31.14
30.95
30.13
16.70
16.67
16.64
16.61
CF3
SO2F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


DXR2370987B-1.3.fid
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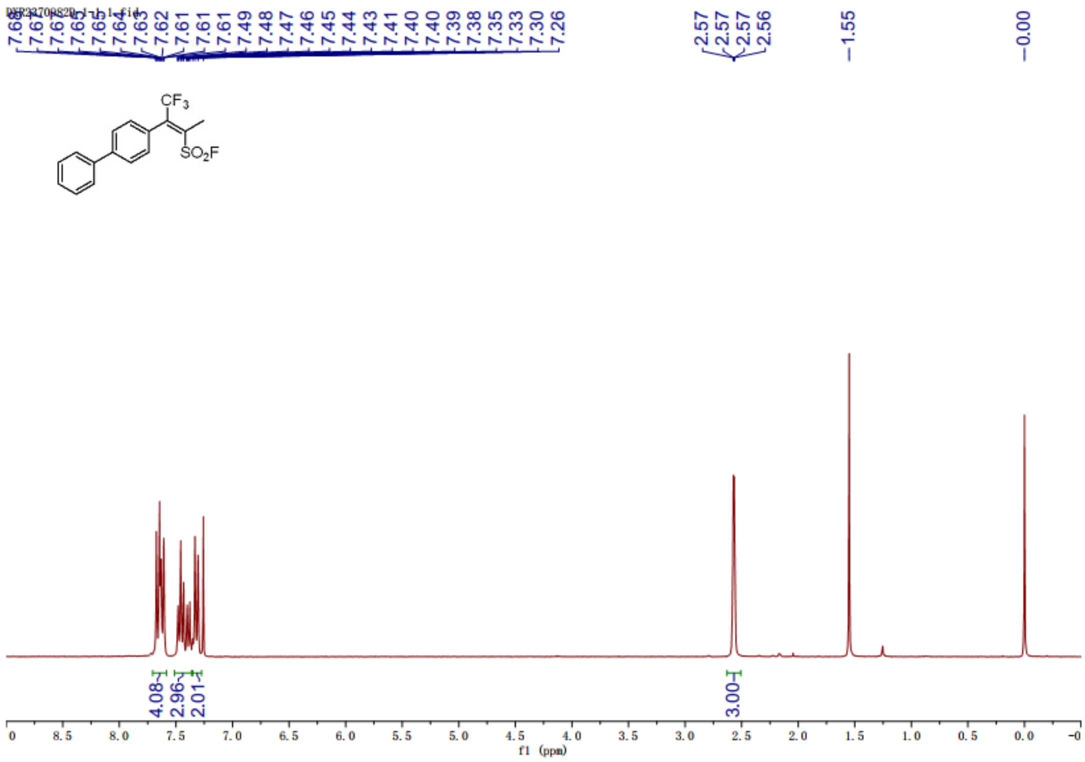
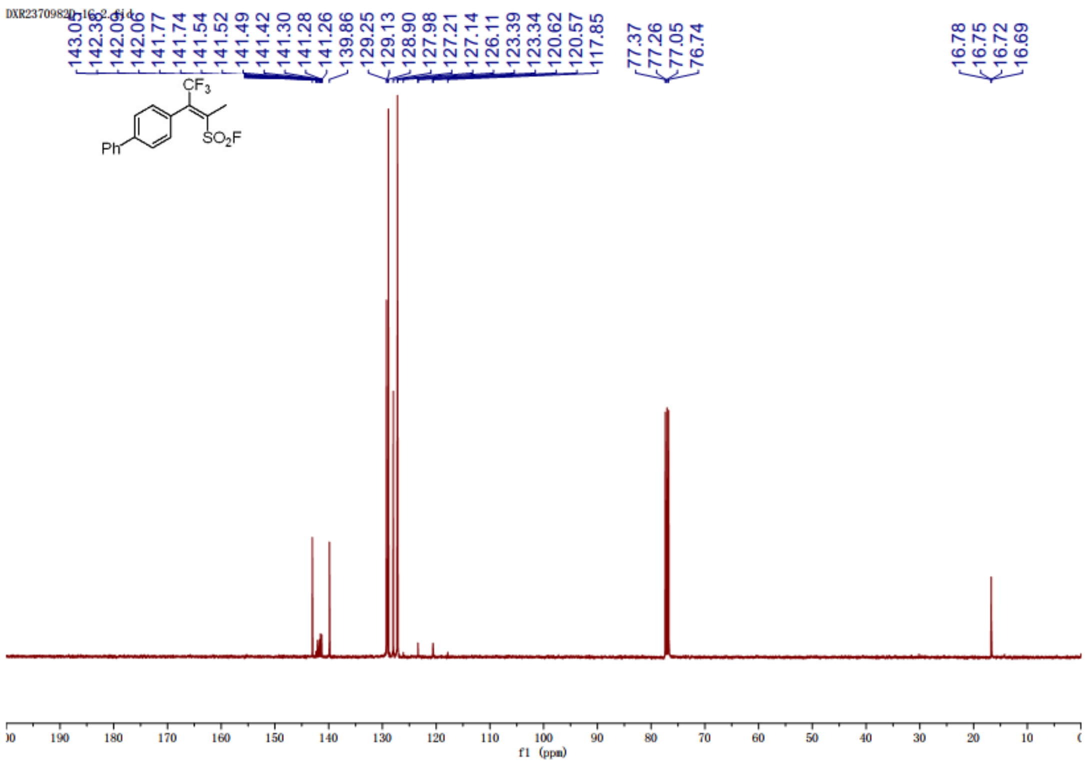
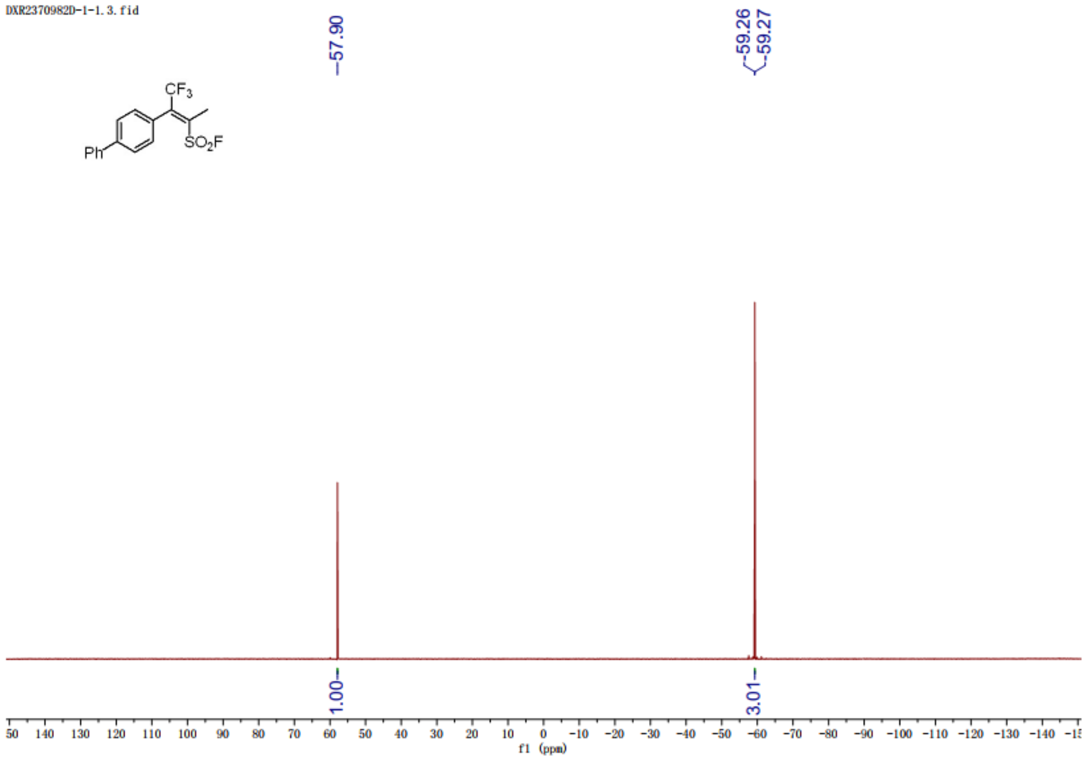
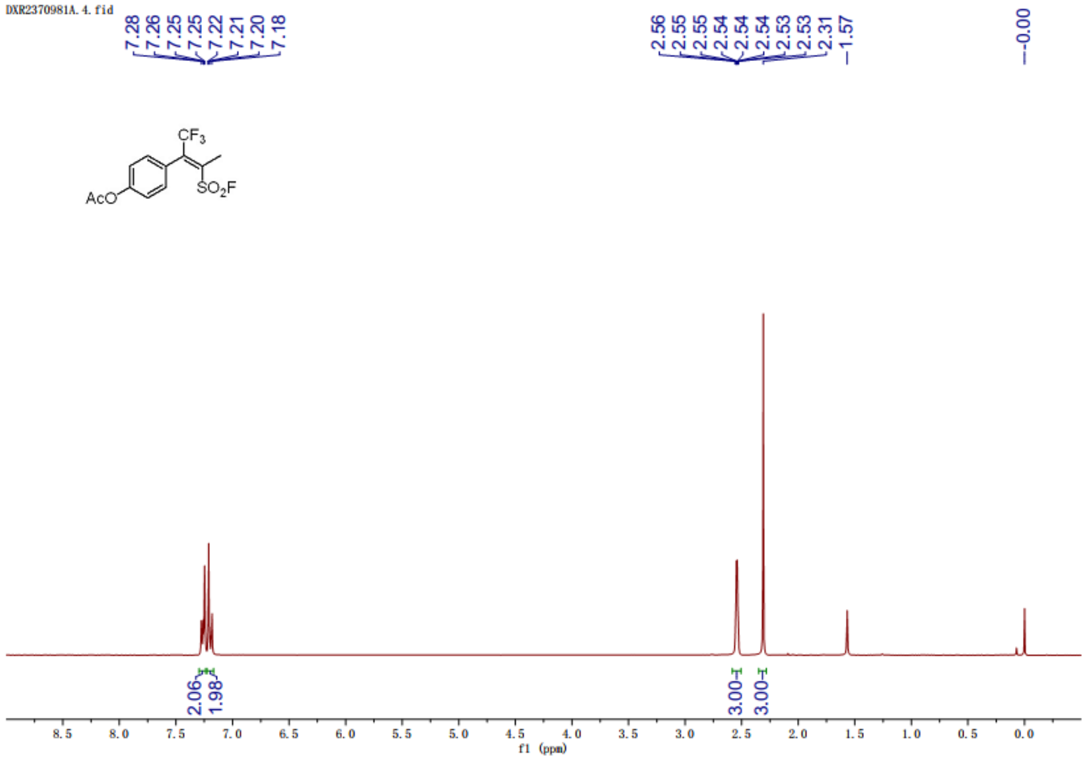
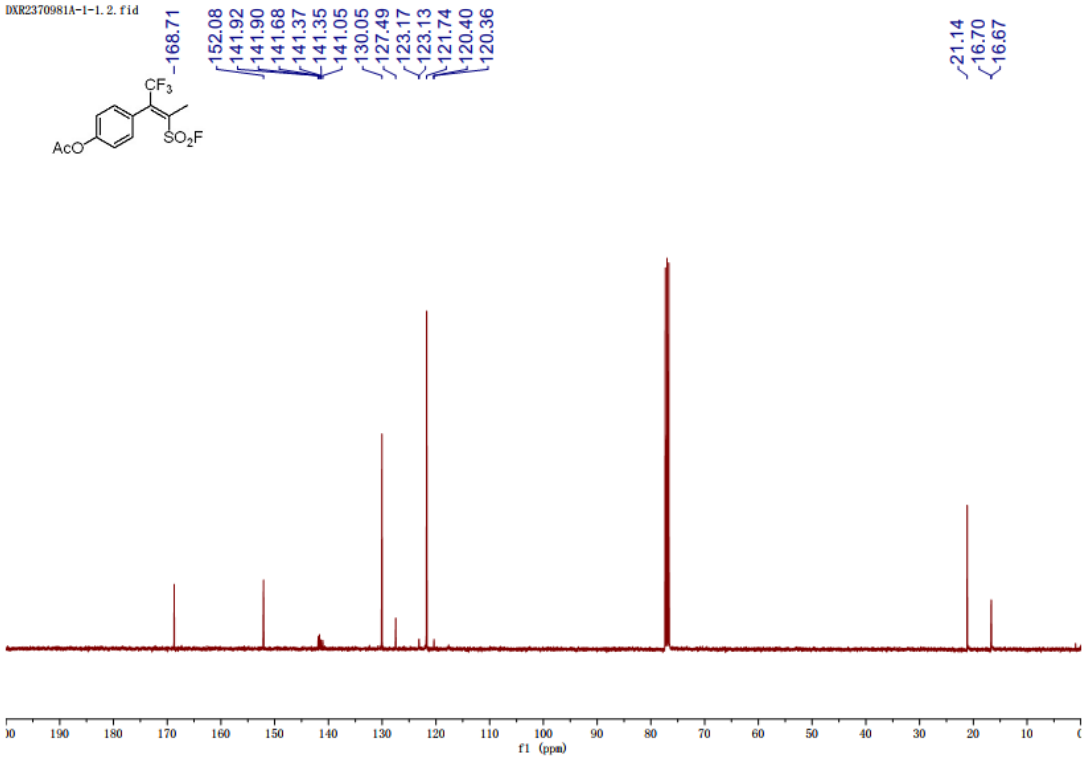
-59.43
-59.44
CF3
SO2F
1.00
2.98
f1 (ppm)

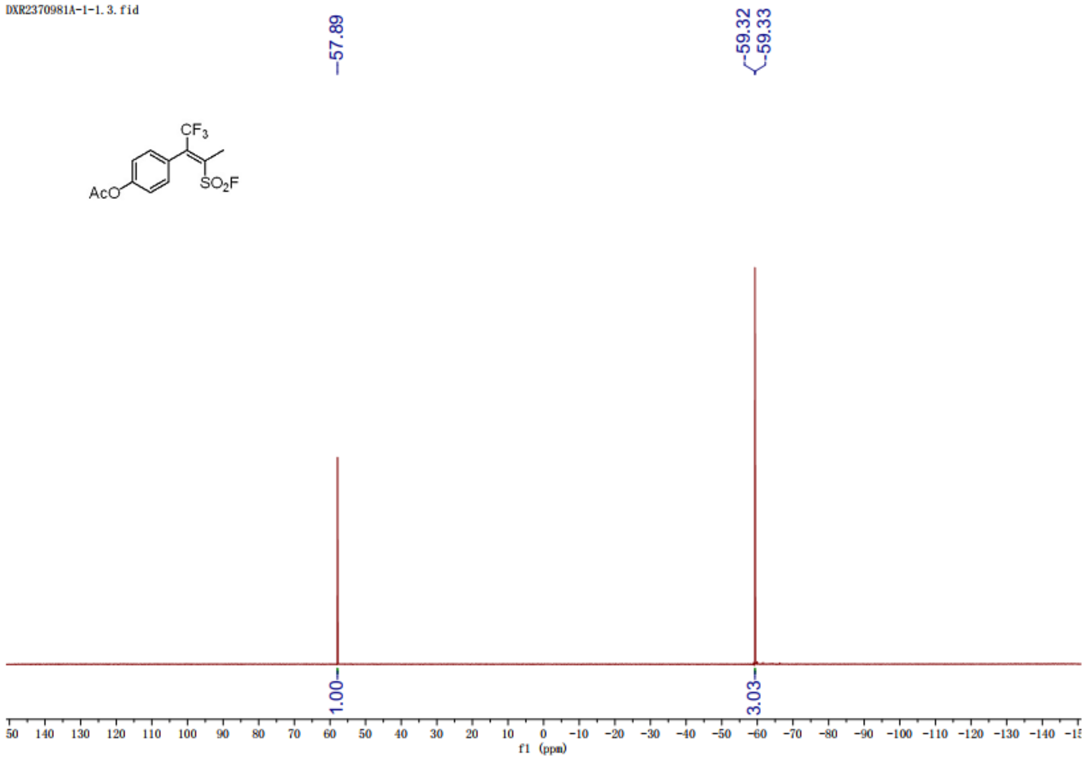

CF3
SO2F
2.57
2.57
2.57
2.56
1.55
0.00
4.08
2.96
2.01
3.00
f1 (ppm)






DXR2370981A.4.fid
7.28
7.26
7.25
7.25
7.22
7.21
7.20
7.18
2.56
2.55
2.55
2.54
2.54
2.54
2.53
2.53
2.31
1.57
0.00
2.06
1.98
3.00
3.00
f1 (ppm)


DXR2370981A-1-1.2.fid
168.71
152.08
141.92
141.90
141.68
141.37
141.35
141.05
130.05
127.49
123.17
123.13
121.74
120.40
120.36
21.14
16.70
16.67
f1 (ppm)


DXR2370981A-1-1.3.fid
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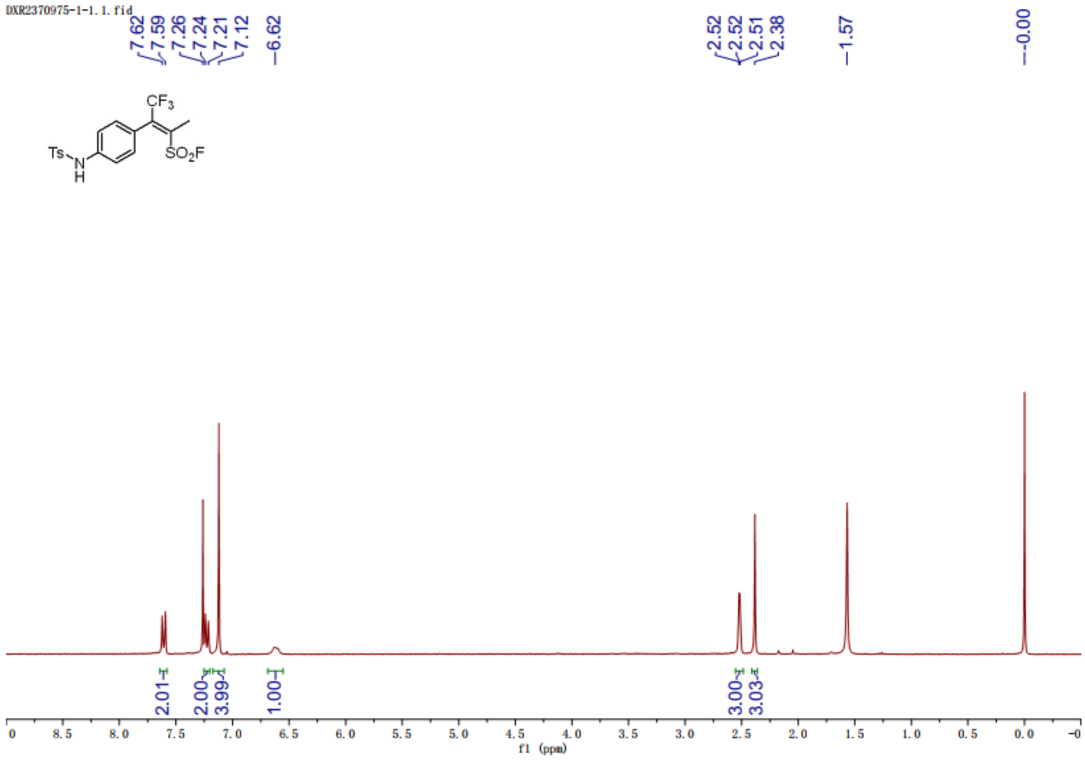
-59.32
-59.33
CF3
AcO
SO2F
1.00
3.03
f1 (ppm)


DXR2370975-1-1.1.fid
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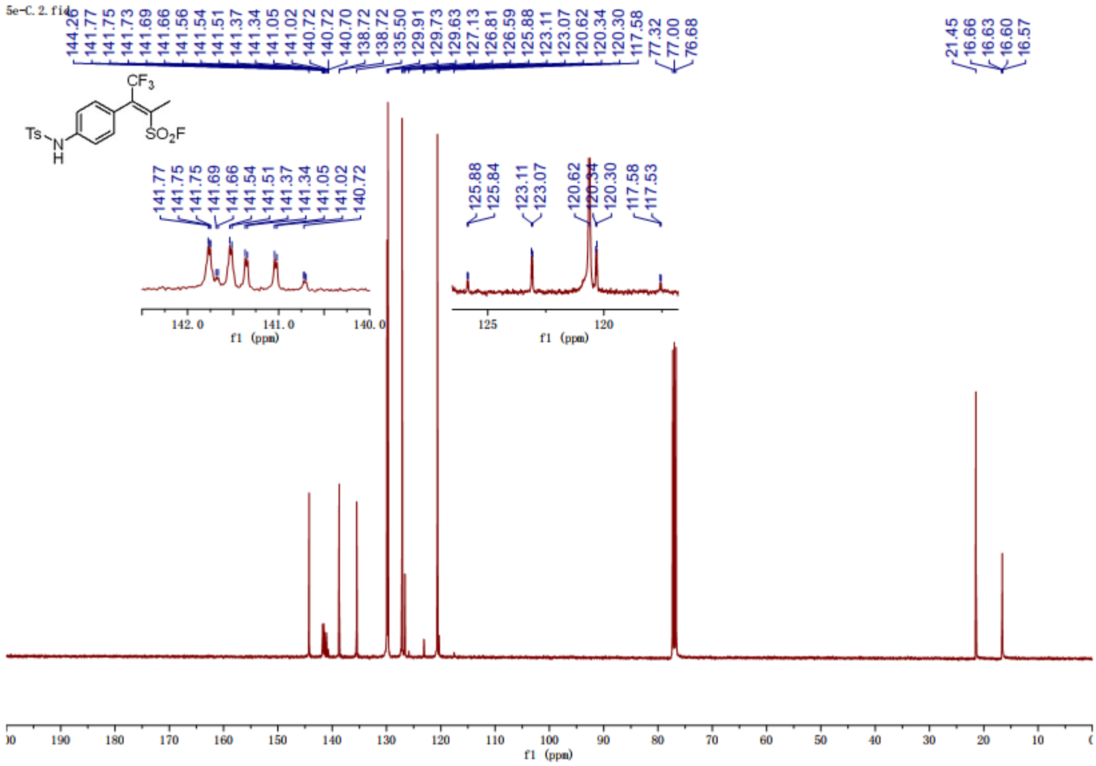
7.59
7.26
7.24
7.21
7.12
6.62
2.52
2.52
2.51
2.38
1.57
0.00
CF3
Ts
N
H
SO2F
2.01
2.00
3.99
1.00
3.00
3.03
f1 (ppm)


5e-C.2.fid
144.26
141.77
141.75
141.73
141.69
141.66
141.56
141.54
141.51
141.37
141.34
141.05
141.02
140.72
140.72
140.70
138.72
138.72
135.50
129.91
129.73
129.63
127.13
126.81
126.59
125.88
123.11
123.07
120.62
120.34
120.30
117.58
77.32
77.00
76.68
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16.66
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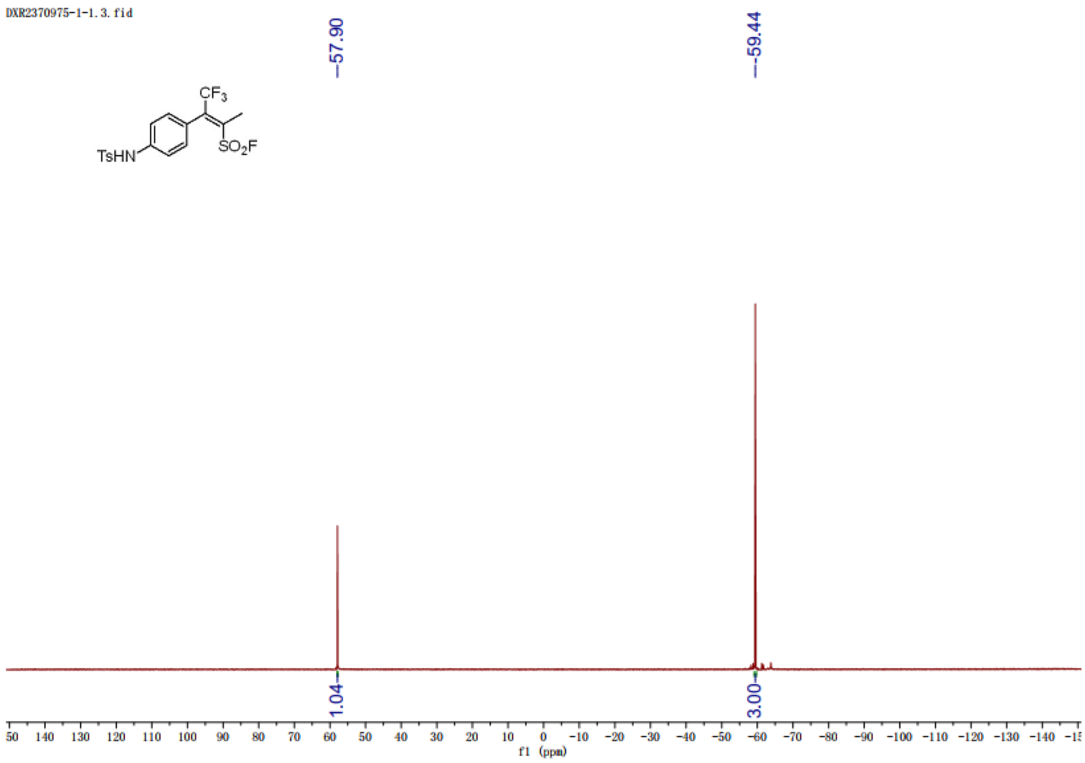
CF3
Ts
N
H
SO2F
f1 (ppm)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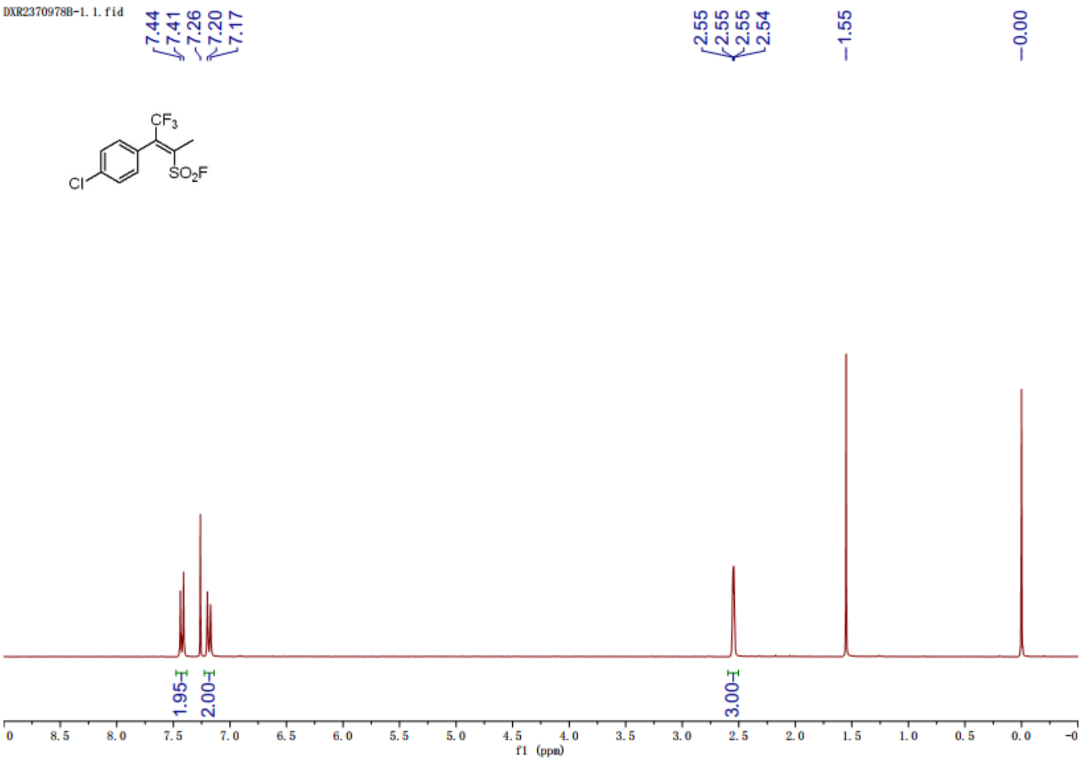
-59.44
CF3
TsHN
SO2F
1.04
3.00
f1 (ppm)


DXR2370978B-1.1.fid
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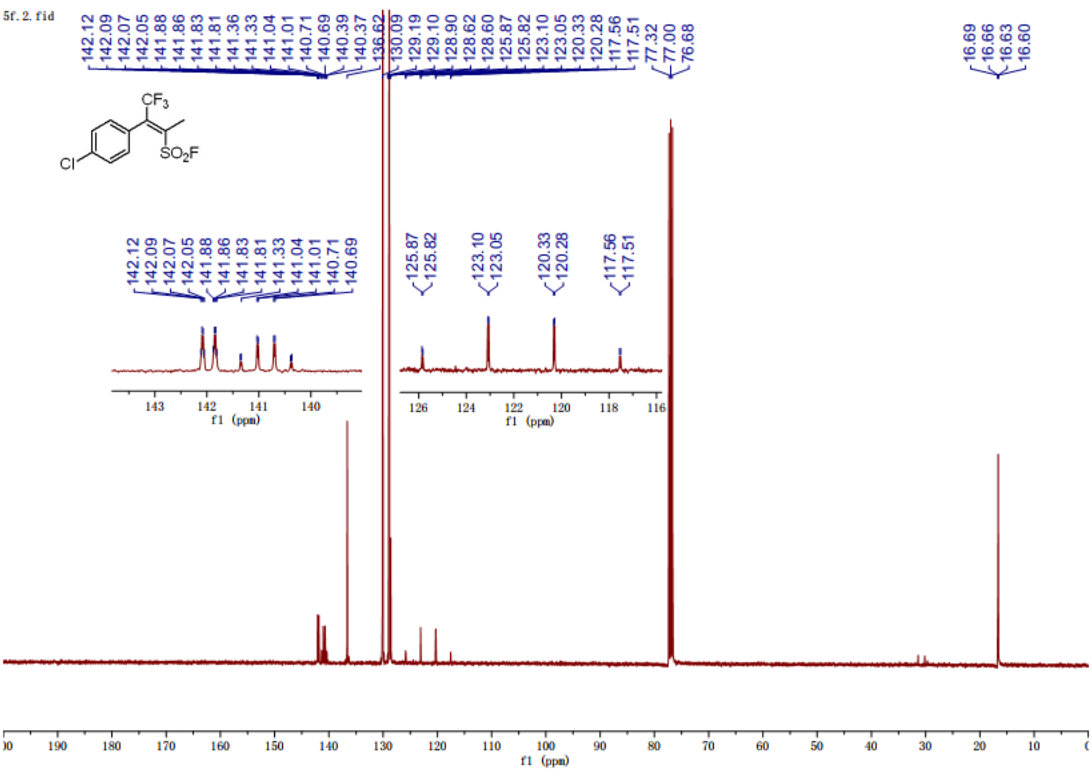
7.41
7.26
7.20
7.17
2.55
2.55
2.55
2.54
1.55
0.00
CF3
Cl
SO2F
1.95
2.00
3.00
f1 (ppm)


5f.2.fid
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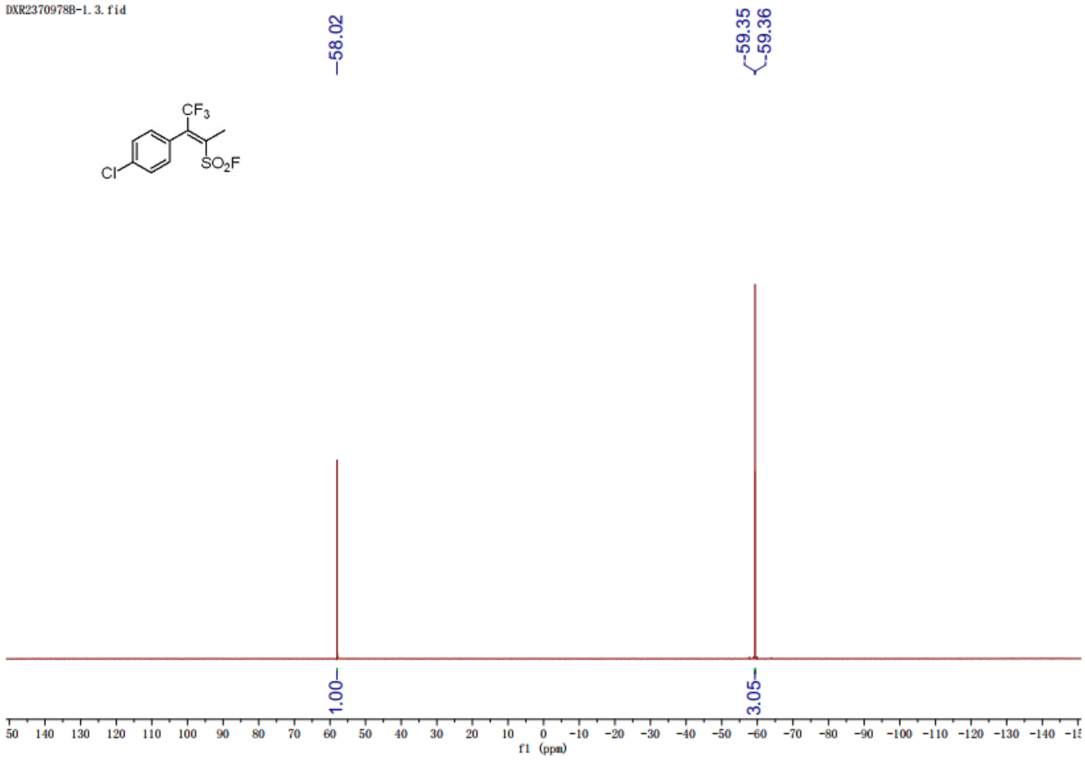
142.09
142.07
142.05
141.88
141.86
141.83
141.81
141.36
141.33
141.04
141.01
140.71
140.69
140.39
140.37
136.62
130.09
129.19
129.10
128.90
128.62
128.60
125.87
125.82
123.10
123.05
120.33
120.28
117.56
117.51
77.32
77.00
76.68
16.69
16.66
16.63
16.60
CF3
Cl
SO2F
f1 (ppm)


DXR2370978B-1.3.fid
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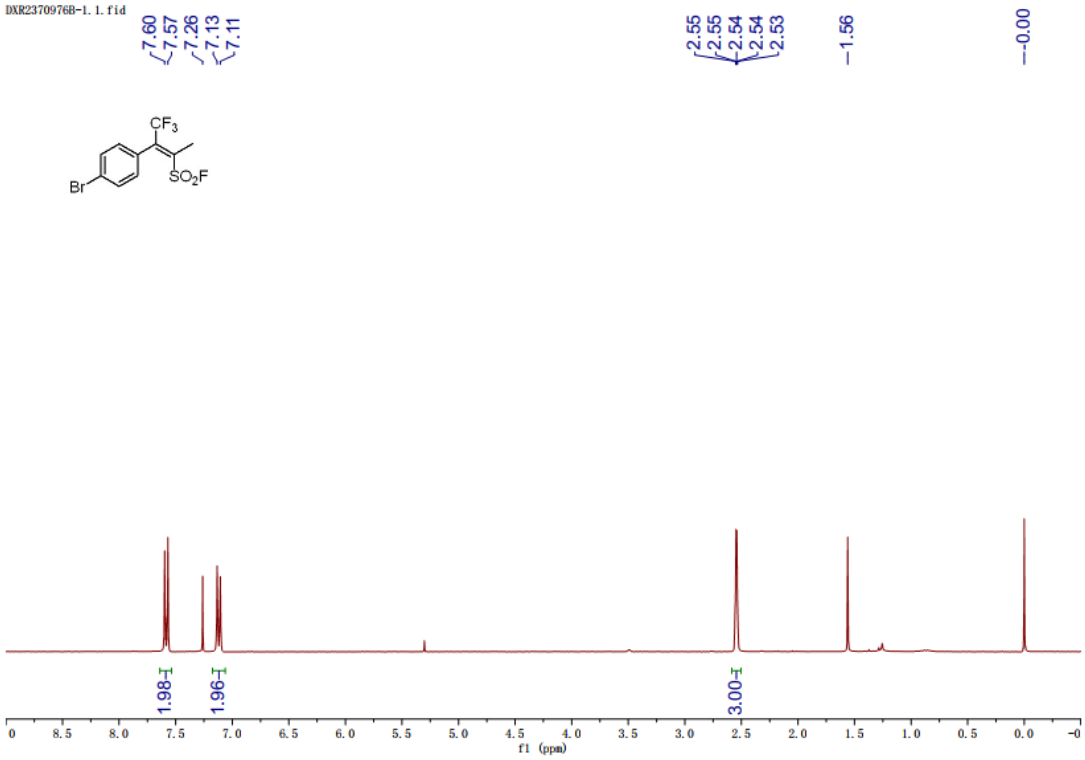
-59.35
-59.36
CF3
Cl
SO2F
1.00
3.05
f1 (ppm)


DXR2370976B-1.1.fid
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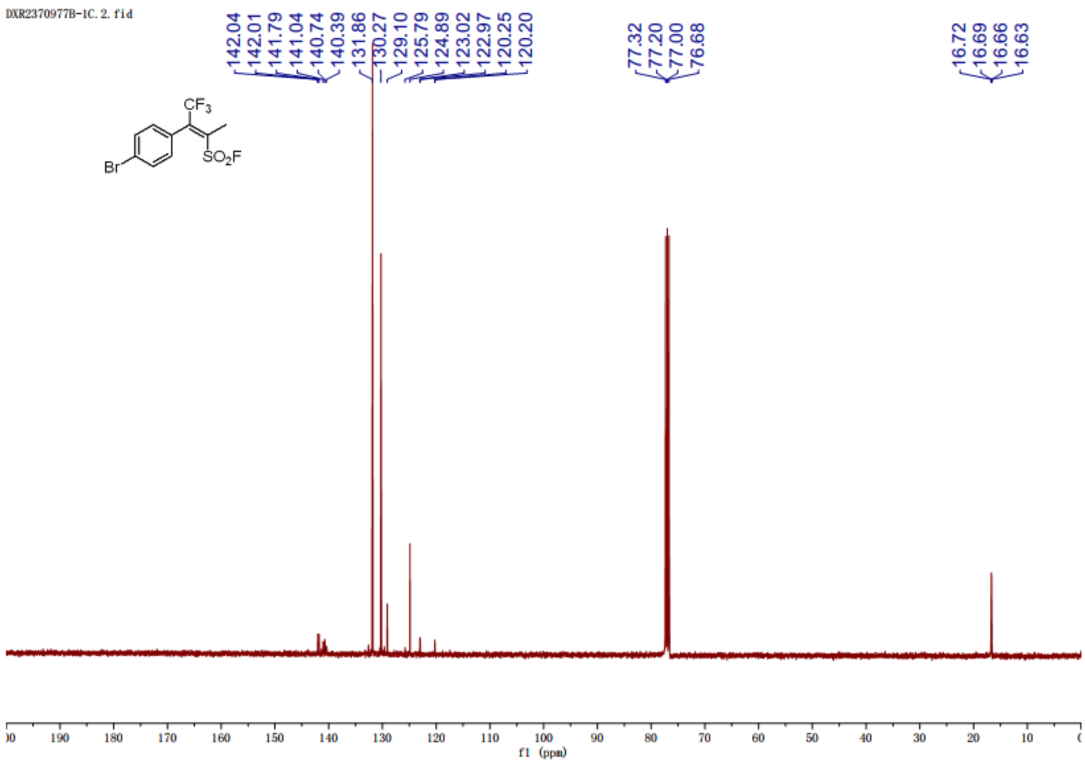
7.57
7.26
7.13
7.11
2.55
2.55
2.54
2.54
2.53
1.56
-0.00
CF3
Br
SO2F
1.98
1.96
3.00
f1 (ppm)


DXR2370977B-1C.2.fid
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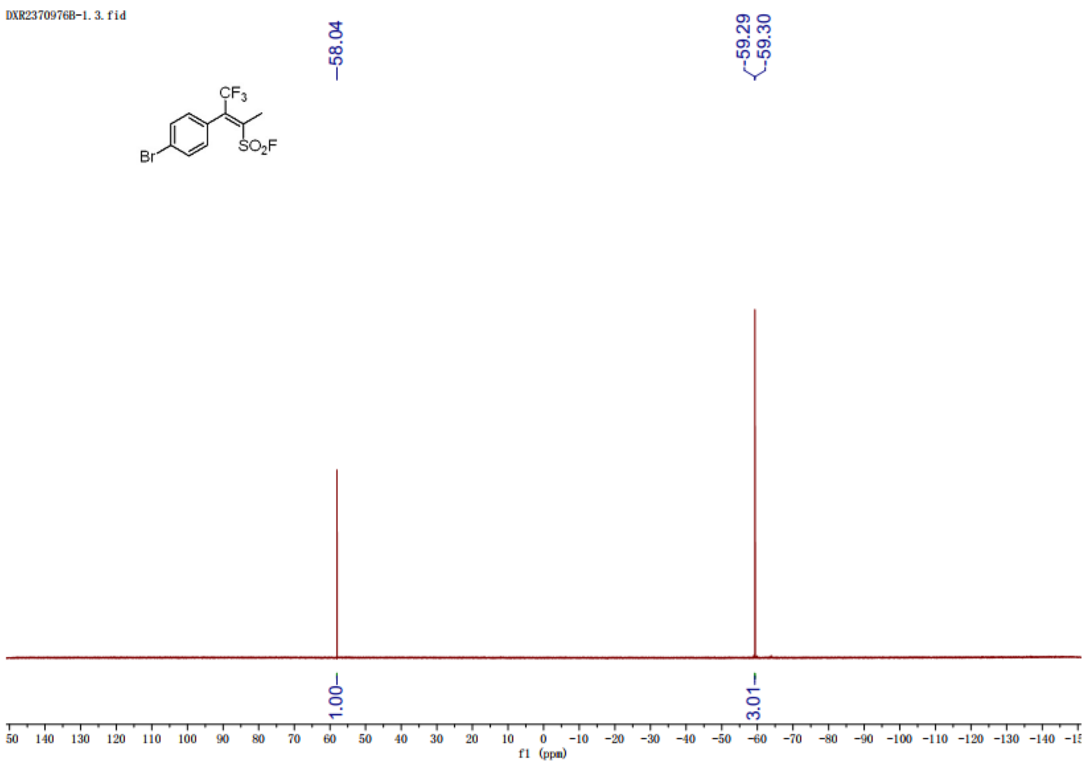
142.01
141.79
141.04
140.74
140.39
131.86
130.27
129.10
125.79
124.89
123.02
122.97
120.25
120.20
77.32
77.20
77.00
76.68
16.72
16.69
16.66
16.63
CF3
Br
SO2F
f1 (ppm)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CF3
Br
SO2F
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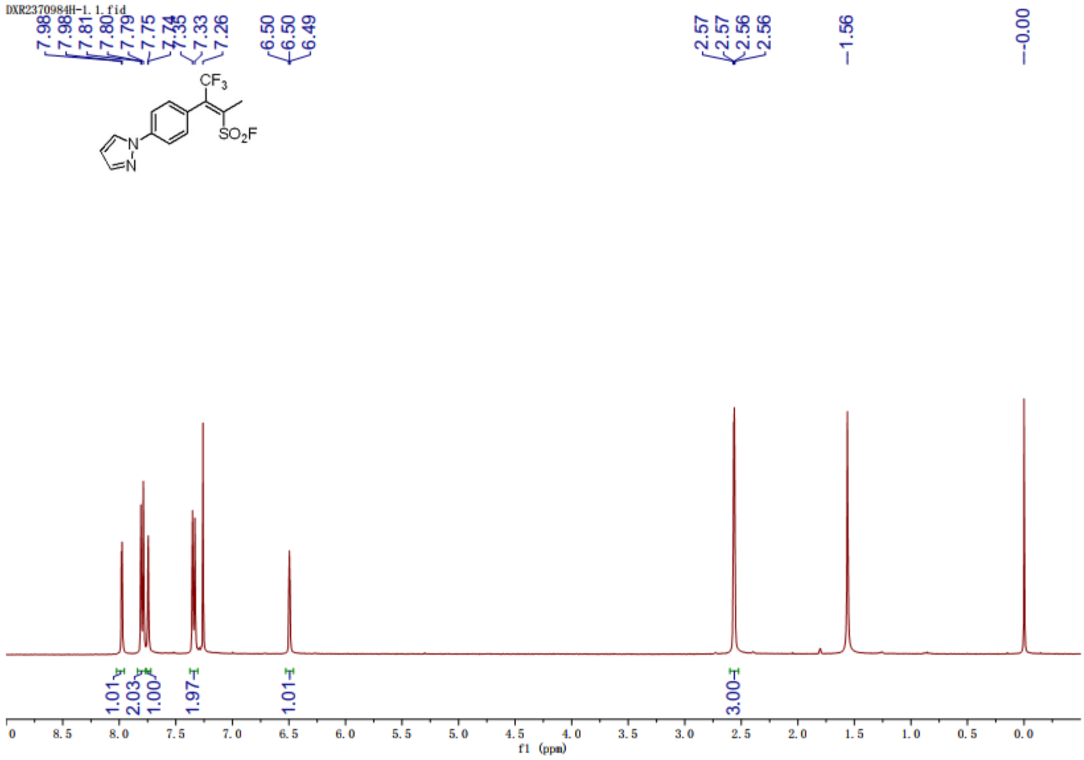
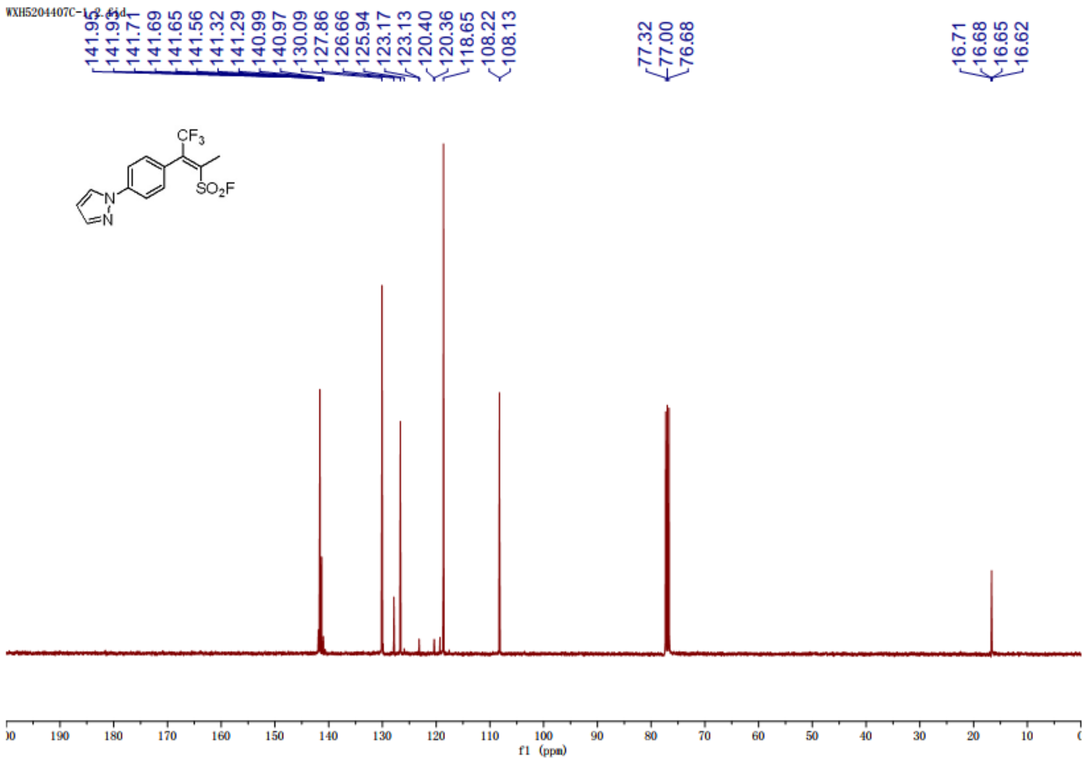
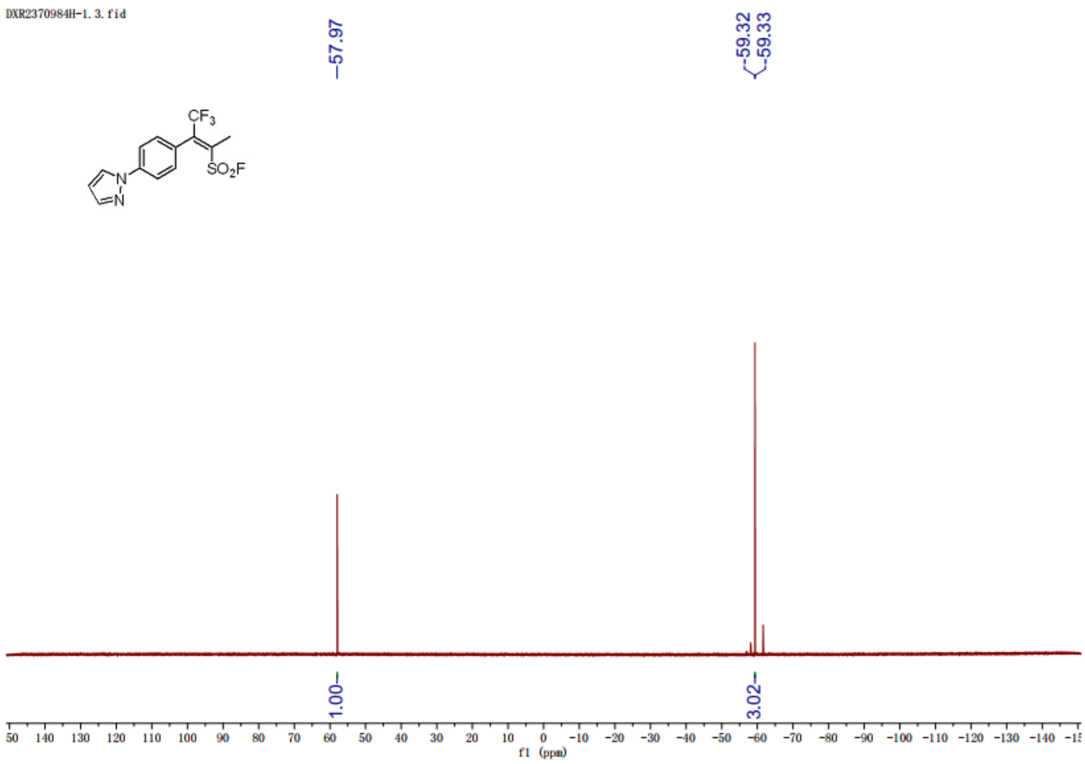
3.01
f1 (ppm)






DXR2370984H-1.3.fid
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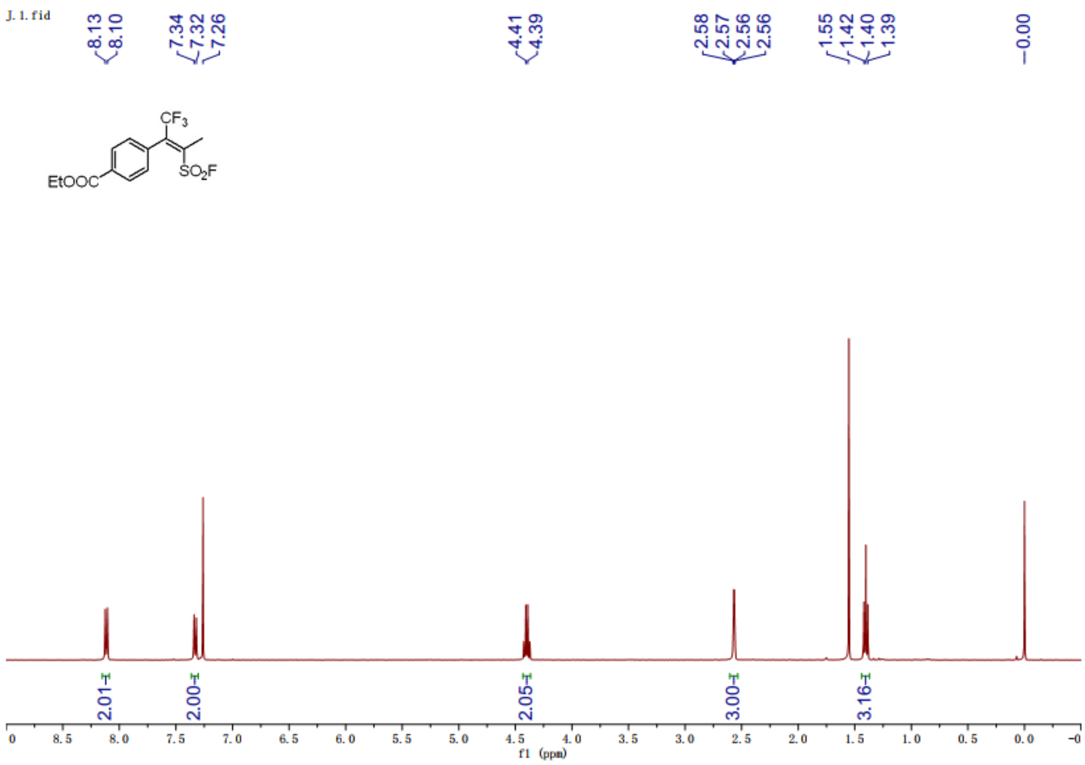
-59.33
CF3
SO2F
N
N
1.00
3.02
f1 (ppm)


J.1.fid
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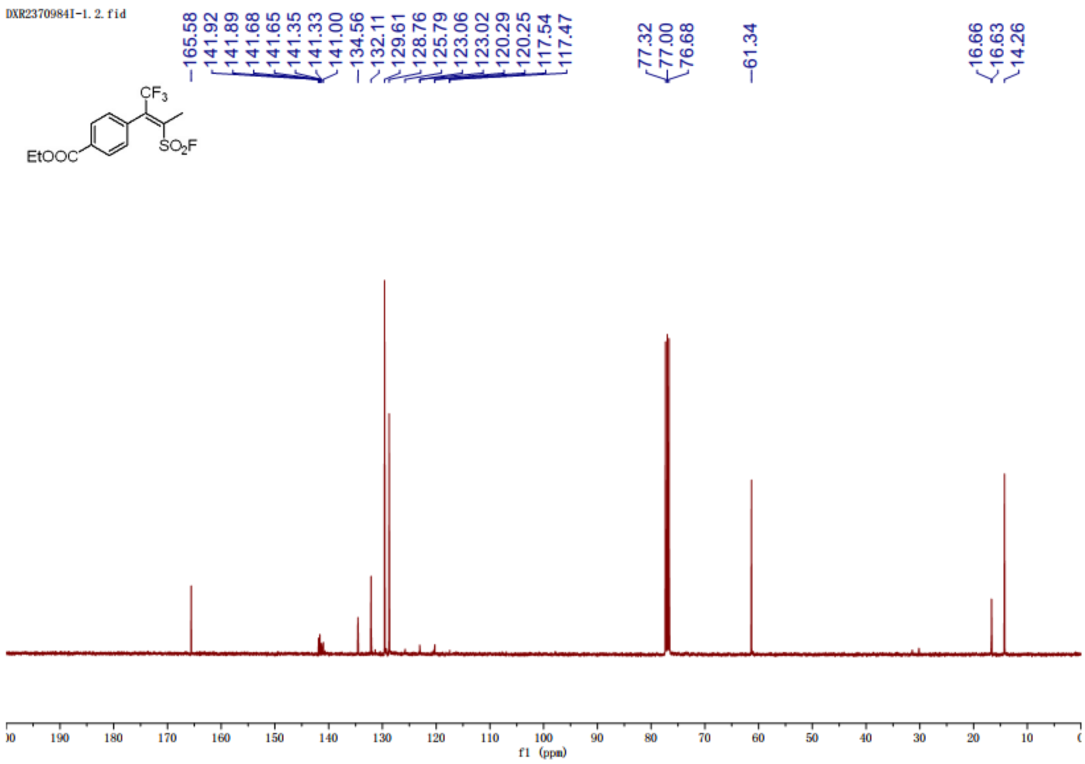
8.10
7.34
7.32
7.26
4.41
4.39
2.58
2.57
2.56
2.56
1.55
1.42
1.40
1.39
0.00
CF3
EtOOC
SO2F
2.01
2.00
2.05
3.00
3.16
f1 (ppm)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141.00
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123.06
123.02
120.29
120.25
117.54
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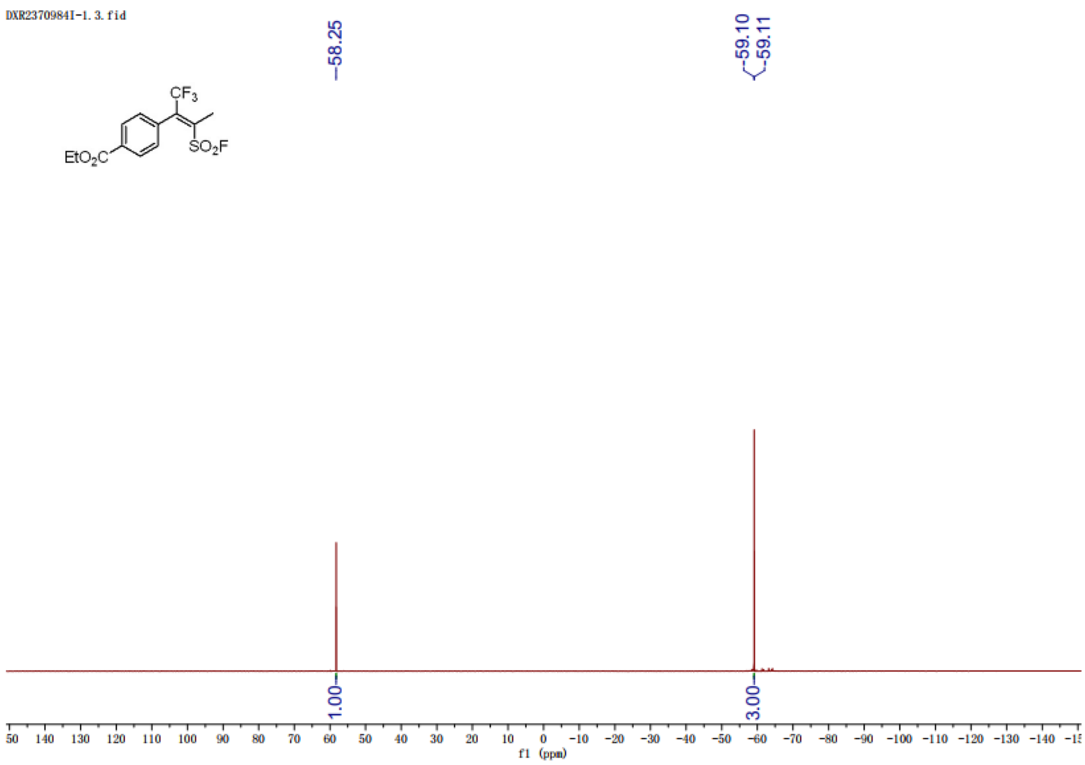
76.68
61.34
16.66
16.63
14.26
CF3
EtOOC
SO2F
f1 (ppm)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CF3
EtO2C
SO2F
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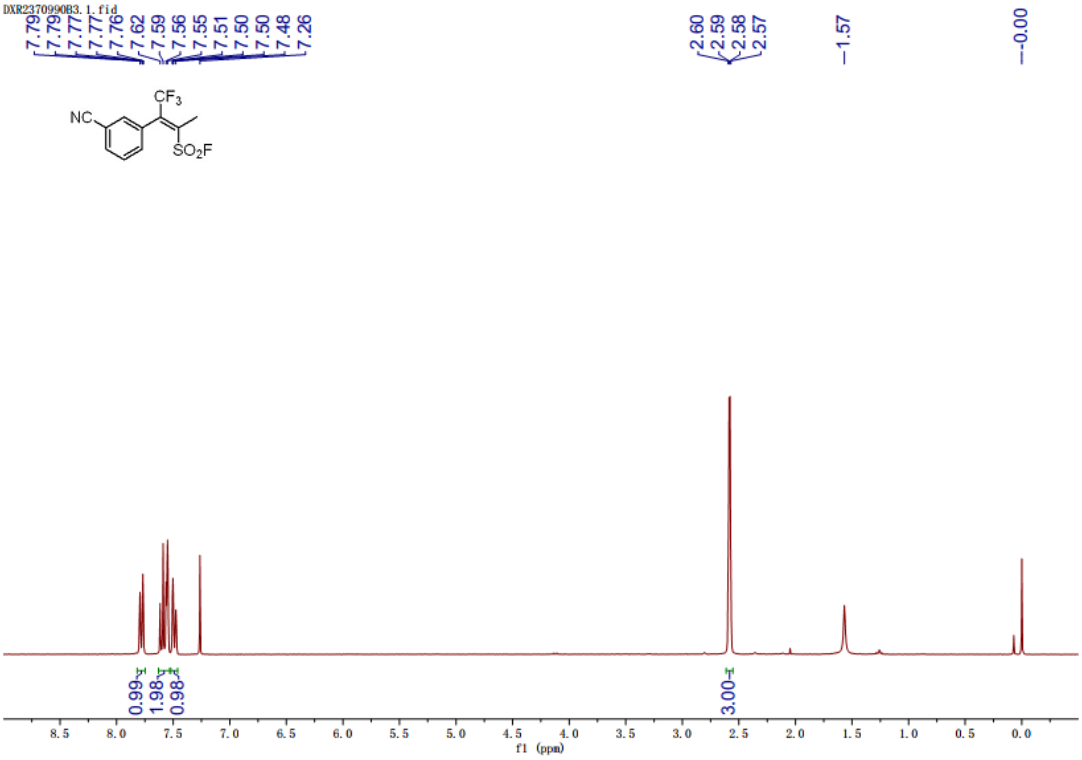
3.00
f1 (ppm)


DXR2370990B3.1.fid
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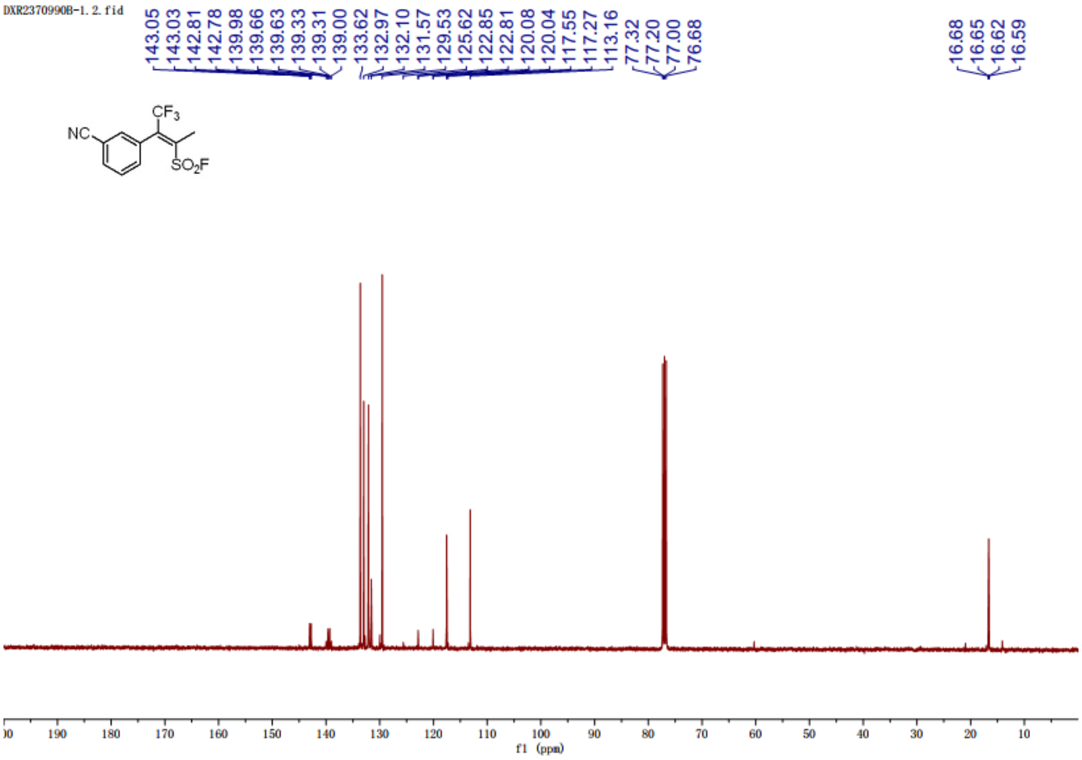
7.79
7.77
7.77
7.76
7.62
7.59
7.56
7.55
7.51
7.50
7.50
7.48
7.26
2.60
2.59
2.58
2.57
1.57
0.00
CF3
NC
SO2F
0.99
1.98
0.98
3.00
f1 (ppm)


DXR2370990B-1.2.fid
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143.03
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139.63
139.33
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139.00
133.62
132.97
132.10
131.57
129.53
125.62
122.85
122.81
120.08
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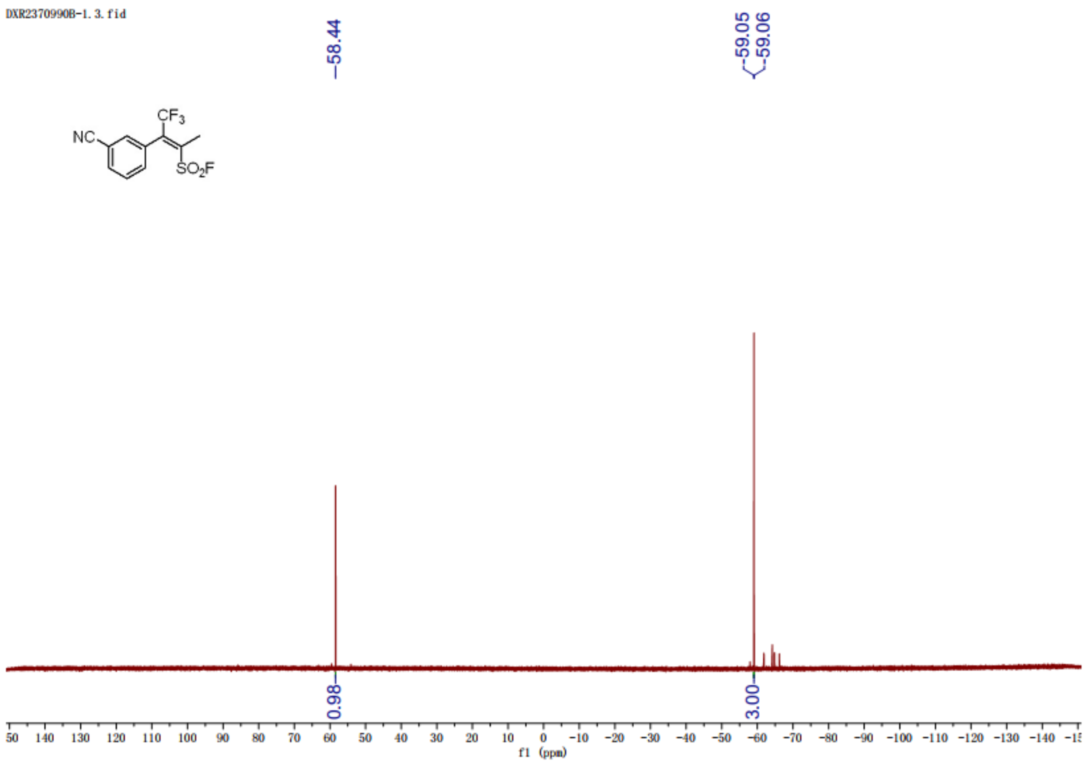
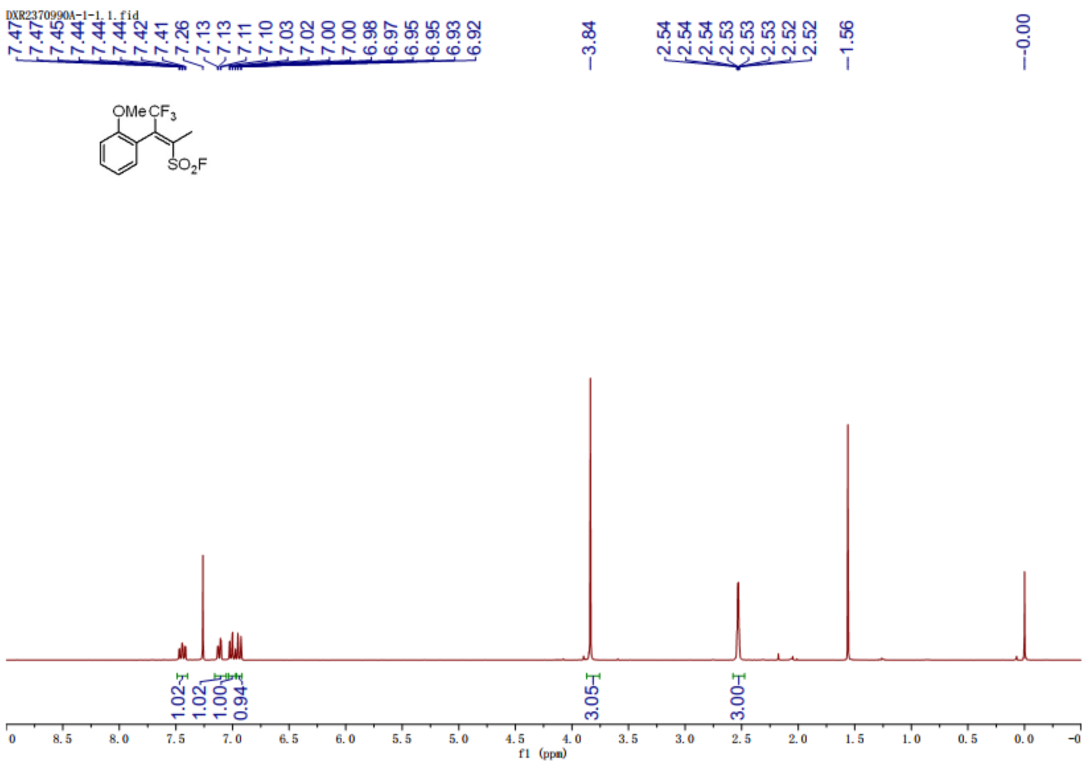
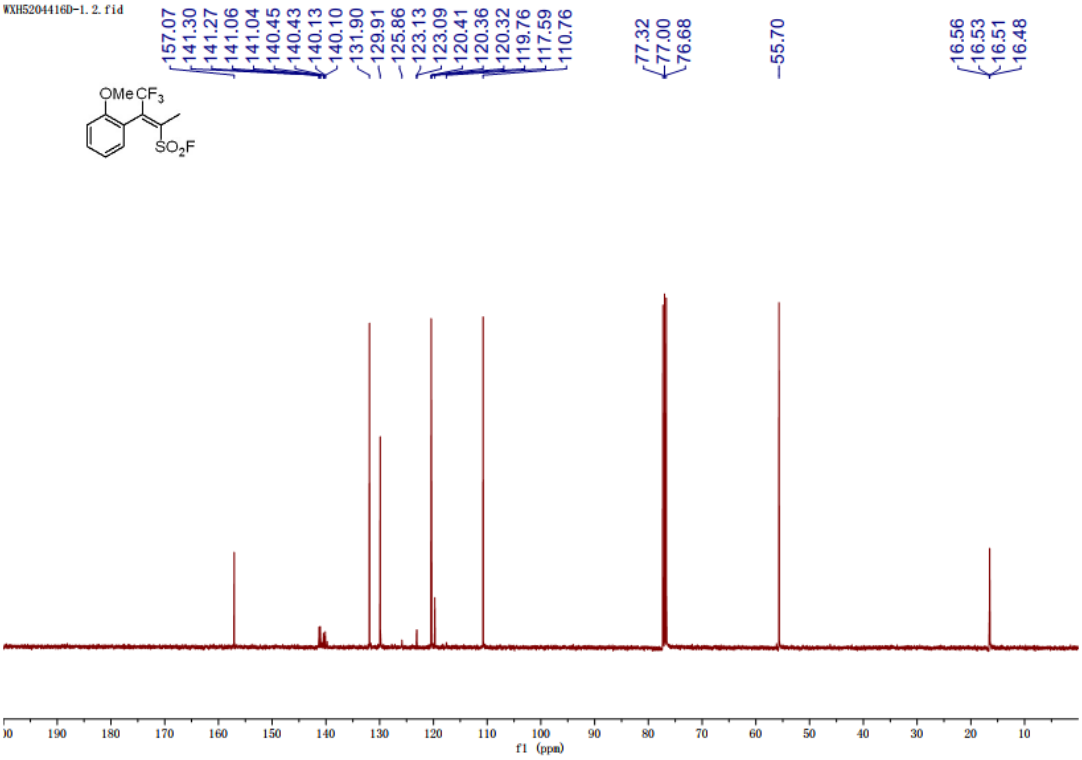
NC
SO2F
f1 (ppm)






WXH5204416D-1.2.fid
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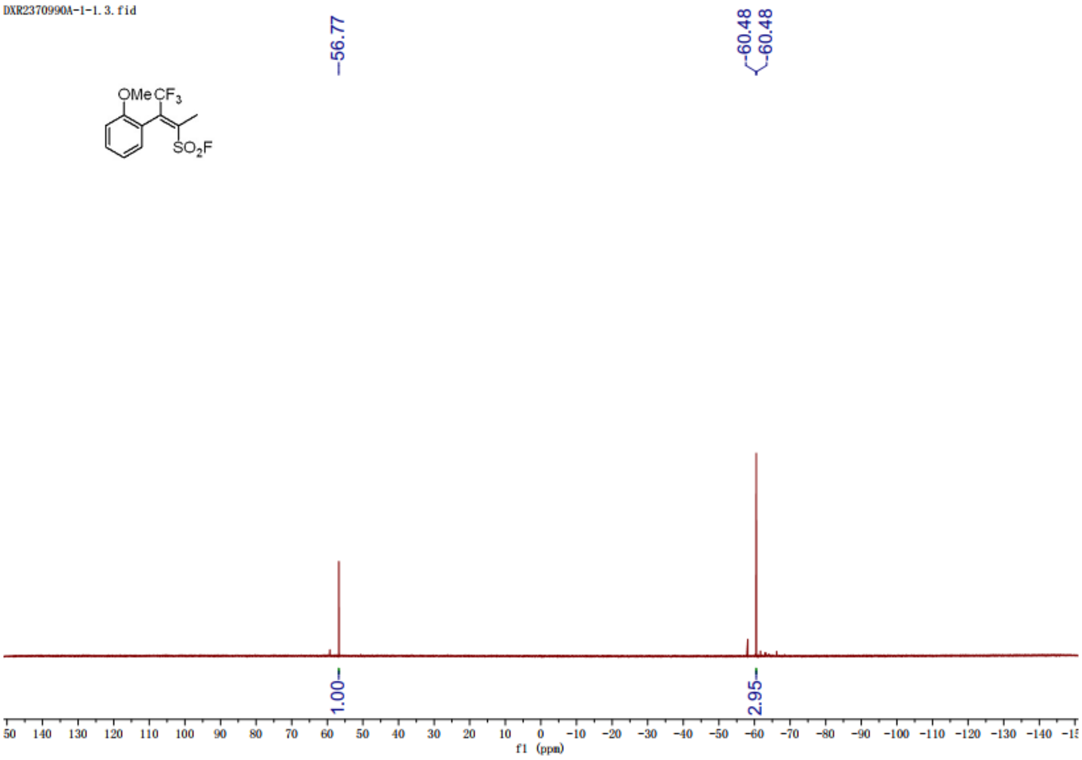
141.06
141.04
140.45
140.43
140.13
140.10
131.90
129.91
125.86
123.13
123.09
120.41
120.36
120.32
119.76
117.59
110.76
77.32
77.00
76.68
55.70
16.56
16.53
16.51
16.48
OMe
CF3
SO2F
f1 (ppm)


DXR2370990A-1-1.3.fid
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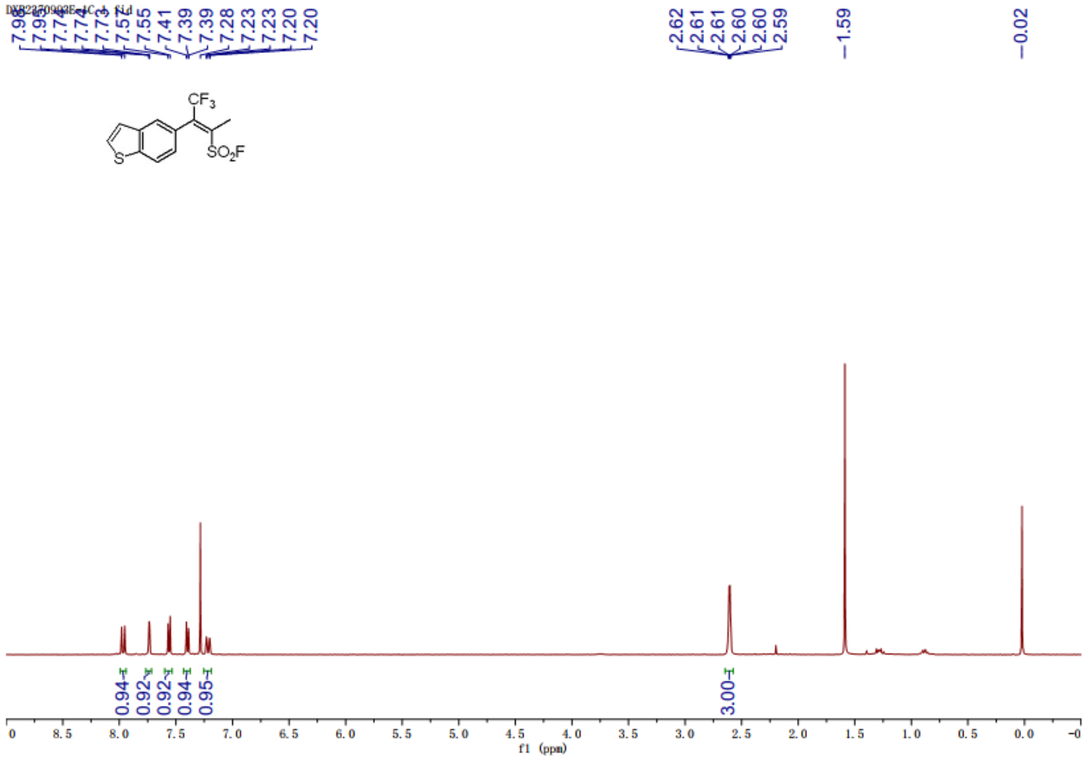
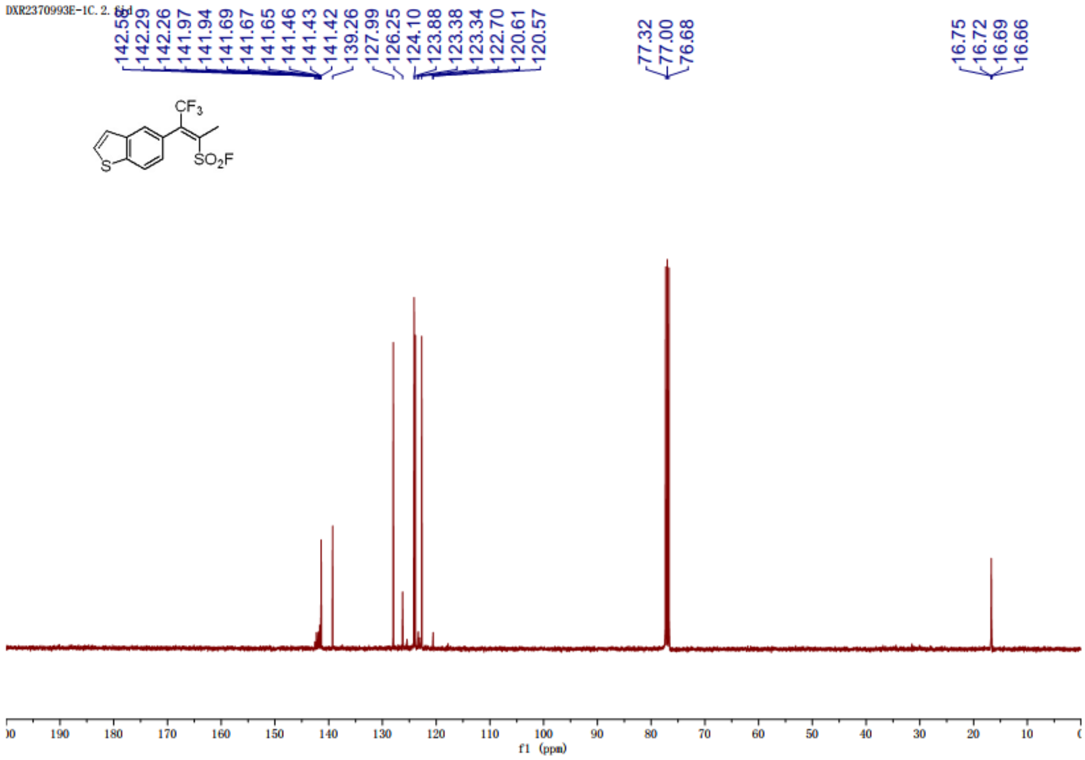
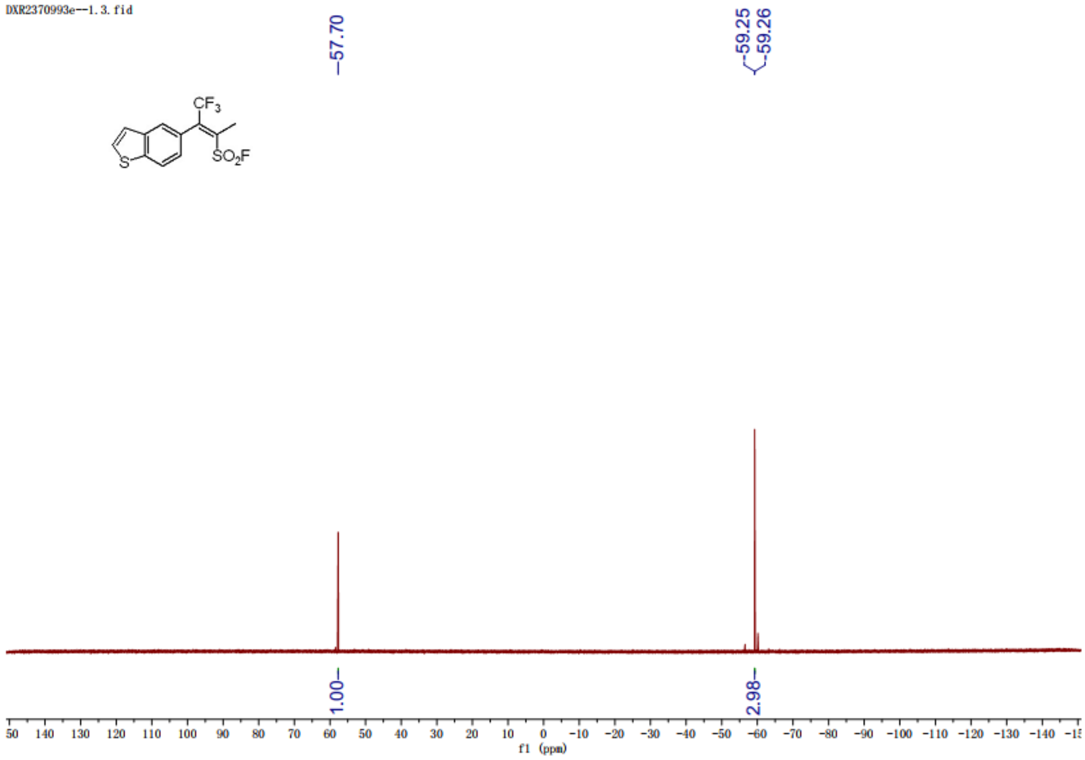
-60.48
OMe
CF3
SO2F
1.00
2.95
f1 (ppm)






DXR2370993e--1.3.fid
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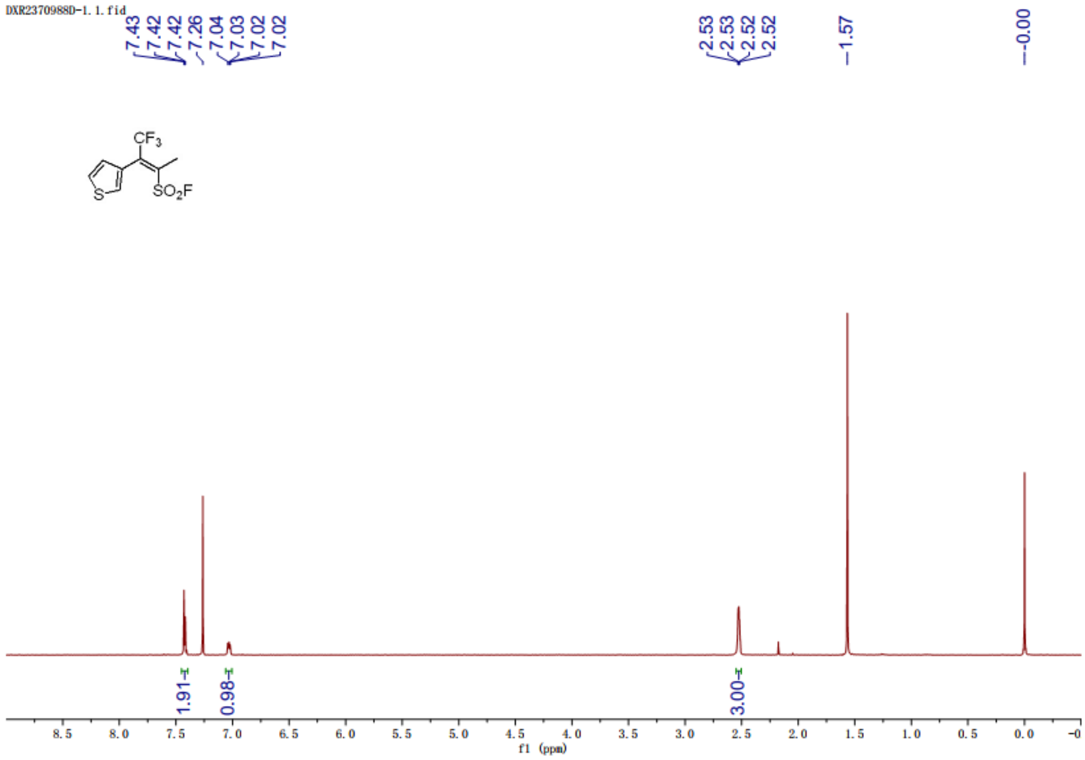
-59.25
-59.26
CF3
SO2F
S
1.00
2.98
f1 (ppm)


DXR2370988D-1.1.fid
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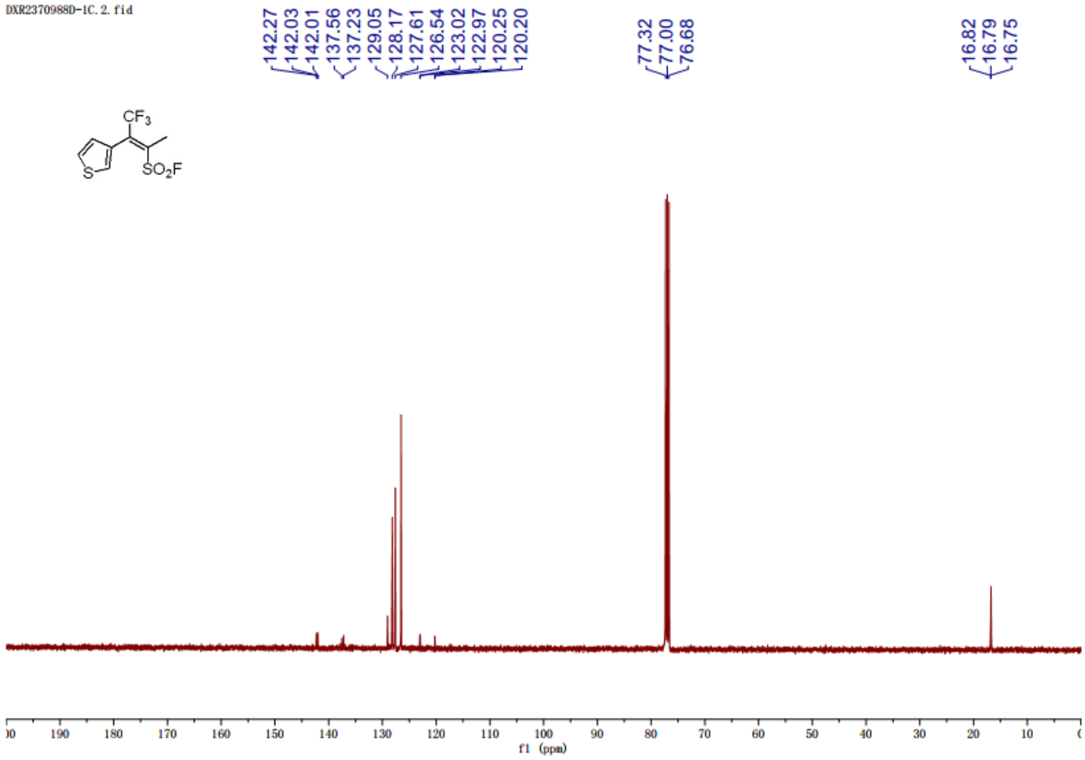
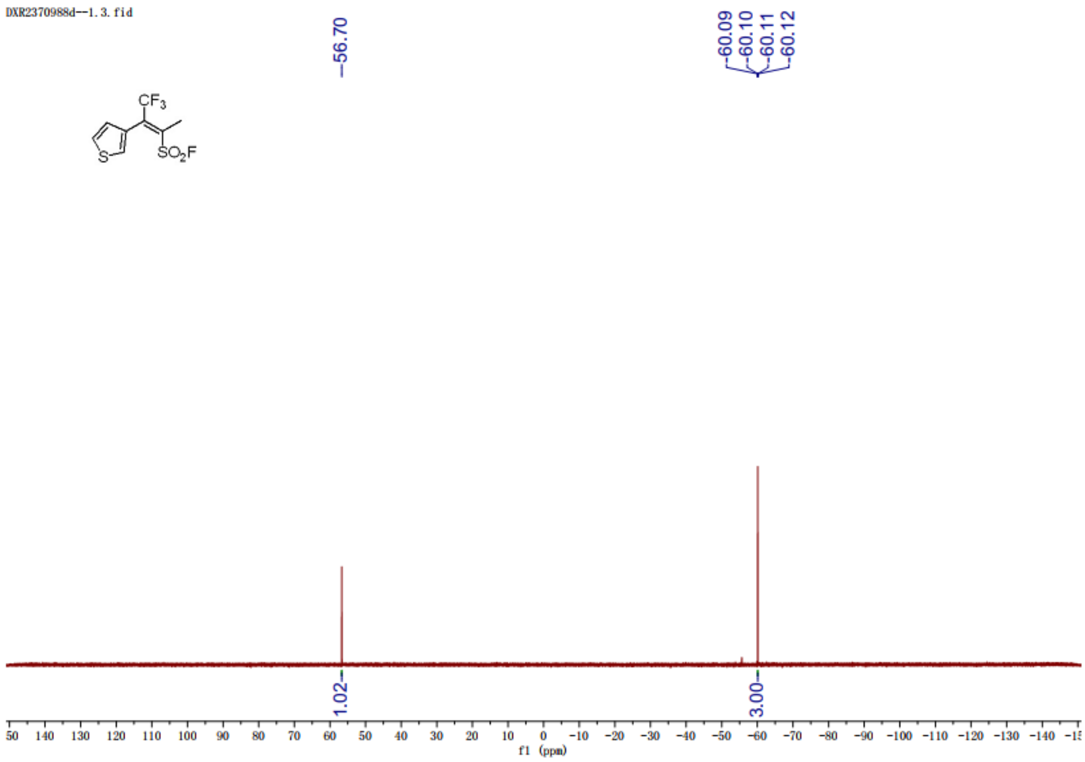
7.42
7.42
7.26
7.04
7.03
7.02
7.02
2.53
2.53
2.52
2.52
1.57
-0.00
CF3
SO2F
S
1.91
0.98
3.00
f1 (ppm)


DXR2370988D-1C.2.fid
142.27
142.03
142.01
137.56
137.23
129.05
128.17
127.61
126.54
123.02
122.97
120.25
120.20
77.32
77.00
76.68
16.82
16.79
16.75
CF3
S
SO2F
f1 (ppm)


DXR2370988d--1.3.fid
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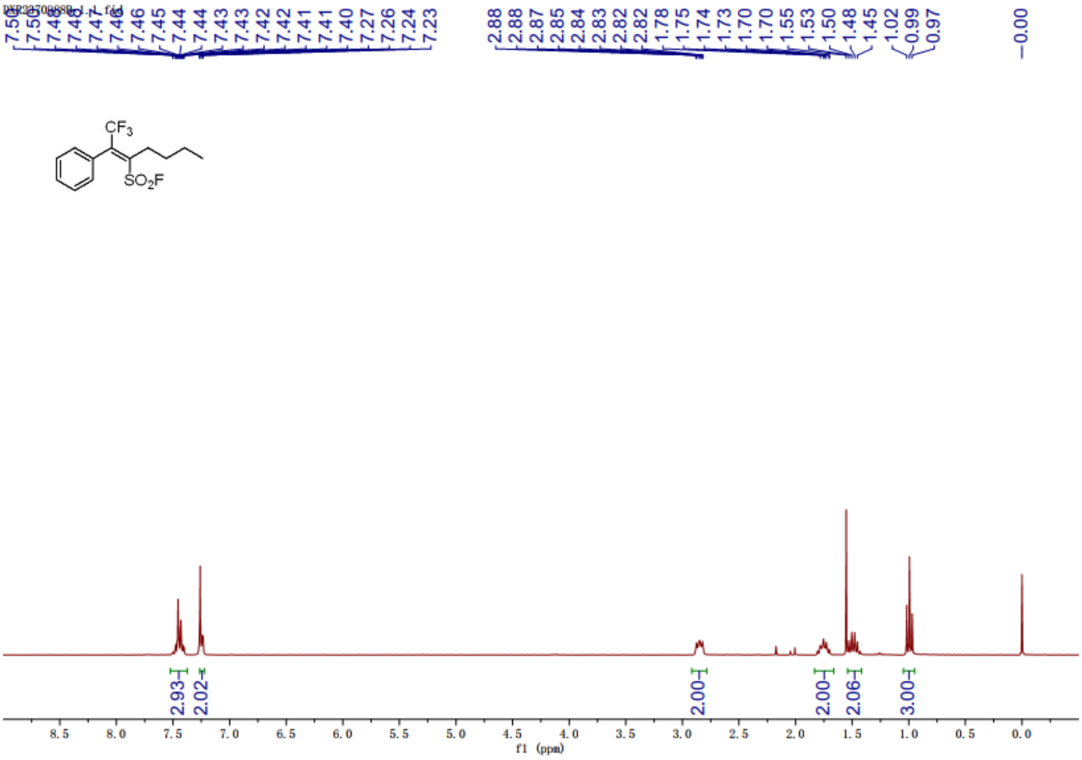
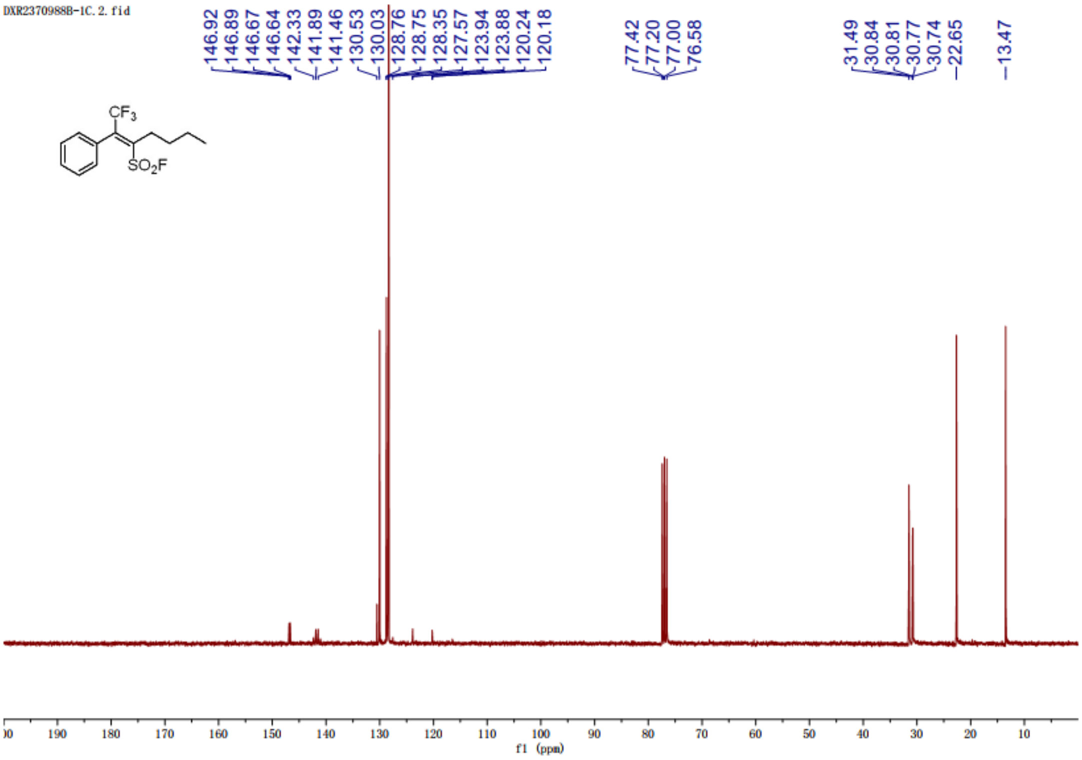
-60.10
-60.11
-60.12
CF3
S
SO2F
1.02
3.00
f1 (ppm)


7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.27
7.26
7.24
7.23
2.88
2.88
2.87
2.85
2.84
2.83
2.82
2.82
1.78
1.75
1.74
1.73
1.70
1.70
1.55
1.53
1.50
1.48
1.45
1.02
0.99
0.97
0.00
CF3
SO2F
2.93
2.02
2.00
2.00
2.06
3.00
f1 (ppm)


DXR2370988B-1C.2.fid
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146.67
146.64
142.33
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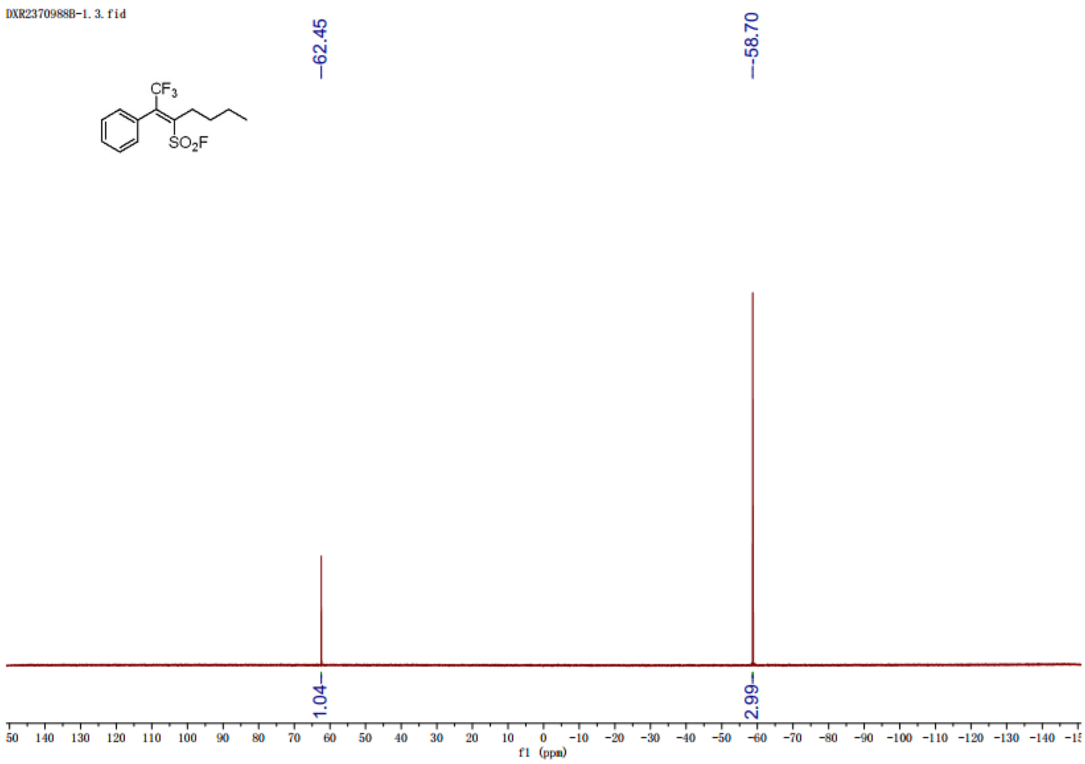
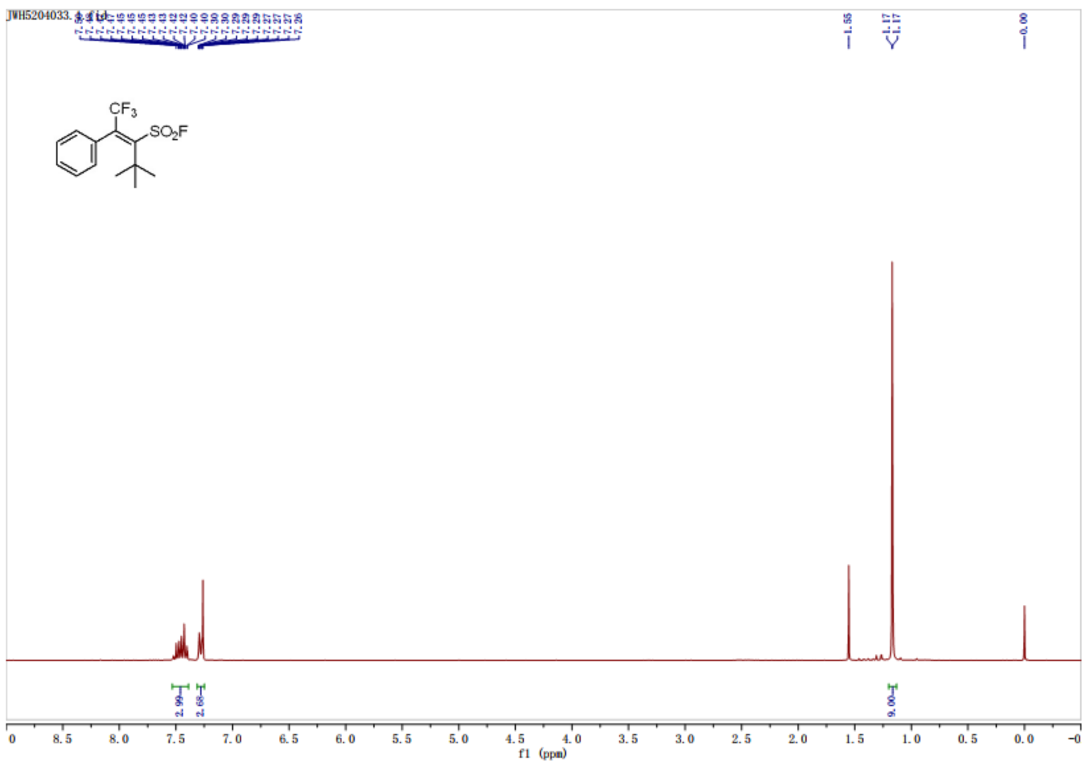
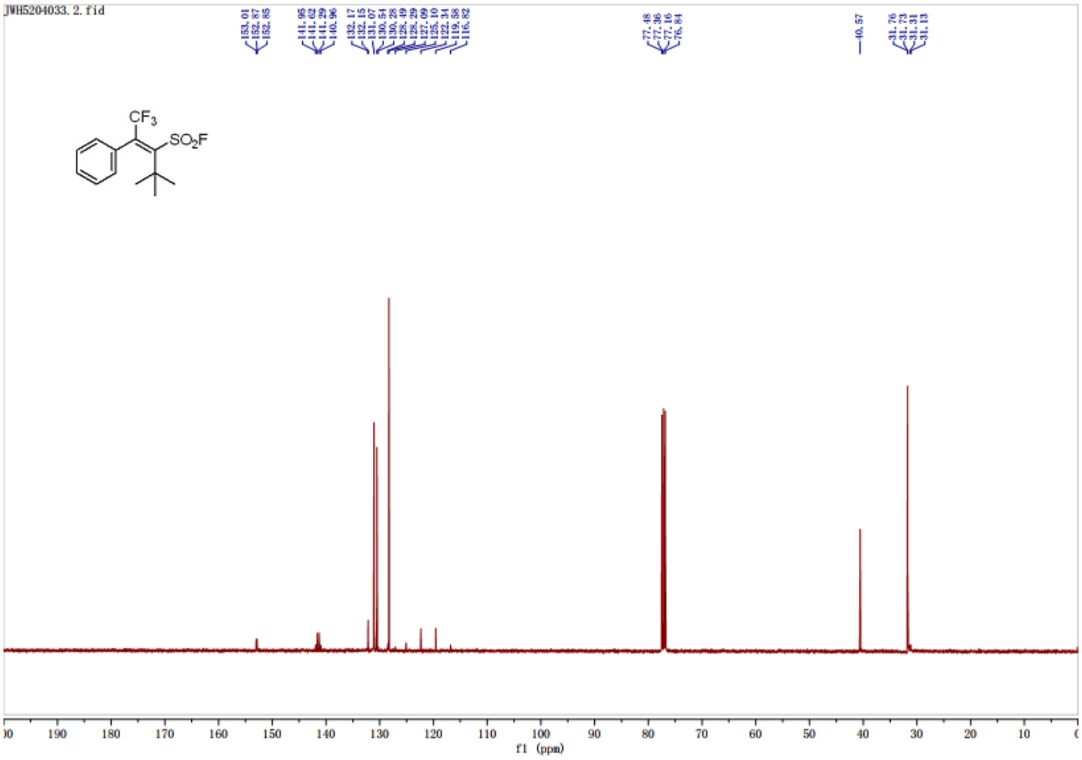
141.46
130.53
130.03
128.76
128.75
128.35
127.57
123.94
123.88
120.24
120.18
77.42
77.20
77.00
76.58
31.49
30.84
30.81
30.77
30.74
22.65
13.47
CF3
SO2F
f1 (ppm)


DXR2370988B-1.3.fid
CF3
SO2F
-62.45
-58.70
1.04
2.99
f1 (ppm)


CF3
SO2F
1.55
1.17
1.17
0.00
2.99
2.08
9.00
f1 (ppm)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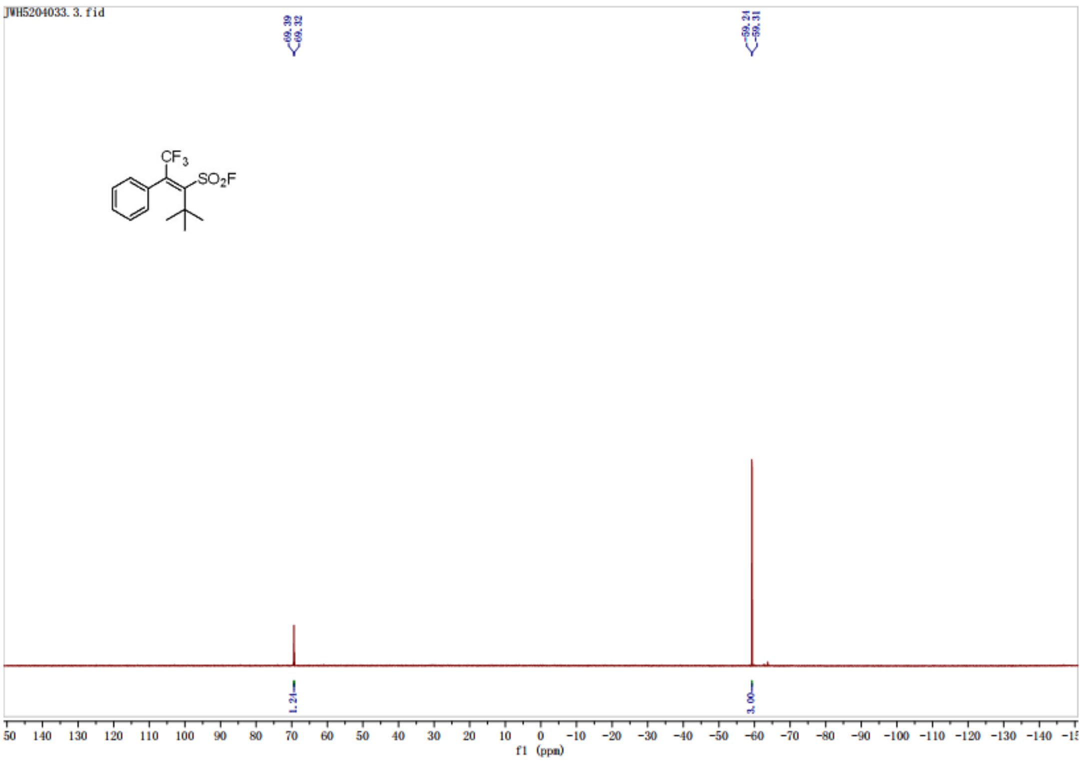
CF3
SO2F
f1 (ppm)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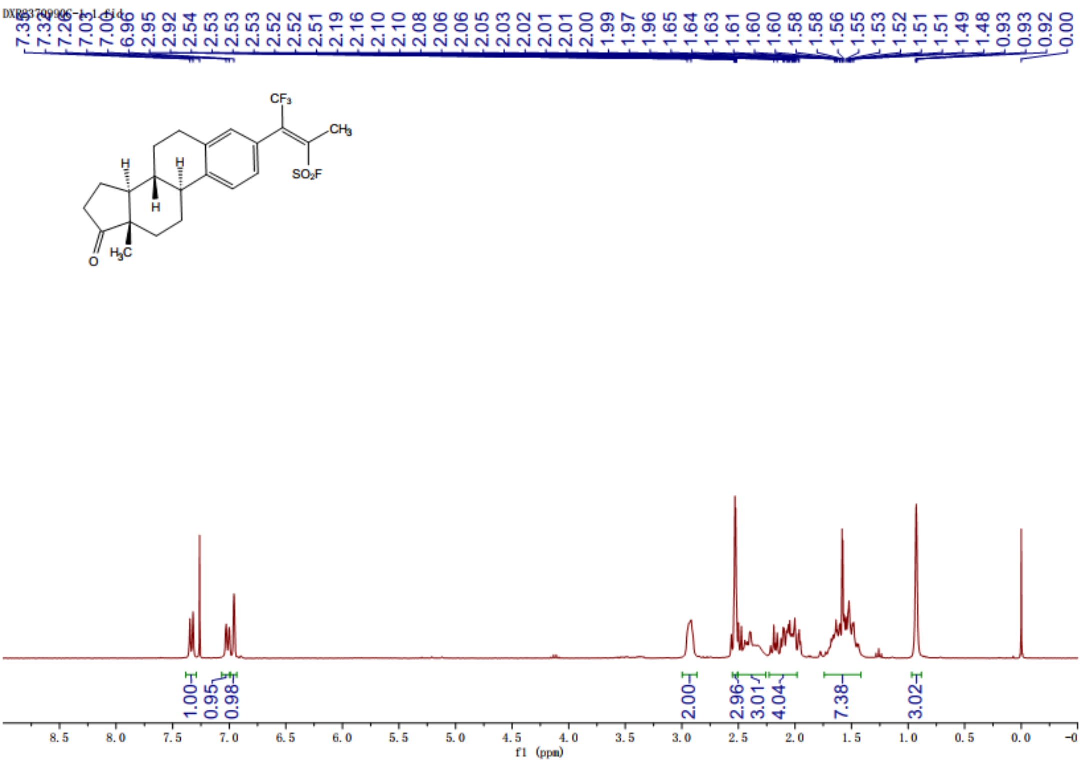
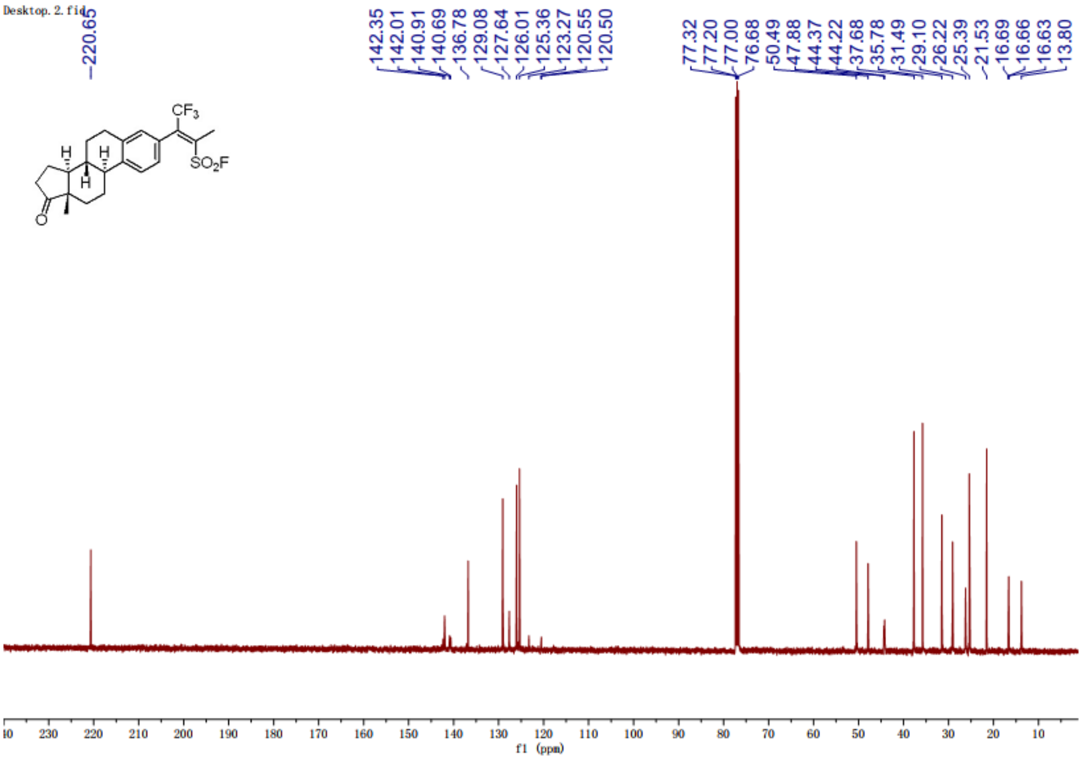
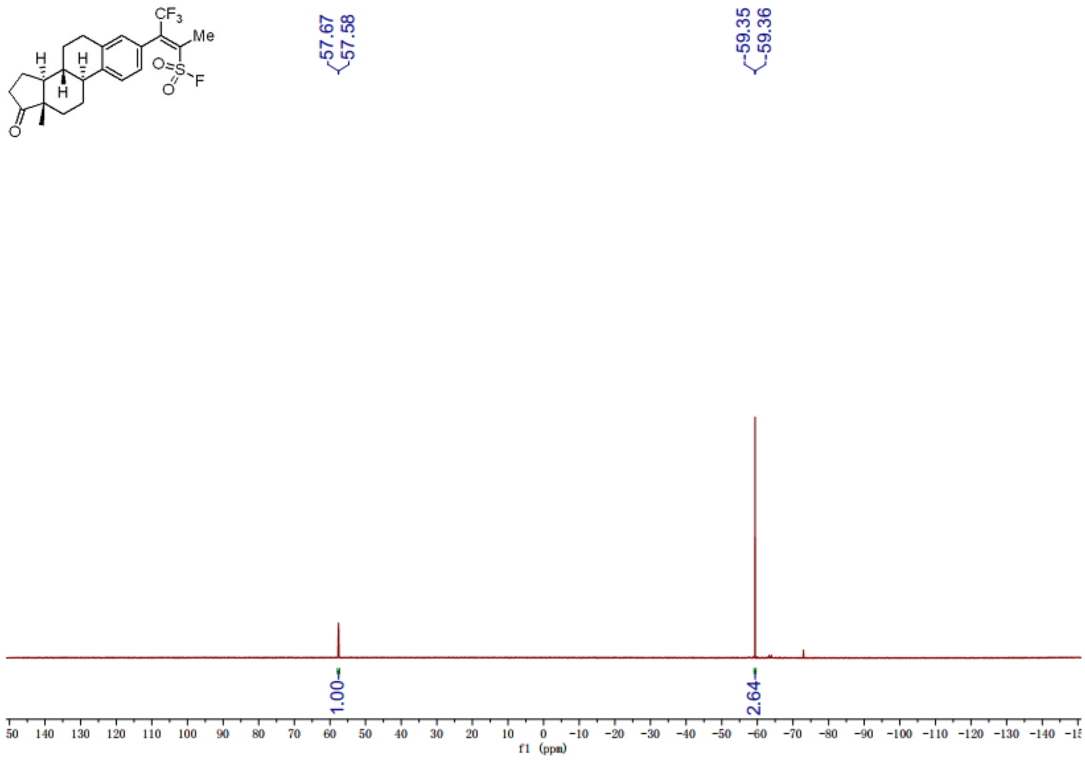
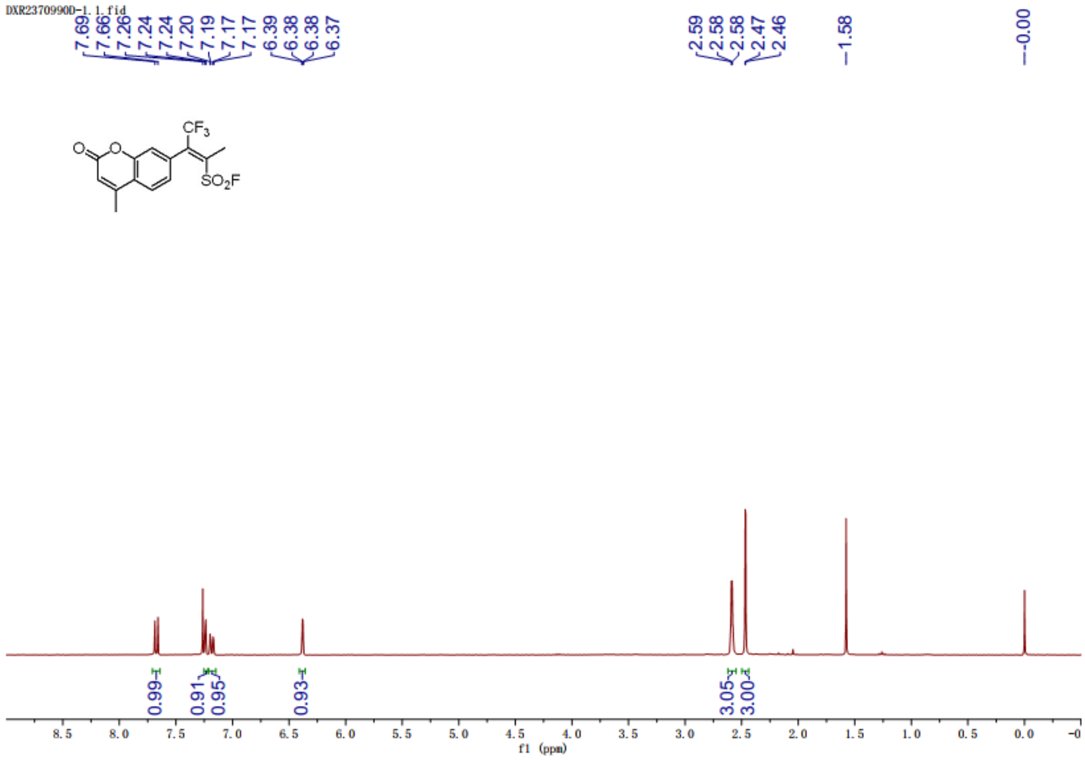
CF3
SO2F
f1 (ppm)


CF3
CH3
SO2F
H
H
H
O
H3C
2.00
2.96
3.01
4.04
7.38
3.02
1.00
0.95
0.98
f1 (ppm)


Desktop.2.fid
220.65
142.35
142.01
140.91
140.69
136.78
129.08
127.64
126.01
125.36
123.27
120.55
120.50
77.32
77.20
77.00
76.68
50.49
47.88
44.37
44.22
37.68
35.78
31.49
29.10
26.22
25.39
21.53
16.69
16.66
16.63
13.80
CF3
SO2F
H
H
H
O
f1 (ppm)


CF3
Me
H
H
H
O
S
O
F
57.67
57.58
59.35
59.36
1.00
2.64
f1 (ppm)


DXR23709900-1.1.fid
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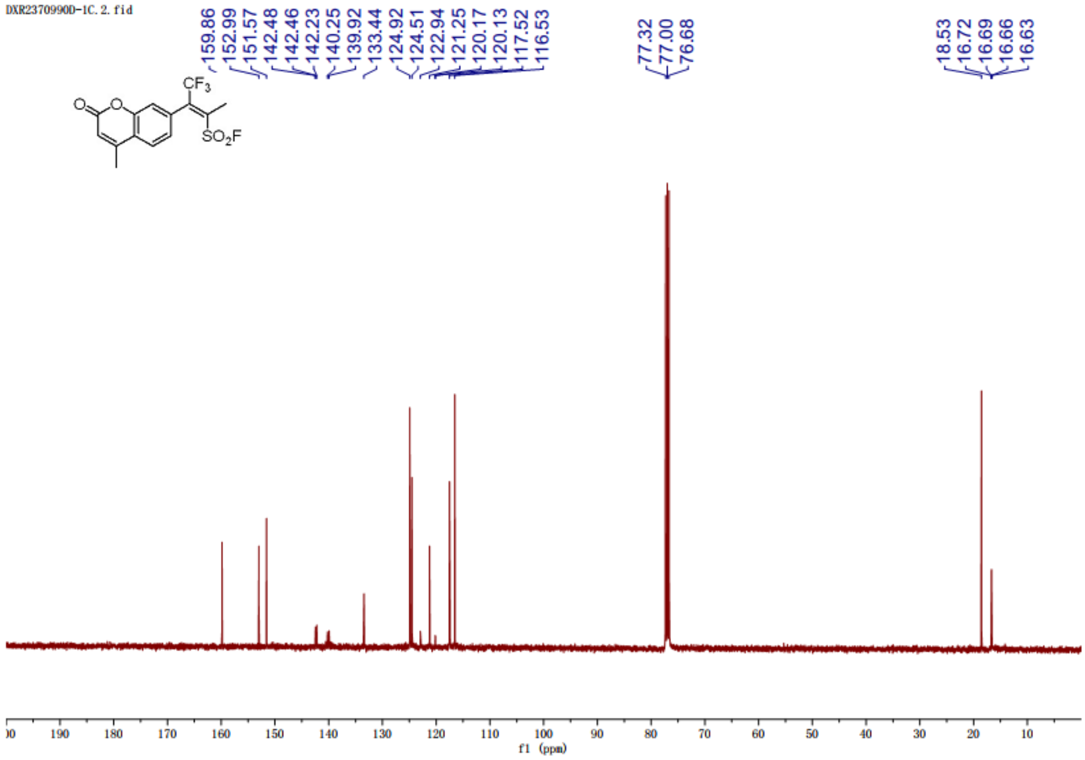
7.66
7.26
7.24
7.24
7.20
7.19
7.17
7.17
6.39
6.38
6.38
6.37
2.59
2.58
2.58
2.47
2.46
1.58
0.00
CF3
SO2F
0.99
0.91
0.95
0.93
3.05
3.00
f1 (ppm)


DXR2370990D-1C.2.fid
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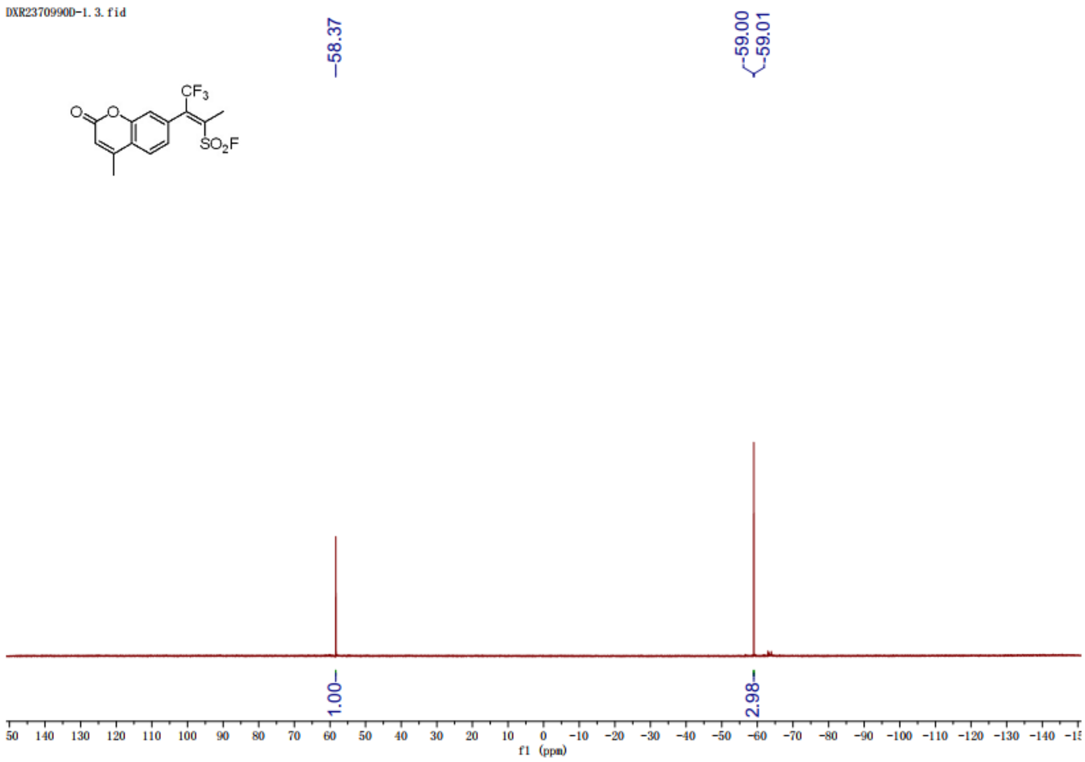
152.99
151.57
142.48
142.46
142.23
140.25
139.92
133.44
124.92
124.51
122.94
121.25
120.17
120.13
117.52
116.53
77.32
77.00
76.68
18.53
16.72
16.69
16.66
16.63
CF3
SO2F
f1 (ppm)


DXR2370990D-1.3.fid
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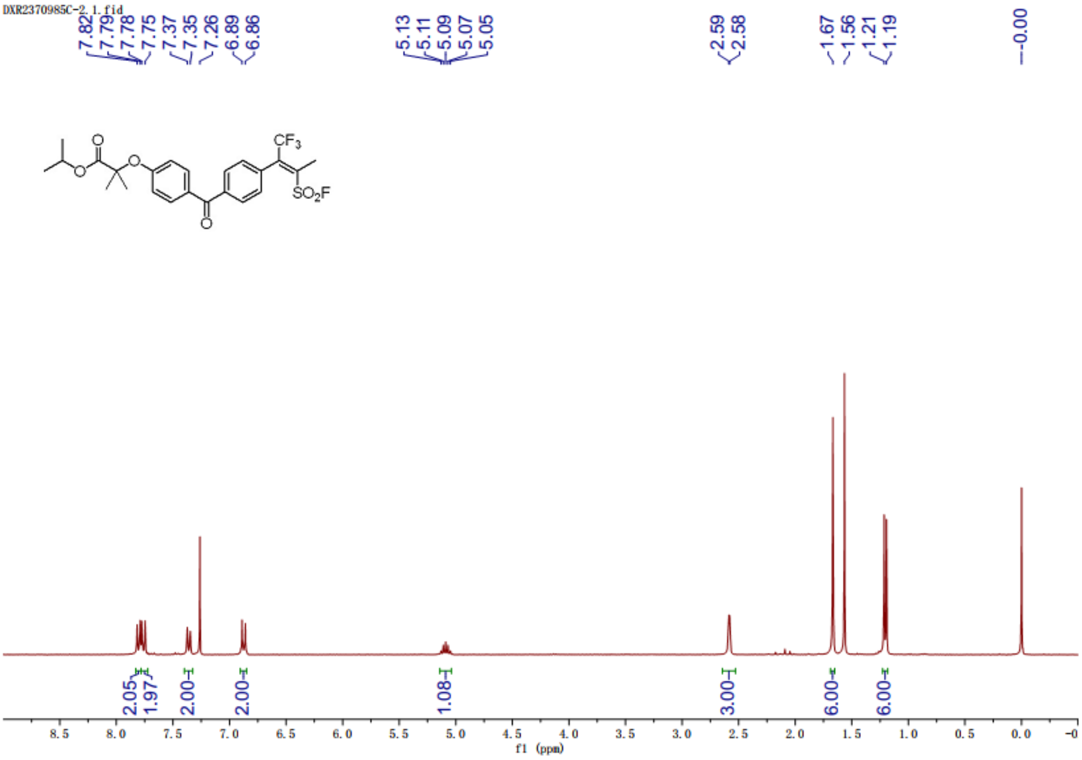
-59.00
-59.01
CF3
SO2F
1.00
2.98
f1 (ppm)


DXR2370985C-2.1.fid
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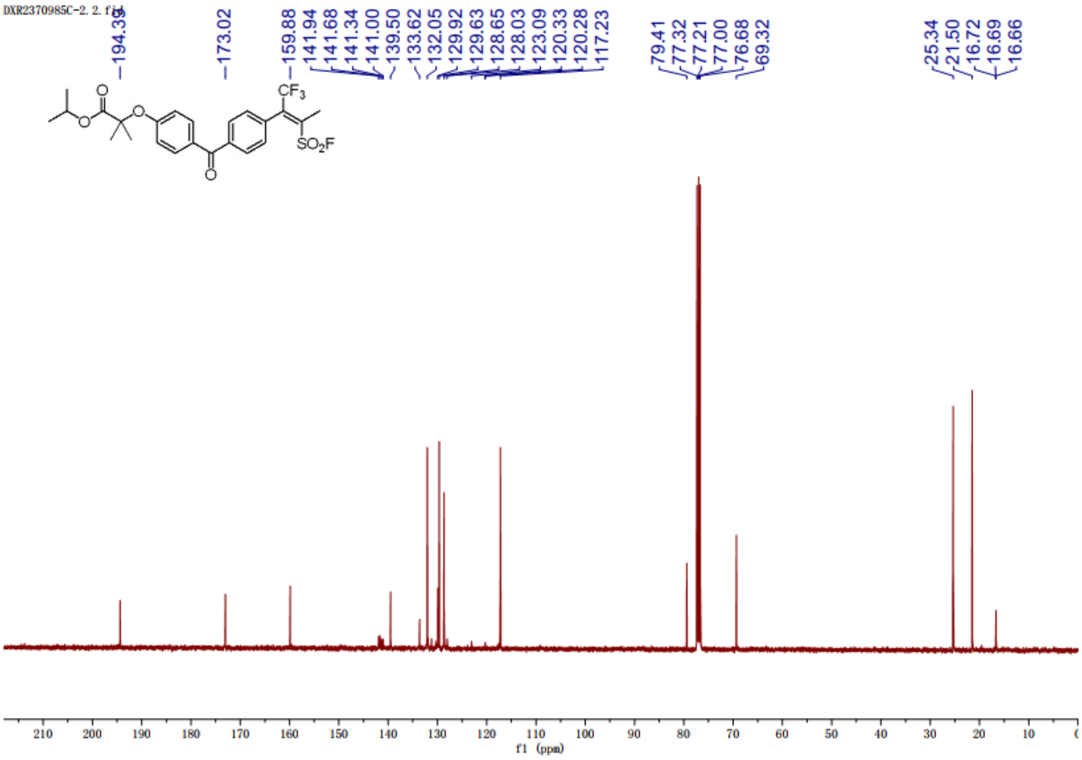
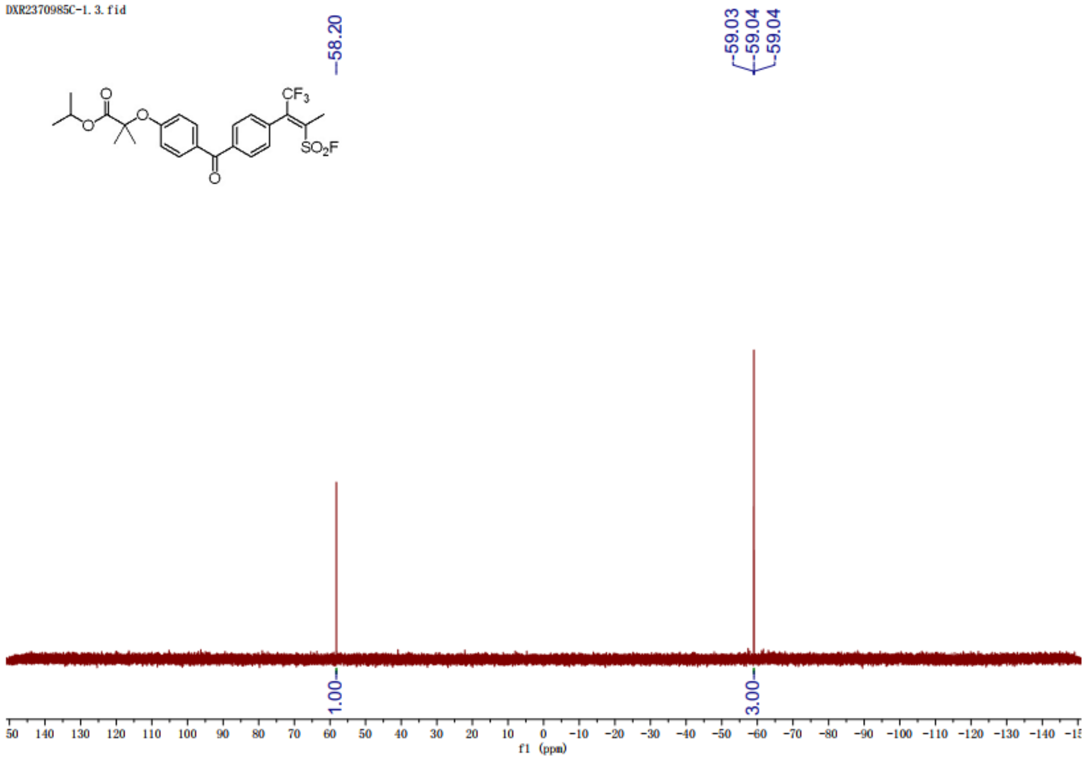
7.79
7.78
7.75
7.37
7.35
7.26
6.89
6.86
5.13
5.11
5.09
5.07
5.05
2.59
2.58
1.67
1.56
1.21
1.19
-0.00
CF3
SO2F
2.05
1.97
2.00
2.00
1.08
3.00
6.00
6.00
f1 (ppm)


DXR2370985C-2.2.fid
194.39
173.02
159.88
141.94
141.68
141.34
141.00
139.50
133.62
132.05
129.92
129.63
128.65
128.03
123.09
120.33
120.28
117.23
79.41
77.32
77.21
77.00
76.68
69.32
25.34
21.50
16.72
16.69
16.66
CF3
SO2F
f1 (ppm)


DXR2370985C-1.3.fid
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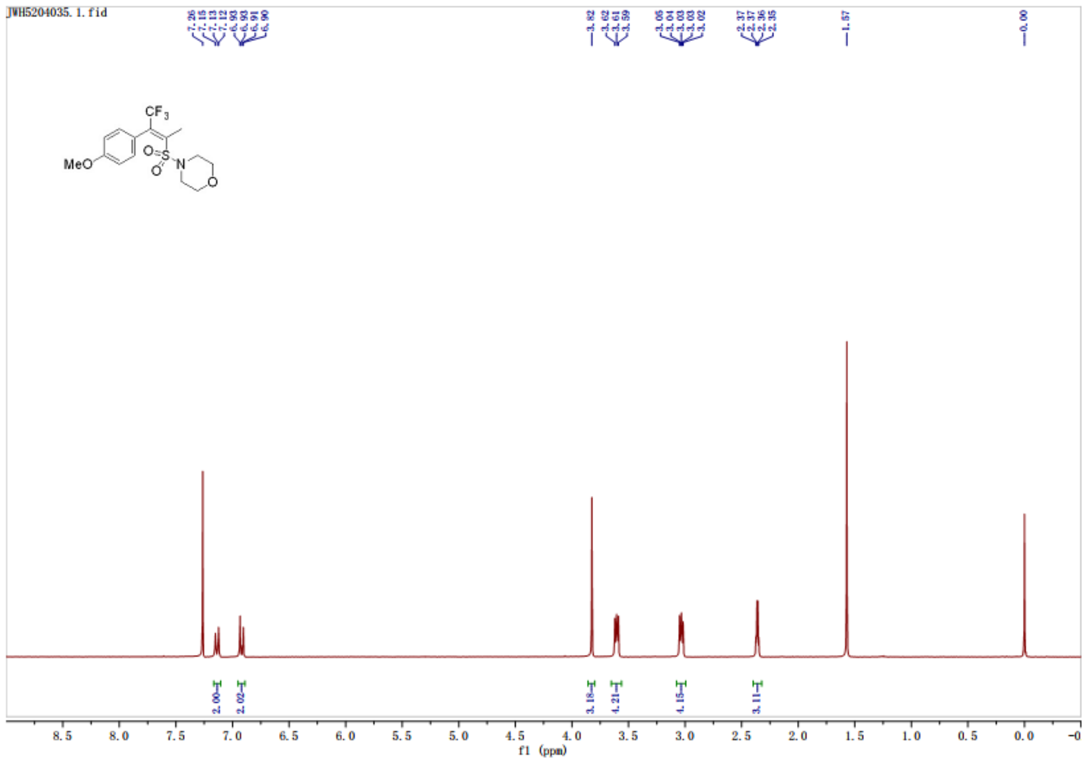
-59.04
-59.04
1.00
3.00
f1 (ppm)


JWH5204035.1.fid
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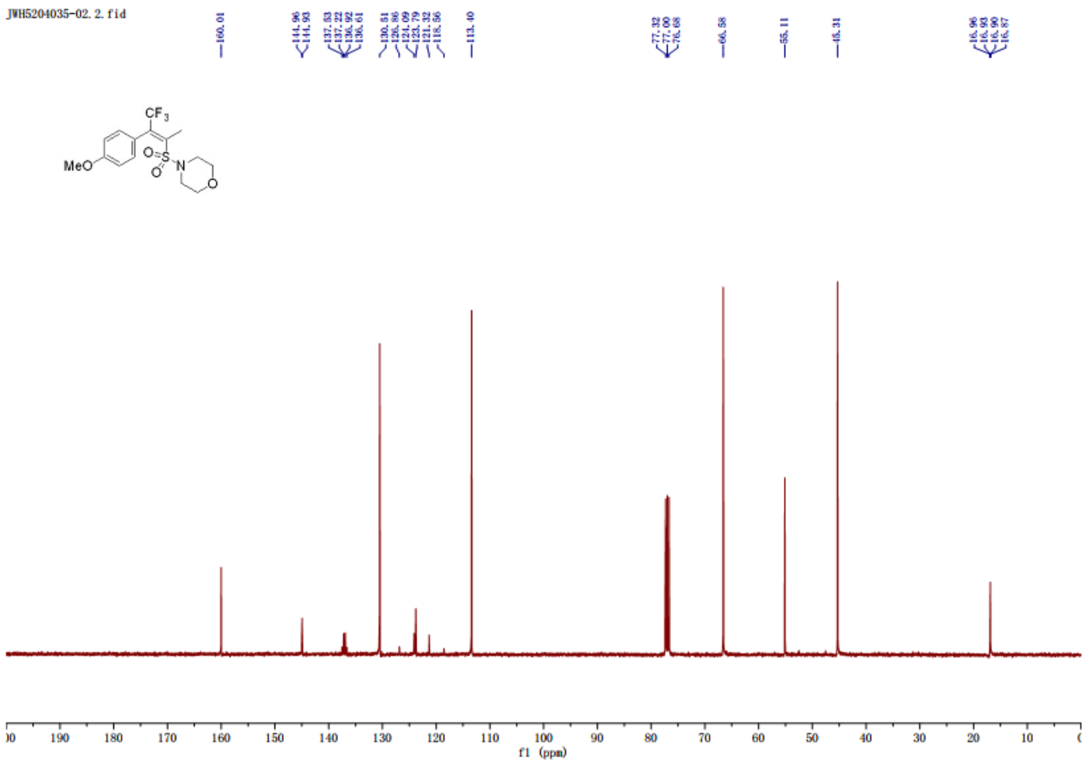
7.15
7.13
7.12
6.93
6.93
6.91
6.90
3.82
3.62
3.61
3.59
3.05
3.04
3.03
3.03
3.02
2.37
2.37
2.36
2.35
1.57
0.00
MeO
2.00
2.02
3.18
4.21
4.15
3.11
f1 (ppm)


JWH5204035-02.2.fid
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144.93
137.53
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136.61
130.51
126.86
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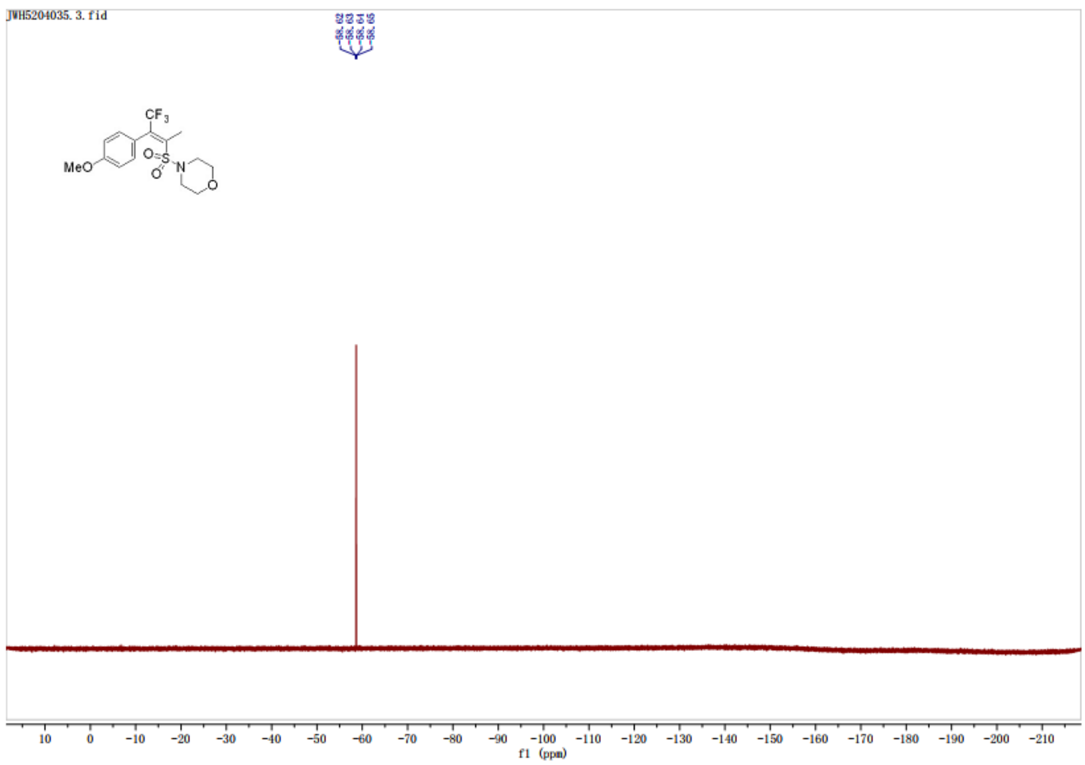
123.79
121.32
118.56
113.40
77.32
77.00
76.68
66.58
55.11
45.31
16.96
16.93
16.90
16.87
CF3
MeO
O
S
O
N
O
f1 (ppm)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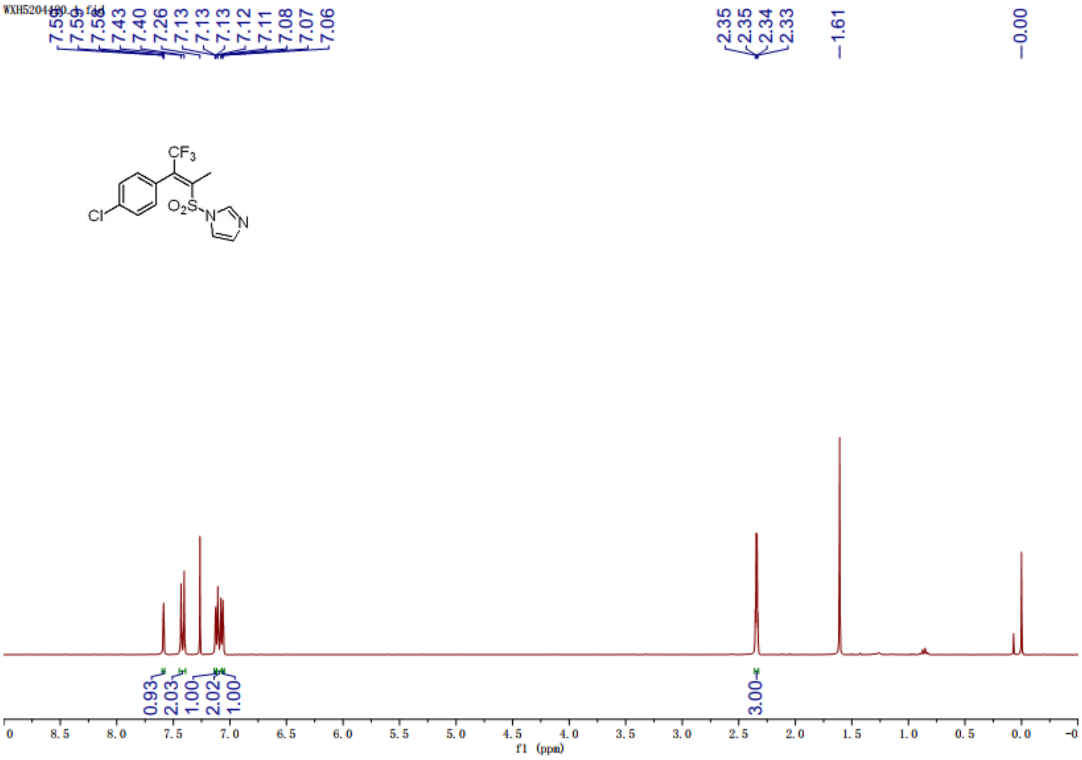
CF3
MeO
O
S
O
N
O
f1 (ppm)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7.53
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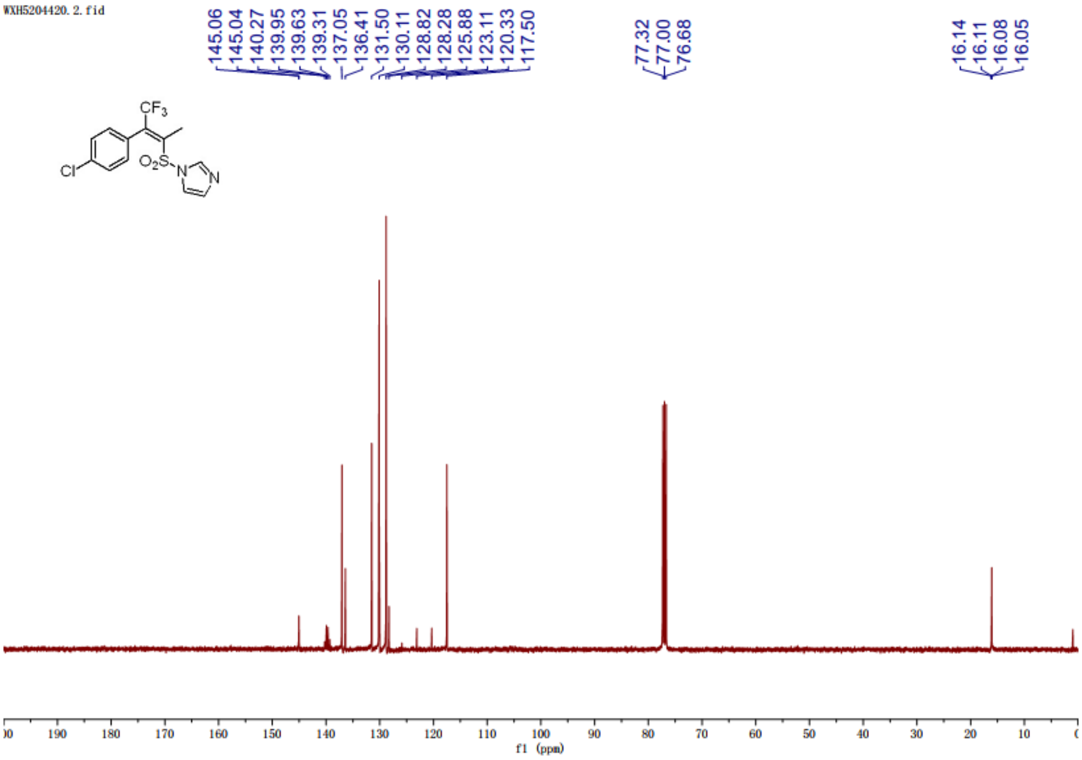
7.26
7.13
7.13
7.13
7.12
7.11
7.08
7.07
7.06
2.35
2.35
2.34
2.33
1.61
0.00
CF3
Cl
O2S
N
N
0.93
2.03
1.00
2.02
1.00
3.00
f1 (ppm)


WXH5204420.2.fid
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139.63
139.31
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136.41
131.50
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128.28
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123.11
120.33
117.50
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CF3
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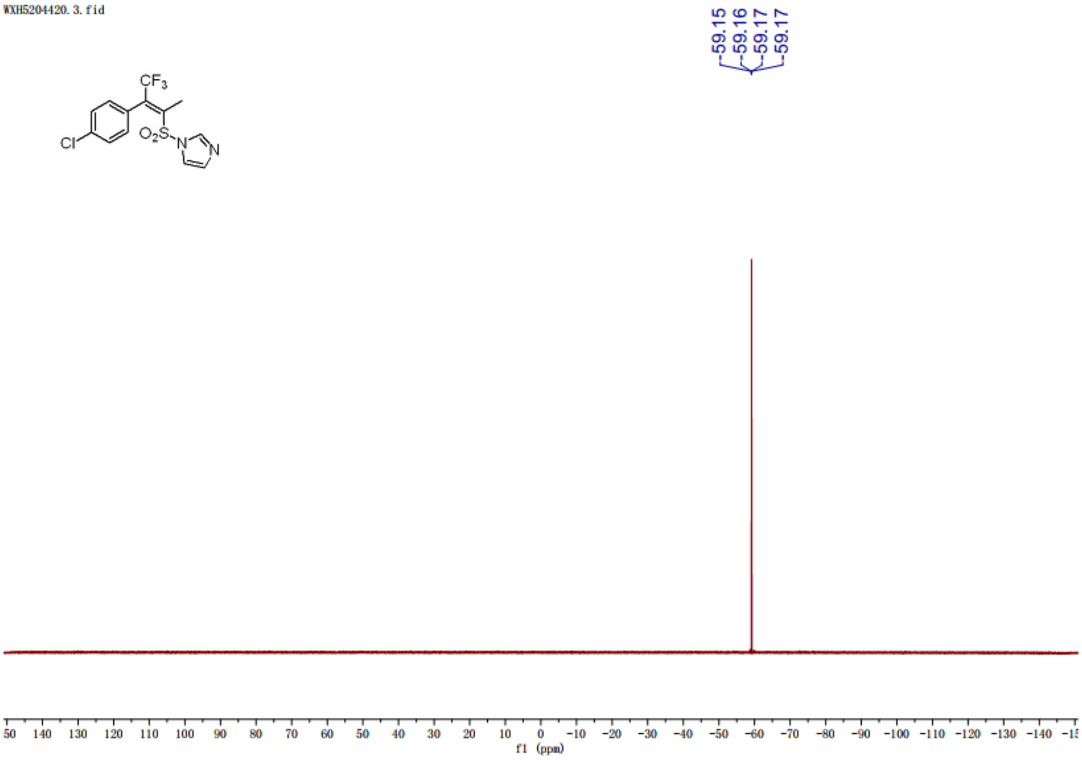
O2S
N
N
f1 (ppm)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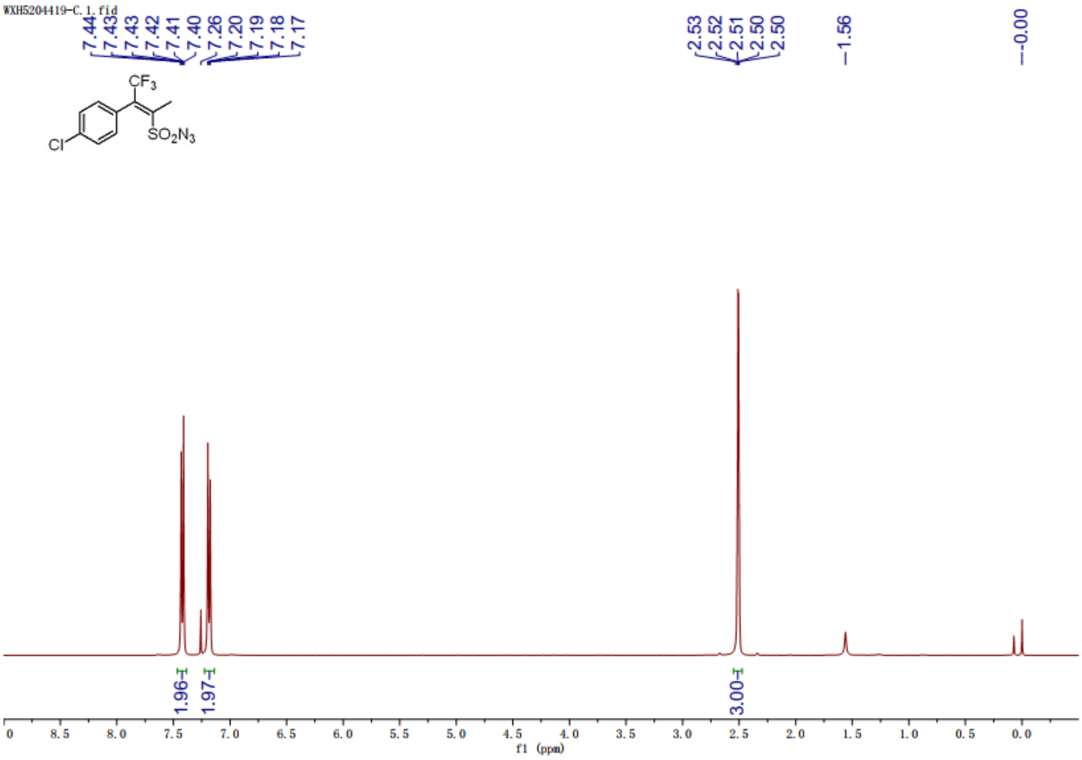
-59.17
-59.17
CF3
O2S
N
N
Cl
f1 (ppm)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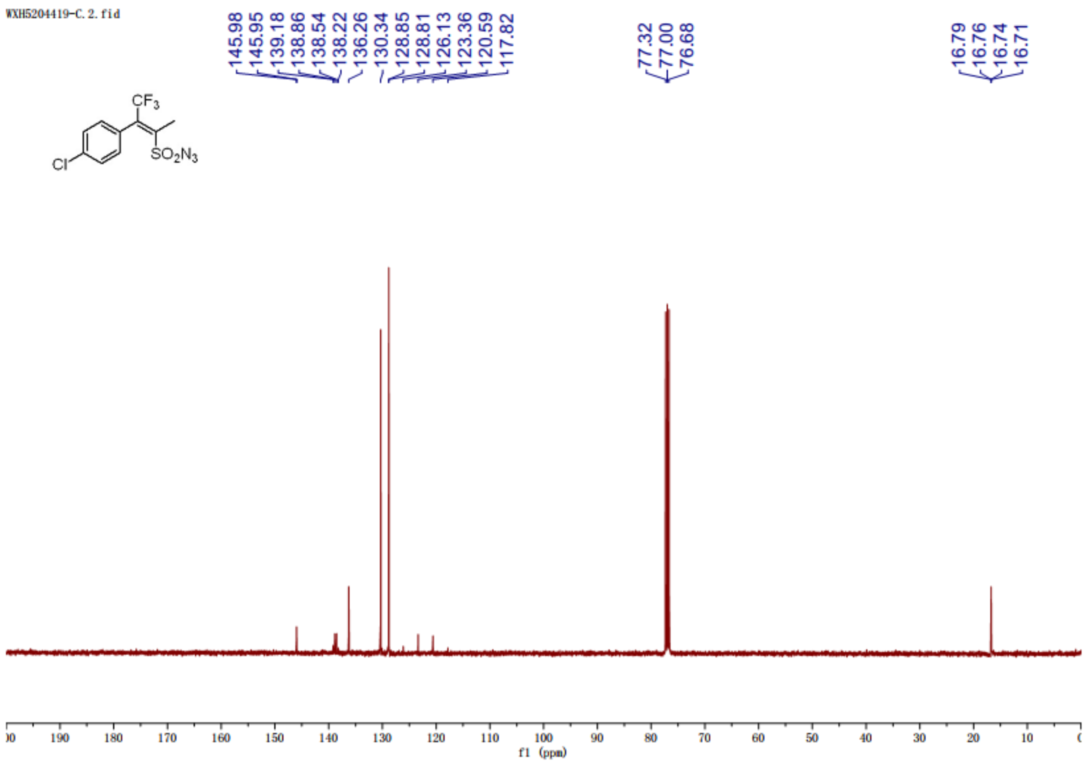
7.43
7.42
7.41
7.40
7.26
7.20
7.19
7.18
7.17
2.53
2.52
2.51
2.50
2.50
1.56
-0.00
CF3
SO2N3
Cl
1.96
1.97
3.00
f1 (ppm)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130.34
128.85
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126.13
123.36
120.59
117.82
77.32
77.00
76.68
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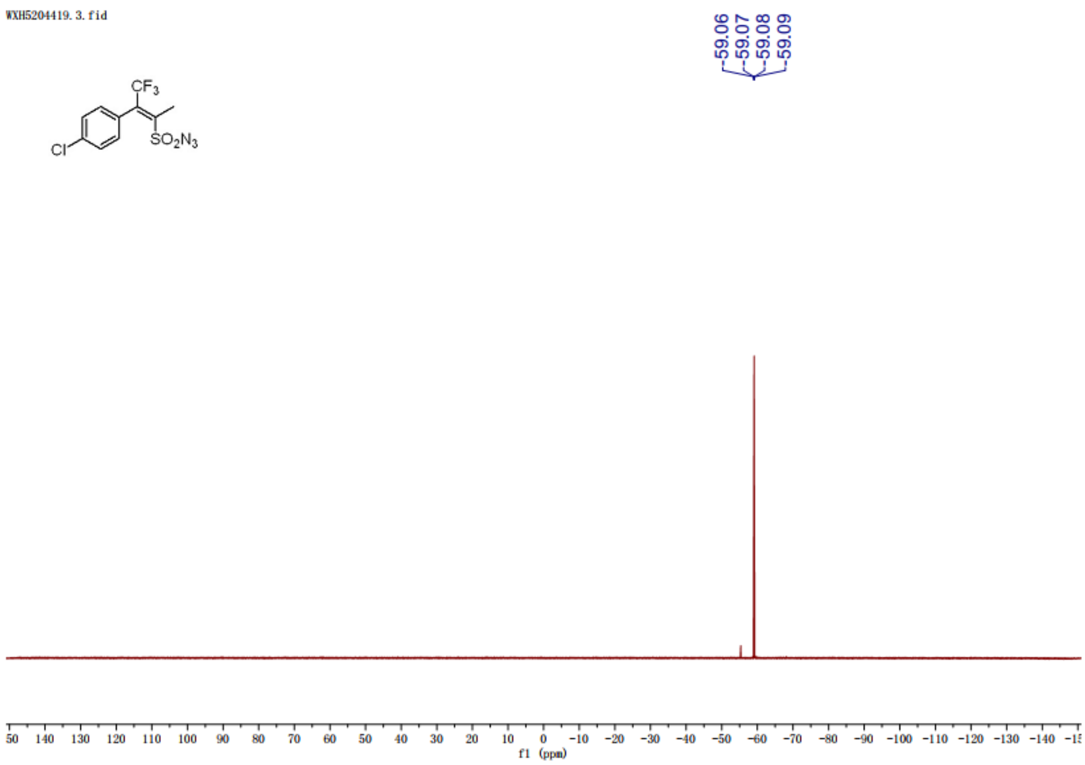
16.76
16.74
16.71
CF3
Cl
SO2N3
f1 (ppm)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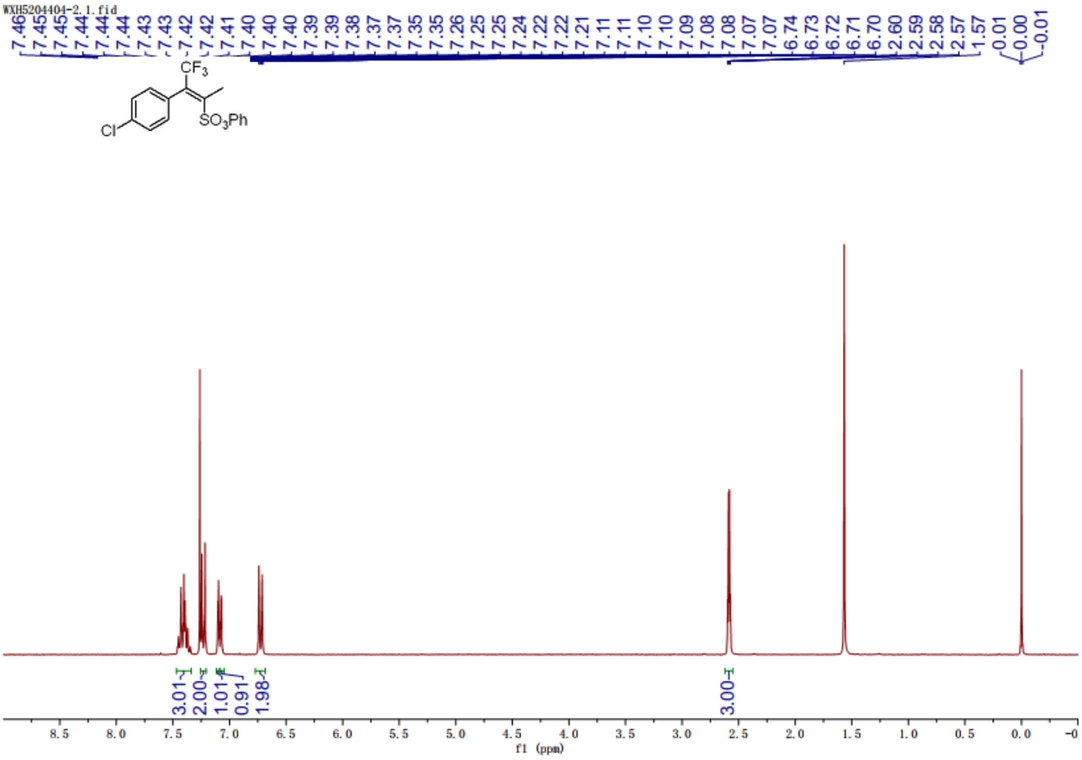
CF3
Cl
SO2N3
f1 (ppm)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7.44
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7.43
7.42
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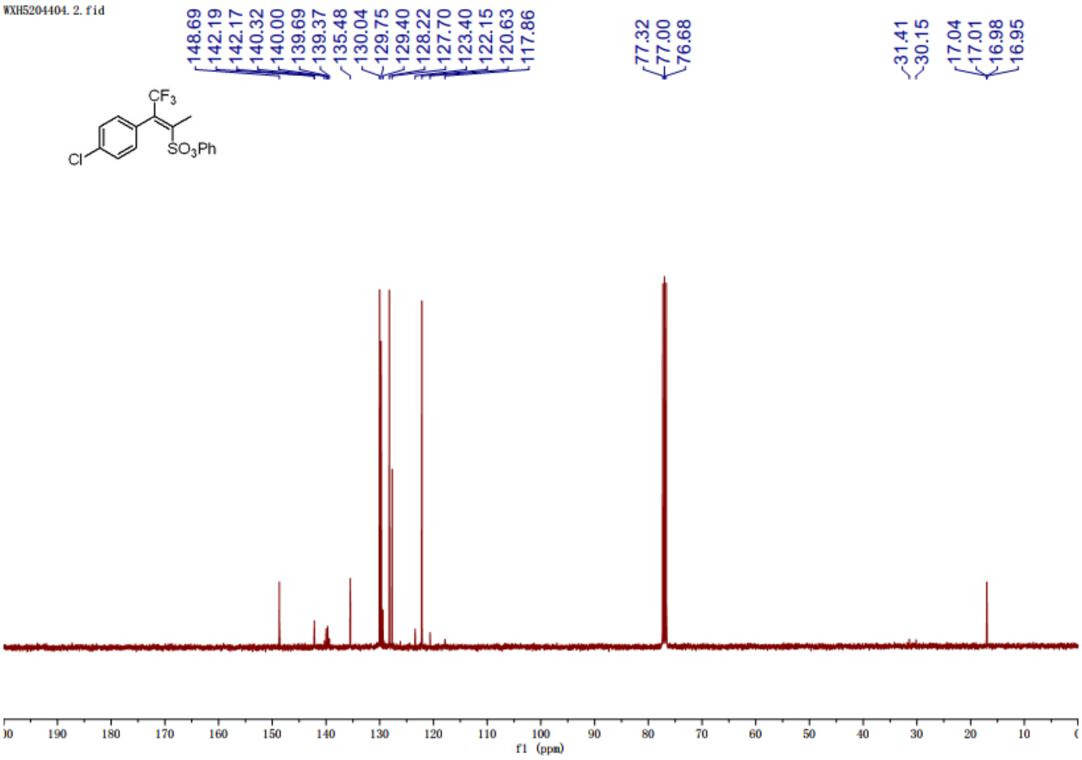
7.08
7.07
7.07
6.74
6.73
6.72
6.71
6.70
2.60
2.59
2.58
2.57
1.57
0.01
0.00
-0.01
CF3
SO3Ph
Cl
3.01
2.00
1.01
0.91
1.98
3.00
f1 (ppm)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139.37
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128.22
127.70
123.40
122.15
120.63
117.86
77.32
77.00
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31.41
30.15
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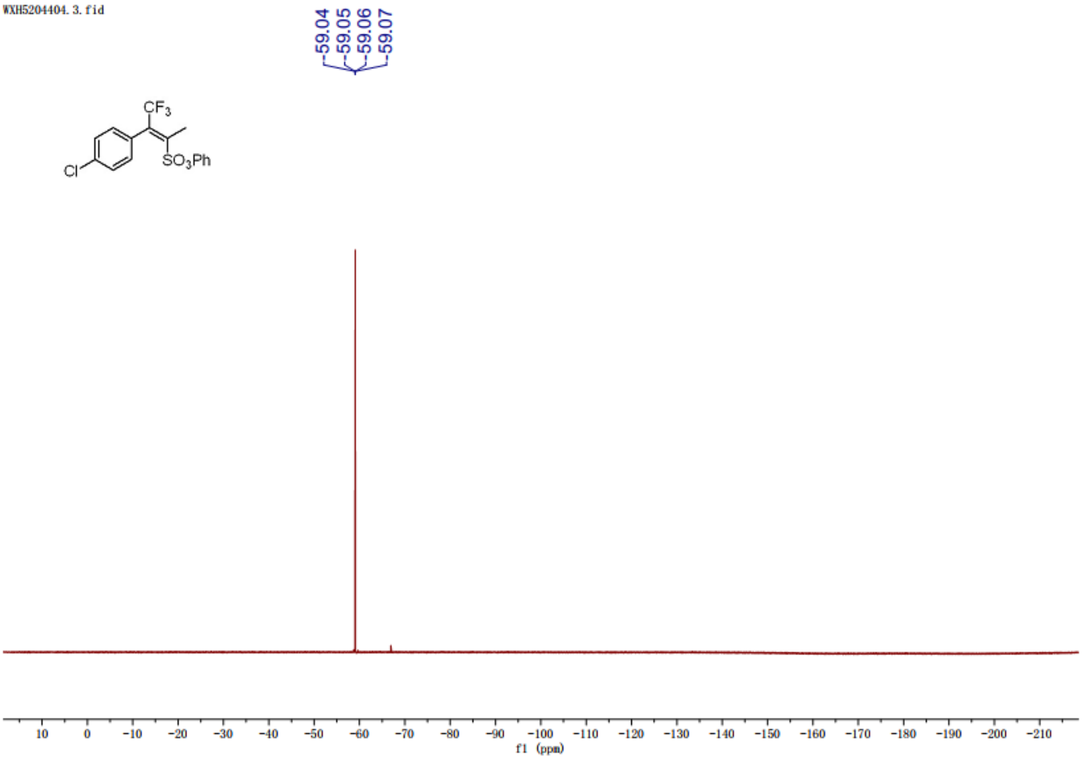
17.01
16.98
16.95
CF3
SO3Ph
Cl
f1 (ppm)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-59.06
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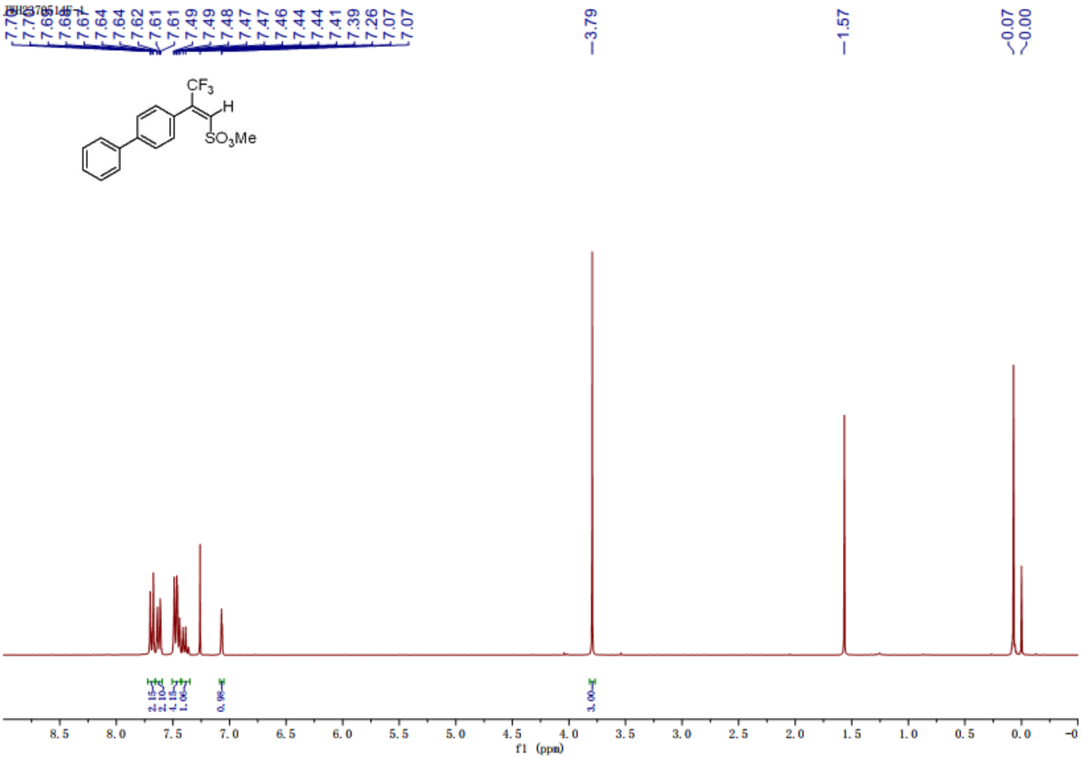
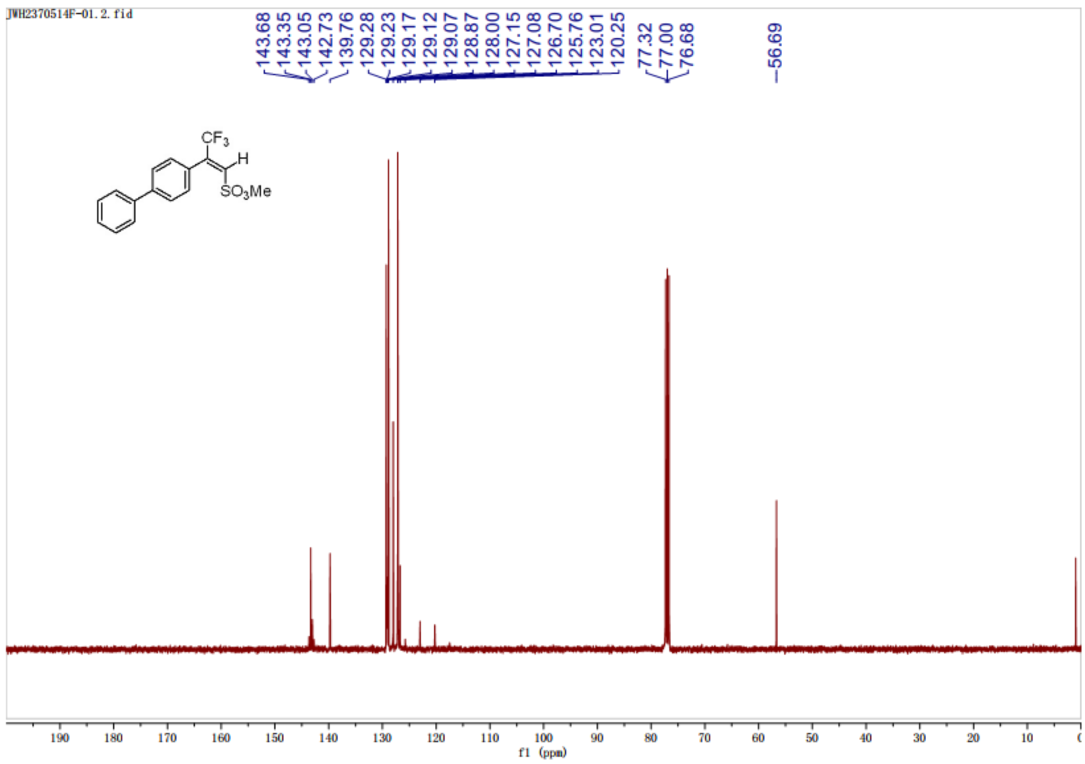
CF3
Cl
SO3Ph
f1 (ppm)


3.79
1.57
0.07
0.00
CF3
H
SO3Me
f1 (ppm)


JWH2370514F-01.2.fid
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143.05
142.73
139.76
129.28
129.23
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128.00
127.15
127.08
126.70
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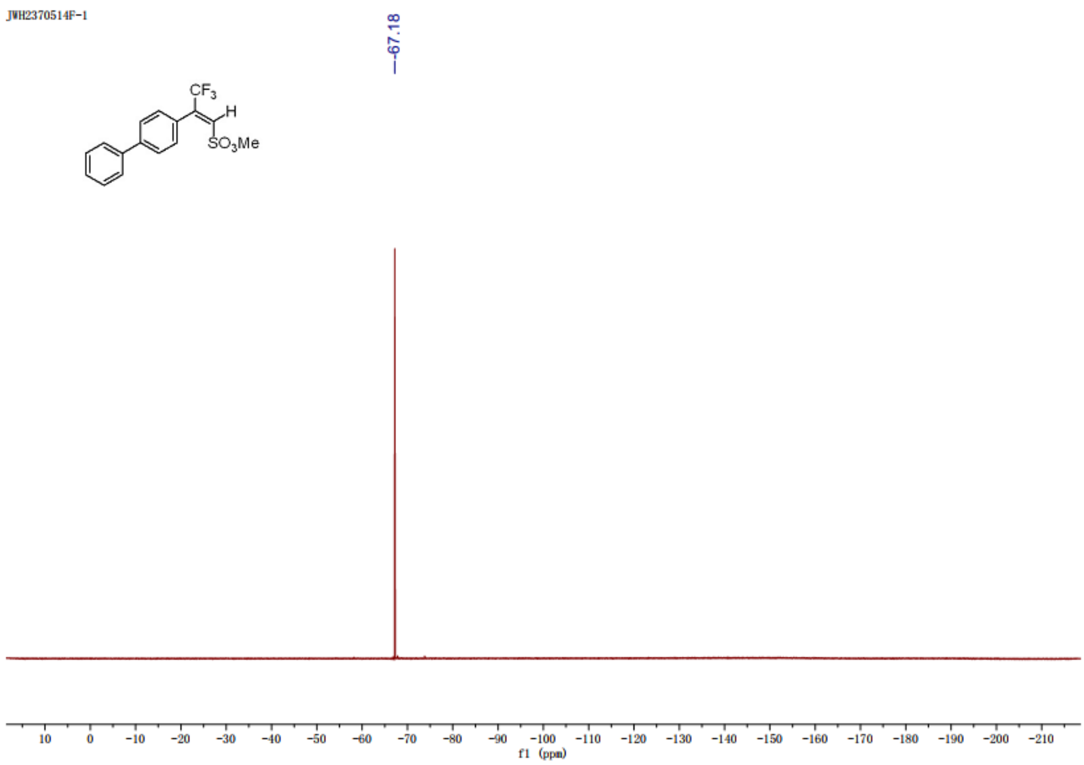
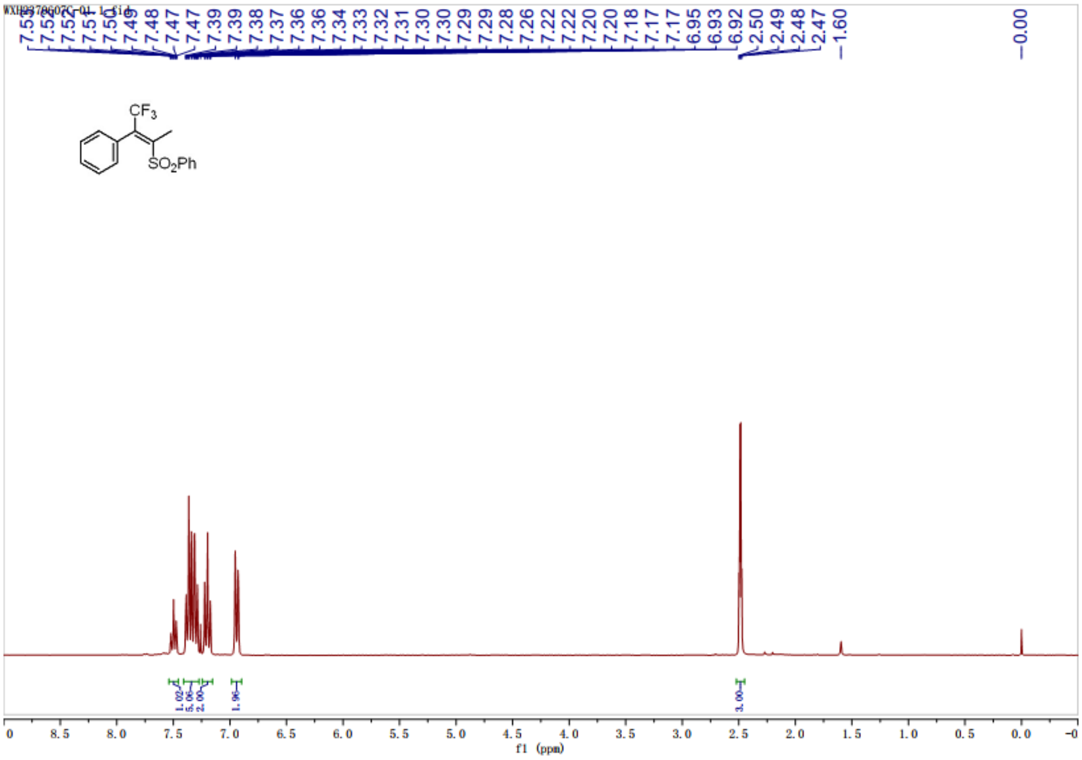
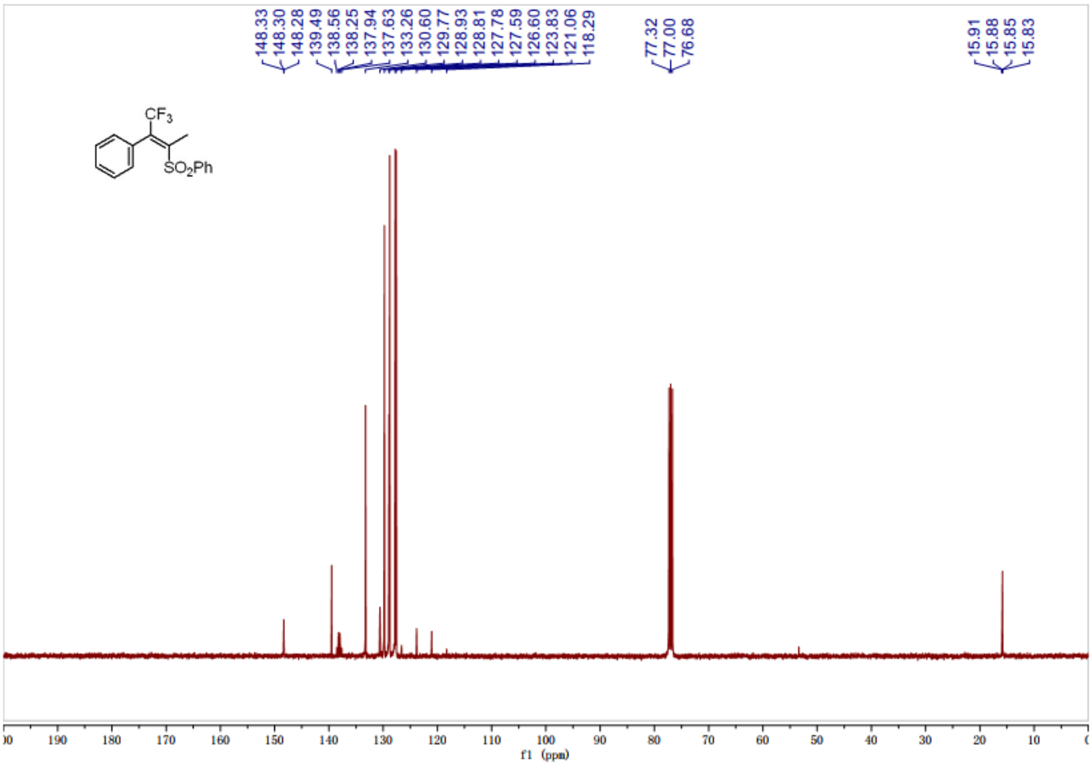
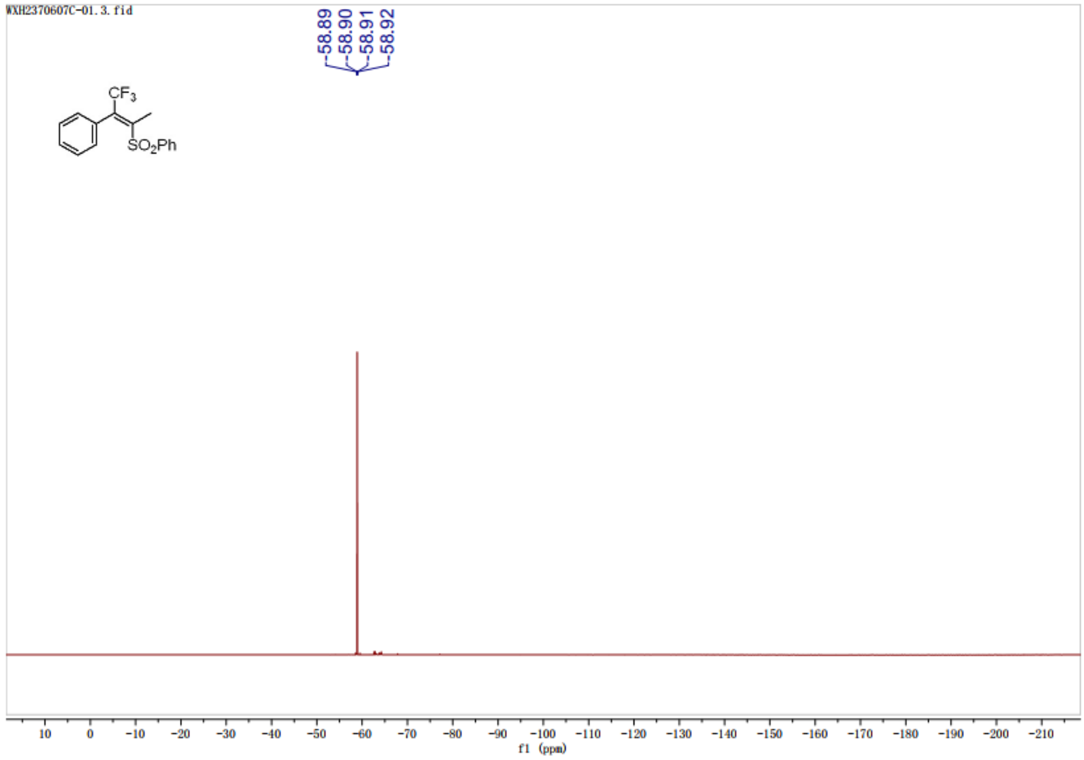
123.01
120.25
77.32
77.00
76.68
56.69
CF3
H
SO3Me
f1 (ppm)


JWH2370514F-1
-67.18
CF3
H
SO3Me
f1 (ppm)






WXH2370607C-01.3.fid
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-58.90
-58.91
-58.92
CF3
SO2Ph
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)