Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

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1. General information:

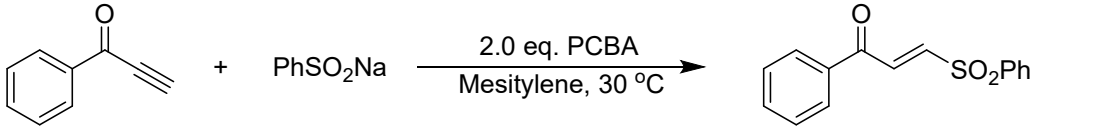
All experiments were carried out under an atmosphere of air. Flash column chromatography was performed over silica gel 48-75 μm. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (500 MHz and 126 MHz, respectively) instrument internally referenced to $SiMe_4$ or chloroform signals. HRMS was recorded using waters G2-Xs qtof mass spectrometer. The new compounds were characterized by ^{1}H NMR, ^{13}C NMR, MS and HRMS. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. The Substrates **1**[1] was synthesized according to the reported methods. All reagents and solvents were used as received from commercial sources without further purification.

2. Experimental procedures

a) General procedure: (E)-1-phenyl-3-(phenylsulfonyl)prop-2-en-1-one (3a):

A 10 mL oven-dried reaction vessel was charged with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2mmol), sodium benzosulfinate (**2a**, 65.7 mg, 0.4 mmol) and 4-chlorobenzoic acid (62.7 mg, 0.4 mmol). The reaction with mesitylene (2.0 mL) was added to the sealed reaction vessel by syringe. The resulting solution was stirred at 30 °C for 48 h. After cooling to room temperature, the volatiles were removed under vacuum and the residue was purified by column chromatography (petroleum ether/ethyl acetate = 5:1) to give **3aq** as white solid; yield: 52.8 mg (97%, E:Z = 98:02).

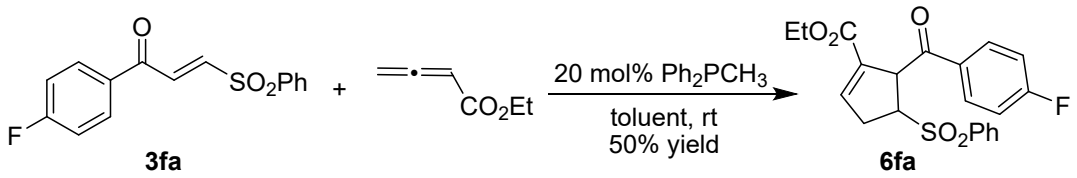
b) Scaled-up Version of the



1a 10 mmol | **2a** 20 mmol | **3aa** 2.21 g, 78% yield, E/Z = 95/05

To a dried round bottle flask with a magnetic stirring bar were added the 1-phenylprop-2-yn-1-one **1a** (10 mmol), sodium benzosulfinate **2a** (20 mmol), and 4-chlorobenzoic acid (20 mmol), followed by the addition of mesitylene (50 mL). The reaction mixture was stirred at room temperature for 50 h. The solvent was removed under reduced pressure, and theresidue was purified by column chromatography on silica gel to afford **3aa** in 2.21 g (78% yield).

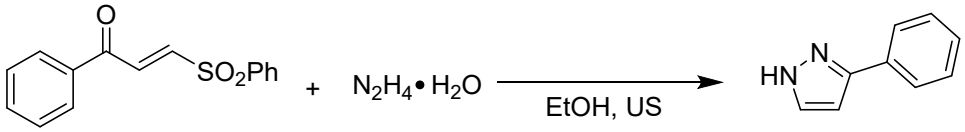
c) Procedure for the synthesis of derivative 6a



3fa 6fa

Under air, a stirred solution of **3fa** (0.2 mmol) and Ph_2PCH_3 (0.04 mmol) in toluene (2 mL). Subsequently, ethyl buta-2,3-dienoate (0.24 mmol) was added in one portion. The reaction mixture was stirred for 24 h in room temperature , the solvents were removed in vacuo and the residue was directly purified by silica gel chromatography using petroleum ether/EtOAc as the eluent to afford the desired cycloaddition product **6fa**.

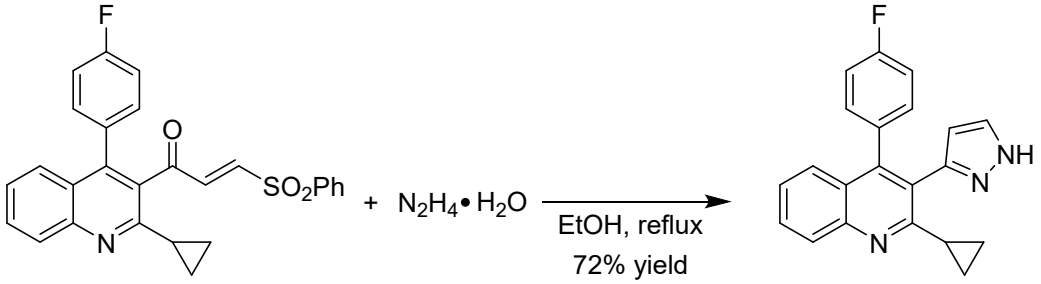
d) Procedure for the synthesis of derivative 6b



3aa 6b

A round-bottom flask was charged with **3aa** (0.20 mmol), N_2H_4 H_2O (0.60 mmol) and EtOH (2 mL). The resultant mixture was allowed to react for 15 minutes under ultrasound irradiation (40 kHz / 50 W). Then the mixture was extracted with ethyl acetate (3 × 20 mL). The organic phase was dried over anhydrous Na_2SO_4, and the organic solvent was removed under reduced pressure. The crude products were purified by flash column chromatography to give the desired product **6b** in 70% yield.

e) Procedure for the synthesis of derivative 6c

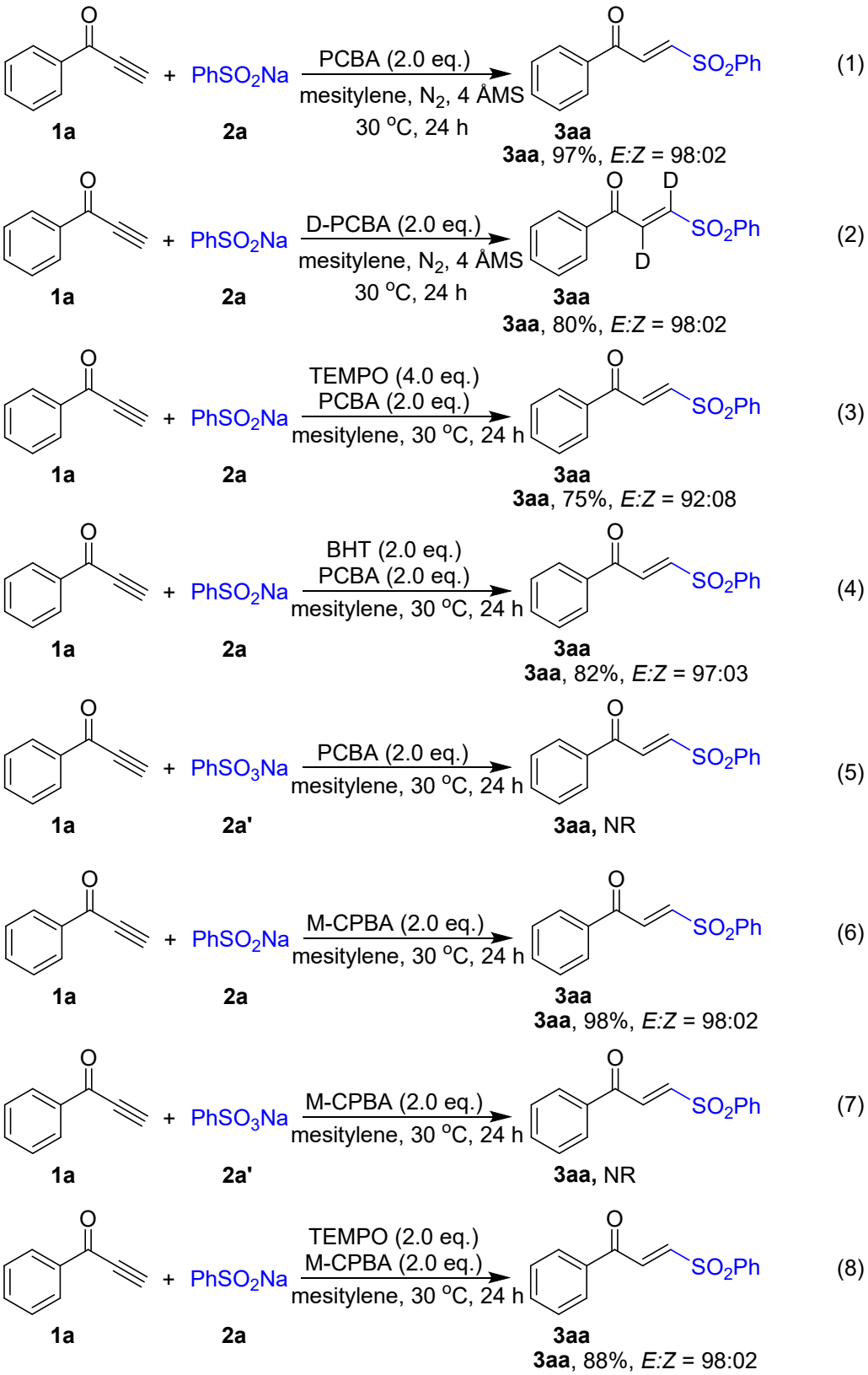


3pa 6c

A round-bottom flask was charged with **3pa** (0.30 mmol), N_2H_4 H_2O (4.5 mmol) and EtOH (10

mL). The resultant mixture was refluxed for 6 h, and then extracted with ethyl acetate (3 × 20 mL). The organic phase was dried over anhydrous Na_2SO_4, and the organic solvent was removed under reduced pressure. The crude products were purified by flash column chromatography to give the desired product **6c** in 72% yield.

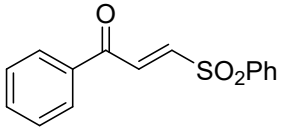
3. Control experiments[a]



[a] Reaction conditions: **1a** (0.05 mmol), **2a** (0.125 mmol), mesitylene (1.0 mL), 30 °C. The yield was dtermined by ^{1}H NMR. E/Z ratio was determined by RP-HPLC.

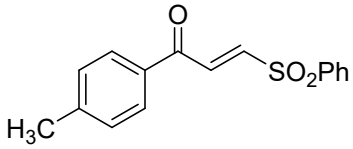
4. Characterization data of the products

(E)-1-phenyl-3-(phenylsulfonyl)prop-2-en-1-one (3aa)[2]



m.p.: 105-109 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.5 Hz, 1H), 8.00-7.92 (m, 4H), 7.70-7.59 (m, 3H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.46 (d, *J* = 8.5 Hz, 1H), 7.36 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.63, 141.97, 138.56, 135.95, 134.51, 134.38, 133.03, 129.66, 129.09, 128.98, 128.29; IR: 3041, 1669, 1592, 1324, 1146, 1086 cm^{-1}.

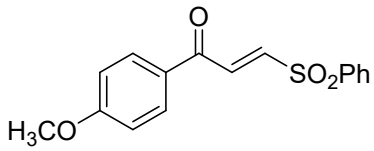
(E)-3-(phenylsulfonyl)-1-(p-tolyl)prop-2-en-1-one (3ba)



The reaction was conducted with 1-(p-tolyl) prop-2-yn-1-one (**1b**, 28.4 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ba** as white solid; yield 98%, E:Z = 90:10.

m.p.: 116-120 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97-7.88 (m, 5H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 2H), 7.34 (dd, *J* = 18.4, 11.4 Hz, 3H), 2.44 (s, 3H)；^{13}C NMR (126 MHz, CDCl3) δ 187.09, 145.81, 141.63, 138.72, 134.35, 133.57, 133.32, 129.82, 129.67, 129.16, 128.28, 21.89. HRMS (ESI) m/z calcd. for $C_{16}H_{14}O_3NaS$ $[M+Na]^+$ = 309.0561, found 309.0569; IR: 3058, 3027, 1661, 1315, 1155, 1089 cm^{-1}.

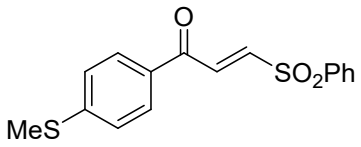
(E)-1-(4-methoxyphenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3ca)[3]



The reaction was conducted with 1-(4-methoxyphenyl)prop-2-yn-1-one (**1c**, 32.0 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ca** as viscous liquid; yield 71%, E:Z = 81:19.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93-7.85 (m, 5H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 7.28-7.19 (m, 1H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 184.70, 163.71, 140.25, 137.83, 133.23, 132.37, 130.51, 128.60, 128.13, 127.22, 113.34, 54.65.

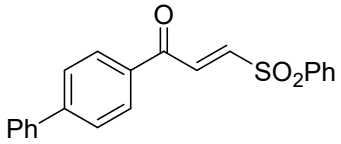
(E)-1-(4-(methylthio)phenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3da)



The reaction was conducted with 1-(4-(methylthio)phenyl)prop-2-yn-1-one (**1d**, 35.3 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3da** as yellow solid; yield 82%, E:Z = 94:06.

m.p.: 137-140 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 28.5, 8.2 Hz, 5H), 7.60 (t, *J* = 7.1 Hz, 1H), 7.51 (t, *J* = 7.3 Hz, 2H), 7.28 (d, *J* = 14.8 Hz, 1H), 7.21 (d, *J* = 8.1 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.22, 148.51, 141.64, 138.65, 134.39, 133.04, 132.14, 129.69, 129.36, 128.29, 125.06, 14.62. HRMS (ESI) m/z calcd. for $C_{16}H_{14}O_3NS_2$ $[M+Na]^+$ = 341.0282, found 341.0284; IR: 3047, 1656, 1586, 1320, 1148, 817 cm^{-1}.

(E)-1-([1,1'-biphenyl]-4-yl)-3-(phenylsulfonyl)prop-2-en-1-one (3ea)

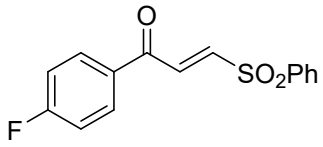


The reaction was conducted with 1-([1,1'-biphenyl]-4-yl)prop-2-yn-1-one (**1e**, 41.25 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ea** as yellow solid; yield 94%, E:Z = 83:17.

m.p.: 191-198 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-7.96 (m, 5H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 7.2 Hz, 2H), 7.60 (dd, *J* = 15.8, 8.1 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.46-7.38 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.10, 147.24, 141.92, 139.37, 138.63, 134.69, 134.43, 133.09, 129.72, 129.68, 129.12, 128.72, 128.34, 127.71, 127.38. HRMS (ESI) m/z

calcd. for $C_{21}H_{16}O_3SNa$ $[M+Na]^+$ = 371.0718, found 371.0722; IR: 2978, 1686, 1592, 1426, 1322, 1093 cm^{-1}.

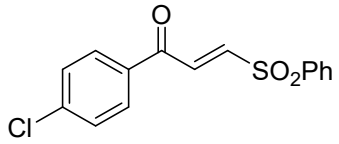
(E)-1-([1,1'-biphenyl]-4-yl)-3-(phenylsulfonyl)prop-2-en-1-one (3fa)



The reaction was conducted with 1-(4-fluorophenyl)prop-2-yn-1-one (**1f**, 29.6 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (76.8 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3fa** as yellow solid; yield 85%, E:Z = 95:05.

m.p.: 114-118 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05-8.03 (m, 2H), 7.96 (d, *J* = 7.8 Hz, 2H), 7.91 (d, *J* = 14.9 Hz, 1H), 7.70 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 7.37 (d, *J* = 14.9 Hz, 1H), 7.21 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.02, 166.54 (d, *J* = 257.8 Hz), 142.25, 138.58, 134.43, 132.68, 132.49 (d, *J* = 2.8 Hz), 131.81 (d, *J* = 9.8 Hz), 129.70, 128.32, 116.42 (d, *J* = 22.1 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -101.93. HRMS (ESI) m/z calcd. for $C_{15}H_{11}O_3NaSF$ $[M+Na]^+$ = 313.0311, found 313.0317; IR: 3078, 1664, 1591, 1310, 1155, 837 cm^{-1}.

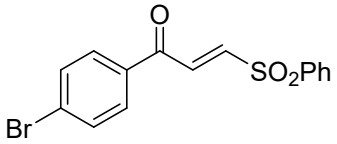
(E)-1-(4-chlorophenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3ga)[4]



The reaction was conducted with 1-(4-chlorophenyl)prop-2-yn-1-one (**1g**, 32.9 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **3ga** as white solid; yield 93%, E:Z = 97:03.

m.p.: 130-137 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97-7.89 (m, 5H), 7.70 (t, *J* = 7.3 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.44, 142.44, 141.20, 138.47, 134.50, 134.31, 132.45, 130.37, 129.74, 129.50, 128.34; IR: 3045, 1683, 185, 1321, 1254, 1009 cm^{-1}.

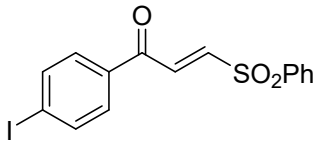
(E)-1-(4-bromophenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3ha)



The reaction was conducted with 1-(4-bromophenyl)prop-2-yn-1-one (**1h**, 41.8 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ha** as white solid; yield 97%, E:Z = 98:02.

m.p.: 140-144 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.7 Hz, 2H), 7.79 (dd, *J* = 13.9, 11.9 Hz, 3H), 7.61 (dd, *J* = 16.1, 7.9 Hz, 3H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.31-7.19 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 185.63, 141.47, 137.50, 133.70, 133.42, 131.45, 131.38, 129.33, 128.99, 128.67, 127.29. HRMS (ESI) m/z calcd. for $C_{15}H_{12}O_3SBr$ $[M+H]^+$ = 350.9691, found 350.9686; IR: 3043, 1685, 1580, 1321, 1154, 999 cm^{-1}.

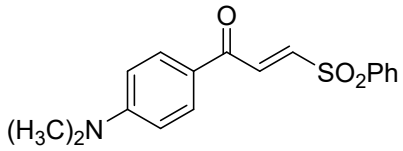
(E)-1-(4-iodophenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3ia)



The reaction was conducted with 1-(4-iodophenyl)prop-2-yn-1-one (**1i**, 51.2 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **3i** as white solid; yield 86%, E:Z = 85:15.

m.p.: 165-170 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 6.4 Hz, 2H), 7.81 (t, *J* = 10.8 Hz, 3H), 7.62 (d, *J* = 6.6 Hz, 3H), 7.53 (s, 2H), 7.32-7.19 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.01, 142.48, 138.48, 138.24, 135.23, 134.51, 132.34, 130.16, 129.74, 128.35, 103.15. HRMS (ESI) m/z calcd. for $C_{15}H_{11}O_3NaSI$ $[M+Na]^+$ = 420.9371, found 420.9377; IR: 3034, 1682, 1575, 1320, 1149, 1001 cm^{-1}.

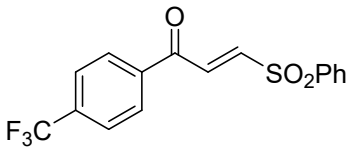
(E)-1-(4-(dimethylamino)phenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3ja)



The reaction was conducted with 1-(4-(dimethylamino)phenyl)prop-2-yn-1-one (**1j**, 34.7 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ja** as red solid; yield 73%, E:Z = 82:18.

m.p.: 45-58 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99-7.91 (m, 5H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 2H), 7.34 -7.27 (m, 1H), 6.67 (d, *J* = 8.7 Hz, 2H), 3.10 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 184.09, 154.26, 139.87, 139.10, 134.14, 134.12, 131.61, 129.57, 128.80, 128.18, 124.01, 111.00, 40.11. HRMS (ESI) m/z calcd. for $C_{17}H_{17}NO_3NaS$ $[M+Na]^+$ = 338.0827, found 338.0833; IR: 2924, 1684, 1593, 1322, 1176, 853 cm^{-1}.

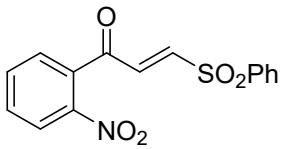
(E)-3-(phenylsulfonyl)-1-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (3ka)



The reaction was conducted with 1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (**1k**, 39.6 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ka** as yellow solid; yield 95%, E:Z = 98:02.

m.p.: 146-150 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.8 Hz, 2H), 7.95 (dd, *J* = 21.2, 11.5 Hz, 4H), 7.79 (d, *J* = 7.9 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 2H), 7.42 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.95, 143.05, 138.60, 138.36, 135.46 (d, *J* = 32.9 Hz), 134.57, 132.21, 129.76, 129.30, 128.36, 126.14 (q, *J* = 3.8 Hz), 123.35 (q, *J* = 273.0 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.22; HRMS (ESI) m/z calcd. for $C_{16}H_{11}O_3NaSF_3$ $[M+Na]^+$ = 363.0279, found 363.0273; IR: 3045, 1671, 1415, 1319, 1131, 751 cm^{-1}.

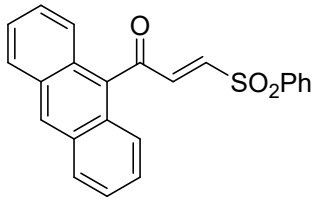
(E)-1-(2-nitrophenyl)-3-(phenylsulfonyl)prop-2-en-1-one (3la)



The reaction was conducted with 1-(2-nitrophenyl)prop-2-yn-1-one (**1l**, 35.0 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 2:1) to give **3la** as white solid; yield 71%, E:Z = 97:03.

m.p.: 121-128 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.2 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 2H), 7.80 (t, *J* = 7.5 Hz, 1H), 7.71 (dd, *J* = 11.9, 7.5 Hz, 2H), 7.60 (t, *J* = 7.8 Hz, 2H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.29-7.26 (m, 1H), 7.04 (d, *J* = 15.3 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.52, 146.20, 141.24, 138.18, 135.71, 134.90, 134.81, 134.59, 132.00, 129.76, 128.82, 128.34, 124.76. HRMS (ESI) m/z calcd. for $C_{15}H_{11}NO_5SNa$ $[M+Na]^+$ = 340.0256, found 340.0264; IR: 3054, 1692, 1523, 1348, 1150, 794 cm^{-1}.

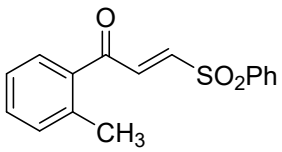
(E)-1-(anthracen-9-yl)-3-(phenylsulfonyl)prop-2-en-1-one (3ma)



The reaction was conducted with 1-(anthracen-9-yl)prop-2-yn-1-one (**1m**, 46.1 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ma** as red solid; yield 94%, E:Z = 98:02.

m.p.: 112-122 ^{o}C;^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.05-8.03 (m, 2H), 7.86 (d, *J* = 7.6 Hz, 2H), 7.76-7.74 (m, 2H), 7.66 (t, *J* = 7.3 Hz, 1H), 7.56-7.48 (m, 7H), 7.07 (d, *J* = 15.3 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.41, 142.94, 138.38, 137.90, 134.48, 131.95, 130.94, 130.59, 129.68, 129.07, 128.40, 128.31, 127.69, 125.81, 124.28. HRMS (ESI) m/z calcd. for $C_{23}H_{16}O_3SNa$ $[M+Na]^+$ = 395.0718, found 395.0713; IR: 2923, 1679, 1592, 1284, 1092, 762 cm^{-1}.

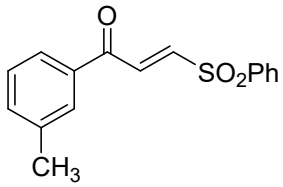
(E)-3-(phenylsulfonyl)-1-(o-tolyl)prop-2-en-1-one (3na)



The reaction was conducted with 1-(o-tolyl)prop-2-yn-1-one (**1n**, 28.8 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3na** as white solid; yield 82%, E:Z = 95:05.

m.p.: 82-84 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.8 Hz, 2H), 7.71-7.58 (m, 5H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.33-7.27 (m, 2H), 7.22 (d, *J* = 15.0 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.07, 141.73, 139.41, 138.61, 136.14, 135.88, 134.42, 132.80, 132.27, 129.78, 129.70, 128.31, 126.02, 21.19. HRMS (ESI) m/z calcd. for $C_{16}H_{14}O_3NaS$ $[M+Na]^+$ = 309.0561, found 309.0560; IR: 3038, 1673, 1600, 1306, 1147, 970 cm^{-1}.

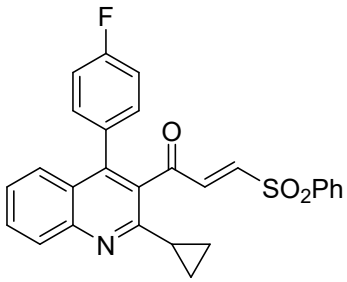
(E)-3-(phenylsulfonyl)-1-(m-tolyl)prop-2-en-1-one (3oa)



The reaction was conducted with 1-(m-tolyl)prop-2-yn-1-one (**1o**, 28.8 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3oa** as yellow solid; yield 94%, E:Z = 95:05.

m.p.: 94-100 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 10.7, 5.9 Hz, 3H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.69 (t, *J* = 7.1 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.43-7.35 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.74, 141.79, 139.10, 138.63, 136.01, 135.38, 134.41, 133.27, 129.70, 129.46, 128.99, 128.31, 126.28, 21.39. HRMS (ESI) m/z calcd. for $C_{16}H_{14}O_3Na$ $[M+Na]^+$ = 309.0561, found 309.0562; IR: 3037, 1663, 1592, 1284, 1144, 837 cm^{-1}.

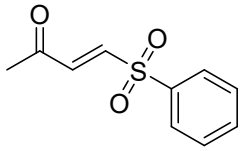
(E)-1-(2-cyclopropyl-4-(4-fluorophenyl)quinolin-3-yl)-3-(phenylsulfonyl)prop-2-en-1-one (3pa)



The reaction was conducted with 1-(2-cyclopropyl-4-(4-fluorophenyl)quinolin-3-yl)prop-2-yn-1-one (**1p**, 63.1 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3pa** as yellow solid; yield 87%, E:Z = 97:03.

m.p.: 133-140 ^{o}C;^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.70 (t, *J* = 8.7 Hz, 4H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.17 (dd, *J* = 8.0, 5.4 Hz, 2H), 7.05 (t, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 3.1 Hz, 1H), 2.01-1.96 (m, 1H), 1.32 (dd, *J* = 6.5, 3.7 Hz, 2H), 0.98-0.95 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.89, 163.05 (d, *J* = 250.1 Hz), 158.36, 148.41, 144.45, 142.19, 138.41, 136.69, 134.44, 132.10 (d, *J* = 8.3 Hz), 131.55, 130.76, 130.60 (d, *J* = 3.5 Hz), 129.63, 129.30, 128.32, 126.52, 125.80, 124.46, 115.97 (d, *J* = 21.5 Hz), 15.58, 10.93; ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.94; HRMS (ESI) m/z calcd. for $C_{27}H_{21}NO_3SF$ $[M+H]^+$ = 458.1226, found 458.1235; IR: 3047, 1662, 1512, 1327, 1159, 848 cm^{-1}.

(E)-4-(phenylsulfonyl)but-3-en-2-one (3qa)[12]

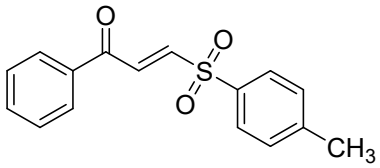


The reaction was conducted with but-3-yn-2-one (**1q**, 13.6 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3qa** as yellow solid; yield 65%, E:Z = 97:03.

m.p.: 50-55 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96-7.90 (m, 2H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.61 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 15.4 Hz, 1H), 7.02 (d, *J* = 15.4 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (126

MHz, $CDCl_3$) δ 195.51, 141.00, 138.52, 136.06, 134.45, 129.69, 128.33, 29.12; IR: 3045, 1692, 1448, 1320, 1148, 757 cm^{-1}.

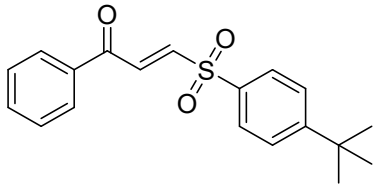
(E)-1-phenyl-3-tosylprop-2-en-1-one (3ab)[2]



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-methylbenzenesulfinate (**2b**, 89 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ab** as yellow solid; yield 70%, E:Z = 94:06.

m.p.: 94-100 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.8 Hz, 2H), 7.90 (d, *J* = 14.9 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 7.36 (dd, *J* = 15.4, 11.6 Hz, 3H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.77, 145.61, 142.33, 136.08, 135.70, 134.41, 132.66, 130.31, 129.07, 128.96, 128.34, 21.73; IR: 3045, 1668, 1313, 1148, 1003, 981 cm^{-1}.

(E)-3-((4-(tert-butyl)phenyl)sulfonyl)-1-phenylprop-2-en-1-one (3ac)

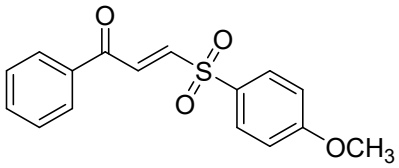


The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-(tert-butyl)benzenesulfinate (**2c**, 55.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **3ac** as white solid; yield 60%, E:Z = 89:11.

m.p.: 123-128 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92-7.75 (m, 5H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.53-7.44 (m, 4H), 7.3007.18 (m, 1H), 1.28 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.49, 141.28, 135.03, 134.46, 133.40, 131.59, 128.35, 128.04, 127.94, 127.79, 127.17, 125.69, 125.18, 34.35,

29.99; HRMS calcd. for: $C_{19}H_{20}O_3NaS$ $[M+Na]^+$ = 351.1031, found 351.01035; IR: 2963, 1693, 1671, 1447, 1196, 690 cm^{-1}.

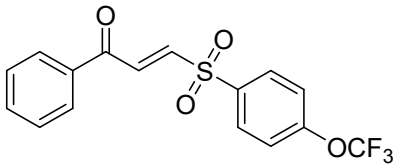
(E)-3-((4-methoxyphenyl)sulfonyl)-1-phenylprop-2-en-1-one (3ad)[4]



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-methoxybenzenesulfinate (**2d**, 48.5 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ad** as yellow solid; yield 61%, E:Z = 86:14.

m.p.: 88-93 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.7 Hz, 2H), 7.89-7.86 (m, 3H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.36-7.26 (m, 1H), 7.04 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.89, 164.38, 142.59, 136.13, 134.39, 132.09, 130.64, 129.96, 129.07, 128.97, 114.94, 55.82; IR: 3063, 1685, 1665, 1592, 1268, 762 cm^{-1}.

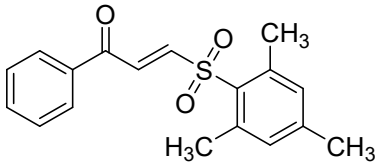
(E)-1-phenyl-3-((4-(trifluoromethoxy)phenyl)sulfonyl)prop-2-en-1-one (3ae)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-(trifluoromethoxy)benzenesulfinate (**2e**, 124.0 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **3ae** as white solid; yield 70%, E:Z = 95:05.

m.p.: 114-120 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03-7.95 (m, 5H), 7.68-7.65 (m, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.44, 153.48, 153.47, 141.49, 136.94, 135.91, 134.61, 133.78, 130.68, 129.15, 129.02, 121.36; ^{19}F NMR (471 MHz, $CDCl_3$) δ -57.64; HRMS calcd. for: $C_{16}H_{11}O_4NaSF_3$ $[M+Na]^+$ = 379.0228, found 379.0223; IR: 3052, 2320, 1670, 1270, 1151, 1006 cm^{-1}.

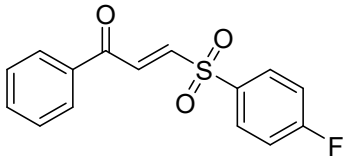
(E)-3-(mesitylsulfonyl)-1-phenylprop-2-en-1-one (3af)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 2,4,6-trimethylbenzenesulfinate (**2f**, 103.0 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3af** as white solid; yield 73%, E:Z = 91:09.

m.p.: 95-105 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99- 7.98 (m, 2H), 7.88 (d, *J* = 14.9 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 14.9 Hz, 1H), 6.99 (s, 2H), 2.65 (s, 6H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.96, 144.42, 142.53, 140.55, 136.18, 134.40, 132.53, 131.86, 131.56, 129.09, 128.94, 22.97, 21.13; HRMS calcd. for: $C_{18}H_{18}O_3NaS$ $[M+Na]^+$ = 337.0874, found 337.0876; IR: 3040, 1666, 1447, 1318, 1075, 694 cm^{-1}.

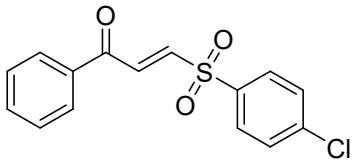
(E)-3-((4-fluorophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3ag)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-fluorobenzenesulfinate (**2g**, 45.5 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ag** as yellow solid; yield 67%, E:Z = 93:07.

m.p.: 92-100 °C; ^{1}H NMR (500 MHz, CDCl3) δ 8.00-7.92 (m, 5H), 7.67 (t, J = 7.2 Hz, 1H), 7.54 (t, J = 7.7 Hz, 2H), 7.34 (d, J = 14.9 Hz, 1H), 7.j27 (dd, J = 11.3, 5.2 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.55, 166.25 (d, *J* = 258.1 Hz), 141.81, 135.96, 134.56, 133.28, 131.32, 131.24, 129.13, 129.00, 117.09 (d, *J* = 22.8 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -101.93; HRMS calcd. for: $C_{15}H_{11}O_3NaSF$ $[M+Na]^+$ = 313.0311, found 313.0317; IR: 3054, 1668, 1590, 1322, 1146, 838 cm^{-1}.

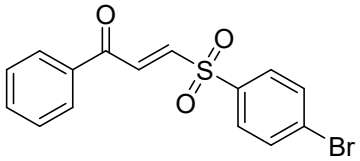
(E)-3-((4-chlorophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3ah)[4]



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-chlorobenzenesulfinate (**2h**, 49.7 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ah** as yellow solid; yield 72%, E:Z = 80:20.

m.p.: 102-110 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00-7.98 (m, 1H), 7.96-7.89 (m, 3H), 7.67 (dd, *J* = 10.6, 4.2 Hz, 1H), 7.58-7.52(m, 4H), 7.35 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.47, 141.59, 141.31, 137.19, 135.93, 134.58, 133.58, 130.05, 129.77, 129.14, 129.00; IR: 3054, 1672, 1449, 1317, 1141, 1083 cm^{-1}.

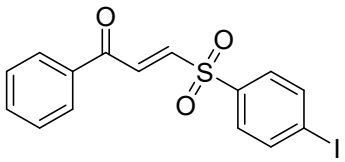
(E)-3-((4-bromophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3ai)[4]



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-bromobenzenesulfinate (**2i**, 121.5 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ai** as white solid; yield 51%, E:Z = 52:48.

m.p.: 97-105 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.86 (d, *J* = 14.9 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.27 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.43, 140.51, 136.73, 134.91, 133.53, 132.62, 132.00, 128.88, 128.75, 128.10, 127.96; IR: 3051, 1667, 1573, 1389, 1321, 967 cm^{-1}.

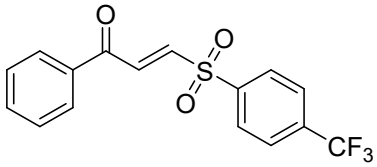
(E)-3-((4-iodophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3aj)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-iodobenzenesulfinate (**2j**, 145.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3aj** as white solid; yield 85%, E:Z = 94:06.

m.p.: 114-124 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99-7.91 (m, 5H), 7.66-7.64 (m, 3H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.46, 141.54, 139.00, 138.42, 135.95, 134.55, 133.65, 129.53, 129.13, 128.99, 102.58; HRMS calcd. for: $C_{15}H_{11}O_3NaSI$ $[M+Na]^+$ = 420.9371, found 420.9370; IR: 3041, 1669, 1563, 1320, 1142, 818 cm^{-1}.

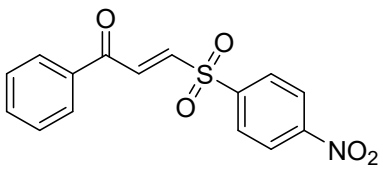
(E)-1-phenyl-3-((4-(trifluoromethyl)phenyl)sulfonyl)prop-2-en-1-one (3ak)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-(trifluoromethyl)benzenesulfinate (**2k**, 116.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **3ak** as yellow solid; yield 83%, E:Z = 80:20.

m.p.: 122-127 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 2H), 8.01-7.99 (m, 3H), 7.87 (d, *J* = 8.2 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 2H), 7.35 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.26, 142.35, 141.05, 135.98 (q, *J* = 34.2 Hz), 135.84, 134.67, 134.49, 129.18, 129.02, 128.92, 126.82 (q, *J* = 3.6 Hz), 123.00 (q, *J* = 273.1 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.28; HRMS calcd. for: $C_{16}H_{11}O_3NaSF_3$ $[M+H]^+$ = 363.0279, found 363.0285; IR: 3052, 1668, 1325, 1152, 1063, 714 cm^{-1}.

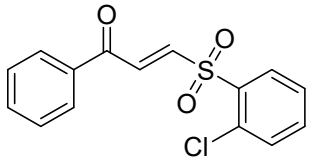
(E)-3-((4-nitrophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3al, CAS: 100961-84-0)[5]



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 4-nitrobenzenesulfinate (**2l**, 104.6 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 3:1) to give **3al** as white solid; yield 85%, E:Z = 55:45.

m.p.: 137-146 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.7 Hz, 2H), 8.10 (d, *J* = 8.7 Hz, 2H), 7.95 (dd, *J* = 19.8, 11.2 Hz, 3H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.05, 151.10, 144.42, 140.54, 135.71, 135.19, 134.83, 129.76, 129.24, 129.06, 124.85; IR: 3049, 1685, 1592, 1324, 1284, 853 cm^{-1}.

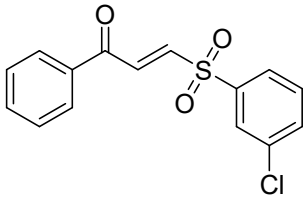
(E)-3-((2-chlorophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3am)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 2-chlorobenzenesulfinate (**2m**, 99.3 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **3am** as white solid; yield 77%, E:Z = 98:02.

m.p.: 129-134 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 7.2 Hz, 1H), 8.03 (dd, *J* = 24.1, 11.0 Hz, 3H), 7.67-7.50 (m, 7H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.57, 140.16, 136.33, 135.96, 135.91, 135.52, 134.58, 133.28, 132.16, 131.43, 129.15, 129.05, 127.78; HRMS calcd. for: C15H11O3NaSCl $[M+Na]^{+}$ = 329.0015, found 329.0021; IR: 3042, 1685, 1592, 1323, 1093, 853 cm^{-1}.

(E)-3-((3-chlorophenyl)sulfonyl)-1-phenylprop-2-en-1-one (3an)

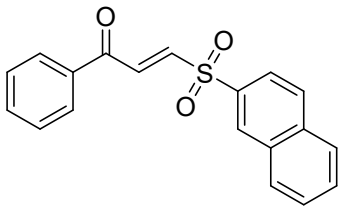


The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium 3-chlorobenzenesulfinate (**2n**, 99.3 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol).

The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3an** as viscous liquid; yield 81%, E:Z = 97:03.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99-7.93 (m, 4H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 2H), 7.56-7.52 (m, 3H), 7.35 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.40, 141.35, 140.51, 135.91, 134.59, 134.50, 134.00, 130.99, 129.14, 129.02, 128.29, 126.41; HRMS calcd. for: $C_{15}H_{11}O_3NaSCl$ $[M+Na]^+$ = 329.0015, found 329.0026; IR: 3034, 1669, 1579, 1324, 1154, 797.

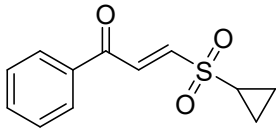
(E)-3-(naphthalen-2-ylsulfonyl)-1-phenylprop-2-en-1-one (3ao)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium naphthalene-2-sulfinate (**2o**, 107.0 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3ao** as yellow solid; yield 87%, E:Z = 95:05.

m.p.: 120-127 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.03-7.97 (m, 5H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.88 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.70 (dd, *J* = 11.1, 4.0 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 2H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.43 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.71, 142.05, 136.03, 135.58, 135.39, 134.50, 133.14, 132.31, 130.44, 130.08, 129.78, 129.56, 129.11, 129.01, 128.09, 127.98, 122.56; HRMS calcd. for: $C_{16}H_{11}O_4NaSF_3$ $[M+Na]^+$ = 379.0228, found 379.0223; IR: 3047, 1675, 1446, 1316, 1148, 767 cm^{-1}.

(E)-3-(cyclopropylsulfonyl)-1-phenylprop-2-en-1-one (3ap)

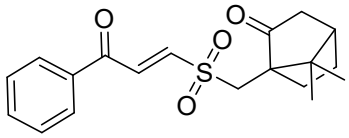


The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium cyclopropanesulfinate (**2p**, 64.0 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol).

The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 3:1) to give **3ap** as white solid; yield 85%, E:Z = 94:06.

m.p.: 64-72 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.4 Hz, 2H), 7.86 (d, *J* = 15.0 Hz, 1H), 7.66 (t, *J* = 7.3 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 15.0 Hz, 1H), 2.49-2.46 (m, 1H), 1.37-1.34 (m, 2H), 1.16-1.15 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 185.91, 138.42, 134.15, 132.62, 132.35, 127.23, 127.13, 28.71, 3.78; HRMS calcd. for: $C_{12}H_{13}O_3S$ $[M+H]^+$ = 237.0585, found 237.0589; IR: 3051, 2918, 1683, 1592, 1321, 1093 cm^{-1}.

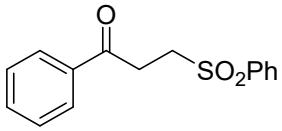
(E)-7,7-dimethyl-1-(((3-oxo-3-phenylprop-1-en-1-yl)sulfonyl)methyl)bicyclo[2.2.1]heptan-2-one (3aq)



The reaction was conducted with 1-phenylprop-2-yn-1-one (**1a**, 26.0 mg, 0.2 mmol), sodium (7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfinate (**2q**, 119.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3aq** as yellow solid; yield 75%, E:Z = 70:30.

m.p.: 42-52 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.6 Hz, 2H), 7.81 (d, *J* = 15.0 Hz, 1H), 7.65 (t, *J* = 6.9 Hz, 1H), 7.58 (d, *J* = 15.0 Hz, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 3.53 (d, *J* = 14.9 Hz, 1H), 2.99 (d, *J* = 14.9 Hz, 1H), 2.42 (dd, *J* = 31.3, 16.7 Hz, 1H), 2.15 (s, 1H), 1.94 (d, *J* = 18.4 Hz, 1H), 1.09 (s, 2H), 0.89 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 214.57, 187.96, 142.01, 136.09, 134.31, 133.85, 129.04, 58.86, 52.44, 48.65, 42.56, 42.52, 27.10, 25.14, 19.74, 19.67; HRMS calcd. for: $C_{19}H_{22}O_4NaS$ $[M+Na]^+$ = 369.1136, found 369.1139; IR: 3055, 2960, 1744, 1680, 1423, 1130 cm^{-1}.

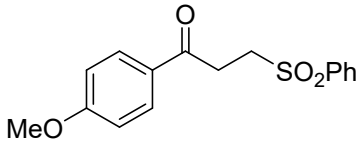
1-phenyl-3-(phenylsulfonyl)propan-1-one (5aa, CAS: 65885-28-1)[6]



The reaction was conducted with 1-phenylprop-2-en-1-one (**4a**, 26.4 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5aa** as white solid; yield 84%.

m.p.: 100-104 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99-7.95 (m, 2H), 7.93-7.92 (m, 2H), 7.68 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.61-7.58 (m, 3H), 7.48 (t, *J* = 7.7 Hz, 2H), 3.59-3.56 (m, 2H), 3.53-3.49 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.46, 139.07, 135.81, 133.98, 133.84, 129.46, 128.83, 128.09, 128.02, 51.05, 31.39 cm^{-1}.

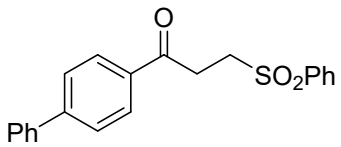
1-(4-methoxyphenyl)-3-(phenylsulfonyl)propan-1-one (5ba)[7]



The reaction was conducted with 1-(4-methoxyphenyl)prop-2-en-1-one (**4b**, 32.4 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 3:1) to give **5ba** as white solid; yield 98%.

m.p.: 104-108 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.4 Hz, 2H), 7.90 (d, *J* = 7.3 Hz, 2H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.58 (t, *J* = 7.1 Hz, 2H), 6.93 (d, *J* = 7.3 Hz, 2H), 3.87 (s, 3H), 3.57-3.54 (m, 2H), 3.46-3.43 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.88, 164.01, 139.08, 133.95, 130.42, 129.44, 128.87, 128.01, 113.96, 55.57, 51.17, 30.95; ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.88, 164.01, 139.08, 133.95, 130.42, 129.44, 128.87, 128.01, 113.96, 55.57, 51.17, 30.95; IR: 3434, 3017, 1678, 1602, 1254, 1110 cm^{-1}.

1-([1,1'-biphenyl]-4-yl)-3-(phenylsulfonyl)propan-1-one (5ca, Cas: 1375496-17-5)[7]

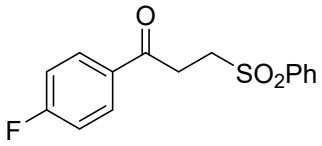


The reaction was conducted with 1-([1,1'-biphenyl]-4-yl)prop-2-en-1-one (**4c**, 41.7 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol).

The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ca** as white solid; yield 88%.

m.p.: 170-174 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92-7.89 (m, 3H), 7.62-7.58 (m, 3H), 7.55-7.50 (m, 3H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.34 (d, *J* = 7.3 Hz, 1H), 3.51-3.45 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.99, 145.45, 138.54, 138.07, 133.45, 132.94, 128.43, 127.99, 127.66, 127.42, 126.99, 126.38, 126.25, 50.05, 30.36; IR: 2991, 1681, 1604, 1262, 1143, 802 cm^{-1}.

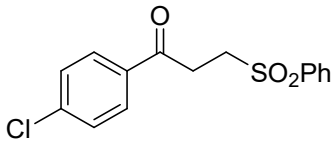
1-(4-fluorophenyl)-3-(phenylsulfonyl)propan-1-one (5da)[7]



The reaction was conducted with 1-(4-fluorophenyl)prop-2-en-1-one (**4d**, 30.0 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5da** as white solid; yield 97%.

m.p.: 132-138°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97-7.95 (m, 4H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.14 (t, *J* = 8.5 Hz, 2H), 3.56 (d, *J* = 7.3 Hz, 2H), 3.48 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.89, 166.11 (d, *J* = 256.3 Hz), 139.02, 134.02, 132.27 (d, *J* = 2.8 Hz), 130.81 (d, *J* = 9.3 Hz), 129.48, 128.00, 116.09, 115.91, 50.97, 31.27; ^{19}F NMR (471 MHz, $CDCl_3$) δ -103.59; IR: 2926, 1680, 1600, 1306, 1152, 843 cm^{-1}.

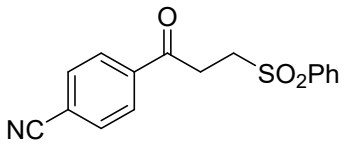
1-(4-chlorophenyl)-3-(phenylsulfonyl)propan-1-one (5ea)[7]



The reaction was conducted with 1-(4-chlorophenyl)prop-2-en-1-one (**4e**, 33.3 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ea** as white solid; yield 87%.

m.p.: 144-154 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.5 Hz, 2H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.68 (t, *J* = 7.1 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 3.57-3.55 (m, 2H), 3.49-3.46 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.31, 140.37, 138.99, 134.10, 134.05, 131.55, 129.50, 129.18, 128.00, 50.92, 31.34; IR: 2926, 1683, 1590, 1306, 1151, 744 cm^{-1}.

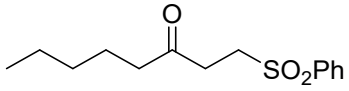
4-(3-(phenylsulfonyl)propanoyl)benzonitrile (5fa)[8]



The reaction was conducted with 4-acryloylbenzonitrile (**4f**, 31.4 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 2:1) to give **5fa** as white solid; yield 95%.

m.p.: 140-144 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.3 Hz, 2H), 7.87 (d, *J* = 7.8 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 3.49 (d, *J* = 6.5 Hz, 2H), 3.45 (d, *J* = 7.0 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.32, 137.89, 137.65, 133.12, 131.68, 128.52, 127.51, 126.95, 116.67, 116.03, 49.70, 30.69; IR: 2962, 2235, 1691, 1298, 1152, 845 cm^{-1}.

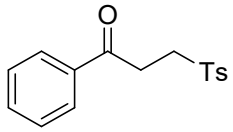
1-(phenylsulfonyl)octan-3-one (5ga, CAS: 82972-50-7)[9]



The reaction was conducted with oct-1-en-3-one (**4g**, 25.2 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ga** as white solid; yield 95%.

m.p.: 34-37 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.4 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.58 (t, *J* = 7.7 Hz, 2H), 3.40-3.37 (m, 2H), 2.91-2.88 (m, 2H), 2.42 (t, *J* = 7.4 Hz, 1H), 1.56-1.51 (dm, 2H), 1.31-1.22 (m, 4H), 0.87 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.25, 139.06, 133.89, 129.39, 127.96, 50.56, 42.81, 34.88, 31.22, 23.35, 22.34, 13.83; IR: 2991, 1681, 1604, 1262, 1143, 802 cm^{-1}.

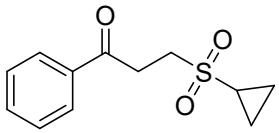
1-phenyl-3-tosylpropan-1-one (5ab, CAS: 52481-46-6)[2]



The reaction was conducted with 1-phenylprop-2-en-1-one (**4a**, 26.0 mg, 0.2 mmol), sodium 4-methylbenzenesulfinate (**2b**, 89.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ab** as yellow solid; yield 95%.

m.p.: 130-138 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, J = 7.5 Hz, 2H), 7.83 (d, J = 8.1 Hz, 2H), 7.59 (t, J = 7.3 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.37 (d, J = 7.9 Hz, 2H), 3.54 (d, J = 7.4 Hz, 2H), 3.49 (d, J = 7.6 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.58, 145.04, 136.01, 135.81, 133.82, 130.08, 128.82, 128.09, 128.05, 51.11, 31.53, 21.70; IR: 3052, 2939, 1681, 1316, 1147, 852 cm^{-1}.

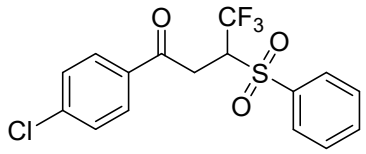
3-(cyclopropylsulfonyl)-1-phenylpropan-1-one (5ap)



The reaction was conducted with 1-phenylprop-2-en-1-one (**4a**, 26.0 mg, 0.2 mmol), sodium cyclopropanesulfinate (**2p**, 64.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ap** as white solid; yield 95%.

m.p.: 97-100 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, J = 7.9 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H), 3.60-3.52 (m, 4H), 2.52-2.43 (m, 1H), 1.29-26 (m, 2H), 1.09-1.05 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.83, 135.86, 133.85, 128.86, 128.13, 48.43, 31.02, 29.98, 4.89; HRMS calcd. for: $C_{12}H_{14}O_3NaS$ $[M+Na]^+$ = 261.0561, found 261.0562; IR: 3056, 2984, 1676, 1597, 1278, 1117 cm^{-1}

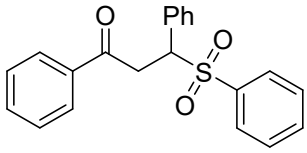
1-(4-chlorophenyl)-4,4,4-trifluoro-3-(phenylsulfonyl)butan-1-one (5ha)



The reaction was conducted with (E)-1-(4-chlorophenyl)-4,4,4-trifluorobut-2-en-1-one (**4h**, 46.9 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ga** as white solid; yield 60%.

m.p.: 123-126 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 16.6, 8.1 Hz, 4H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 4.94-4.91 (m, 1H), 4.04 (dd, *J* = 18.4, 7.0 Hz, 1H), 3.34 (dd, *J* = 18.4, 4.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.81, 140.76, 138.36, 134.75, 133.68, 129.79, 129.49, 129.29, 128.92, 123.18 (q, *J* = 280.2 Hz), 62.09 (q, *J* = 28.7 Hz), 32.55; ^{19}F NMR (471 MHz, $CDCl_3$) δ -65.19; HRMS calcd. for: $C_{16}H_{12}O_3NaSClF_3$ $[M+Na]^+$ = 399.0045, found 399.0044; IR: 2950, 1695, 1589, 1324, 1148, 843 cm^{-1}

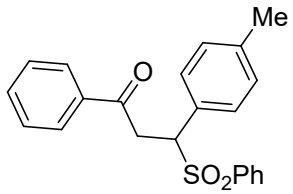
1,3-diphenyl-3-(phenylsulfonyl)propan-1-one (5ia, CAS: 300376-97-0)[10]



The reaction was conducted with (E)-chalcone (**4i**, 41.7 mg, 0.2 mmol), sodium benzenesulfinate (**2a**, 82.1 mg, 0.5 mmol) and 4-chlorobenzoic acid (62.6 mg, 0.4 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ia** as white solid; yield 61%.

m.p.: 154-158 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 23.7, 11.2 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.66 (d, *J* = 8.5 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H), 7.25 (d, *J* = 15.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.43, 140.51, 136.73, 134.91, 133.53, 132.62, 132.00, 128.88, 128.75, 128.10, 127.96; IR: 3059, 1685, 1592, 1306, 1094, 762 cm^{-1}

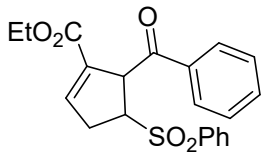
1,3-diphenyl-3-tosylpropan-1-one (5ja)[13]



The reaction was conducted with (E)-1-phenyl-3-(p-tolyl)prop-2-en-1-one (**4j**, 22.3 mg, 0.1 mmol), sodium benzenesulfinate (**2a**, 41.0 mg, 0.25 mmol) and 4-chlorobenzoic acid (31.3 mg, 0.2 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **5ja** as white solid; yield 57%.

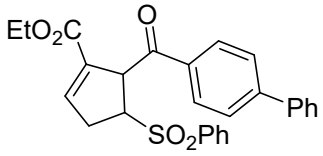
m.p.: 160-164 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.7 Hz, 2H), 7.56 (dd, *J* = 13.5, 7.0 Hz, 4H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 7.9 Hz, 2H), 4.91 (dd, *J* = 9.7, 3.4 Hz, 1H), 4.09 (dd, *J* = 17.8, 3.5 Hz, 1H), 3.91 (dd, *J* = 17.8, 9.8 Hz, 1H), 2.27 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.94, 138.75, 137.08, 136.19, 133.67, 133.66, 129.73, 129.62, 129.34, 129.21, 129.06, 128.74, 128.15, 66.22, 36.97, 21.17.

Ethyl 5-benzoyl-4-(phenylsulfonyl)cyclopent-1-ene-1-carboxylate (6aa)



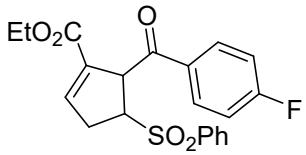
m.p.: 104-117 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.58-7.52 (m, 2H), 7.46-7.41 (m, 5H), 6.87 (d, *J* = 1.6 Hz, 1H), 5.35 (s, 1H), 4.16-4.12 (m, 1H), 4.02 (q, *J* = 7.1 Hz, 2H), 3.13 (d, *J* = 19.3 Hz, 1H), 2.98 (dd, *J* = 19.3, 9.0 Hz, 1H), 1.02 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.28, 162.78, 142.91, 137.12, 135.99, 135.64, 134.16, 133.62, 129.38, 129.09, 128.57, 128.53, 66.91, 60.91, 51.02, 34.15, 13.81; HRMS (ESI) m/z calcd. for $C_{21}H_{20}NaO_5S[M+Na]^+$ = 407.0929, found 407.0918; IR: 2964, 1679, 1644, 1282, 1146, 747 cm^{-1}

Ethyl 5-([1,1'-biphenyl]-4-carbonyl)-4-(phenylsulfonyl)cyclopent-1-ene-1-carboxylate (6ea)



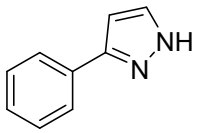
m.p.: 164-171 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.3 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 2H), 7.65 (t, *J* = 7.7 Hz, 4H), 7.53-7.48 (m, 3H), 7.46-7.42 (m, 3H), 6.88 (d, *J* = 1.7 Hz, 1H), 5.39 (d, *J* = 2.4 Hz, 1H), 4.20-4.15 (m, 1H), 4.07-4.02 (m, 2H), 3.16-3.12 (m, 1H), 3.03-2.97 (m, 1H), 1.06 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.88, 162.86, 146.23, 142.87, 139.80, 137.19, 135.70, 134.70, 134.15, 129.72, 129.41, 129.04, 128.59, 128.39, 127.30, 127.16, 66.96, 60.96, 51.05, 34.20, 13.89; HRMS (ESI) m/z calcd. for C27H24O5S [M+H] + = 461.1423, found 461.1445; IR: 2972, 1710, 1649, 1279, 1140, 760 cm^{-1}

Ethyl 5-(4-fluorobenzoyl)-4-(phenylsulfonyl)cyclopent-1-ene-1-carboxylate (6fa)



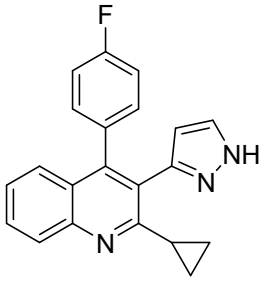
m.p.: 115-124 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 8.2, 5.6 Hz, 2H), 7.83 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.11 (t, *J* = 8.5 Hz, 2H), 6.88 (s, 1H), 5.32-5.30 (m, 1H), 4.16-4.12 (m, 1H), 4.06-4.01 (m, 2H), 3.11 (d, *J* = 19.3 Hz, 1H), 2.97 (dd, *J* = 19.3, 9.0 Hz, 1H), 1.06 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.77, 163.90 (d, *J* = 288.8 Hz), 167.08, 142.93, 137.06, 135.46, 134.20, 132.44 (d, *J* = 2.7 Hz), 131.88, 131.81, 129.40, 128.52, 115.66 (d, *J* = 22.0 Hz), 66.83, 60.95, 50.86, 34.21, 13.85; ^{19}F NMR (471 MHz, $CDCl_3$) δ -104.09; HRMS (ESI) m/z calcd. for $C_{21}H_{19}FNaO_5S$ [M+Na] $^{+}$ = 425.0835, found 425.0824; IR: 2965, 1715, 1597, 1279, 1146, 745 cm^{-1}

3-phenyl-1H-pyrazole (6b, CAS: 2458-26-6)[11]



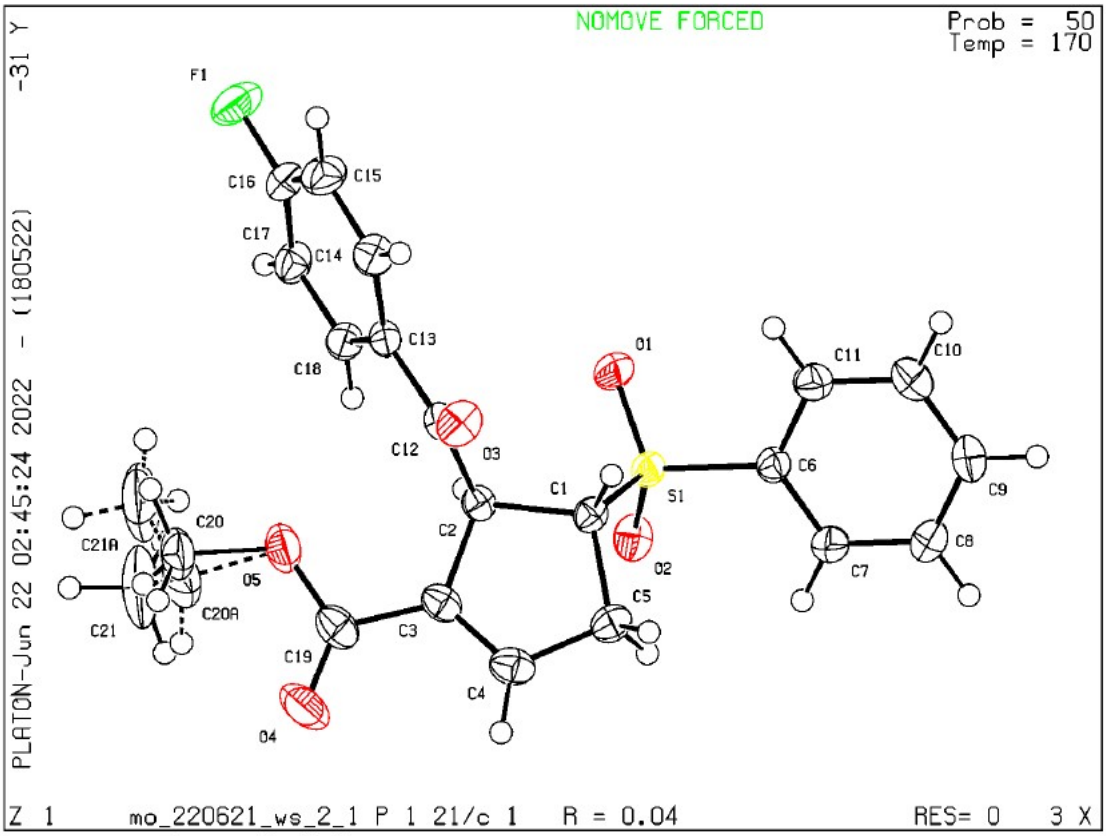
m.p.: 38-47 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.54 (s, 1H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.60 (s, 1H), 7.44-7.38 (m, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 6.61 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 132.03, 131.44, 128.82, 128.69, 128.12, 125.88, 102.76; IR: 2924, 1594, 1456, 1093, 955, 759 cm^{-1}.

2-cyclopropyl-4-(4-fluorophenyl)-3-(1H-pyrazol-3-yl)quinoline (6c)



m.p.: 93-112 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.63 (dd, *J* = 11.2, 4.0 Hz, 1H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.37-7.32 (m, 2H), 7.08-7.05 (m, 2H), 6.98-6.94 (m, 2H), 6.07 (s, 1H), 2.04-2.01 (m, 1H), 1.29 (d, *J* = 2.2 Hz, 3H), 0.87 (dd, *J* = 4.8, 3.1 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.07, 161.67, 161.10, 147.32 (d, *J* = 115.8 Hz), 133.37, 132.60 (d, *J* = 3.2 Hz), 131.37 (d, *J* = 7.9 Hz), 129.52, 128.97, 126.25, 125.58, 125.50, 124.77, 114.99, 114.82, 107.79, 15.53, 10.98; ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.1; HRMS calcd. for: $C_{21}H_{17}N_3F$ $[M+H]^+$ = 330.1407, found 330.1414; IR: 2929, 1605, 1513, 1132, 922, 841 cm^{-1}.

5. X-ray Crystal Structure for 6fa



6. Reference

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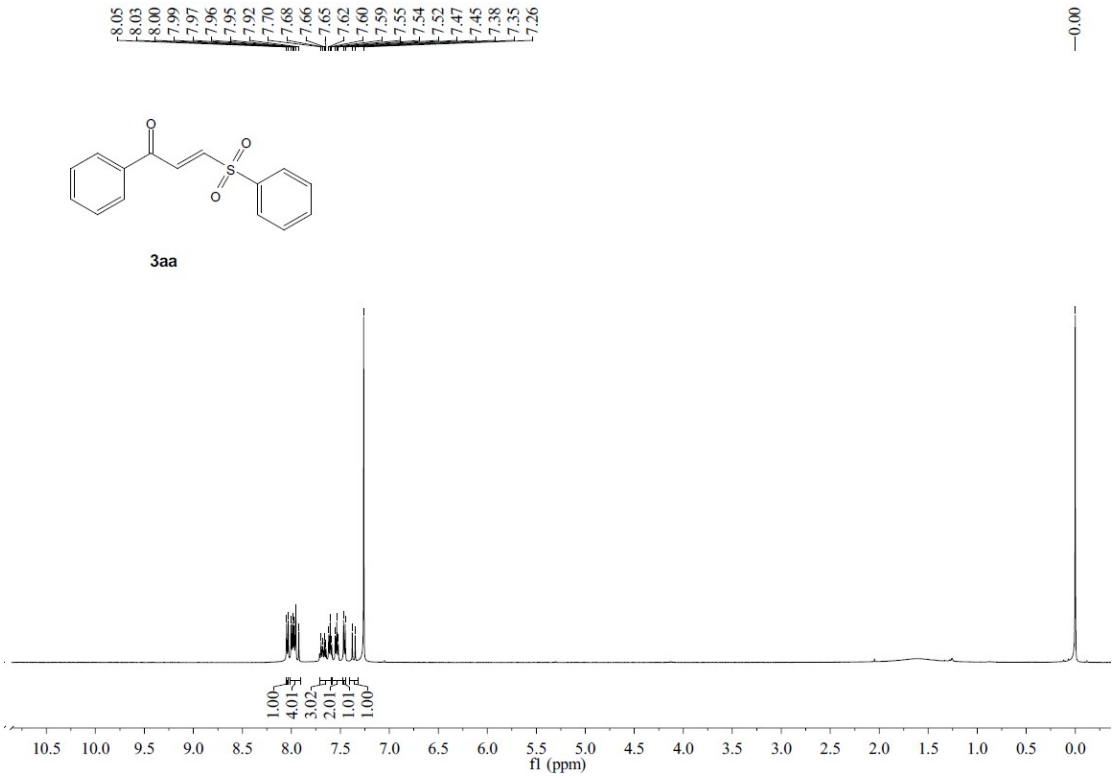
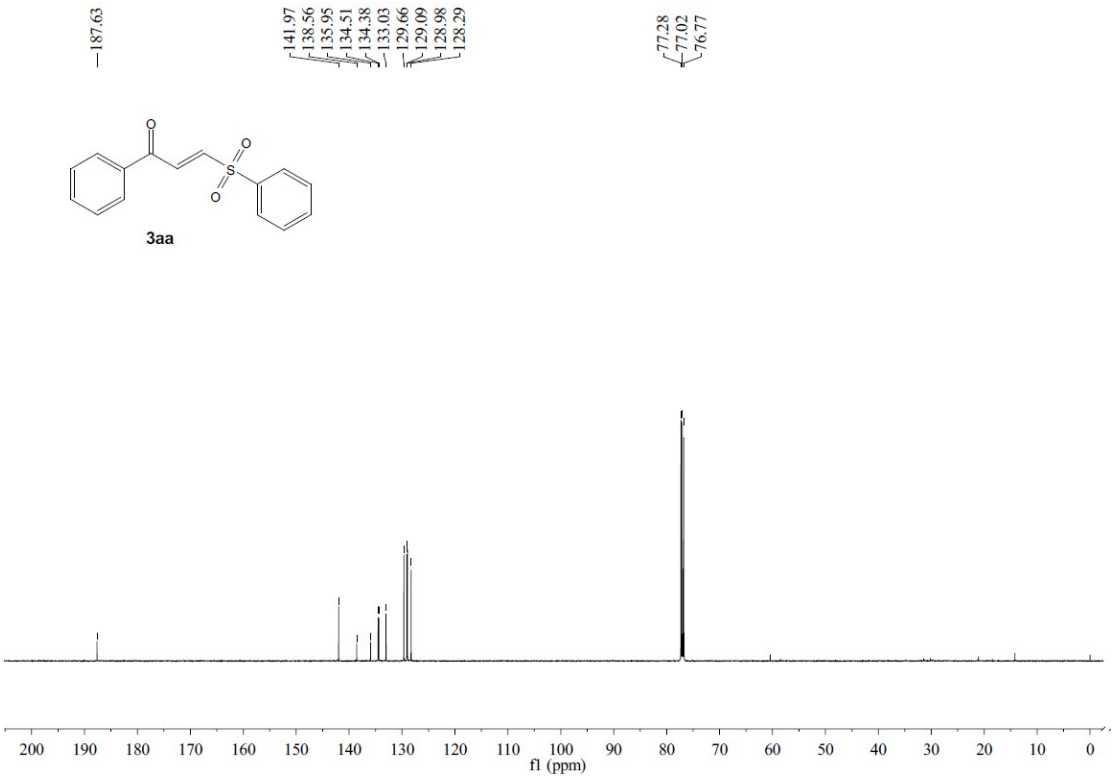
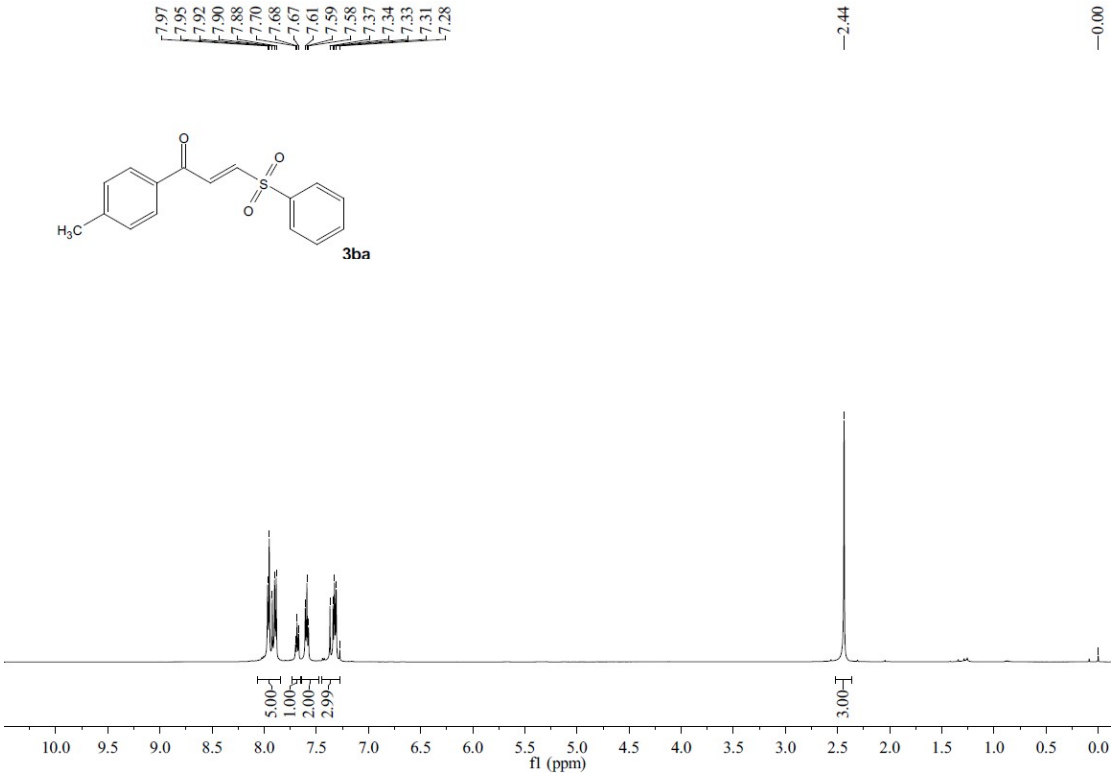
7. ^{1}H, ^{13}C, ^{19}F NMR spectra of compounds.



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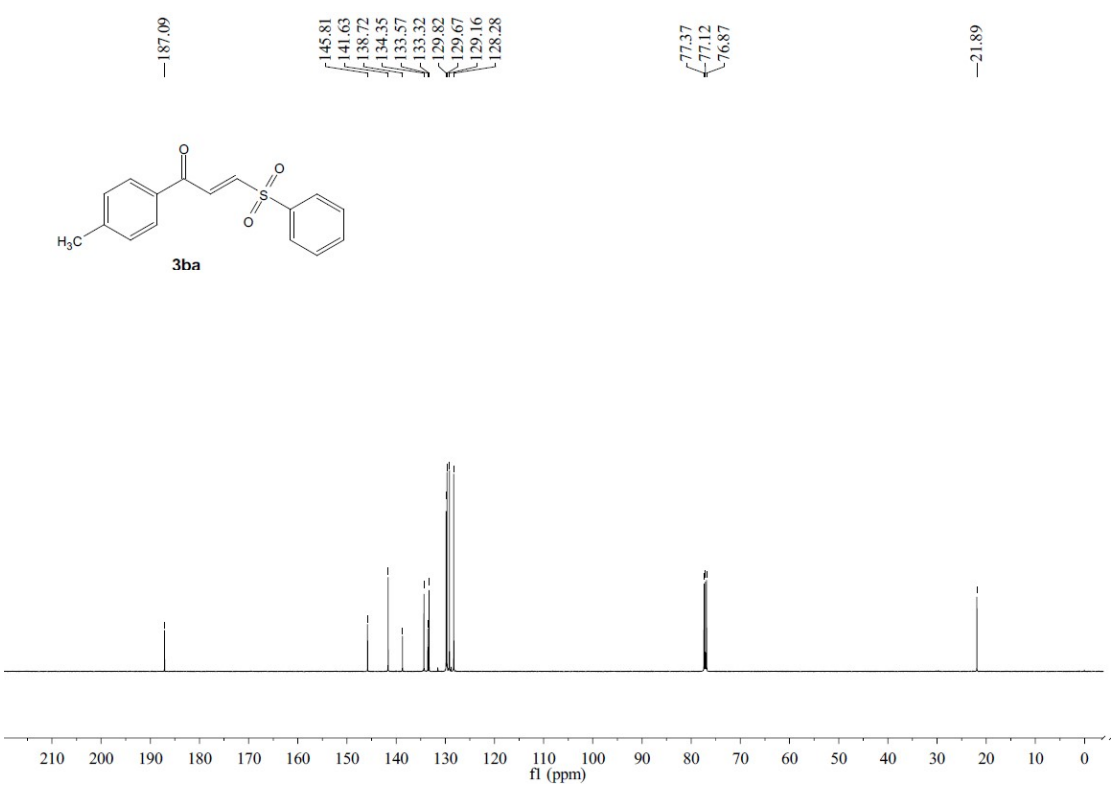
7.95
7.92
7.90
7.88
7.70
7.68
7.67
7.61
7.59
7.58
7.37
7.34
7.33
7.31
7.28
2.44
0.00
O
O
S
O
H3C
3ba
5.00
1.00
2.00
2.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.32
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129.16
128.28
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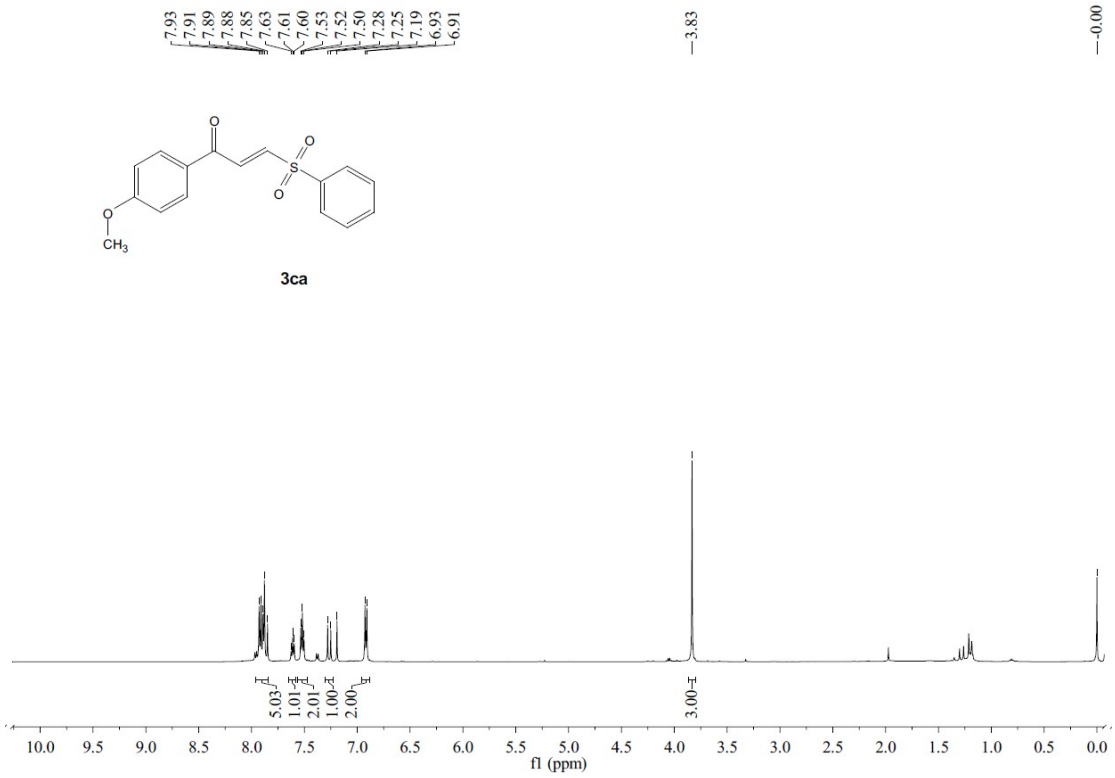
77.12
76.87
21.89
O
O
S
O
H3C
3ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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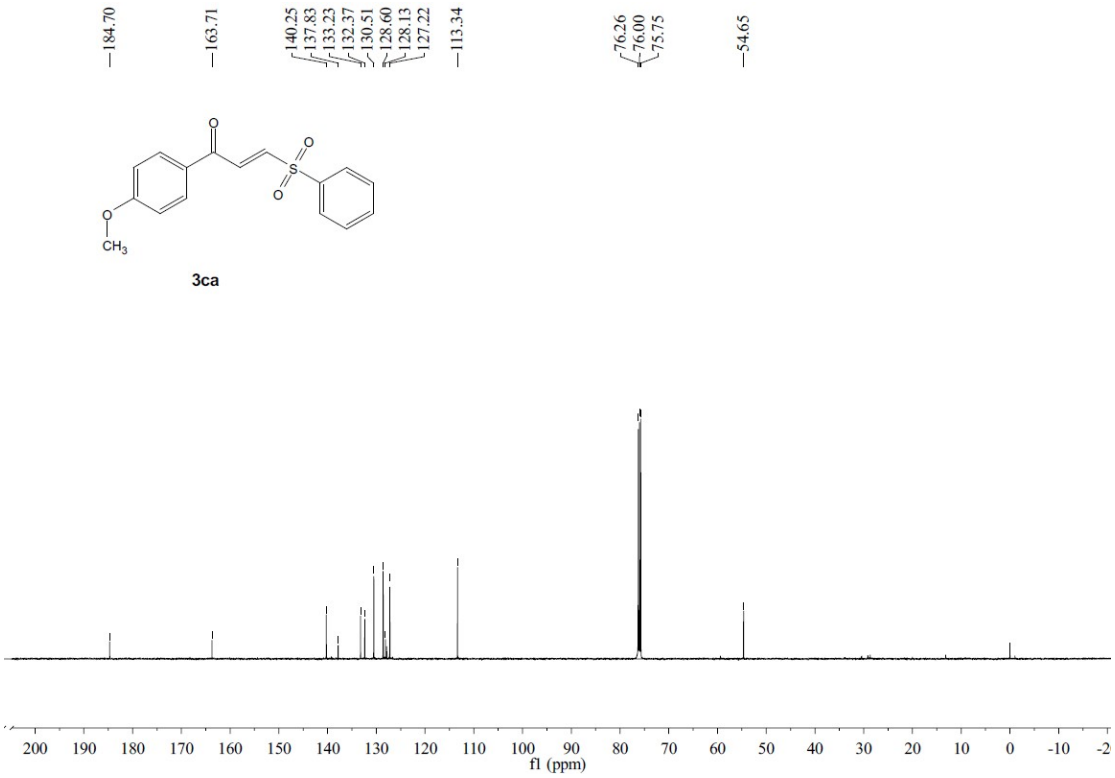
7.85
7.63
7.61
7.60
7.53
7.52
7.50
7.28
7.25
7.19
6.93
6.91
3.83
0.00
O
O
S
O
O
CH3
5.03
1.01
2.01
1.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ca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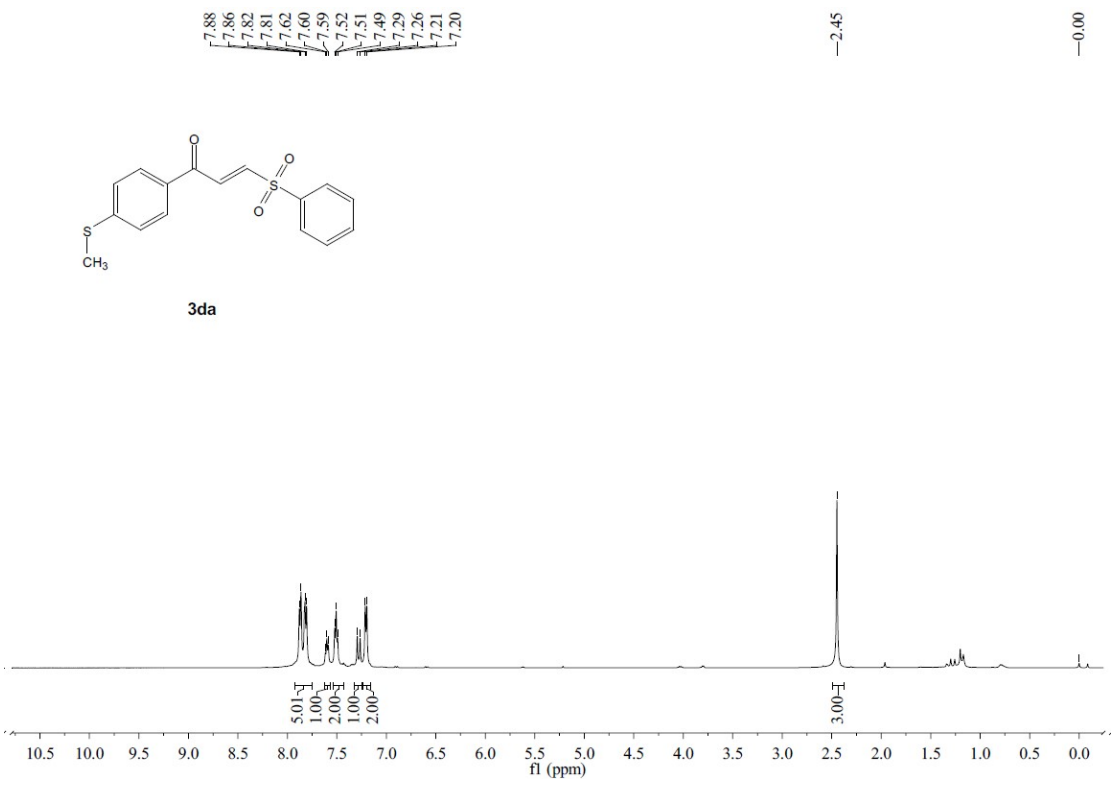
132.37
130.51
128.60
128.13
127.22
113.34
76.26
76.00
75.75
54.65
O
O
S
O
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)

3ca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7.49
7.29
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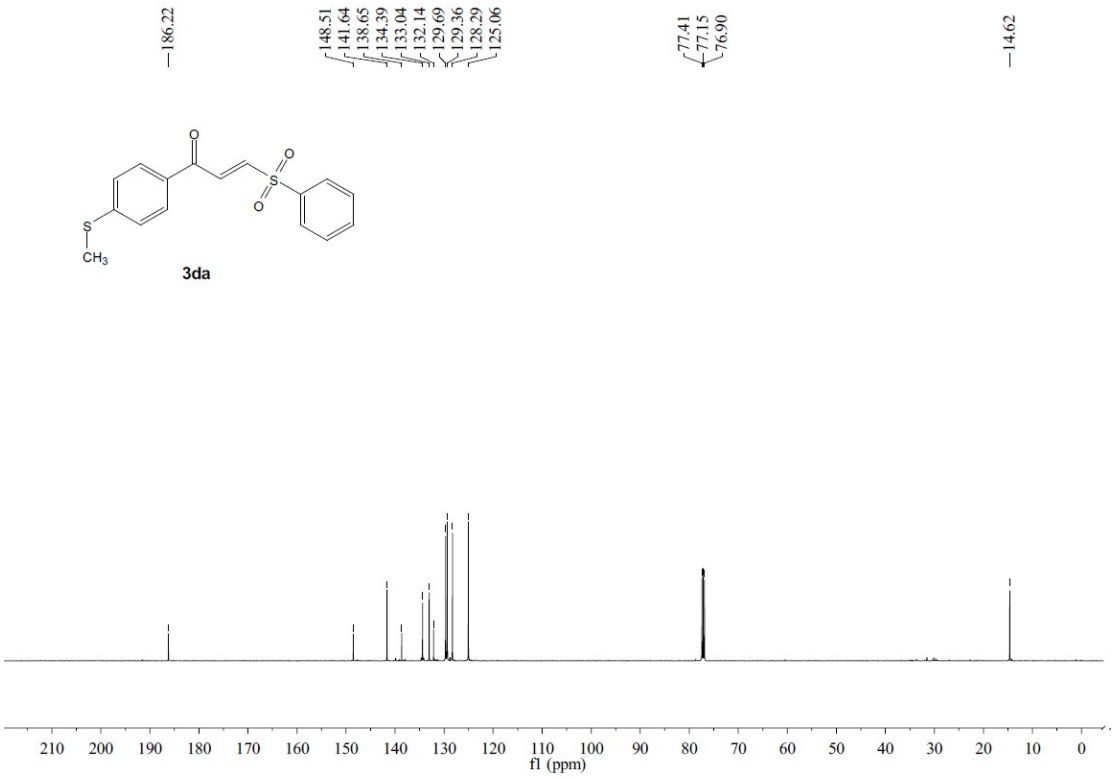
7.21
7.20
2.45
0.00
O
O
S
O
S
CH3
5.01
1.00
2.00
1.00
2.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3da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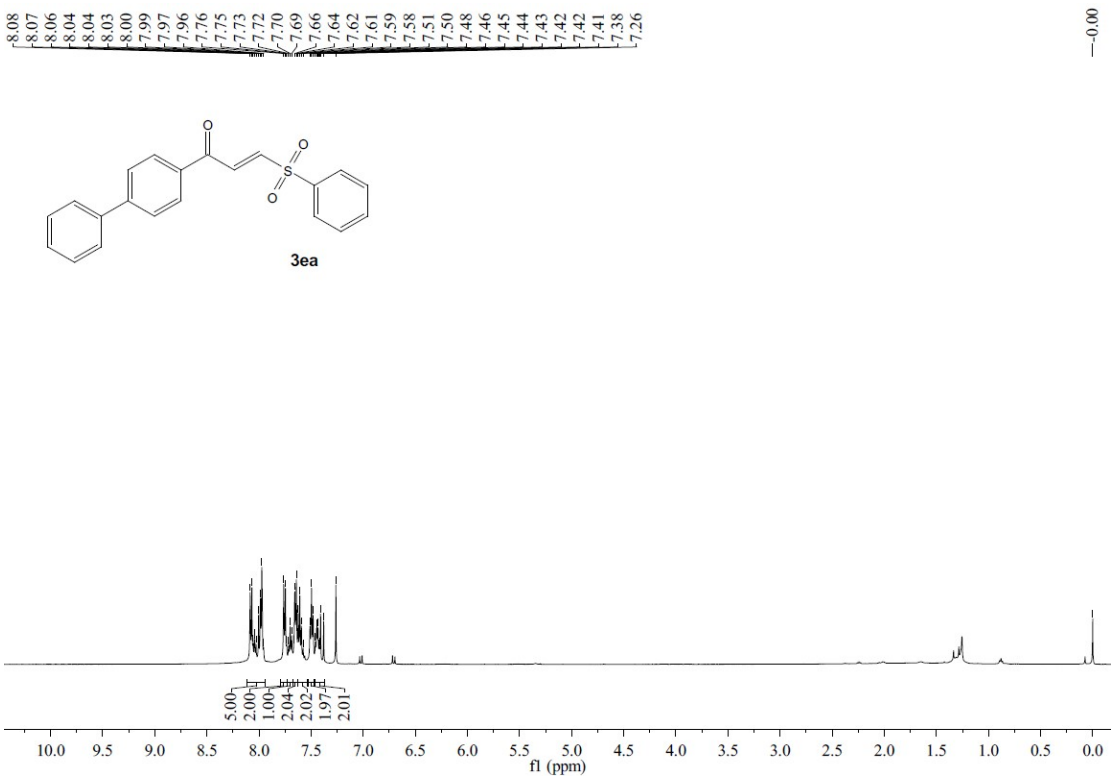
77.15
76.90
14.62
3da
fl (ppm)


8.08
8.07
8.06
8.04
8.04
8.03
8.00
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7.97
7.96
7.76
7.75
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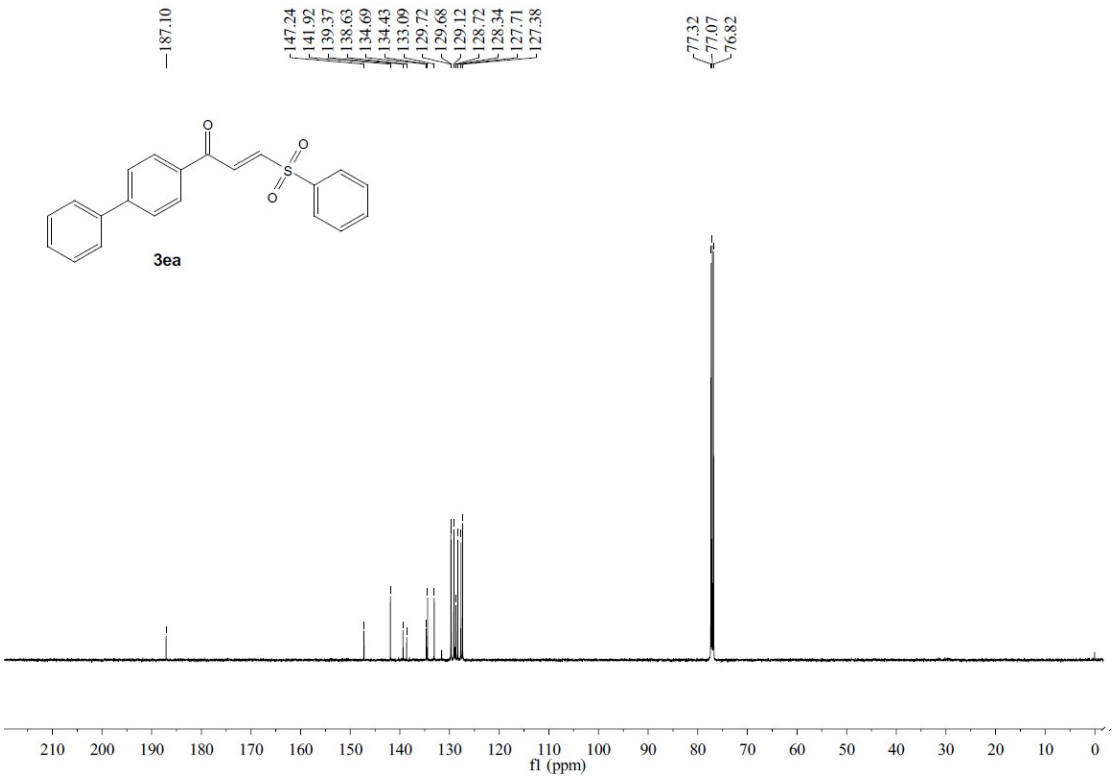
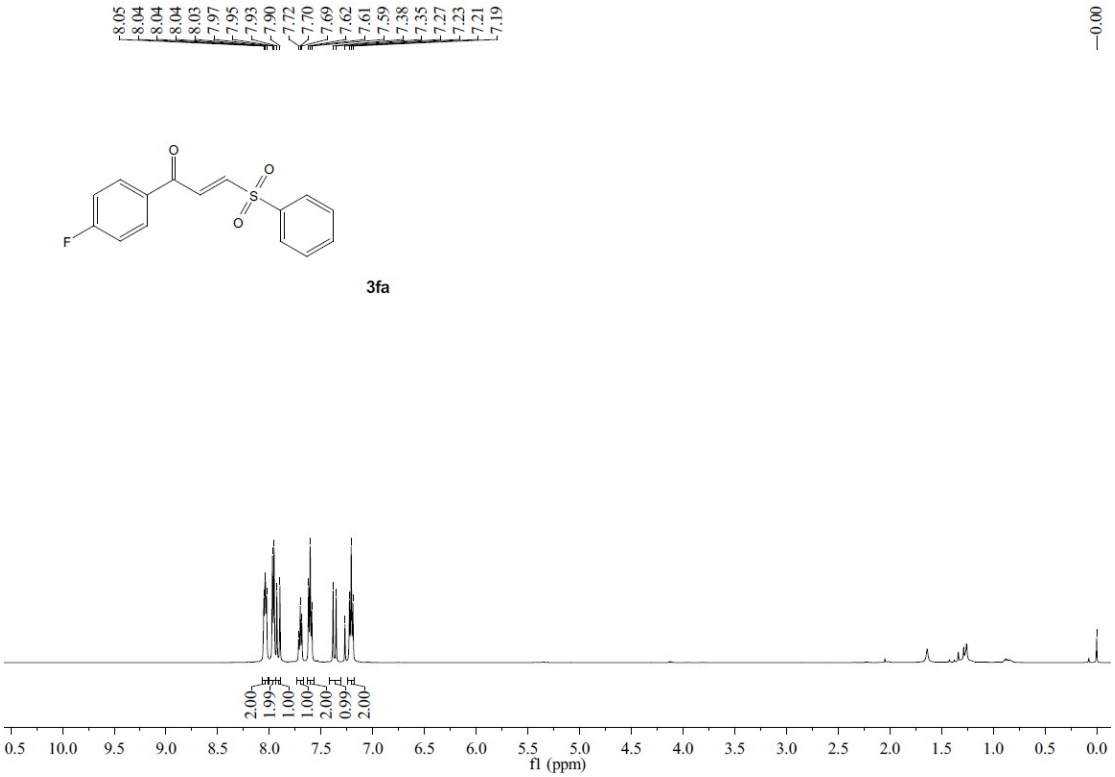
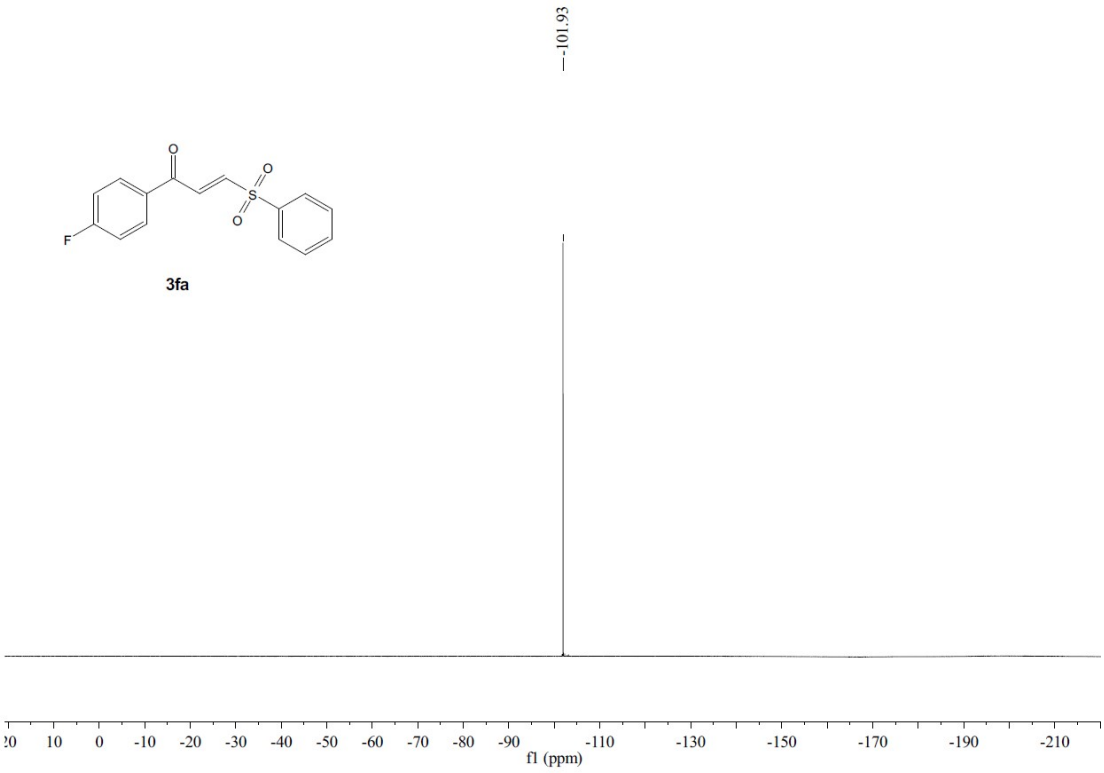
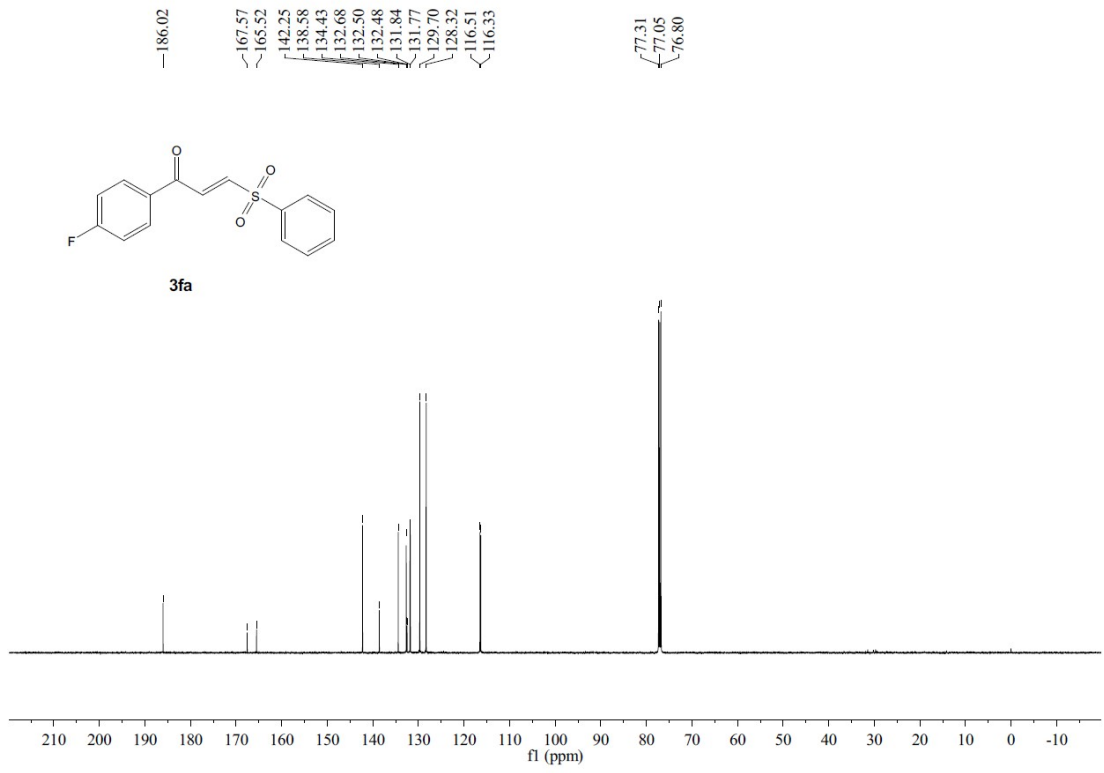
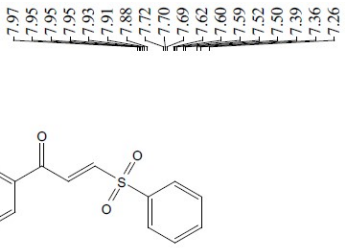
7.72
7.70
7.69
7.66
7.64
7.62
7.61
7.59
7.58
7.51
7.50
7.48
7.46
7.45
7.44
7.43
7.42
7.42
7.41
7.38
7.26
0.00
3ea
5.00
2.00
1.00
2.04
2.02
1.97
2.01
fl (ppm)


187.10
147.24
141.92
139.37
138.63
134.69
134.43
133.09
129.72
129.68
129.12
128.72
128.34
127.71
127.38
77.32
77.07
76.82
3ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

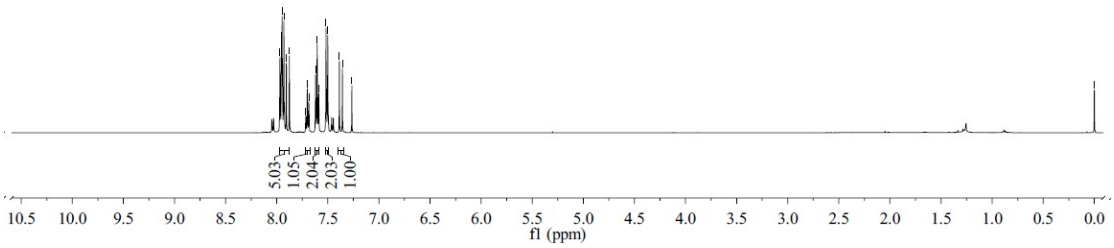

8.05
8.04
8.04
8.04
8.03
7.97
7.95
7.93
7.90
7.72
7.70
7.69
7.62
7.61
7.59
7.38
7.35
7.27
7.23
7.21
7.19
0.00
F
3fa
2.00
1.99
1.00
1.00
2.00
0.99
2.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

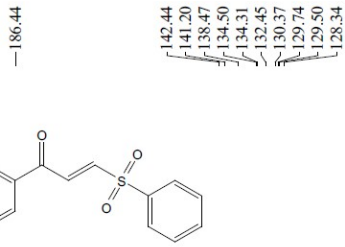

-101.93
3fa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


186.02
167.57
165.52
142.25
138.58
134.43
132.68
132.50
132.48
131.84
131.77
129.70
128.32
116.51
116.33
77.31
77.05
76.80
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

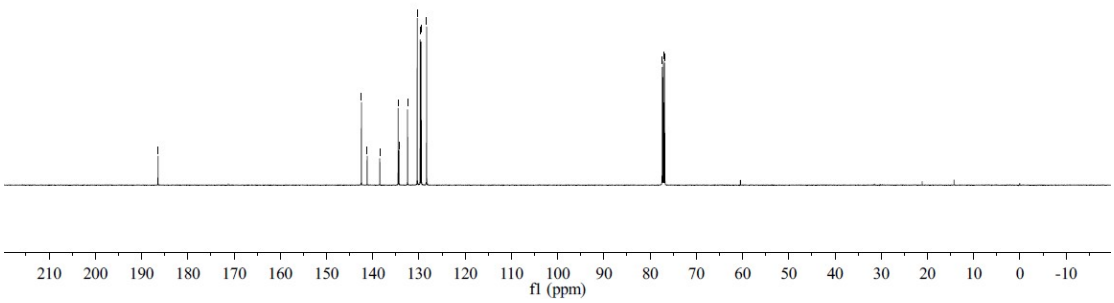

7.97
7.95
7.95
7.95
7.93
7.91
7.88
7.72
7.70
7.69
7.62
7.60
7.59
7.52
7.50
7.39
7.36
7.26
0.00
O
O
S
O
Cl

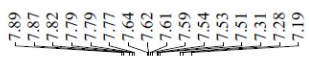
3ga

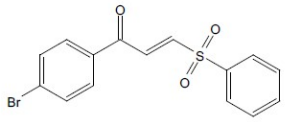

5.03
1.05
2.04
2.03
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


186.44
142.44
141.20
138.47
134.50
134.31
132.45
130.37
129.74
129.50
128.34
77.35
77.10
76.85
O
O
S
O
Cl

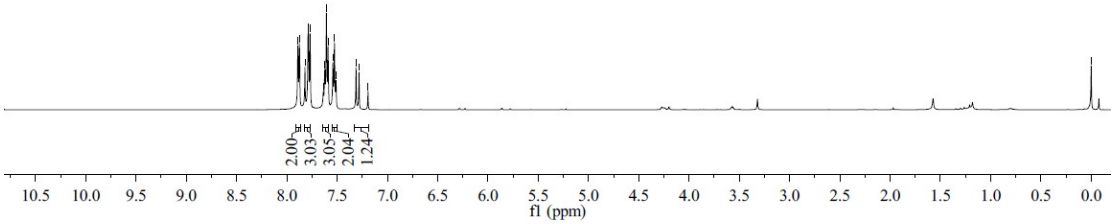
3ga

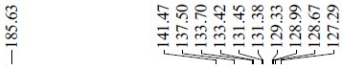

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

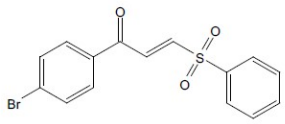

7.89
7.87
7.82
7.79
7.79
7.79
7.77
7.64
7.62
7.61
7.59
7.54
7.53
7.51
7.31
7.28
7.19
0.00


O
O
S
O
Br

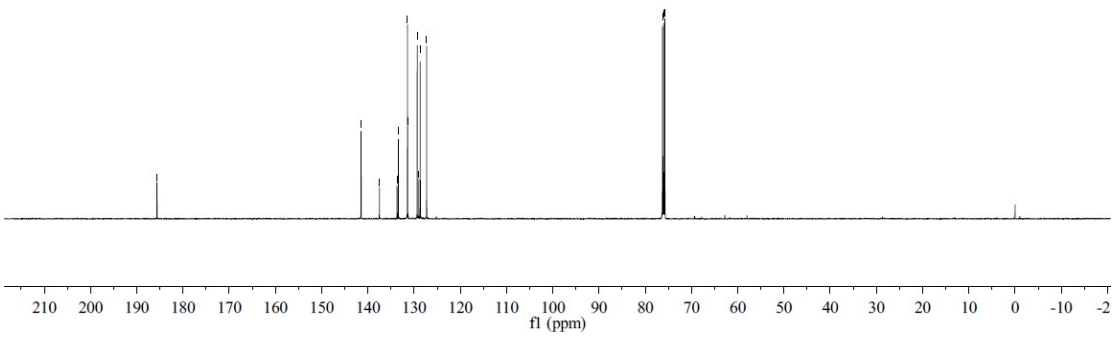
3ha

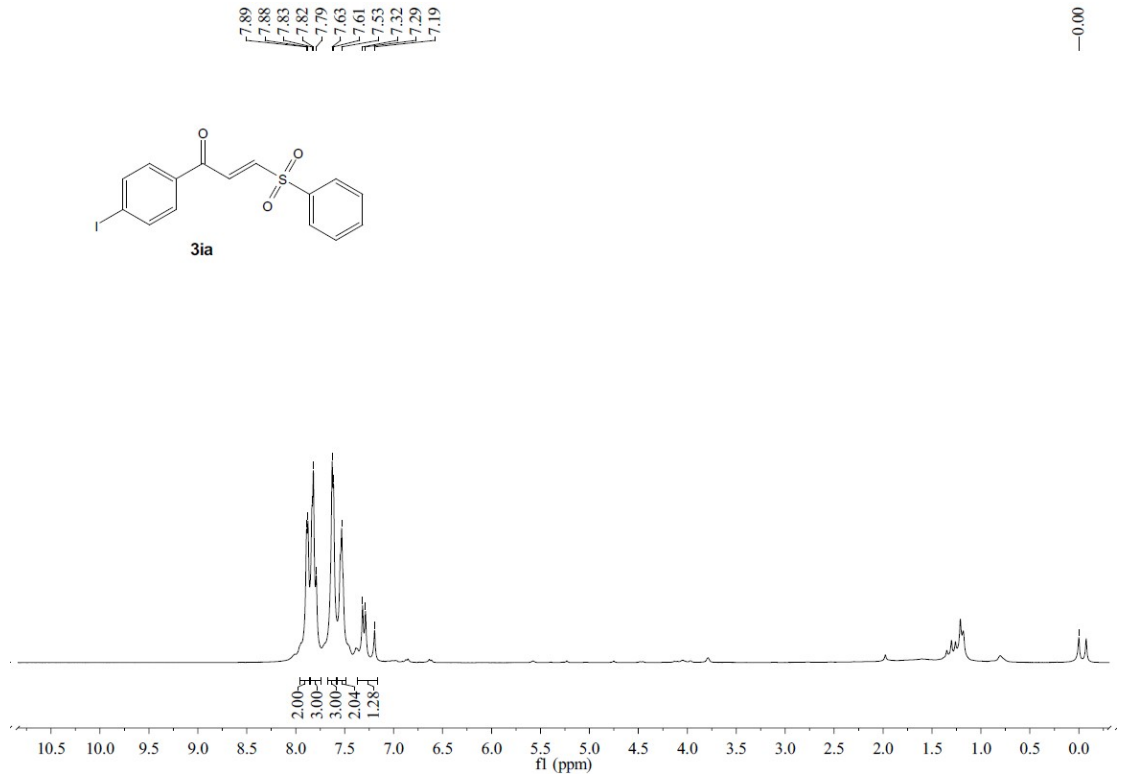

2.00
3.03
3.05
2.04
1.24
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

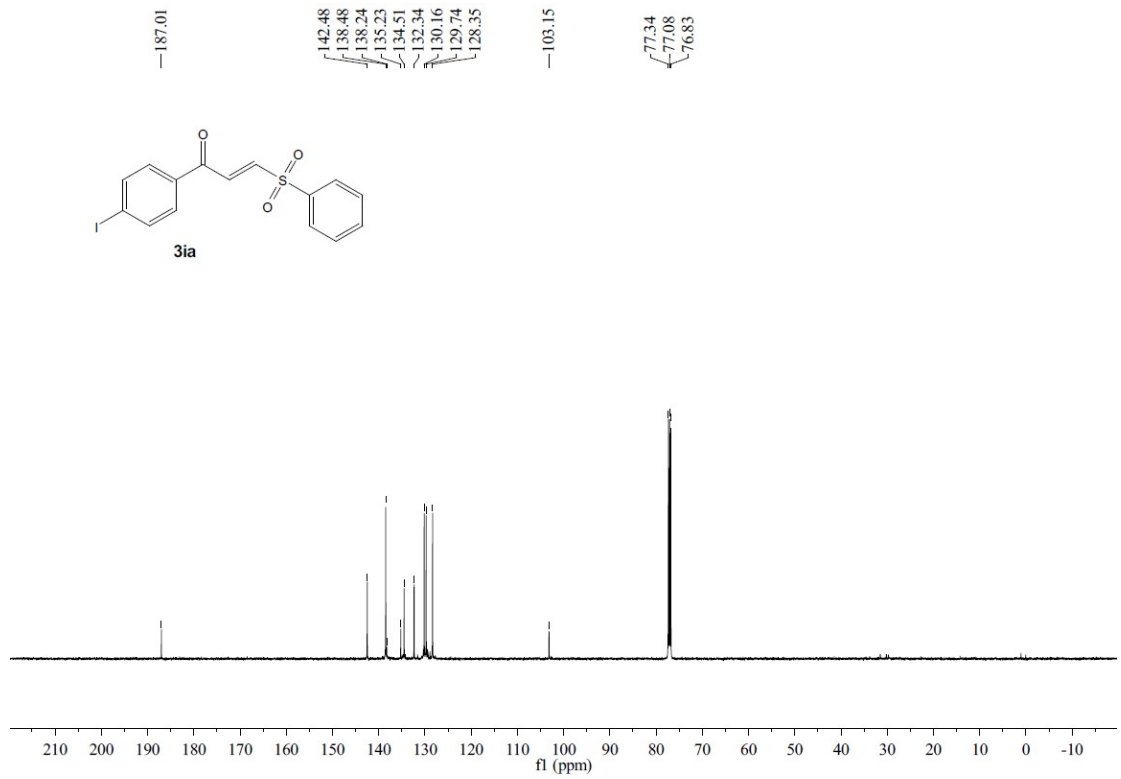

185.63
141.47
137.50
133.70
133.42
131.45
131.38
129.33
128.99
128.67
127.29
76.27
76.02
75.77

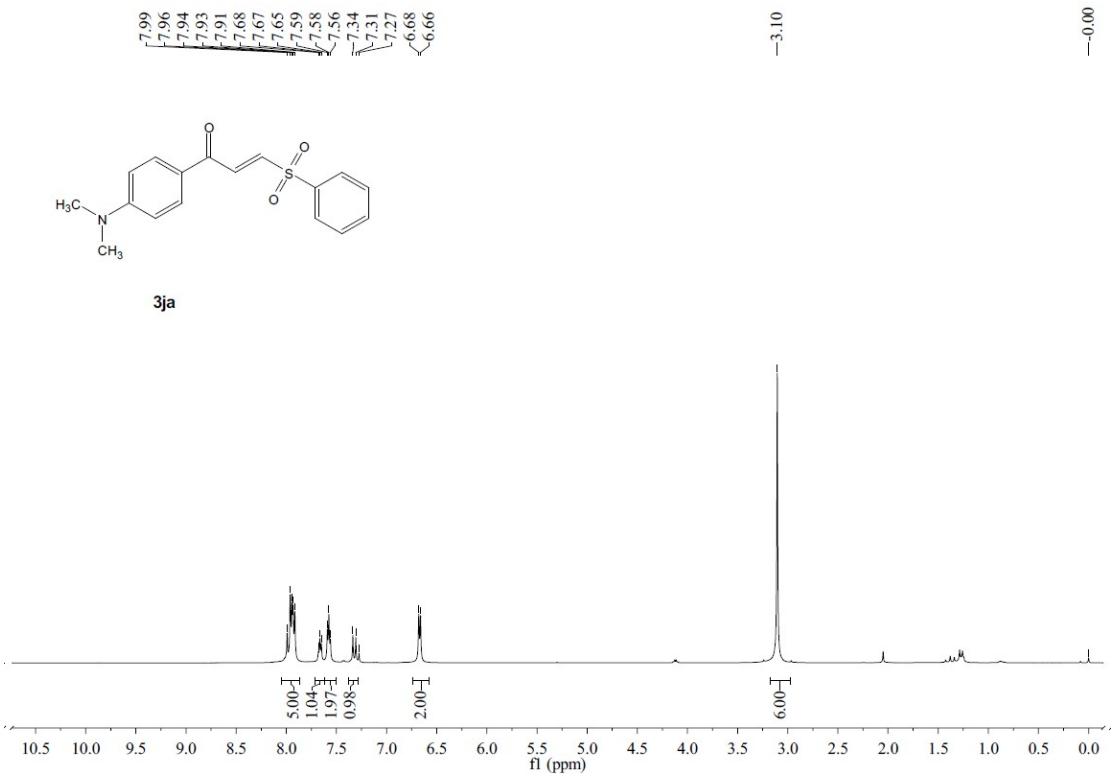

O
O
S
O
Br

3ha

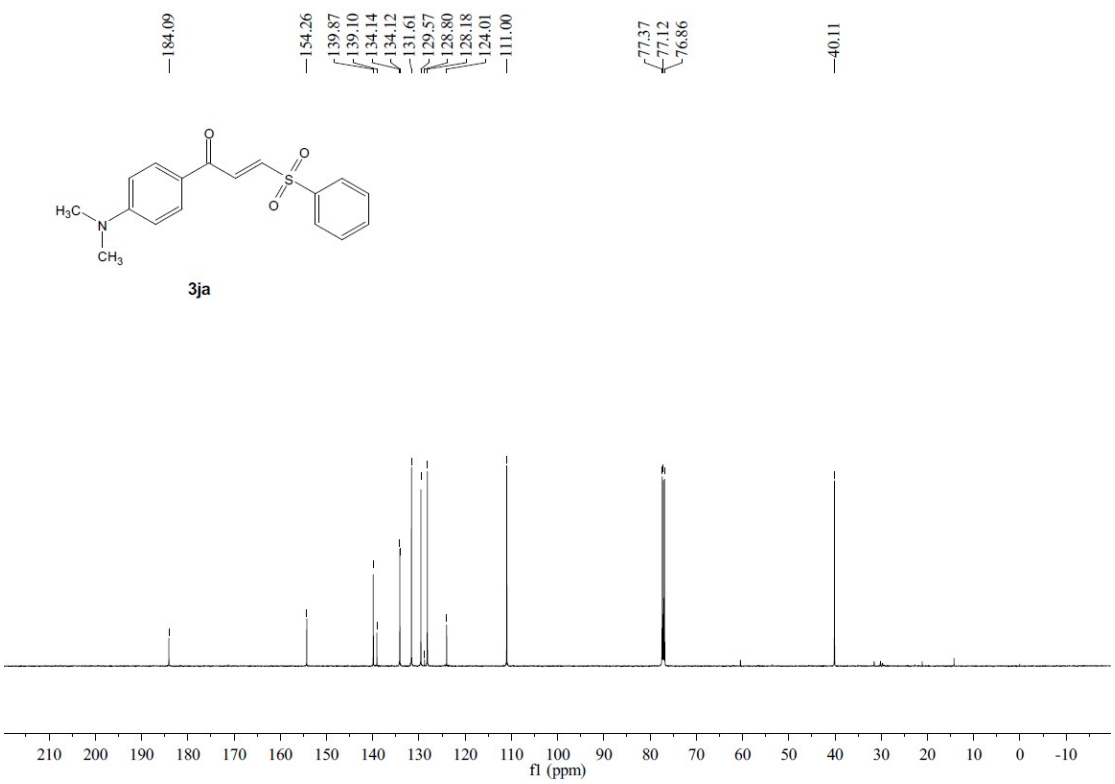

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)


7.89
7.88
7.83
7.82
7.79
7.63
7.61
7.53
7.32
7.29
7.19
0.00
3ia
2.00
3.00
3.00
2.04
1.28
f1 (ppm)

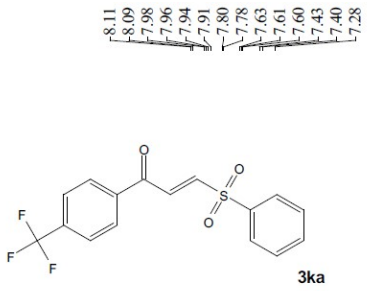

187.01
142.48
138.48
138.24
135.23
134.51
132.34
130.16
129.74
128.35
103.15
77.34
77.08
76.83
3ia
f1 (ppm)


7.99
7.96
7.94
7.93
7.91
7.68
7.67
7.65
7.59
7.58
7.56
7.34
7.31
7.27
6.68
6.66
3.10
0.00
O
O
S
O
H3C
N
CH3
5.00
1.04
1.97
0.98
2.00
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

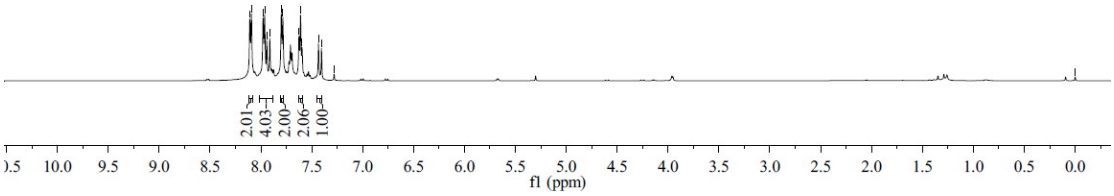
3ja

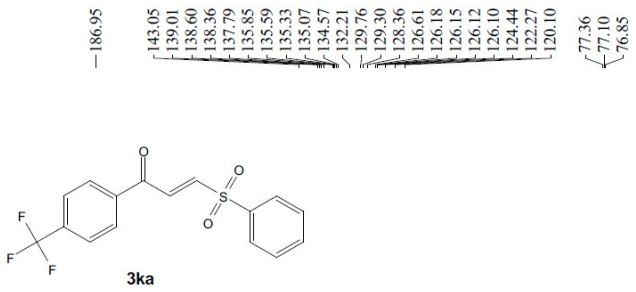

184.09
154.26
139.87
139.10
134.14
134.12
131.61
129.57
128.80
128.18
124.01
111.00
77.37
77.12
76.86
40.11
O
O
S
O
H3C
N
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ja

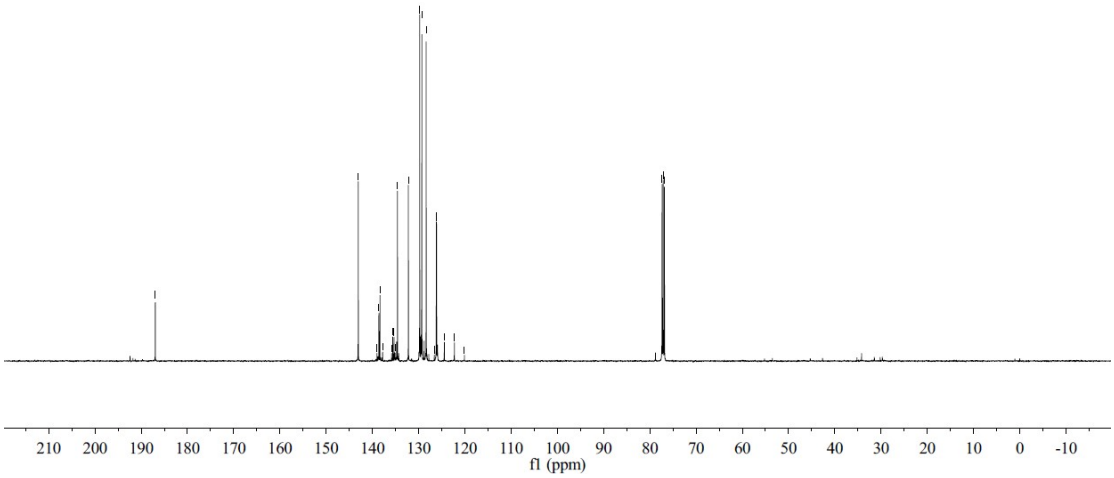

8.11
8.09
7.98
7.96
7.94
7.91
7.80
7.78
7.63
7.61
7.60
7.43
7.40
7.28
0.00
O
O
S
O
F
F
F

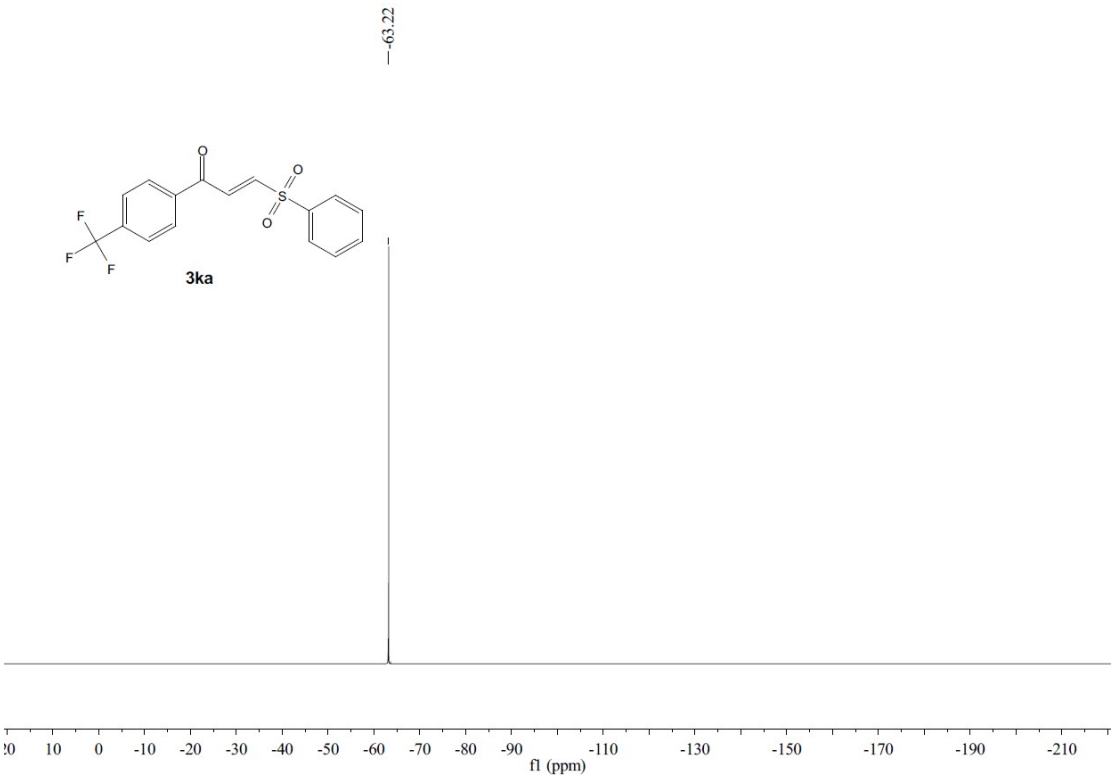
3ka

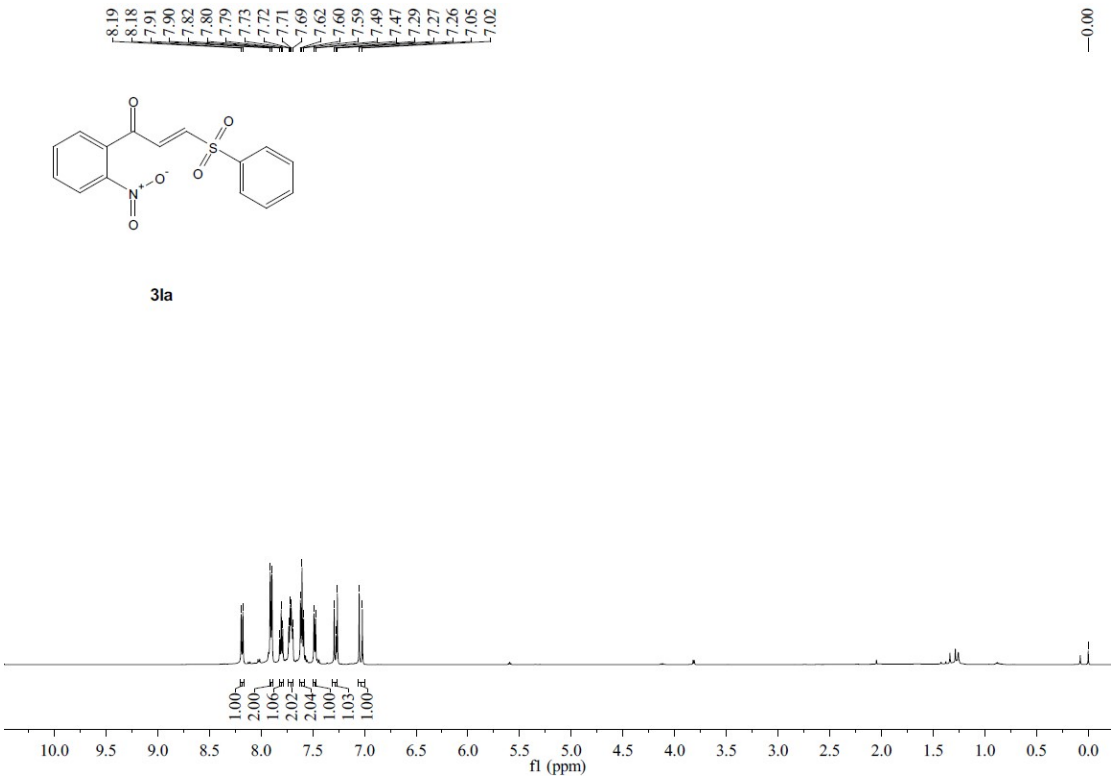

2.01
4.03
2.00
2.06
1.00
f1 (ppm)

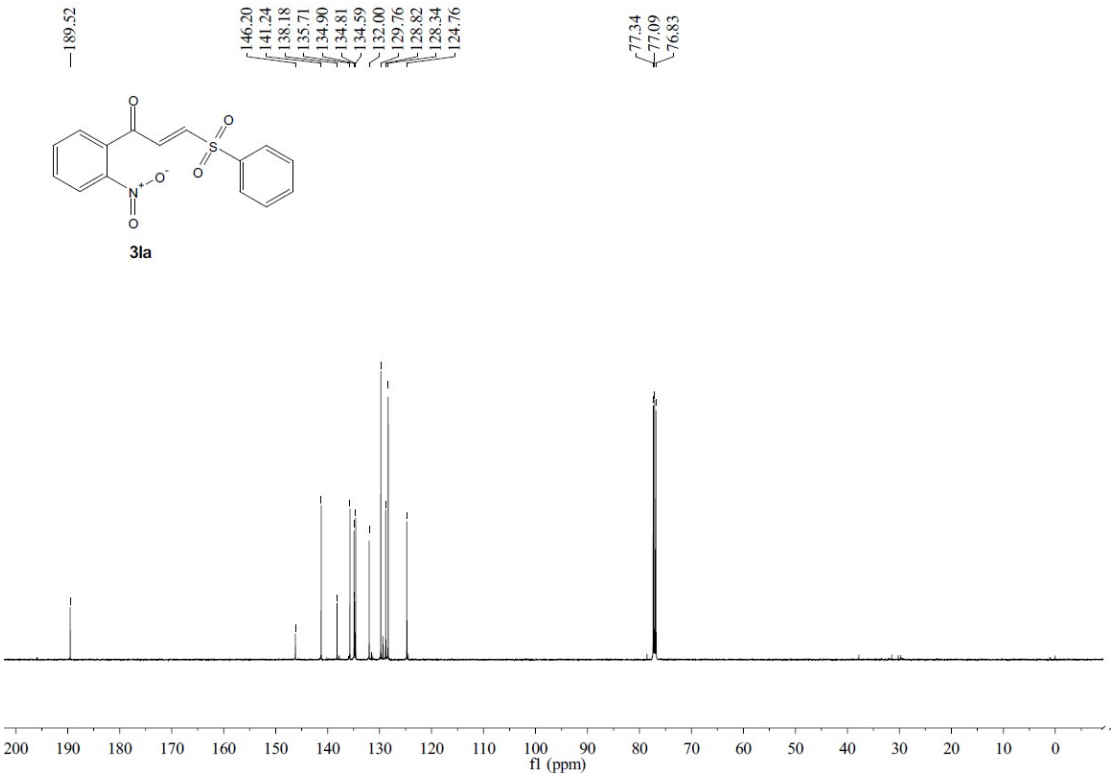

186.95
143.05
139.01
138.60
138.36
137.79
135.85
135.59
135.33
135.07
134.57
132.21
129.76
129.30
128.36
126.61
126.18
126.15
126.12
126.10
124.44
122.27
120.10
77.36
77.10
76.85
O
O
S
O
F
F
F

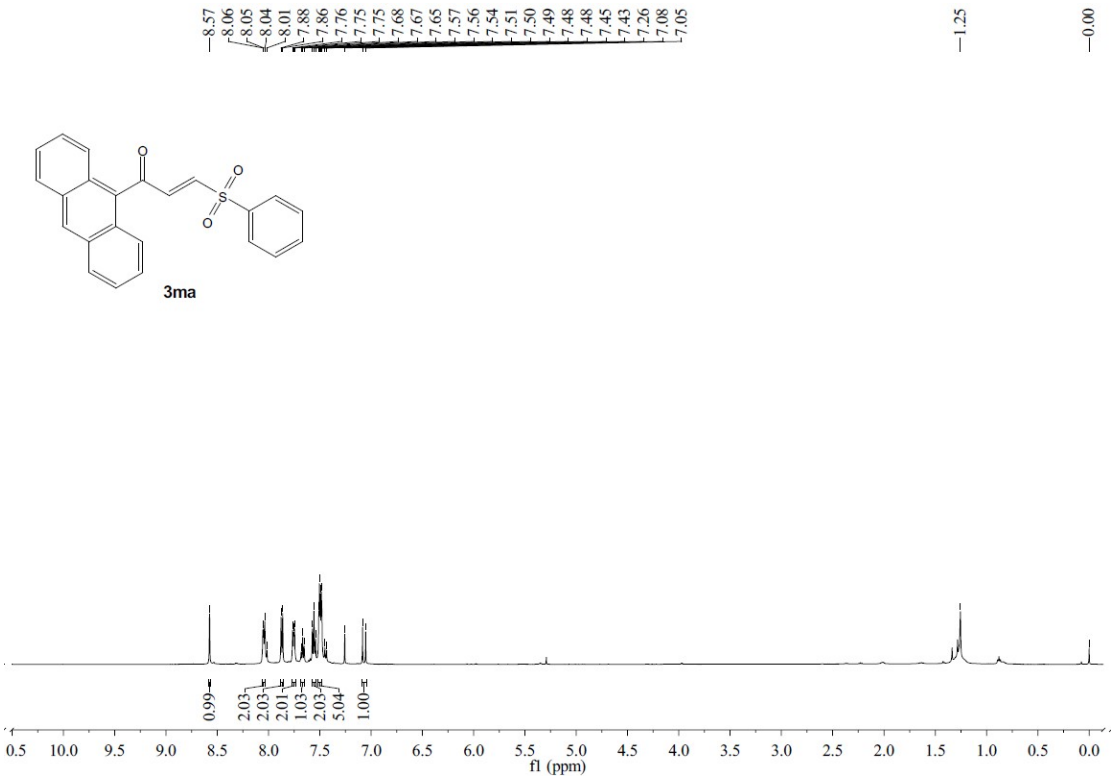
3ka

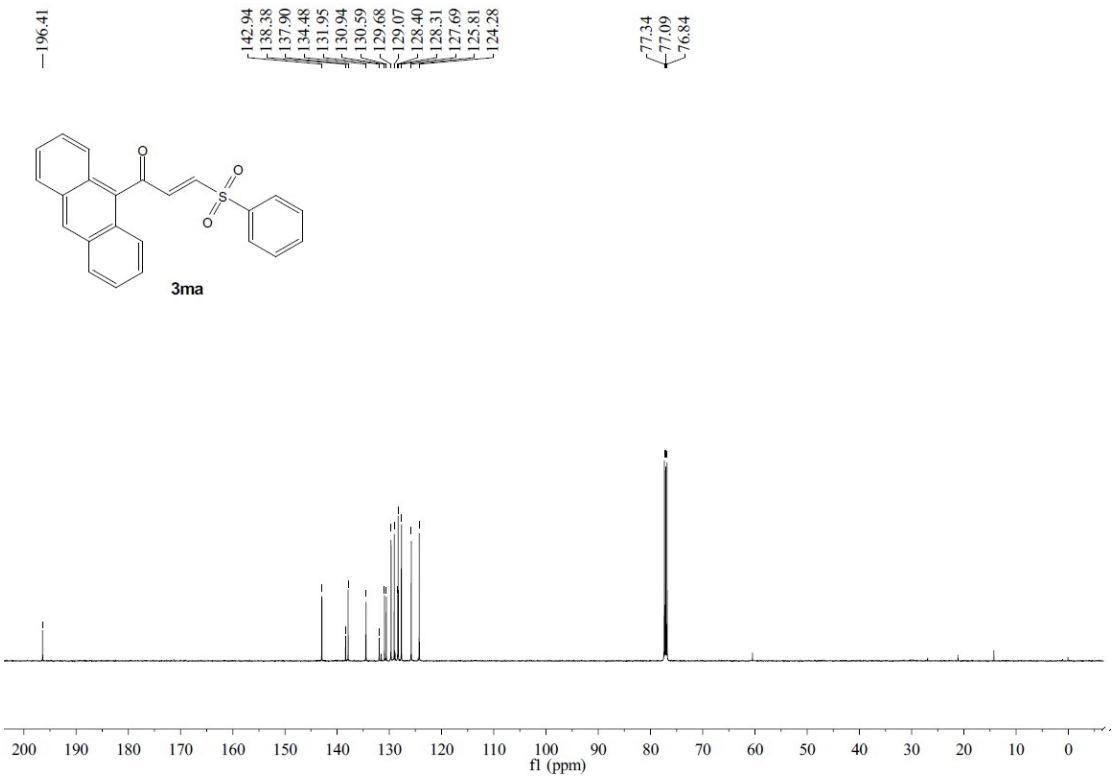

f1 (ppm)


-63.22
3ka
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


8.19
8.18
7.91
7.90
7.82
7.80
7.79
7.73
7.72
7.71
7.69
7.62
7.60
7.59
7.49
7.47
7.29
7.27
7.26
7.05
7.02
0.00
3la
1.00
2.00
1.06
2.02
2.04
1.00
1.03
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


189.52
146.20
141.24
138.18
135.71
134.90
134.81
134.59
132.00
129.76
128.82
128.34
124.76
77.34
77.09
76.83
3la
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.57
8.06
8.05
8.04
8.01
7.88
7.86
7.76
7.75
7.75
7.68
7.67
7.65
7.57
7.56
7.54
7.51
7.50
7.49
7.48
7.48
7.45
7.43
7.26
7.08
7.05
1.25
0.00
3ma
0.99
2.03
2.03
2.01
1.03
2.03
5.04
1.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


196.41
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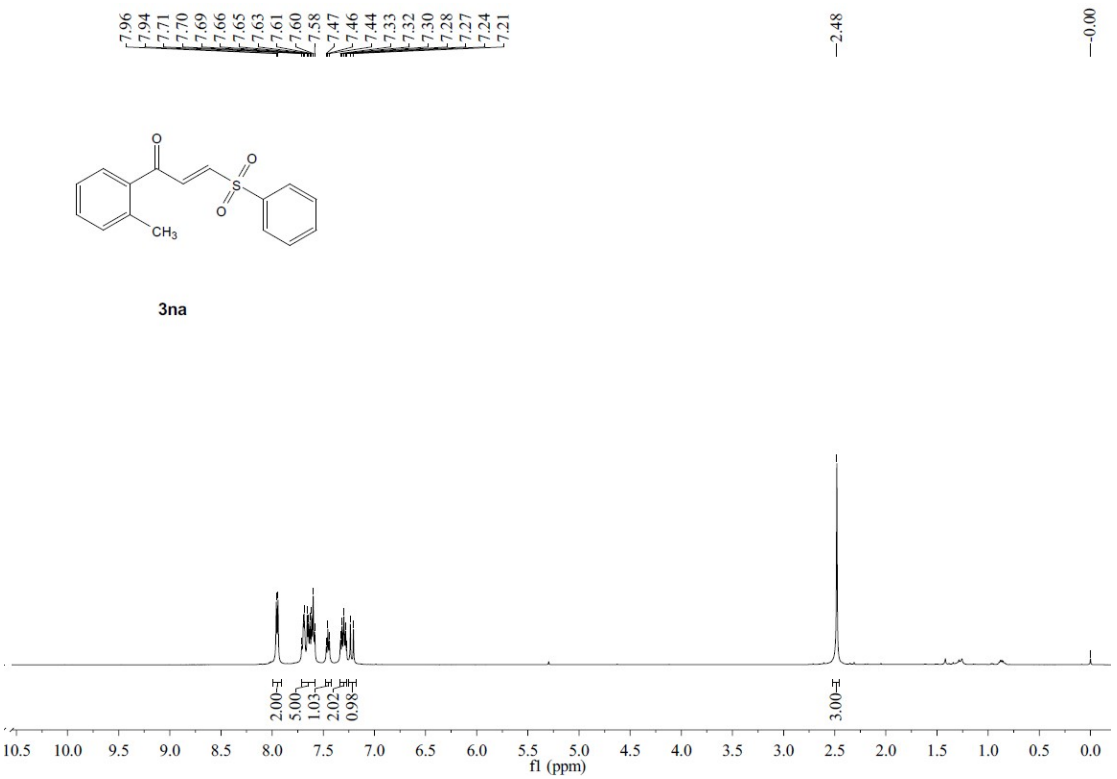
137.90
134.48
131.95
130.94
130.59
129.68
129.07
128.40
128.31
127.69
125.81
124.28
77.34
77.09
76.84
3ma
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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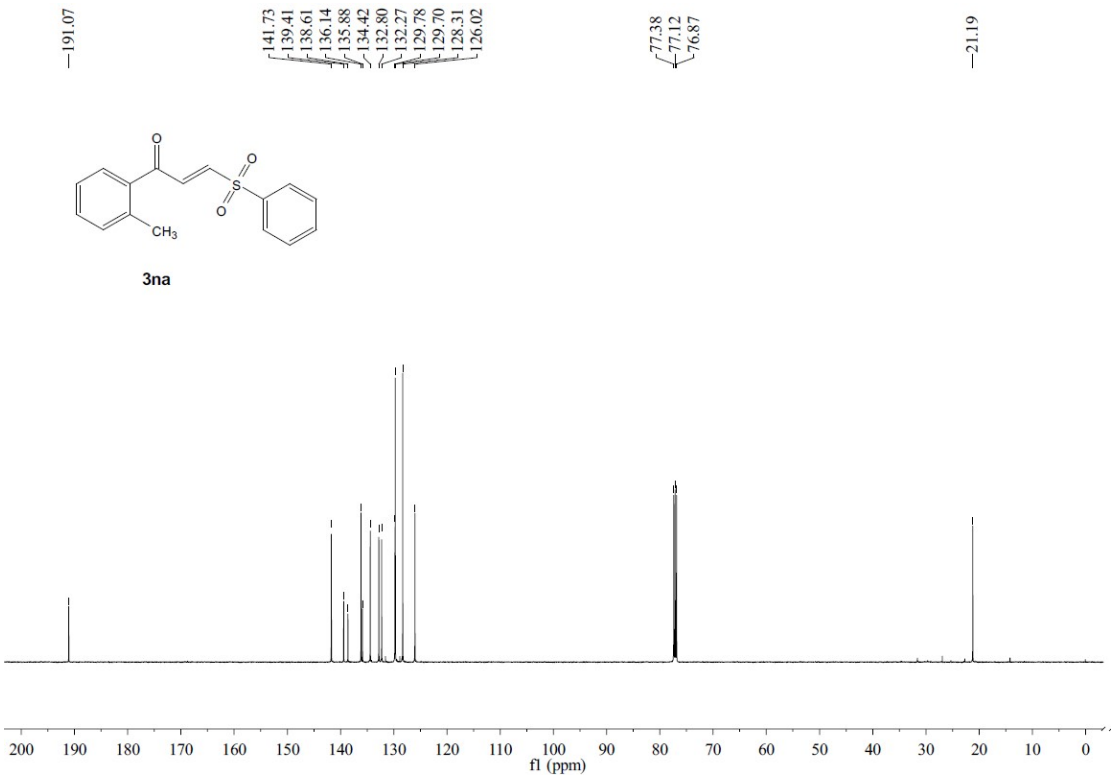
7.70
7.69
7.66
7.65
7.63
7.61
7.60
7.58
7.47
7.46
7.44
7.33
7.32
7.30
7.28
7.27
7.24
7.21
2.48
0.00
CH3
3na
2.00
5.00
1.03
2.02
0.98
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


191.07
141.73
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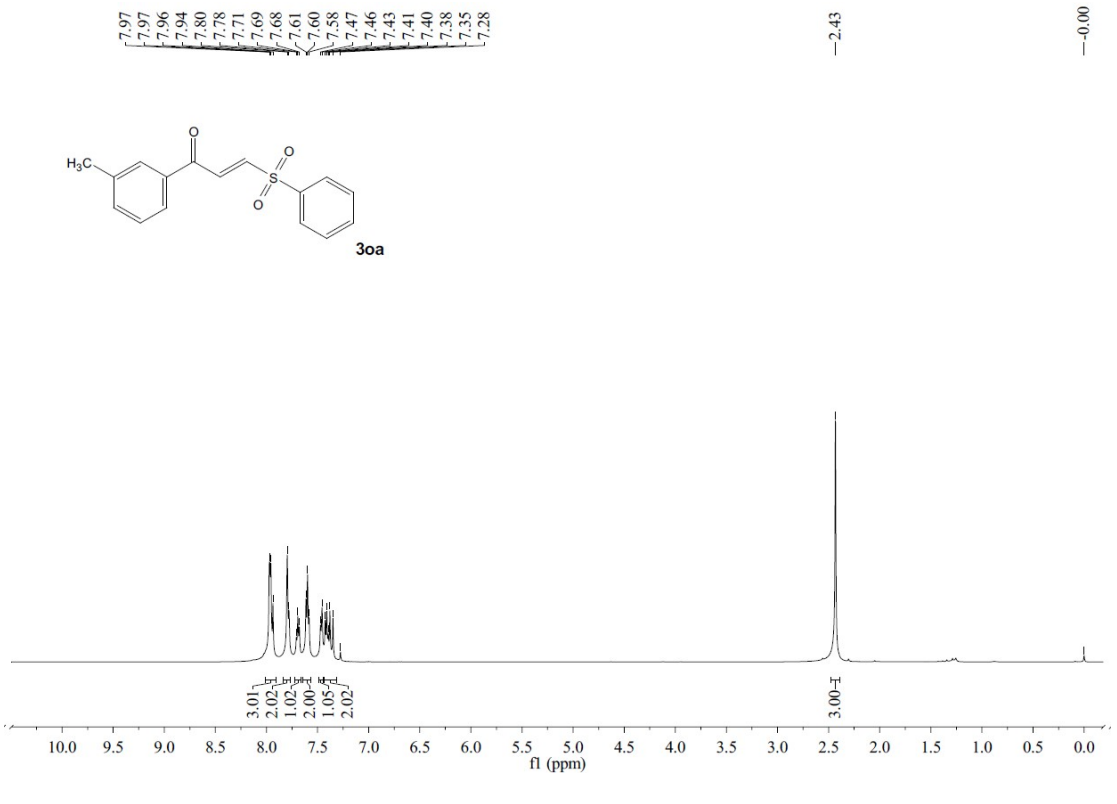
135.88
134.42
132.80
132.27
129.78
129.70
128.31
126.02
77.38
77.12
76.87
21.19
O
O
S
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3na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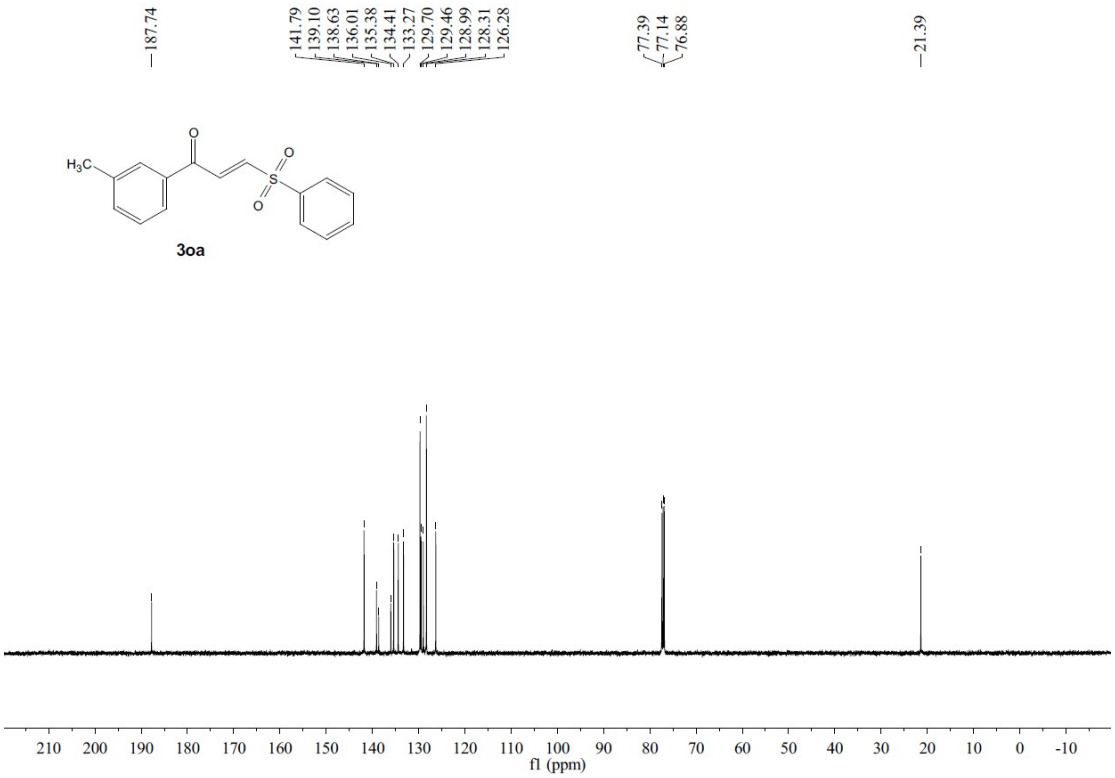
7.97
7.96
7.94
7.80
7.78
7.71
7.69
7.68
7.61
7.60
7.58
7.47
7.46
7.43
7.41
7.40
7.38
7.35
7.28
2.43
0.00
H3C
O
O
S
O
3.01
2.02
1.02
2.00
1.05
2.02
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3oa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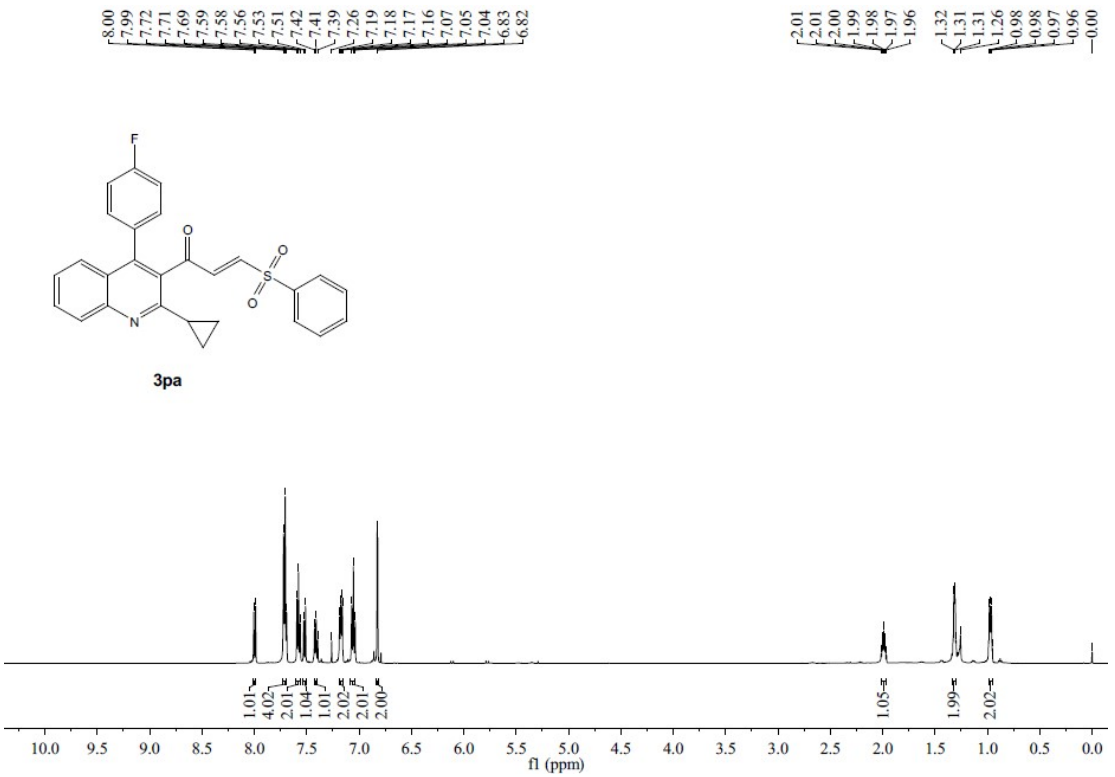
134.41
133.27
129.70
129.46
128.99
128.31
126.28
77.39
77.14
76.88
21.39
H3C
O
O
S
O
3oa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.00
7.99
7.72
7.71
7.69
7.59
7.58
7.56
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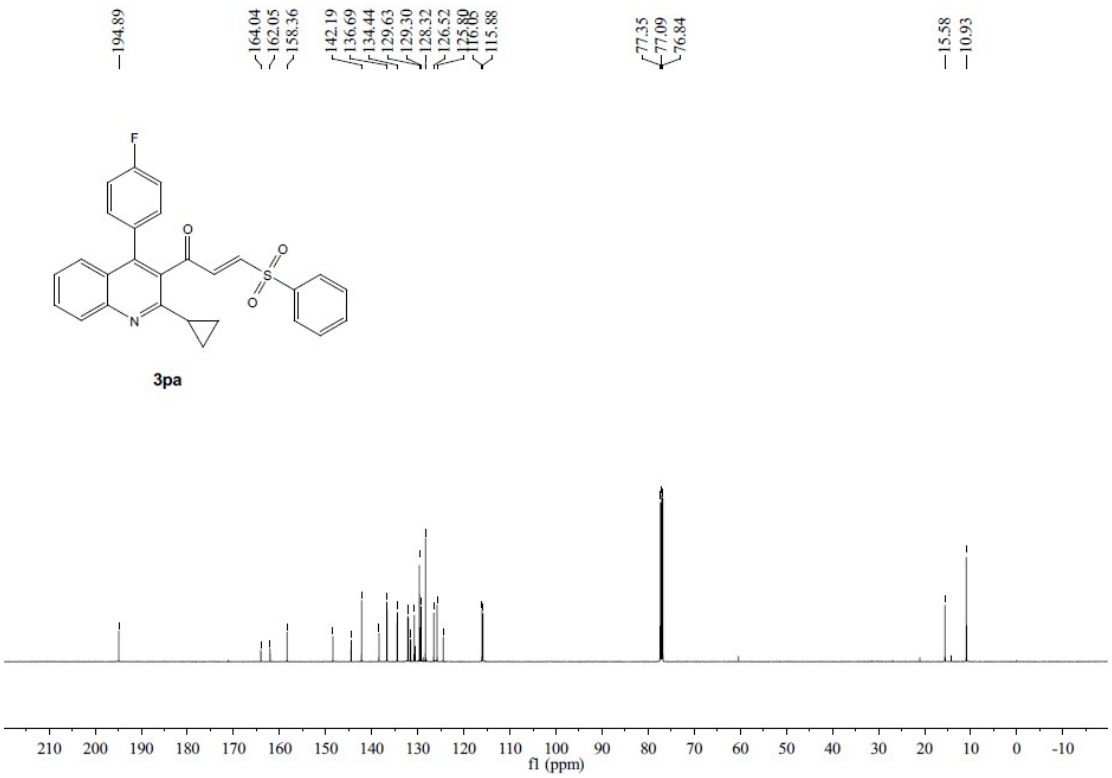
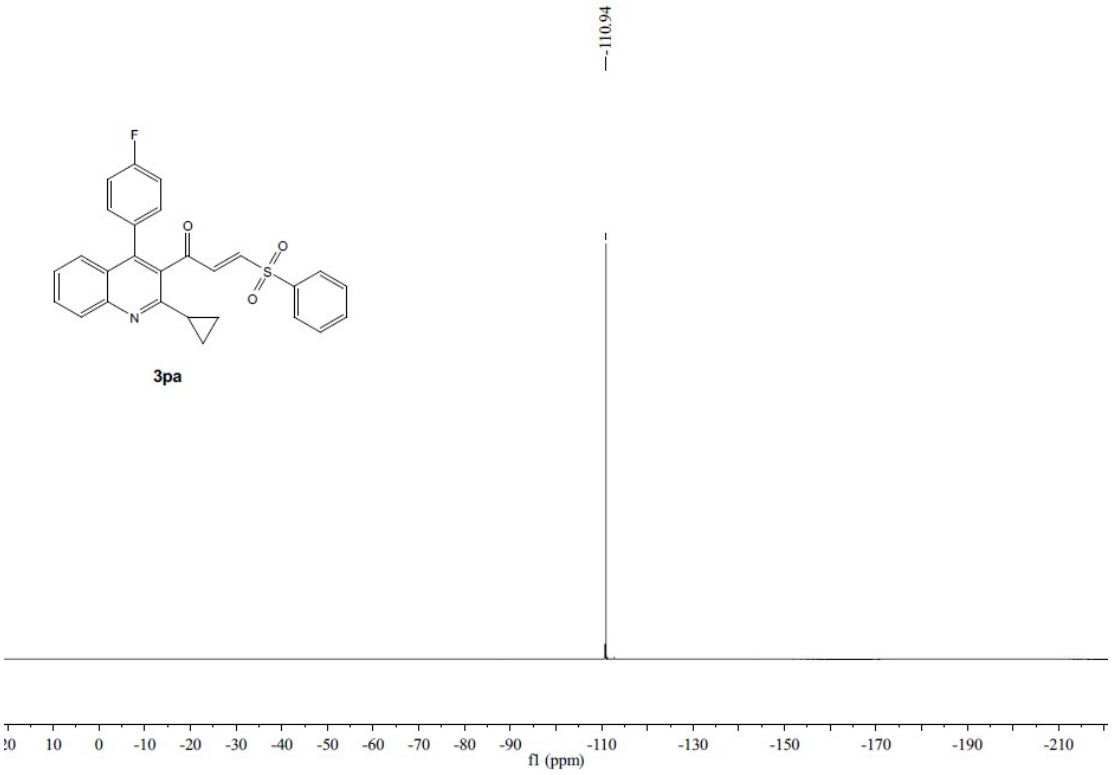
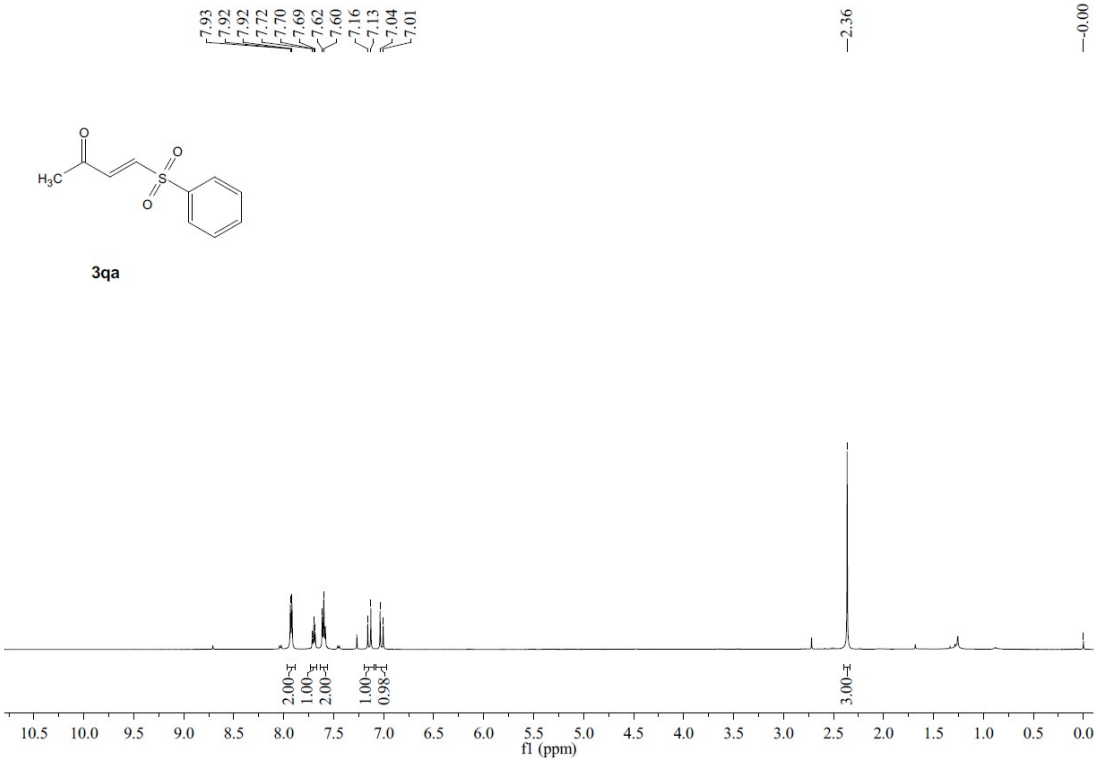
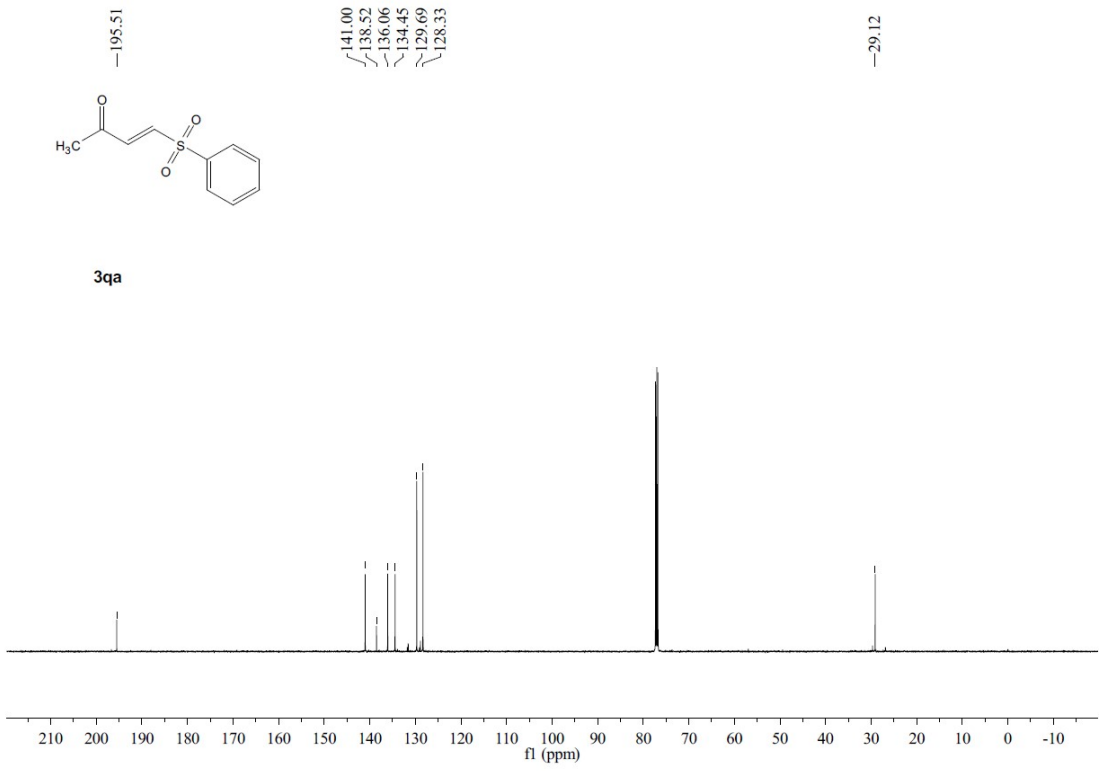
7.51
7.42
7.41
7.39
7.26
7.19
7.18
7.17
7.16
7.07
7.05
7.04
6.83
6.82
2.01
2.01
2.00
1.99
1.98
1.97
1.96
1.32
1.31
1.31
1.26
0.98
0.98
0.97
0.96
0.00
F
O
O
S
O
N
3pa
1.01
4.02
2.01
1.04
1.01
2.02
2.01
2.00
1.05
1.99
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.89
164.04
162.05
158.36
142.19
136.69
134.44
129.63
129.30
128.32
126.52
125.89
116.08
115.88
77.35
77.09
76.84
15.58
10.93
F
O
O
O
S
N
3pa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

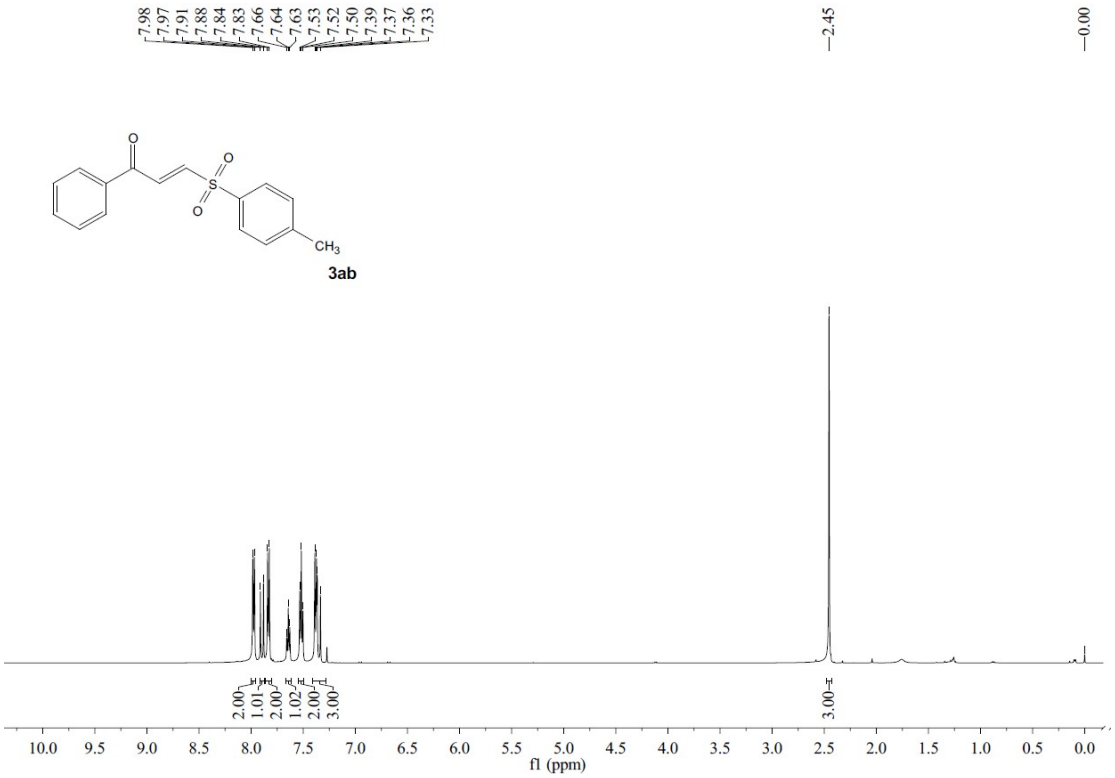

-110.94
F
O
O
O
S
N
3pa
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

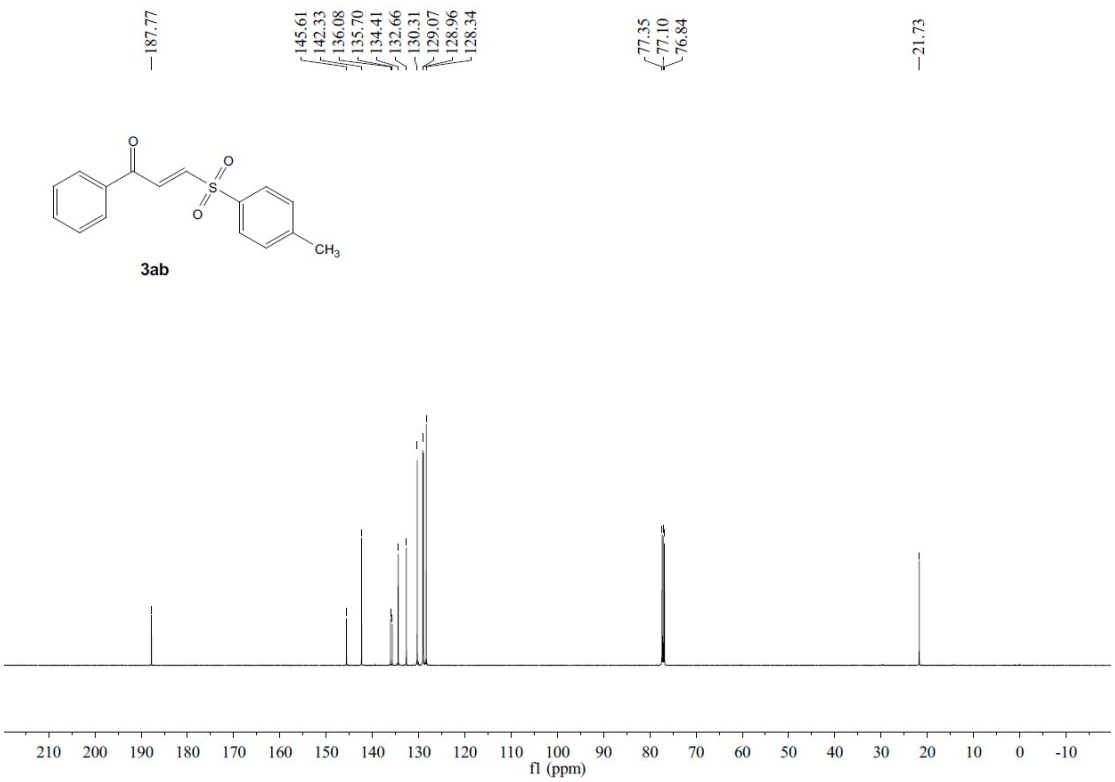

7.93
7.92
7.92
7.72
7.70
7.69
7.62
7.60
7.16
7.13
7.04
7.01
2.36
0.00
2.00
1.00
2.00
1.00
0.98
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

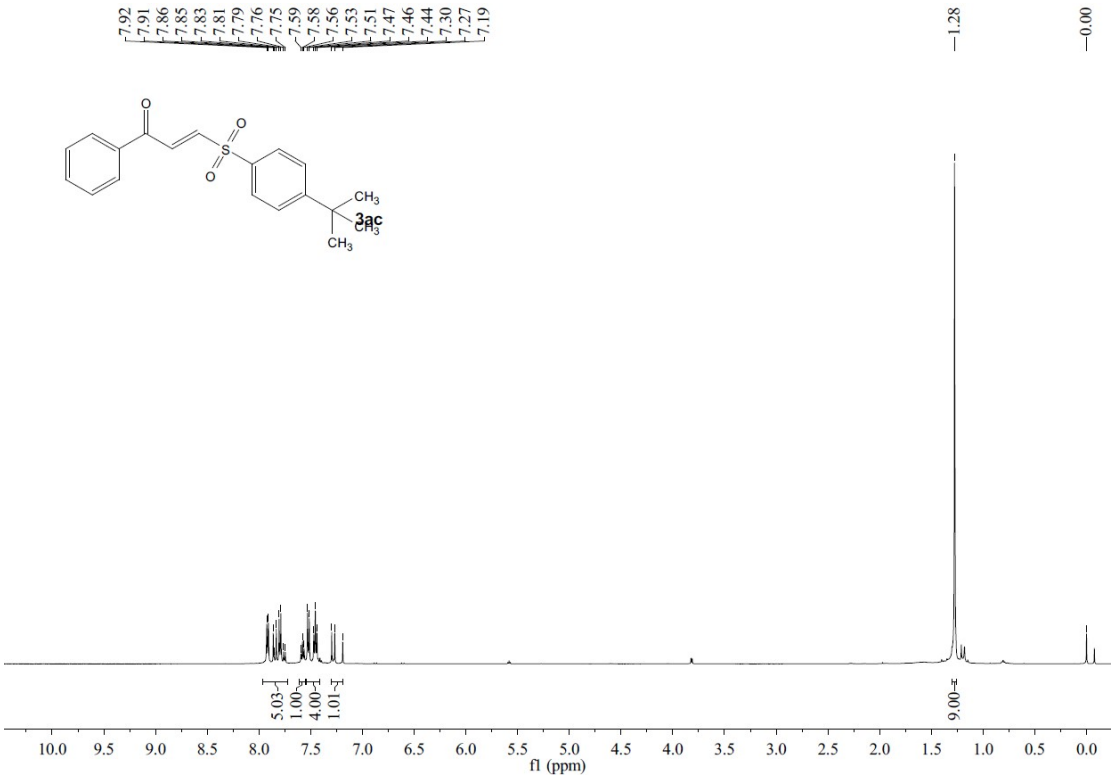
3qa

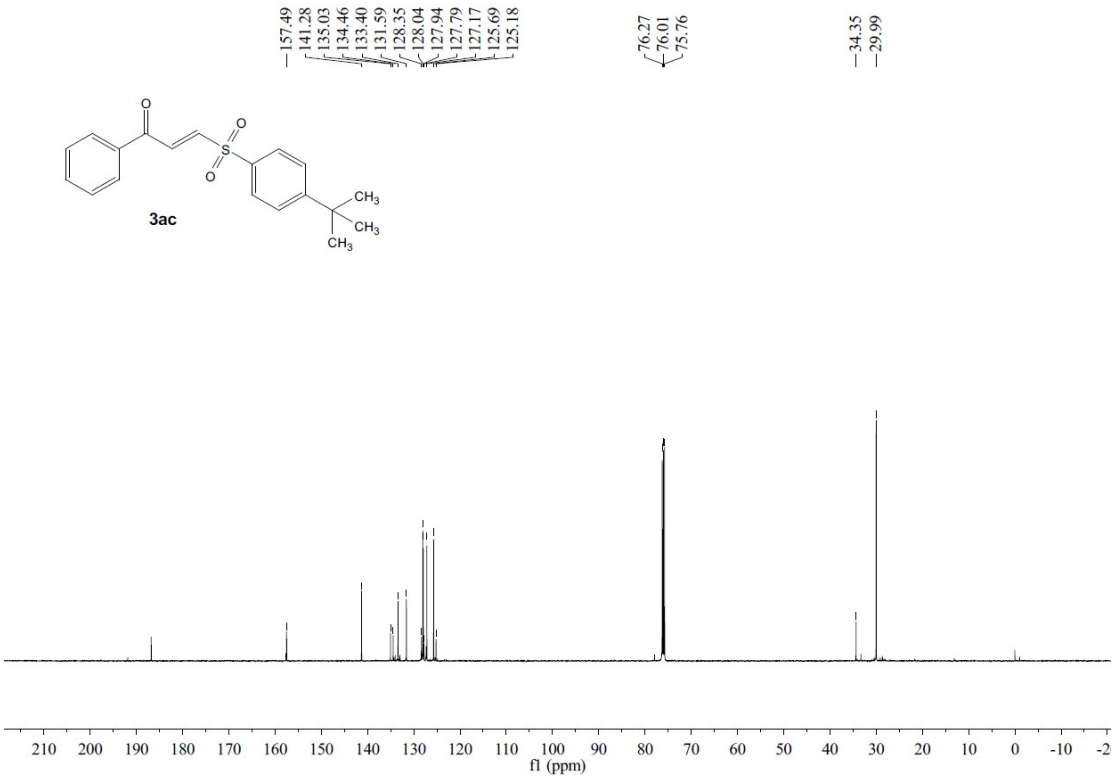

195.51
141.00
138.52
136.06
134.45
129.69
128.33
29.12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

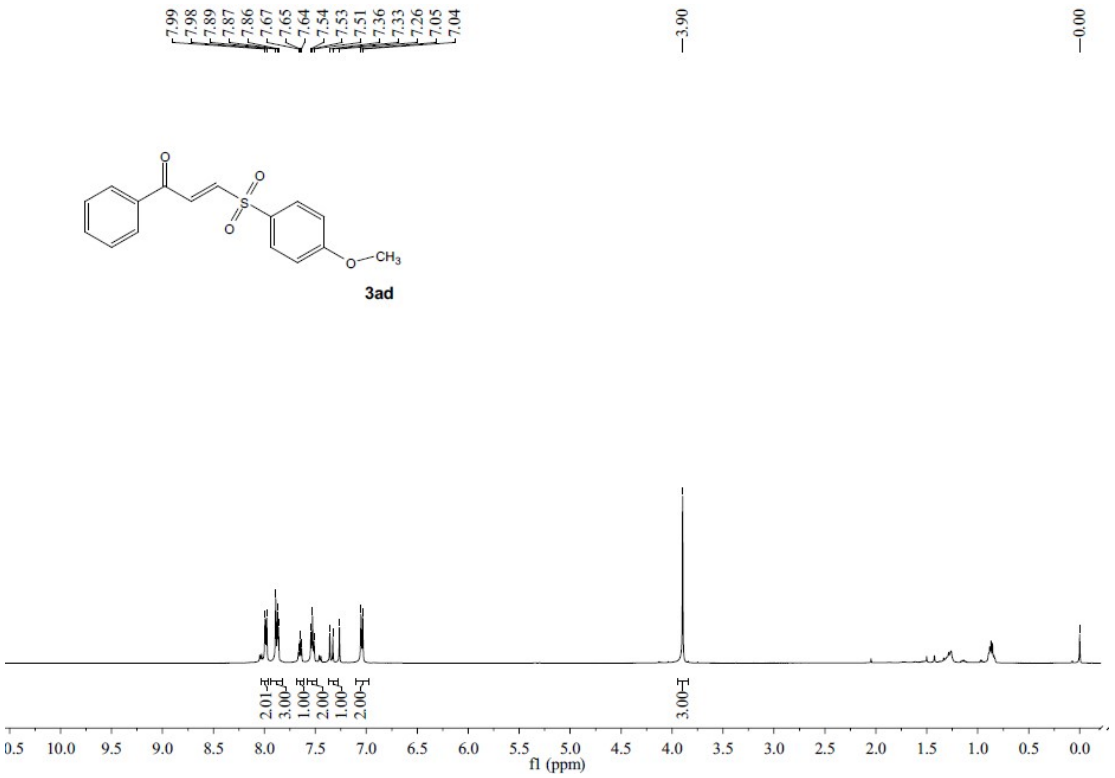
3qa

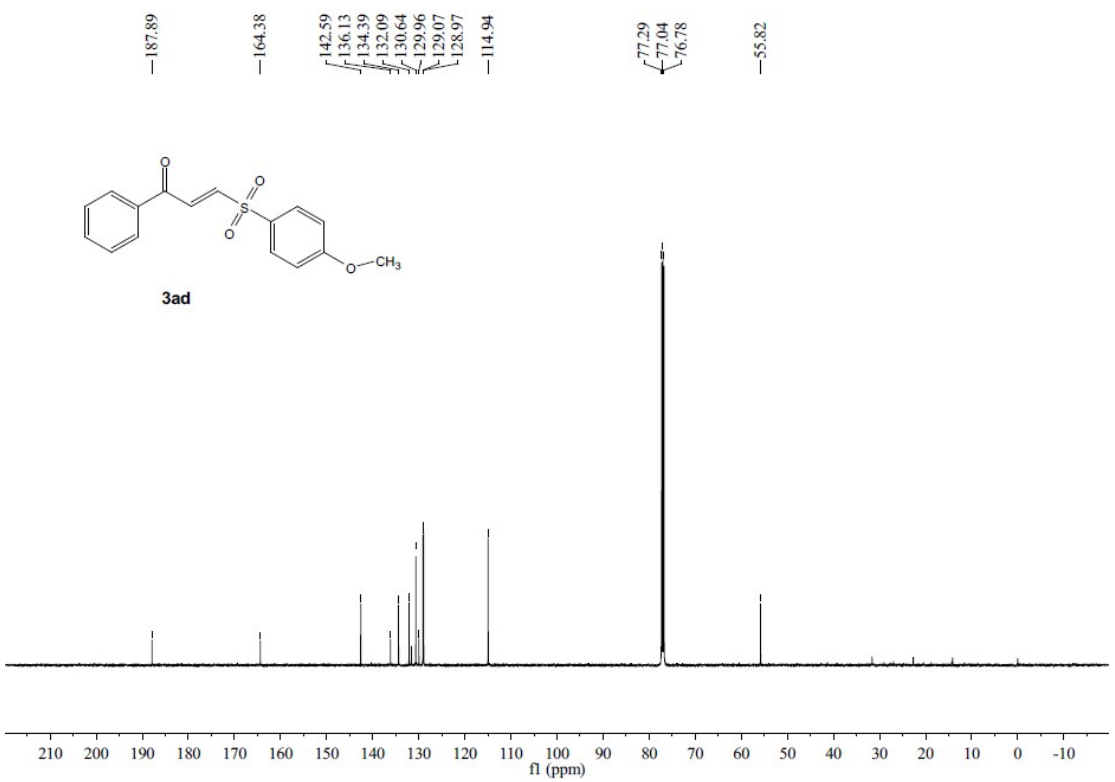

7.98
7.97
7.91
7.88
7.84
7.83
7.66
7.64
7.63
7.53
7.52
7.50
7.39
7.37
7.36
7.33
2.45
0.00
3ab
2.00
1.01
2.00
1.02
2.00
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

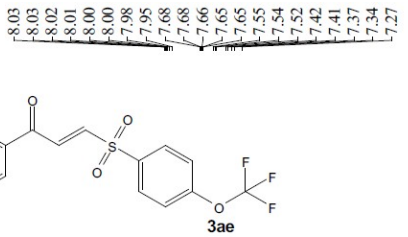

187.77
145.61
142.33
136.08
135.70
134.41
132.66
130.31
129.07
128.96
128.34
77.35
77.10
76.84
21.73
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

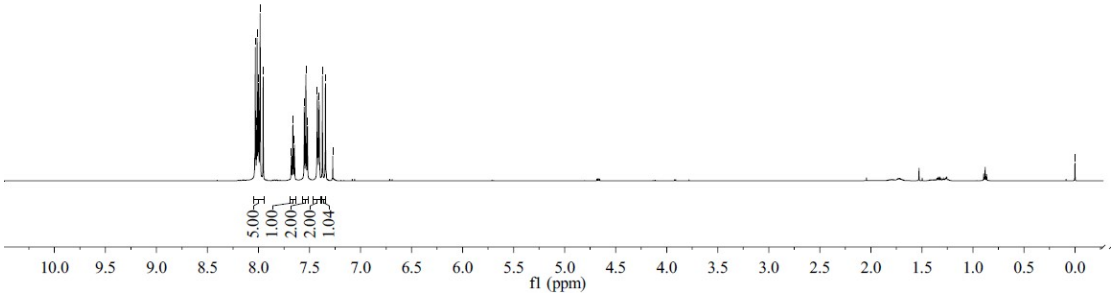

7.92
7.91
7.86
7.85
7.83
7.81
7.79
7.76
7.75
7.59
7.58
7.56
7.53
7.51
7.47
7.46
7.44
7.30
7.27
7.19
1.28
0.00
3ac
5.03
1.00
4.00
1.01
9.00
f1 (ppm)

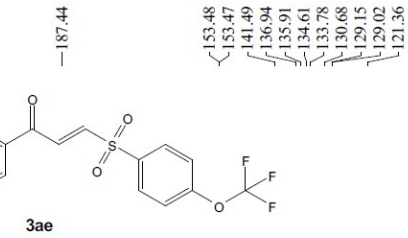

157.49
141.28
135.03
134.46
133.40
131.59
128.35
128.04
127.94
127.79
127.17
125.69
125.18
76.27
76.01
75.76
34.35
29.99
3ac
f1 (ppm)

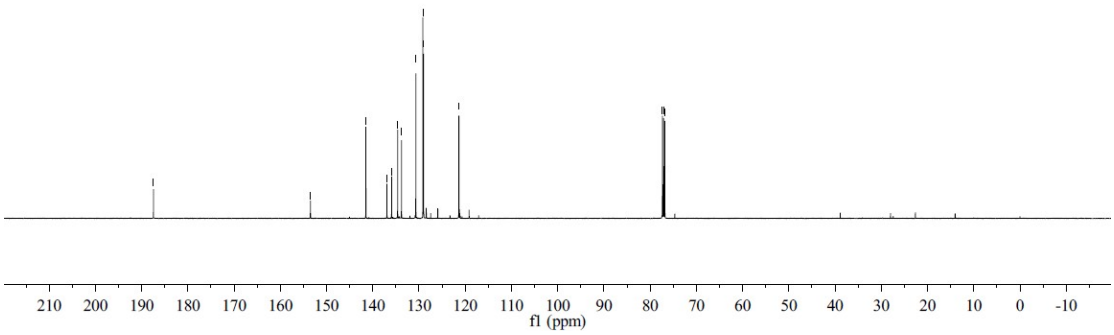

7.99
7.98
7.89
7.87
7.86
7.67
7.65
7.64
7.54
7.53
7.51
7.36
7.33
7.26
7.05
7.04
3.90
0.00
3ad
2.01
3.00
1.00
2.00
1.00
2.00
3.00
f1 (ppm)

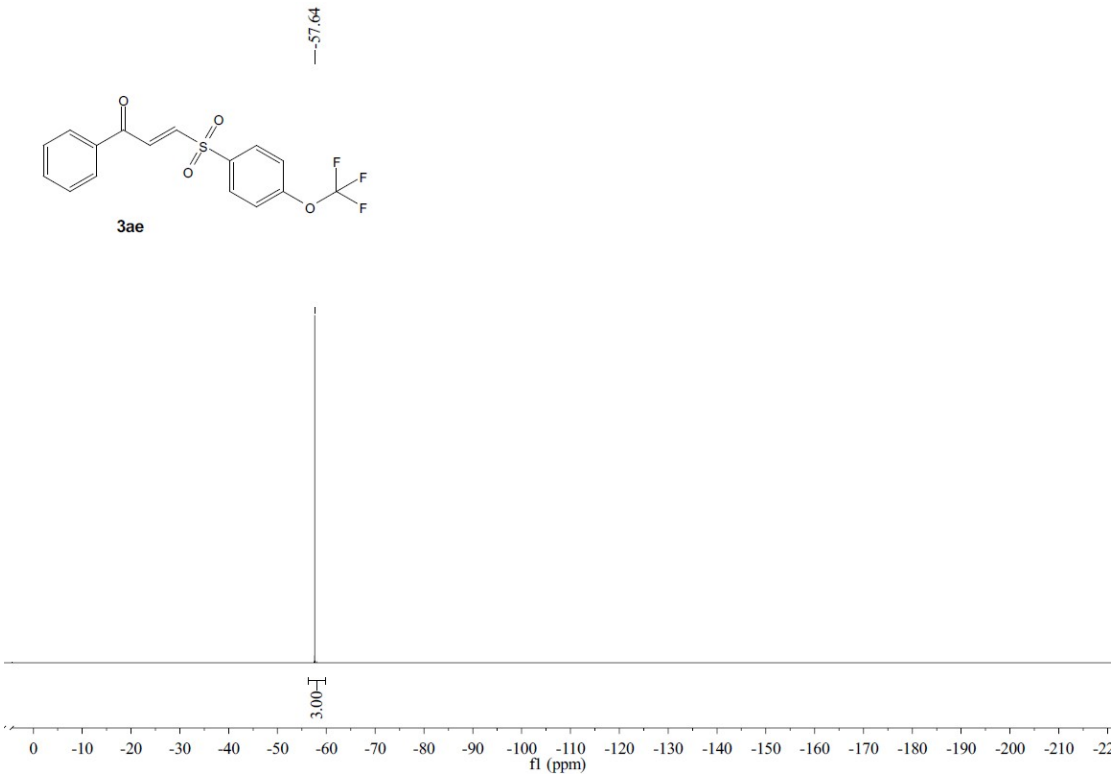

187.89
164.38
142.59
136.13
134.39
132.09
130.64
129.96
129.07
128.97
114.94
77.29
77.04
76.78
55.82
3ad
f1 (ppm)

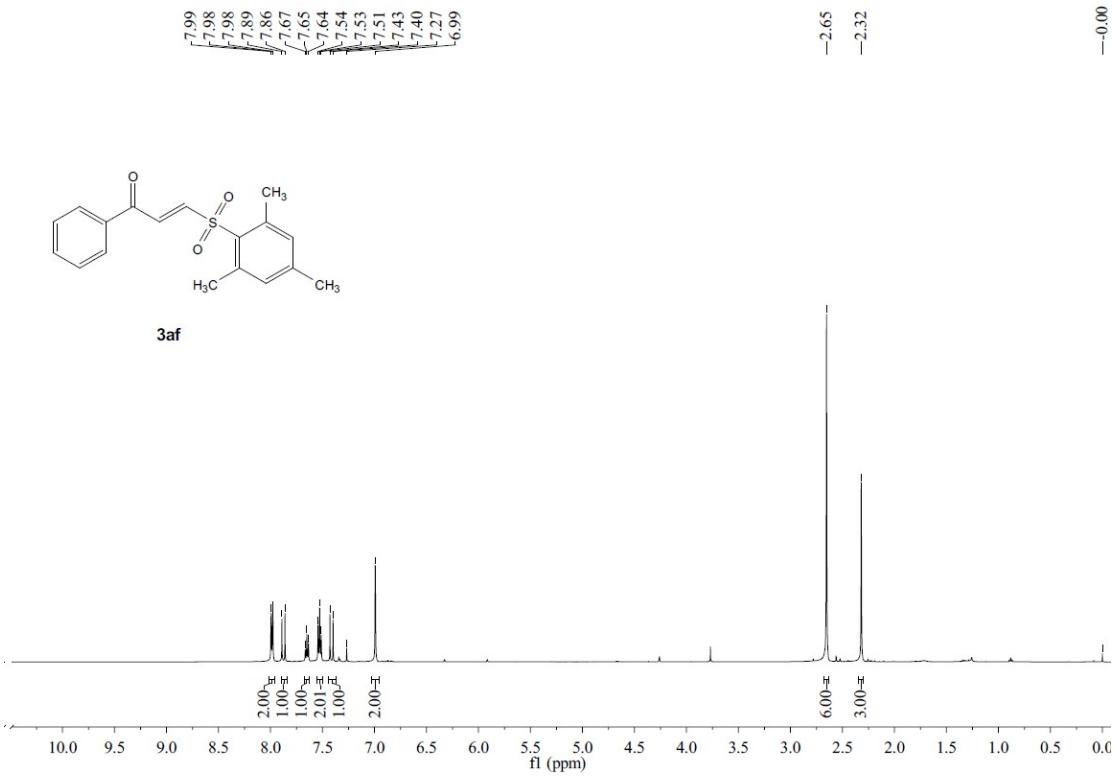

8.03
8.03
8.02
8.01
8.00
8.00
7.98
7.95
7.68
7.66
7.65
7.65
7.55
7.54
7.52
7.42
7.41
7.37
7.34
7.27
0.00
O
O
S
O
F
F
F
O
3ae

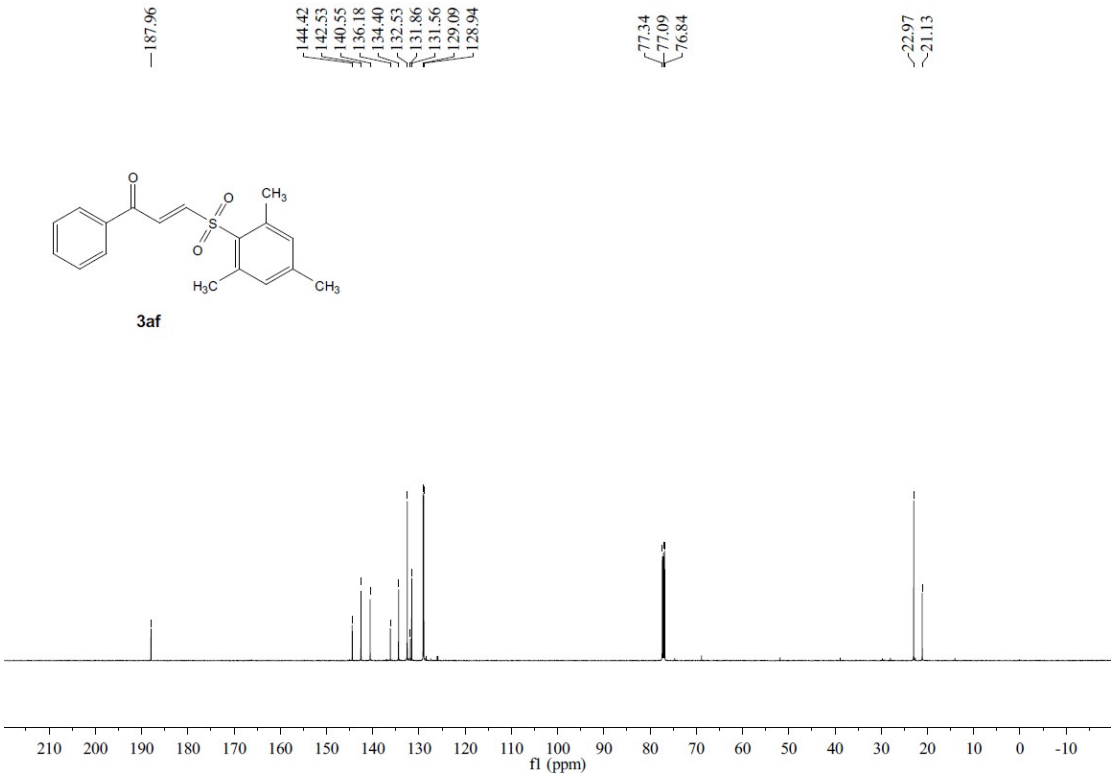

5.00
1.00
2.00
2.00
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

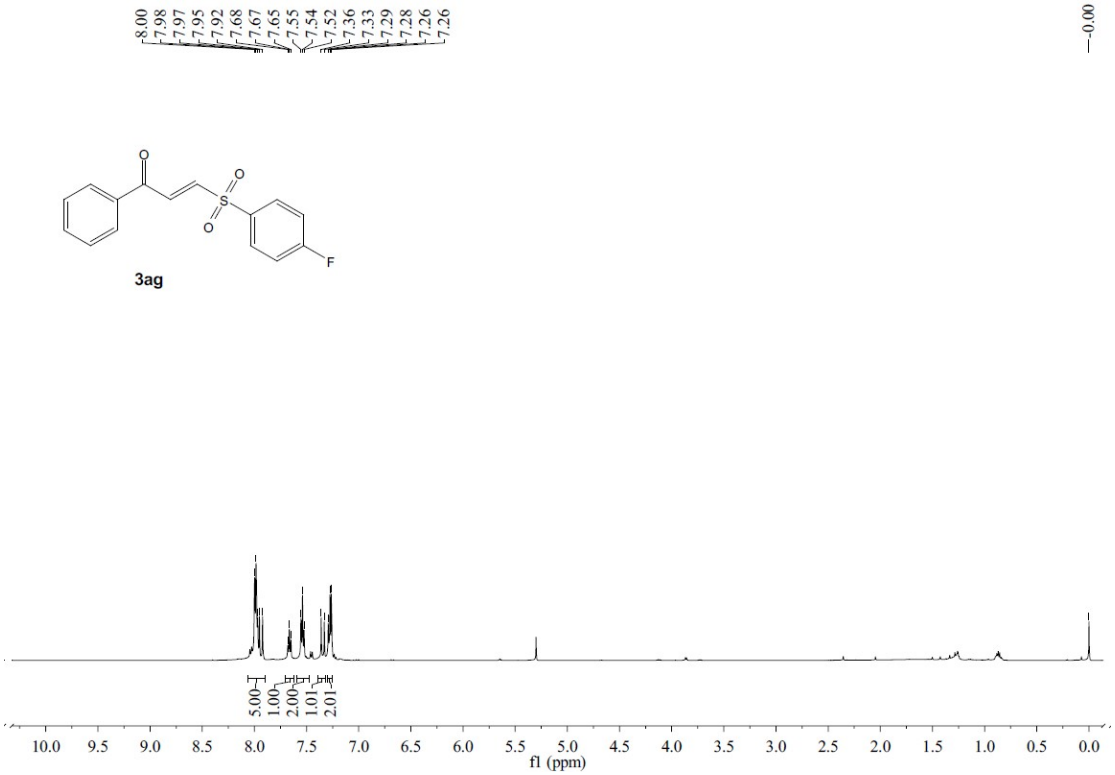

187.44
153.48
153.47
141.49
136.94
135.91
134.61
133.78
130.68
129.15
129.02
121.36
77.34
77.08
76.83
O
O
S
O
F
F
F
O
3ae


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

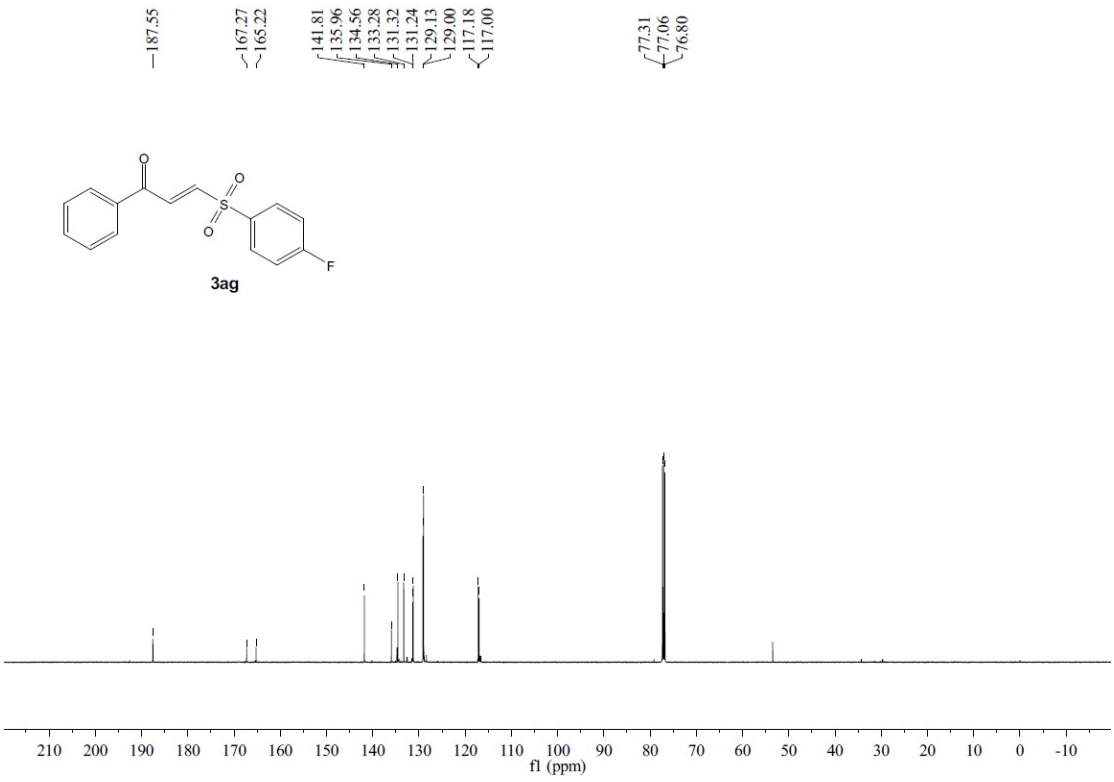

-57.64
3ae
3.00
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

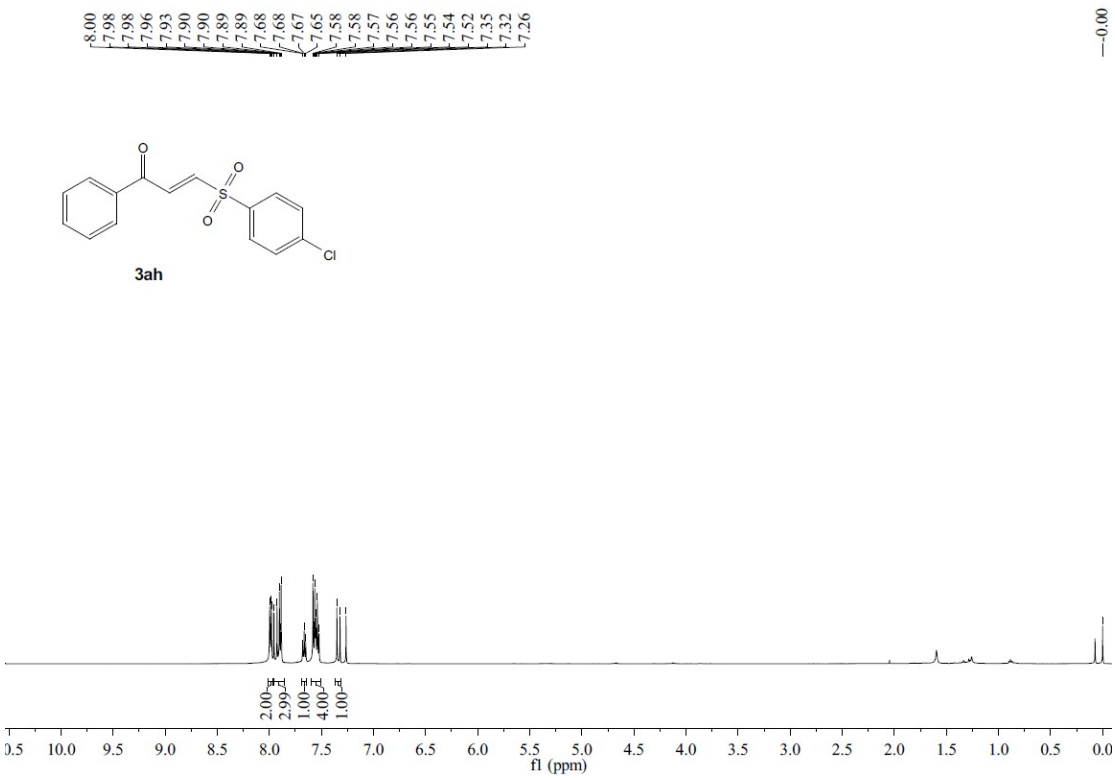

7.99
7.98
7.98
7.89
7.86
7.67
7.65
7.64
7.54
7.53
7.51
7.43
7.40
7.27
6.99
2.65
2.32
0.00
3af
2.00
1.00
1.00
2.01
1.00
2.00
6.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

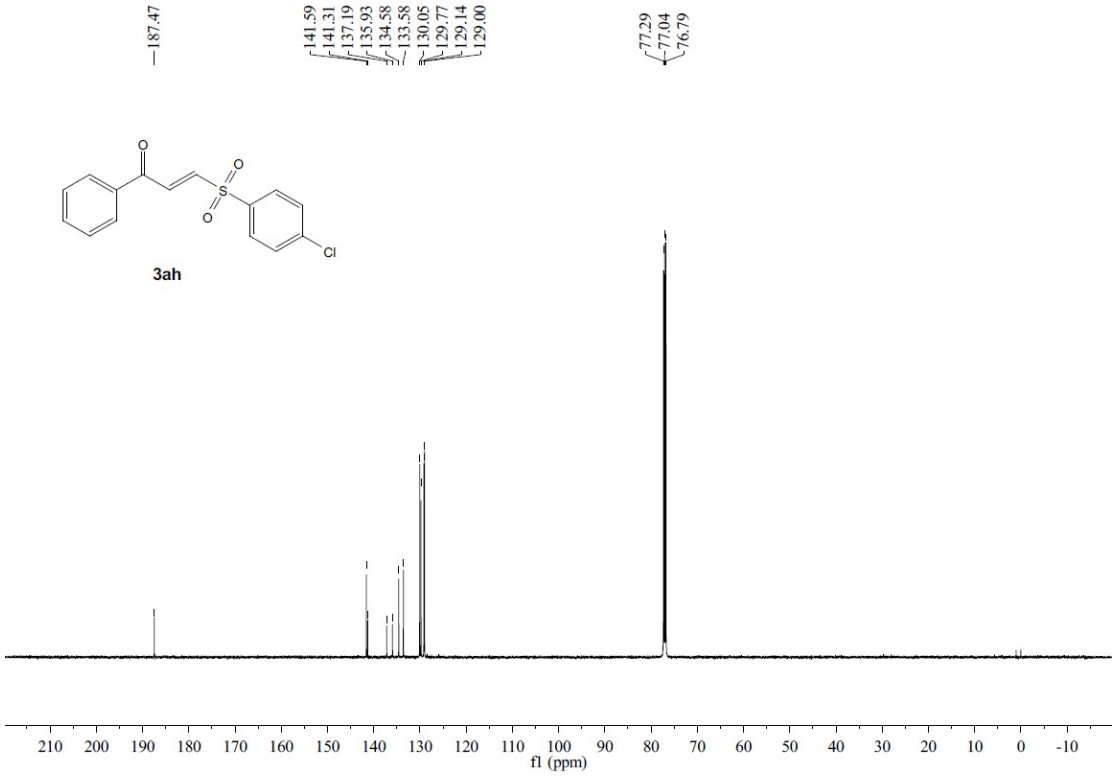

187.96
144.42
142.53
140.55
136.18
134.40
132.53
131.86
131.56
129.09
128.94
77.34
77.09
76.84
22.97
21.13
O
O
S
O
CH3
H3C
CH3
3af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

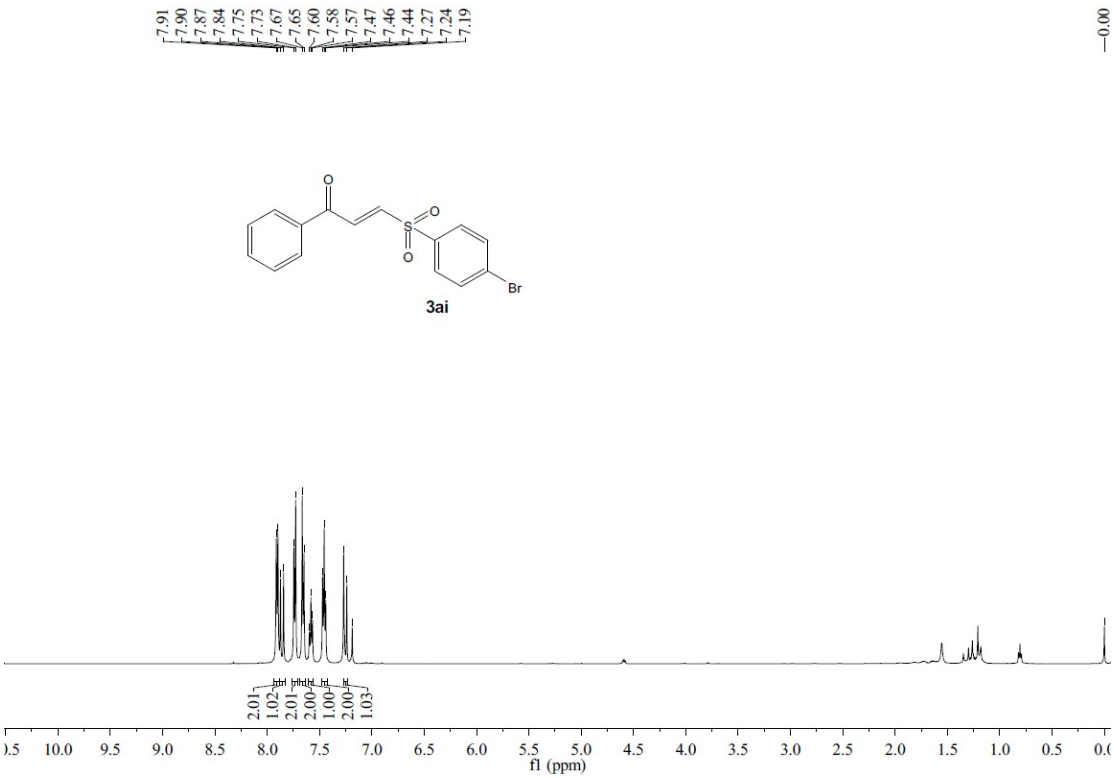

8.00
7.98
7.97
7.95
7.92
7.68
7.67
7.65
7.55
7.54
7.52
7.36
7.33
7.29
7.28
7.26
7.26
-0.00
O
O
S
O
F
3ag
5.00
1.00
2.00
1.01
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

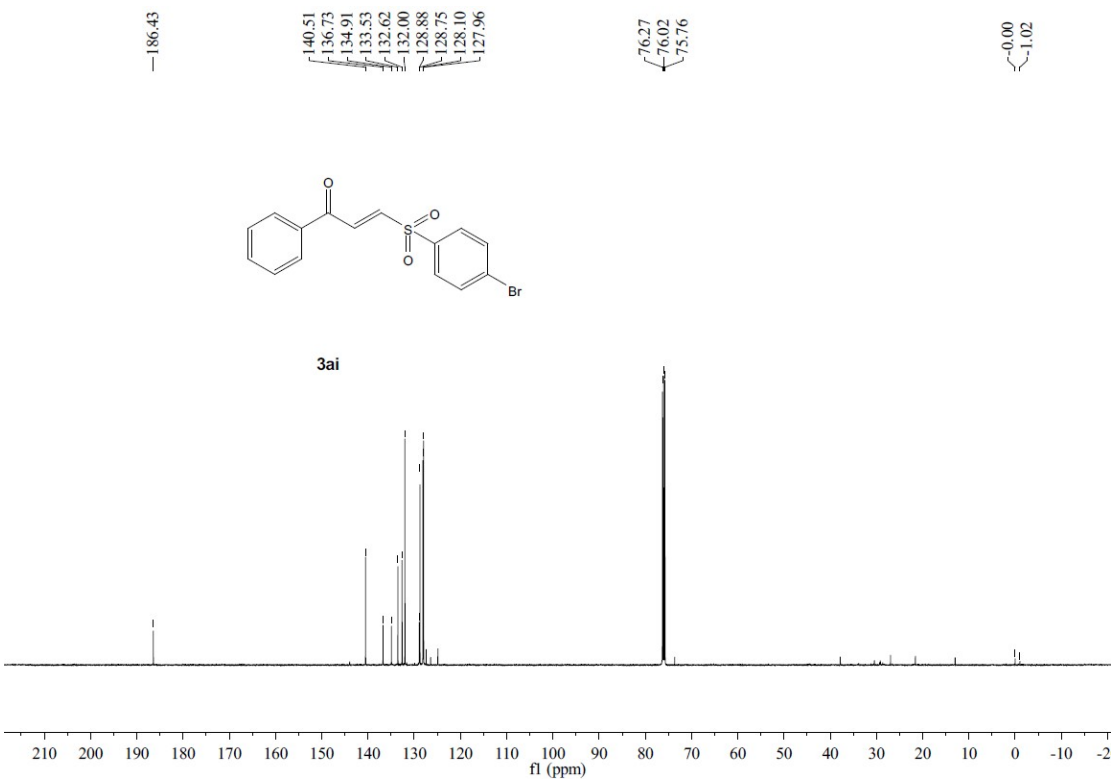

-101.93
3ag
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

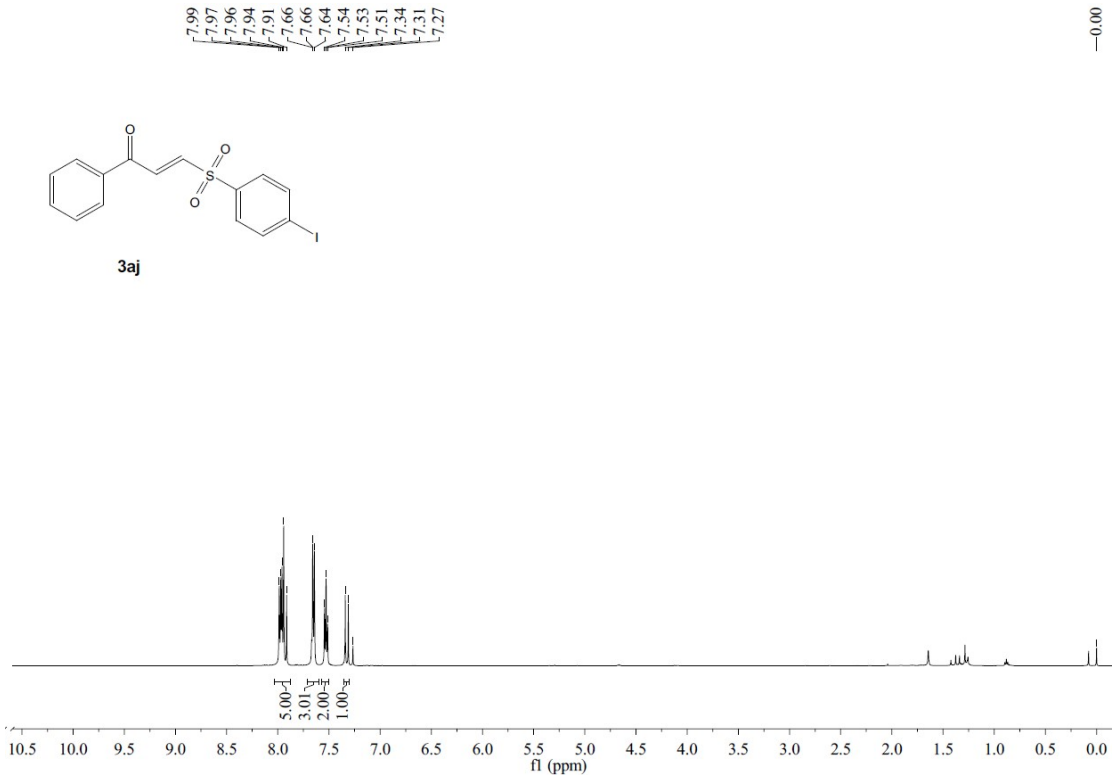

187.55
167.27
165.22
141.81
135.96
134.56
133.28
131.32
131.24
129.13
129.00
117.18
117.00
77.31
77.06
76.80
3ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

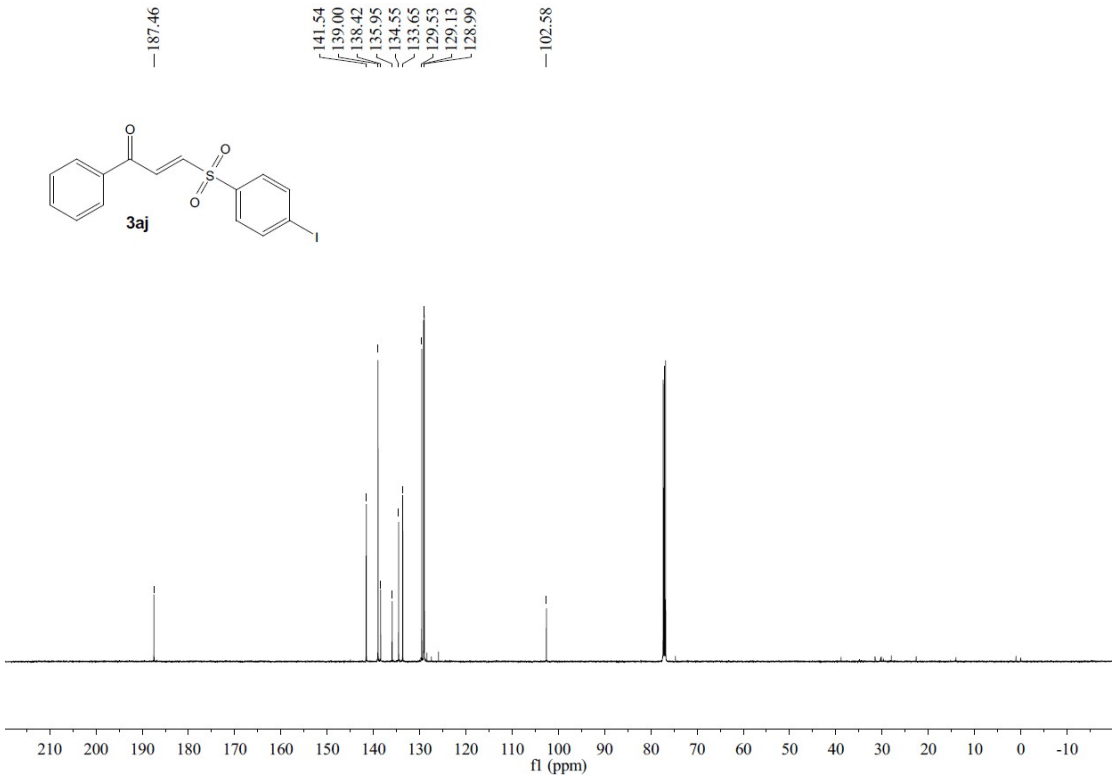

8.00
7.98
7.98
7.96
7.93
7.90
7.90
7.89
7.89
7.68
7.68
7.67
7.65
7.58
7.58
7.57
7.56
7.56
7.55
7.54
7.52
7.35
7.32
7.26
0.00
3ah
2.00
2.99
1.00
4.00
1.00
f1 (ppm)

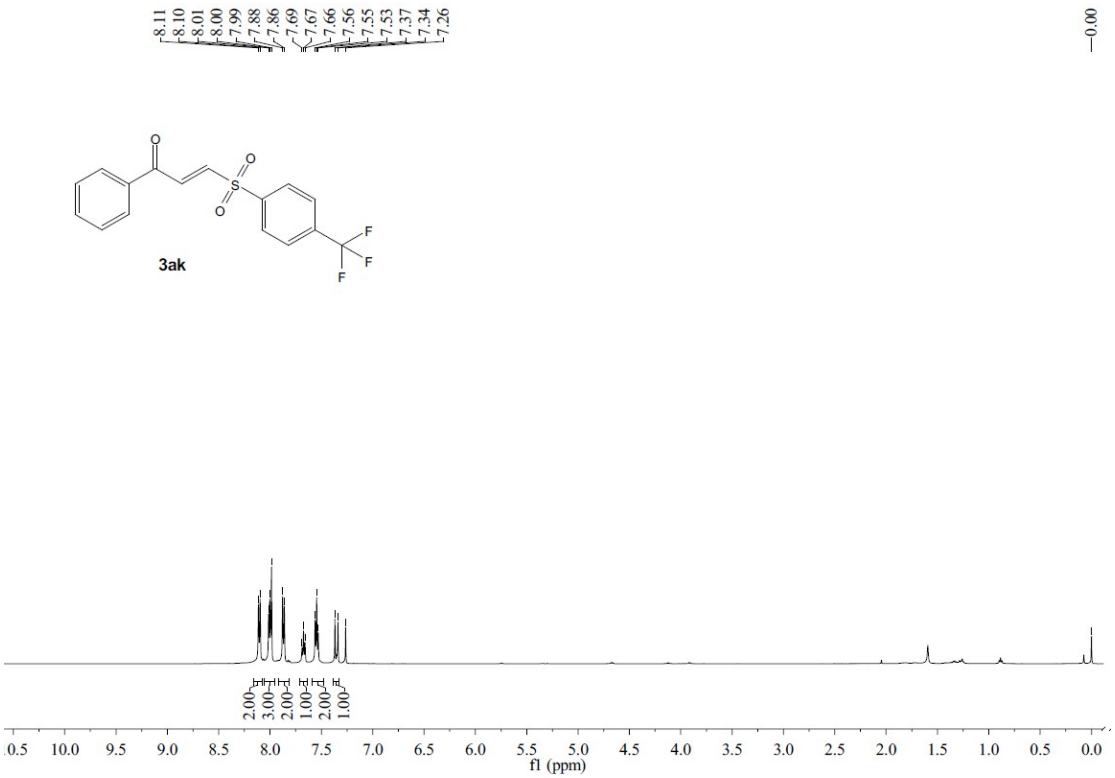

187.47
141.59
141.31
137.19
135.93
134.58
133.58
130.05
129.77
129.14
129.00
77.29
77.04
76.79
3ah
f1 (ppm)

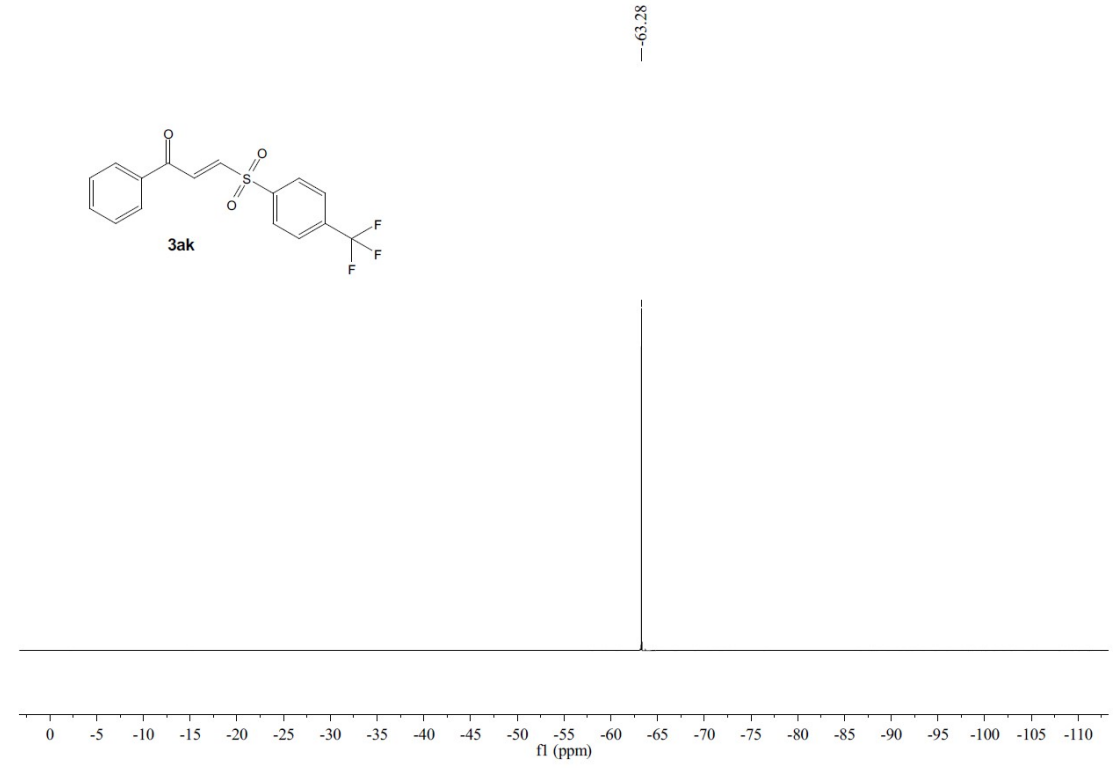

7.91
7.90
7.87
7.84
7.75
7.73
7.67
7.65
7.60
7.58
7.57
7.47
7.46
7.44
7.27
7.24
7.19
0.00
O
O
S
O
Br
3ai
2.01
1.02
2.01
2.00
1.00
2.00
1.03
f1 (ppm)

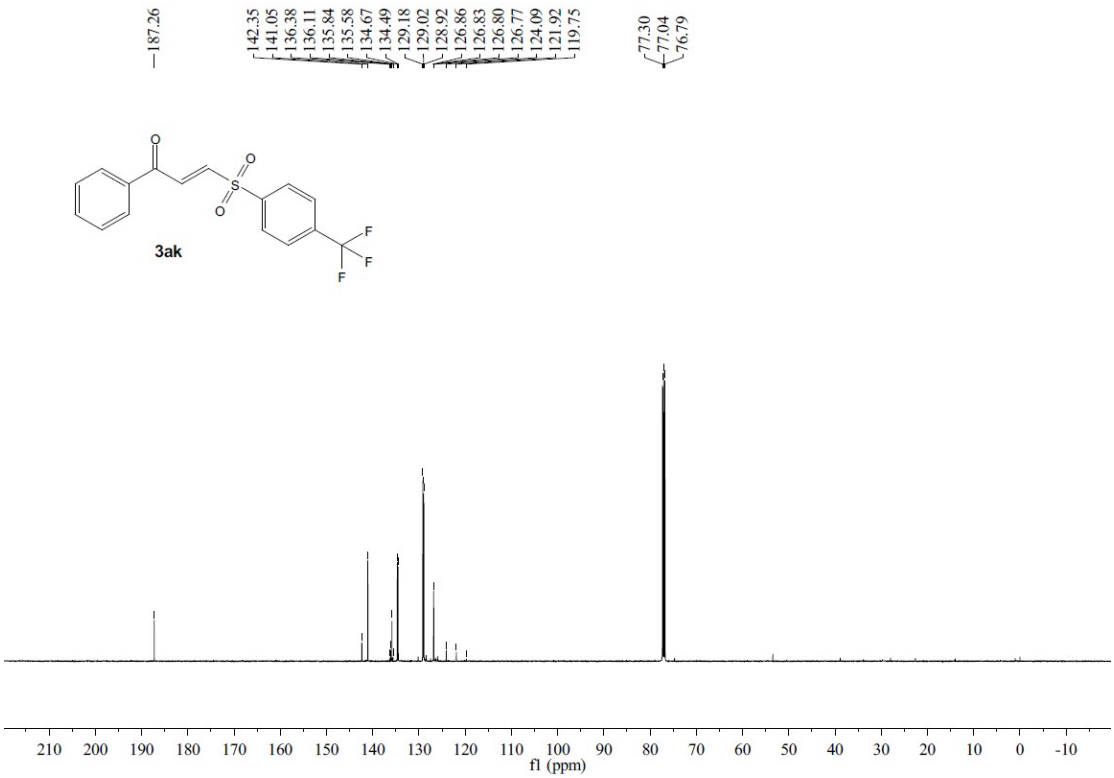

186.43
140.51
136.73
134.91
133.53
132.62
132.00
128.88
128.75
128.10
127.96
76.27
76.02
75.76
0.00
1.02
O
O
S
O
Br
3ai
f1 (ppm)

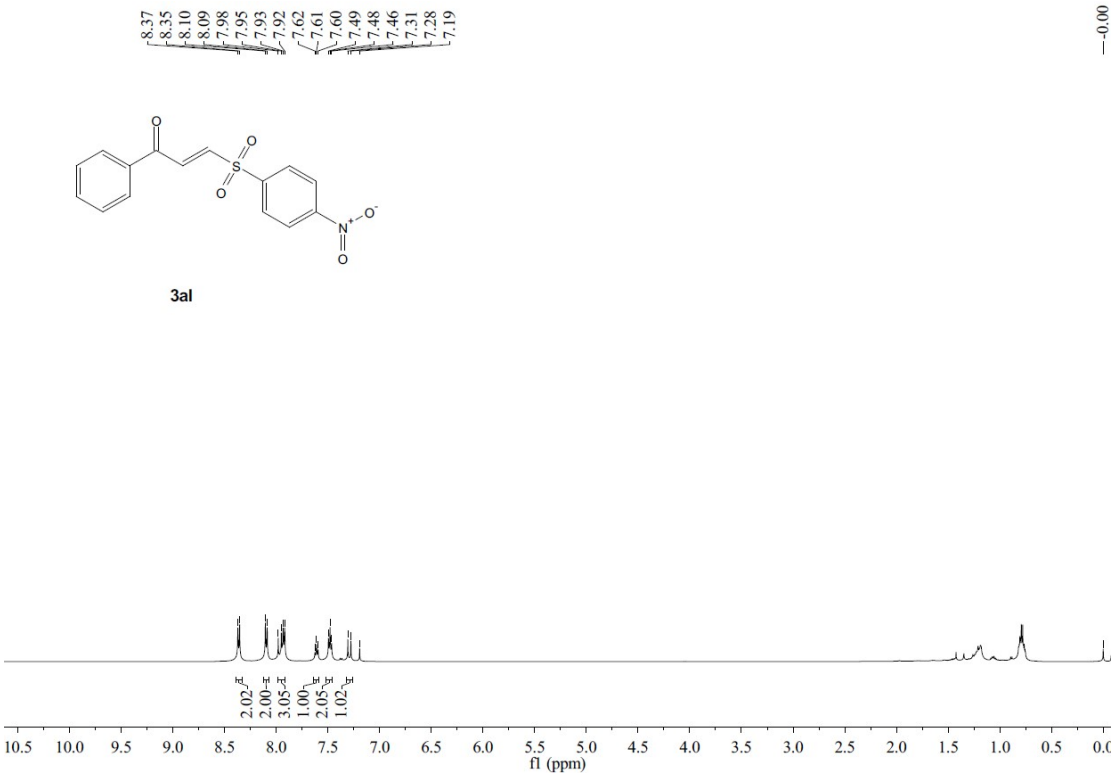

7.99
7.97
7.96
7.94
7.91
7.66
7.66
7.64
7.54
7.53
7.51
7.34
7.31
7.27
0.00
3aj
5.00
3.01
2.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

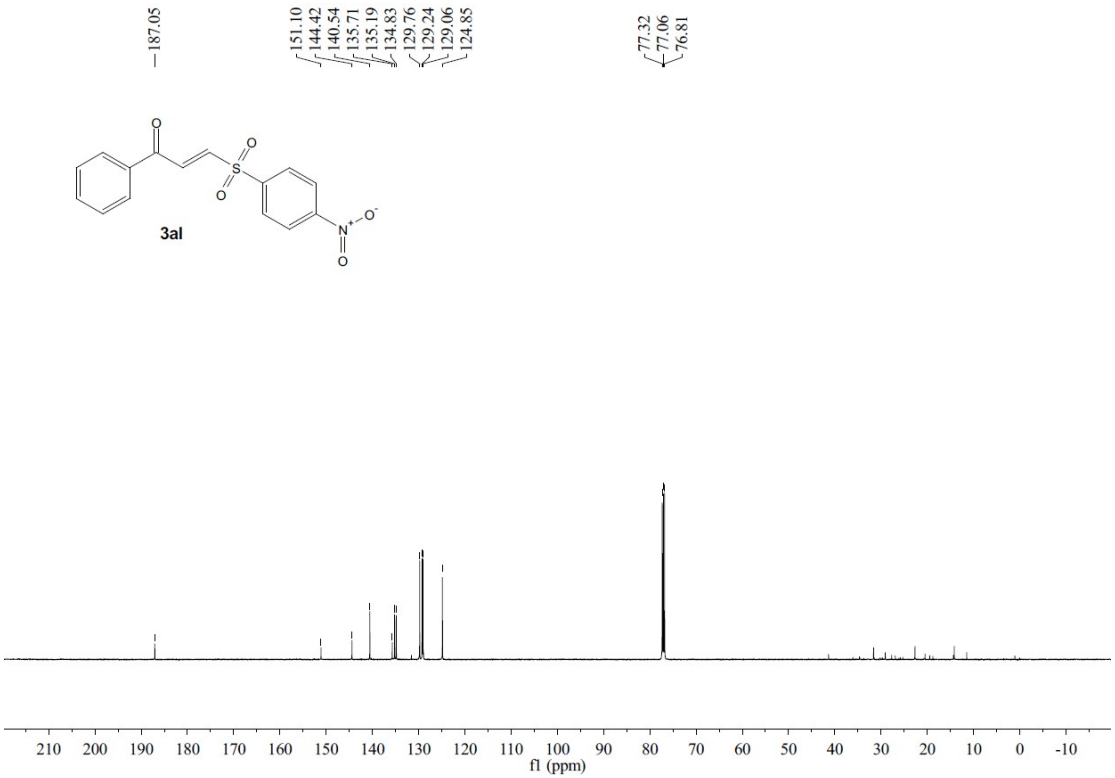

187.46
141.54
139.00
138.42
135.95
134.55
133.65
129.53
129.13
128.99
102.58
3aj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

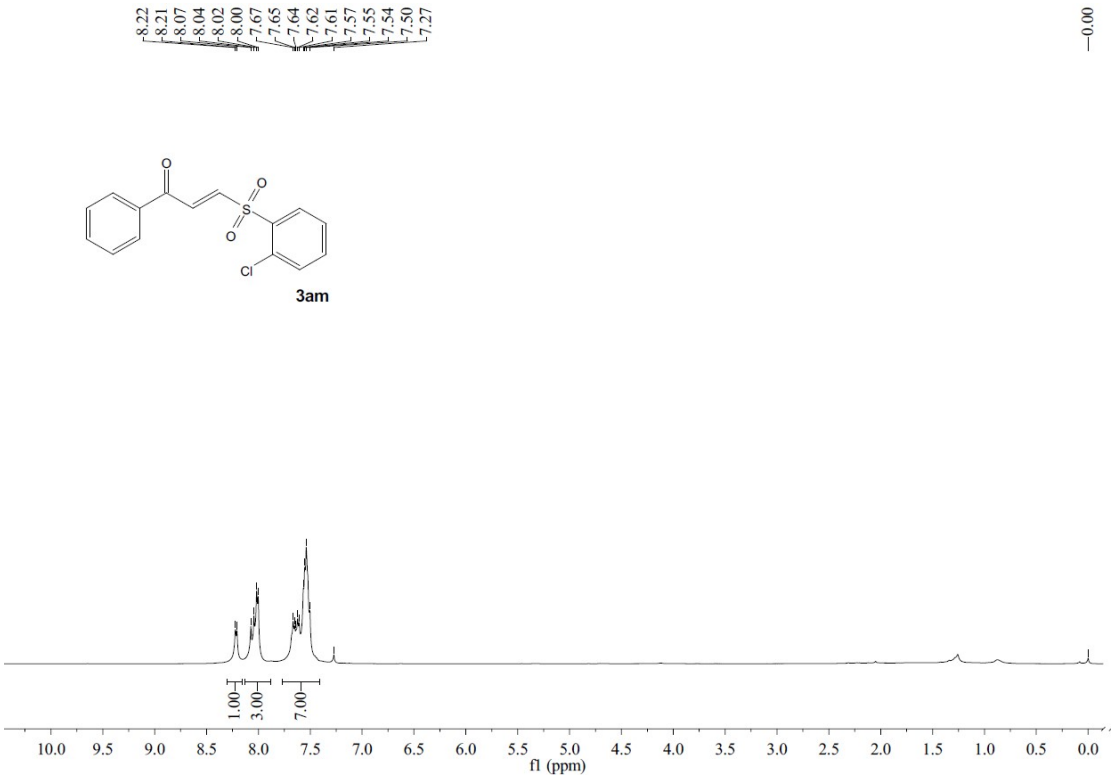

8.11
8.10
8.01
8.00
7.99
7.88
7.86
7.69
7.67
7.66
7.56
7.55
7.53
7.37
7.34
7.26
0.00
3ak
2.00
3.00
2.00
1.00
1.00
2.00
1.00
fl (ppm)

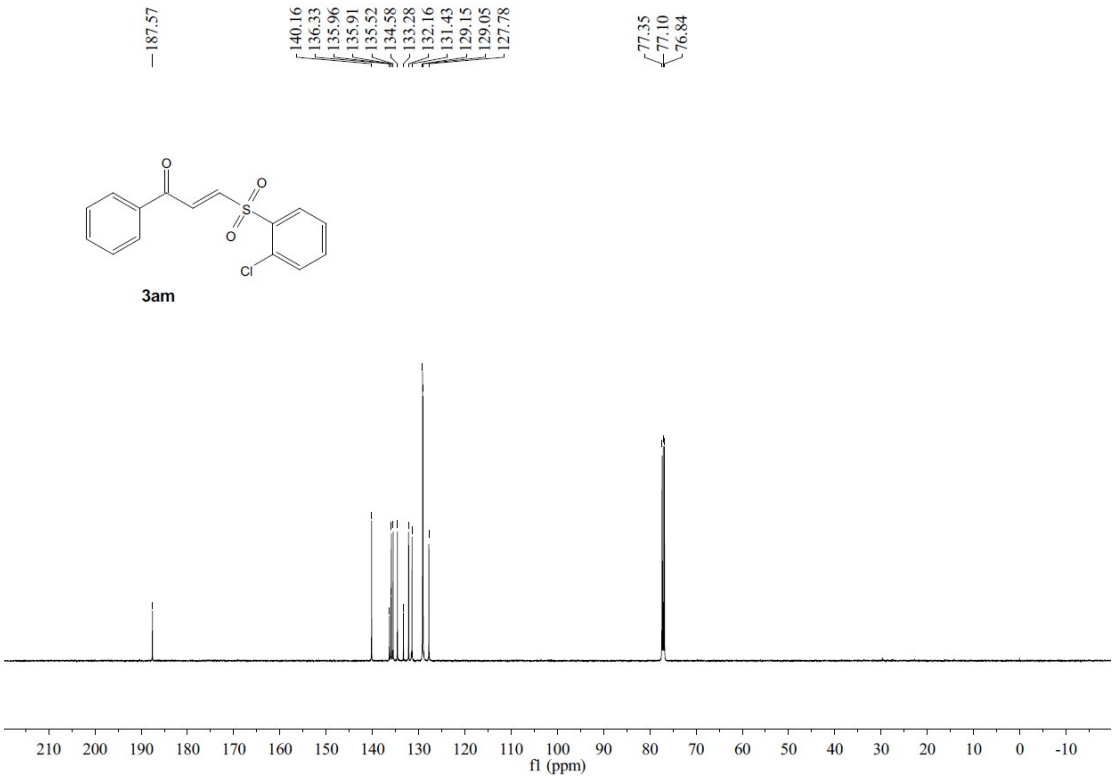

-63.28
3ak
fl (ppm)

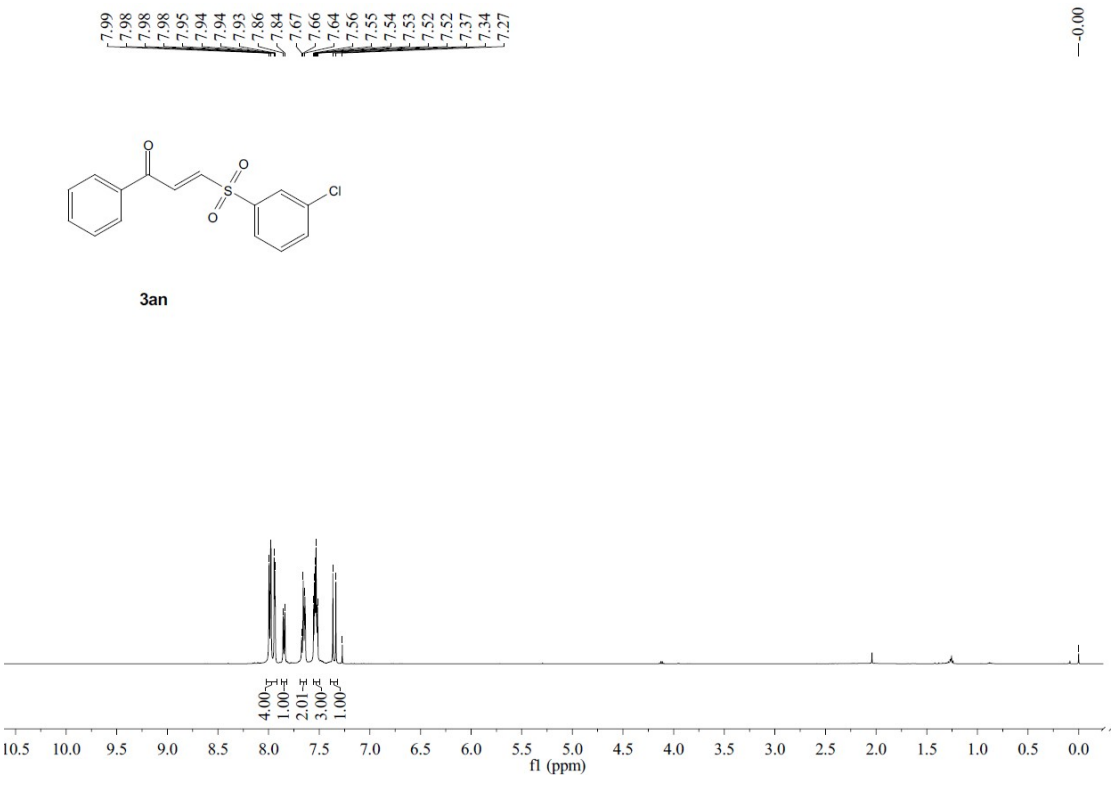

187.26
142.35
141.05
136.38
136.11
135.84
135.58
134.67
134.49
129.18
129.02
128.92
126.86
126.83
126.80
126.77
124.09
121.92
119.75
77.30
77.04
76.79
3ak
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

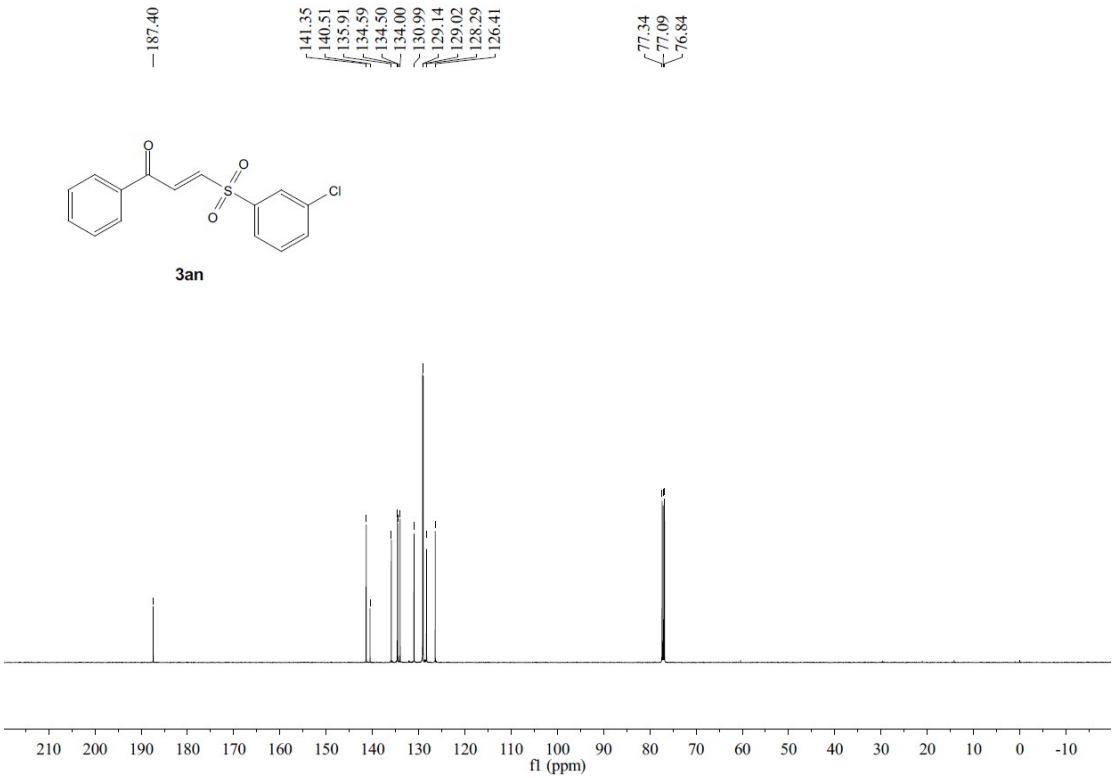

8.37
8.35
8.10
8.09
7.98
7.95
7.93
7.92
7.62
7.61
7.60
7.49
7.48
7.46
7.31
7.28
7.19
-0.00
3al
2.02
2.00
3.05
1.00
2.05
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

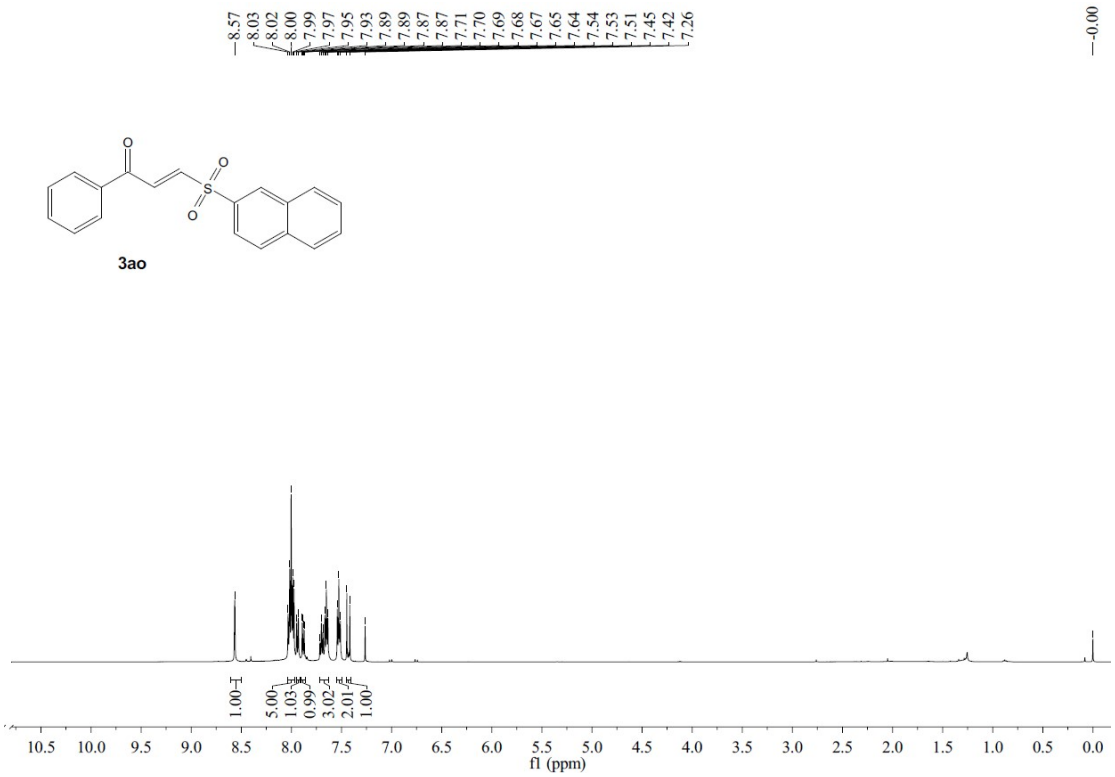

187.05
151.10
144.42
140.54
135.71
135.19
134.83
129.76
129.24
129.06
124.85
77.32
77.06
76.81
3al
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

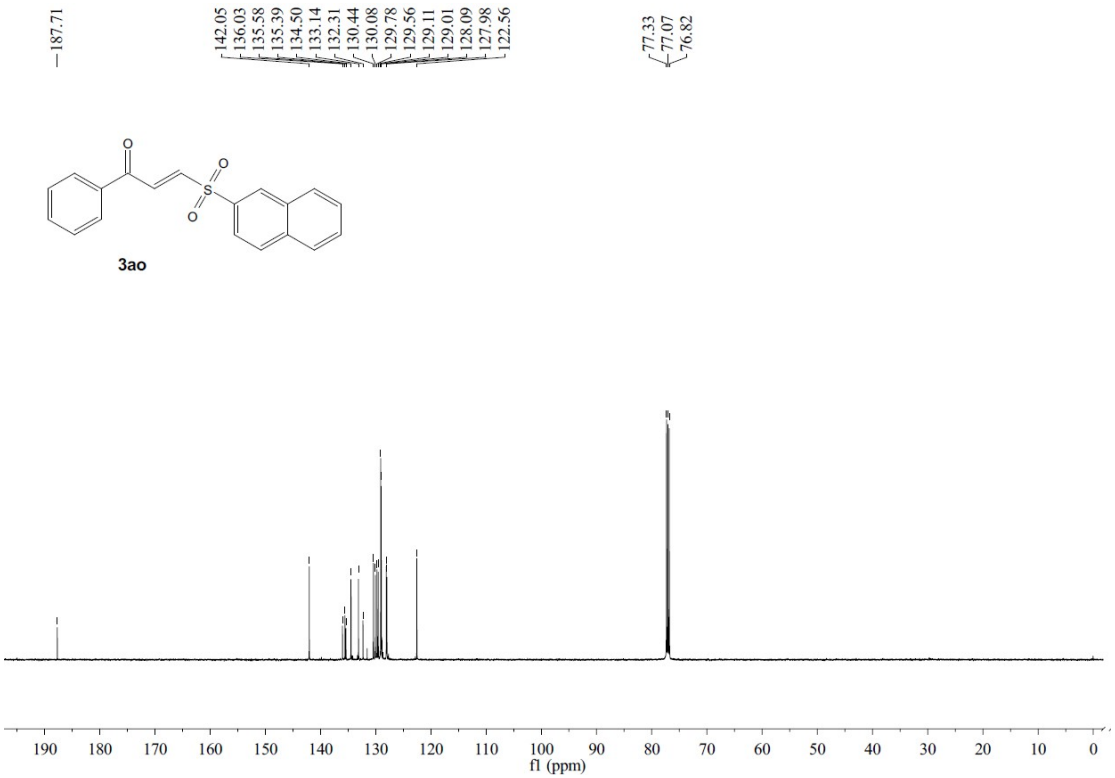

8.22
8.21
8.07
8.04
8.02
8.00
7.67
7.65
7.64
7.62
7.61
7.57
7.55
7.54
7.50
7.27
0.00
3am
1.00
3.00
7.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

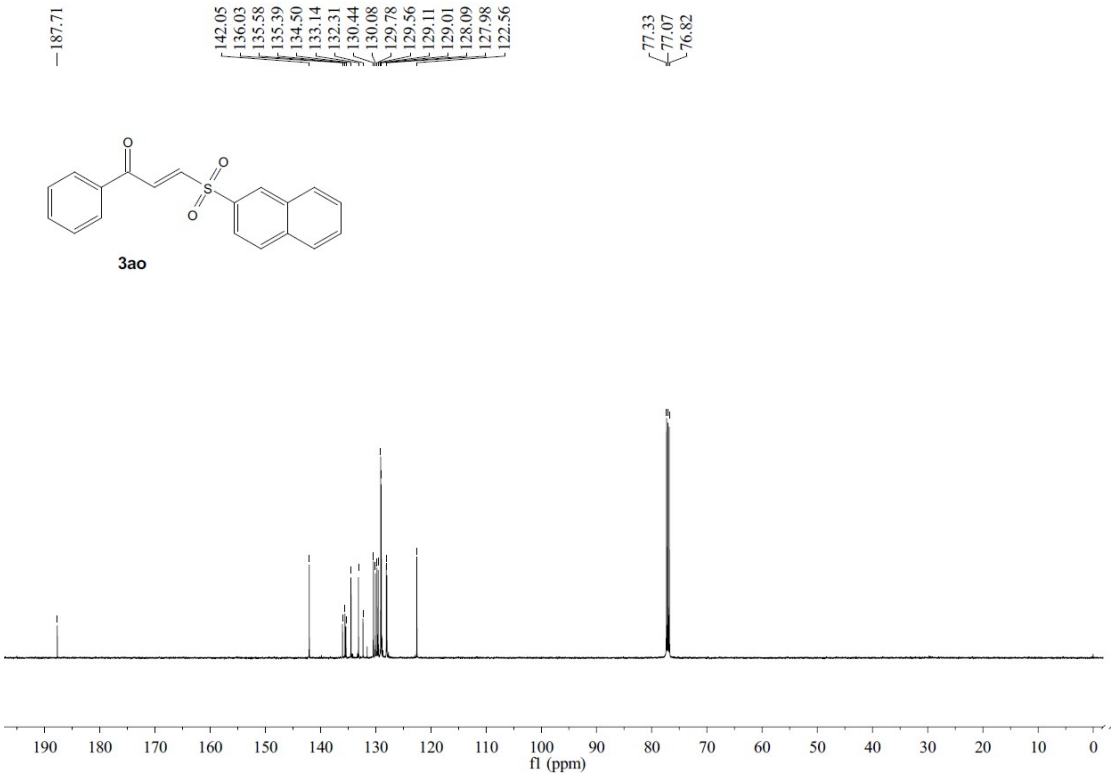

187.57
140.16
136.33
135.96
135.91
135.52
134.58
133.28
132.16
131.43
129.15
129.05
127.78
77.35
77.10
76.84
O
O
S
O
Cl
3am
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.99
7.98
7.98
7.98
7.95
7.94
7.94
7.93
7.86
7.84
7.67
7.66
7.64
7.56
7.55
7.54
7.54
7.53
7.52
7.52
7.37
7.34
7.27
0.00
O
O
S
O
Cl
3an
4.00
1.00
2.01
3.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


187.40
141.35
140.51
135.91
134.59
134.50
134.00
130.99
129.14
129.02
128.29
126.41
77.34
77.09
76.84
O
O
S
O
Cl
3an
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

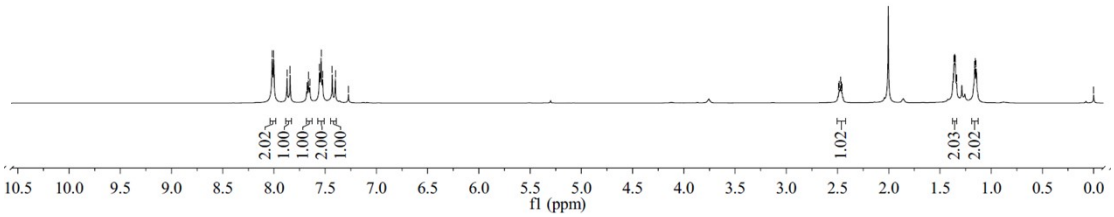

8.57
8.03
8.02
8.00
7.99
7.97
7.95
7.93
7.89
7.89
7.87
7.87
7.71
7.70
7.69
7.68
7.67
7.65
7.64
7.54
7.53
7.51
7.45
7.42
7.26
0.00
O
O
S
O
3ao
1.00
5.00
1.03
0.99
3.02
2.01
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

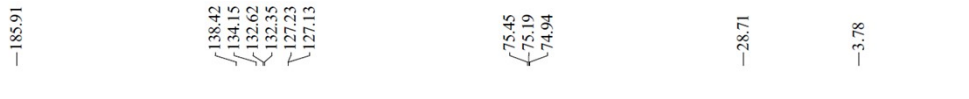

187.71
142.05
136.03
135.58
135.39
134.50
133.14
132.31
130.44
130.08
129.78
129.56
129.11
129.01
128.09
127.98
122.56
77.33
77.07
76.82
O
O
S
O
3ao
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

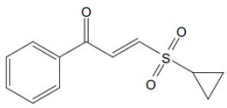

187.71
142.05
136.03
135.58
135.39
134.50
133.14
132.31
130.44
130.08
129.78
129.56
129.11
129.01
128.09
127.98
122.56
77.33
77.07
76.82
O
O
S
O
3ao
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.02
8.00
7.87
7.84
7.68
7.66
7.65
7.56
7.54
7.53
7.43
7.40
7.27
2.49
2.48
2.47
2.46
2.46
1.37
1.36
1.36
1.35
1.35
1.34
1.16
1.16
1.15
0.00

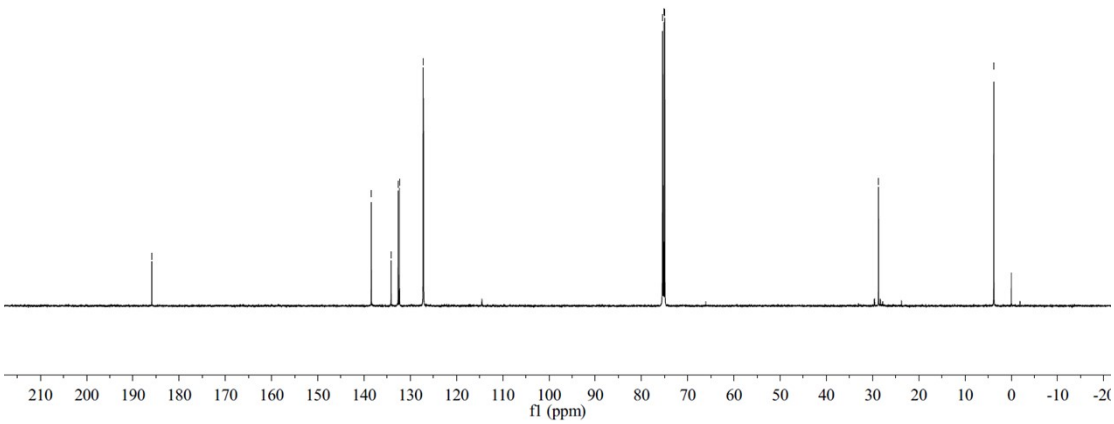
3ap

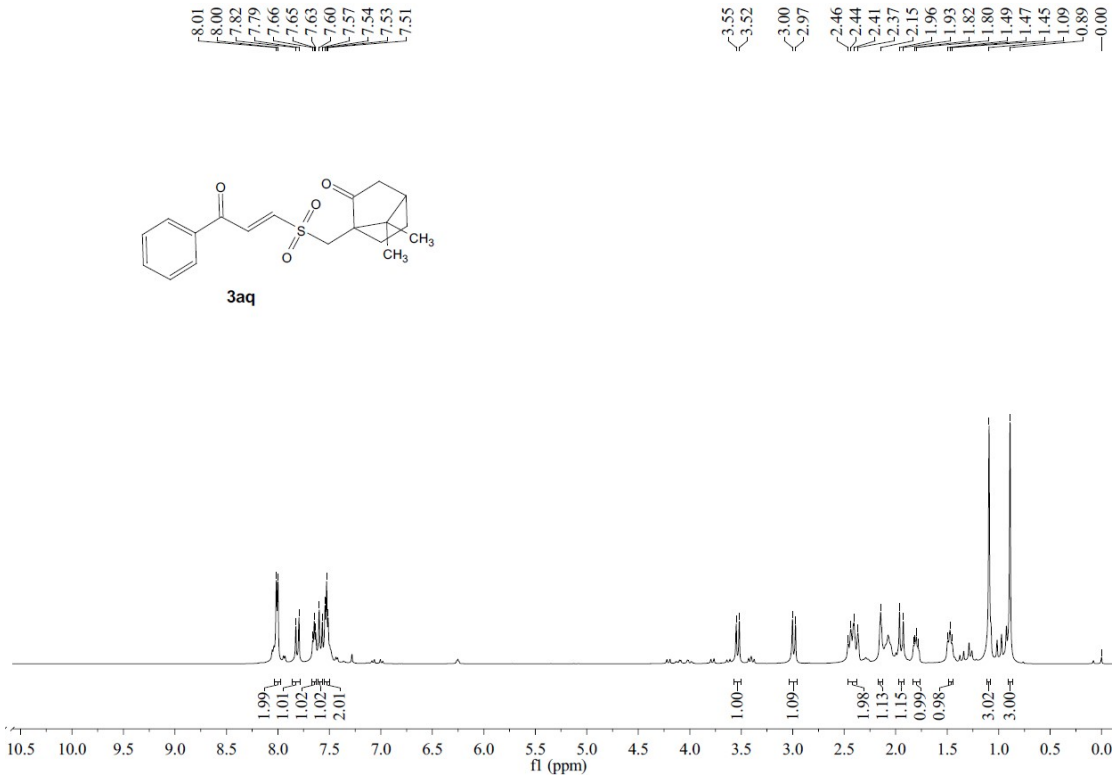

2.02
1.00
1.00
2.00
1.00
1.02
2.03
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


185.91
138.42
134.15
132.62
132.35
127.23
127.13
75.45
75.19
74.94
28.71
3.78

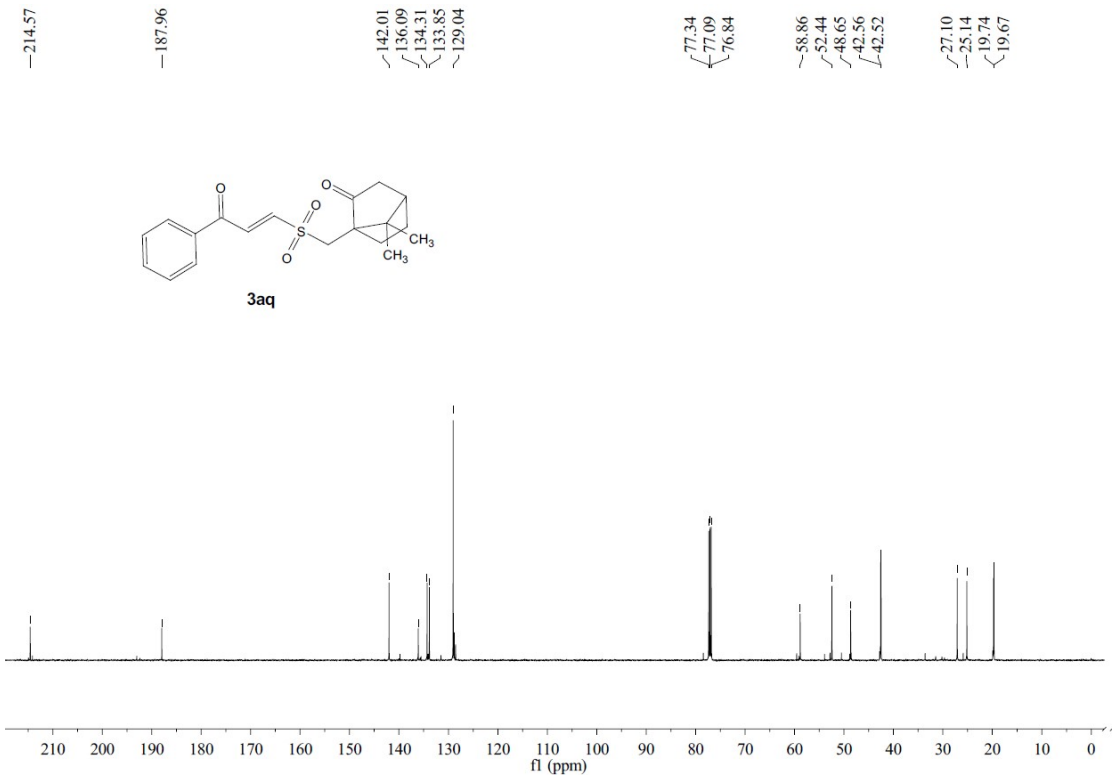


3ap


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.01
8.00
7.82
7.79
7.66
7.65
7.63
7.60
7.57
7.54
7.53
7.51
3.55
3.52
3.00
2.97
2.46
2.44
2.41
2.37
2.15
1.96
1.93
1.82
1.80
1.49
1.47
1.45
1.09
0.89
0.00
O
O
O
S
O
O
CH3
CH3
1.99
1.01
1.02
1.02
2.01
1.00
1.09
1.98
1.13
1.15
0.99
0.98
3.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3aq


214.57
187.96
142.01
136.09
134.31
133.85
129.04
77.34
77.09
76.84
58.86
52.44
48.65
42.56
42.52
27.10
25.14
19.74
19.67
O
O
O
S
O
O
CH3
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3aq


7.97
7.96
7.95
7.93
7.92
7.92
7.70
7.69
7.68
7.67
7.61
7.61
7.60
7.60
7.59
7.58
7.58
7.49
7.48
7.46
7.44
7.27
3.59
3.59
3.58
3.57
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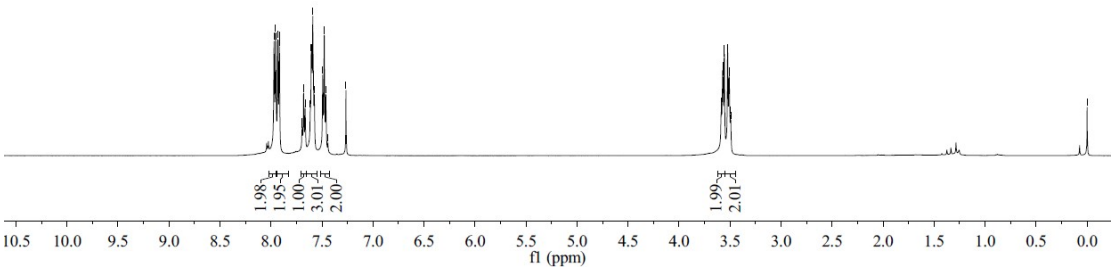
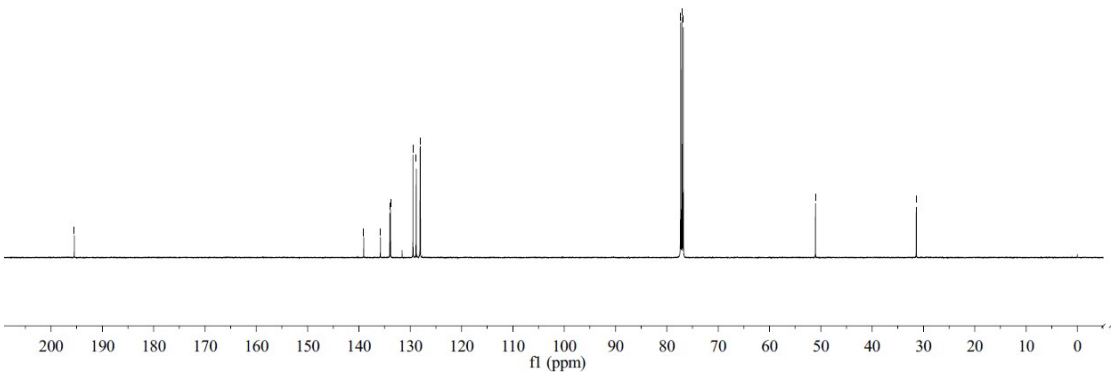
3.51
3.51
3.51
3.50
3.49
0.00

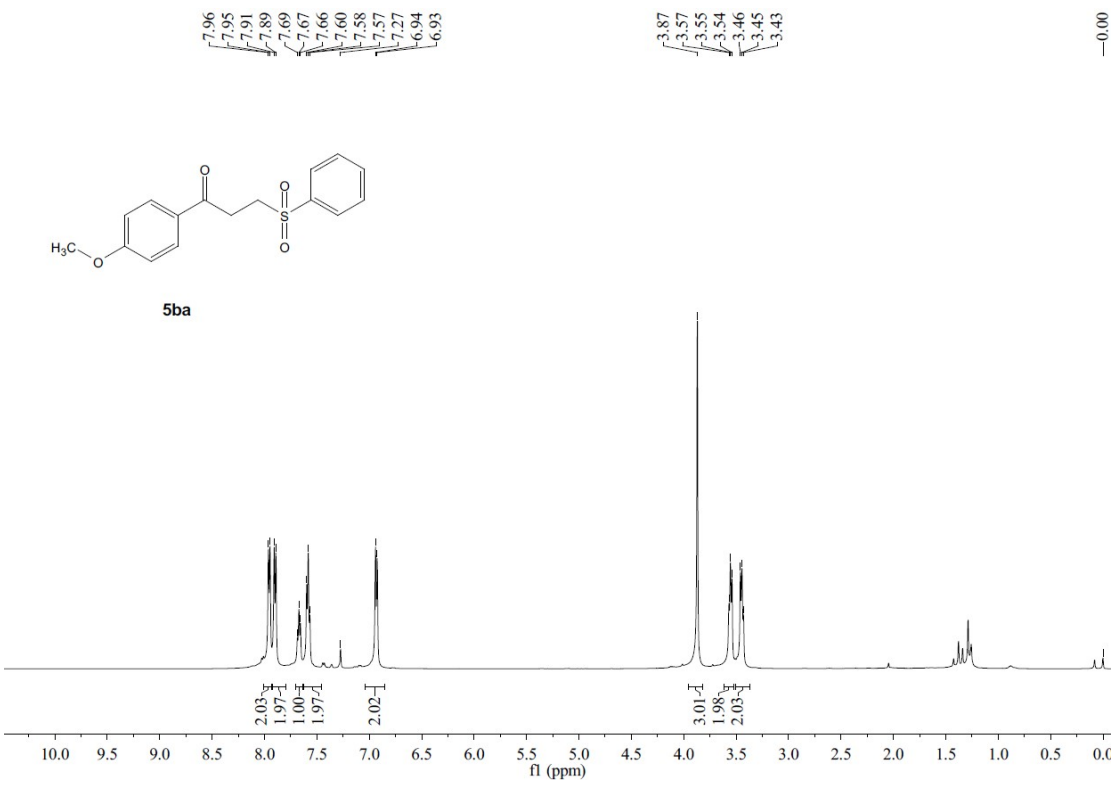
5aa


1.98
1.95
1.00
3.01
2.00
1.99
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

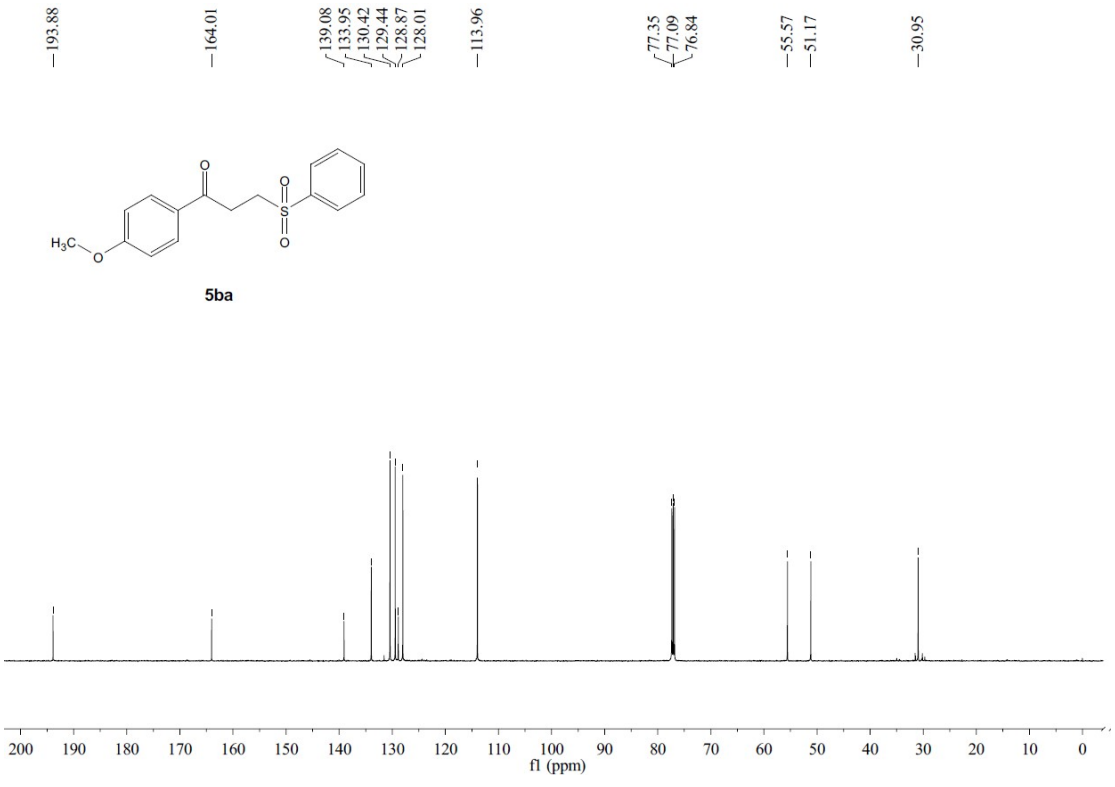

195.46
139.07
135.81
133.98
133.84
129.46
128.83
128.09
128.02
77.30
77.05
76.80
51.05
31.39

5aa

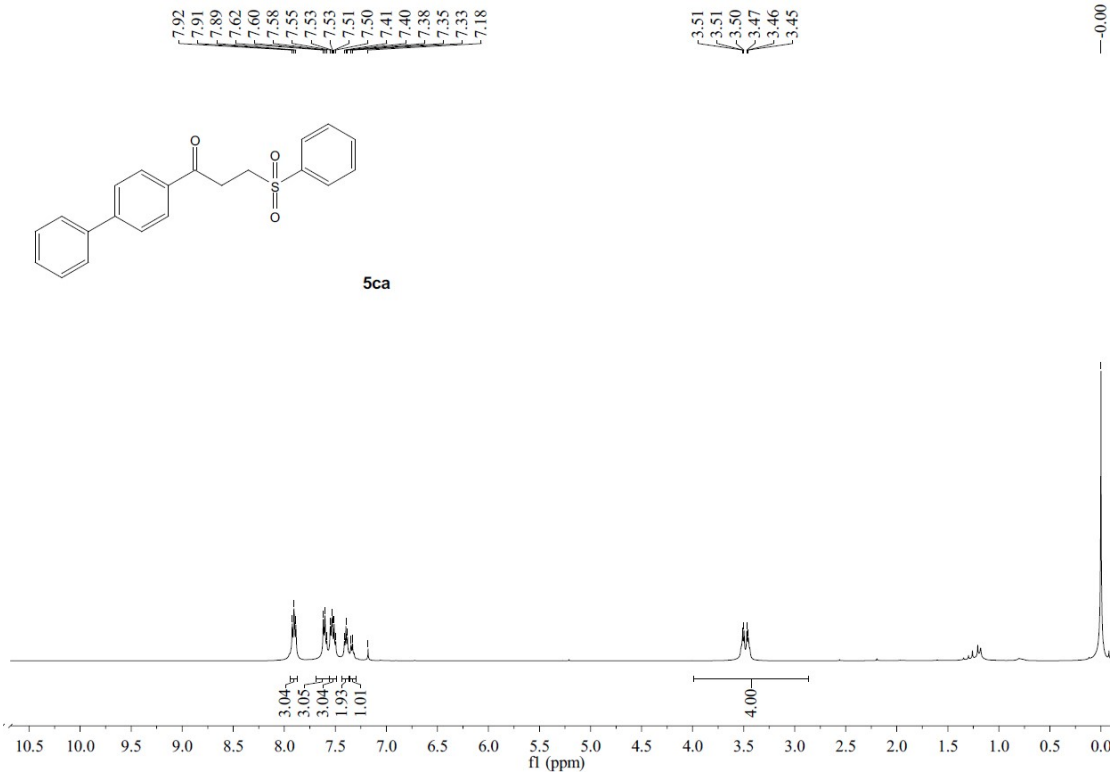

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

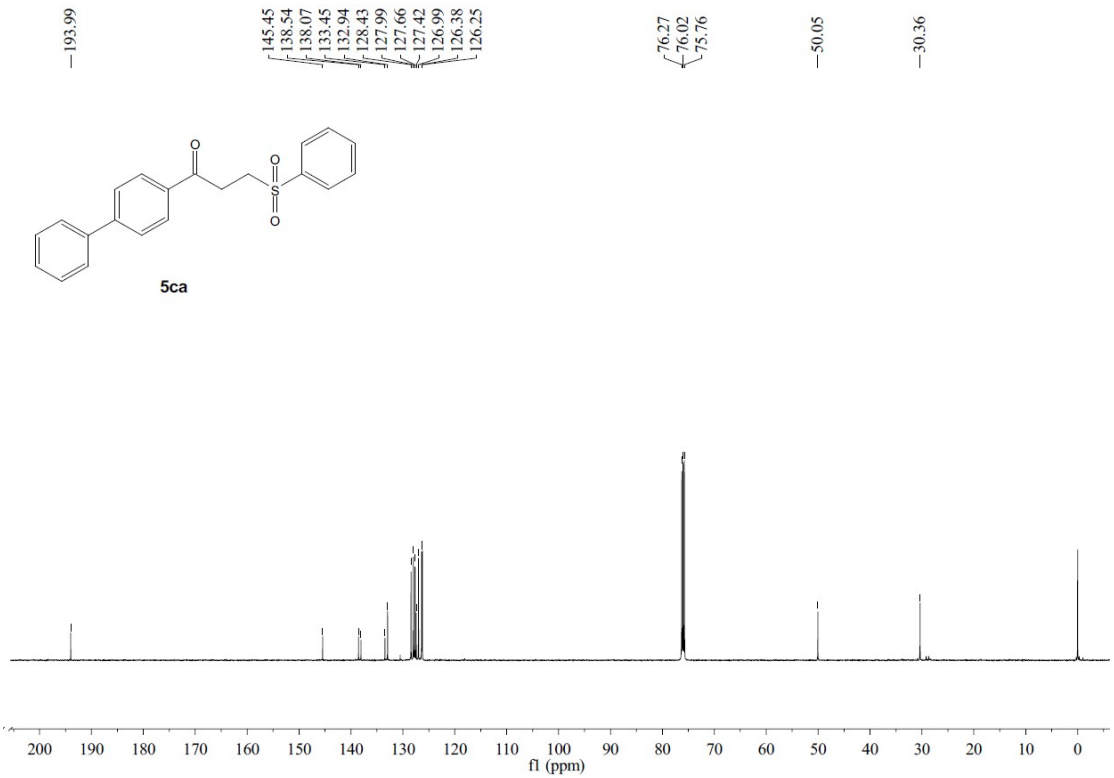

7.96
7.95
7.91
7.89
7.69
7.67
7.66
7.60
7.58
7.57
7.27
6.94
6.93
3.87
3.57
3.55
3.54
3.46
3.45
3.43
0.00
O
O
S
O
O
H3C
O
2.03
1.97
1.00
1.97
2.02
3.01
1.98
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

5ba


193.88
164.01
139.08
133.95
130.42
129.44
128.87
128.01
113.96
77.35
77.09
76.84
55.57
51.17
30.95
O
O
S
O
O
H3C
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

5ba


7.92
7.91
7.89
7.62
7.60
7.58
7.55
7.53
7.53
7.51
7.50
7.41
7.40
7.38
7.35
7.33
7.18
3.51
3.51
3.50
3.47
3.46
3.45
0.00
5ca
3.04
3.05
3.04
1.93
1.01
4.00
f1 (ppm)


193.99
145.45
138.54
138.07
133.45
132.94
128.43
127.99
127.66
127.42
126.99
126.38
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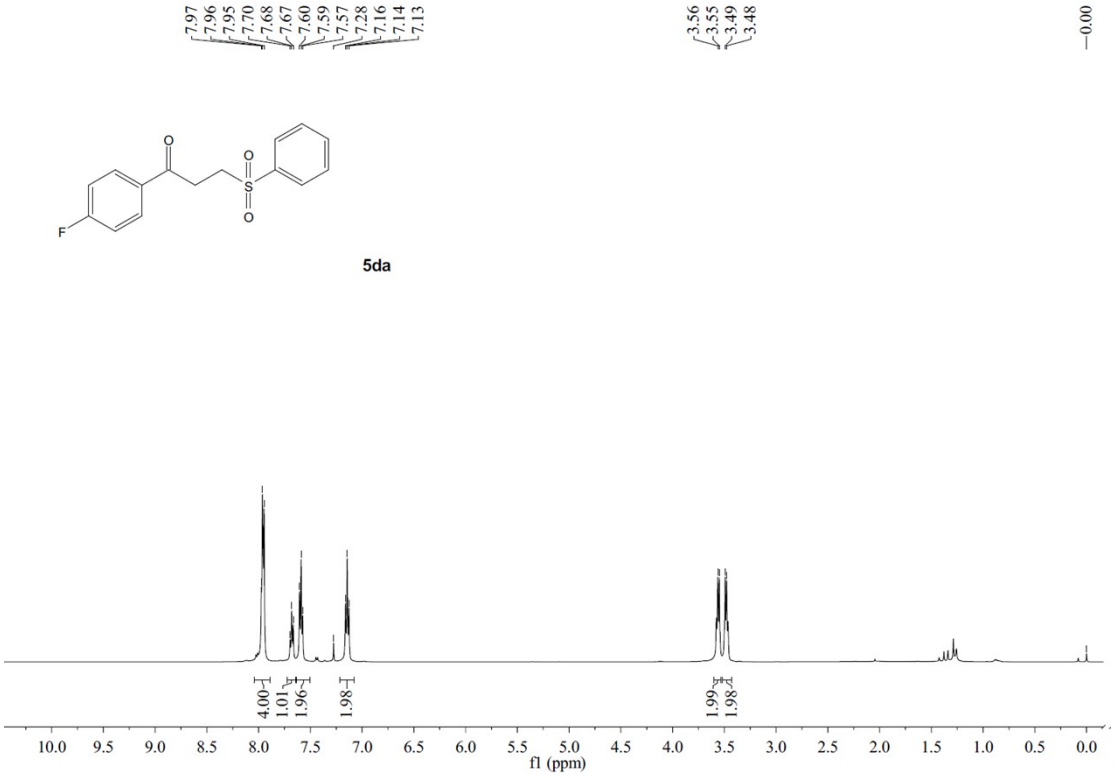
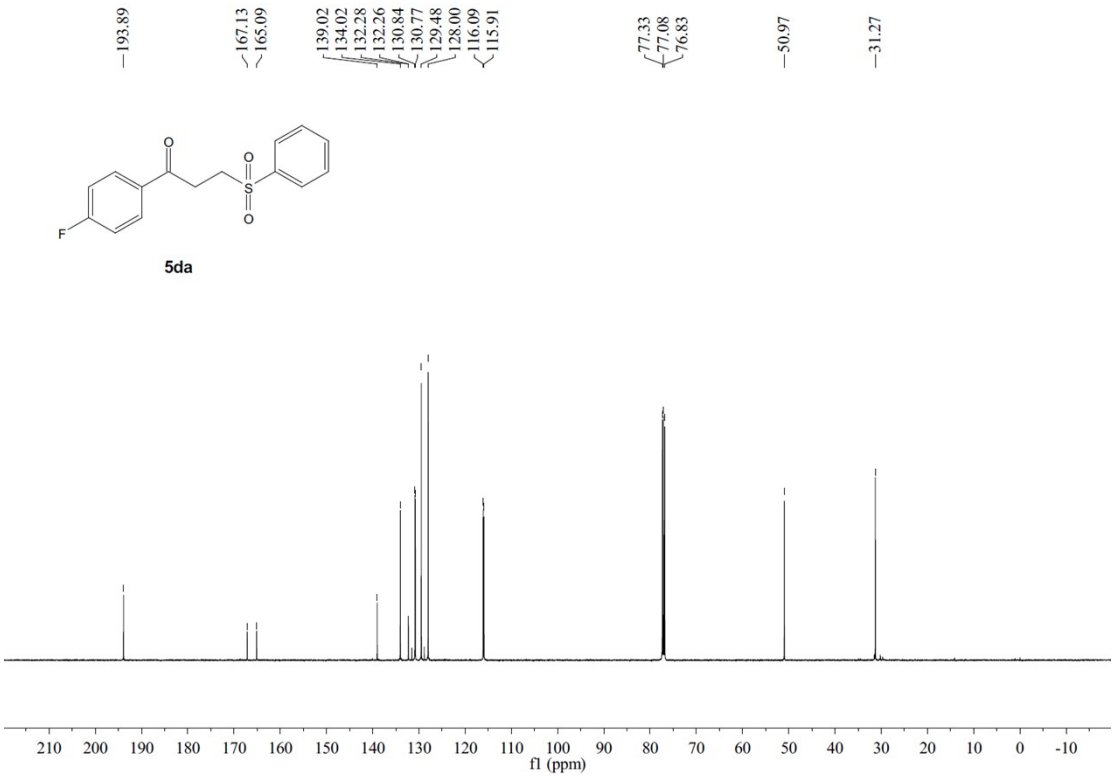
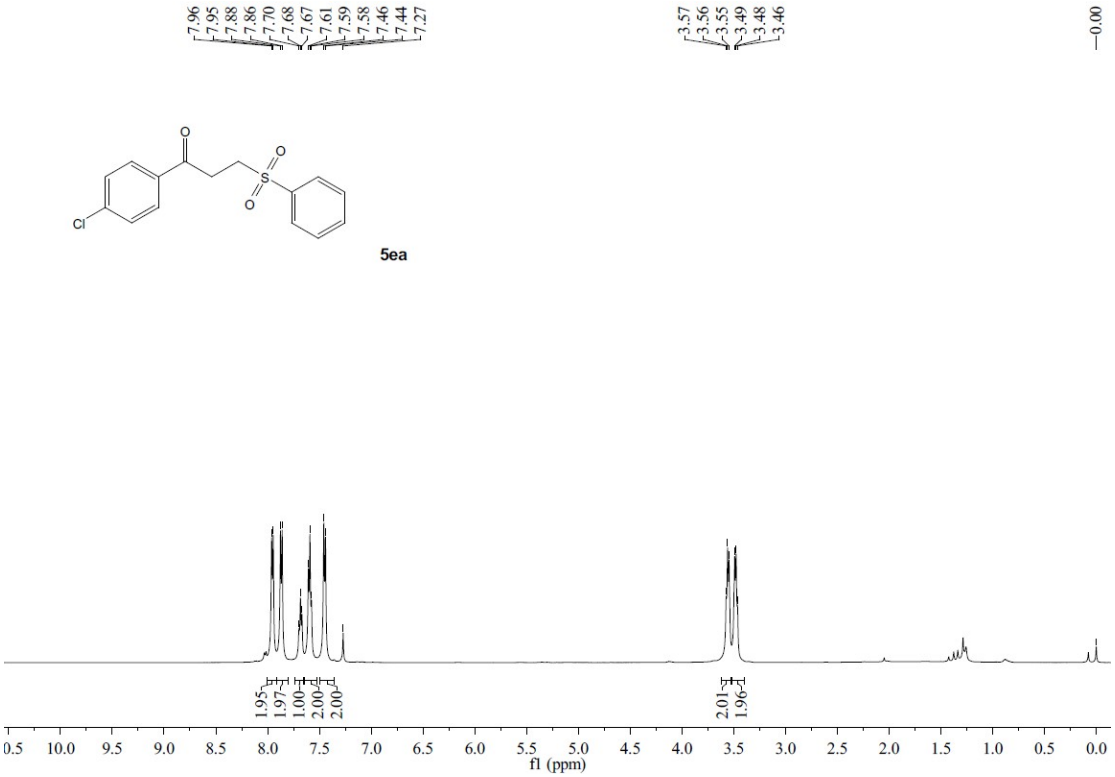
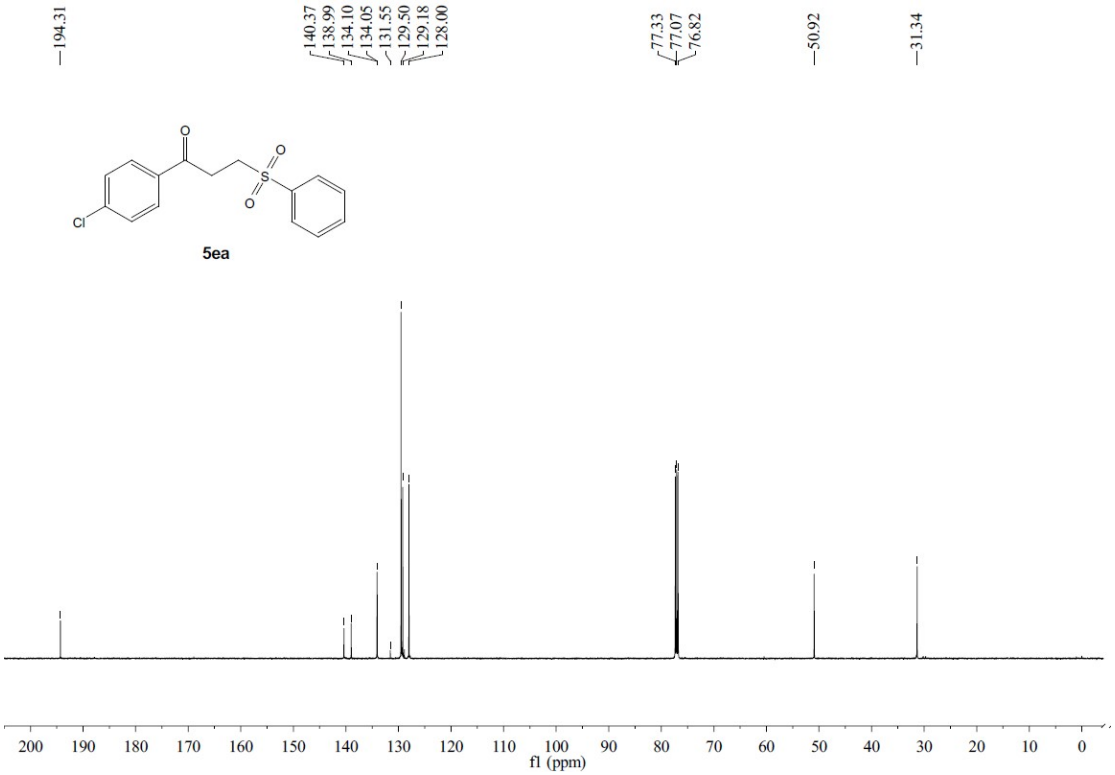
75.76
50.05
30.36
5ca
f1 (ppm)

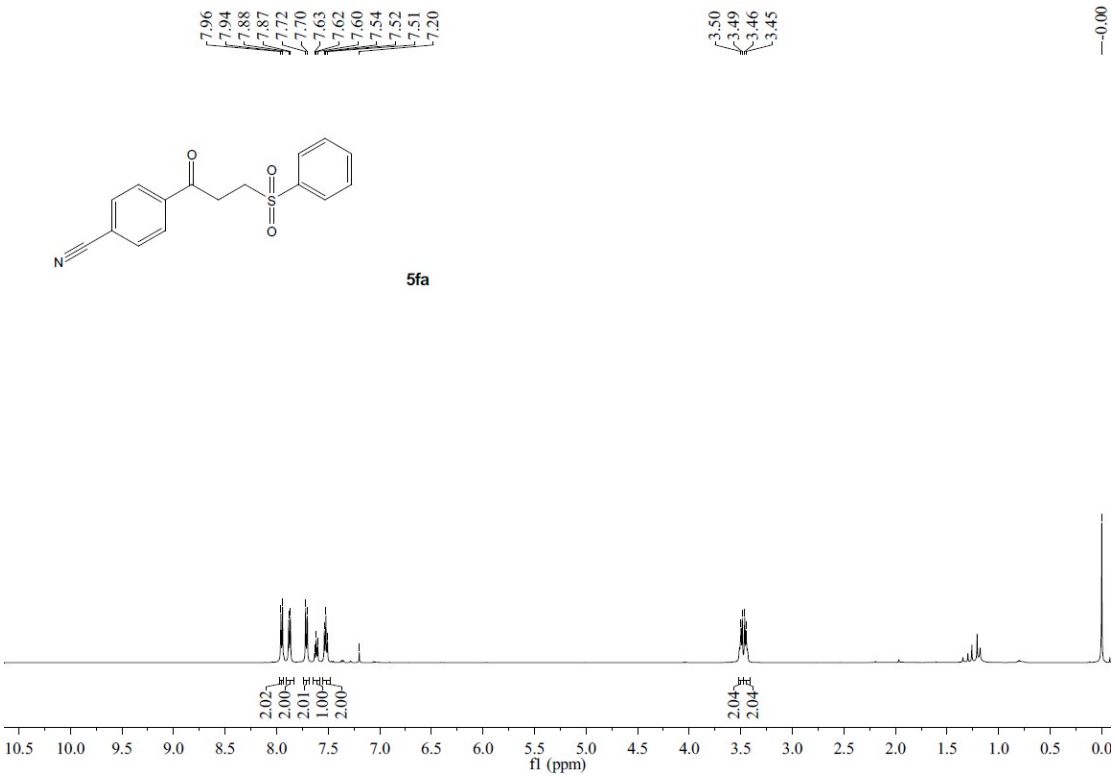

7.97
7.96
7.95
7.70
7.68
7.67
7.60
7.59
7.57
7.28
7.16
7.14
7.13
3.56
3.55
3.49
3.48
0.00
O
O
S
O
O
F
4.00
1.01
1.96
1.98
1.99
1.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
-103.59
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

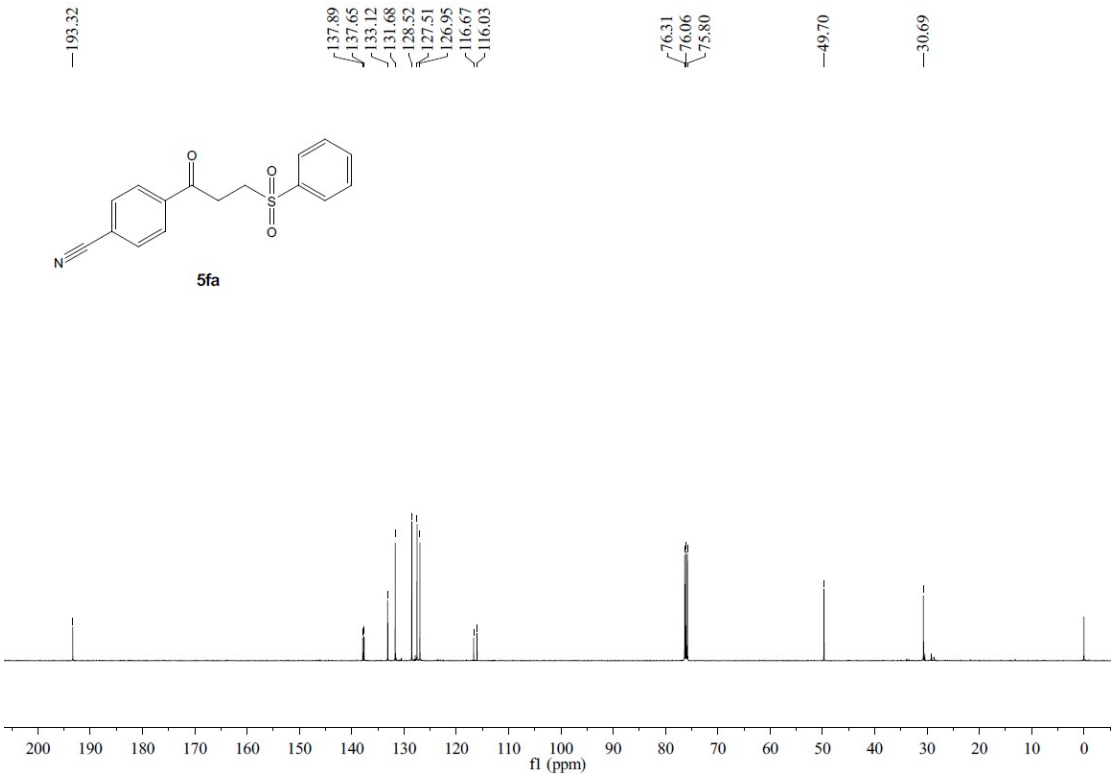
5da

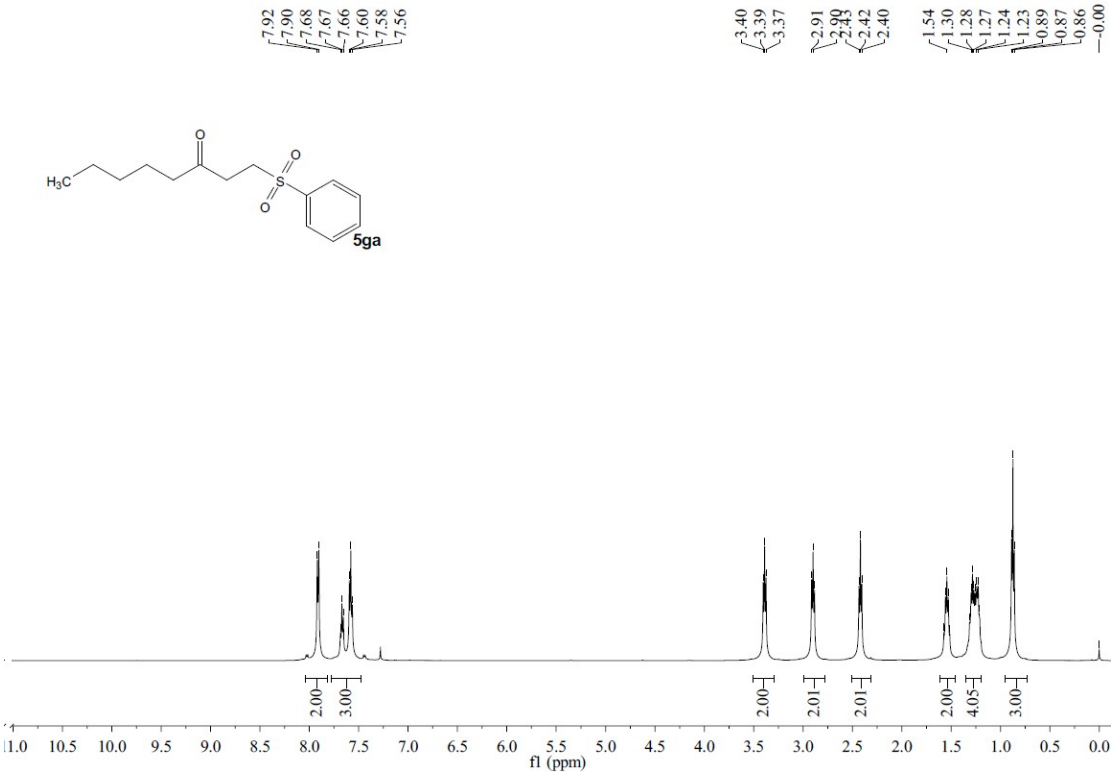

193.89
167.13
165.09
139.02
134.02
132.28
132.26
130.84
130.77
129.48
128.00
116.09
115.91
77.33
77.08
76.83
50.97
31.27
F
5da
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

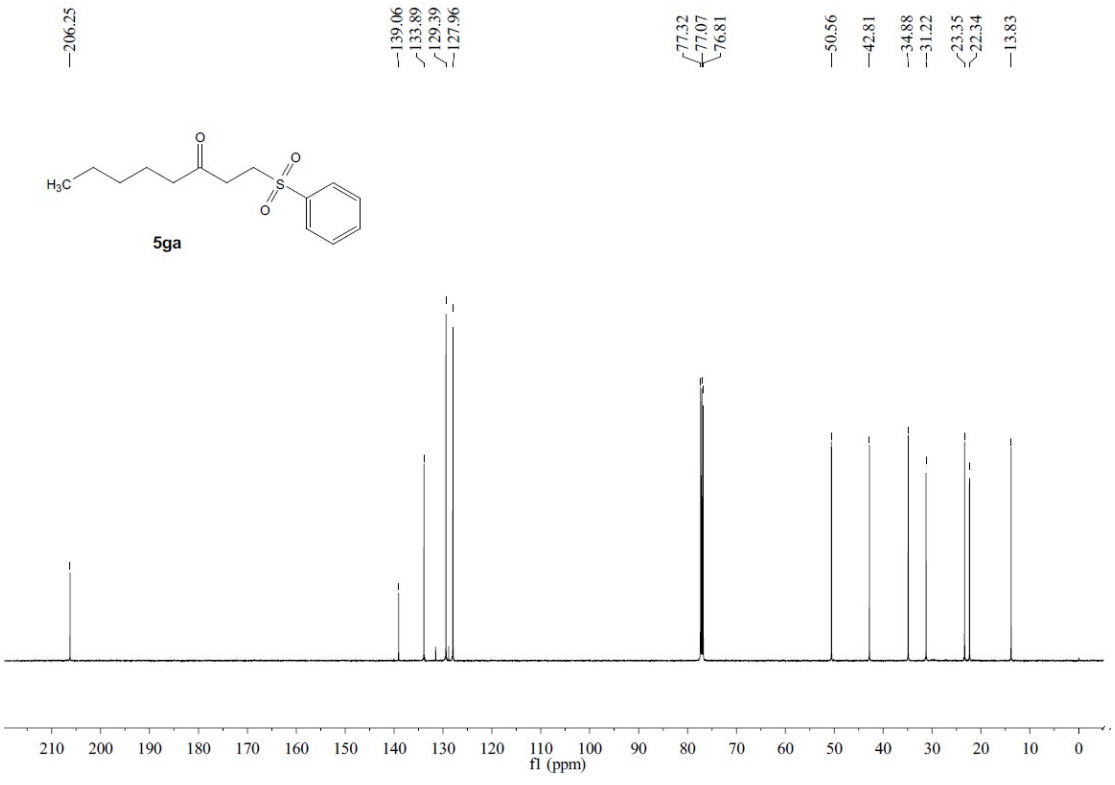

7.96
7.95
7.88
7.86
7.70
7.68
7.67
7.61
7.59
7.58
7.46
7.44
7.27
3.57
3.56
3.55
3.49
3.48
3.46
0.00
Cl
5ea
1.95
1.97
1.00
2.00
2.00
2.01
1.96
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

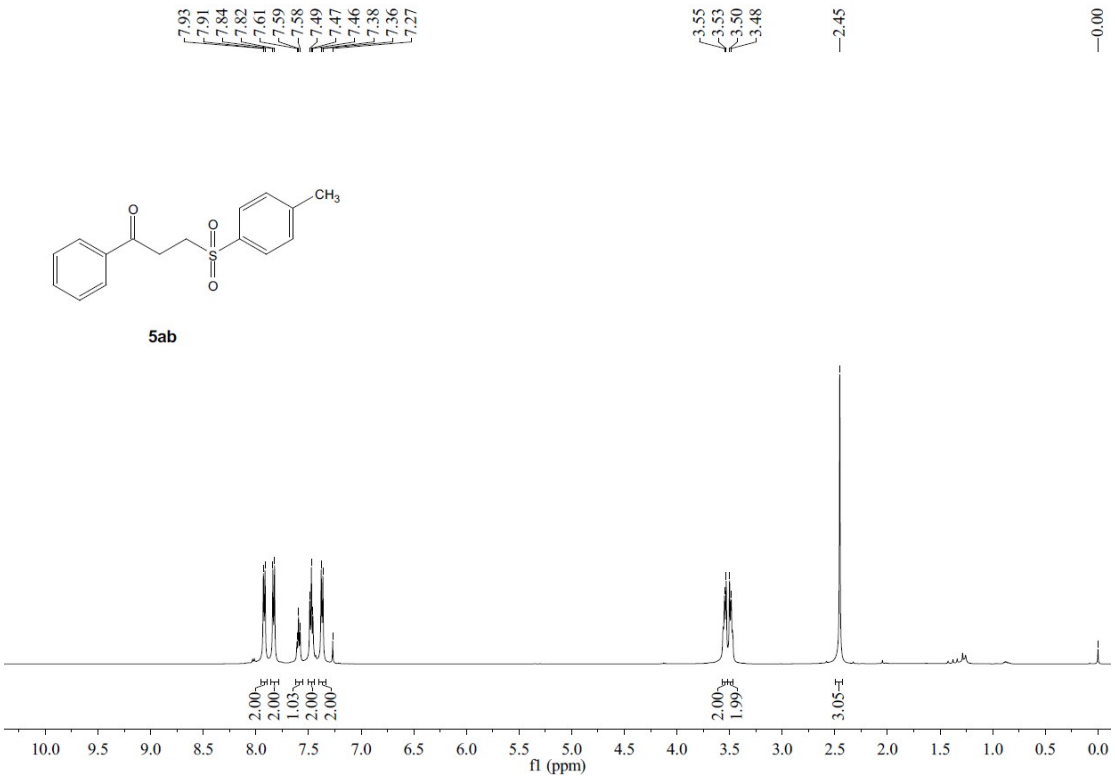

194.31
140.37
138.99
134.10
134.05
131.55
129.50
129.18
128.00
77.33
77.07
76.82
50.92
31.34
O
O
S
O
Cl
5ea
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.96
7.94
7.88
7.87
7.72
7.70
7.63
7.62
7.60
7.54
7.52
7.51
7.20
3.50
3.49
3.46
3.45
0.00
O
O
S
O
N
5fa
2.02
2.00
2.01
1.00
2.00
2.04
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


193.32
137.89
137.65
133.12
131.68
128.52
127.51
126.95
116.67
116.03
76.31
76.06
75.80
49.70
30.69
5fa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.92
7.90
7.68
7.67
7.66
7.60
7.58
7.56
3.40
3.39
3.37
2.91
2.90
2.43
2.42
2.40
1.54
1.30
1.28
1.27
1.24
1.23
0.89
0.87
0.86
0.00
5ga
2.00
3.00
2.00
2.01
2.01
2.00
4.05
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


206.25
139.06
133.89
129.39
127.96
77.32
77.07
76.81
50.56
42.81
34.88
31.22
23.35
22.34
13.83
5ga
fl (ppm)


7.93
7.91
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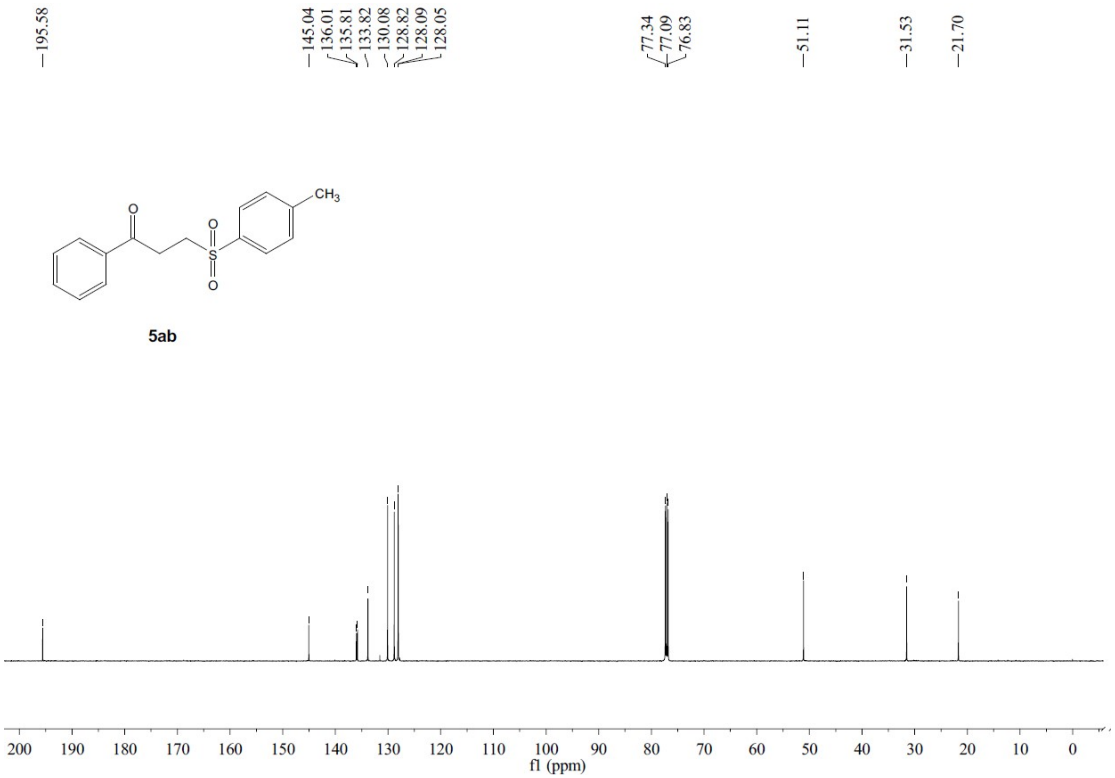
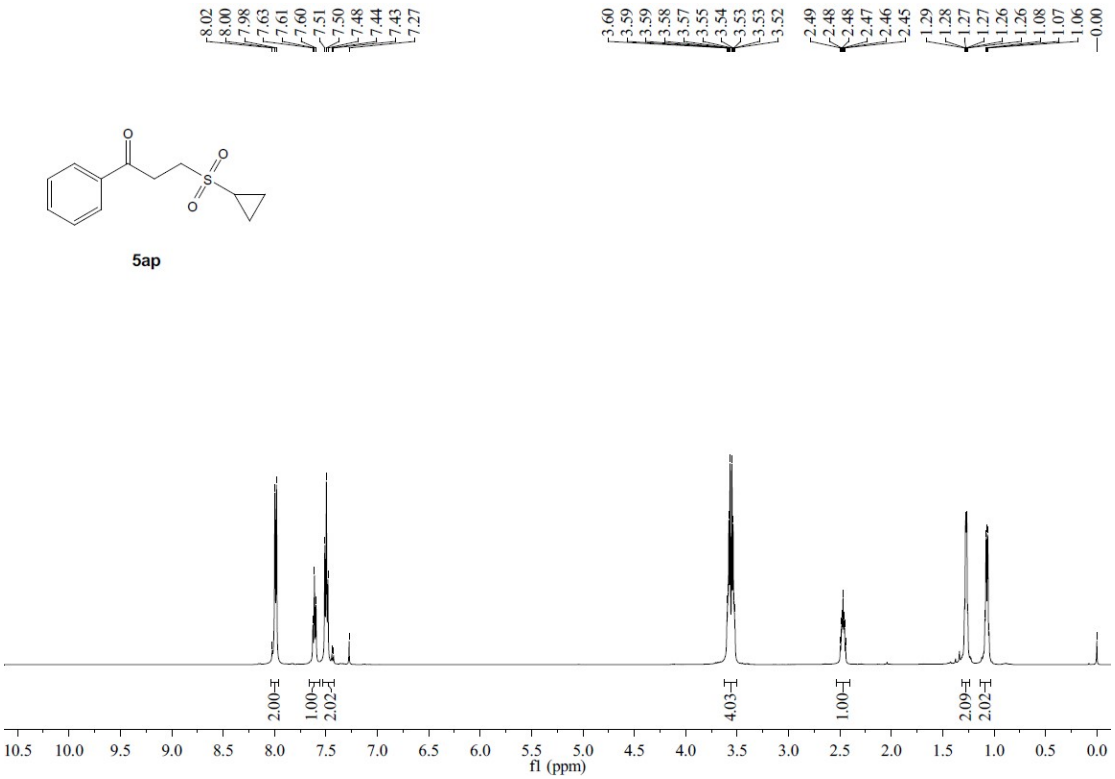
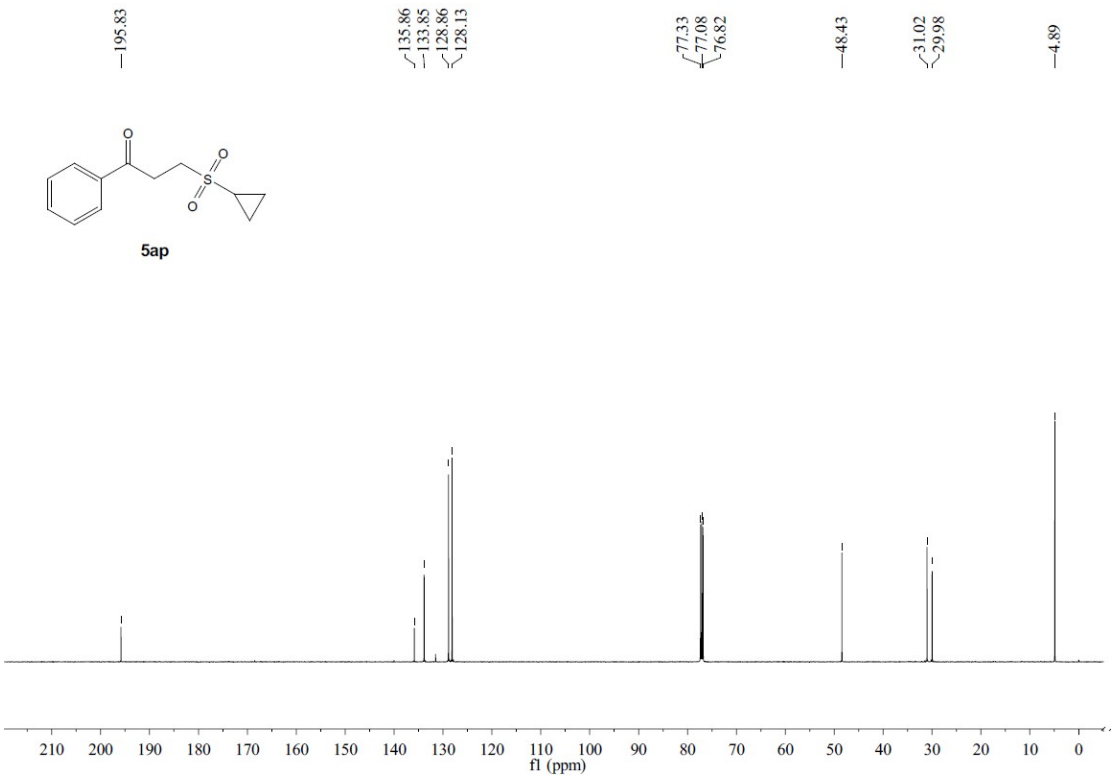
7.82
7.61
7.59
7.58
7.49
7.47
7.46
7.38
7.36
7.27
3.55
3.53
3.50
3.48
2.45
0.00
5ab
2.00
2.00
1.03
2.00
2.00
2.00
1.99
3.05
fl (ppm)

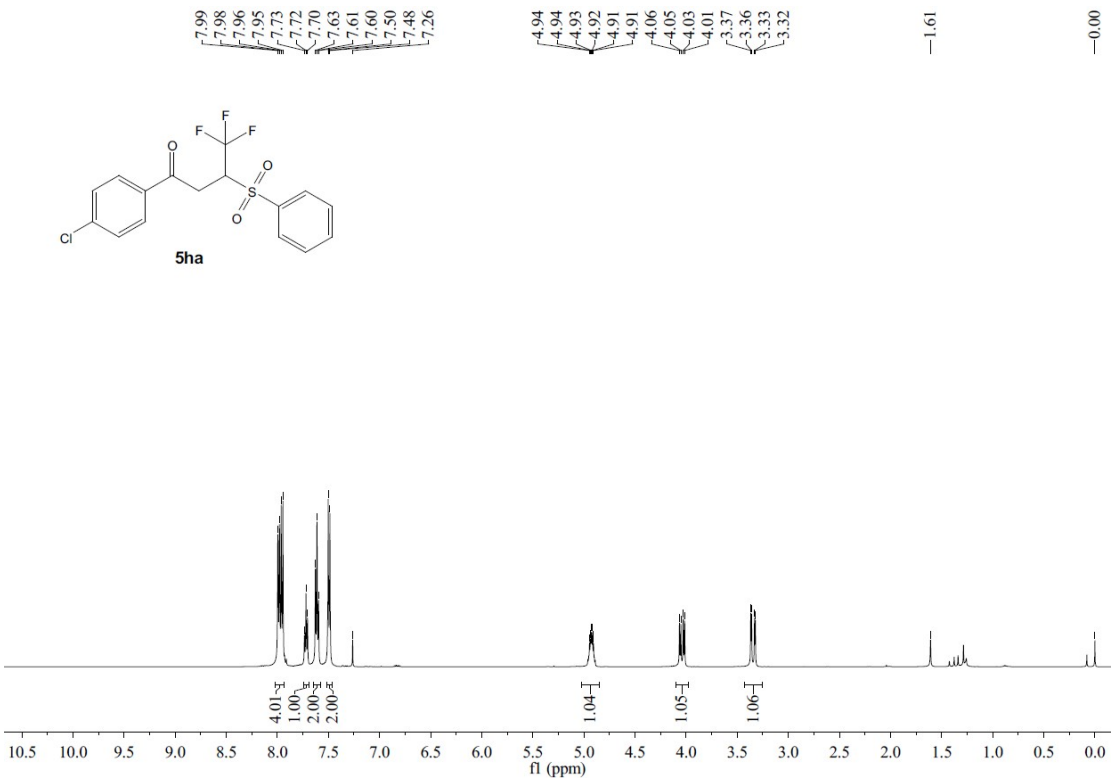

195.58
145.04
136.01
135.81
133.82
130.08
128.82
128.09
128.05
77.34
77.09
76.83
51.11
31.53
21.70
CH3
O
O
S
O
fl (ppm)

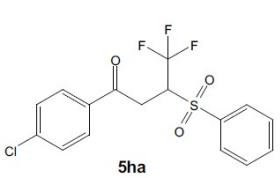
5ab


8.02
8.00
7.98
7.63
7.61
7.60
7.51
7.50
7.48
7.44
7.43
7.27
3.60
3.59
3.59
3.58
3.57
3.55
3.54
3.53
3.53
3.52
2.49
2.48
2.48
2.47
2.46
2.45
1.29
1.28
1.27
1.27
1.26
1.26
1.08
1.07
1.06
0.00
O
O
S
O
2.00
1.00
2.02
4.03
1.00
2.09
2.02
fl (ppm)

5ap

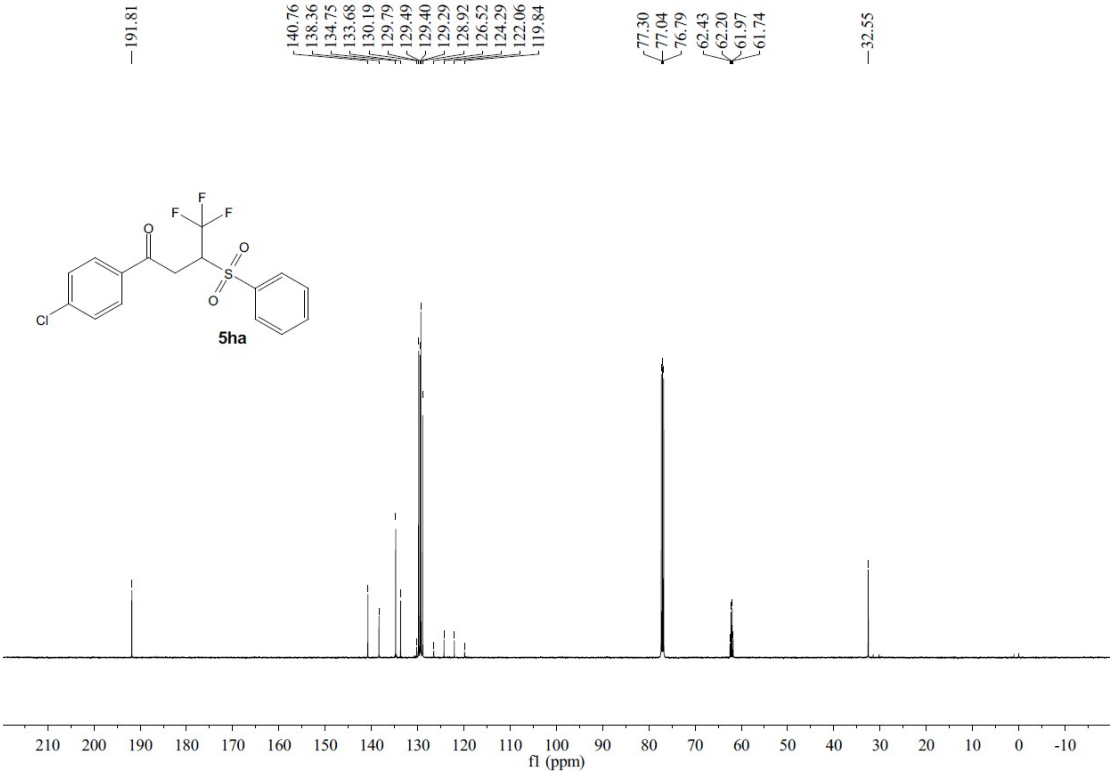

195.83
135.86
133.85
128.86
128.13
77.33
77.08
76.82
48.43
31.02
29.98
4.89
5ap
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

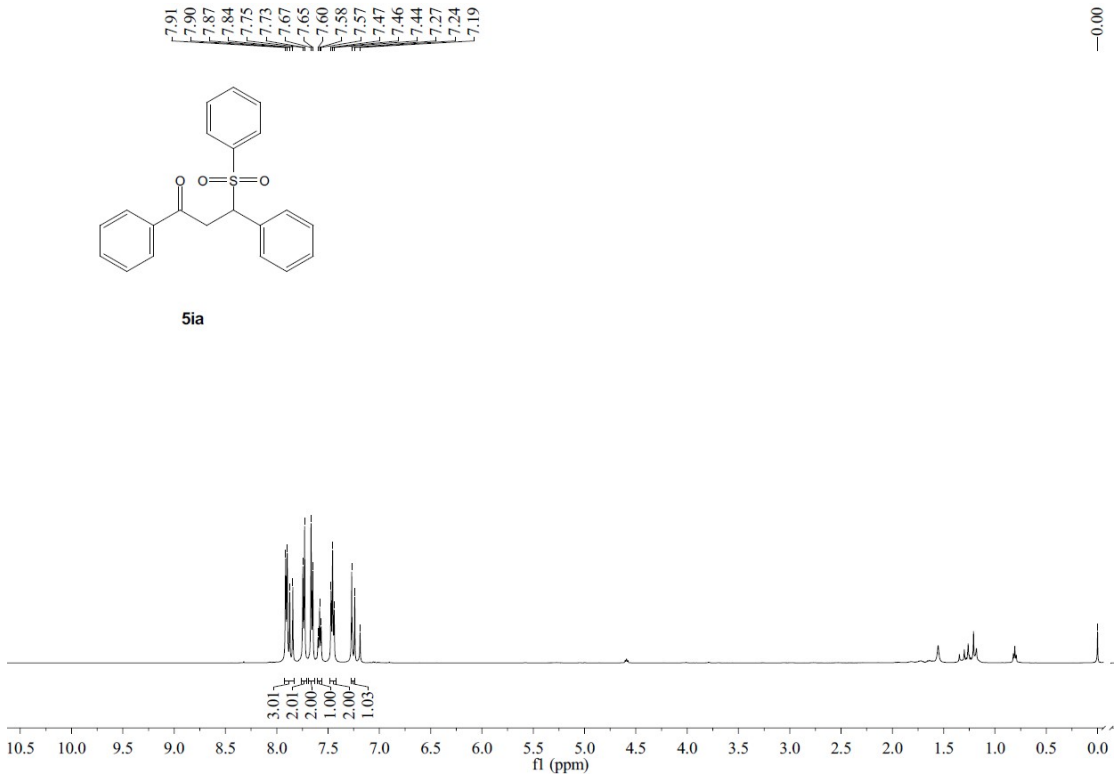

7.99
7.98
7.96
7.95
7.73
7.72
7.70
7.63
7.61
7.60
7.50
7.48
7.26
4.94
4.94
4.93
4.92
4.91
4.91
4.06
4.05
4.03
4.01
3.37
3.36
3.33
3.32
1.61
0.00
5ha
4.01
1.00
2.00
2.00
1.04
1.05
1.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

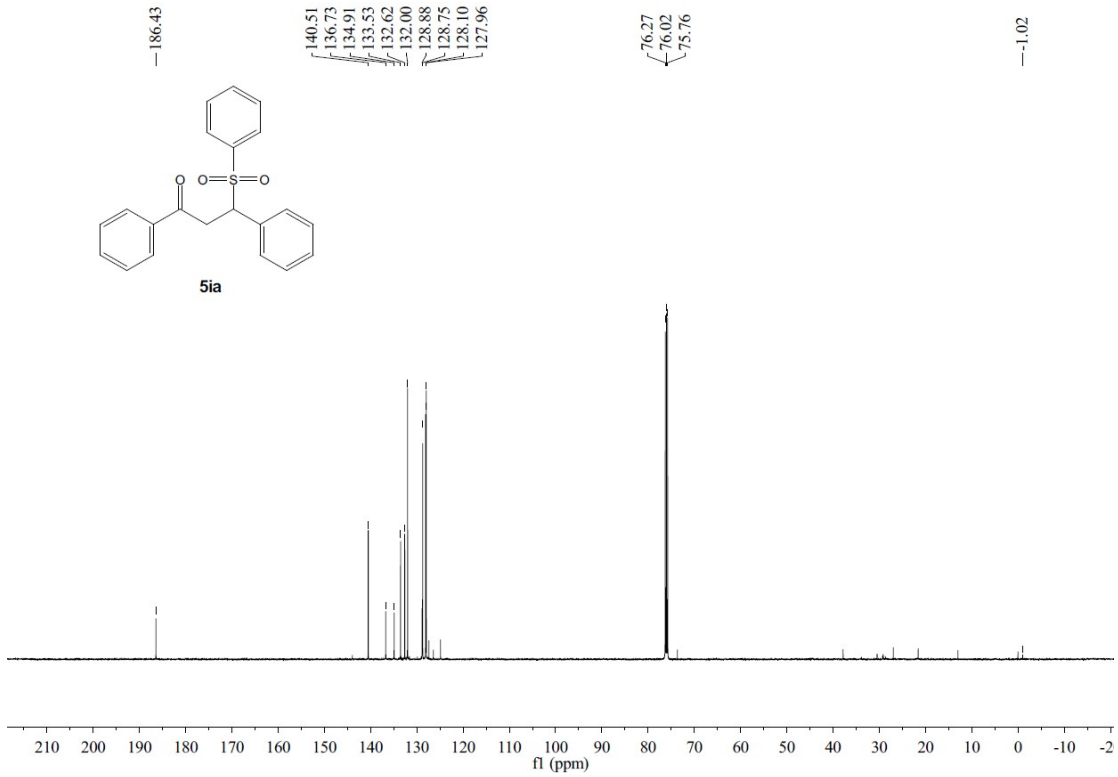

F
F
F
O
O
S
O
Cl

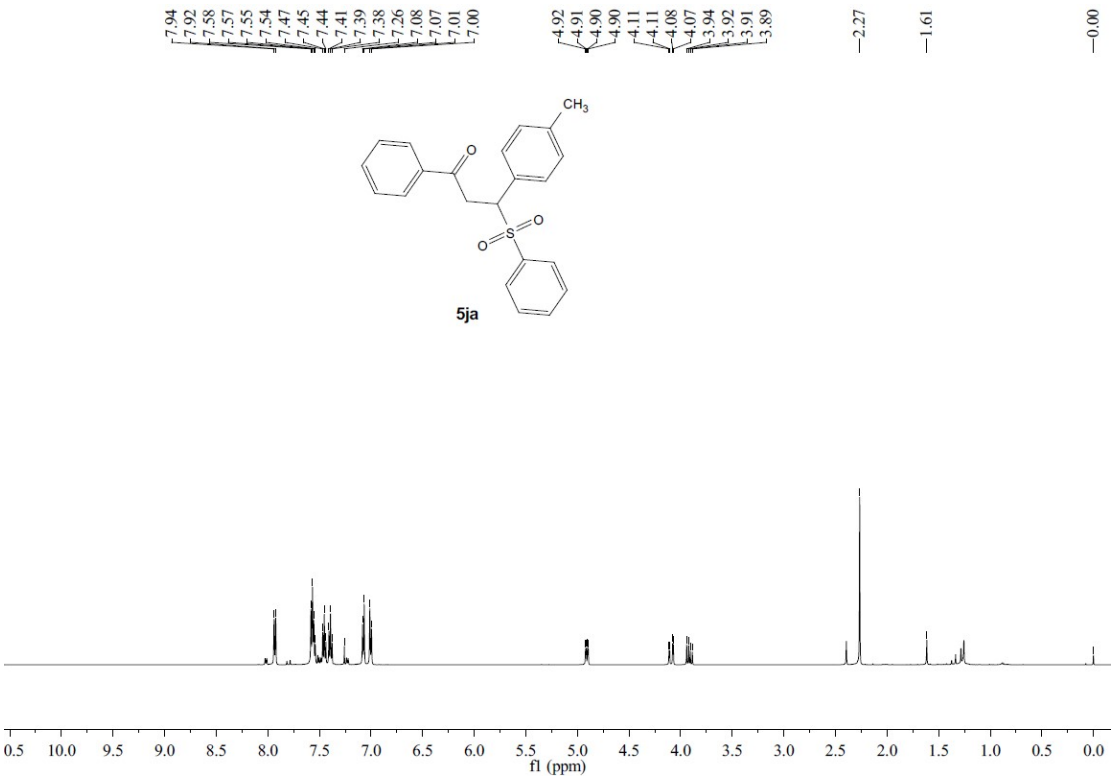
5ha

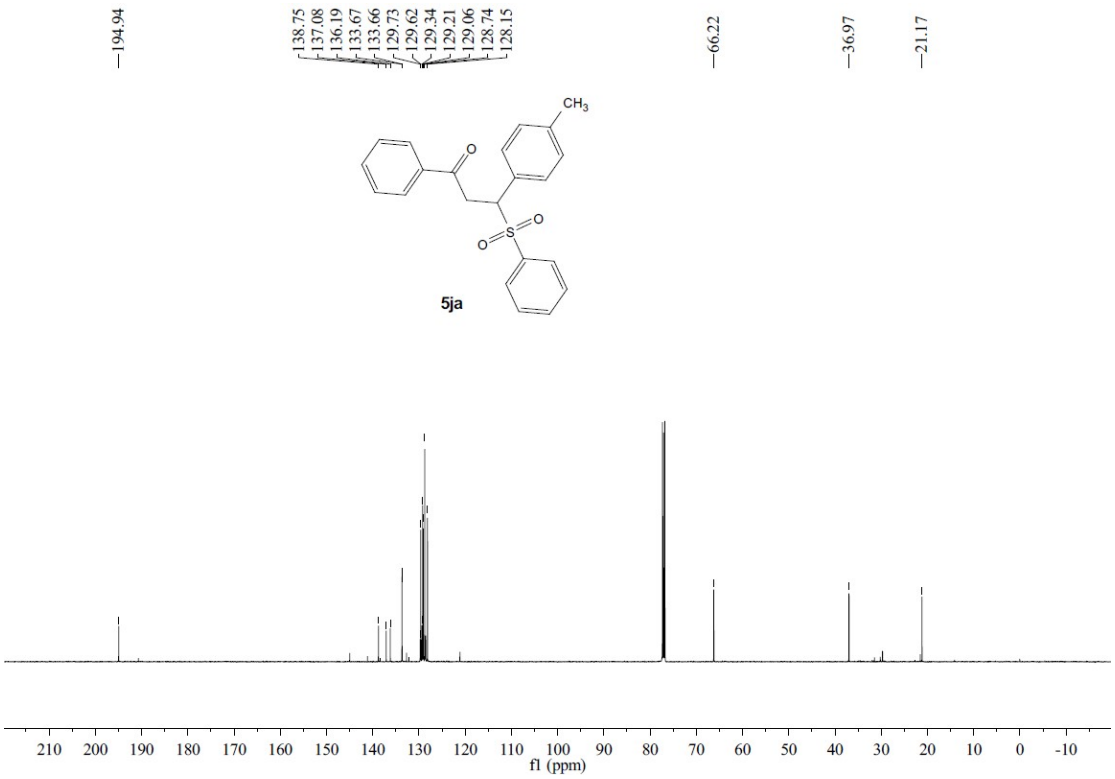
-65.19
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

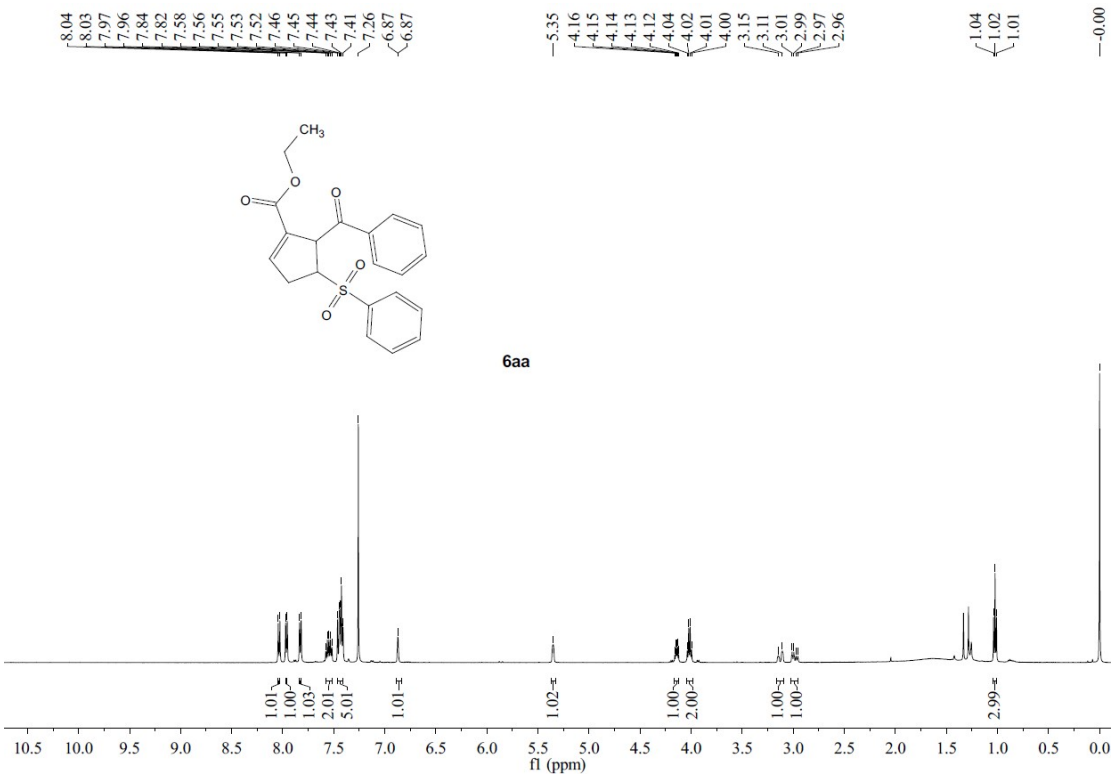

191.81
140.76
138.36
134.75
133.68
130.19
129.79
129.49
129.40
129.29
128.92
126.52
124.29
122.06
119.84
77.30
77.04
76.79
62.43
62.20
61.97
61.74
32.55
F
F
F
O
O
S
O
Cl
5ha
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

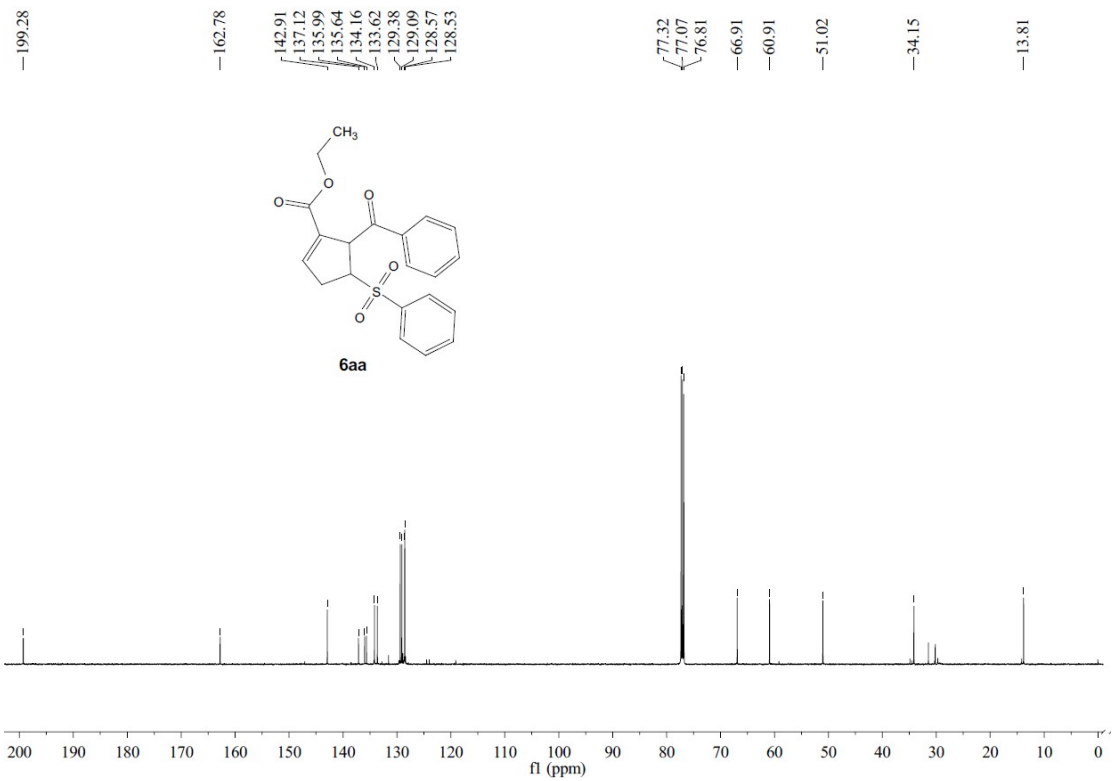

7.91
7.90
7.87
7.84
7.75
7.73
7.67
7.65
7.60
7.58
7.57
7.47
7.46
7.44
7.27
7.24
7.19
0.00
5ia
3.01
2.01
2.00
1.00
2.00
1.03
fl (ppm)

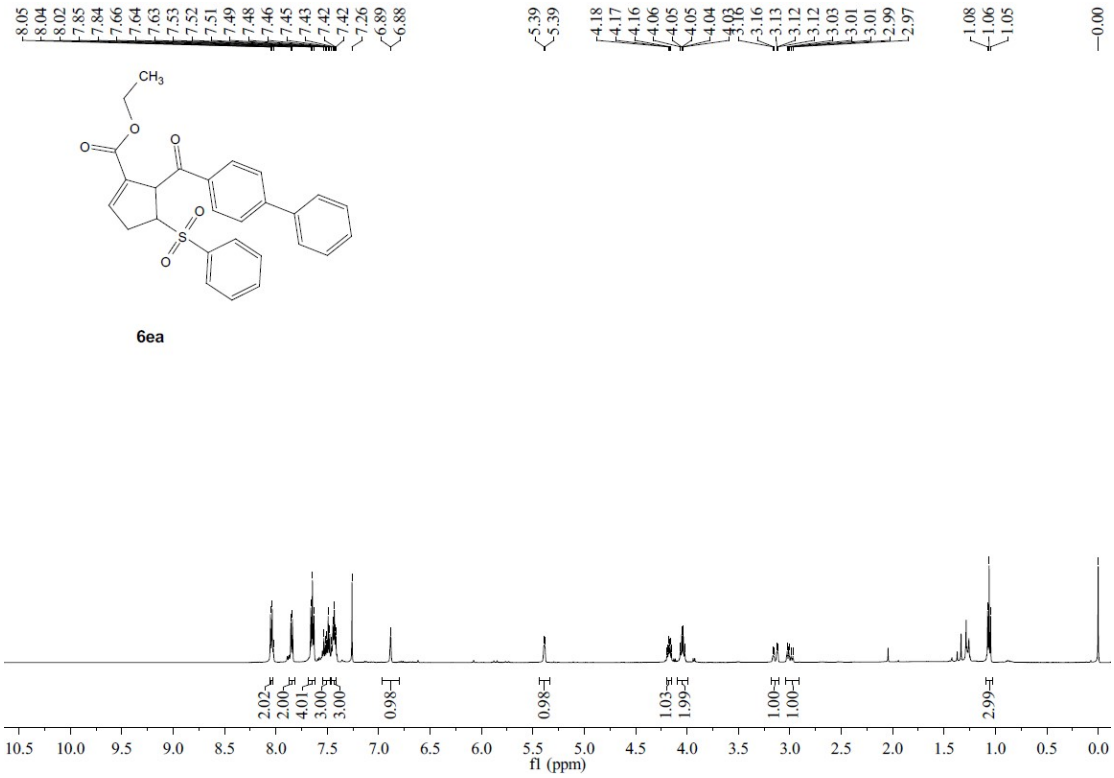

186.43
140.51
136.73
134.91
133.53
132.62
132.00
128.88
128.75
128.10
127.96
76.27
76.02
75.76
1.02
5ia
fl (ppm)

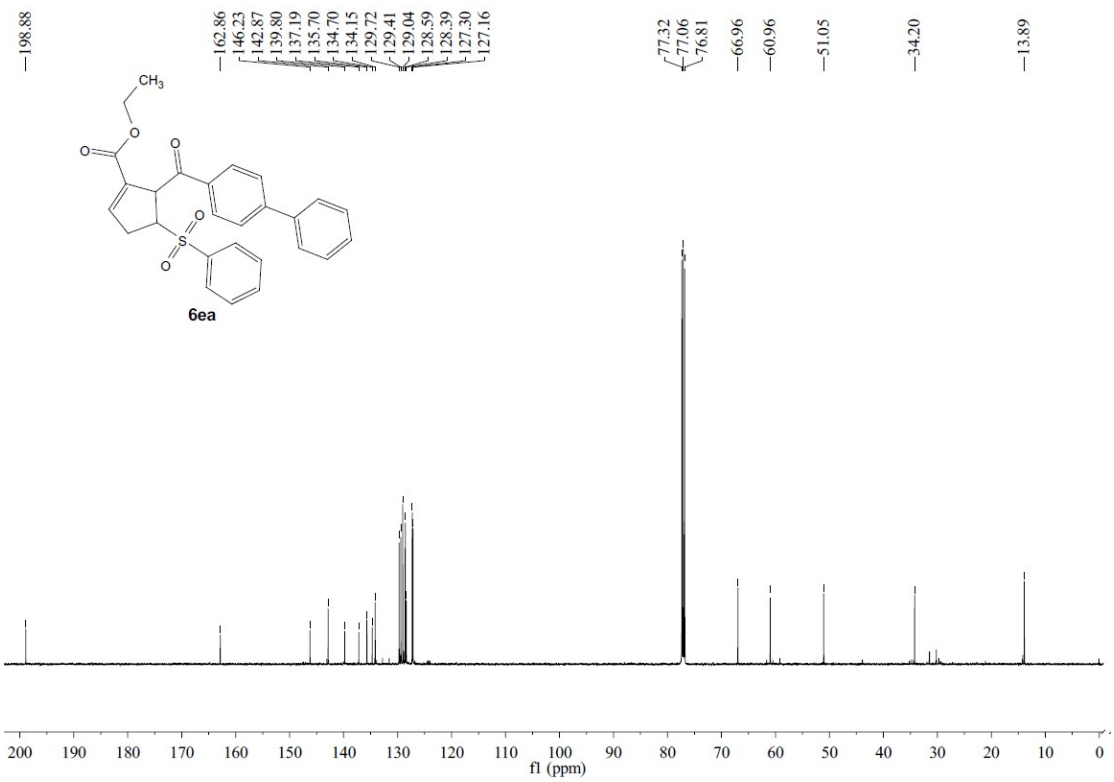

7.94
7.92
7.58
7.57
7.55
7.54
7.47
7.45
7.44
7.41
7.39
7.38
7.26
7.08
7.07
7.01
7.00
4.92
4.91
4.90
4.90
4.11
4.11
4.08
4.07
3.94
3.92
3.91
3.89
2.27
1.61
0.00
CH3
O
O
S
O
5ja
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.94
138.75
137.08
136.19
133.67
133.66
129.73
129.62
129.34
129.21
129.06
128.74
128.15
66.22
36.97
21.17
CH3
O
O
S
O
5ja
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.04
8.03
7.97
7.96
7.84
7.82
7.58
7.56
7.55
7.53
7.52
7.46
7.45
7.44
7.43
7.41
7.26
6.87
6.87
5.35
4.16
4.15
4.14
4.13
4.12
4.04
4.02
4.01
4.00
3.15
3.11
3.01
2.99
2.97
2.96
1.04
1.02
1.01
0.00
CH3
O
O
O
O
S
O
6aa
1.01
1.00
1.03
2.01
5.01
1.01
1.02
1.00
2.00
1.00
1.00
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


199.28
162.78
142.91
137.12
135.99
135.64
134.16
133.62
129.38
129.09
128.57
128.53
77.32
77.07
76.81
66.91
60.91
51.02
34.15
13.81
CH3
O
O
O
O
S
O
6aa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.05
8.04
8.02
7.85
7.84
7.66
7.64
7.63
7.53
7.52
7.51
7.49
7.48
7.46
7.45
7.43
7.42
7.42
7.26
6.89
6.88
5.39
5.39
4.18
4.17
4.16
4.06
4.05
4.05
4.04
4.03
3.16
3.16
3.13
3.12
3.12
3.03
3.01
3.01
2.99
2.97
1.08
1.06
1.05
0.00
CH3
O
O
O
O
S
O
6ea
2.02
2.00
4.01
3.00
3.00
0.98
0.98
1.03
1.99
1.00
1.00
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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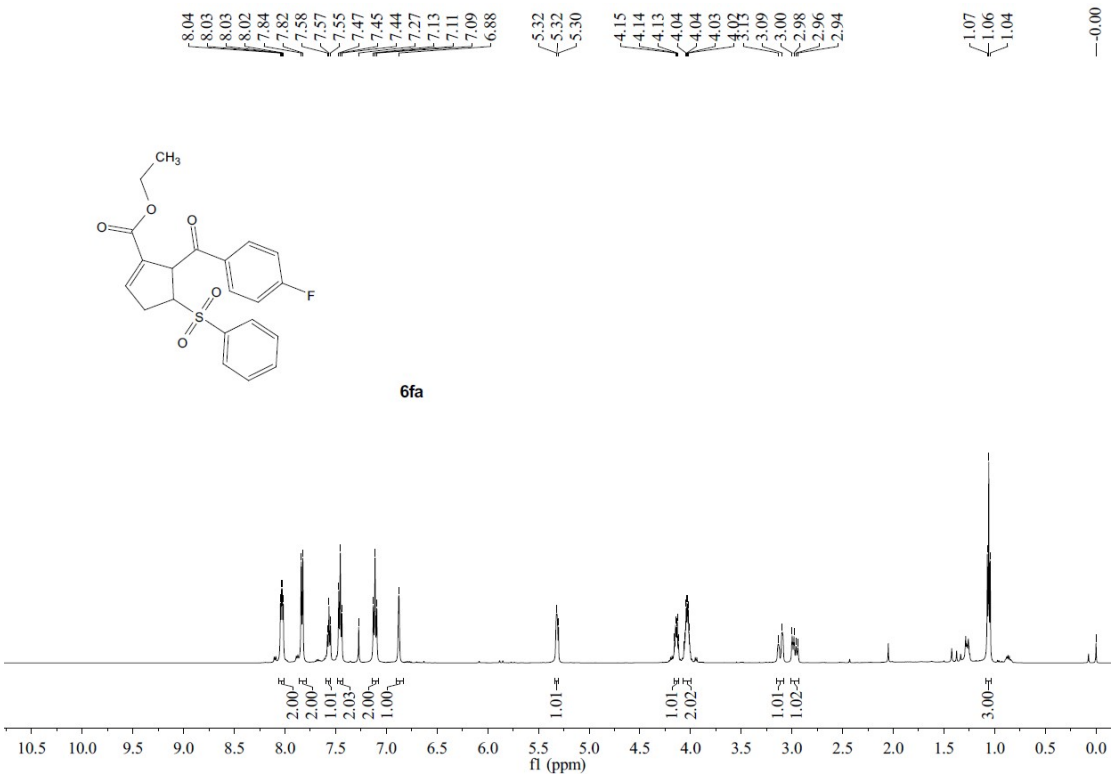
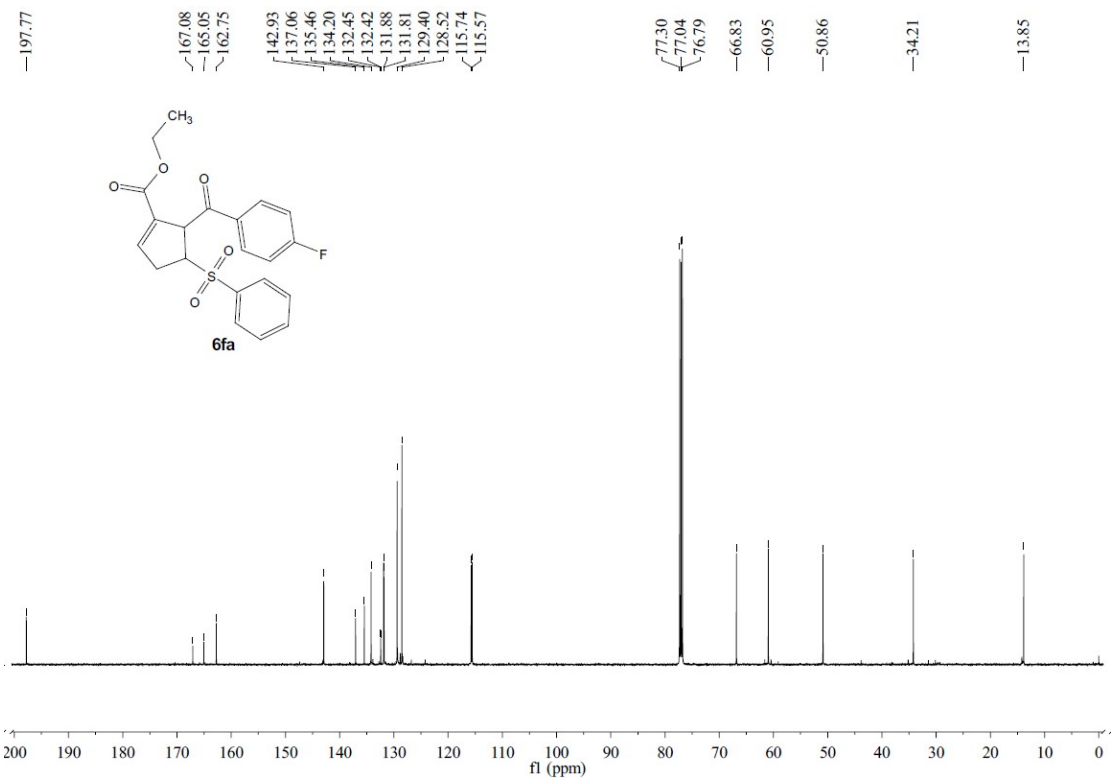
146.23
142.87
139.80
137.19
135.70
134.70
134.15
129.72
129.41
129.04
128.59
128.39
127.30
127.16
77.32
77.06
76.81
66.96
60.96
51.05
34.20
13.89
CH3
O
O
O
O
S
O
6ea
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.04
8.03
8.03
8.02
7.84
7.82
7.58
7.57
7.55
7.47
7.45
7.44
7.27
7.13
7.11
7.09
6.88
5.32
5.32
5.30
4.15
4.14
4.13
4.04
4.04
4.03
4.02
3.15
3.09
3.00
2.98
2.96
2.94
1.07
1.06
1.04
0.00
CH3
O
O
O
O
S
O
F
6fa
2.00
2.00
1.01
2.03
2.00
1.00
1.01
1.01
2.02
1.01
1.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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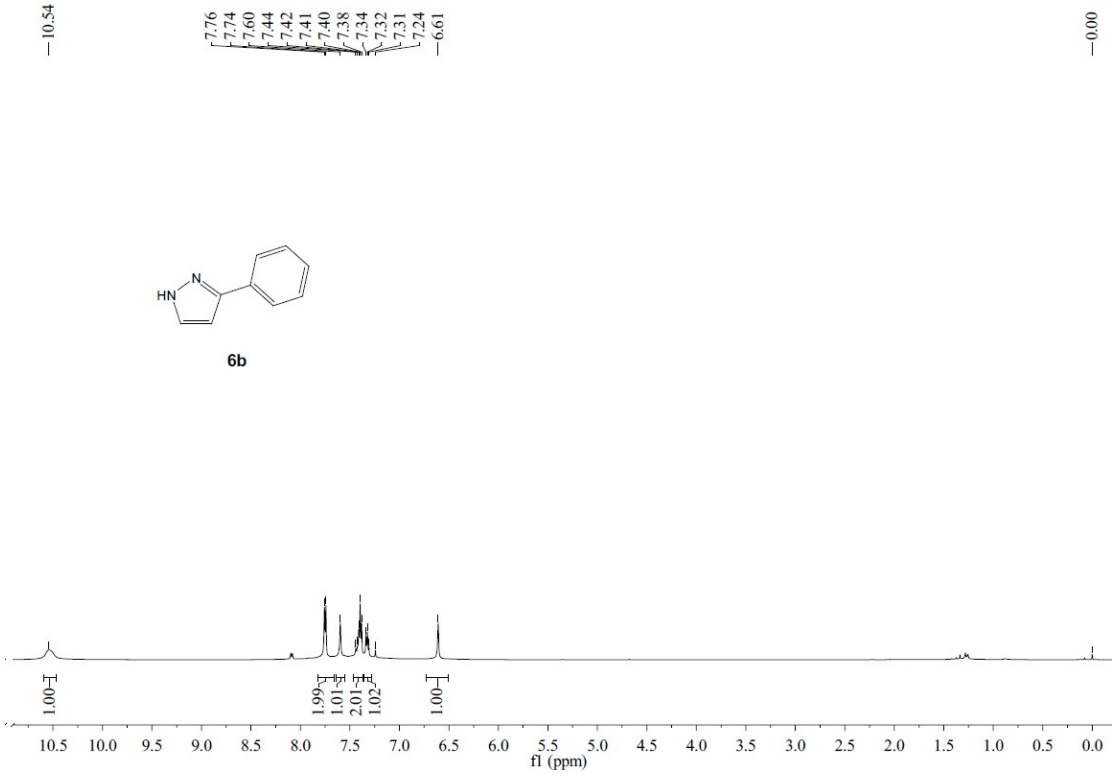
167.08
165.05
162.75
142.93
137.06
135.46
134.20
132.45
132.42
131.88
131.81
129.40
128.52
115.74
115.57
77.30
77.04
76.79
66.83
60.95
50.86
34.21
13.85
CH3
O
O
O
O
S
O
F
6fa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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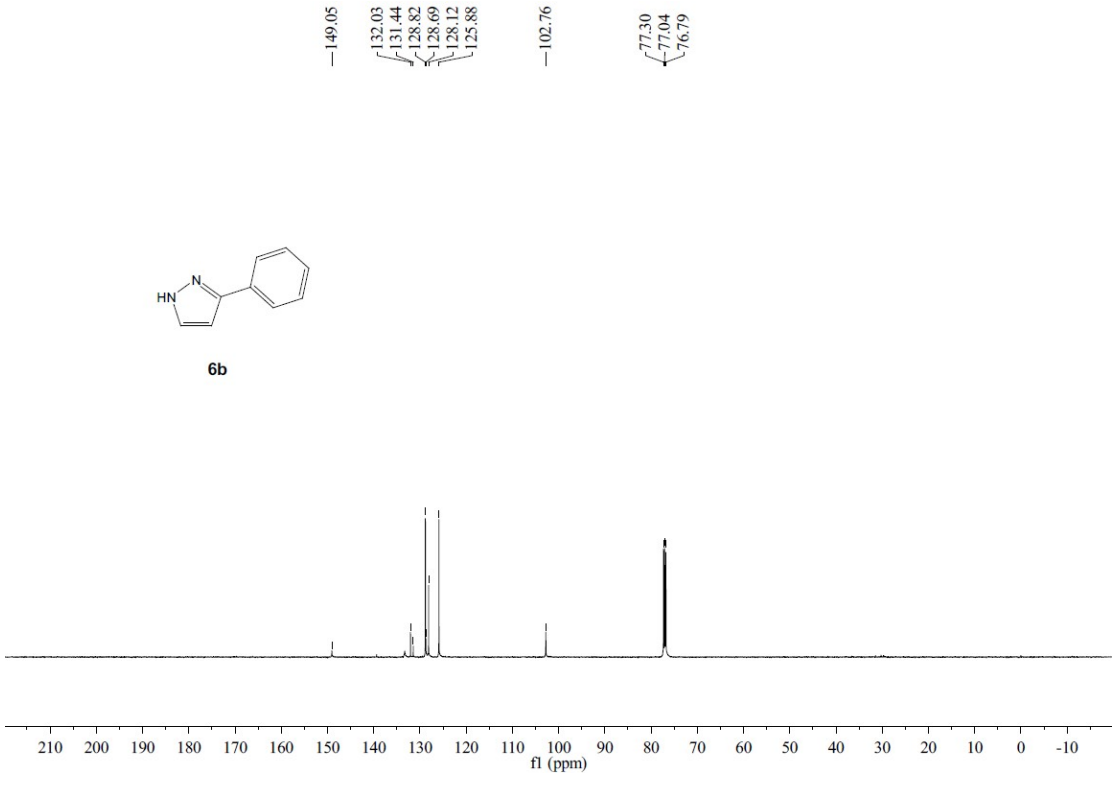
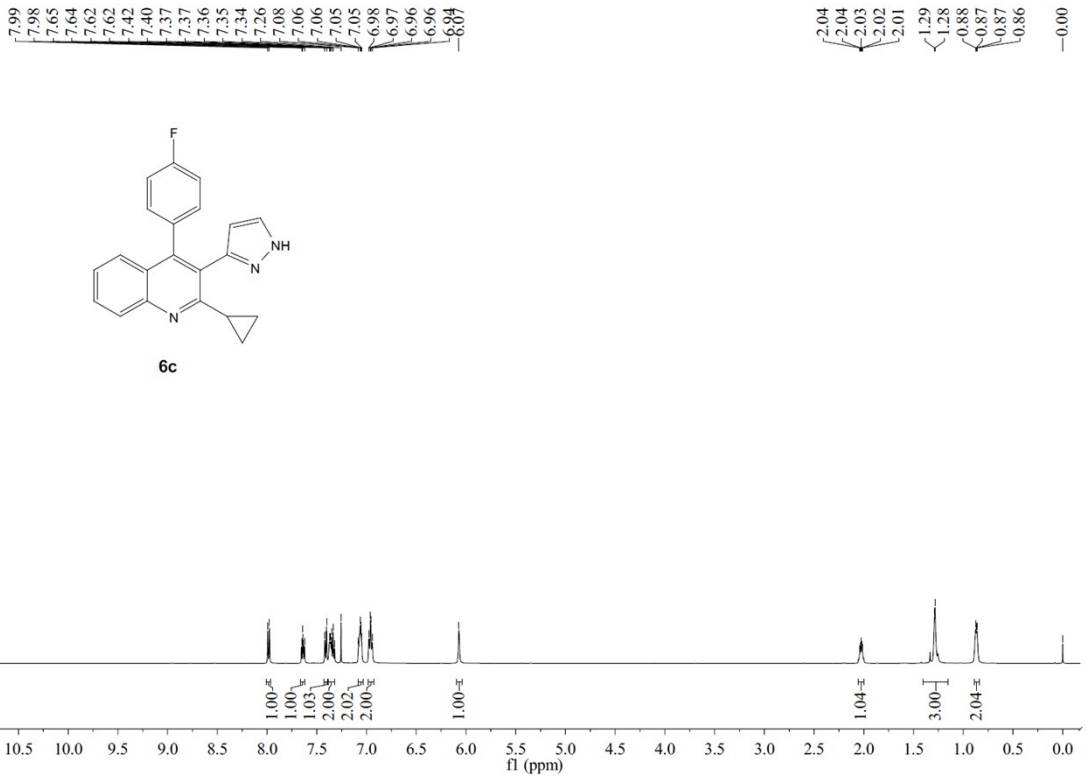
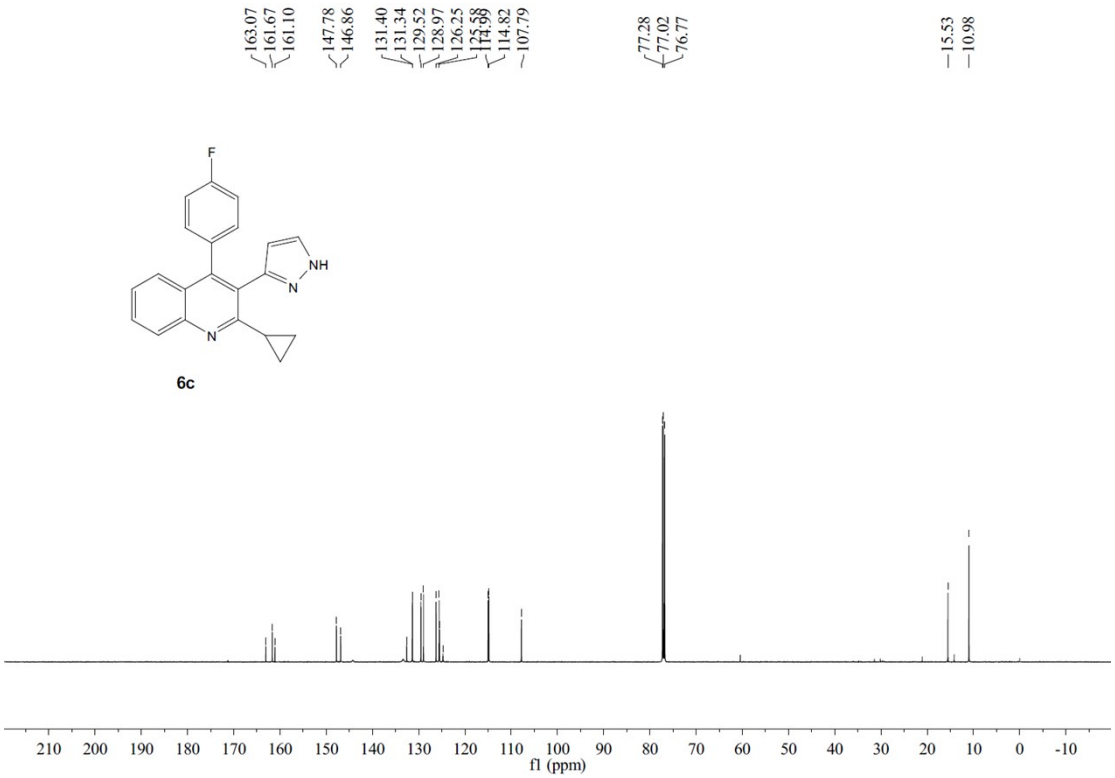
7.76
7.74
7.60
7.44
7.42
7.41
7.40
7.38
7.34
7.32
7.31
7.24
6.61
0.00
HN
N
6b
1.00
1.99
1.01
2.01
1.02
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


149.05
132.03
131.44
128.82
128.69
128.12
125.88
102.76
77.30
77.04
76.79
HN
N
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.99
7.98
7.65
7.64
7.62
7.62
7.42
7.40
7.37
7.37
7.36
7.35
7.34
7.26
7.08
7.06
7.06
7.05
7.05
6.98
6.97
6.96
6.96
6.94
6.07
2.04
2.04
2.03
2.02
2.01
1.29
1.28
0.88
0.87
0.87
0.86
0.00
F
NH
N
N
6c
1.00
1.00
1.03
2.00
2.02
2.00
1.00
1.04
3.00
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
-114.10
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


163.07
161.67
161.10
147.78
146.86
131.40
131.34
129.52
128.97
126.25
125.58
114.82
107.79
77.28
77.02
76.77
15.53
10.98
F
NH
N
N
6c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)