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Supporting Information

Direct carbonylative difunctional of terminal alkynes with sodium sulfinates to access olefin sulfonyl methyl esters under metal-free conditions

Bo Chen[a], Han Yin[a], Zhi-Peng Bao,[a,b] Chang-Sheng Kuai[a] and Xiao-Feng Wu*[a,b]

[a.] *Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, Liaoning, China, e-mail: xwu2020@dicp.ac.cn*

[b.] *Leibniz-Institut für Katalyse e.V., 18059 Rostock, Germany*

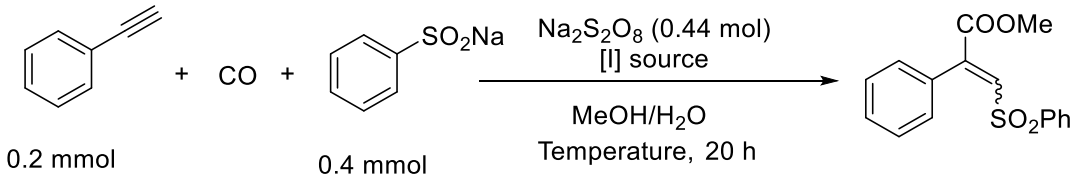
1 General information

Reagents, solvents and analytical methods:

Unless otherwise noted, all reactions were carried out under a carbon monoxide or nitrogen atmosphere. All reagents were commercially available. All solvents were dried by standard techniques, and distilled prior to use. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (b. p. 30-60 °C) and ethyl acetate as eluent. ^{1}H and ^{13}C NMR spectra were taken on Bruker AVANCE III 400 MHz spectrometers and $CDCl_3$ (^{1}H NMR δ 7.26, ^{13}C NMR δ 77.0) as solvent. All coupling constants (*J*) are reported in Hz with the following abbreviations: s = singlet, d = doublet, dd = double doublet , t = triplet, dt = double triplet, q = quatriplet, m = multiplet, br = broad. Gas chromatography (GC) analyses were performed on an Agilent HP-7890A instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d. 0.25 μm film thickness) using argon as carrier gas. Gas chromatography mass spectrometer (GC-MS) analyses were performed on an Shimadzu QP2020 NX instrument. High resolution mass spectra (HRMS) were recorded on Agilent 8890-7250 and Agilent Q-TOF 6540.

Because of the high toxicity of carbon monoxide, all of the reactions should be performed in an autoclave. The laboratory should well-equipped with a CO detector and alarm system.

2 Optimization of reaction conditions



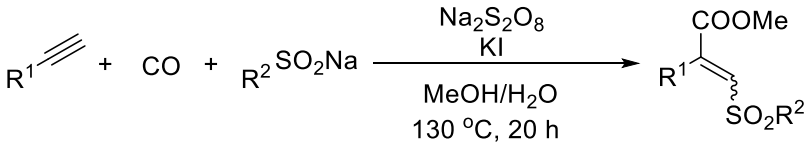
Entry	[I] source	solvent	temperature	CO pressure	Yield %[a]
1	KI (10 mol%)	MeOH (1.6 mL)/H_2O (0.4 mL)	110°C	60 bar	trace
2	KI (50 mol%)	MeOH (1.6 mL)/H_2O (0.4 mL)	110°C	60 bar	39
3	KI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	110°C	60 bar	61
4	KI (2 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	110°C	60 bar	54
5	KI (3 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	110°C	60 bar	trace
6	KI (1.5 eq.)	MeOH (2.0 mL)	110°C	60 bar	ND

7	KI (1.5 eq.)	MeOH (1.9 mL)/H_2O (0.1 mL)	110°C	60 bar	trace
8	KI (1.5 eq.)	MeOH (1.8 mL)/H_2O (0.2 mL)	110°C	60 bar	trace
9	KI (1.5 eq.)	MeOH (1.0 mL)/H_2O (1.0 mL)	110°C	60 bar	55
10	KI (1.5 eq.)	1,4-dioxane (1.0 mL)/MeOH (0.5 mL)/H_2O (0.5 mL)	110°C	60 bar	trace
11	KI (1.5 eq.)	1,4-dioxane (1.5 mL)/MeOH (0.2 mL)/H_2O (0.2 mL)	110°C	60 bar	trace
12	KI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	90°C	60 bar	trace
13	KI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	60 bar	64
14	KI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	81
15	KI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	20 bar	71
16	KI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	10 bar	43
17	CaI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	33
18	NaI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	79
19	LiI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	80
20	TBAI (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	62
21	I_2 (1.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	trace
22	KI (1.5 eq.)/[1.2 eq. $PhSO_2Na$]	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	30
23	KI (1.5 eq.)/[1.5 eq. $PhSO_2Na$]	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	51
24	KI (1.1 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	80 (68[b])
25	LiI (1.1 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	79
26	KI (1.1 eq.)/[$K_2S_2O_8$ 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130°C	40 bar	61

27	KI (1.1 eq.)/[$(NH_4)_2S_2O_8$ 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	41
28	I_2 (0.5 eq.)	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	72
29	KI (1.1 eq.)/[H_2O_2 5.0 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	ND
30	KI (1.1 eq.)/[Ag_2CO_3 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	ND
31	KI (1.1 eq.)/[BQ 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	ND
32	KI (1.1 eq.)/[$Mn(OAc)_3$ 2H2O 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	ND
33	KI (1.1 eq.)/[Oxone 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	20
34	KI (1.1 eq.)/[$PhI(OAc)_2$ 2.2 eq.]	MeOH (1.6 mL)/H_2O (0.4 mL)	130^{o}C	40 bar	ND

a) The yields were determined by GC using hexadecane as the internal standard. b) Isolated yield.

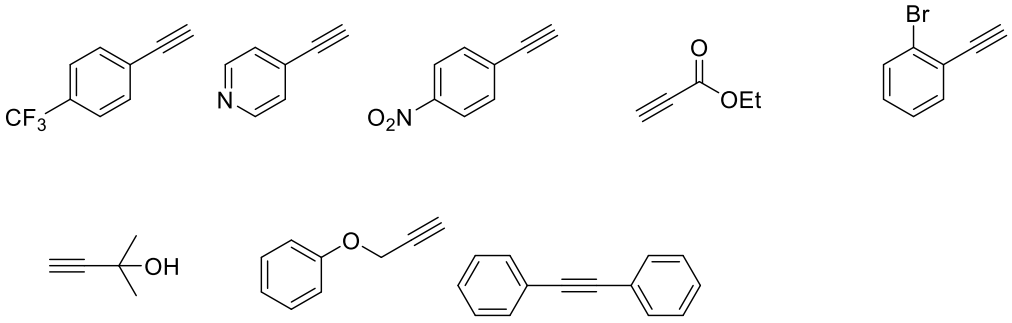
3 General procedure



A 4 mL screw-cap vial was charged with alkynes (0.2 mmol), sodium sulfinates (0.4 mmol), $Na_2S_2O_8$ (0.44 mmol, 105 mg), KI (0.22 mmol, 36 mg) and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After MeOH (1.6 mL) and water (0.4 mL) were added with a syringe under N_2 atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under N_2 atmosphere. At room temperature, the autoclave was flushed with CO three times and charged with 40 bar CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer. The reaction mixture was heated to 130 °C for 20 h. The reaction mixture was then diluted with EtOAc, filtered through silica gel with copious washings (Et_2O or EtOAc), concentrated, and purified by column chromatography.

4 failed examples

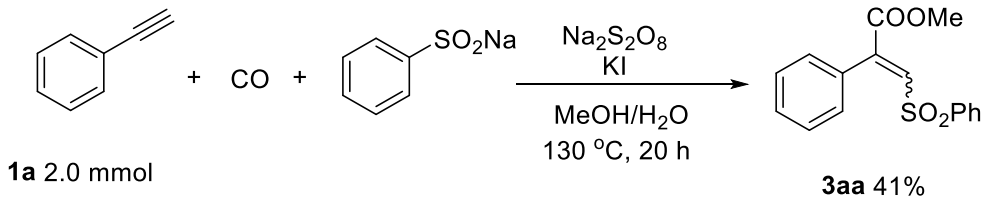
Alkynes



Sodium sulfinates

CF_3SO_2Na

5 Millimole Scale Experiment



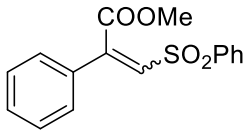
1a 2.0 mmol

3aa 41%

A 100 mL beaker was charged with ethynylbenzene (2.0 mmol), sodium benzenesulfinate (4 mmol), $Na_2S_2O_8$ (4.4 mmol, 1050 mg), KI (2.2 mmol, 360 mg) and an oven-dried stirring bar. After MeOH (16 mL) and water (4 mL) were added with a syringe under N_2 atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under N_2 atmosphere. At room temperature, the autoclave was flushed with CO three times and charged with 40 bar CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer. The reaction mixture was heated to 130 °C for 20 h. The reaction mixture was then diluted with EtOAc, filtered through silica gel with copious washings, concentrated, and purified by column chromatography(EtOAc/PE = 1:4 v/v), obtained **3aa** 248 mg (yield 41%).

6 Spectroscopic data of products

methyl 2-phenyl-3-(phenylsulfonyl)acrylate



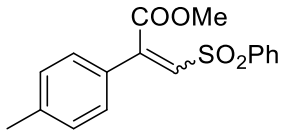
3aa, a mixture of *E* and *Z* = 3:1, yellow oil, yield 68%.

^{1}H NMR (700 MHz, Chloroform-*d*) δ 7.98 – 7.92 (m, 0.65H), 7.51 (s, 1.00H), 7.48 (dd, *J* = 8.4, 1.5 Hz, 2.31H), 7.46 – 7.44 (m, 1.02H), 7.36 – 7.31 (m, 1.60H), 7.29 (tt, *J* = 7.4, 1.6 Hz, 2.96H), 7.22 (dd, *J* = 8.5, 7.0 Hz, 1.96H), 7.08 – 7.03 (m, 1.95H), 6.55 (s, 0.34H) 3.94 (s, 1.01H), 3.69 (s, 3.00H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 166.5, 165.5, 146.1, 143.1, 140.5, 140.2, 139.7, 133.9, 133.7, 132.1, 131.3, 130.8, 129.4, 129.4, 129.3, 129.2, 129.0, 128.0, 127.8, 127.0, 126.5, 53.4, 53.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{14}O_4S$ 303.0686; Found: 303.0685.

methyl 3-(phenylsulfonyl)-2-(p-tolyl)acrylate



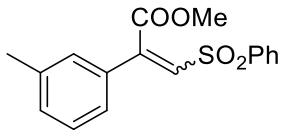
3ba, a mixture of *E* and *Z* = 3:1, yellow oil, yield 41%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.91 (m, 0.6H), 7.55 – 7.50 (m, 2.30H), 7.49 – 7.44 (m, 2.32H), 7.34 – 7.27 (m, 2.11H), 7.23 (d, *J* = 8.3 Hz, 0.79H), 7.11 (d, *J* = 8.2 Hz, 0.68H), 7.04 (d, *J* = 8.0 Hz, 2.04H), 6.98 (d, *J* = 8.2 Hz, 2.05H), 6.52 (s, 0.30H), 3.94 (s, 0.88H), 3.69 (s, 3.00H), 2.30 (s, 2.99H), 2.28 (s, 0.87H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 165.7, 143.1, 142.0, 140.4, 139.9, 139.9, 139.5, 133.8, 133.6, 129.9, 129.4, 129.4, 128.9, 128.5, 128.0, 128.0, 127.9, 127.0, 125.3, 53.4, 53.1, 21.5, 21.4.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{17}H_{16}O_4S$ 317.0842; Found: 317.0840.

methyl 3-(phenylsulfonyl)-2-(m-tolyl)acrylate



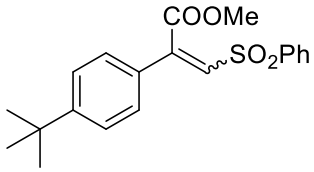
3ca, a mixture of *E* and *Z* = 3:1, yellow oil, yield 57%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.90 (m, 0.70H), 7.52 – 7.41 (m, 4.70H), 7.32 – 7.24 (m, 2.22H), 7.21 – 7.06 (m, 3.83H), 6.87 (dt, *J* = 7.3, 1.8 Hz, 0.99H), 6.74 (d, *J* = 2.0 Hz, 0.99H), 6.53 (s, 0.35H), 3.94 (s, 1.00H), 3.69 (s, 3.00H), 2.26 (s, 1.09H), 2.20 (s, 3.01H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 165.6, 146.3, 143.3, 140.4, 140.3, 139.8, 139.1, 137.4, 133.8, 133.5, 132.1, 132.0, 130.7, 130.0, 129.7, 129.4, 129.1, 128.8, 128.1, 128.0, 127.7, 127.5, 126.5, 126.3, 124.2, 53.4, 53.2, 21.4, 21.3.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{17}H_{16}O_4S$ 317.0842; Found: 317.0843.

methyl 2-(4-(tert-butyl)phenyl)-3-(phenylsulfonyl)acrylate



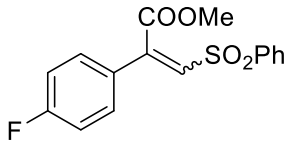
3da, a mixture of *E* and *Z* = 10:3, yellow oil, yield 55%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.91 (m, 0.60H), 7.56 – 7.46 (m, 2.05H), 7.45 – 7.38 (m, 3.15H), 7.35 – 7.26 (m, 1.59H), 7.25 – 7.17 (m, 4.30H), 6.53 (s, 0.28H) 7.01 – 6.94 (m, 1.96H), 3.94 (s, 0.9H), 3.70 (s, 3.00H), 1.25 (s, 9.24H), 1.22 (d, *J* = 3.2 Hz, 2.98H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 165.7, 155.1, 152.5, 146.0, 143.3, 140.4, 139.7, 133.8, 133.4, 129.4, 129.3, 128.7, 128.0, 127.9, 127.7, 126.8, 126.2, 125.4, 124.7, 53.3, 53.1, 34.9, 34.7, 31.3, 31.0.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{20}H_{22}O_4S$ 359.1312; Found: 359.1314.

methyl 2-(4-fluorophenyl)-3-(phenylsulfonyl)acrylate



3ea, a mixture of *E* and *Z* = 15:1, yellow oil, yield 50%.

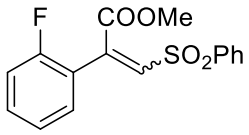
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.46 (m, 4H), 7.37 – 7.31 (m, 2H), 7.11 – 7.05 (m, 2H), 6.92 (t, *J* = 8.7 Hz, 2H), 3.71 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 164.3 (d, *J* = 251.48 Hz), 141.9, 140.8, 139.7, 133.9, 131.6 (d, *J* = 8.39 Hz), 129.1, 128.0, 126.7 (d, *J* = 3.39 Hz), 115.0 (d, *J* = 22.32 Hz), 53.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.15.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{13}FO_4S$ 321.0591; Found: 321.0596.

methyl 2-(2-fluorophenyl)-3-(phenylsulfonyl)acrylate



3fa, a mixture of *E* and *Z* = 4:1, yellow oil, yield 42%.

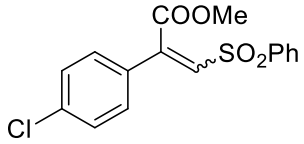
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.92 (m, 0.61H), 7.62 – 7.47 (m, 4.97H), 7.38 – 7.27 (m, 3.97H), 7.23 (td, *J* = 7.4, 1.8 Hz, 1.19H), 7.11 (td, *J* = 7.5, 1.1 Hz, 1.40H), 6.86 (ddd, *J* = 9.5, 8.3, 1.1 Hz, 1.16H), 6.78 (s, 0.30H), 3.93 (s, 0.85H), 3.70 (s, 3.00H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 164.5, 159.4 (d, *J* = 247.49 Hz), 142.0, 139.3, 137.6, 133.9, 131.8 (d, *J* = 2.58 Hz), 131.6 (d, *J* = 8.27 Hz), 129.4, 129.1, 128.1, 128.0, 124.9 (d, *J* = 3.68 Hz), 123.7 (d, *J* = 3.68 Hz), 119.1 (d, *J* = 16.11 Hz), 116.7 (d, *J* = 22.55 Hz), 115.1 (d, *J* = 21.34 Hz), 53.5, 53.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.1, -111.8.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{13}FO_4S$ 321.0591; Found: 321.0599.

methyl 2-(4-chlorophenyl)-3-(phenylsulfonyl)acrylate

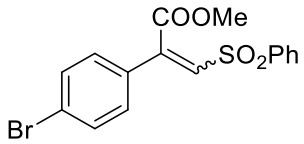


3ga, a mixture of *E* and *Z* > 20:1, yellow oil, yield 31%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.51 (m, 3H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.23 – 7.19 (m, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 3.71 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 141.7, 140.9, 139.6, 135.6, 133.9, 130.9, 129.1, 128.1, 128.0, 53.5.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{13}ClO_4S$ 337.0296; Found: 337.0299.



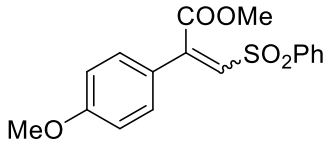
3ha, a mixture of *E* and *Z* > 20:1, yellow oil, yield 49%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 – 7.48 (m, 4H), 7.40 – 7.33 (m, 4H), 6.98 – 6.90 (m, 2H), 3.70 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 141.7, 140.9, 139.6, 133.9, 129.7, 129.1, 128.0, 123.9, 53.5.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{13}BrO_4S$ 380.9791; Found: 380.9787.

methyl 2-(4-methoxyphenyl)-3-(phenylsulfonyl)acrylate



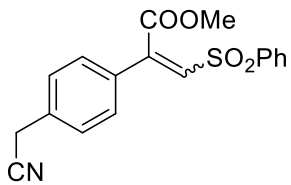
3ia, a mixture of *E* and *Z* = 9:4, yellow oil, yield 18%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.91 (m, 0.87H), 7.56 – 7.50 (m, 2.68H), 7.49 – 7.43 (m, 2.63H), 7.36 – 7.26 (m, 2.95H), 7.10 – 7.03 (m, 2.03H), 6.84 – 6.79 (m, 0.95H), 6.78 – 6.73 (m, 2.04H), 6.46 (s, 0.44H), 3.95 (s, 1.25H), 3.76 (s, 3.04H), 3.75 (s, 1.33H), 3.71 (s, 3.00H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 160.6, 142.8, 140.0, 139.5, 133.7, 133.6, 131.2, 129.3, 128.9, 128.8, 128.0, 127.9, 123.7, 123.0, 114.7, 113.3, 55.5, 55.3, 53.3, 53.1.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{17}H_{16}O_5S$ 333.0791; Found: 333.0790.

methyl 2-(4-(cyanomethyl)phenyl)-3-(phenylsulfonyl)acrylate



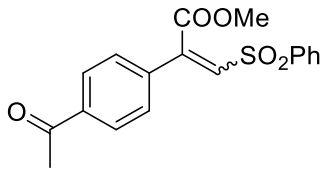
3ja, a mixture of *E* and *Z* = 3:2, yellow oil, yield 26%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.92 (m, 1.47H), 7.58 – 7.49 (m, 6.36H), 7.36 (td, *J* = 6.8, 5.7, 1.7 Hz, 4.54H), 7.30 (d, *J* = 8.3 Hz, 2.00H), 7.22 (d, *J* = 8.0 Hz, 2.46H), 7.15 – 7.09 (m, 2.13H), 6.56 (s, 0.64H), 3.95 (s, 1.91H), 3.71 (s, 5.00H), 3.70 (s, 1.36H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 165.2, 145.1, 141.9, 140.8, 140.0, 139.6, 134.0, 134.0, 133.2, 132.1, 131.1, 130.9, 130.2, 129.5, 129.1, 128.8, 128.1, 128.0, 127.8, 127.5, 127.3, 117.4, 117.0, 53.5, 53.3, 23.6, 23.5.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{18}H_{15}NO_4S$ 342.0795; Found: 342.0796.

methyl 2-(4-acetylphenyl)-3-(phenylsulfonyl)acrylate



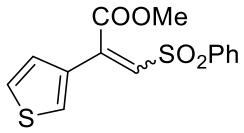
3ka, a mixture of *E* and *Z* = 5:2, yellow oil, yield 44%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (dd, *J* = 8.7, 1.6 Hz, 1.01H), 7.90 – 7.83 (m, 3.24H), 7.59 – 7.48 (m, 5.62H), 7.44 (d, *J* = 8.5 Hz, 0.99H), 7.39 – 7.33 (m, 2.39H), 7.21 (dt, *J* = 9.0, 2.1 Hz, 2.19H), 6.63 (s, 0.46H), 3.96 (s, 1.21H), 3.70 (s, 3.00H), 2.56 (s, 3.01H), 2.52 (s, 1.21H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.5, 197.0, 166.0, 164.9, 144.8, 141.7, 140.8, 139.8, 139.6, 138.7, 137.3, 136.3, 135.7, 134.1, 134.1, 129.7, 129.5, 129.2, 129.0, 128.6, 128.1, 128.0, 127.7, 127.3, 53.6, 53.4, 26.7, 26.7.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{18}H_{16}O_5S$ 345.0791; Found: 345.0794.

methyl 3-(phenylsulfonyl)-2-(thiophen-3-yl)acrylate



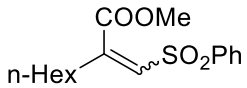
3la, a mixture of *E* and *Z* = 10:3, yellow oil, yield 55%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.89 (m, 0.62H), 7.59 – 7.53 (m, 2.31H), 7.52 – 7.44 (m, 3.58H), 7.43 – 7.39 (m, 0.34H), 7.37 – 7.26 (m, 2.43H), 7.13 (dd, *J* = 5.1, 3.0 Hz, 0.99H), 7.08 – 7.04 (m, 0.35H) 6.83 (dd, *J* = 5.0, 1.3 Hz, 0.97H), 6.05 (s, 0.30H), 3.96 (s, 0.91H), 3.72 (s, 3.00H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 165.2, 140.3, 139.7, 138.2, 133.8, 133.7, 130.2, 129.4, 129.2, 128.9, 128.8, 128.2, 127.9, 127.8, 127.7, 125.0, 125.0, 124.7, 53.4, 53.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{14}H_{12}O_4S_2$ 309.0250; Found: 309.0250.

methyl 2-((phenylsulfonyl)methylene)octanoate



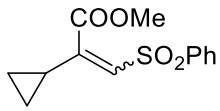
3ma, a mixture of *E* and *Z* = 20:3, yellow oil, yield 60%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (dq, *J* = 7.1, 2.0 Hz, 2.32H), 7.63 – 7.57 (m, 1.04H), 7.53 – 7.48 (m, 2.24H), 7.08 (s, 0.90H), 6.09 (s, 0.16H), 3.84 (s, 0.46H), 3.70 (s, 3.00H), 2.76 (dd, *J* = 8.8, 6.4 Hz, 2.05H), 1.40 – 1.12 (m, 11.00H), 0.81 (t, *J* = 6.7 Hz, 4.17H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.0, 145.8, 140.8, 136.7, 134.0, 129.5, 127.7, 52.9, 31.4, 29.4, 29.1, 27.3, 22.5, 14.0.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{22}O_4S$ 311.1312; Found: 311.1316.

methyl 2-cyclopropyl-3-(phenylsulfonyl)acrylate



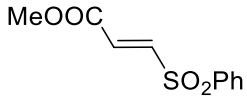
3na, a mixture of *E* and *Z* = 15:1, colorless oil, yield 12%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ7.96 – 7.92 (m, 0.41H), 7.91 – 7.86 (m, 2.17H), 7.62 – 7.57 (m, 1.17H), 7.53 – 7.48 (m, 2.57H), 6.83 (s, 0.95H), 3.83 (s, 0.21H), 3.63 (s, 3.00H), 2.69 (tt, *J* = 8.6, 5.2 Hz, 1.11H), 1.11 – 1.05 (m, 1.99H), 0.91 (dt, *J* = 8.6, 3.2 Hz, 2.10H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 164.6, 152.2, 148.3, 141.1, 134.7, 133.8, 133.5, 133.2, 129.4, 129.2, 129.0, 128.2, 127.5, 127.1, 52.5, 25.8, 10.9, 10.7, 9.5, 9.3.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{13}H_{14}O_4S$ 267.0686; Found: 267.0691.

methyl (E)-3-(phenylsulfonyl)acrylate



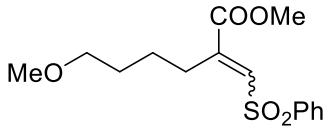
3oa, the product was obtained from ethynyltrimethylsilane, colorless oil, yield 13%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.80 (m, 2H), 7.68 – 7.57 (m, 1H), 7.58 – 7.49 (m, 2H), 7.28 (d, *J* = 15.2 Hz, 1H), 6.78 (d, *J* = 15.1 Hz, 1H), 3.74 (s, 3H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 163.9, 143.5, 138.4, 134.4, 130.5, 129.7, 128.4, 52.8.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{10}H_{10}O_4S$ 227.0373; Found: 223.0375.

methyl 6-methoxy-2-((phenylsulfonyl)methylene)hexanoate



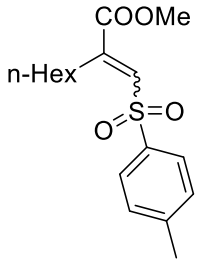
3pa, the product was obtained from 6-iodohex-1-yne, A mixture of *E* and *Z* > 20:1, colorless oil, yield 27%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.85 (m, 2H), 7.64 – 7.57 (m, 1H), 7.55 – 7.47 (m, 2H), 7.09 (s, 1H), 3.70 (s, 3H), 3.33 (t, *J* = 6.4 Hz, 2H), 3.26 (s, 3H), 2.87 – 2.76 (m, 2H), 1.59 (ddt, *J* = 7.2, 5.9, 1.6 Hz, 2H), 1.49 – 1.43 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 145.3, 140.6, 137.0, 134.0, 129.5, 127.7, 72.2, 58.5, 53.0, 29.5, 26.9, 25.8.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{15}H_{20}O_5S$ 313.1104; Found: 313.1113.

methyl 3-oxo-2-(tosylmethylene)octanoate



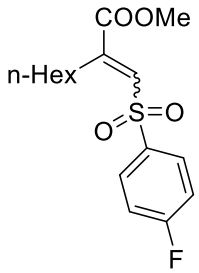
3mb, a mixture of *E* and *Z* = 10:1, colorless oil, yield 67%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.64 (m, 2.53H), 7.29 (d, *J* = 8.1 Hz, 2.57H), 7.07 (s, 0.95H), 6.08 (s, 0.11H), 3.83 (s, 0.30H), 3.69 (s, 3.00H), 2.74 (dd, *J* = 8.8, 6.4 Hz, 2.02H), 2.38 (s, 3.97H), 1.39 – 1.10 (m, 10.89H), 0.89 – 0.73 (m, 4.20H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 145.3, 145.1, 137.8, 137.1, 130.1, 127.8, 52.9, 31.5, 29.4, 29.1, 27.3, 22.5, 21.7, 14.1.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{17}H_{24}O_4S$ 325.1468; Found: 325.1477.

methyl 2-(((4-fluorophenyl)sulfonyl)methylene)-3-oxooctanoate



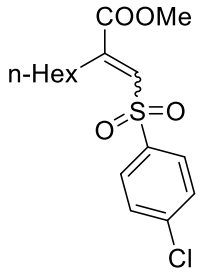
3mc, a mixture of *E* and *Z* = 5:1, colorless oil, yield 81%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.84 (m, 2.37H), 7.27 – 7.11 (m, 2.60H), 7.05 (s, 0.95H), 6.08 (s, 0.18H), 3.84 (s, 0.56H), 3.71 (s, 3.00H), 2.80 – 2.70 (m, 2.02H), 2.32 – 2.26 (m, 0.38H), 1.42 – 1.10 (m, 10.50H), 0.92 – 0.71 (m, 3.93H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.6, 166.0 (d, *J* = 258.34 Hz), 165.9, 149.7, 145.9, 136.8 (d, *J* = 3.03 Hz), 136.5, 130.9 (d, *J* = 9.75 Hz), 130.7 (d, *J* = 9.48 Hz), 127.4, 116.8 (d, *J* = 23.11 Hz), 116.6 (d, *J* = 22.54 Hz), 53.0, 52.8, 34.8, 31.4, 31.3, 29.4, 29.2, 28.4, 27.3, 26.5, 22.5, 22.4, 14.0, 13.9.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{21}FO_4S$ 329.1217; Found: 329.1222.

methyl 2-(((4-chlorophenyl)sulfonyl)methylene)-3-oxooctanoate



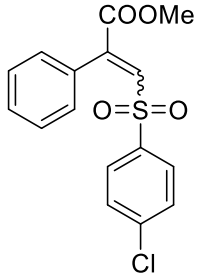
3md, a mixture of *E* and *Z* = 5:1, colorless oil, yield 58%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.77 (m, 2.22H), 7.51 – 7.43 (m, 2.38H), 7.05 (s, 0.89H), 6.07 (s, 0.18H), 3.84 (s, 0.57H), 3.71 (s, 3.00H), 2.82 – 2.69 (m, 2.03H), 2.33 – 2.25 (m, 0.40H), 1.44 – 1.11 (m, 11.14H), 0.80 (dt, *J* = 17.0, 6.7 Hz, 4.16H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.5, 165.9, 150.1, 146.3, 140.8, 139.2, 136.2, 129.8, 129.6, 129.4, 129.2, 127.2, 53.0, 52.8, 34.8, 31.4, 31.3, 29.4, 29.2, 28.4, 27.4, 26.5, 22.5, 22.4, 14.0, 13.9.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{21}ClO_4S$ 345.0922; Found: 345.0926.

methyl 3-((4-chlorophenyl)sulfonyl)-2-phenylacrylate



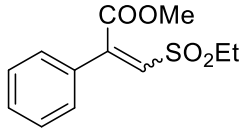
3ad, a mixture of *E* and *Z* = 20:3, yellow oil, yield 16%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ7.91 – 7.86 (m, 0.34H), 7.51 (s, 0.99H), 7.50 – 7.45 (m, 0.38H), 7.41 – 7.35 (m, 2.28H), 7.35 – 7.29 (m, 1.61H), 7.27 – 7.21 (m, 3.96H), 7.05 – 7.01 (m, 1.88H), 6.53 (s, 0.15H), 3.95 (s, 0.44), 3.71 (s, 3.00H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 143.4, 140.5, 140.3, 138.1, 130.7, 129.7, 129.5, 129.5, 129.4, 129.4, 129.3, 129.2, 127.9, 127.0, 53.5.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{16}H_{13}ClO_4S$ 337.0296; Found: 337.0298.

methyl 3-(ethylsulfonyl)-2-phenylacrylate



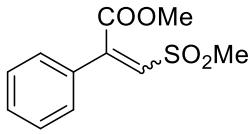
3ae, a mixture of *E* and *Z* = 4:1, yellow oil, yield 45%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.31 (m, 7.31H),6.57 (s, 0.26H) 3.86 (s, 0.77H), 3.76 (s, 3.00H), 3.12 (q, *J* = 7.5 Hz, 0.58H), 2.66 (q, *J* = 7.4 Hz, 2.12H), 1.35 (t, *J* = 7.5 Hz, 0.96H), 1.17 (t, *J* = 7.4 Hz, 3.28H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 143.8, 137.2, 131.4, 131.0, 129.8, 129.4, 129.3, 128.1, 127.0, 124.7, 53.5, 53.1, 50.2, 49.0, 6.8, 6.7.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{12}H_{14}O_4S$ 255.0686; Found: 255.0691.

methyl 3-(methylsulfonyl)-2-phenylacrylate



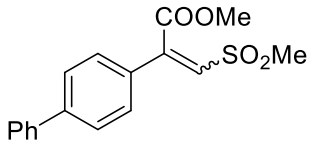
3af, a mixture of *E* and *Z* = 5:1, yellow oil, yield 67%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.30 (m, 7.17H), 6.66 (s, 0.21), 3.87 (s, 0.61H), 3.76 (s, 3.00H), 3.04 (s, 0.60H), 2.58 (s, 3.01H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 165.4, 148.5, 142.9, 139.3, 131.9, 131.5, 130.9, 130.0, 129.5, 129.3, 128.3, 127.1, 126.7, 53.5, 53.2, 43.9, 42.9.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{11}H_{12}O_4S$ 241.0529; Found: 241.0533.

methyl 2-([1,1'-biphenyl]-4-yl)-3-(methylsulfonyl)acrylate



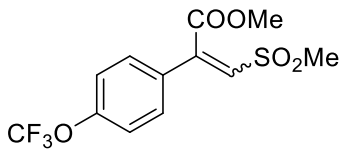
3qf, a mixture of *E* and *Z* = 15:4, yellow oil, yield 44%.

^{1}H NMR (700 MHz, Chloroform-*d*) δ 7.62 – 7.57 (m, 3.11H), 7.56 – 7.51 (m, 3.57H), 7.46 – 7.40 (m, 4.06H), 7.38 (t, *J* = 7.8 Hz, 3.58H), 7.32 – 7.28 (m, 2.12H), 6.70 (s, 0.30), 3.89 (s, 0.80H), 3.79 (s, 3.00H), 3.06 (s, 0.77H), 2.65 (s, 3.06H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 166.2, 165.5, 148.2, 144.4, 142.8, 142.7, 140.0, 139.1, 130.1, 129.9, 129.7, 129.1, 129.0, 128.9, 128.9, 128.8, 128.3, 128.0, 127.9, 127.7, 127.6, 127.4, 127.2, 127.1, 127.1, 126.9, 126.2, 53.6, 53.3, 43.9, 43.0.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{17}H_{16}O_4S$ 317.0842; Found: 317.0850.

methyl 3-(methylsulfonyl)-2-(4-(trifluoromethoxy)phenyl)acrylate



3rf, a mixture of *E* and *Z* > 20:1, colorless oil, yield 43%.

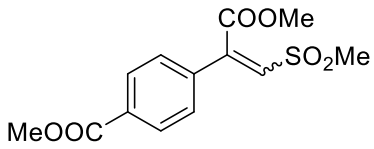
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 (d, *J* = 8.8 Hz, 2H), 7.26 – 7.17 (m, 2H), 3.78 (s, 3H), 2.71 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 150.2, 141.8, 139.3, 131.3, 129.2, 120.3 (t, *J* = 137.69 Hz), 53.6, 43.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -57.7.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{12}H_{11}F_3O_5S$ 325.0352; Found: 325.0355.

methyl 4-(3-methoxy-1-(methylsulfonyl)-3-oxoprop-1-en-2-yl)benzoate



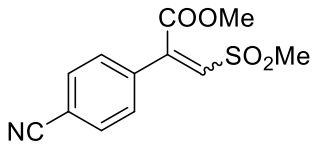
3sf, a mixture of *E* and *Z* > 20:1, colorless oil, yield 50%.

^{1}H NMR (700 MHz, Chloroform-*d*) δ 8.03 (d, *J* = 8.3 Hz, 2H), 7.48 (s, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H), 3.77 (s, 3H), 2.70 (s, 3H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 165.3, 163.8, 141.2, 138.5, 134.4, 130.3, 128.5, 128.3, 52.7, 51.3, 42.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{13}H_{14}O_6S$ 299.0584; Found: 299.0589.

methyl 2-(4-cyanophenyl)-3-(methylsulfonyl)acrylate



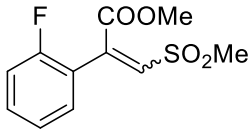
3tf, a mixture of *E* and *Z* > 20:1, yellow oil, yield 23%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 – 7.63 (m, 2H), 7.51 (s, 1H), 7.41 (d, *J* = 8.5 Hz, 2H), 3.78 (s, 3H), 2.83 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 141.5, 139.5, 135.5, 131.7, 130.2, 118.2, 113.6, 53.8, 43.4.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{12}H_{11}NO_4S$ 266.0482; Found: 266.0483.

methyl 2-(2-fluorophenyl)-3-(methylsulfonyl)acrylate



3uf, a mixture of *E* and *Z* = 5:1, yellow oil, yield 64%.

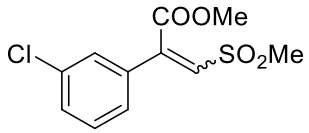
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 (s, 1.02H), 7.37 (ddt, *J* = 12.9, 5.3, 2.6 Hz, 1.32H), 7.30 (qd, *J* = 7.5, 7.0, 1.8 Hz, 1.19H), 7.15 (td, *J* = 7.6, 1.1 Hz, 1.27H), 7.07 (tdd, *J* = 9.5, 8.0, 1.1 Hz, 1.38H), 6.83 (s, 0.23H), 3.85 (s, 0.64H), 3.76 (s, 3.00H), 3.10 (s, 0.64H), 2.78 (s, 3.08H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.5, 164.5, 159.4 (d, *J* = 246.95 Hz), 143.0, 140.2, 138.2, 133.1(d, *J* = 8.57 Hz), 131.9 (d, *J* = 8.57 Hz), 131.6 (d, *J* = 2.34 Hz), 129.9 (d, *J* = 2.61 Hz), 125.0 (d, *J* = 3.75 Hz), 124.0 (d, *J* = 3.75 Hz), 119.1 (d, *J* = 16.03 Hz), 116.7 (d, *J* = 21.58 Hz), 115.4 (d, *J* = 20.98 Hz), 53.7, 53.3, 43.9, 42.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.40, -112.28.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{11}H_{11}FO_4S$ 259.0435; Found: 259.0441.

methyl 2-(3-chlorophenyl)-3-(methylsulfonyl)acrylate



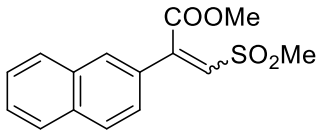
3vf, a mixture of *E* and *Z* = 10:1, yellow oil, yield 46%.

^{1}H NMR (700 MHz, Chloroform-*d*) δ 7.45 (s, 0.90H), 7.36 (ddd, *J* = 8.1, 2.1, 1.1 Hz, 0.93H), 7.32 – 7.27 (m, 1.98H), 7.22 (dt, *J* = 7.7, 1.4 Hz, 0.92H), 6.66 (s, 0.10H), 3.88 (s, 0.28H), 3.78 (s, 3.00H), 3.05 (s, 0.23H) 2.72 (s, 3.00H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 164.9, 141.6, 139.5, 134.2, 132.5, 130.0, 129.5, 129.3, 127.8, 53.7, 43.2.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{11}H_{11}ClO_4S$ 275.0139; Found: 275.0138.

methyl 3-(methylsulfonyl)-2-(naphthalen-2-yl)acrylate



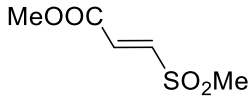
3wf, a mixture of *E* and *Z* = 5:1, yellow oil, yield 47%.

^{1}H NMR (700 MHz, Chloroform-*d*) δ 7.89 – 7.86 (m, 0.97H), 7.84 – 7.77 (m, 3.80H), 7.52 – 7.44 (m, 3.63H), 7.37 (dd, *J* = 8.4, 1.8 Hz, 0.99H), 6.78 (s, 0.23H), 3.92 (s, 0.61H), 3.77 (s, 3.00H), 3.08 (s, 0.60H), 2.57 (s, 3.14H).

^{13}C NMR (176 MHz, $CDCl_3$) δ 165.2, 164.4, 147.5, 141.9, 139.4, 138.4, 133.4, 132.5, 131.9, 131.4, 128.7, 128.3, 128.0, 127.9, 127.6, 127.3, 127.2, 127.1, 127.0, 126.8, 126.8, 126.8, 126.8, 126.4, 126.2, 125.8, 125.6, 125.1, 121.8, 52.5, 52.3, 42.9, 41.9.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{15}H_{14}O_4S$ 291.0686; Found: 291.0681.

methyl (*E*)-3-(methylsulfonyl)acrylate



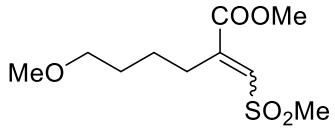
3xf, the product was obtained from ethynyltrimethylsilane, colorless oil, yield 46%.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 (d, *J* = 15.2 Hz, 1H), 6.82 (d, *J* = 15.2 Hz, 1H), 3.79 (s, 3H), 2.96 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.7, 142.1, 132.5, 52.9, 42.4.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_5H_8O_4S$ 165.0216; Found: 165.0218.

methyl 6-methoxy-2-((methylsulfonyl)methylene)hexanoate



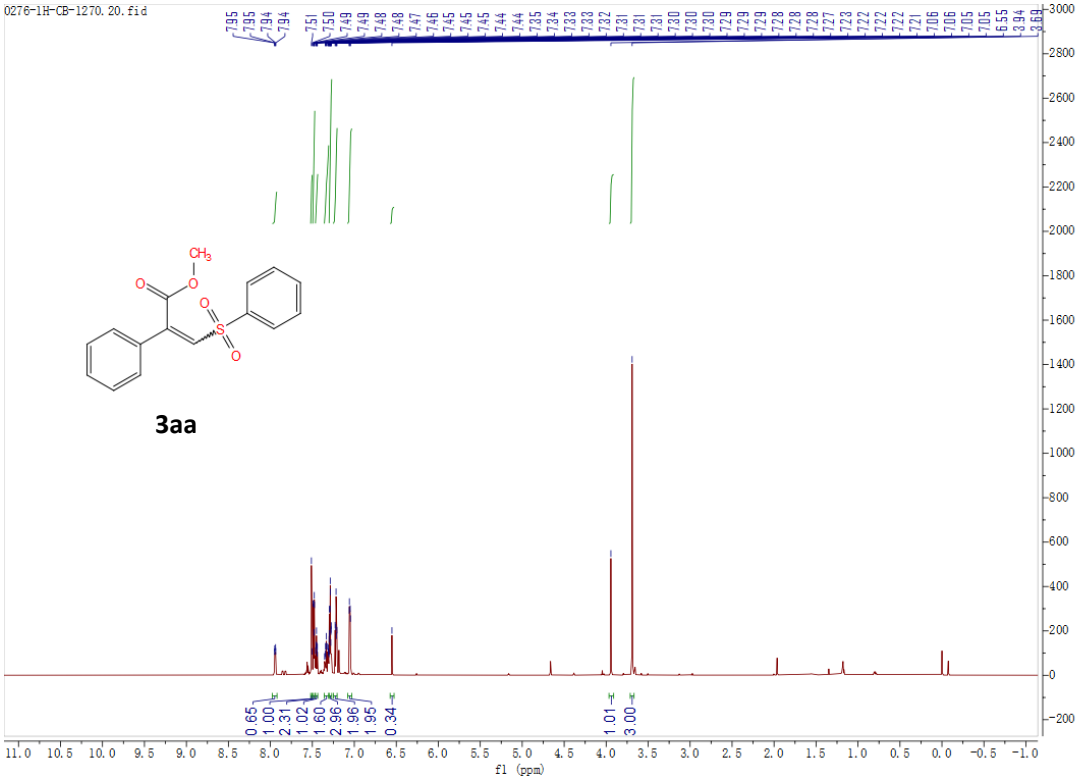
3yf, the product was obtained from 6-iodohex-1-yne, A mixture of *E* and *Z* > 20:1, colorless oil, yield 28%.

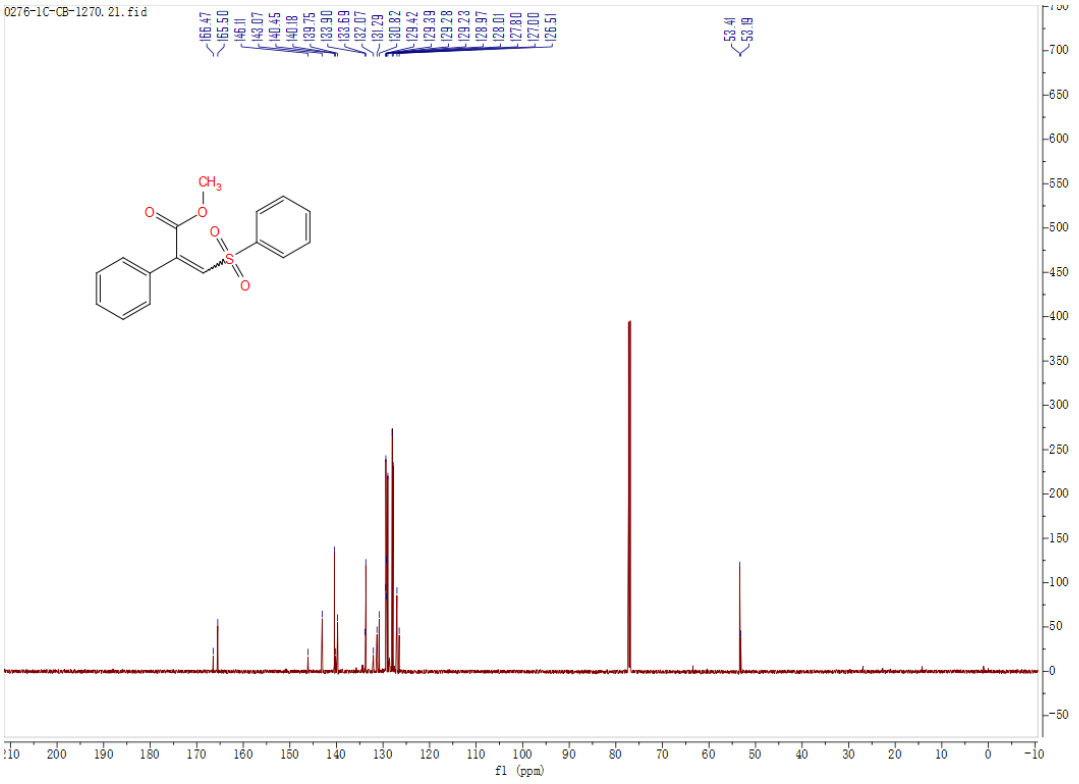
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.11 (s, 1H), 3.77 (s, 3H), 3.33 (t, *J* = 6.2 Hz, 2H), 3.25 (s, 3H), 2.97 (s, 3H), 2.81 – 2.75 (m, 2H), 1.60 – 1.51 (m, 4H).

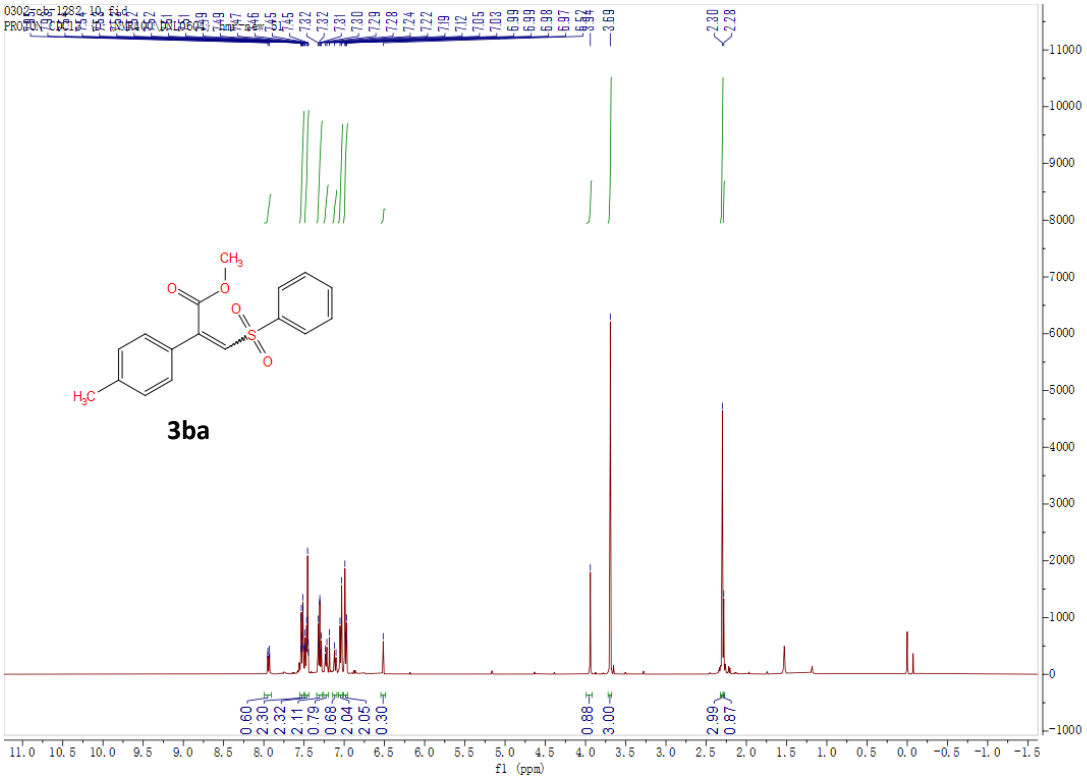
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 146.7, 135.7, 72.1, 58.5, 53.1, 43.8, 29.4, 27.0, 25.9.

HRMS (ESI-TOF) m/z: [M + H]+ Calcd for $C_{10}H_{18}O_5S$ 251.0948; Found: 251.0953.

7 Copies of NMR spectra for compounds



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0.60
2.30
2.32
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0.79
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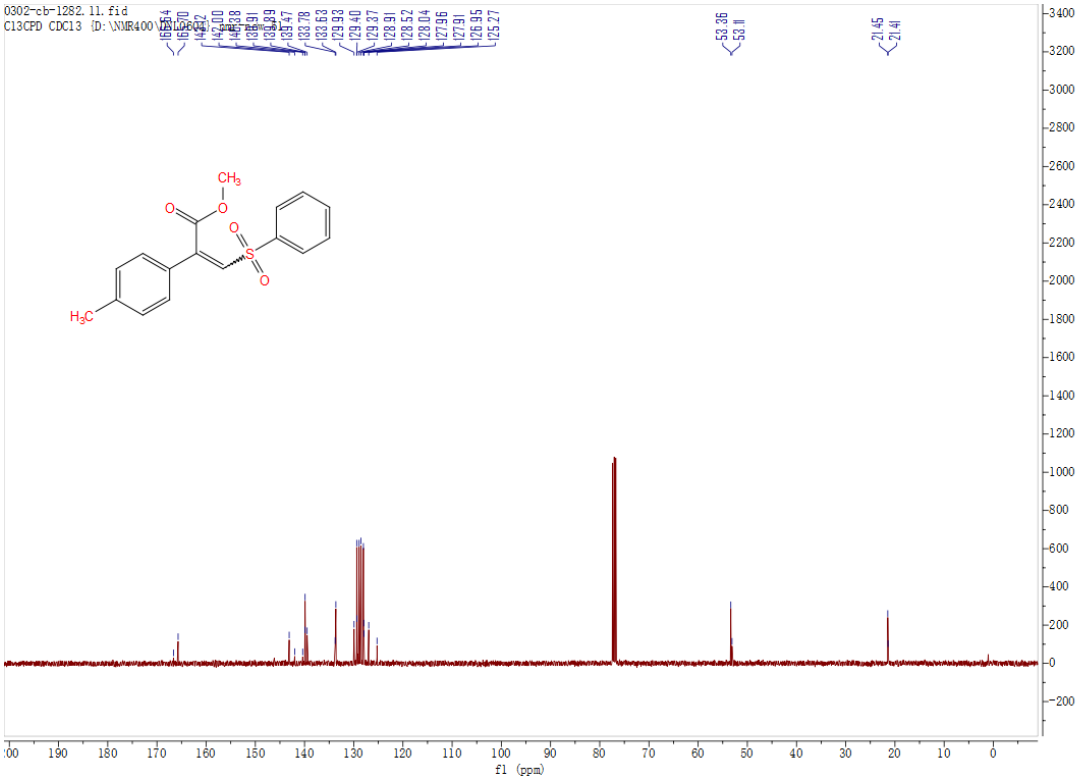
2.04
2.05
0.30
0.88
3.00
2.99
0.87
f1 (ppm)

3ba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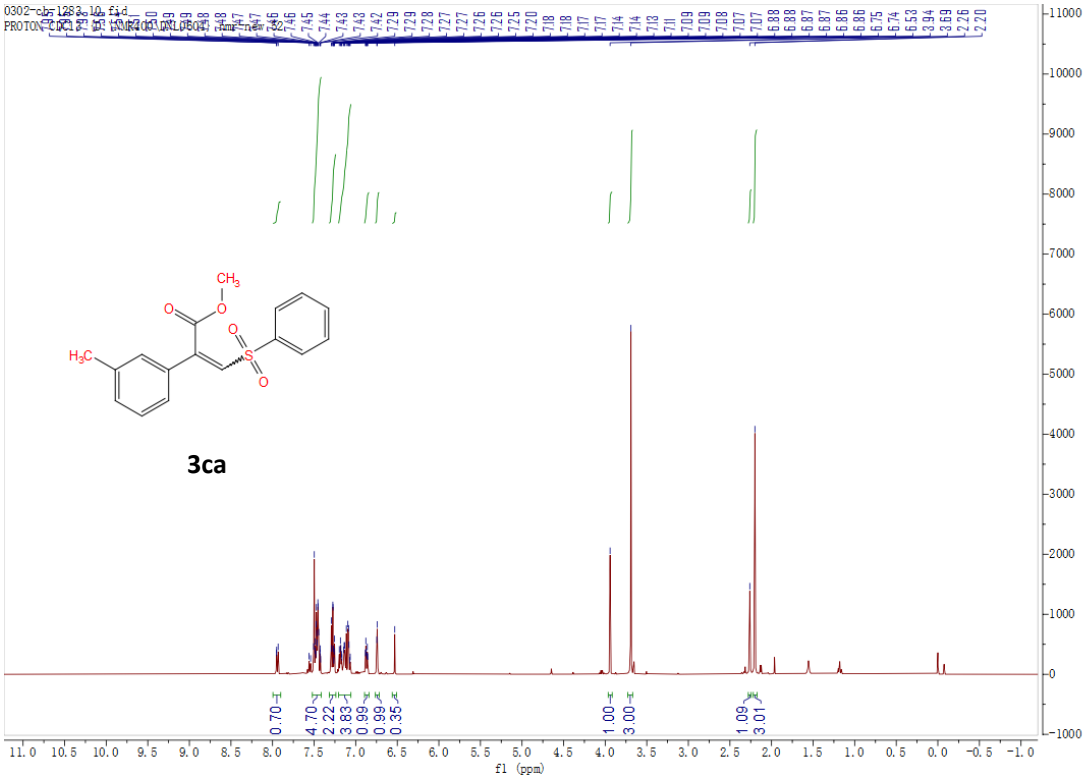
0.70
4.70
2.22
3.83
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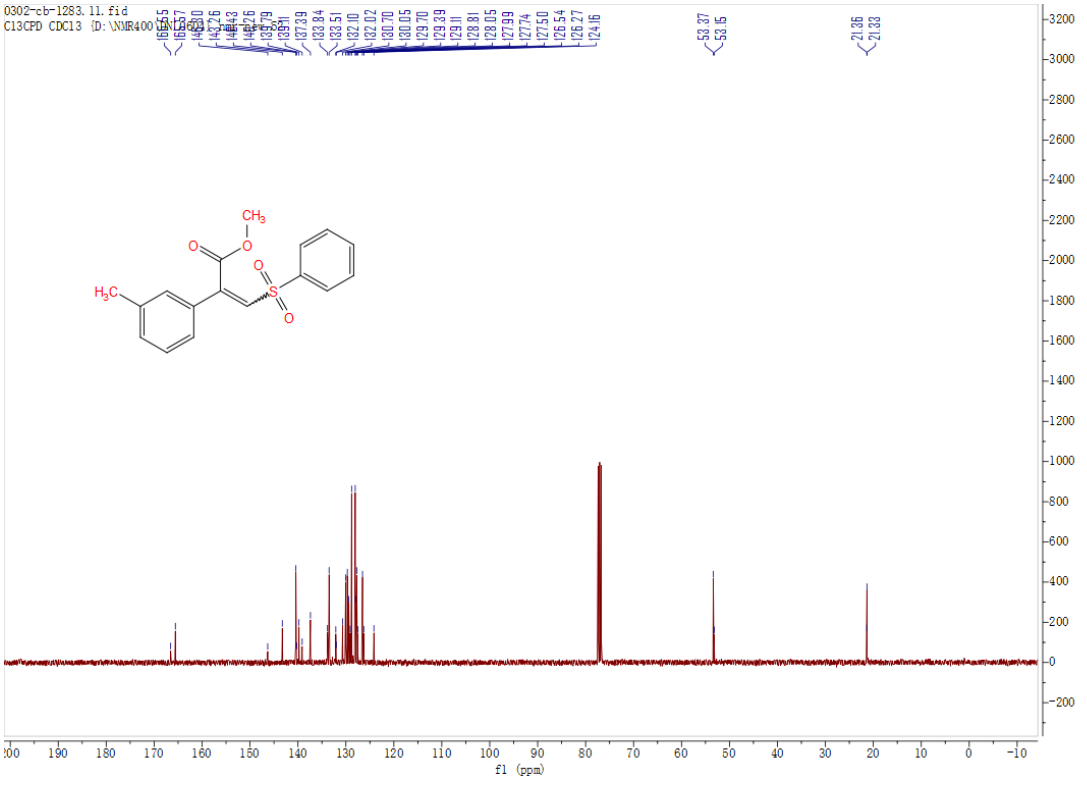
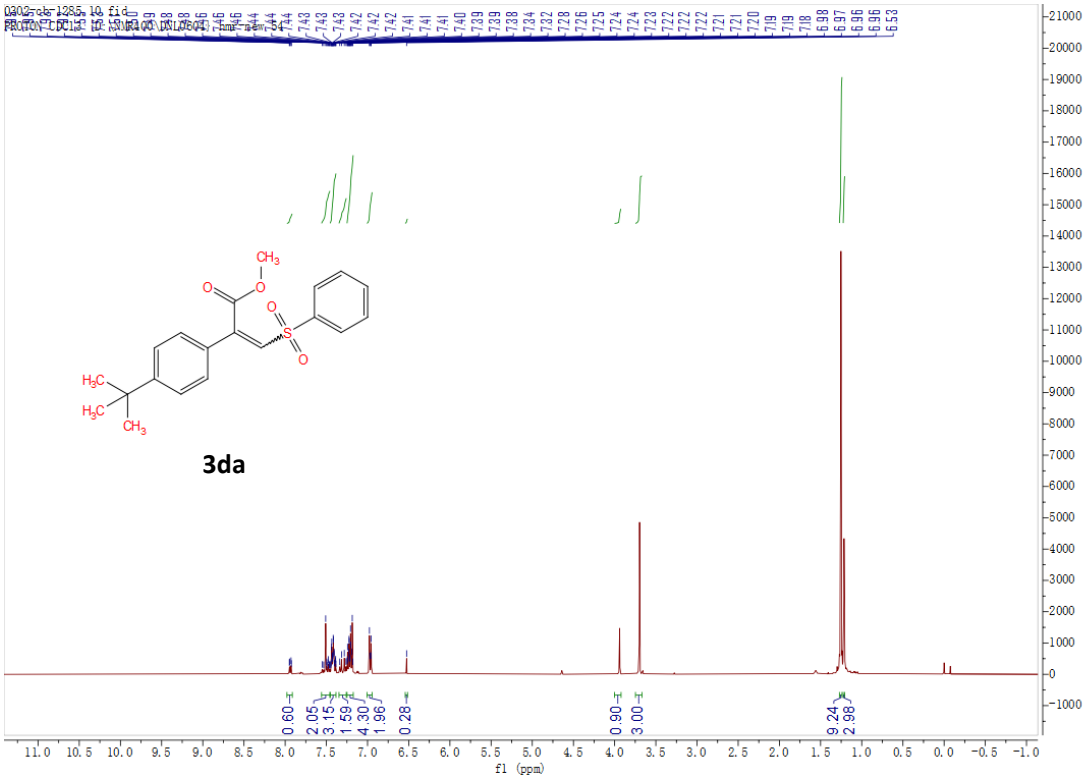
0.99
0.35
1.00
3.00
1.09
3.01
f1 (ppm)

3ca


53.87
53.15
21.36
21.33
f1 (ppm)



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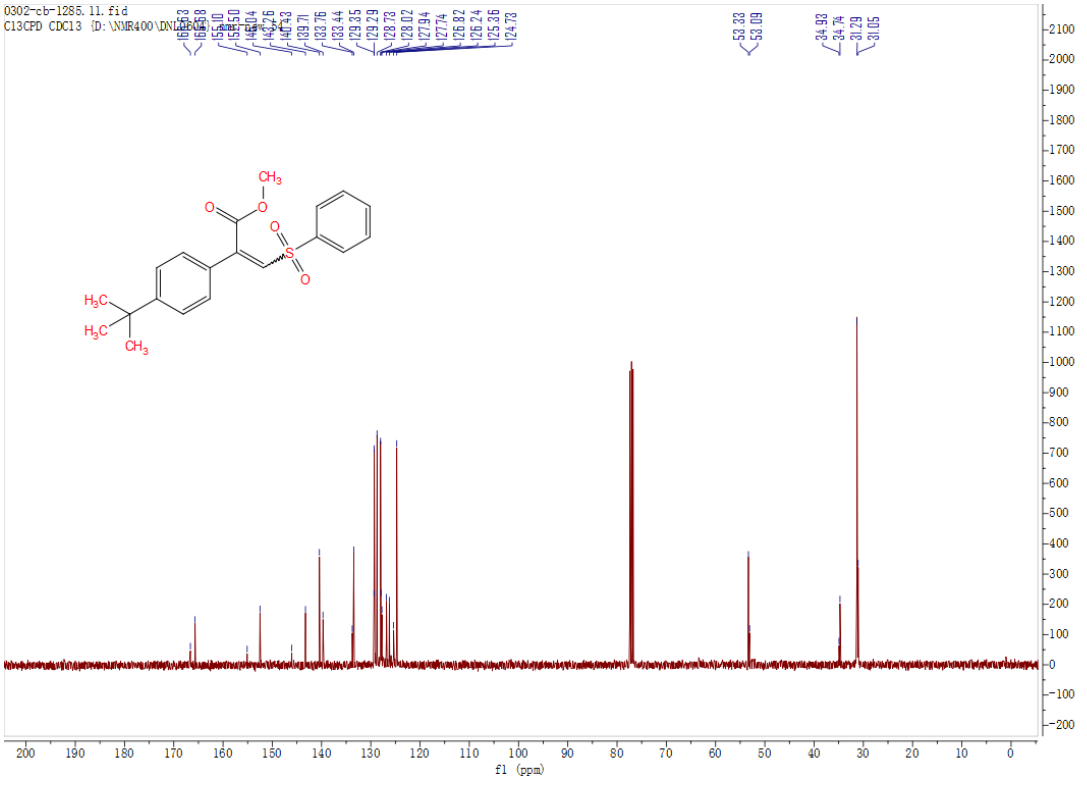

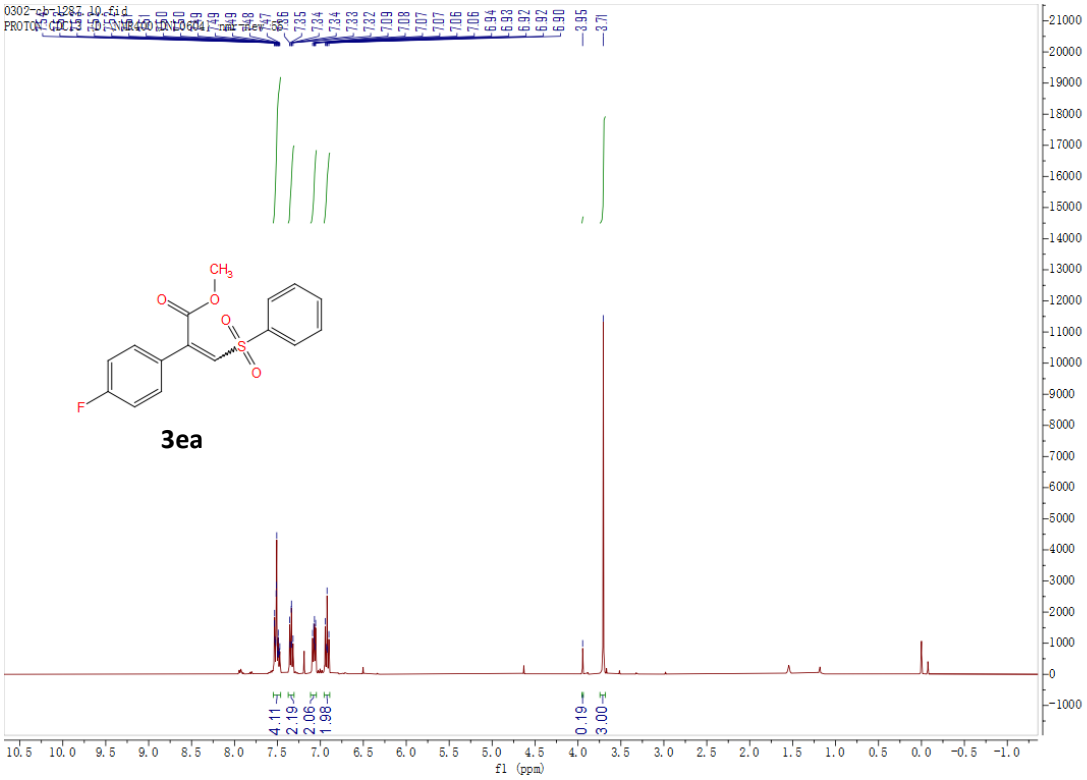
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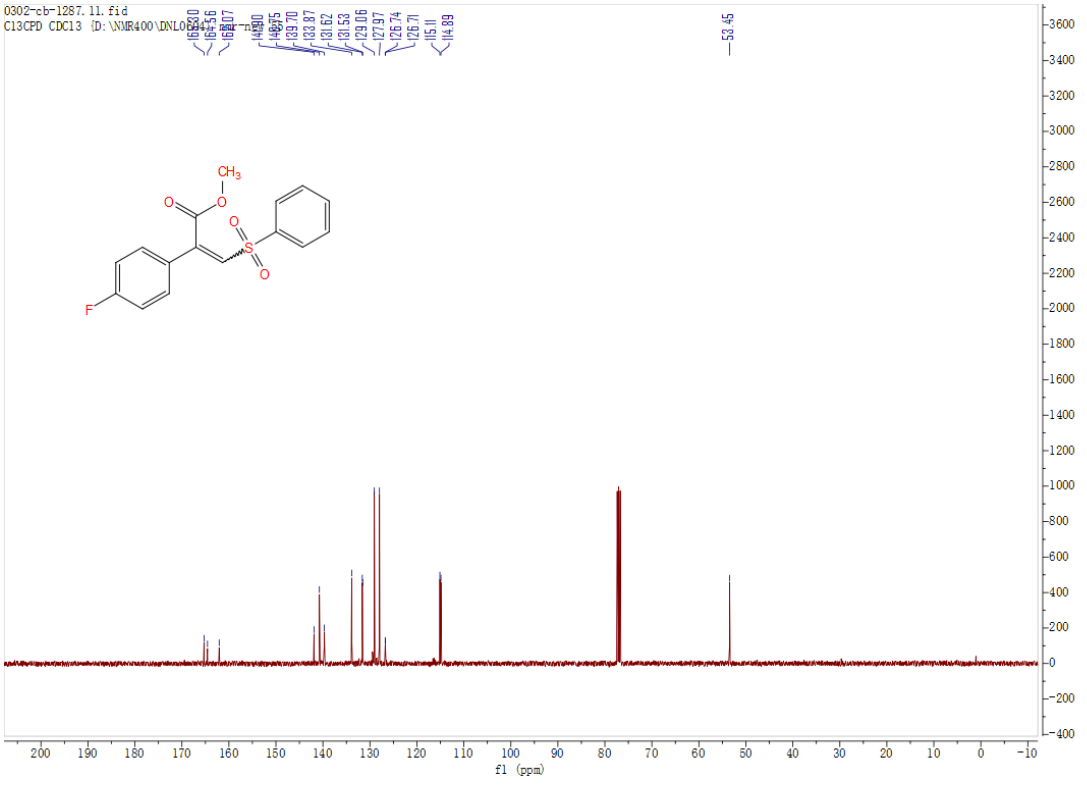
0.19
3.00
f1 (ppm)

3ea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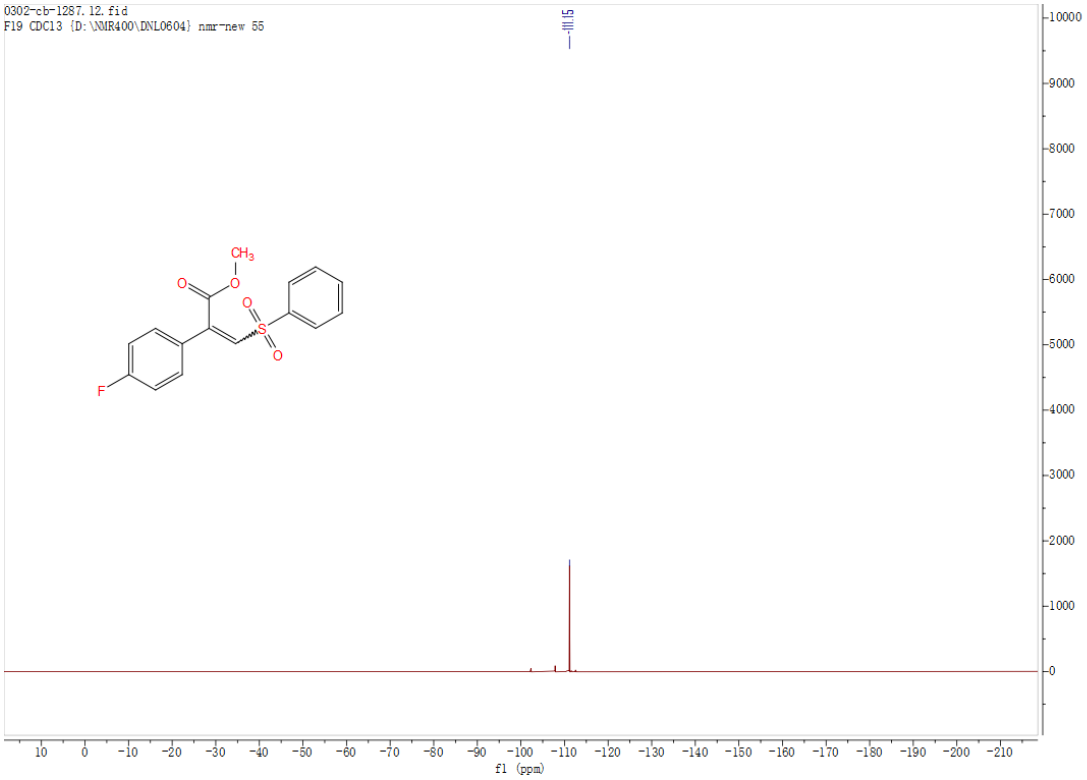
f1 (ppm)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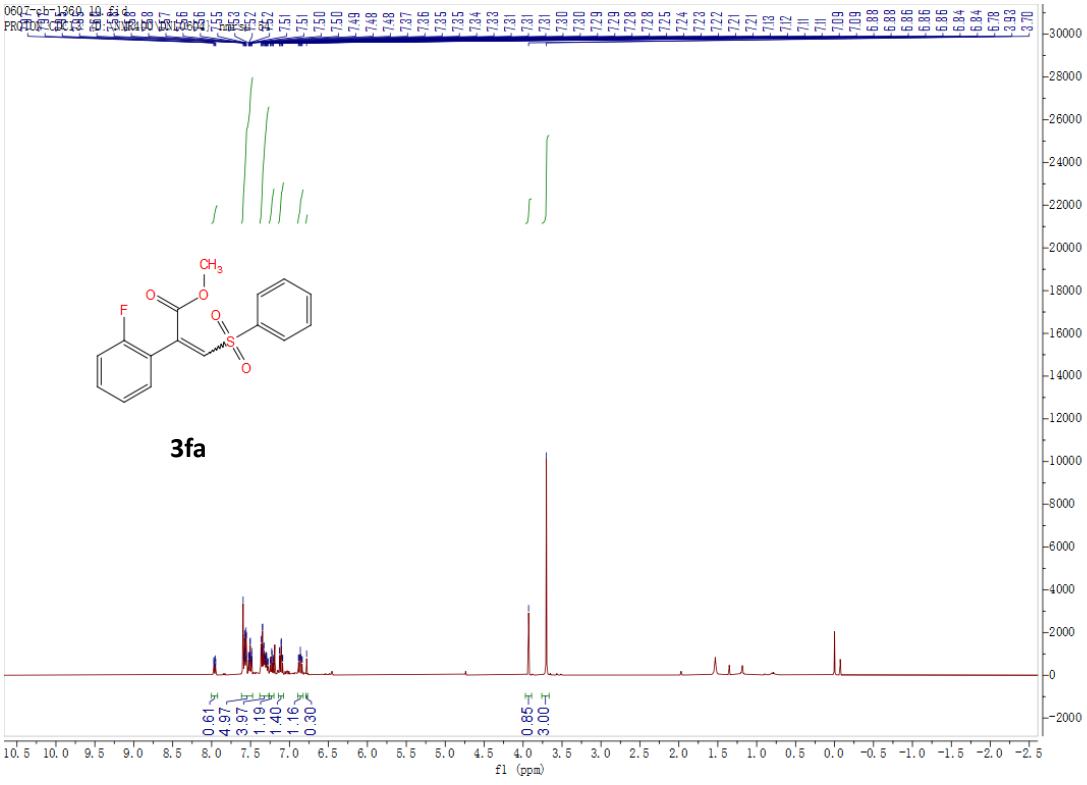
f1 (ppm)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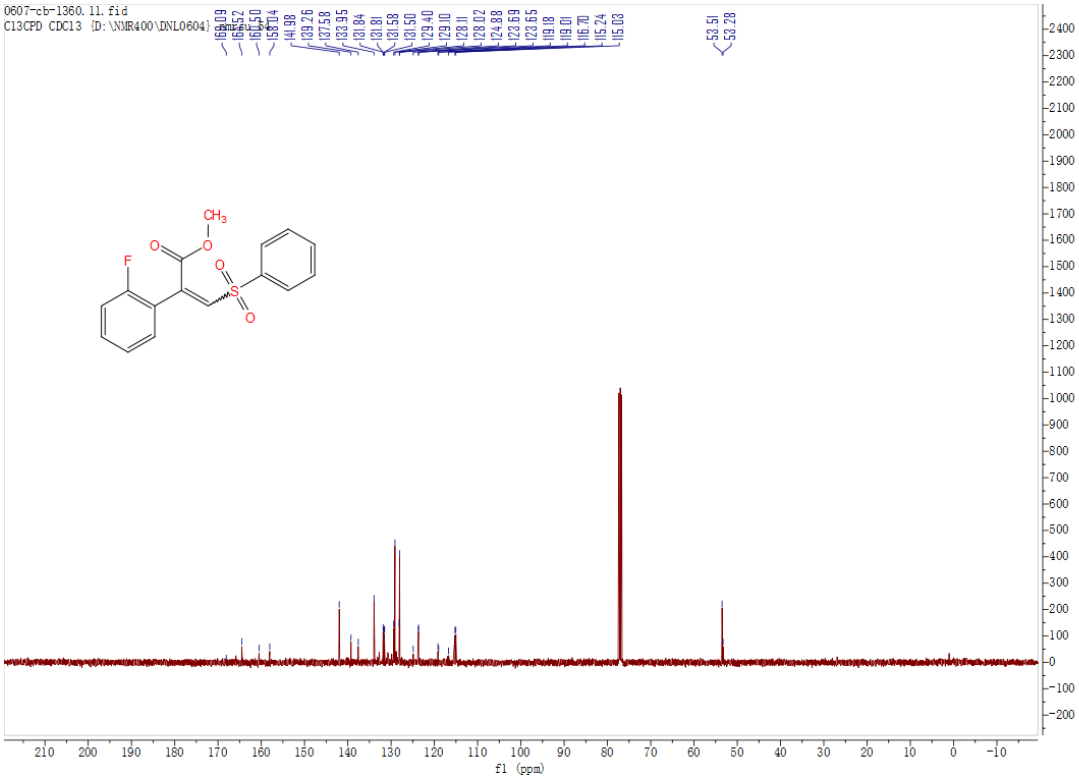
f1 (ppm)

3fa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165.10
159.04
141.98
139.26
137.58
133.95
131.84
131.81
131.58
131.50
129.40
129.10
128.11
126.02
124.88
123.69
123.65
119.18
119.01
116.70
115.24
115.03
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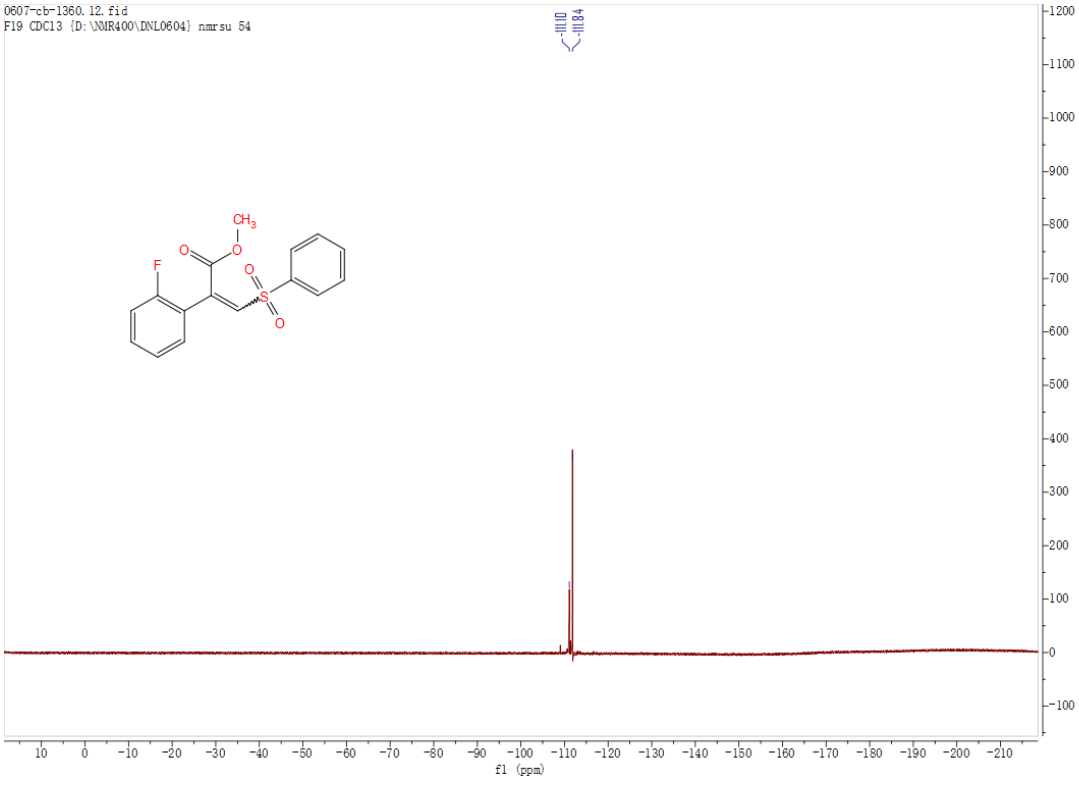
CH3
O
O
F
O
S
O
f1 (ppm)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-111.10
-111.84
CH3
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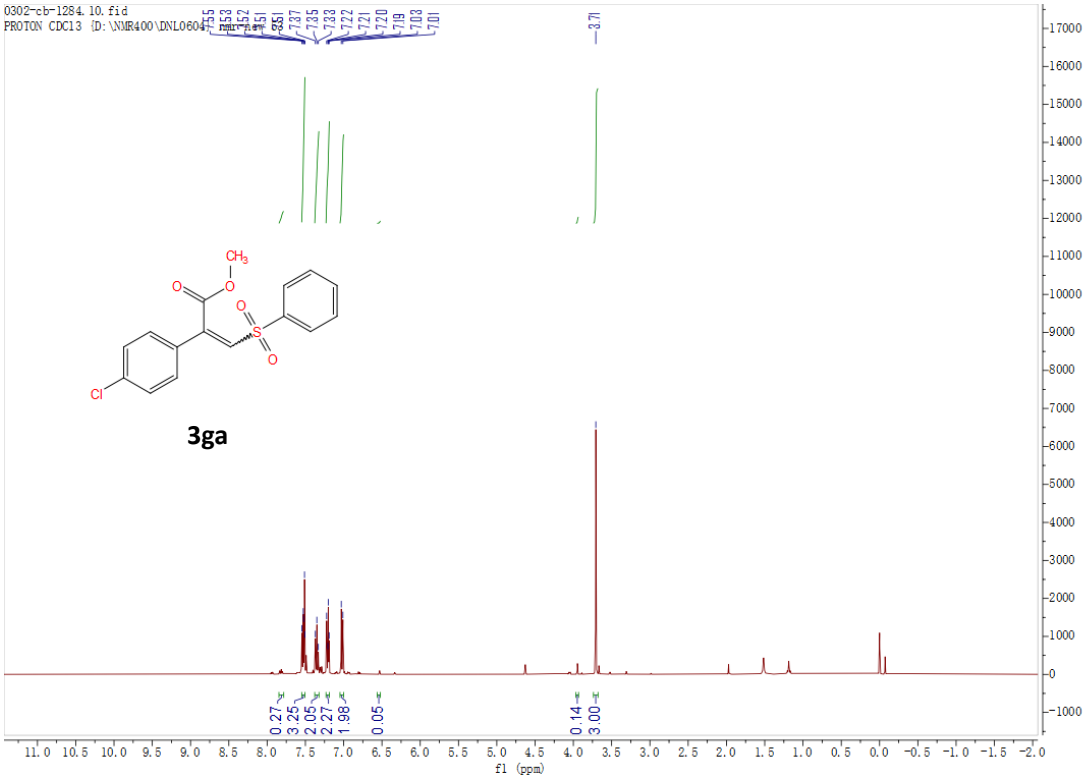
O
F
O
S
O
f1 (ppm)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7.53
7.52
7.51
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7.33
7.22
7.21
7.20
7.19
7.03
7.01
3.71
CH3
O
O
O
S
O
Cl
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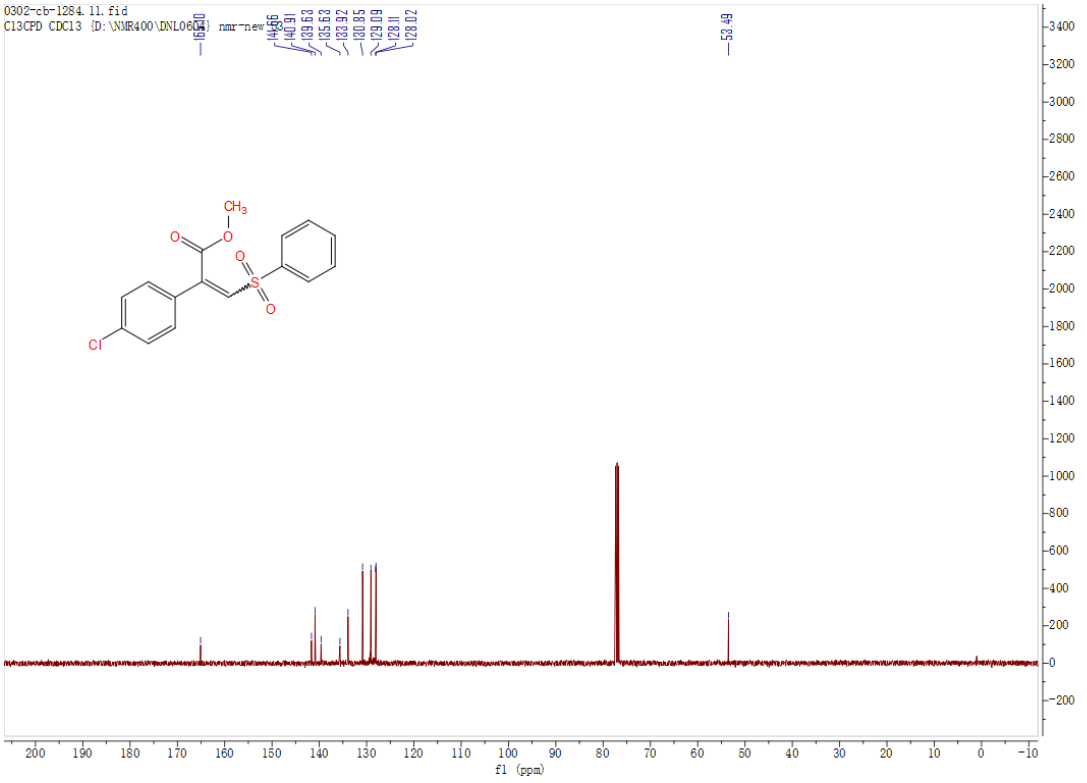
3.25
2.05
2.27
1.98
0.05
0.14
3.00
f1 (ppm)

3ga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140.91
139.63
135.63
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129.09
128.11
128.02
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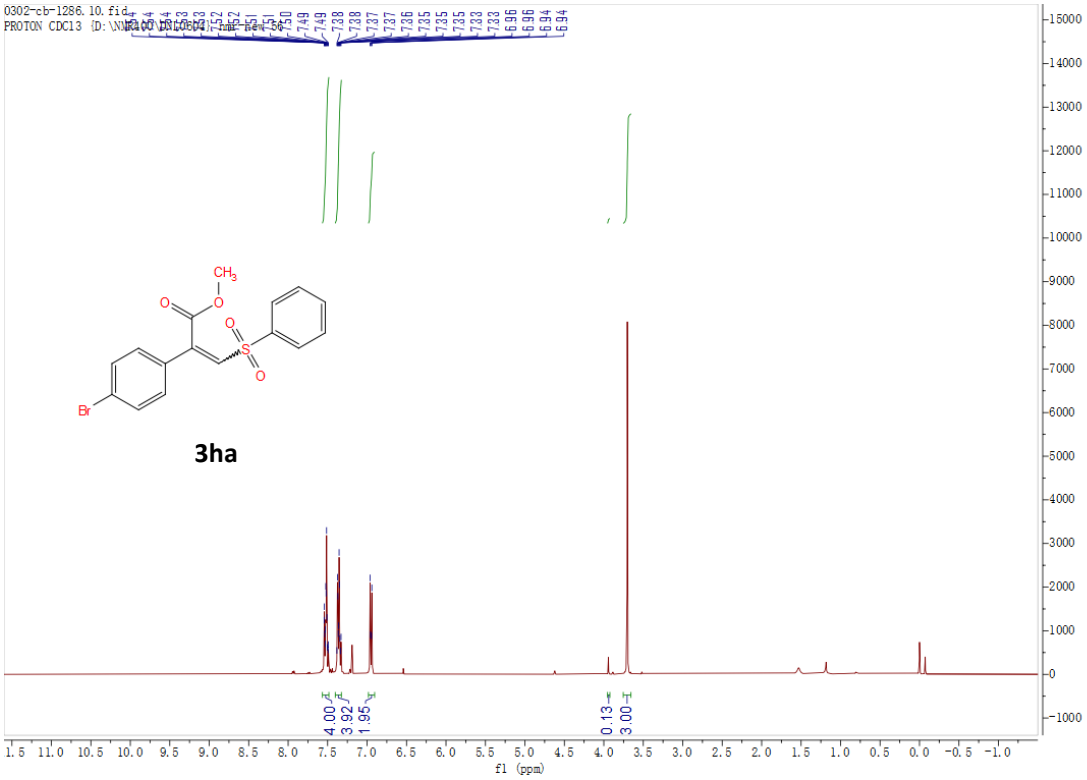
CH3
O
O
O
S
O
Cl
f1 (ppm)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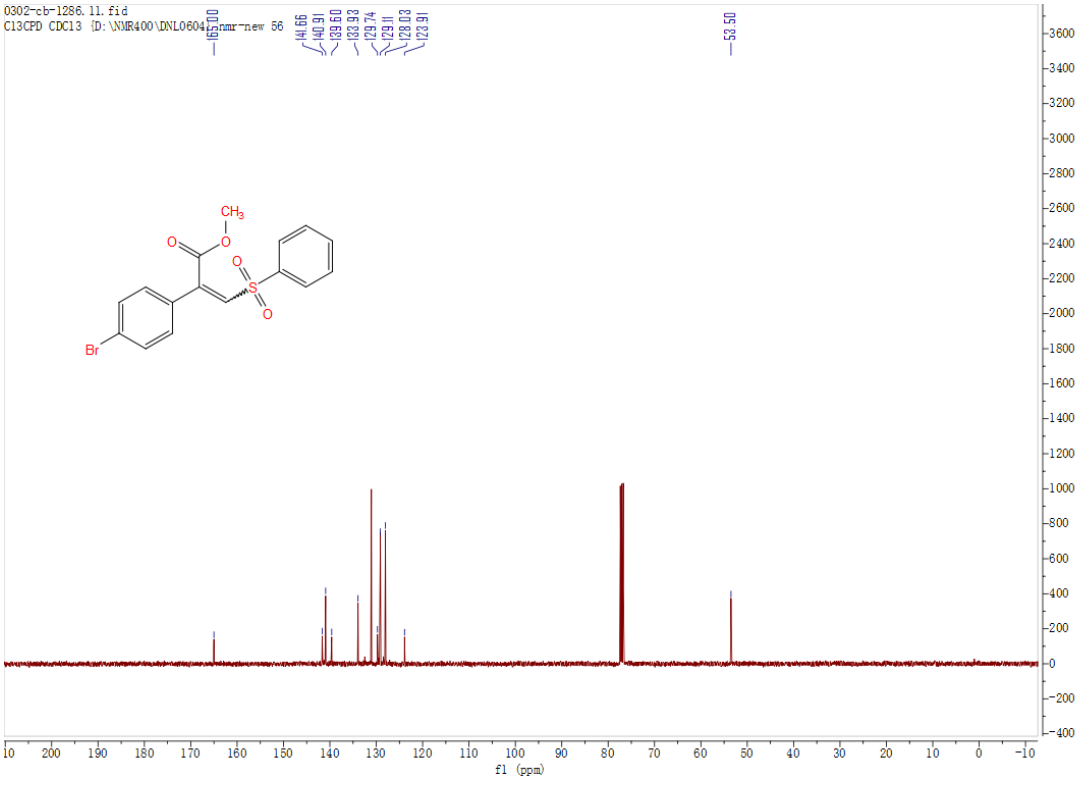
3.92
1.95
0.13
3.00
f1 (ppm)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133.93
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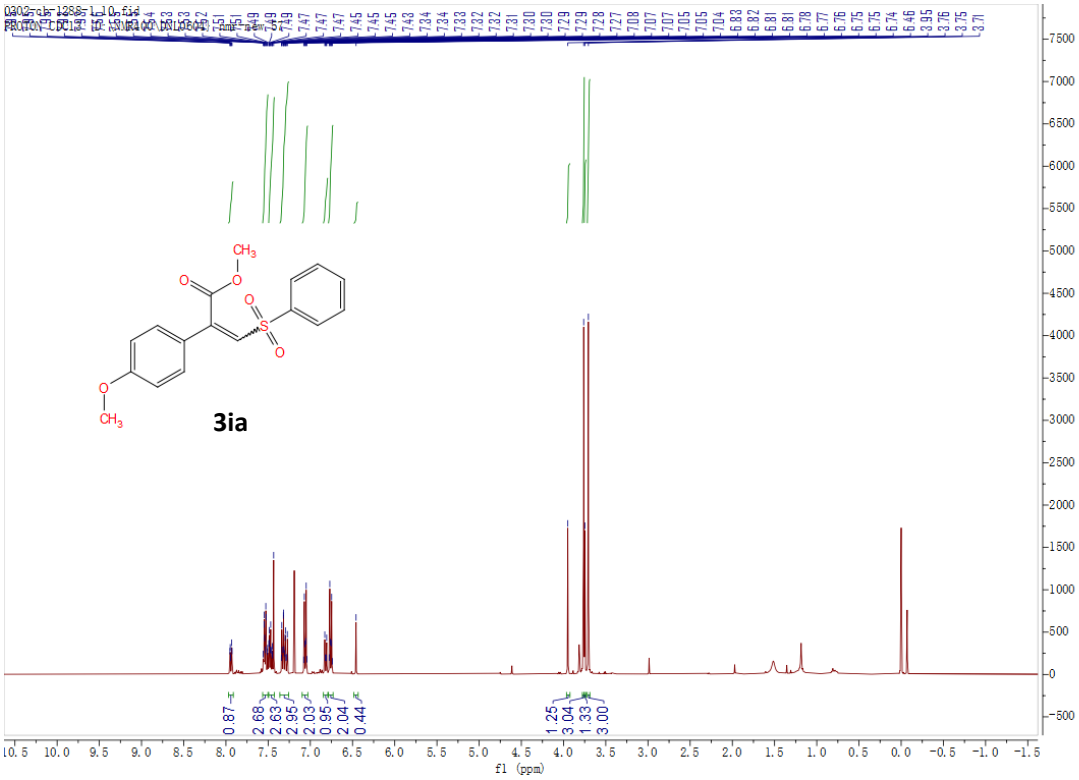
53.50
f1 (ppm)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3.04
1.33
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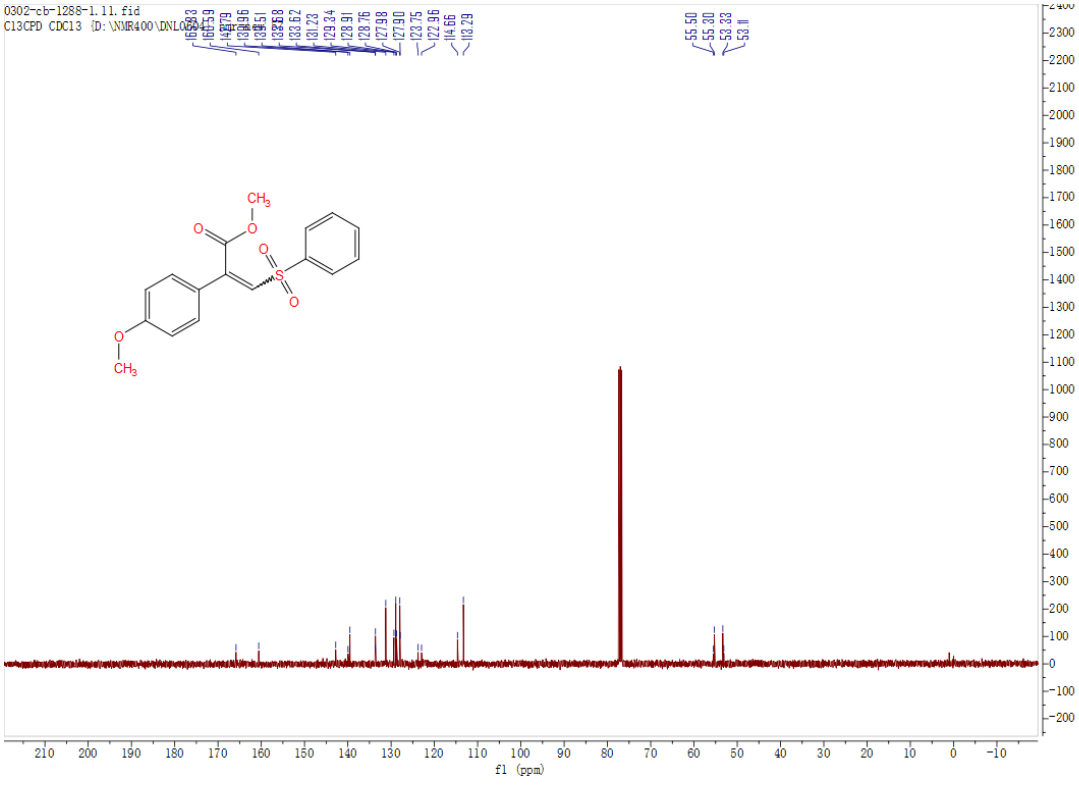
f1 (ppm)

3ia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53.11
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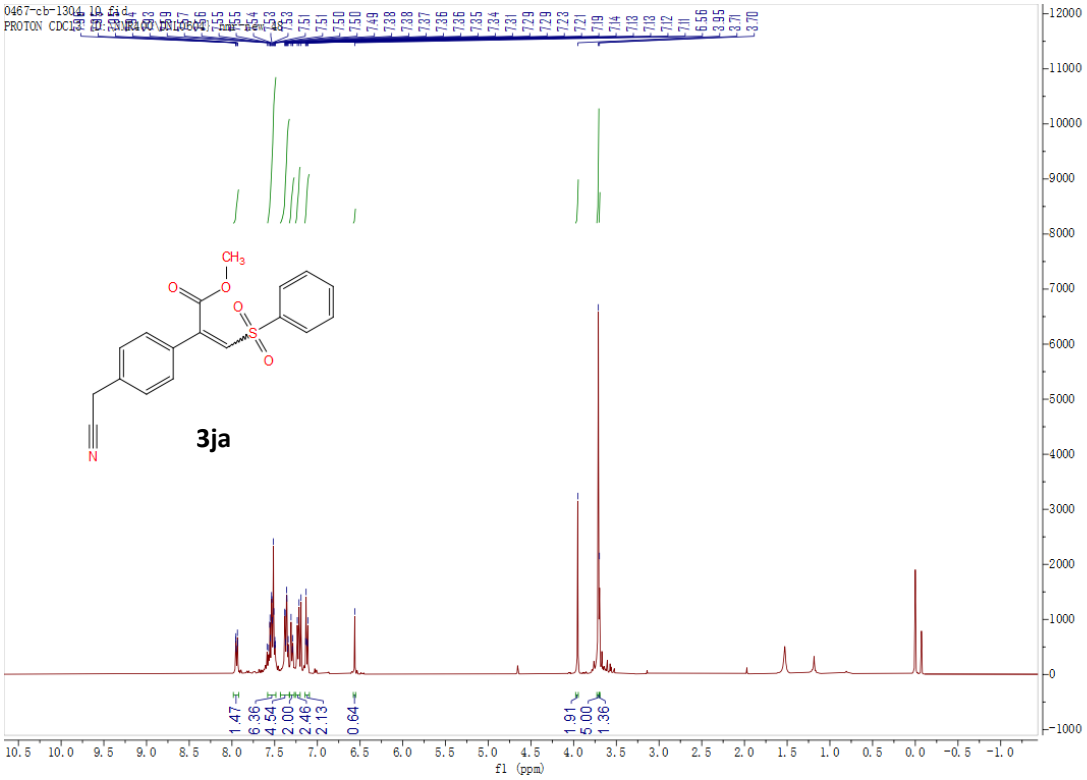
0467-cb-1304-10.fid
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2.13
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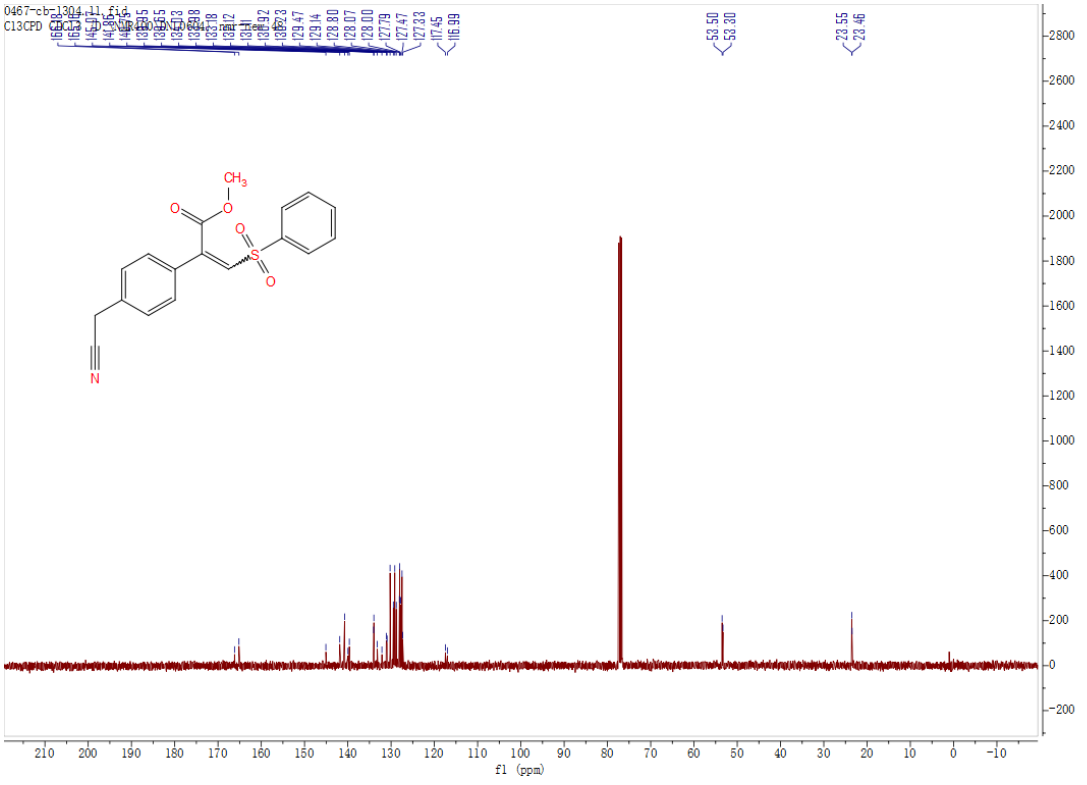
1.91
5.00
1.36
f1 (ppm)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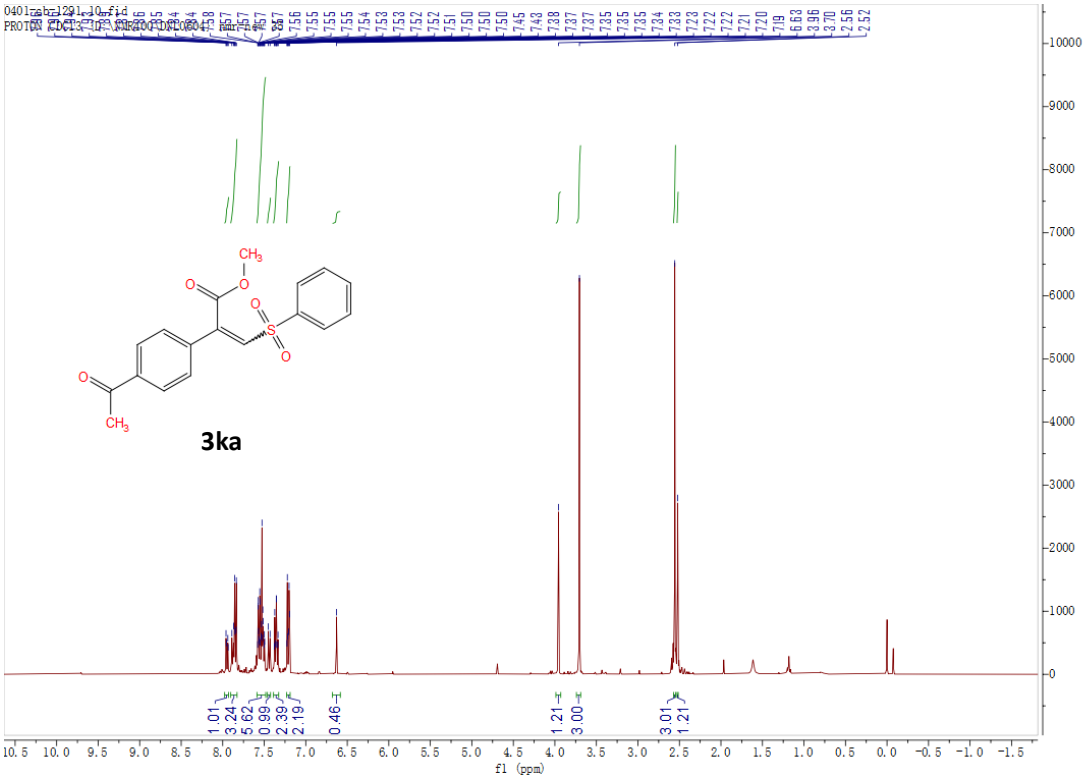
23.55
23.46
f1 (ppm)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3.24
5.62
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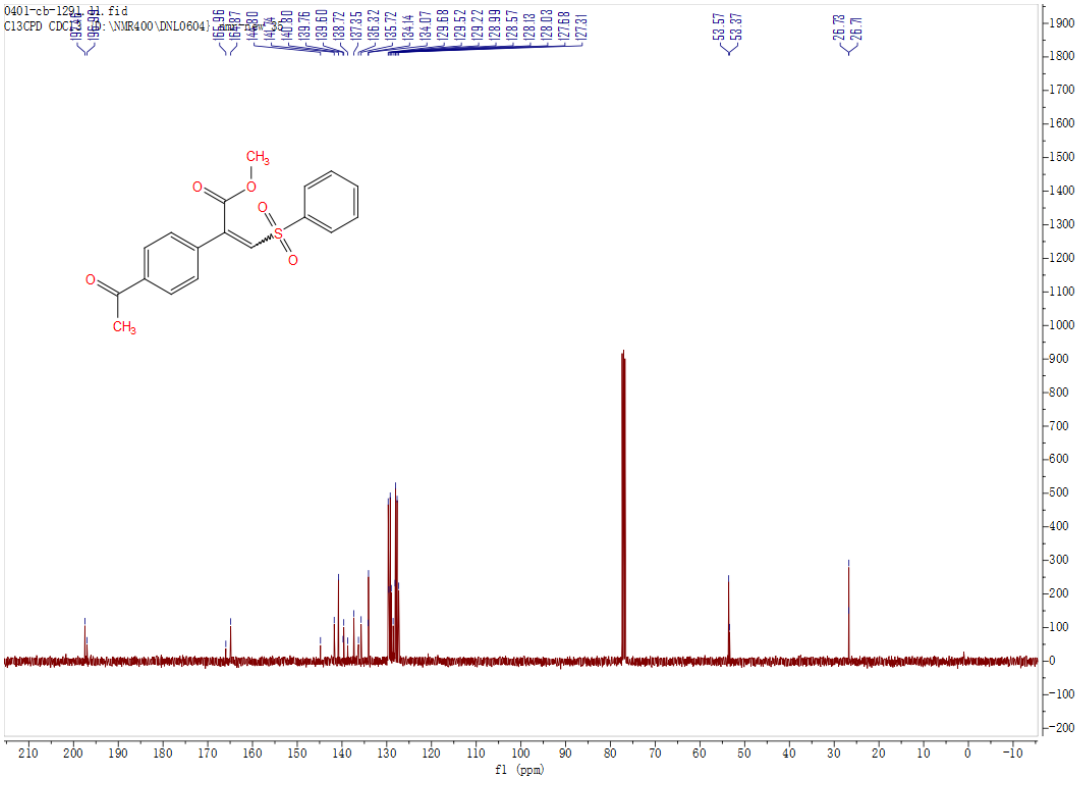
2.39
2.19
0.46
1.21
3.00
3.01
1.21
f1 (ppm)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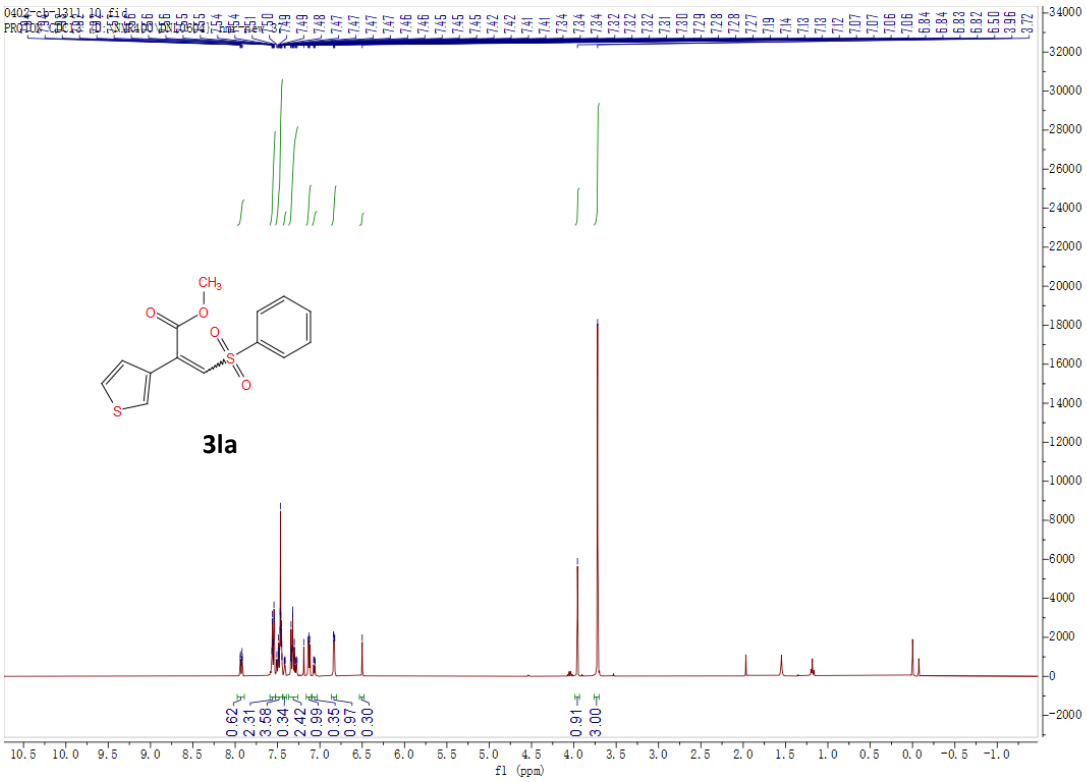
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2.42
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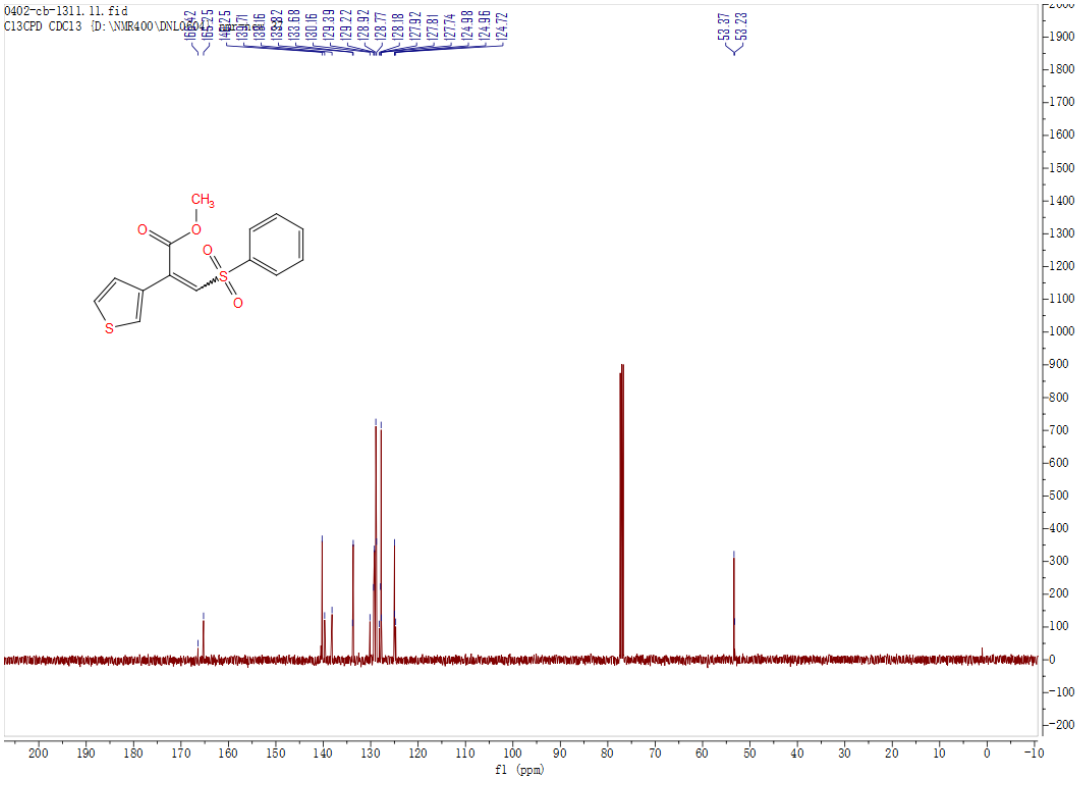
0.35
0.97
0.30
0.91
3.00
f1 (ppm)

3la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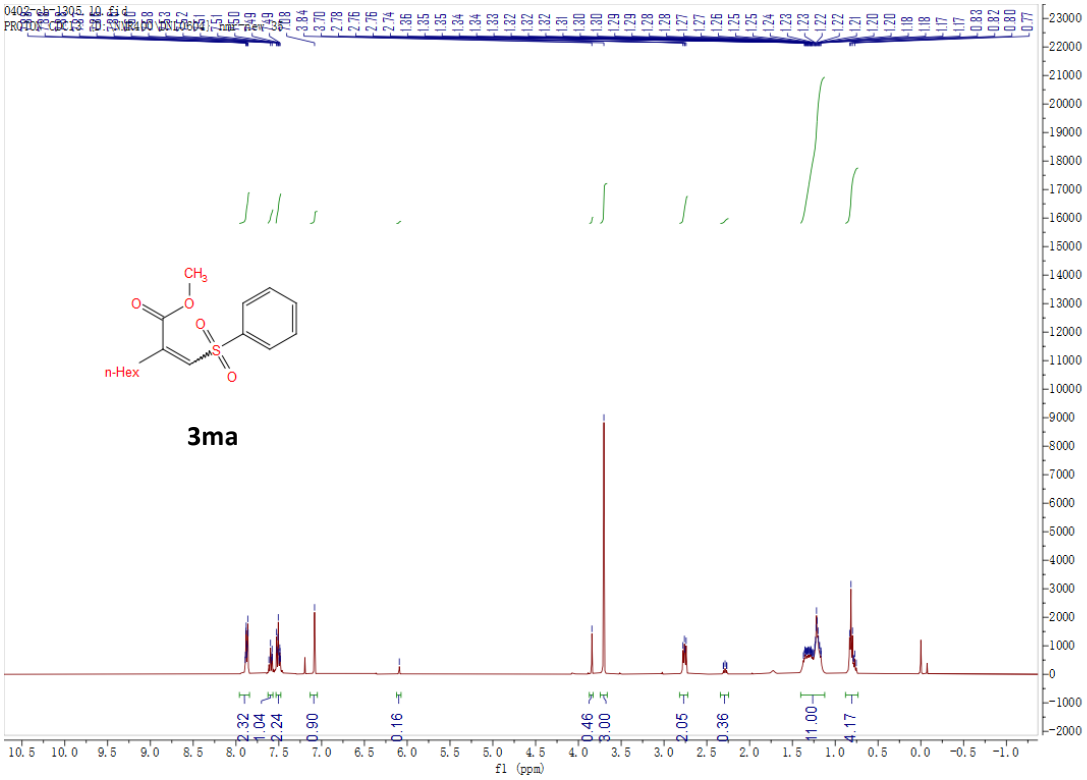
f1 (ppm)



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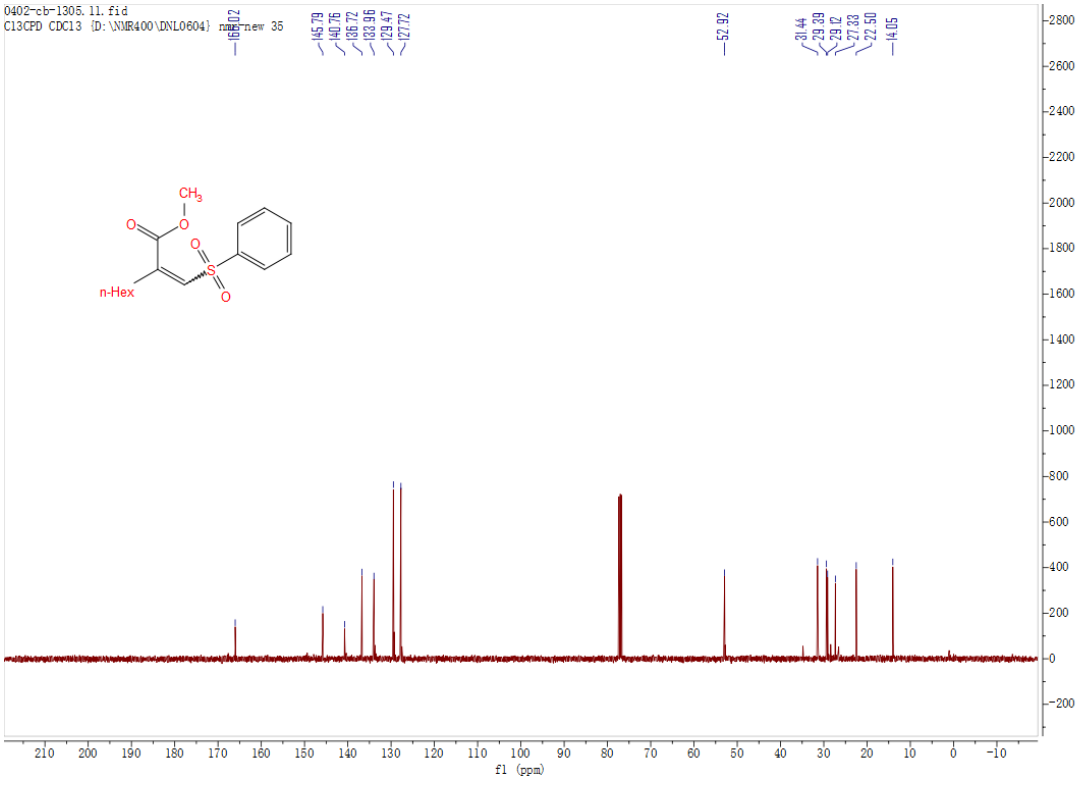
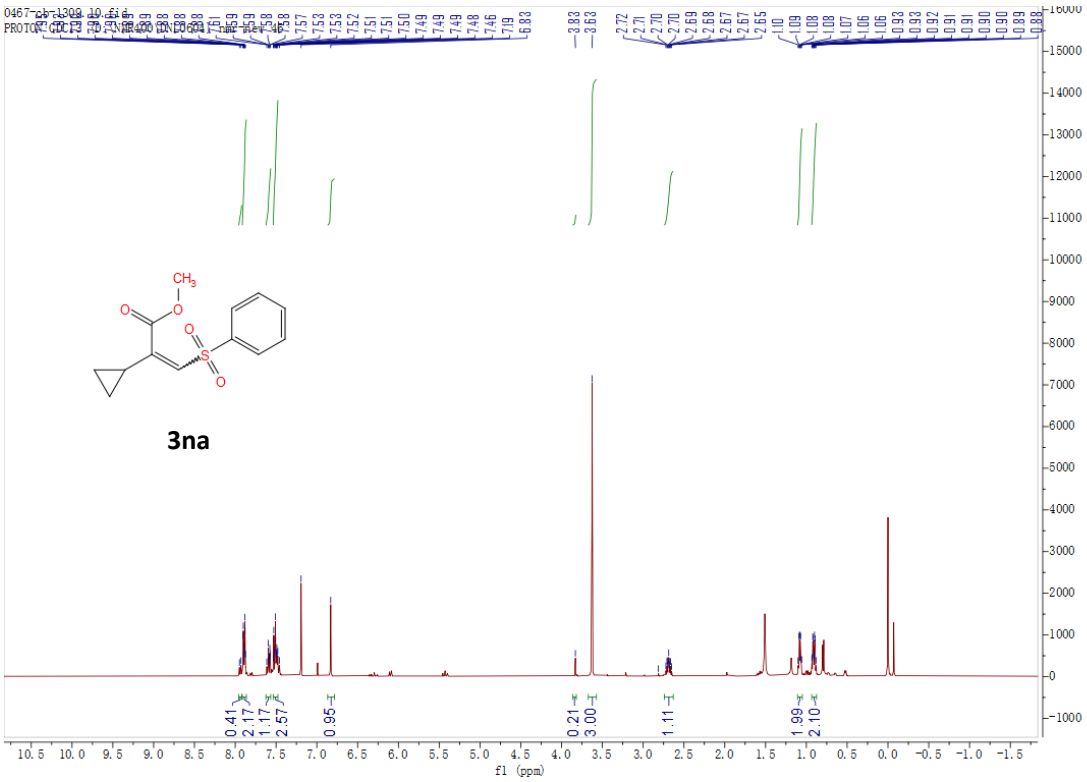
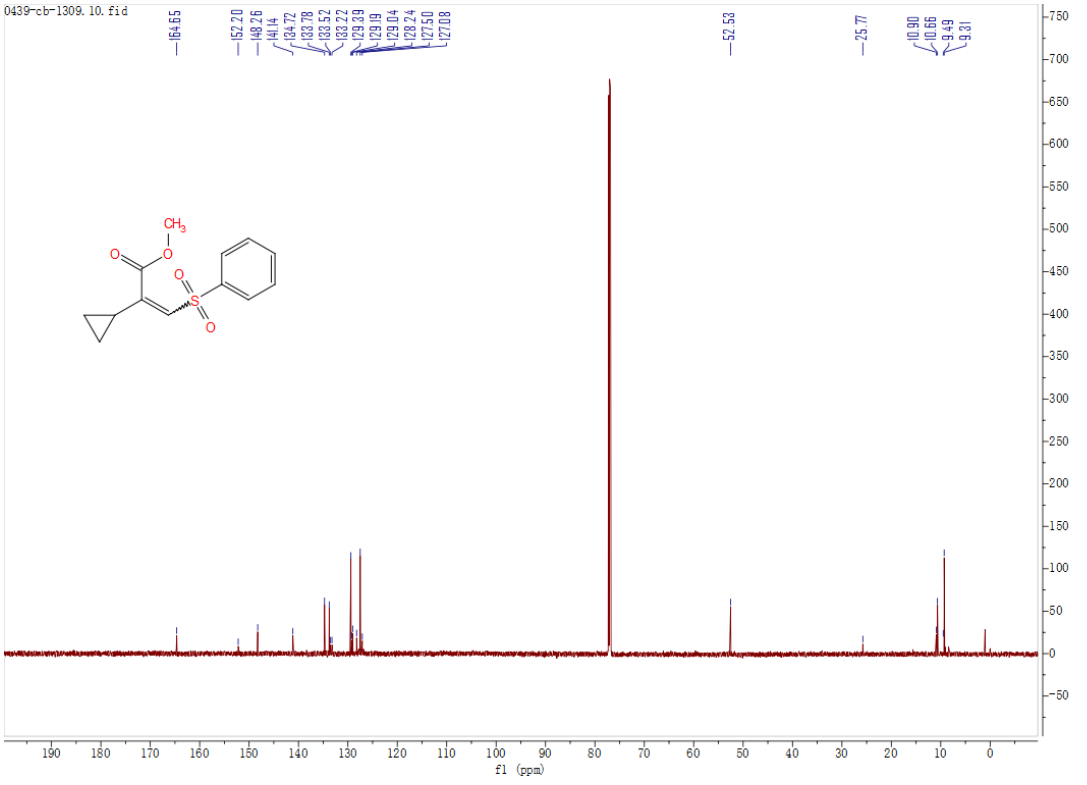
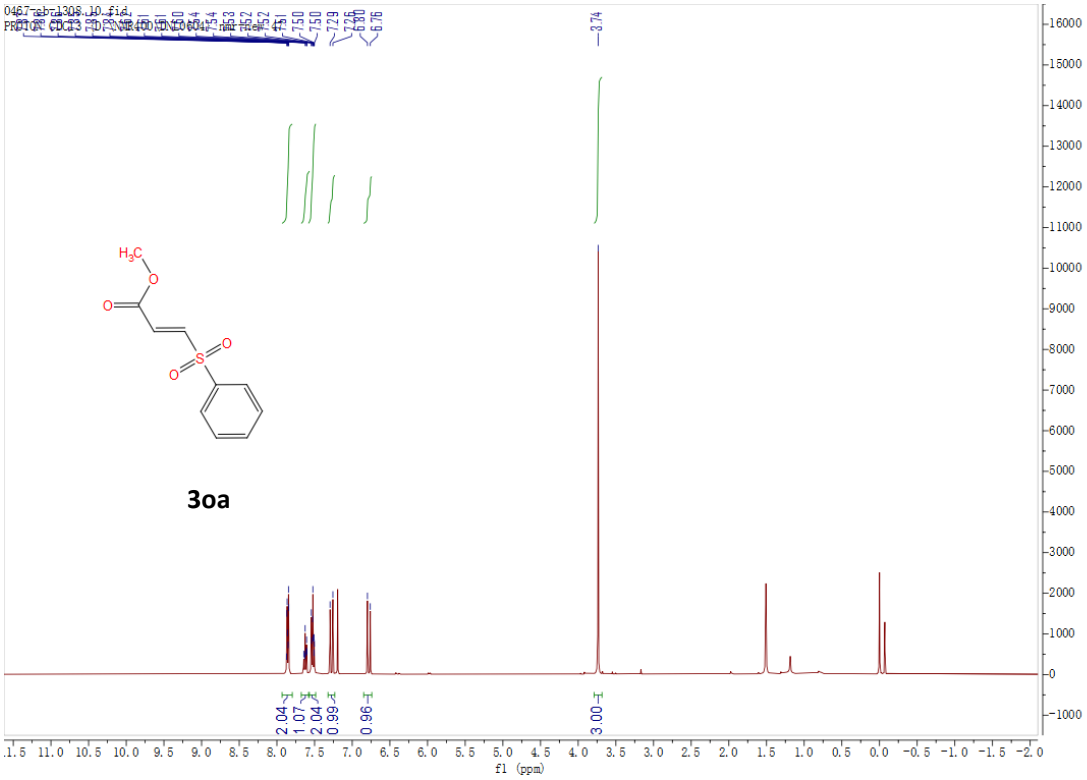




3na

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3.74
7.50
7.50
7.29
7.25
6.80
6.76
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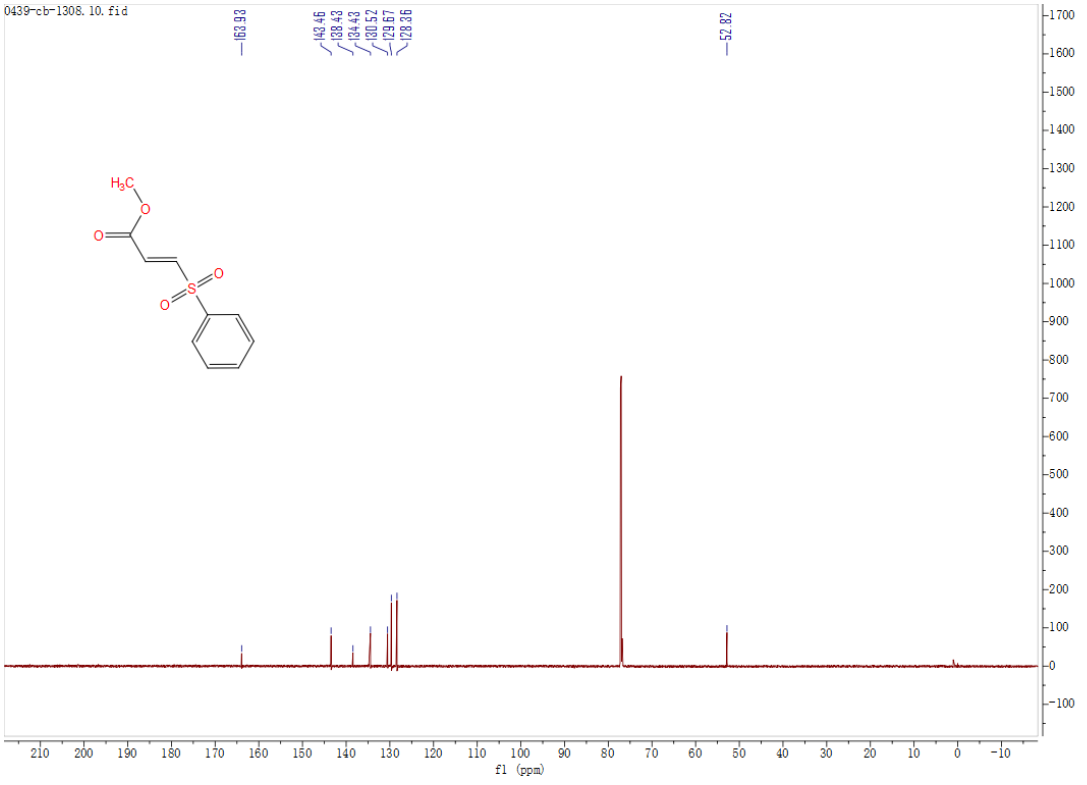
2.04
0.99
0.96
3.00
f1 (ppm)

3oa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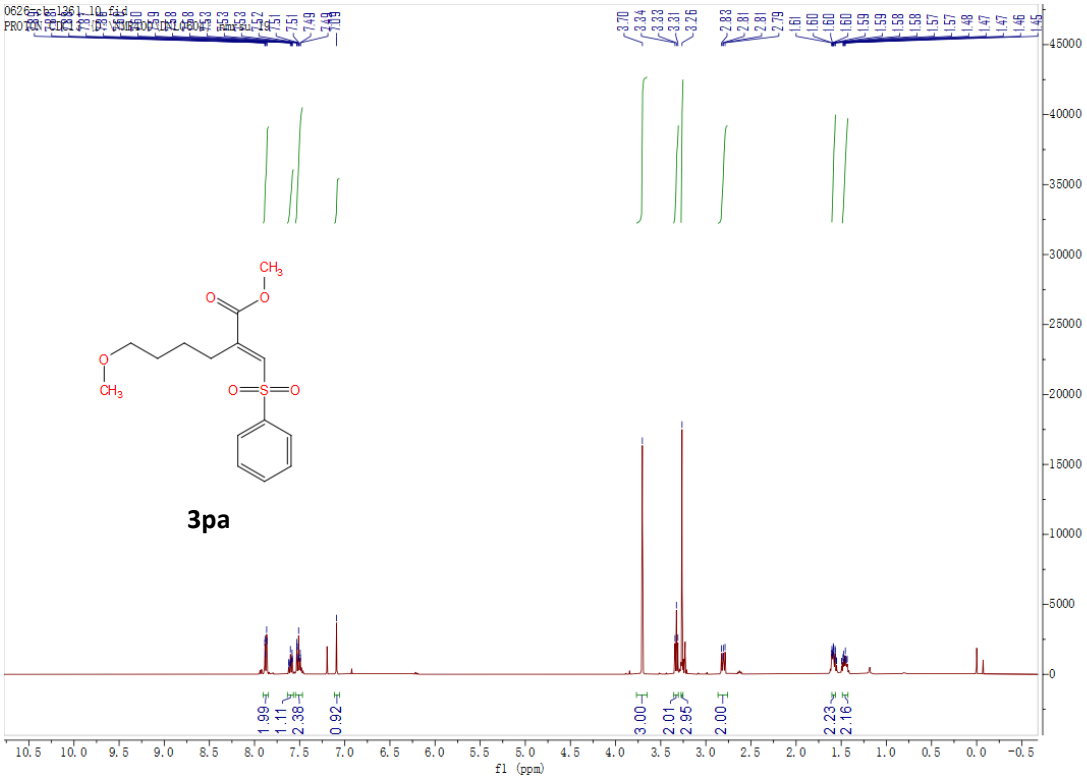
52.82
f1 (ppm)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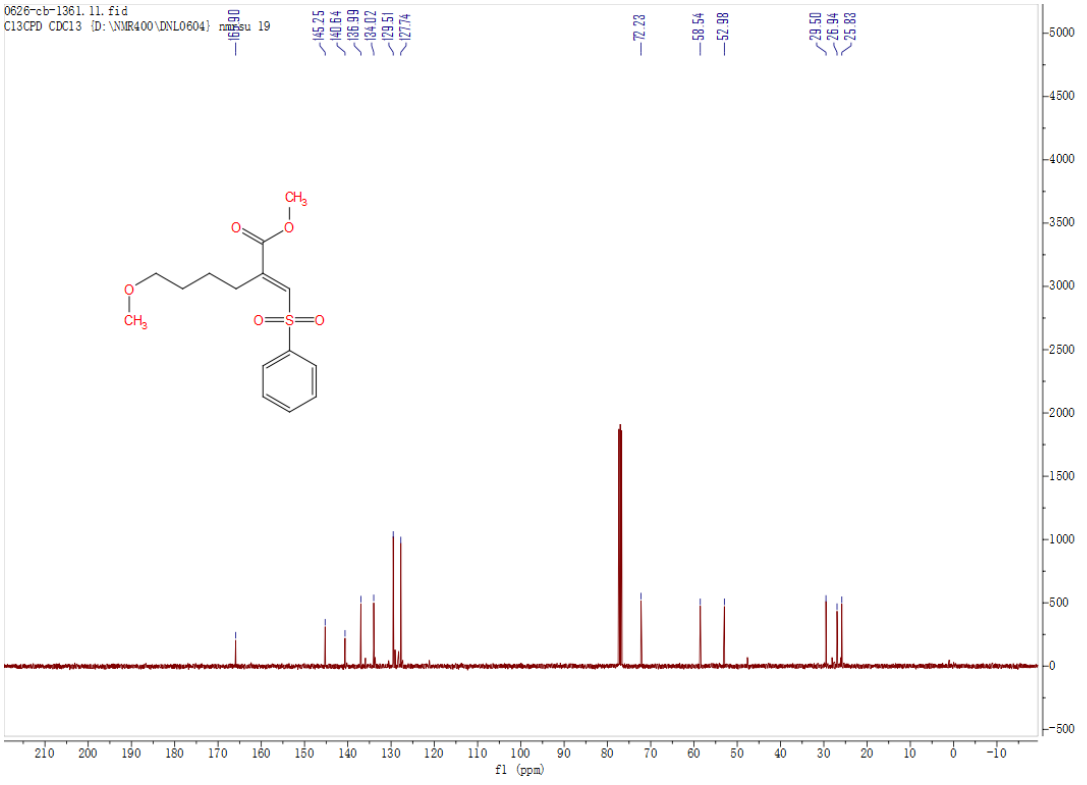
fl (ppm)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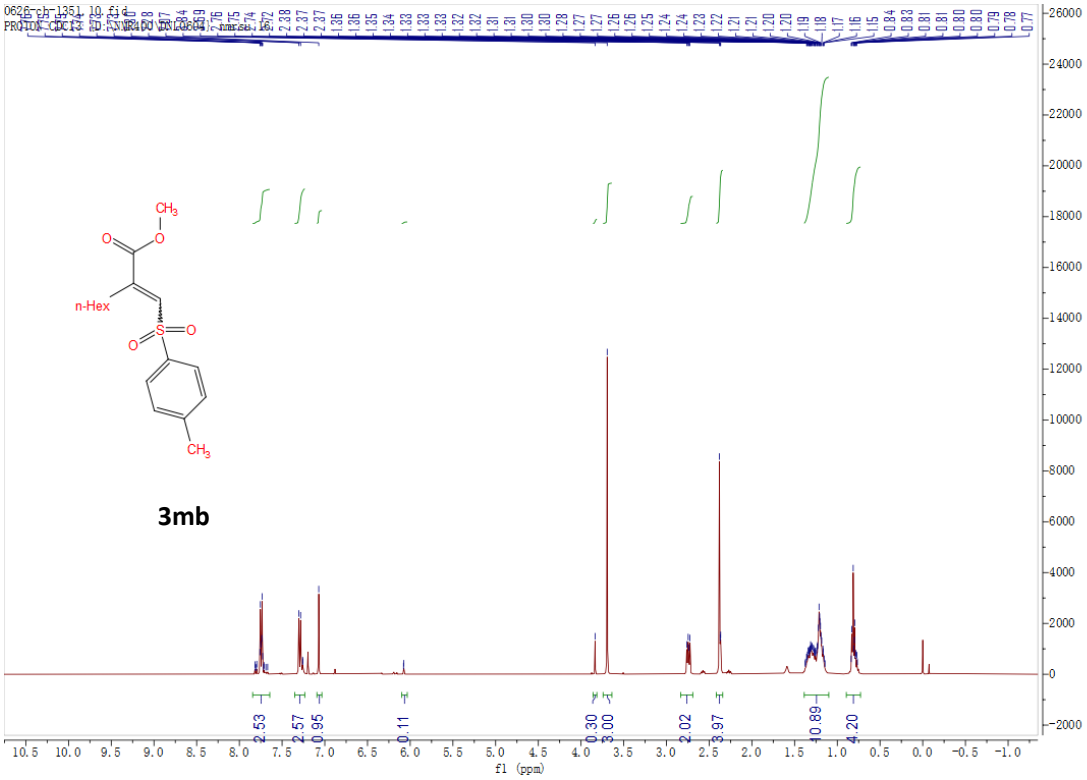
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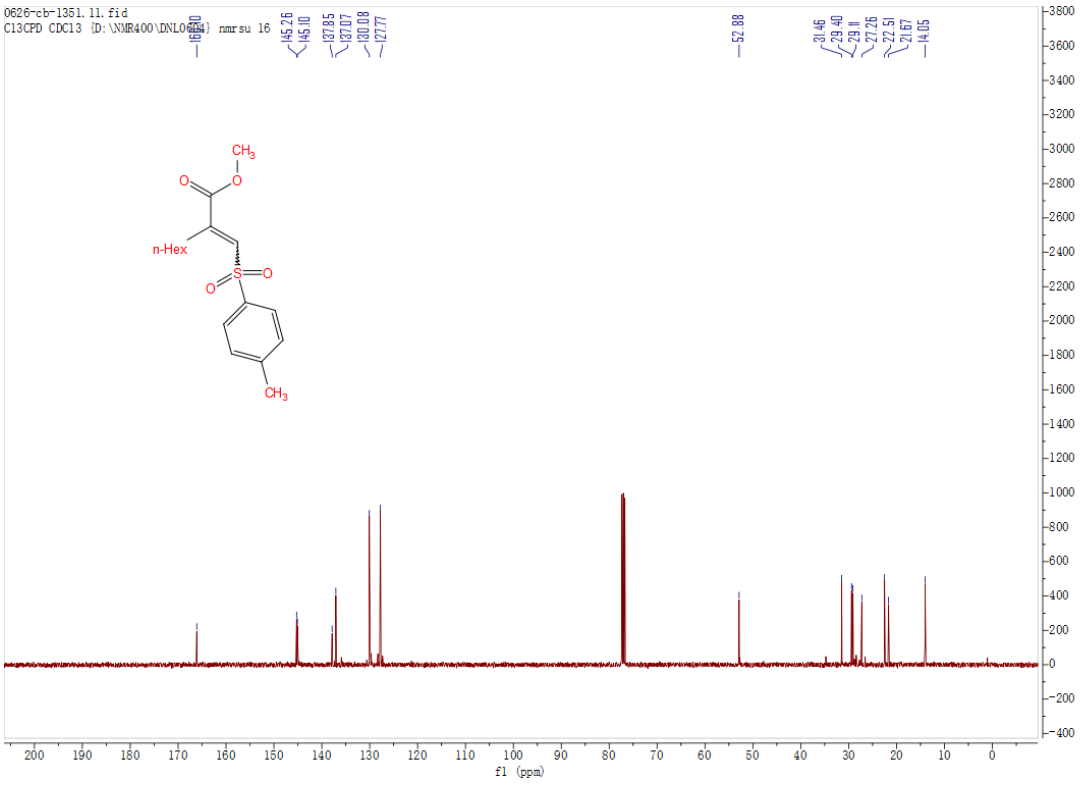
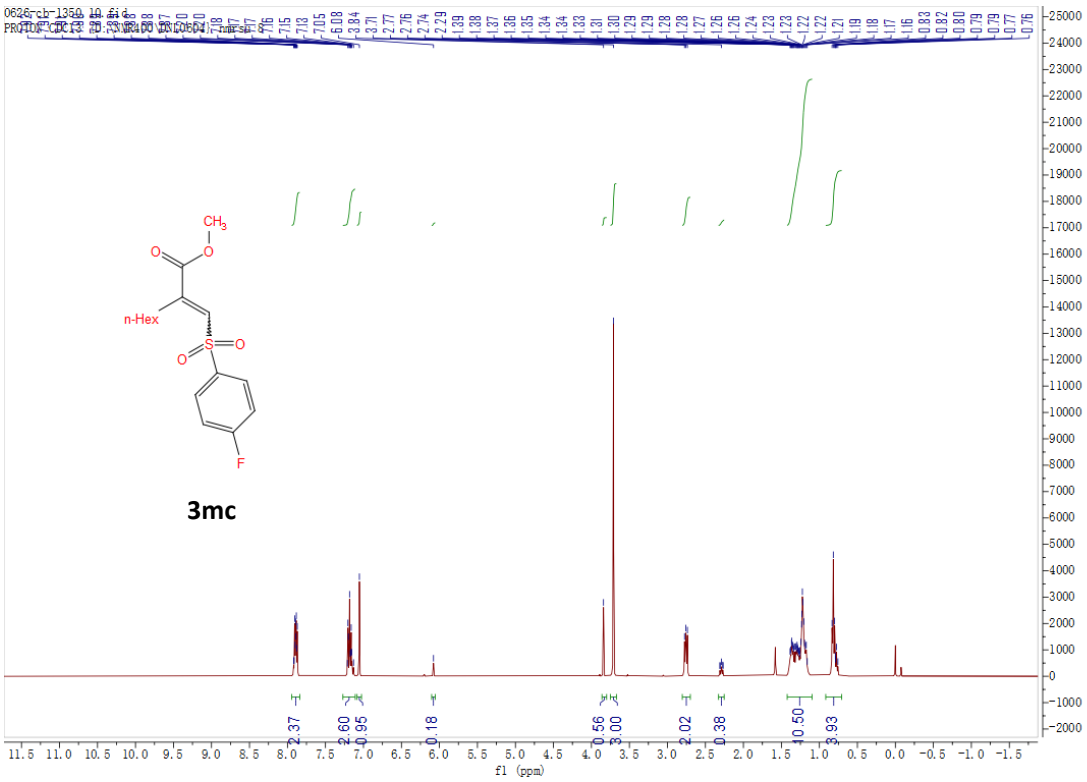
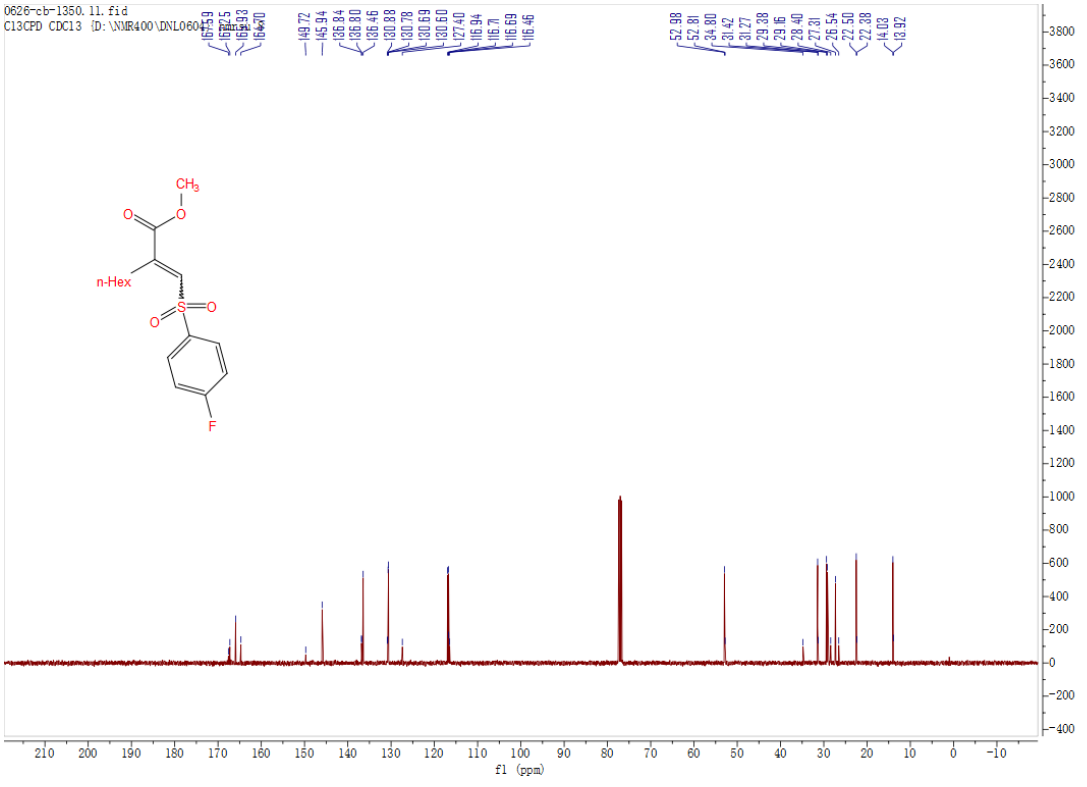
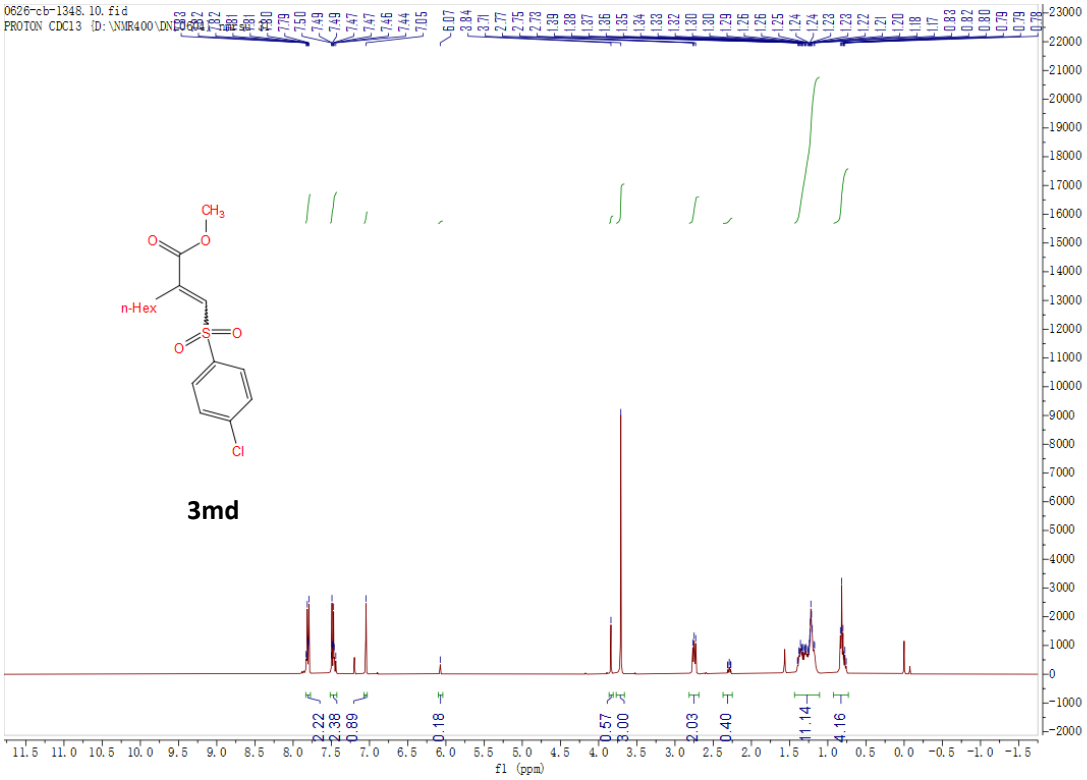
n-Hex
CH3
3mb
2.53
2.57
0.95
0.11
0.30
3.00
2.02
3.97
10.89
4.20
f1 (ppm)

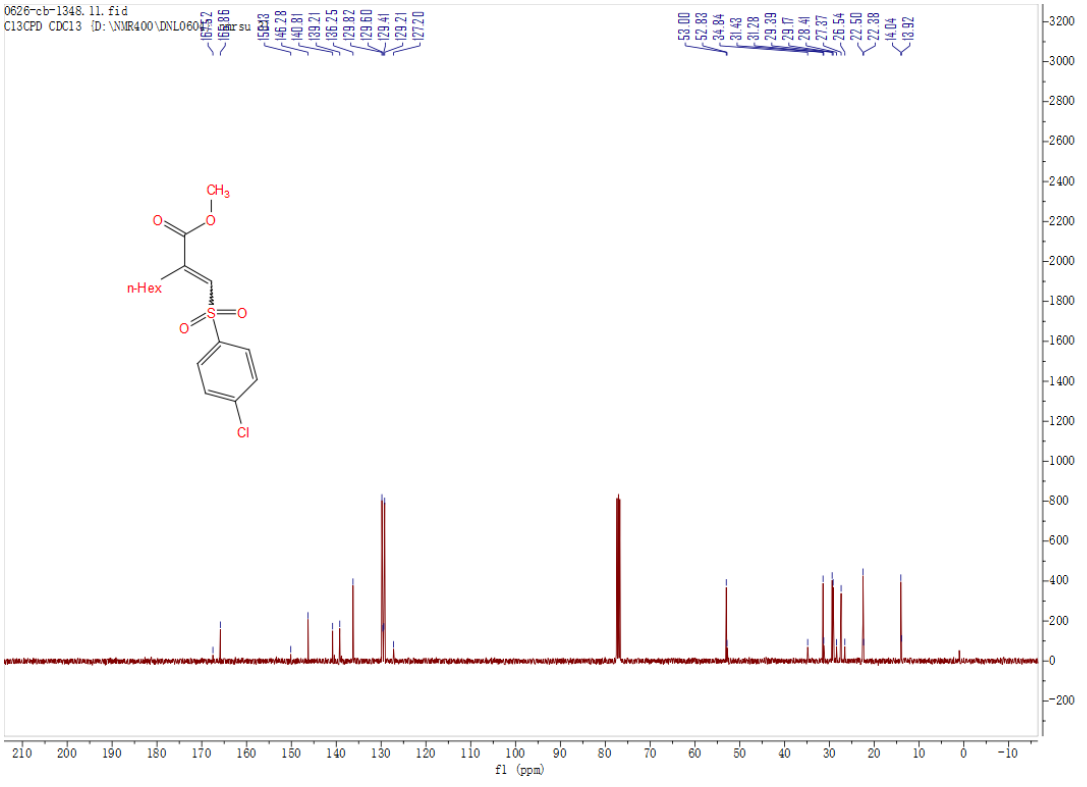

0626-cb-1351.11.fid
C13CPD CDCl3
145.26
145.10
137.85
137.07
130.08
127.77
52.88
31.46
29.40
29.11
27.26
22.51
21.67
14.05
n-Hex
CH3
f1 (ppm)

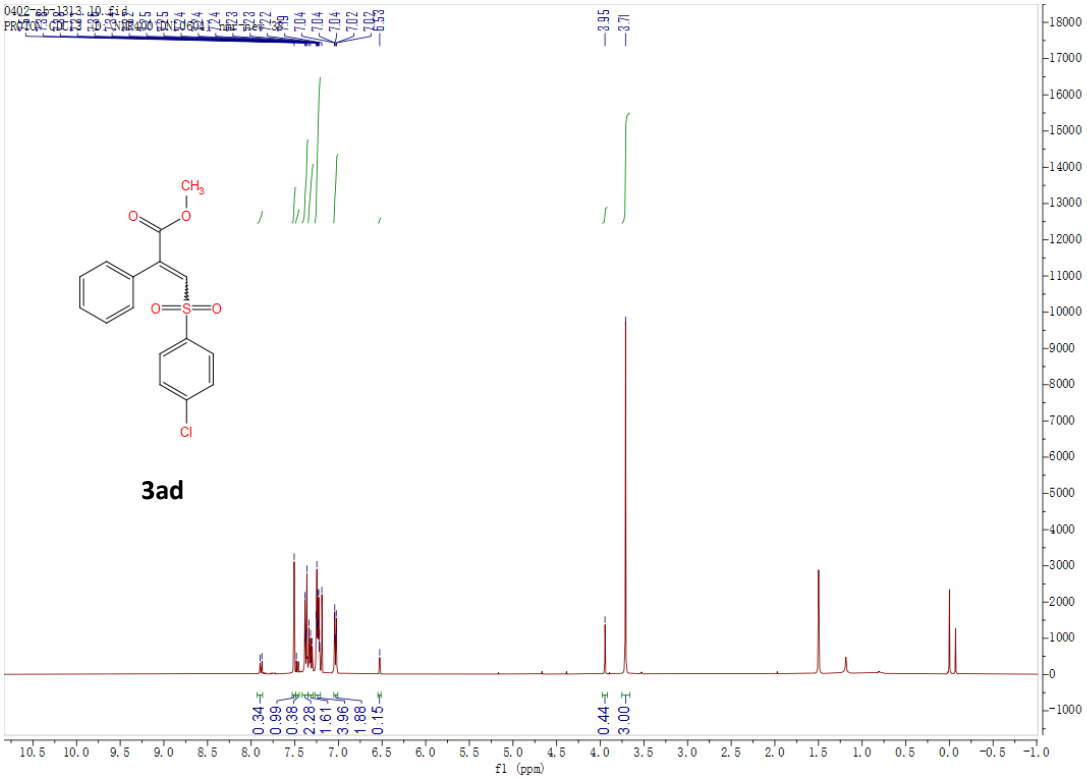

CH3
O
O
n-Hex
S
O
O
F
3mc
2.37
2.60
0.95
0.18
0.56
3.00
2.02
0.38
10.50
3.93
f1 (ppm)


CH3
O
O
n-Hex
S
O
O
F
f1 (ppm)

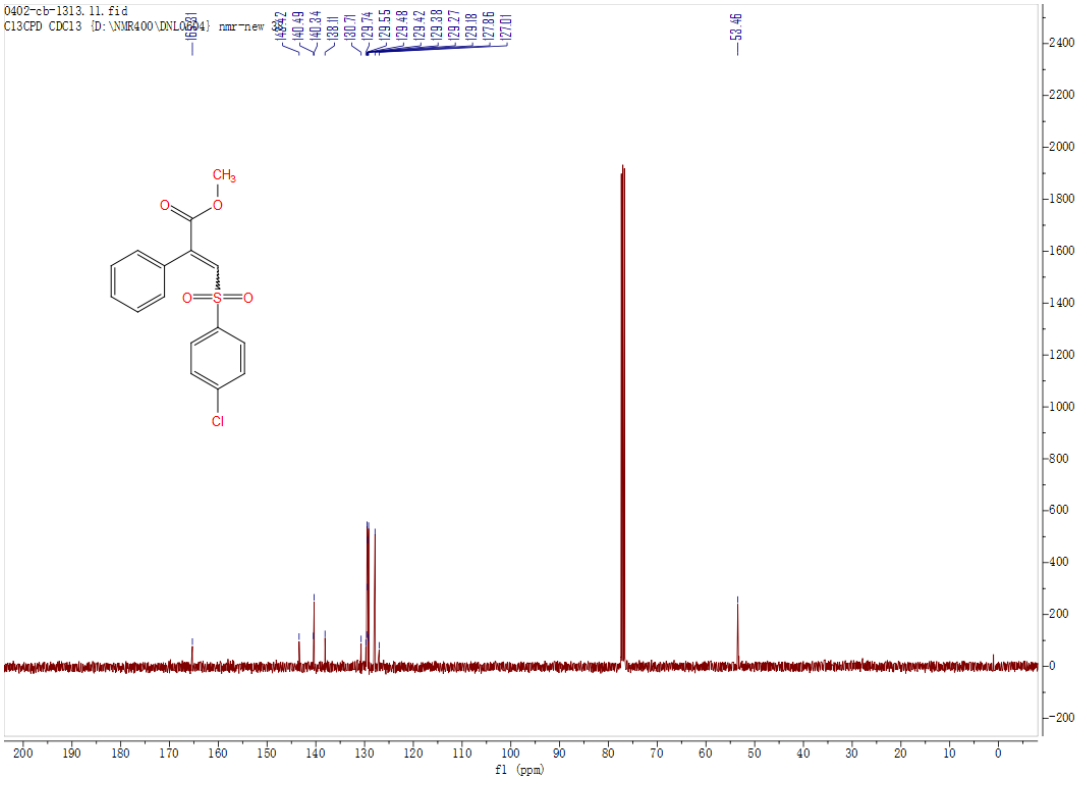

0626-cb-1348.10.fid
PROTON CDCl3 {D:\NMR400\DNL060
n-Hex
Cl
2.22
2.38
0.89
0.18
0.57
3.00
2.03
0.40
11.14
4.16
f1 (ppm)

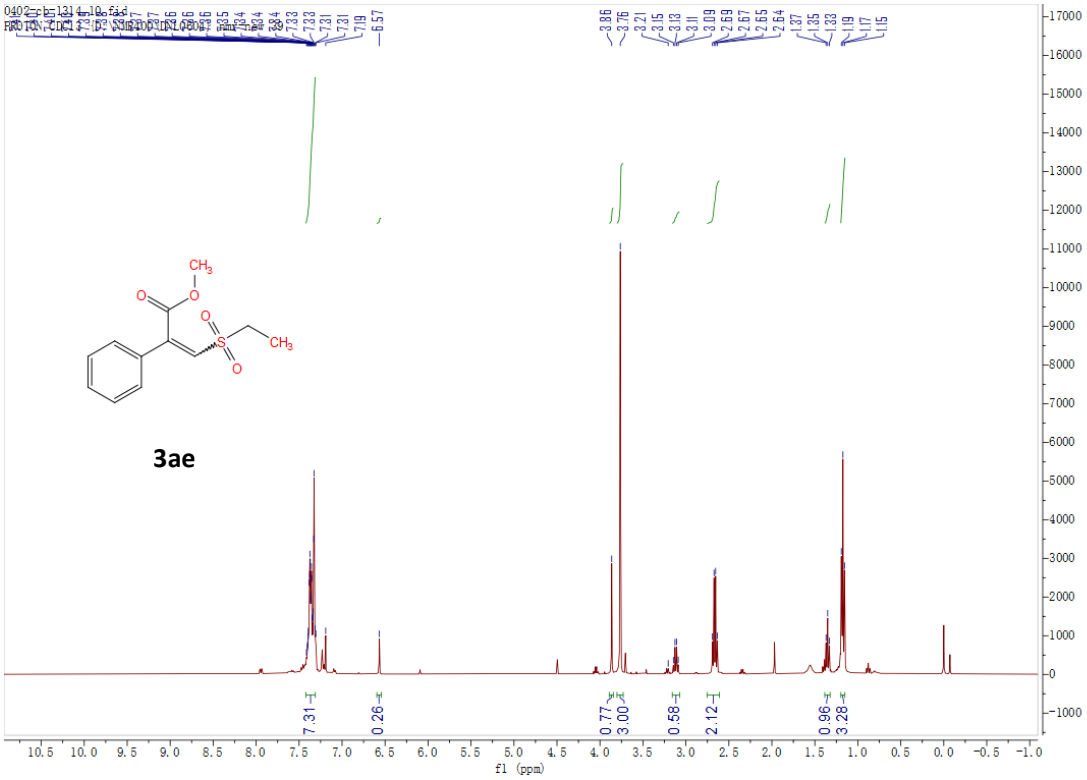
3md


0626-cb-1348.11.fid
C13CPD CDCl3 {D:\NMR400\DNL060
n-Hex
Cl
f1 (ppm)

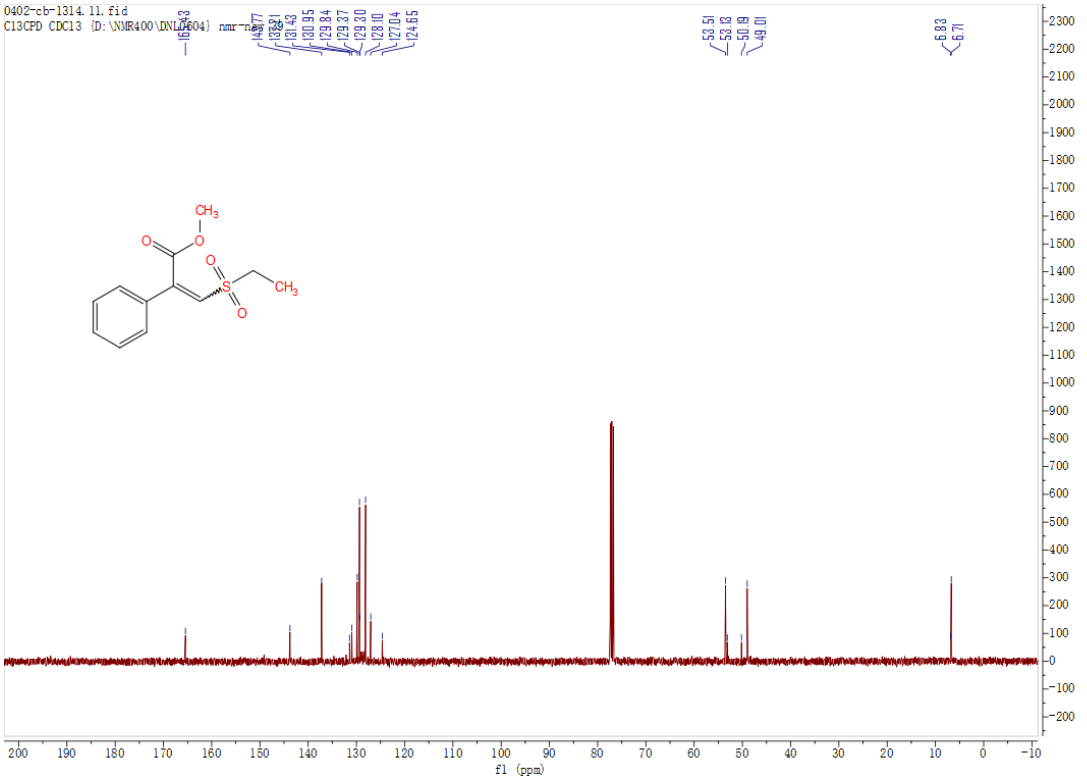

0402-cb-1313.10.fid
3.95
3.71
0.34
0.99
0.38
2.28
1.61
3.96
1.88
0.15
0.44
3.00
f1 (ppm)

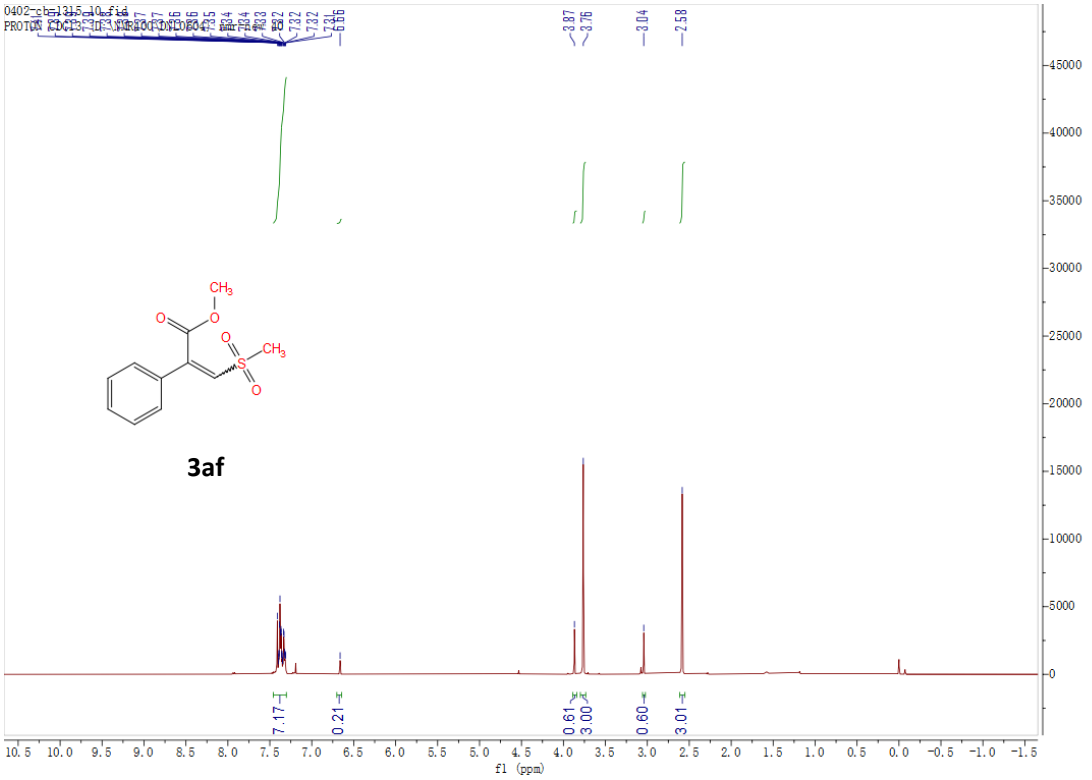
3ad


0402-cb-1313.11.fid
C13CPD CDCl3
53.46
f1 (ppm)

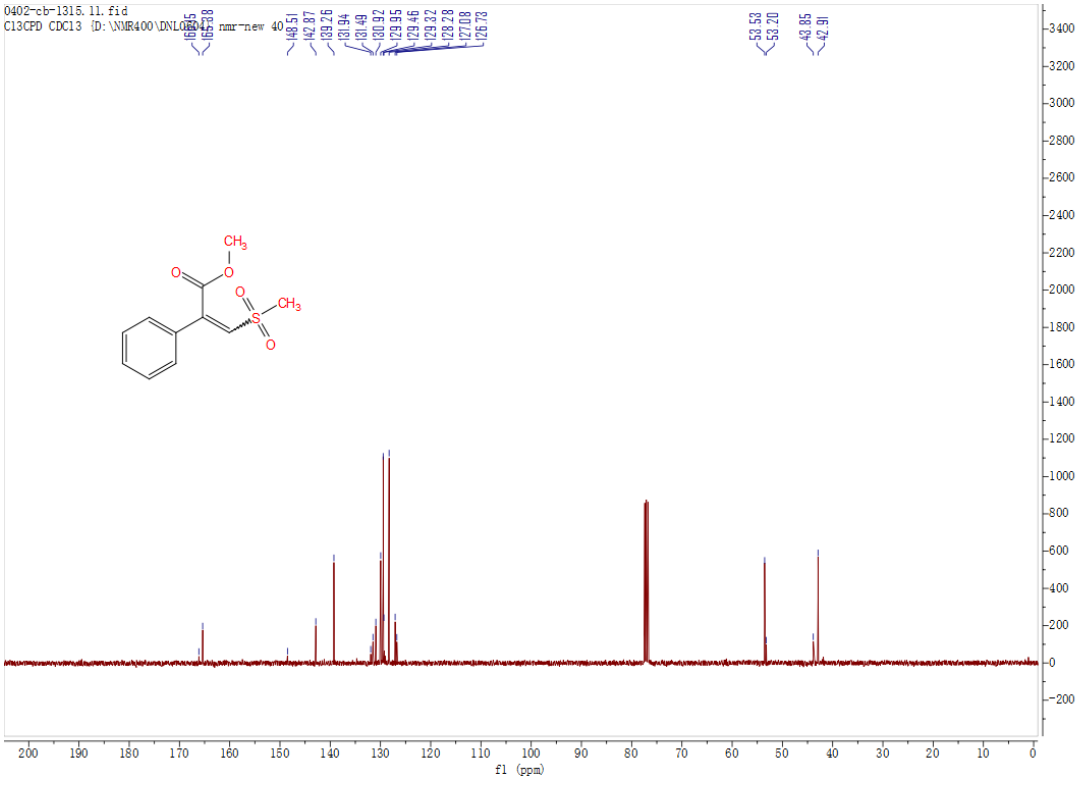

3.86
3.76
3.21
3.15
3.13
3.11
3.09
2.69
2.67
2.65
2.64
1.37
1.35
1.33
1.19
1.17
1.15
7.33
7.31
7.19
6.57
7.31
0.26
0.77
3.00
0.58
2.12
0.96
3.28
fl (ppm)

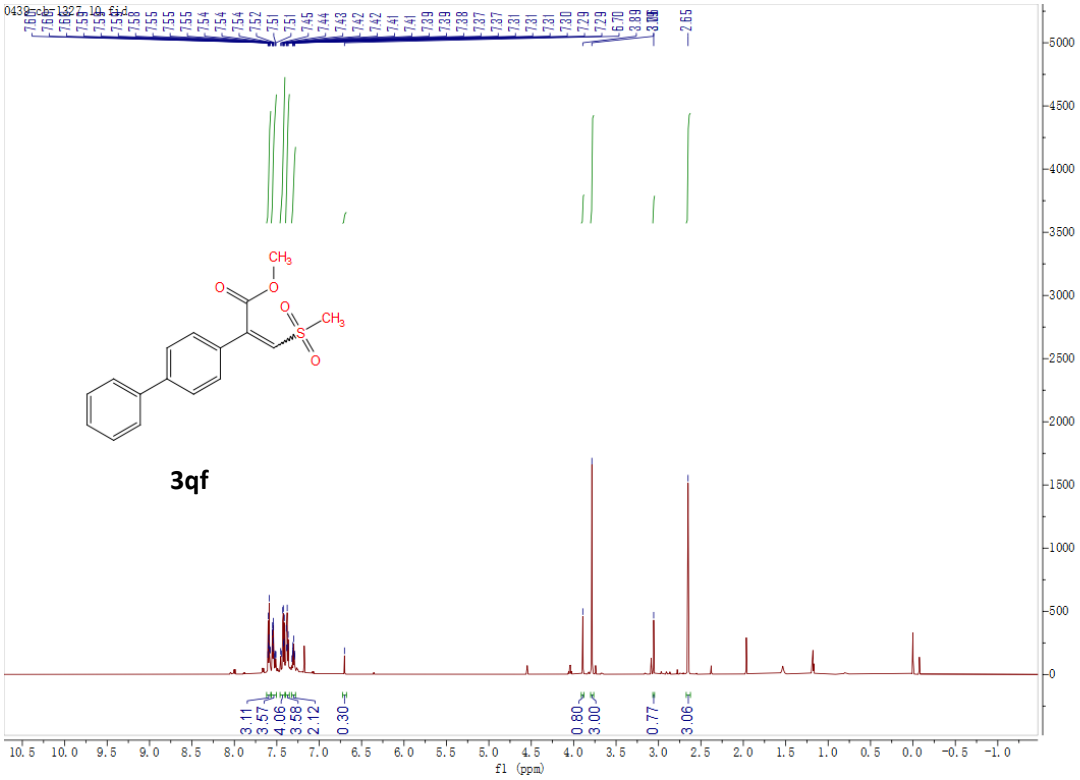
3ae

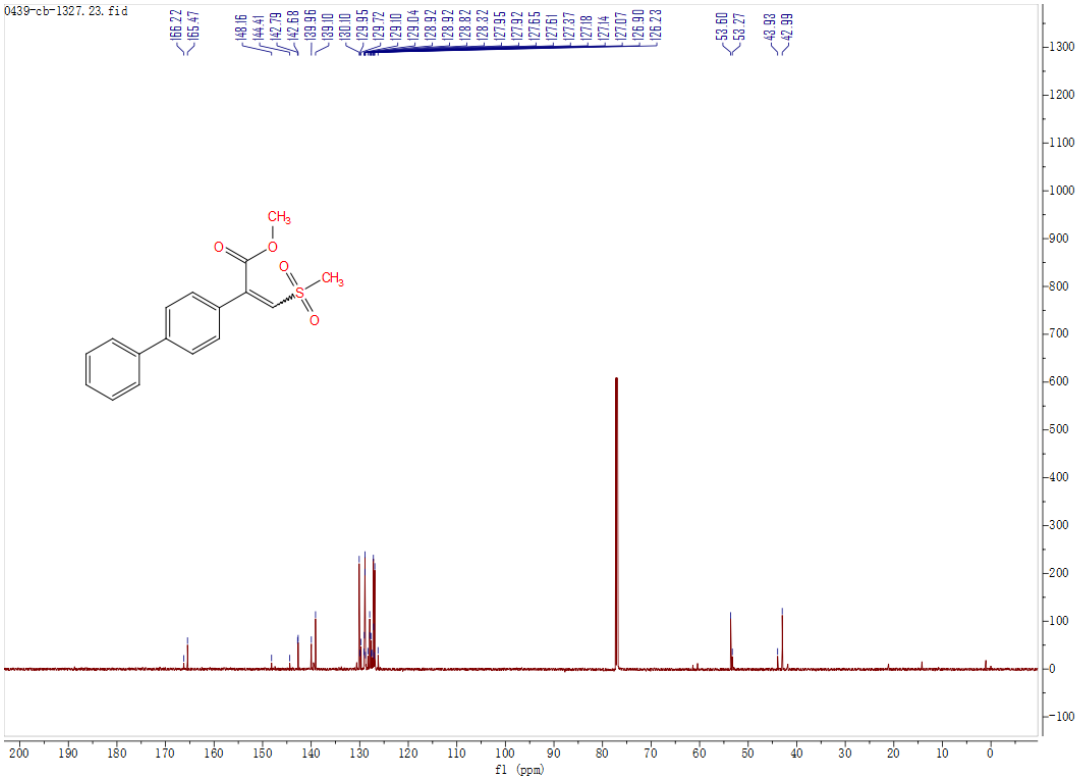

53.51
53.13
50.89
49.01
6.83
6.71
fl (ppm)

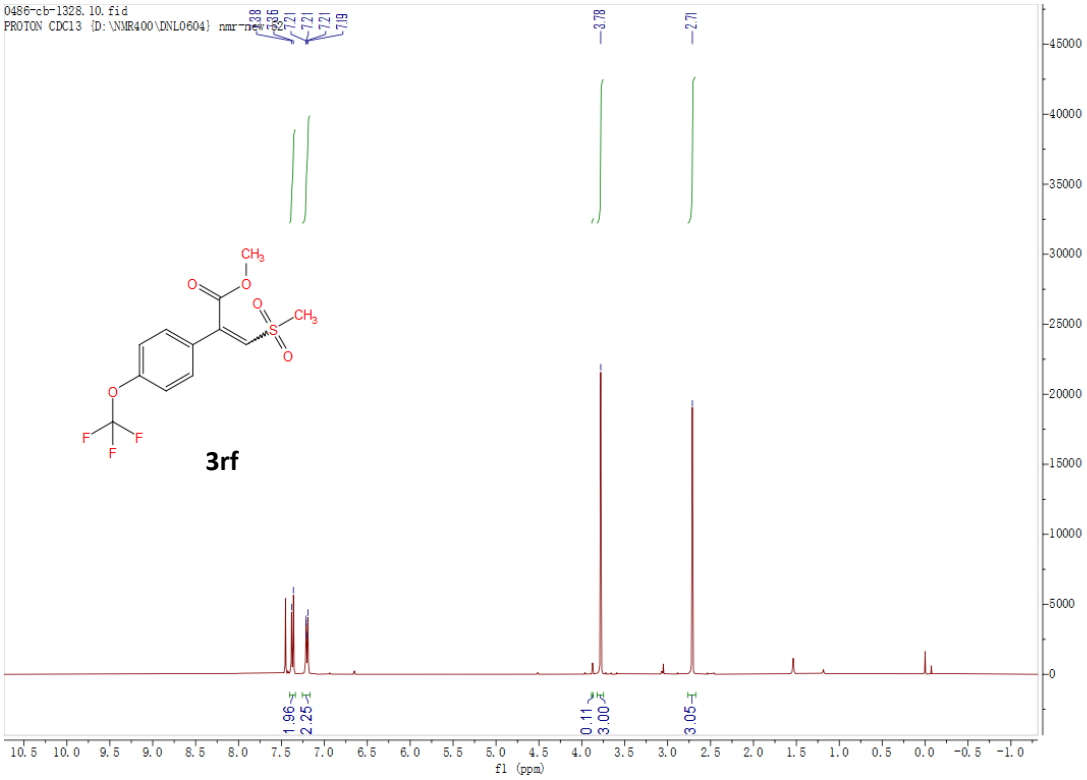

3.87
3.76
3.04
2.58
7.17
0.21
0.61
3.00
0.60
3.01
f1 (ppm)

3af

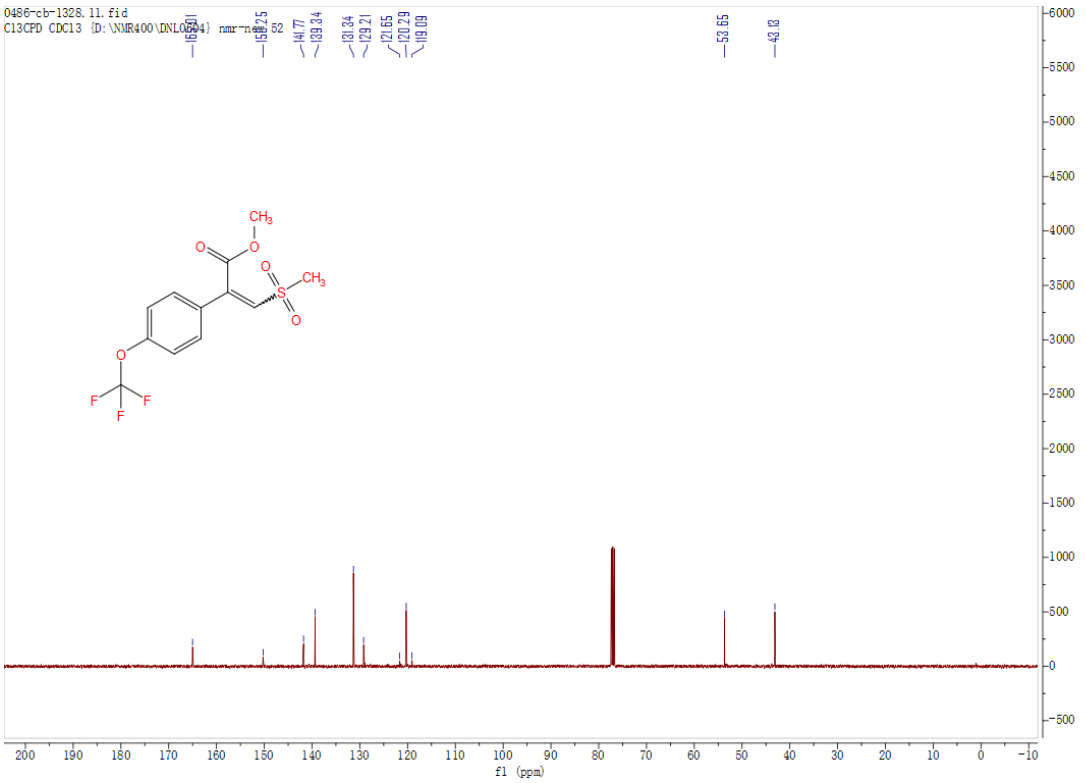

53.53
53.20
43.85
42.91
f1 (ppm)

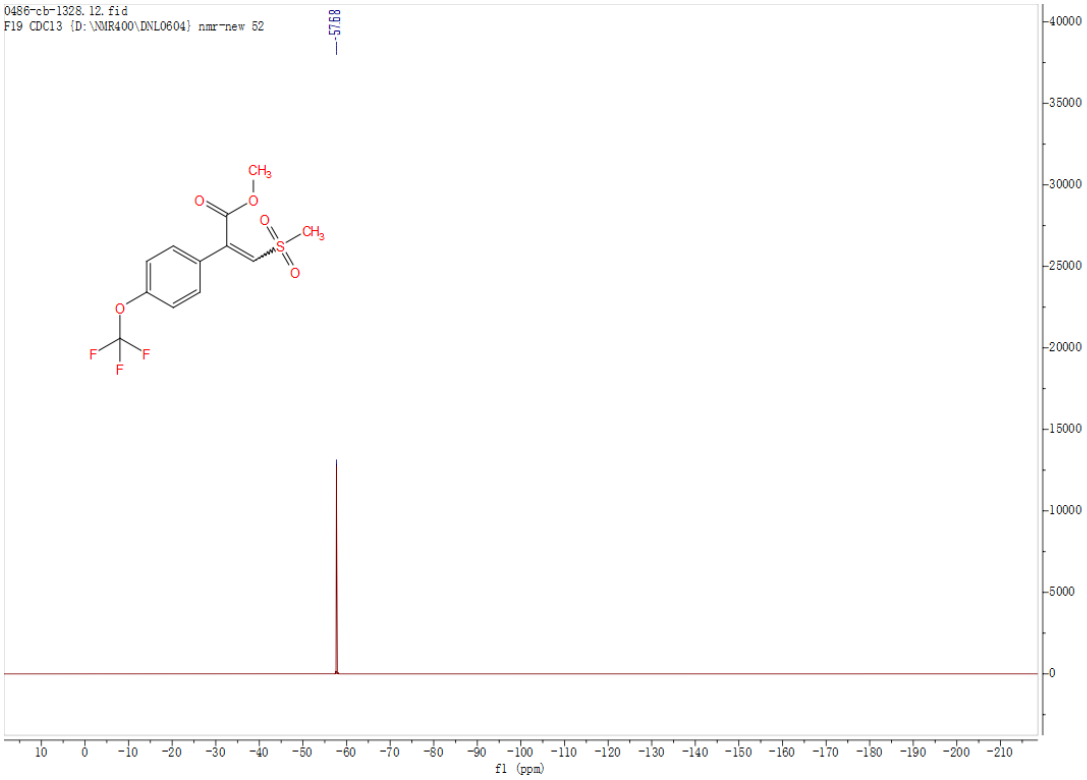

3qf
fl (ppm)

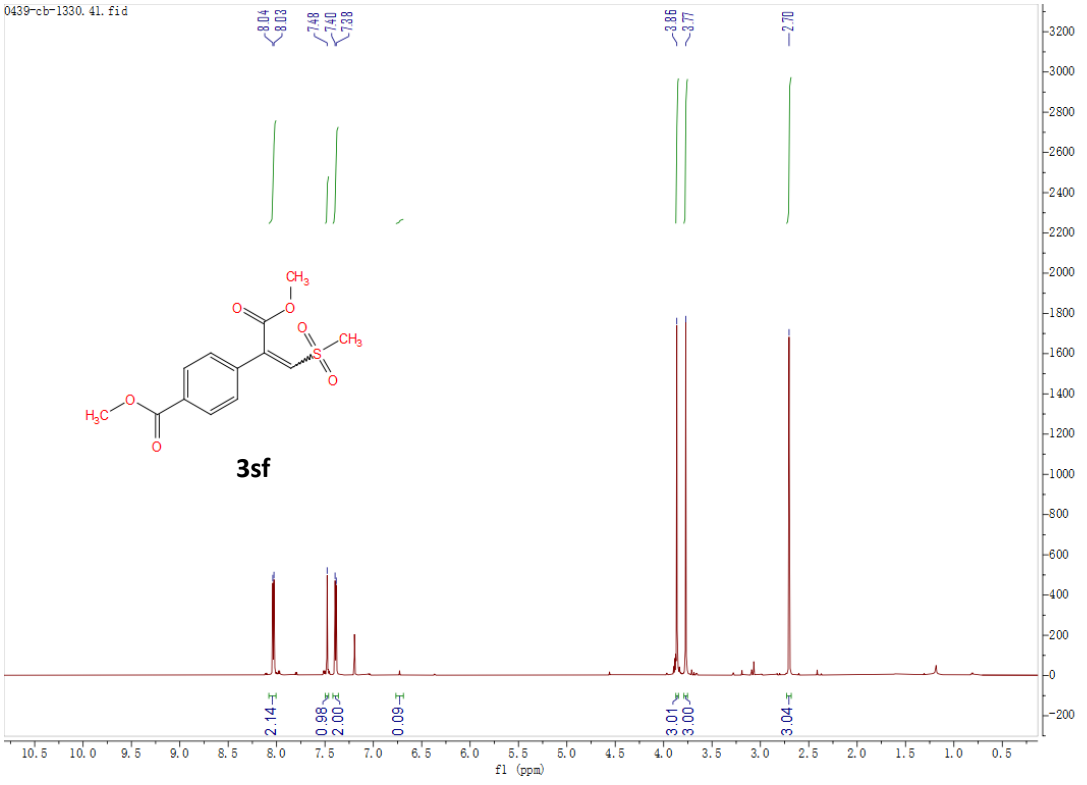

fl (ppm)


0486-cb-1328.10.fid
PROTON CDCl3 {D:\NMR400\DNL0604} nmr-neat
7.38
7.36
7.21
7.21
7.21
7.19
3.78
2.71
1.96
2.25
0.11
3.00
3.05
f1 (ppm)

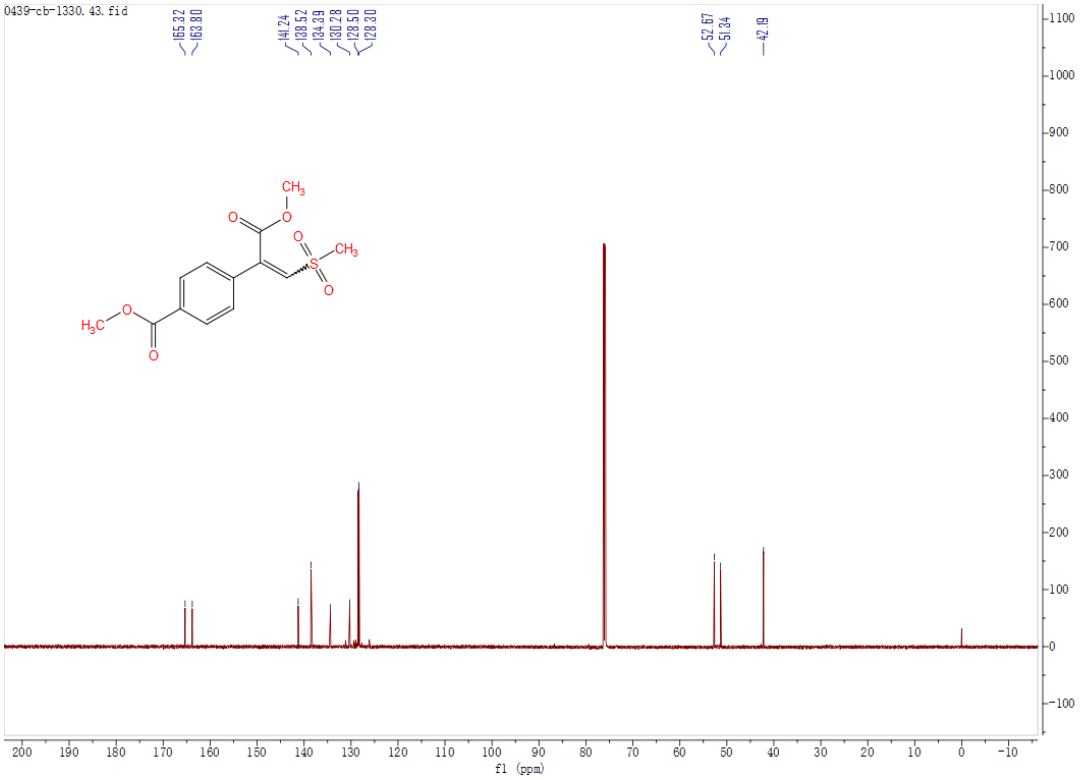
3rf

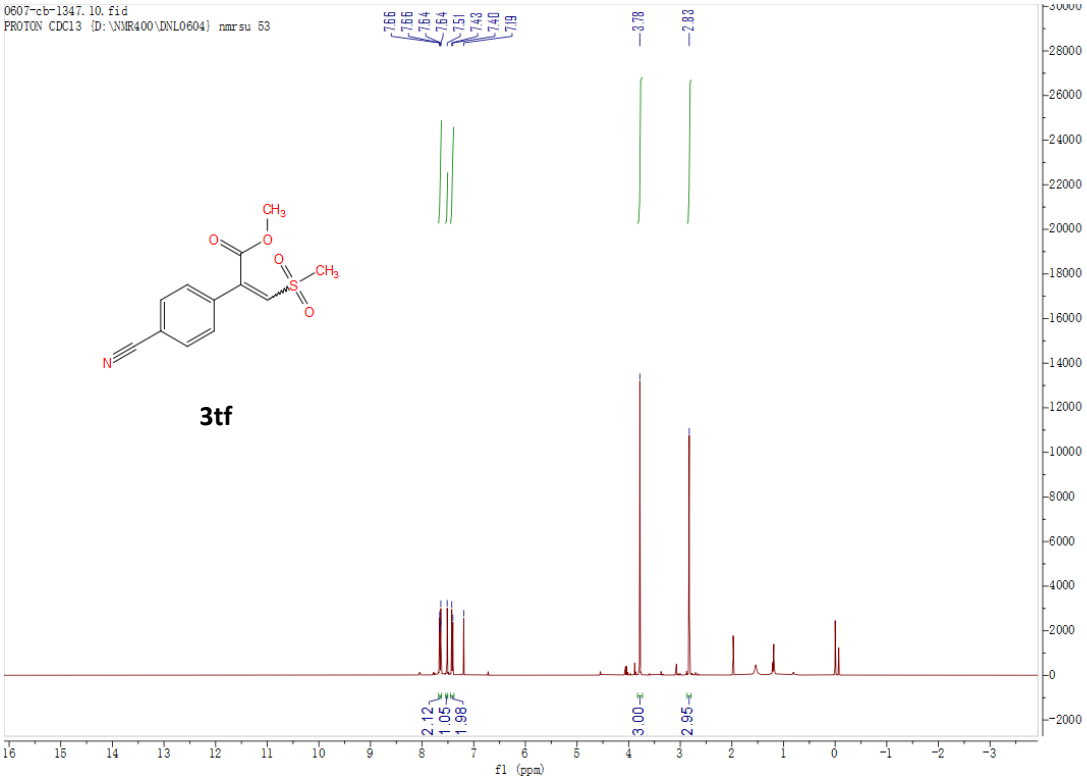

0486-cb-1328.11.fid
C13CPD CDCl3 {D:\NMR400\DNL0604} nmr-neat
165.01
152.25
141.77
139.34
131.34
129.21
121.65
120.29
119.09
53.65
43.13
f1 (ppm)


0486-cb-1328.12.fid
F19 CDCl3 {D:\\NMR400\DNL0604} nmr-new 52
-57.68
fl (ppm)

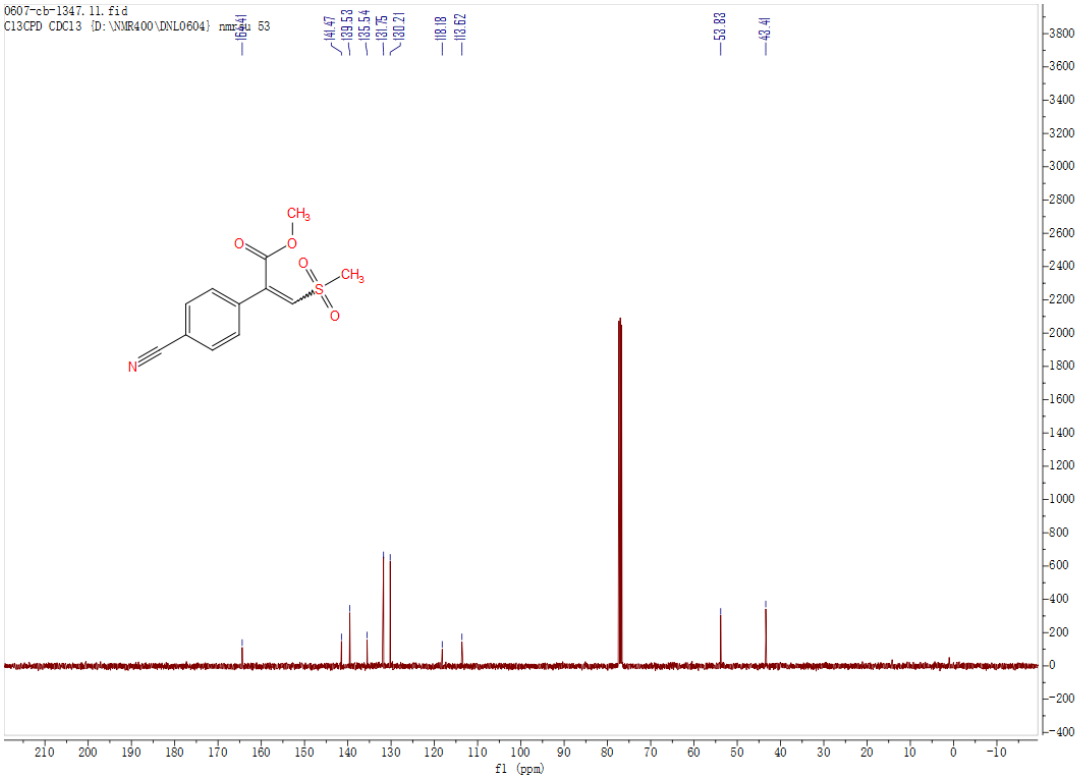

0439-cb-1330.41.fid
8.04
8.03
7.48
7.40
7.38
3.86
3.77
2.70
2.14
0.98
2.00
0.09
3.01
3.00
3.04
fl (ppm)

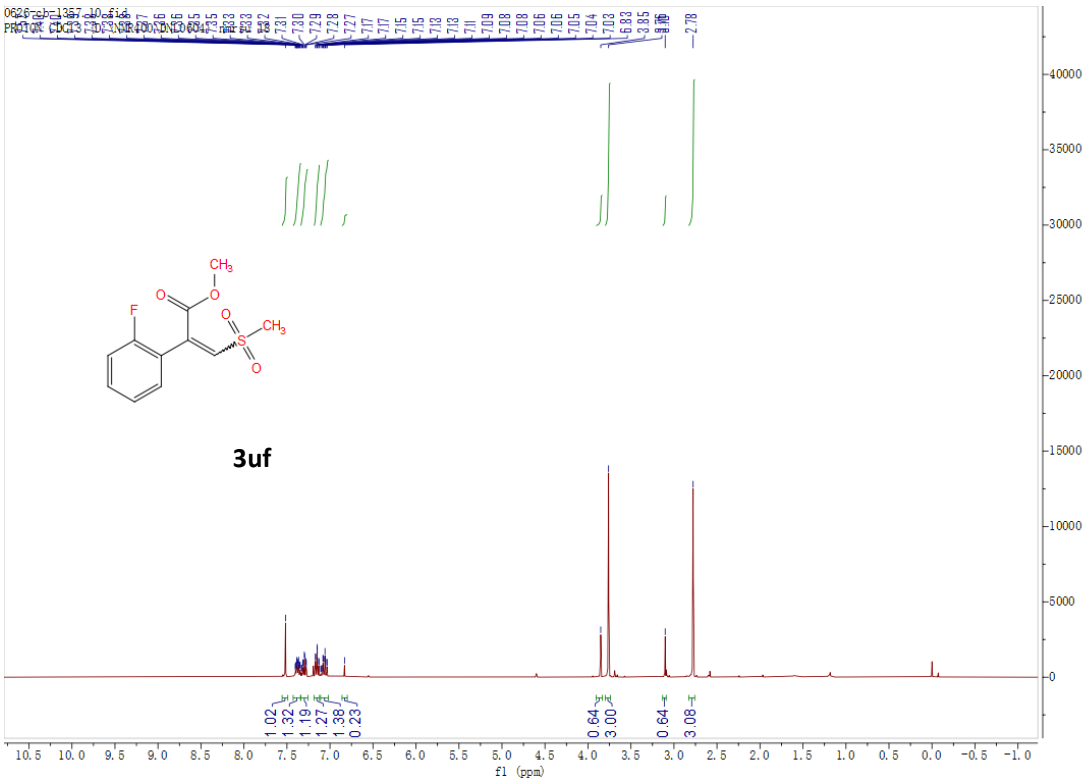
3sf


0439-cb-1330.43.fid
165.32
163.80
141.24
138.52
134.39
130.28
129.50
129.30
52.67
51.34
42.19
f1 (ppm)


0607-cb-1347.10.fid
PROTON CDCl3 {D:\NMR400\DNL0604} nmrsu 53
7.66
7.66
7.64
7.64
7.51
7.43
7.40
7.19
3.78
2.93
2.12
1.05
1.98
3.00
2.95
f1 (ppm)

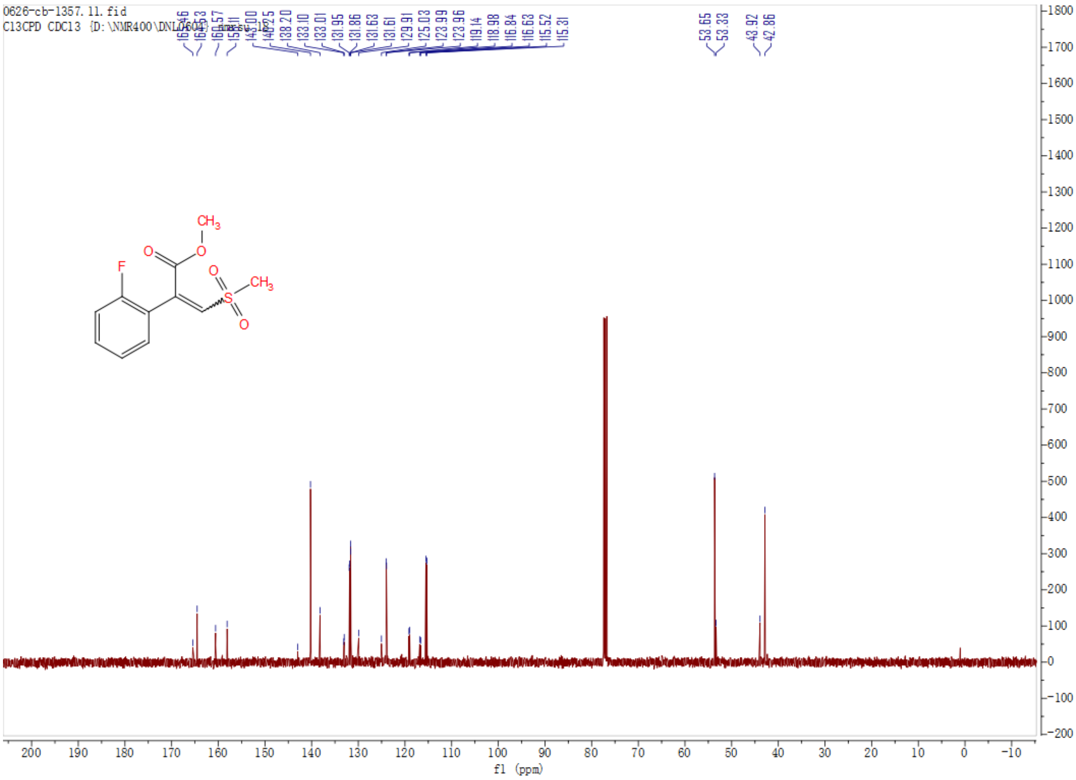
3tf


0607-cb-1347.11.fid
C13CPD CDCl3 (D:\NMR400\DNL0604) nmr
141.47
139.53
135.54
131.75
130.21
118.18
113.62
53.83
43.41
f1 (ppm)

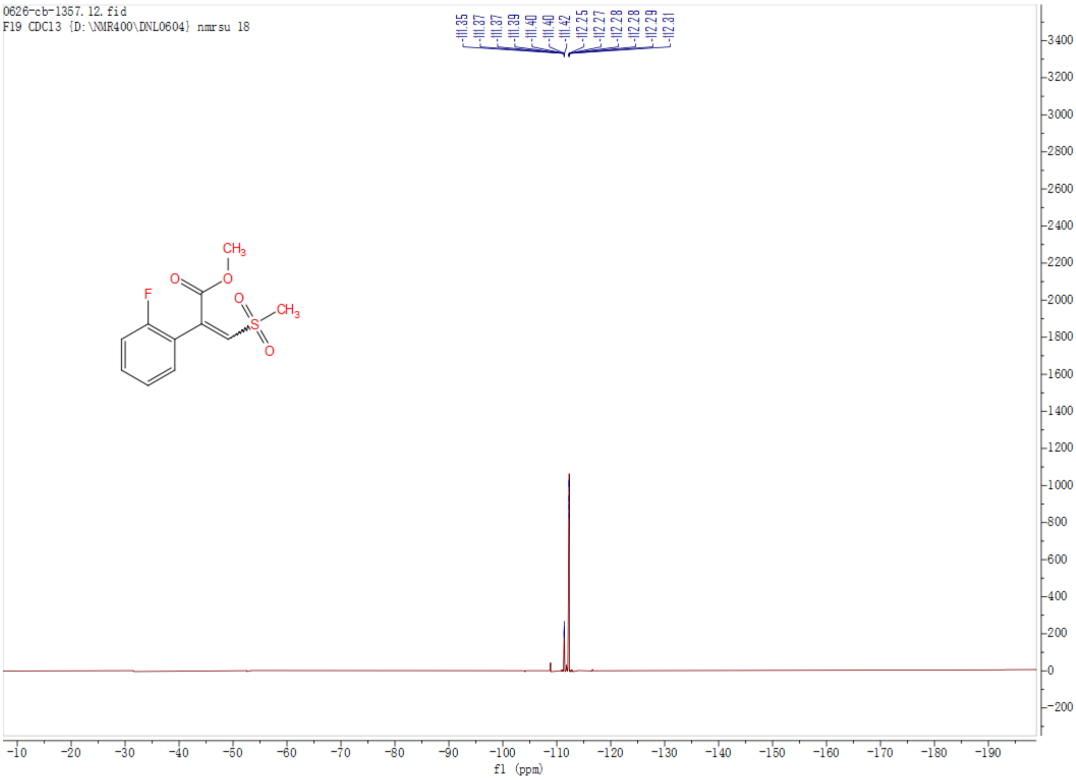

PROTON CDCl3
7.30
7.29
7.28
7.27
7.17
7.15
7.13
7.11
7.09
7.08
7.06
7.05
7.04
7.03
6.83
3.85
2.78
1.02
1.32
1.19
1.27
1.38
0.23
0.64
3.00
0.64
3.08
f1 (ppm)

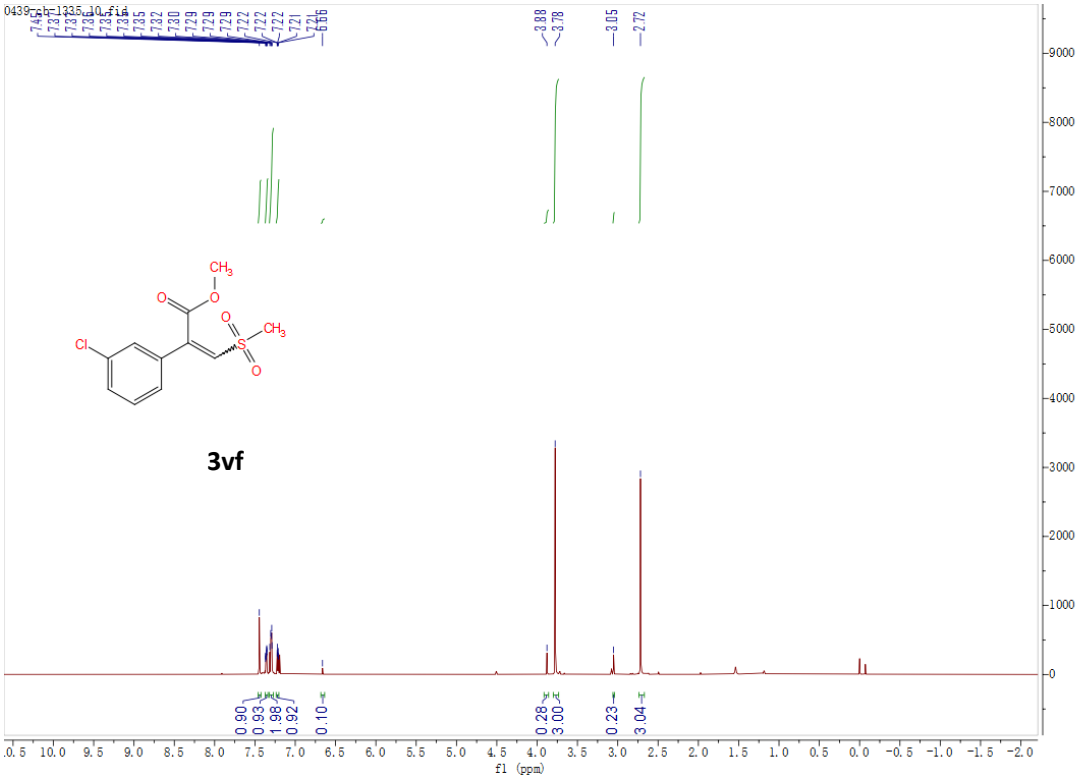
3uf

0626-cb-1357.11.fid
C13CPD CDCl3 {D:\NMR400\DNL0604} nmrsu 18

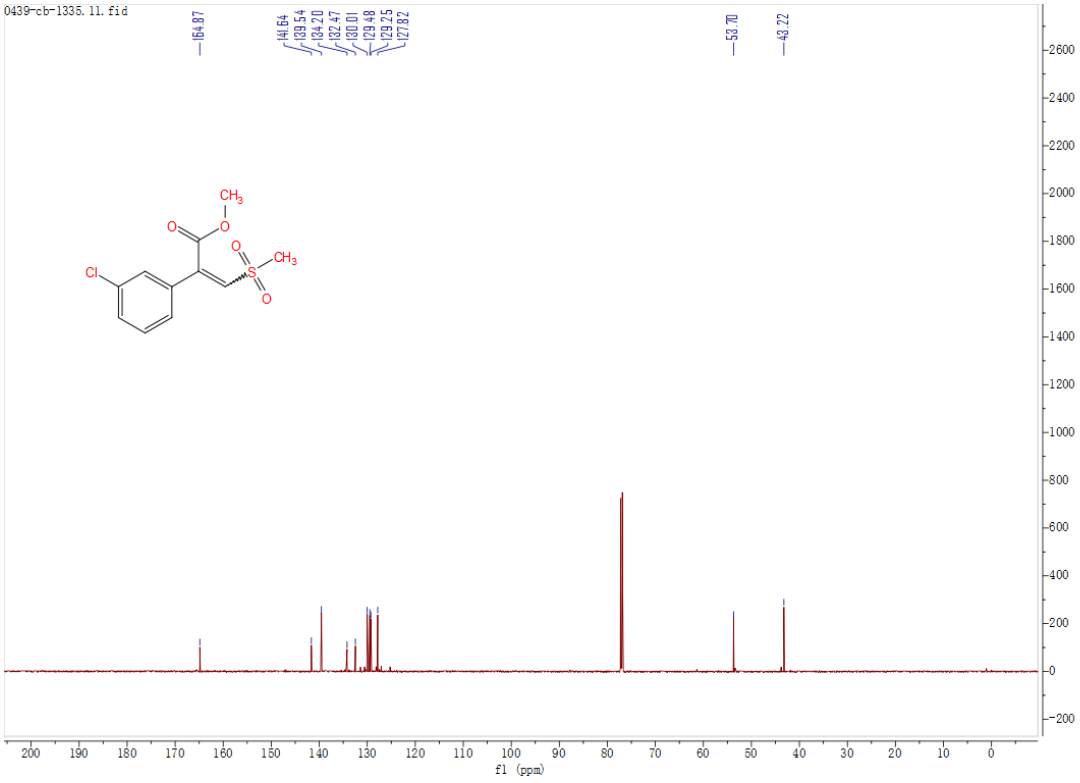


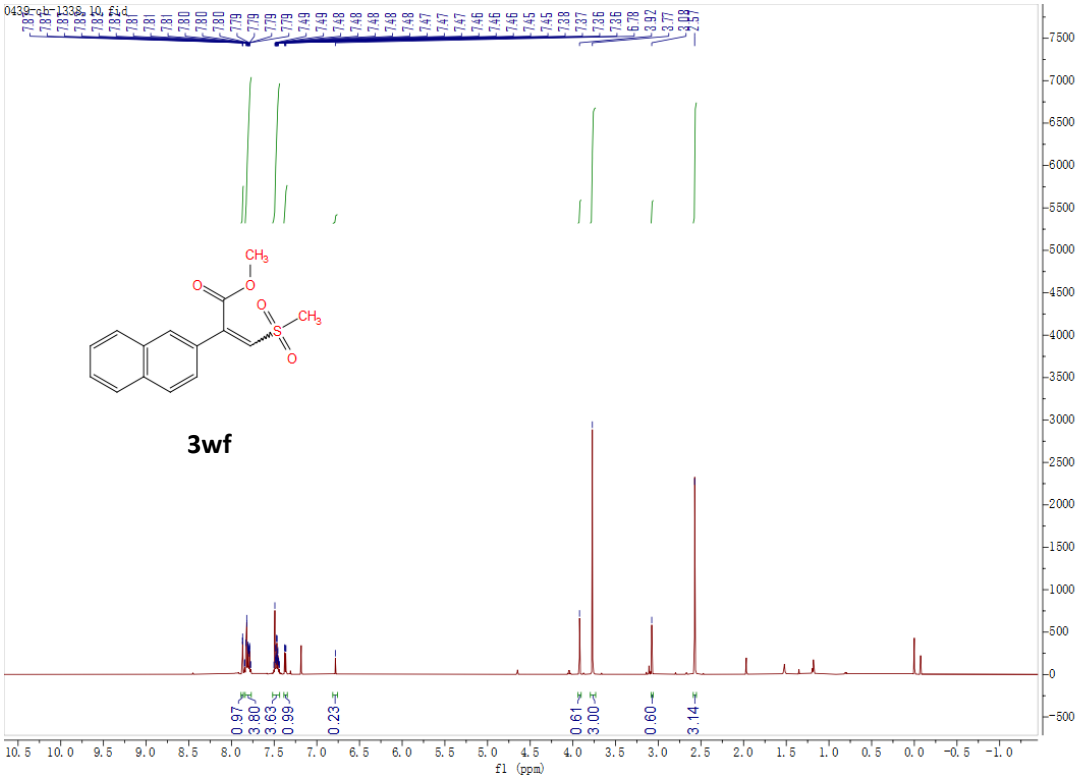
0626-cb-1357.12.fid
F19 CDCl3 {D:\NMR400\DNL0604} nmrsu 18

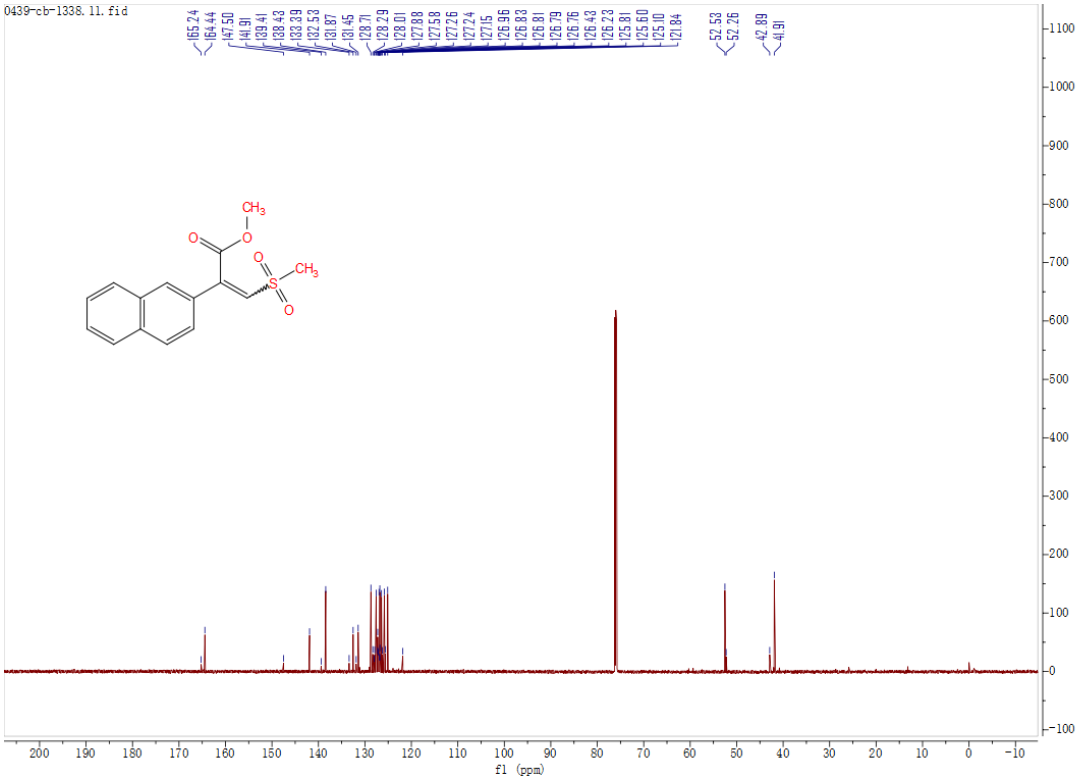


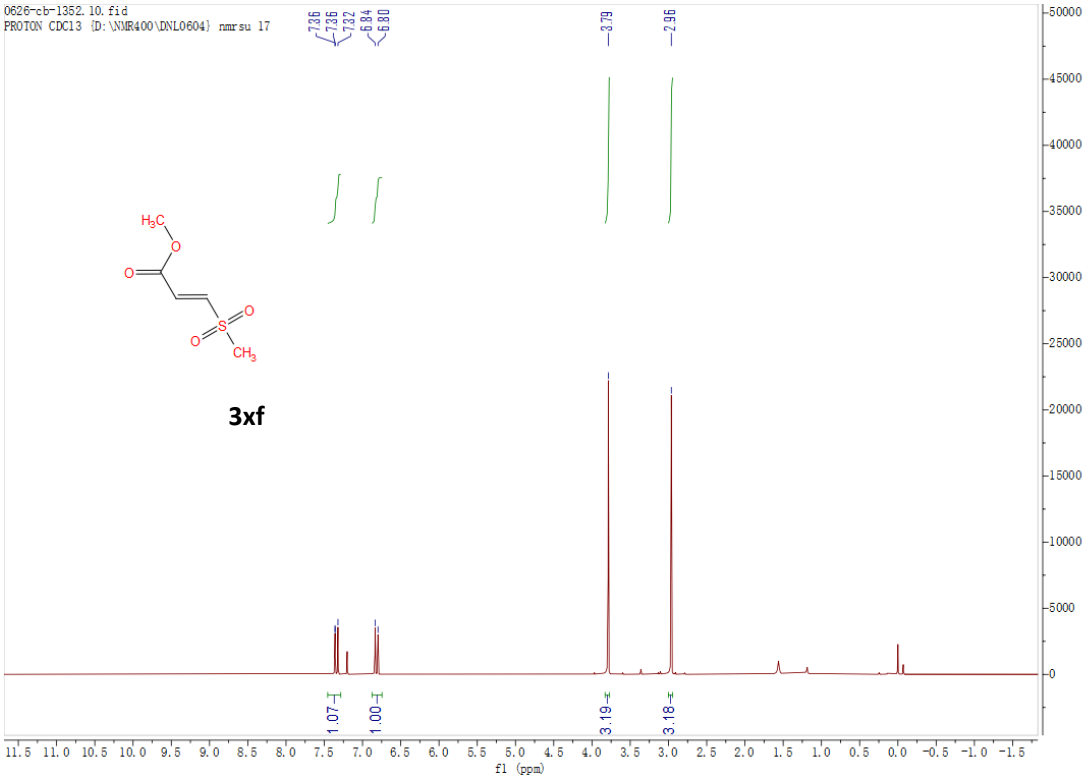

0439-cb-1335.10.fid
3.88
3.78
3.05
2.72
0.90
0.93
1.98
0.92
0.10
0.28
3.00
0.23
3.04
f1 (ppm)

3vf

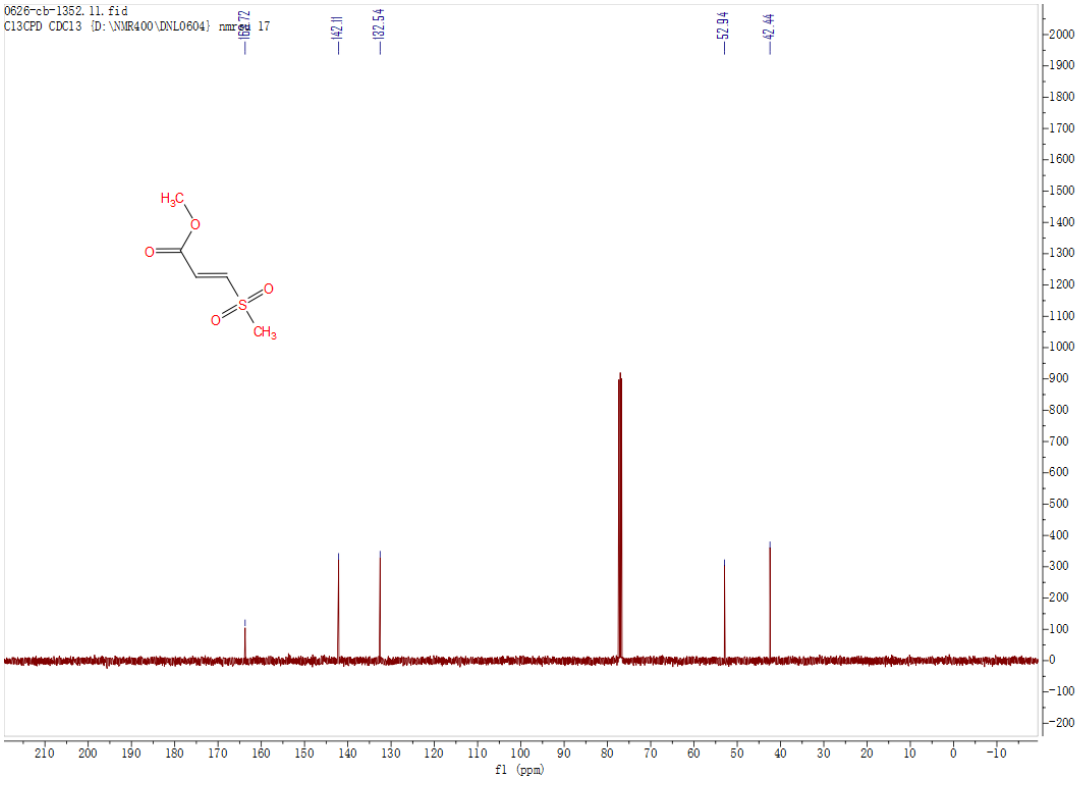

0439-cb-1335.11.fid
164.87
141.64
139.54
134.20
132.47
130.01
129.48
129.25
127.82
53.70
43.22
f1 (ppm)

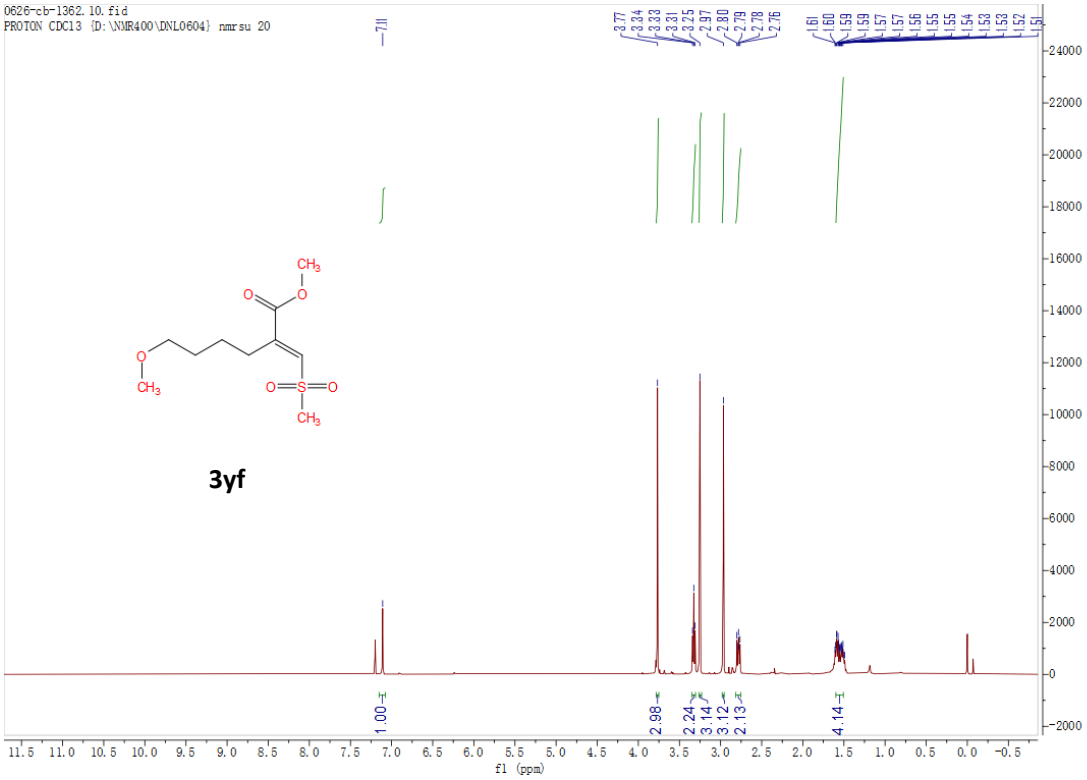

0439-cb-1338.10.fid
3wf
fl (ppm)

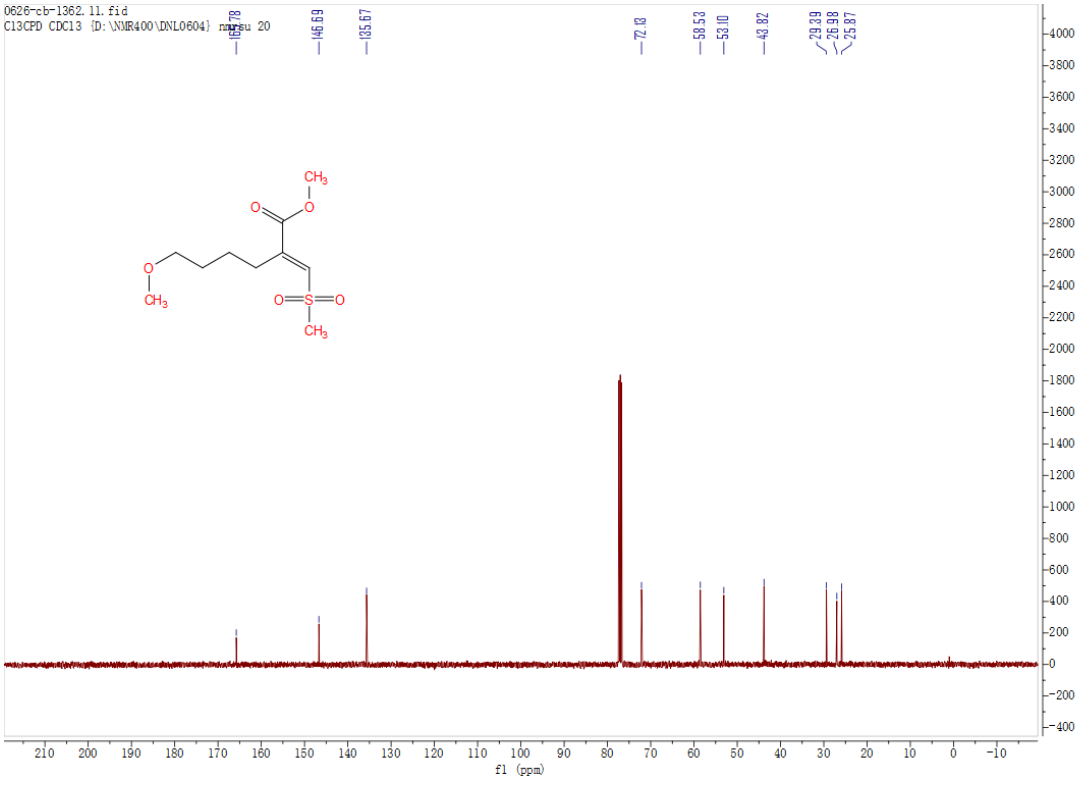

0439-cb-1338.11.fid
fl (ppm)


0626-cb-1352.10.fid
PROTON CDC13 {D:\NMR400\DNL0604} nmrsu 17
7.35
7.35
7.32
6.84
6.80
3.79
2.96
1.07
1.00
3.19
3.18
f1 (ppm)

3xf


0626-cb-1352.11.fid
C13CPD CDC13 {D:\NMR400\DNL0604} nmrsu 17
142.11
132.54
52.94
42.44
f1 (ppm)


0626-cb-1362.10.fid
PROTON CDCl3 {D:\NMR400\DNL0604} nmrsu 20
3yf
1.00
2.98
2.24
3.14
3.12
2.13
4.14
f1 (ppm)


0626-cb-1362.11.fid
C13CPD CDCl3 {D:\NMR400\DNL0604} nmrsu 20
f1 (ppm)