Electronic Supplementary Material (ESI) for RSC Advances.


*Supporting Information*

# Photoredox-Catalyzed Sulfonylation of Diaryliodonium Salts with DABSO and Silyl Enolates Involving the Insertion of $SO_2$

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## I. General remarks

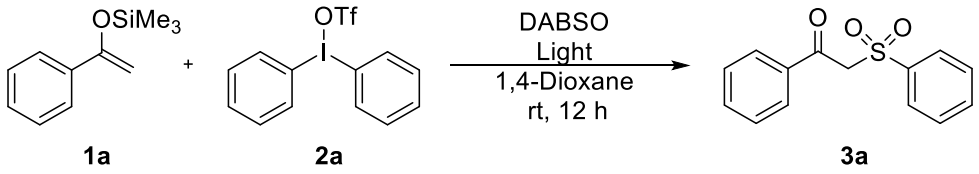
NMR spectra were obtained on Bruker AV-400 MHz and AV-600 MHz spectrometers. The $^{1}H$ NMR chemical shifts were measured relative to $CDCl_3$ as the internal reference ($CDCl_3$: $\delta$ = 7.26 ppm). The $^{13}C$ NMR chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: $\delta$ = 77.16 ppm). High resolution mass spectra (HRMS) were obtained with a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Silyl enolates and diaryliodonium salts were prepared according to the literature procedures.[1] $SO_2$-MeCN solution was prepared according to the literature procedure.[2] All catalytic experiments were carried out using ultra dry solvents purchased from J&K Scientific. The GC internal standard, *n*-$C_{12}H_{26}$ was degassed with nitrogen and dried over activated 4 Å molecular sieve beads before use. Gas chromatography (GC) analysis was performed on a Agilent8890B GC System with Agilent J & W GC column DB-5MS-UI.

## II. Condition optimization

*Procedure without any photocatalyst*: In a nitrogen-filled glove box, **1a** (0.2 mmol, 2.0 equiv), **2a** (0.1 mmol, 1.0 equiv), DABSO (0.2 mmol, 2.0 equiv), GC standard *n*-$C_{12}H_{26}$ (10 μL) and 1,4-dioxane (1.0 mL) were added to a 10-mL Schlenk tube. After stirring at room temperature Under a specific light source for 12 h, the reaction mixture was diluted with 3 mL of EtOAc. Aliquots were taken from the organic phase, and passed through a short plug of silica gel with EtOAc washing (about 1.5 mL). The filtrate was subjected to GC analysis to determine the yield of the product **3a**.

**Table S1.** The effect of light source in the absence of photocatalysts.[a]



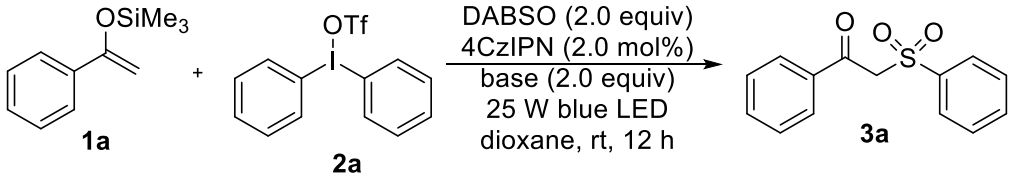

**1a** **2a** **3a**

| Entry | Light | Yield **3a** (%)[b] |
|---|---|---|
| 1 | 25 W blue LED (465 nm) | 47 |

| | | |
|---|---|---|
| 2 | 10 W blue LED **(465 nm)** | 35 |
| 3 | 30 W blue LED **(465 nm)** | 41 |
| 4 | 24 W white-light LED | 0 |
| 5 | 18 W CFL | 0 |
| 6 | Kessil light (390 nmm) | 15 |
| 7 | UV (600W) | 24 |
| 8[c] | 25 W blue LED (465 nm) | 55 |
| 9 | no light | 0 |

[a] For entry 1-6 and 8, the sealed reaction test-tubes were placed in a test-tube rack on a magnetic stirplate that was flanked by two lights. The temperature in the test-tube rack was maintained ⩾30 °C with a DC condensing fan. For entry 7, the mixture, placed around the mercury lamp (purchased from Yuming, Shanghai) with a distance of 10 centimeters, was stirred under UV irradiation (0.67 W cm-1) at room temperature. [b] GC yields. [c] The mixture was stirred for 24 h.

**Table S2.** The effect of base.[a]

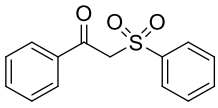



| Entry | base | Yield **3a** (%)[b] |
|---|---|---|
| 1 | NaO$^t$Bu | 71 |
| 2 | NaOH | 65 |
| 3 | $Na_2CO_3$ | 78 |
| 4 | $NaHCO_3$ | 80 |
| 5 | $NEt_3$ | 82 |

[a] Reaction conditions: **1a** (2.0 equiv), **2a** (0.1 mmol, 1.0 equiv), DABSO (2.0 equiv), 4CzIPN (2 mol%), base (2.0 equiv) and *n*-$C_{12}H_{26}$ (10 μL) in dioxane (1.0 mL) at room temperature for 12 h, irradiation with 25 W blue LED, under $N_2$. [b] GC yields.

## III. General procedure for the photoredox-catalyzed sulfonylation of diaryliodonium salts with DABSO and silyl enolates

In a nitrogen-filled glove box, **1a** (0.4 mmol, 2.0 equiv), **2a** (0.2 mmol, 1.0 equiv), DABSO (0.4 mmol, 2.0 equiv), 4CzIPN (2 mol%), and 1,4-dioxane (2.0 mL) were added to a 10-mL Schlenk tube. After stirring at room temperature under 25 W blue-light LED for 12 h, the reaction mixture was extracted with EtOAc. The solvent was removed under reduced pressure and the crude product was purified by silica gel flash chromatography (petroleum ether/EtOAc) to give the corresponding product.



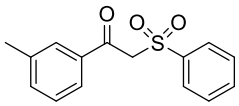
**1-Phenyl-2-(phenylsulfonyl)ethan-1-one** (**3a**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 85% yield. M.p.: 88-89 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.94-7.88 (m, 4H), 7.68-7.60 (m, 2H), 7.56-7.52 (m, 2H), 7.49-7.45 (t, $J$ = 8.0 Hz, 2H), 4.74 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.1, 138.9, 135.8, 134.5, 134.4, 129.4, 129.3, 129.0, 128.7, 63.6.

HRMS (ESI) calcd for $C_{14}H_{13}O_3S$ $[M+H]^+$ 261.0585, found 261.0578.



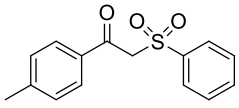
**2-(Phenylsulfonyl)-1-(*m*-tolyl)ethan-1-one** (**3b**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 67% yield. M.p.: 103-105 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.91-7.88 (m, 2H), 7.73-7.71 (m, 2H), 7.68-7.63 (m, 1H), 7.56-7.52 (m, 2H), 7.43-7.41 (m, 1H), 7.37-7.33 (m, 1H), 4.73 (s, 2H), 2.39 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.2, 138.9, 135.9, 135.3, 134.3, 129.8, 129.3, 128.9, 128.7, 126.7, 63.5, 21.4.

HRMS (ESI) calcd for $C_{15}H_{14}NaO_3S$ $[M+Na]^+$ 297.0561, found 297.0557.



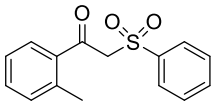
**2-(Phenylsulfonyl)-1-(*p*-tolyl)ethan-1-one** (**3c**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 71% yield. M.p.: 122-124 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.91-7.88 (m, 2H), 7.84-7.82 (m, 2H), 7.68-7.64 (m, 1H), 7.56-7.52 (m, 2H), 7.28-7.26 (m, 2H), 4.71 (s, 2H), 2.42 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.6, 145.8, 138.9, 134.3, 133.5, 129.7, 129.6, 129.3, 128.7, 63.6, 21.9.

HRMS (ESI) calcd for $C_{15}H_{14}NaO_3S$ $[M+Na]^+$ 297.0561, found 297.0557.



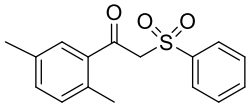
**2-(Phenylsulfonyl)-1-(*o*-tolyl)ethan-1-one** (**3d**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 69% yield. M.p.: 55-57 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.88-7.86 (m, 2H), 7.71-7.69 (d, $J$ = 8.0 Hz, 1H), 7.67-7. 63 (m, 1H), 7.55-7.51 (m, 2H), 7.43-7.40 (m, 1H), 7.28-7.24 (m, 2H), 4.71 (s, 2H), 2.43 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 190.5, 140.2, 139.1, 135.8, 134.3, 133.0, 132.4, 130.5, 129.3, 128.6, 126.1, 65.6, 21.6.

HRMS (ESI) calcd for $C_{15}H_{14}NaO_3S$ $[M+Na]^+$ 297.0561, found 297.0557.



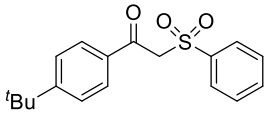
**1-(2,5-Dimethylphenyl)-2-(phenylsulfonyl)ethan-1-one** (**3e**)

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 67% yield. M.p.: 65-66 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.88-7.85 (m, 2H), 7.67-7.63 (m, 1H), 7.55-7.51 (m, 2H), 7.42 (s, 1H), 7.22-7.20 (d, $J$ = 8.0 Hz, 1H), 7.13-7.11 (d, $J$ = 8.0 Hz, 1H), 4.70 (s, 2H), 2.38 (s, 3H), 2.32 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 190.6, 139.1, 137.0, 135.7, 135.6, 134.2, 133.7, 132.3, 130.9, 129.3, 128.6, 65.6, 21.1, 21.0.

HRMS (ESI) calcd for $C_{16}H_{16}NaO_3S$ $[M+Na]^+$ 311.0718, found 311.0712.



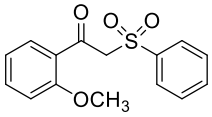
**1-(4-(*tert*-Butyl)phenyl)-2-(phenylsulfonyl)ethan-1-one** (**3f**)[4]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as colorless oil. 67% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.91-7.86 (m, 4H), 7.68-7.64 (m, 1H), 7.56-7.52 (m, 2H), 7.50-7.47 (m, 2H), 4.72 (s, 2H), 1.34 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.6, 158.6, 138.9, 134.3, 133.4, 129.5, 129.3, 128.7, 126.0, 63.6, 35.4, 31.1.

HRMS (ESI) calcd for $C_{18}H_{21}O_3S$ $[M+H]^+$ 317.1211, found 317.1205.



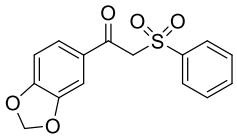
**1-(2-Methoxyphenyl)-2-(phenylsulfonyl)ethan-1-one** (**3g**)[5]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 4/1, v/v) as a white solid. 65% yield. M.p.: 116-118 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.87-7.85 (m, 2H), 7.66-7.64 (dd, $J$ = 7.6, 1.6 Hz, 1H), 7.62-7.58 (m, 1H), 7.51-7.45 (m, 3H), 7.00-6.96 (m, 1H), 6.89-6.86 (d, $J$ = 8.4 Hz, 1H), 4.94 (s, 2H), 3.85 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 189.1, 159.0, 139.7, 135.4, 133.9, 131.3, 129.0, 128.6, 126.3, 121.1, 111.8, 67.5, 55.7.

HRMS (ESI) calcd for $C_{15}H_{14}NaO_4S$ $[M+Na]^+$ 313.0510, found 313.0505.



**1-(Benzo[*d*][1,3]dioxol-5-yl)-2-(phenylsulfonyl)ethan-1-one** (**3h**)[6]

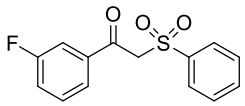
The product was isolated by flash chromatography (petroleum ether/EtOAc = 4/1, v/v) as colorless oil. 65% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.90-7.87 (m, 2H), 7.68-7.64 (m, 1H), 7.57-7.53 (m, 3H), 7.38 (d, $J$ = 1.6 Hz, 1H), 6.86-6.84 (d, $J$ = 8.4 Hz, 1H), 6.06 (s, 2H), 4.65 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 185.9, 153.2, 148.6, 138.8, 134.3, 130.8, 129.3, 128.7,

126.9, 108.6, 108.2, 102.4, 63.6.

HRMS (ESI) calcd for $C_{15}H_{13}O_5S$ $[M+H]^+$ 305.0484, found 305.0478.



**1-(3-Fluorophenyl)-2-(phenylsulfonyl)ethan-1-one** (**3i**)[7]

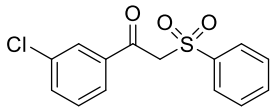
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 66% yield. M.p.: 102-103 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.90-7.88 (m, 2H), 7.75-7.73 (m, 1H), 7.70-7.65 (m, 1H), 7.62-7.59 (m, 1H), 7.58-7.54 (m, 2H), 7.50-7.44 (m, 1H), 7.34-7.29 (m, 1H), 4.71 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.0 (d, $J_{C-F}$ = 2.2 Hz), 164.2, 161.7 (d, $J_{C-F}$ = 250.0 Hz), 138.7, 137.9, 137.8 (d, $J_{C-F}$ = 6.5 Hz), 134.5, 130.8, 130.7, 129.4, 128.7, 125.4 (d, $J_{C-F}$ = 3.1 Hz), 125.4, 121.7, 121.5 (d, $J_{C-F}$ = 21.5 Hz), 116.0, 115.8 (d, $J_{C-F}$ = 23.0 Hz), 63.7.

$^{19}$F NMR (377 MHz, $CDCl_3$): $\delta$ -110.9, -111.0.

HRMS (ESI) calcd for $C_{14}H_{11}FNaO_3S$ $[M+Na]^+$ 301.0311, found 304.0306.



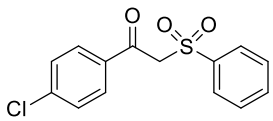
**1-(3-Chlorophenyl)-2-(phenylsulfonyl)ethan-1-one** (**3j**)[7]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 74% yield. M.p.: 98-100 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.90-7.87 (m, 3H), 7.85-7.82 (m, 1H), 7.70-7.66 (m, 1H), 7.60-7.54 (m, 3H), 7.45-7.42 (m, 1H), 4.71 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.0, 138.6, 137.3, 135.4, 134.6, 134.4, 130.3, 129.5, 129.3, 128.7, 127.7, 63.7.

HRMS (ESI) calcd for $C_{14}H_{11}ClNaO_3S$ $[M+Na]^+$ 317.0015, found 317.0007.



**1-(4-Chlorophenyl)-2-(phenylsulfonyl)ethan-1-one** (**3k**)[3]

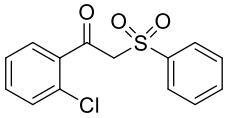
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v)

as a white solid. 75% yield. M.p.: 125-127 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.90-7.86 (m, 4H), 7.69-7.65 (m, 1H), 7.57-7.53 (m, 2H), 7.47-7.43 (m, 2H), 4.71 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.0, 141.3, 138.7, 134.5, 134.2, 130.9, 129.4, 129.4, 128.6, 63.7.

HRMS (ESI) calcd for $C_{14}H_{11}ClNaO_3S$ $[M+Na]^+$ 317.0015, found 317.0007.



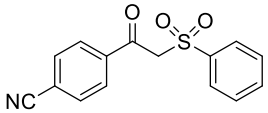
**1-(2-Chlorophenyl)-2-(phenylsulfonyl)ethan-1-one** (**3l**)[8]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 70% yield. M.p.: 58-60 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.90-7.88 (m, 2H), 7.68-7.64 (m, 1H), 7.56-7.52 (m, 3H), 7.45-7.41 (m, 1H), 7.38-7.32 (m, 2H), 4.84 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 190.3, 139.0, 137.4, 134.4, 133.3, 131.7, 130.8, 130.7, 129.4, 128.7, 127.4, 66.4.

HRMS (ESI) calcd for $C_{14}H_{11}ClNaO_3S$ $[M+Na]^+$ 317.0015, found 317.0007.



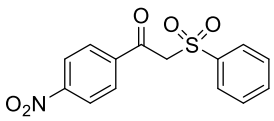
**4-(2-(Phenylsulfonyl)acetyl)benzonitrile** (**3m**)[5]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 4/1, v/v) as a white solid. 62% yield. M.p.: 136-138 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.07-8.05 (m, 2H), 7.88-7.86 (m, 2H), 7.79-7.77 (m, 2H), 7.71-7.67 (m, 1H), 7.59-7.55 (m, 2H), 4.75 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.1, 138.6, 138.5, 134.7, 132.8, 129.8, 129.5, 128.6, 117.7, 117.6, 63.8.

HRMS (ESI) calcd for $C_{15}H_{11}NNaO_3S$ $[M+Na]^+$ 308.0357, found 308.0362.



**1-(4-Nitrophenyl)-2-(phenylsulfonyl)ethan-1-one** (**3n**)[8]

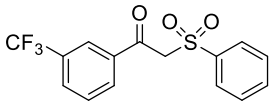
The product was isolated by flash chromatography (petroleum ether/EtOAc = 3/1, v/v)

as a white solid. 55% yield. M.p.: 129-130 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.34-8.33 (t, $J$ = 2.0 Hz, 1H), 8.32-8.31 (t, $J$ = 2.0 Hz, 1H), 8.16-8.15 (t, $J$ = 2.0 Hz, 1H), 8.13-8.12 (t, $J$ = 2.0 Hz, 1H), 7.90-7.87 (m, 2H), 7.73-7.68 (m, 1H), 7.60-7.56 (m, 2H), 4.78 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.0, 151.0, 140.0, 138.5, 134.8, 130.6, 129.6, 128.6, 124.1, 64.1.

HRMS (ESI) calcd for $C_{14}H_{11}NNaO_5S$ $[M+Na]^+$ 328.0256, found 328.0263.



**2-(Phenylsulfonyl)-1-(3-(trifluoromethyl)phenyl)ethan-1-one** (**3o**)[9]

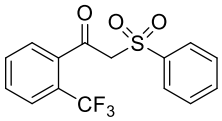
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 62% yield. M.p.: 106-108 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.17-8.15 (m, 2H), 7.89-7.85 (m, 3H), 7.70-7.62 (m, 2H), 7.58-7.54 (t, $J$ = 8.0 Hz, 2H), 4.77 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.1, 138.6, 136.3, 134.6, 132.7, 132.2, 131.9, 131.5, 131.2 (q, $J_{C-F}$ = 33.4 Hz), 130.9, 130.8 (q, $J_{C-F}$ = 3.6 Hz), 129.8, 129.5, 128.7, 127.6, 126.1, 126.0 (q, $J_{C-F}$ = 3.7 Hz), 124.9, 122.2, 119.5 (q, $J_{C-F}$ = 273.8 Hz), 63.7.

$^{19}$F NMR (377 MHz, $CDCl_3$): $\delta$ -62.9.

HRMS (ESI) calcd for $C_{15}H_{11}F_3NaO_3S$ $[M+Na]^+$ 351.0279, found 351.0274.



**2-(Phenylsulfonyl)-1-(2-(trifluoromethyl)phenyl)ethan-1-one** (**3p**)[10]

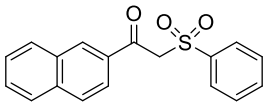
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 68% yield. M.p.: 88-90 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.94-7.91 (m, 2H), 7.71-7.62 (m, 5H), 7.60-7.56 (m, 2H), 4.66 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 191.0, 138.7, 138.0, 134.5, 132.4, 131.6, 129.5, 128.7, 127.9, 127.6, 127.5, 127.3 (q, $J_{C-F}$ = 32.6 Hz), 127.1, 127.0, 126.9 (q, $J_{C-F}$ = 5.1 Hz), 124.8, 122.1, 119.4 (q, $J_{C-F}$ = 274.8 Hz), 66.6, 66.5 (q, $J_{C-F}$ = 2.0 Hz).

$^{19}$F NMR (377 MHz, $CDCl_3$): $\delta$ -57.7.

HRMS (ESI) calcd for $C_{15}H_{11}F_3NaO_3S$ $[M+Na]^+$ 351.0279, found 351.0274.



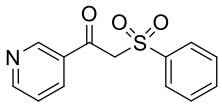
**1-(Naphthalen-2-yl)-2-(phenylsulfonyl)ethan-1-one** (**3q**)[5]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 61% yield. M.p.: 138-140 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.46 (s, 1H), 7.97-7.86 (m, 6H), 7.66-7.62 (m, 2H), 7.59-7.51 (m, 3H), 4.87 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.0, 138.8, 136.1, 134.4, 133.2, 132.4, 132.3, 130.1, 129.5, 129.3, 129.0, 128.7, 127.9, 127.3, 124.0, 63.7.

HRMS (ESI) calcd for $C_{18}H_{15}O_3S$ $[M+H]^+$ 311.0742, found 311.0750.



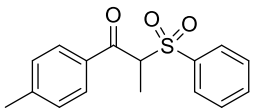
**2-(Phenylsulfonyl)-1-(pyridin-3-yl)ethan-1-one** (**3r**)[10]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 2/1, v/v) as a white solid. 59% yield. M.p.: 108-109 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 9.12-9.11 (d, $J$ = 2.0 Hz, 1H), 8.81-8.79 (d, $J$ = 3.2 Hz, 1H), 8.25-8.22 (dt, $J$ = 8.0, 2.0 Hz, 1H), 7.88-7.86 (m, 2H), 7.69-7.65 (m, 1H), 7.57-7.53 (m, 2H), 7.45-7.42 (dd, $J$ = 8.0, 4.8 Hz, 1H), 4.75 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.3, 154.5, 150.6, 138.5, 136.7, 134.6, 131.3, 129.5, 128.6, 123.8, 63.8.

HRMS (ESI) calcd for $C_{13}H_{12}NO_3S$ $[M+H]^+$ 262.0538, found 262.0532.



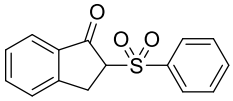
**2-(Phenylsulfonyl)-1-(*p*-tolyl)propan-1-one** (**3s**)[11]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as colorless oil. 62% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.89-7.87 (d, $J$ = 8.4 Hz, 2H), 7.80-7.77 (m, 2H), 7.67-7.63 (m, 1H), 7.54-7.50 (m, 2H), 7.29-7.27 (d, $J$ = 8.0 Hz, 2H), 5.17-5.12 (d, $J$ = 6.8 Hz, 1H), 2.42 (s, 3H), 1.57-1.55 (d, $J$ = 6.8 Hz, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 192.1, 145.4, 136.2, 134.3, 133.9, 130.0, 129.6, 129.5, 129.0, 65.0 21.9, 13.4.

HRMS (ESI) calcd for $C_{16}H_{17}O_3S$ $[M+H]^+$ 289.0898, found 289.0895.



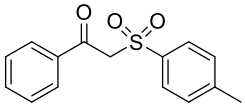
**2-(Phenylsulfonyl)-2,3-dihydro-1*H*-inden-1-one** (**3t**)[12]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as colorless oil. 57% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.94-7.91 (m, 2H), 7.72-7.55 (m, 5H), 7.50-7.48 (m, 1H), 7.40-7.36 (m, 1H), 4.30-4.27 (m, 1H), 3.85-3.79 (m, 1H), 3.57-3.51 (m, 1H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 194.6, 152.0, 137.6, 136.1, 135.9, 134.4, 129.4, 129.2, 128.4, 126.5, 125.0, 68.8, 28.2.

HRMS (ESI) calcd for $C_{15}H_{13}O_3S$ $[M+H]^+$ 273.0585, found 273.0589.



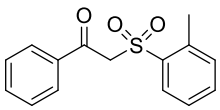
**1-Phenyl-2-tosylethan-1-one** (**4a**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as colorless oil. 68% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.95-7.93 (m, 2H), 7.77-7.75 (m, 2H), 7.64-7.59 (m, 1H), 7.49-7.46 (m, 2H), 7.34-7.32 (d, $J$ = 8.4 Hz, 2H), 4.72 (s, 2H), 2.44 (s, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.3, 145.5, 135.9, 134.5, 130.0, 129.5, 129.0, 128.7, 63.7, 21.8.

HRMS (ESI) calcd for $C_{15}H_{15}O_3S$ $[M+H]^+$ 275.0742, found 275.0748.



**1-Phenyl-2-(*o*-tolylsulfonyl)ethan-1-one** (**4b**)[3]

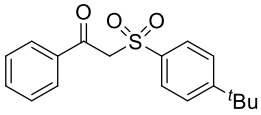
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as colorless oil. 66% yield.

$^1$H NMR (600 MHz, $CDCl_3$): $\delta$ 7.96-7.94 (m, 2H), 7.89-7.87 (dd, $J$ = 7.8, 1.2 Hz, 1H), 7.63-7.60 (m, 1H), 7.54-7.51 (td, $J$ = 7.2, 1.2 Hz, 1H), 7.49-7.46 (m, 2H), 7.35-7.31

(m, 2H), 4.76 (s, 2H), 2.72 (s, 3H).

$^{13}$C NMR (151 MHz, $CDCl_3$): $\delta$ 188.1, 138.4, 137.0, 135.9, 134.5, 134.4, 132.9, 130.7, 129.5, 129.0, 126.7, 63.0, 20.7.

HRMS (ESI) calcd for $C_{15}H_{15}O_3S$ $[M+H]^+$ 275.0742, found 275.0748.



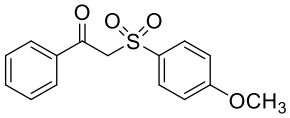

**2-((4-(*tert*-Butyl)phenyl)sulfonyl)-1-phenylethan-1-one** (**4c**)[9]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 70% yield. M.p.: 128-130 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.94-7.91 (m, 2H), 7.82-7.79 (m, 2H), 7.62-7.58 (m, 1H), 7.55-7.51 (m, 2H), 7.48-7.44 (m, 2H), 4.72 (s, 2H), 1.33 (s, 9H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.3, 158.4, 136.0, 135.9, 134.4, 129.4, 129.0, 128.6, 126.4, 63.7, 35.5, 31.2.

HRMS (ESI) calcd for $C_{18}H_{21}O_3S$ $[M+H]^+$ 317.1211, found 317.1205.



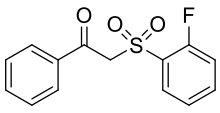

**2-((4-Methoxyphenyl)sulfonyl)-1-phenylethan-1-one** (**4d**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 4/1, v/v) as colorless oil. 62% yield.

$^1$H NMR (600 MHz, $CDCl_3$): $\delta$ 7.96-7.95 (d, $J$ = 7.2 Hz, 2H), 7.82-7.79 (m, 2H), 7.63-7.61 (t, $J$ = 7.2 Hz, 1H), 7.50-7.47 (m, 2H), 7.00-6.98 (m, 2H), 4.71 (s, 2H), 3.88 (s, 3H).

$^{13}$C NMR (151 MHz, $CDCl_3$): $\delta$ 188.5, 164.3, 135.9, 134.5, 131.0, 130.3, 129.5, 129.0, 114.5, 63.9, 55.9.

HRMS (ESI) calcd for $C_{15}H_{14}NaO_4S$ $[M+Na]^+$ 313.0510, found 313.0506.




**2-((2-Fluorophenyl)sulfonyl)-1-phenylethan-1-one** (**4e**)[9]

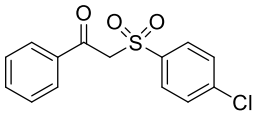
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as colorless oil. 60% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.96-7.94 (m, 2H), 7.90-7.86 (m, 1H), 7.70-7.61 (m, 2H), 7.51-7.47 (t, $J$ = 8.0 Hz, 2H), 7.34-7.24 (m, 3H), 4.92 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.9 161.0, 158.5 (d, $J_{C-F}$ = 256.8 Hz), 136.8, 136.7 (d, $J_{C-F}$ = 8.8 Hz), 135.8, 134.6, 130.9, 129.3, 129.1, 126.8 (d, $J_{C-F}$ = 14.0 Hz), 124.9 (d, $J_{C-F}$ = 3.6 Hz), 117.3, 117.1 (d, $J_{C-F}$ = 21.2 Hz), 62.3 (d, $J_{C-F}$ = 2.3 Hz).

$^{19}$F NMR (377 MHz, $CDCl_3$): $\delta$ -108.9.

HRMS (ESI) calcd for $C_{14}H_{12}FO_3S$ $[M+H]^+$ 279.0491, found 279.0485.



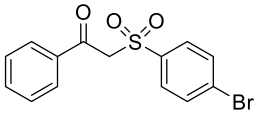

**2-((4-Chlorophenyl)sulfonyl)-1-phenylethan-1-one** (**4f**)[3]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 71% yield. M.p.: 102-104 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.95-7.92 (m, 2H), 7.85-7.82 (m, 2H), 7.66-7.62 (m, 1H), 7.54-7.48 (m, 4H), 4.74 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.0, 141.3, 137.2, 135.7, 134.7, 130.3, 129.7, 129.4, 129.1, 63.5.

HRMS (ESI) calcd for $C_{14}H_{11}ClNaO_3S$ $[M+Na]^+$ 317.0015, found 317.0019.



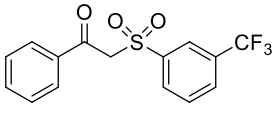

**2-((4-Bromophenyl)sulfonyl)-1-phenylethan-1-one** (**4g**)[4]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 65% yield. M.p.: 112-113 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.95-7.92 (m, 2H), 7.77-7.74 (m, 2H), 7.70-7.62 (m, 3H), 7.52-7.48 (m, 2H), 4.74 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 188.0, 137.7, 135.7, 134.7, 132.7, 130.4, 129.9, 129.4, 129.1, 63.4.

HRMS (ESI) calcd for $C_{14}H_{11}BrNaO_3S$ $[M+Na]^+$ 360.9510, found 360.9507.




**1-Phenyl-2-((3-(trifluoromethyl)phenyl)sulfonyl)ethan-1-one** (**4h**)[9]

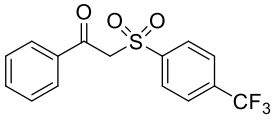
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 62% yield. M.p.: 72-74 ℃.

$^1$H NMR (600 MHz, $CDCl_3$): $\delta$ 8.17 (s, 1H), 8.13-8.11 (d, $J$ = 7.8 Hz, 1H), 7.93-7.91 (m, 3H), 7.73-7.71 (t, $J$ = 7.8 Hz, 1H), 7.66-7.63 (m, 1H), 7.51-7.49 (m, 2H), 4.79 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.9, 140.0, 135.6, 134.8, 132.6, 132.3, 131.9, 131.6 (q, $J_{C-F}$ = 34.1 Hz), 131.1, 131.0 (q, $J_{C-F}$ = 3.2 Hz), 130.1, 129.3, 129.2, 126.1, 126.0 (q, $J_{C-F}$ = 3.8 Hz), 123.8, 121.8, 119.8, 117.9 (q, $J_{C-F}$ = 202.3 Hz), 114.2, 63.3.

$^{19}$F NMR (565 MHz, $CDCl_3$): $\delta$ -62.8.

HRMS (ESI) calcd for $C_{15}H_{12}F_3O_3S$ $[M+H]^+$ 329.0459, found 329.0457.




**1-Phenyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)ethan-1-one** (**4i**)[13]

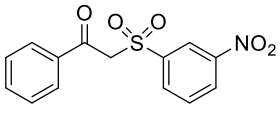
The product was isolated by flash chromatography (petroleum ether/EtOAc = 5/1, v/v) as a white solid. 58% yield. M.p.: 98-99 ℃.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.06-8.04 (d, $J$ = 8.4 Hz, 2H), 7.93-7.91 (m, 2H), 7.83-7.81 (d, $J$ = 8.0 Hz, 2H), 7.66-7.61 (m, 1H), 7.51-7.47 (t, $J$ = 8.0 Hz, 2H), 4.78 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.9, 142.2, 136.5, 136.1, 135.8, 135.6, 135.5 (q, $J_{C-F}$ = 33.0 Hz), 134.8, 129.5, 129.3, 129.1, 128.9, 128.2, 127.3, 127.2, 126.5, 126.4 (q, $J_{C-F}$ = 3.8 Hz), 126.2, 126.1 (q, $J_{C-F}$ = 3.3 Hz), 125.9, 124.5, 121.8, 119.1 (q, $J_{C-F}$ = 274.1 Hz), 63.2.

$^{19}$F NMR (377 MHz, $CDCl_3$): $\delta$ -63.3.

HRMS (ESI) calcd for $C_{15}H_{12}F_3O_3S$ $[M+H]^+$ 329.0459, found 329.0457.




**2-((3-Nitrophenyl)sulfonyl)-1-phenylethan-1-one** (**4j**)[9]

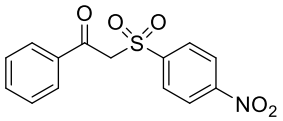
The product was isolated by flash chromatography (petroleum ether/EtOAc = 3/1, v/v) as a white solid. 53% yield. M.p.: 119-121 ℃.

$^1$H NMR (600 MHz, $CDCl_3$): $\delta$ 8.77-8.76 (t, $J$ = 1.8 Hz, 1H), 8.54-8.52 (m, 1H),

8.27-8.26 (m, 1H), 7.94-7.92 (m, 2H), 7.81-7.79 (t, *J* = 7.8 Hz, 1H), 7.68-7.65 (m, 1H), 7.53-7.50 (m, 2H), 4.83 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.9, 148.4, 140.8, 135.5, 135.0, 134.7, 130.7, 129.3, 129.2, 128.8, 124.3, 63.1.

HRMS (ESI) calcd for $C_{14}H_{11}NNaO_5S$ $[M+Na]^+$ 328.0256, found 328.0260.



**2-((4-Nitrophenyl)sulfonyl)-1-phenylethan-1-one** (**4k**)[4]

The product was isolated by flash chromatography (petroleum ether/EtOAc = 3/1, v/v) as colorless oil. 55% yield.

$^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.42-8.38 (m, 2H), 8.14-8.11 (m, 2H), 7.95-7.92 (m, 2H), 7.69-7.64 (m, 1H), 7.54-7.50 (m, 2H), 4.81 (s, 2H).

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 187.8, 144.2, 137.2, 135.5, 135.0, 130.5, 129.3, 129.2, 124.5, 63.1.

HRMS (ESI) calcd for $C_{14}H_{11}NNaO_5S$ $[M+Na]^+$ 328.0256, found 328.0260.

## **IV**. **References**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[3] Liu, T.; Zheng, D.; Ding, Y.; Fan, X.; Wu, J. Synthesis of β-Keto Sulfones by a Catalyst-Free Reaction of Aryldiazonium Tetrafluoroborates, Sulfur Dioxide, and Silyl Enol Ethers. *Chem. Asian J.* **2017**, *12*, 465-469.

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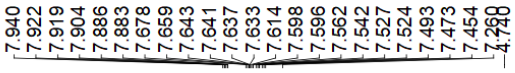
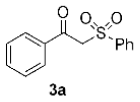
## V. Copies of NMR spectra

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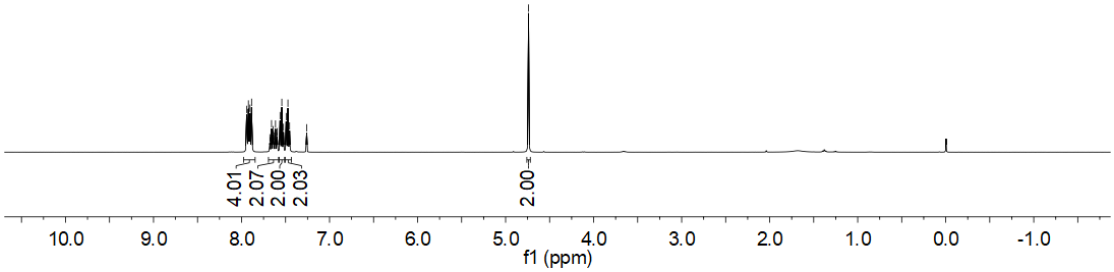



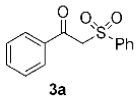


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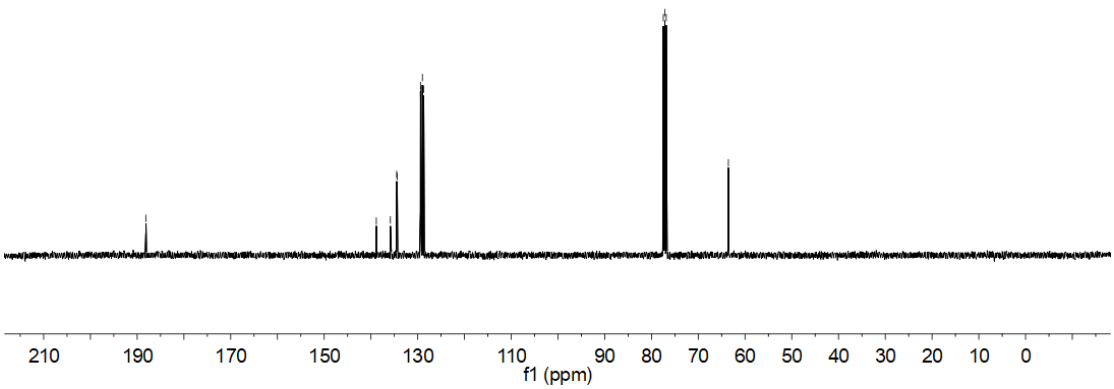


7.907
7.904
7.891
7.886
7.883
7.732
7.710
7.708
7.675
7.656
7.640
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7.634
7.560
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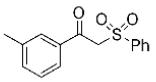
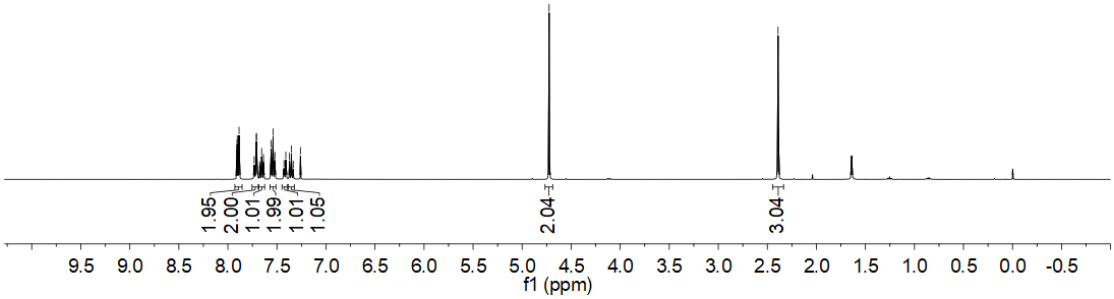
7.353
7.334
7.260
4.725
2.391


O
O
S
O
Ph

3b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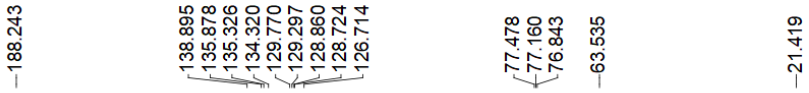
2.00
1.01
1.99
1.01
1.05
2.04
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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135.878
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129.297
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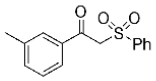
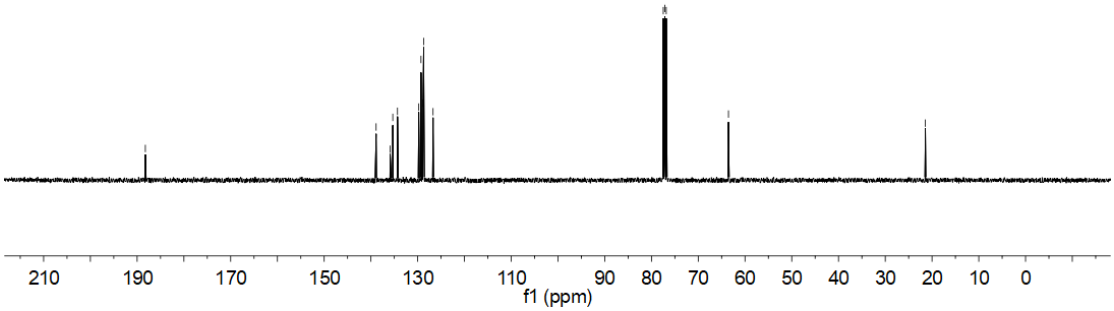
126.714
77.478
77.160
76.843
63.535
21.419


O
O
S
O
Ph

3b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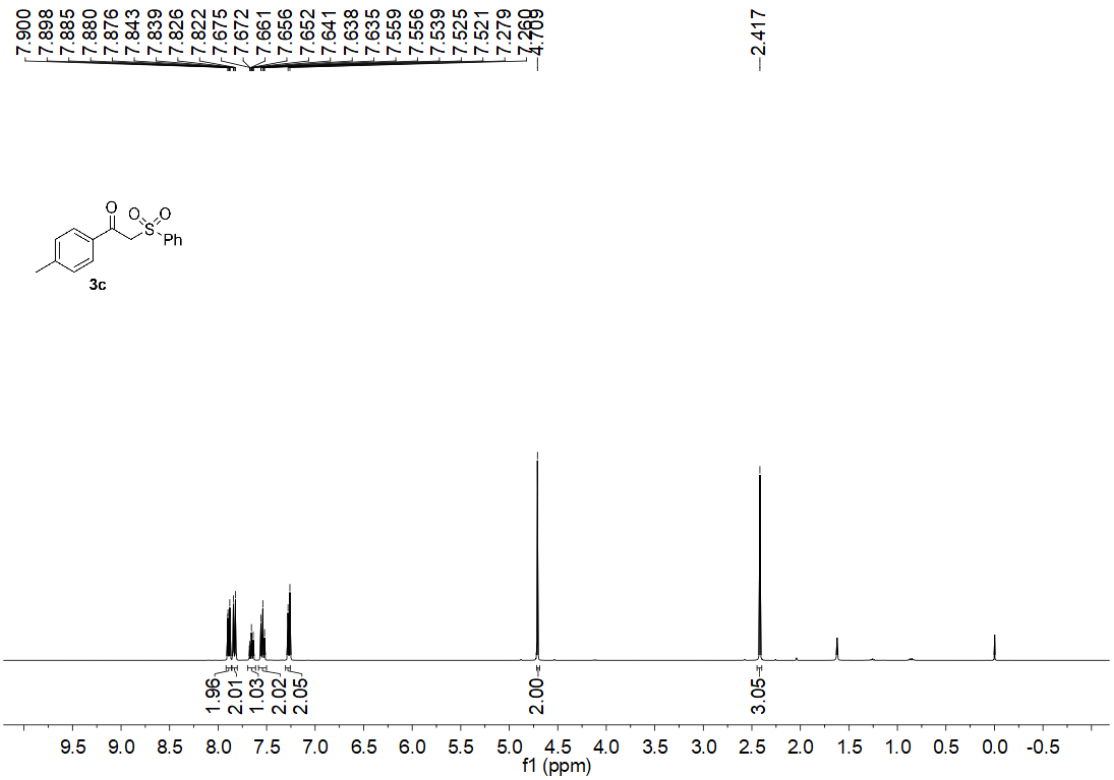
f1 (ppm)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7.661
7.656
7.652
7.641
7.638
7.635
7.559
7.556
7.539
7.525
7.521
7.279
2.417
3c
1.96
2.01
1.03
2.02
2.05
2.00
3.05
f1 (ppm)
187.598
145.753
138.898
134.306
133.448
129.698
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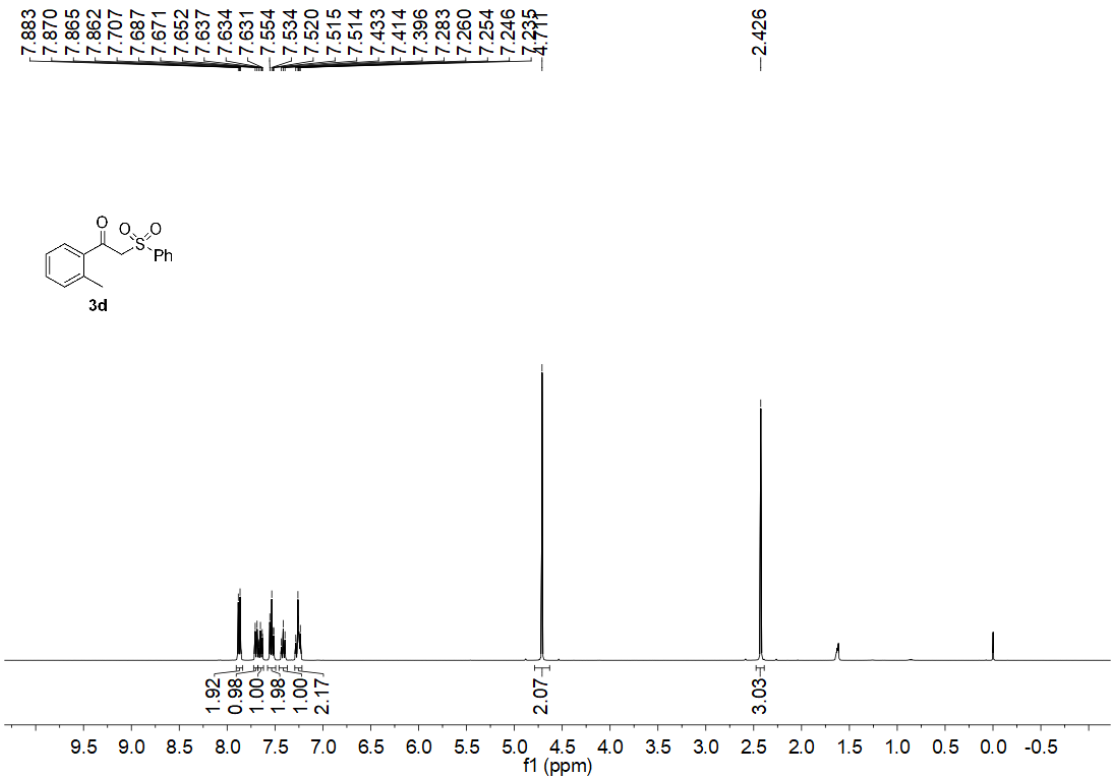
129.301
128.705
77.478
77.160
76.842
63.547
21.904
3c
f1 (ppm)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7.652
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7.520
7.515
7.514
7.433
7.414
7.396
7.283
7.260
7.254
7.246
7.235
4.711
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3d
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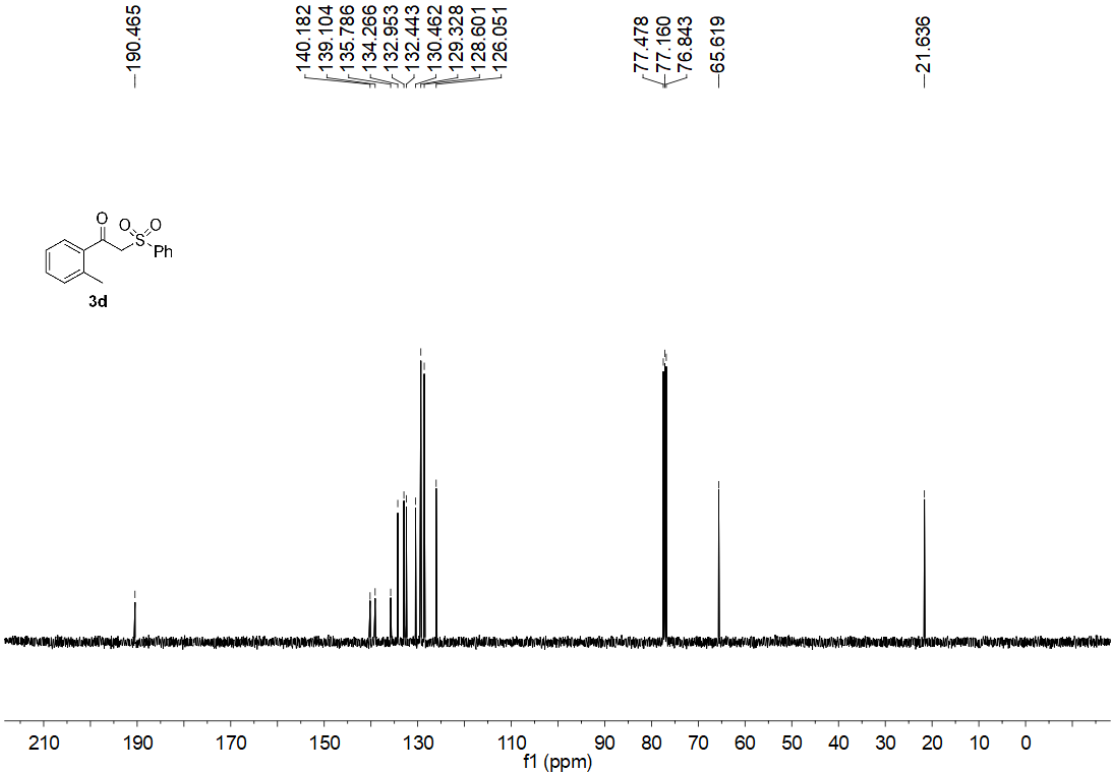
1.00
1.98
1.00
2.17
2.07
3.03
f1 (ppm)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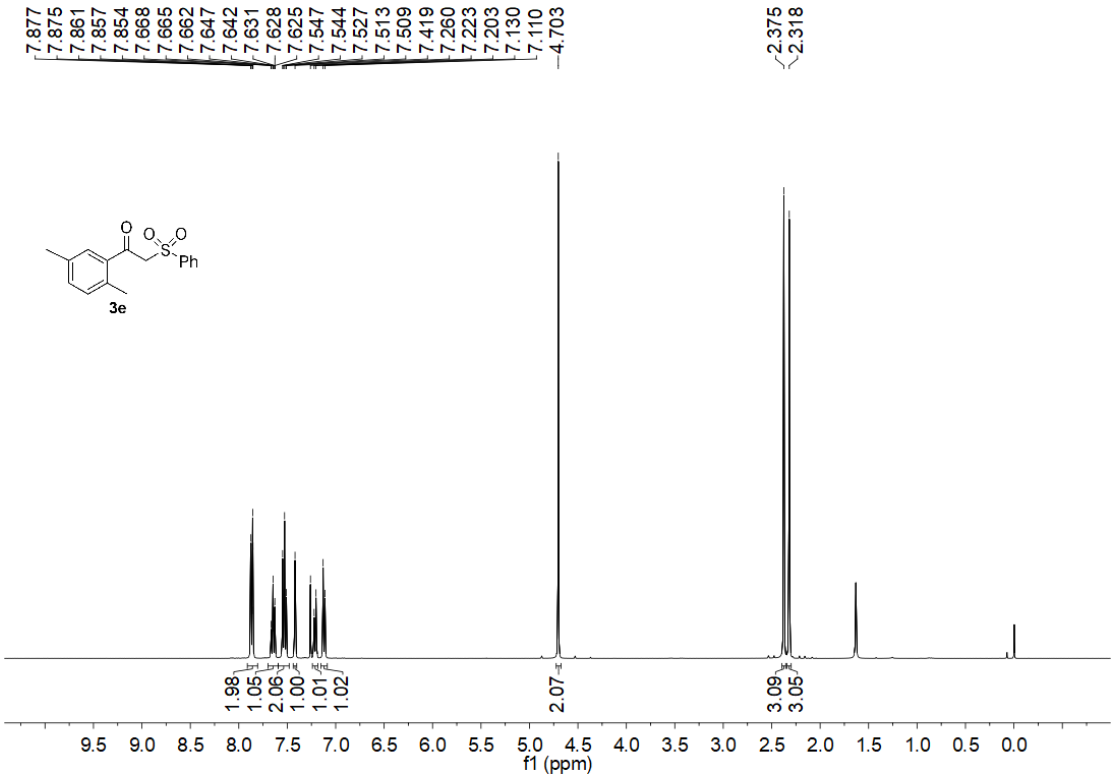
3d
f1 (ppm)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7.668
7.665
7.662
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7.642
7.631
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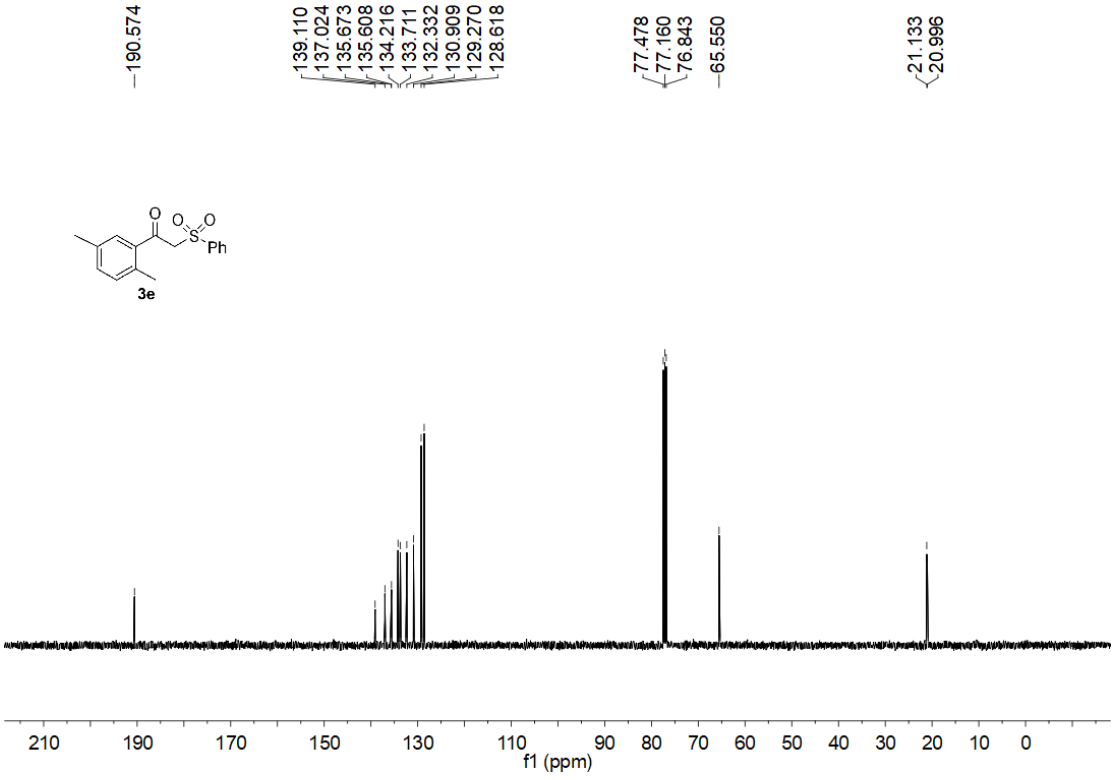
7.625
7.547
7.544
7.527
7.513
7.509
7.419
7.260
7.223
7.203
7.130
7.110
4.703
2.375
2.318
O
O
S
O
Ph
3e
1.98
1.05
2.06
1.00
1.01
1.02
2.07
3.09
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.332
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129.270
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77.160
76.843
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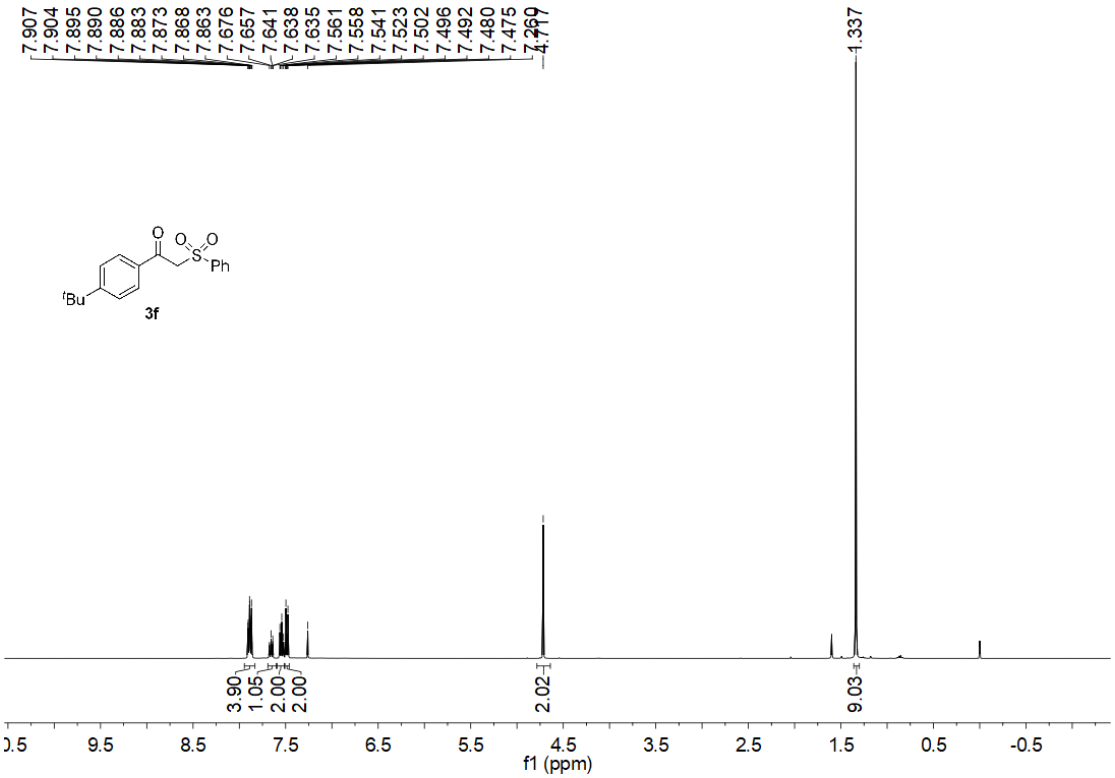
20.996
O
O
S
O
Ph
3e
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.657
7.641
7.638
7.635
7.561
7.558
7.541
7.523
7.502
7.496
7.492
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7.475
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2.00
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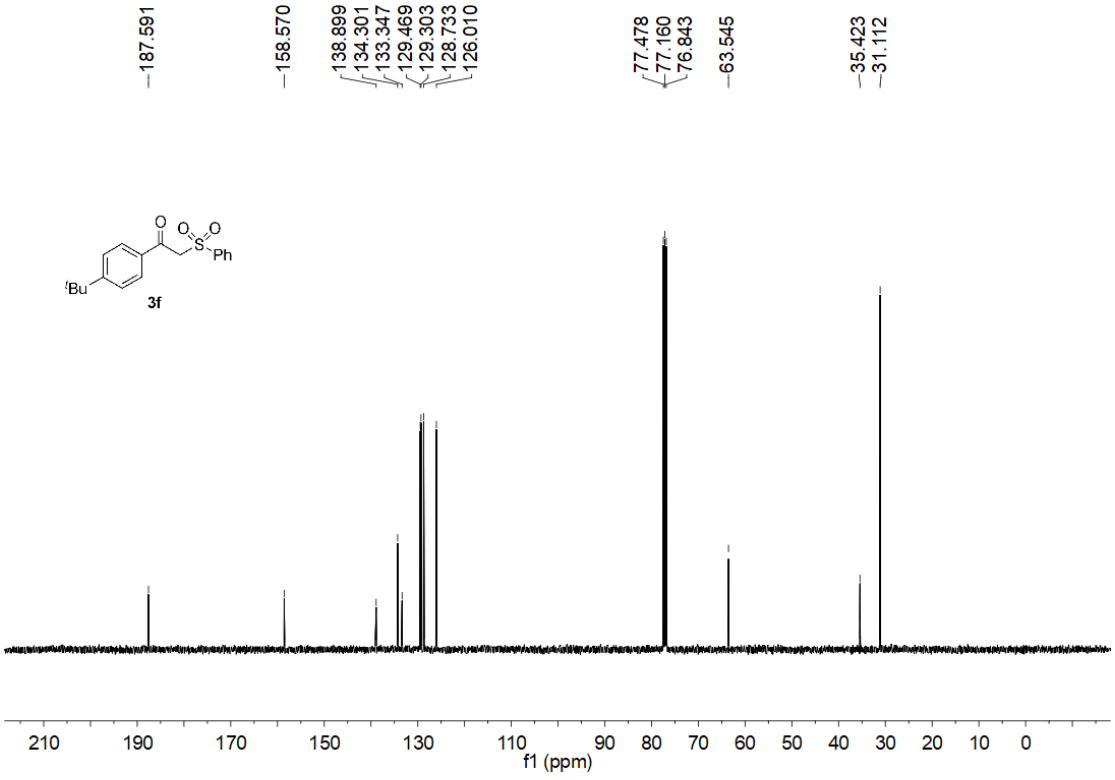
9.03
f1 (ppm)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63.545
35.423
31.112
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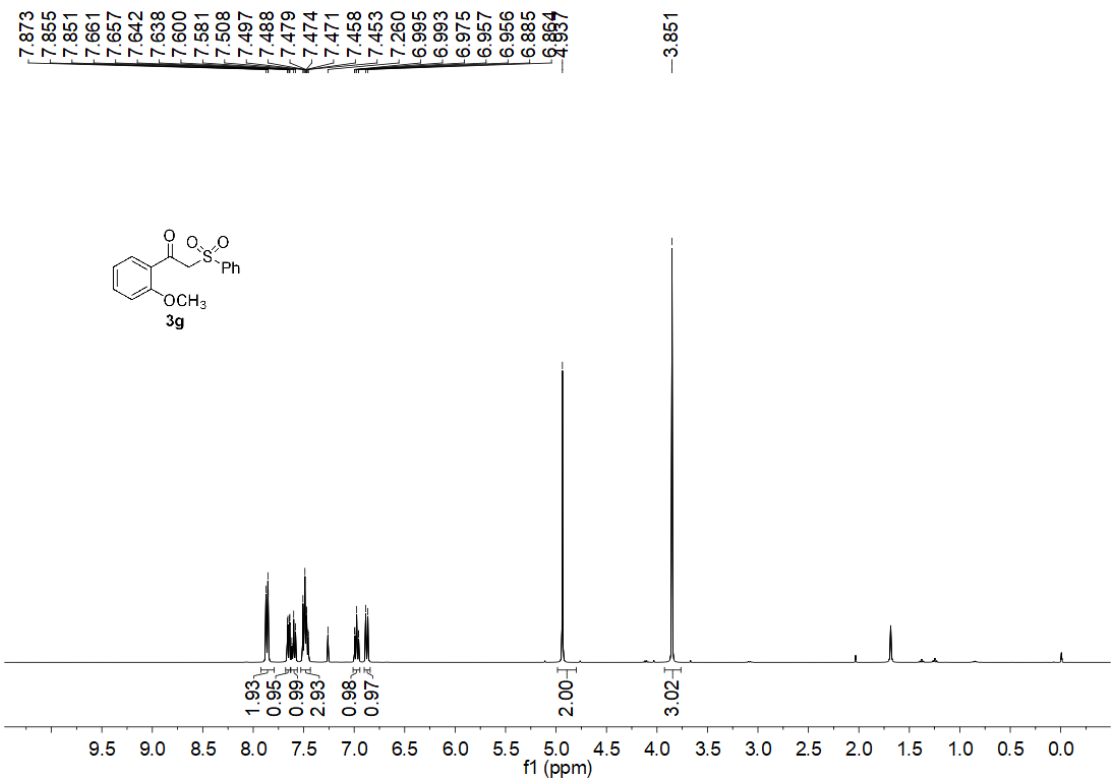
f1 (ppm)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7.508
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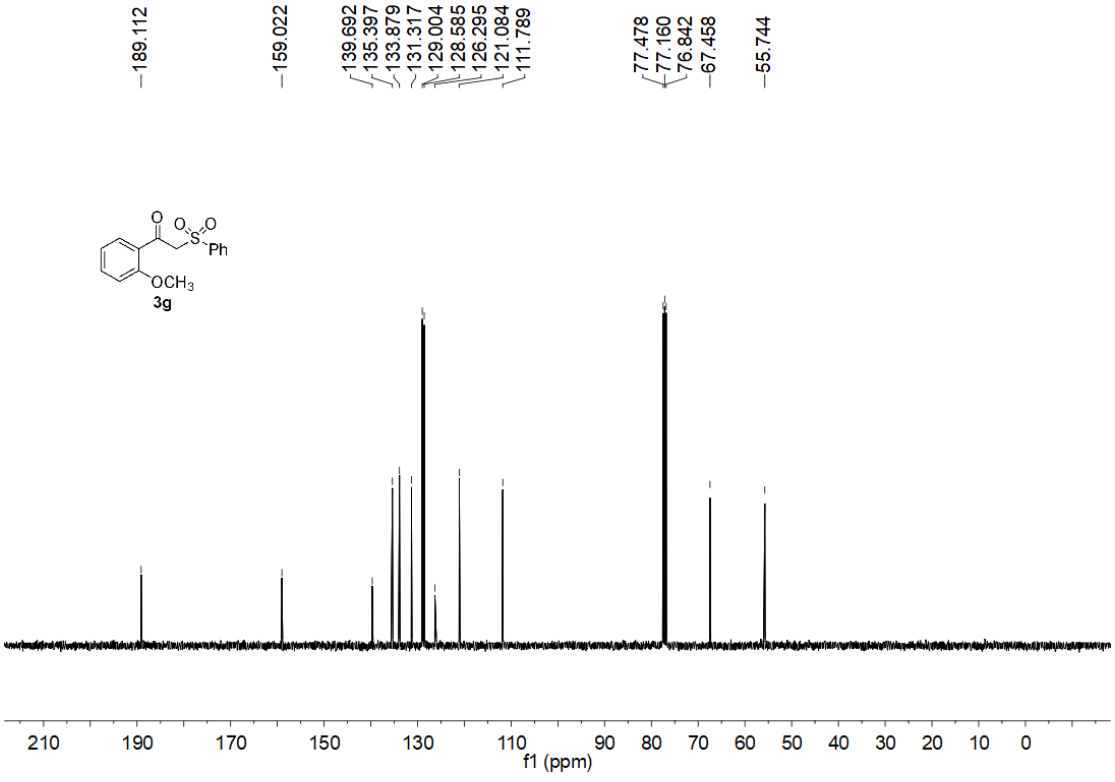
7.479
7.474
7.471
7.458
7.453
7.260
6.995
6.993
6.975
6.957
6.956
6.885
3.851
O
O
S
O
Ph
OCH3
3g
1.93
0.95
0.99
2.93
0.98
0.97
2.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.084
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77.160
76.842
67.458
55.744
O
O
S
O
Ph
OCH3
3g
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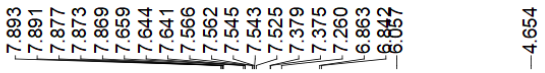
f1 (ppm)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7.641
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7.375
7.260
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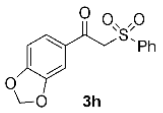
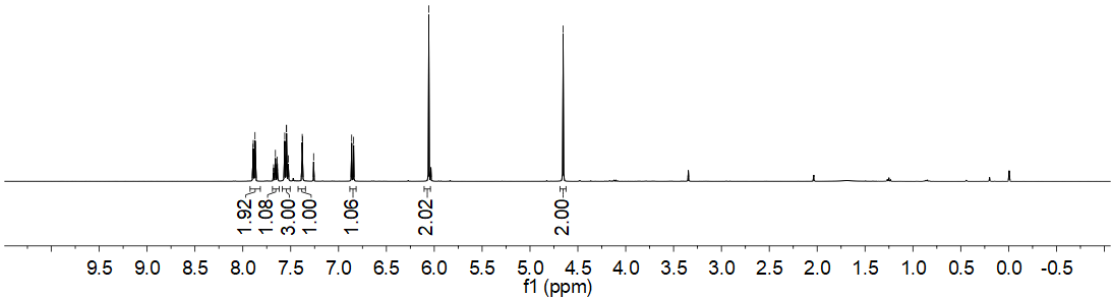
6.842
6.057
4.654


O
O
S
O
Ph
O
O
3h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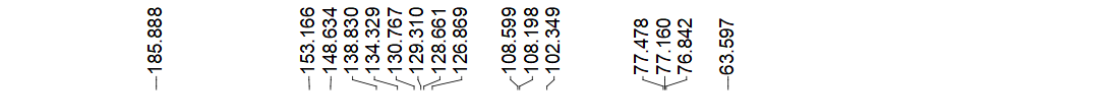
1.08
3.00
1.00
1.06
2.02
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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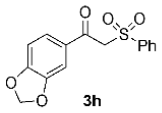
77.160
76.842
63.597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Ph
O
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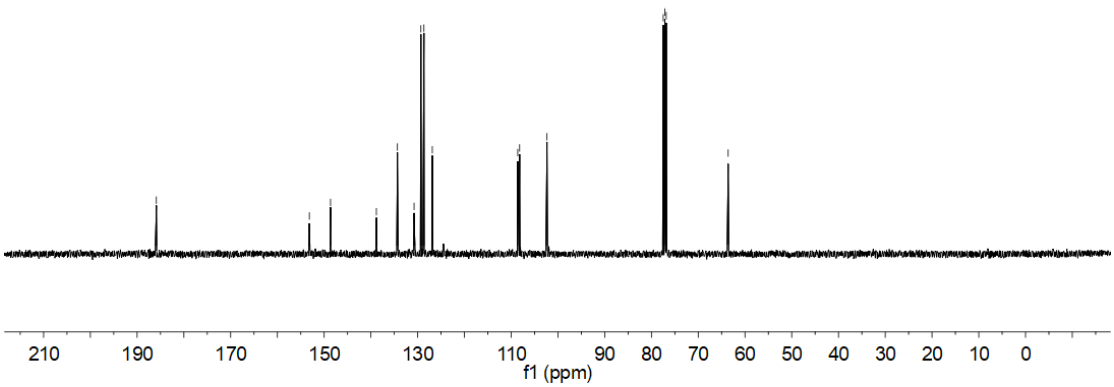
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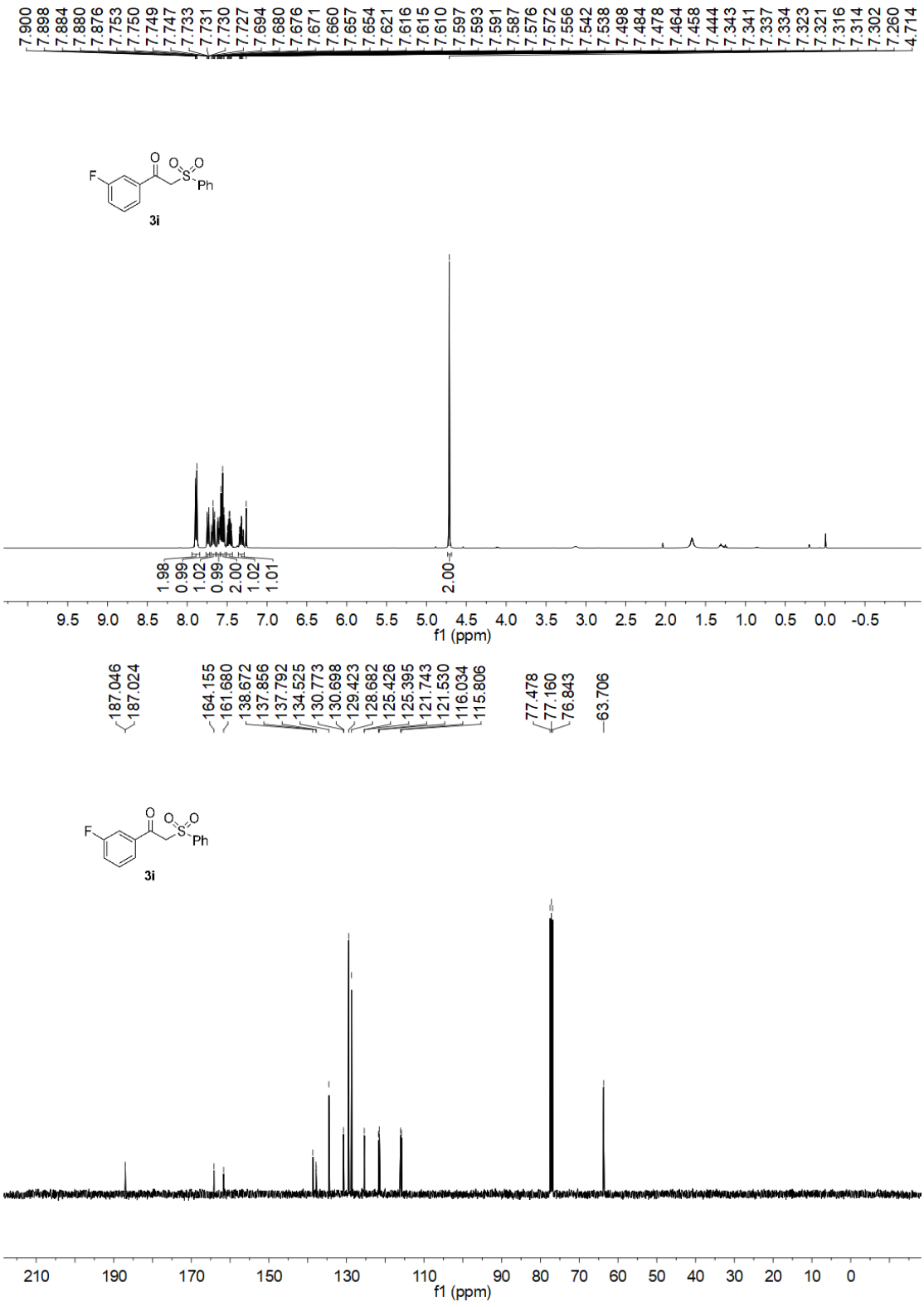
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7.727
7.694
7.680
7.676
7.671
7.660
7.657
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7.610
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7.323
7.321
7.316
7.314
7.302
7.260
4.714
F
O
O
S
O
Ph
3i
1.98
0.99
1.02
0.99
2.00
1.02
1.01
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
187.046
187.024
164.155
161.680
138.672
137.856
137.792
134.525
130.773
130.698
129.423
128.682
125.426
125.395
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121.530
116.034
115.806
77.478
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S
O
Ph
3i
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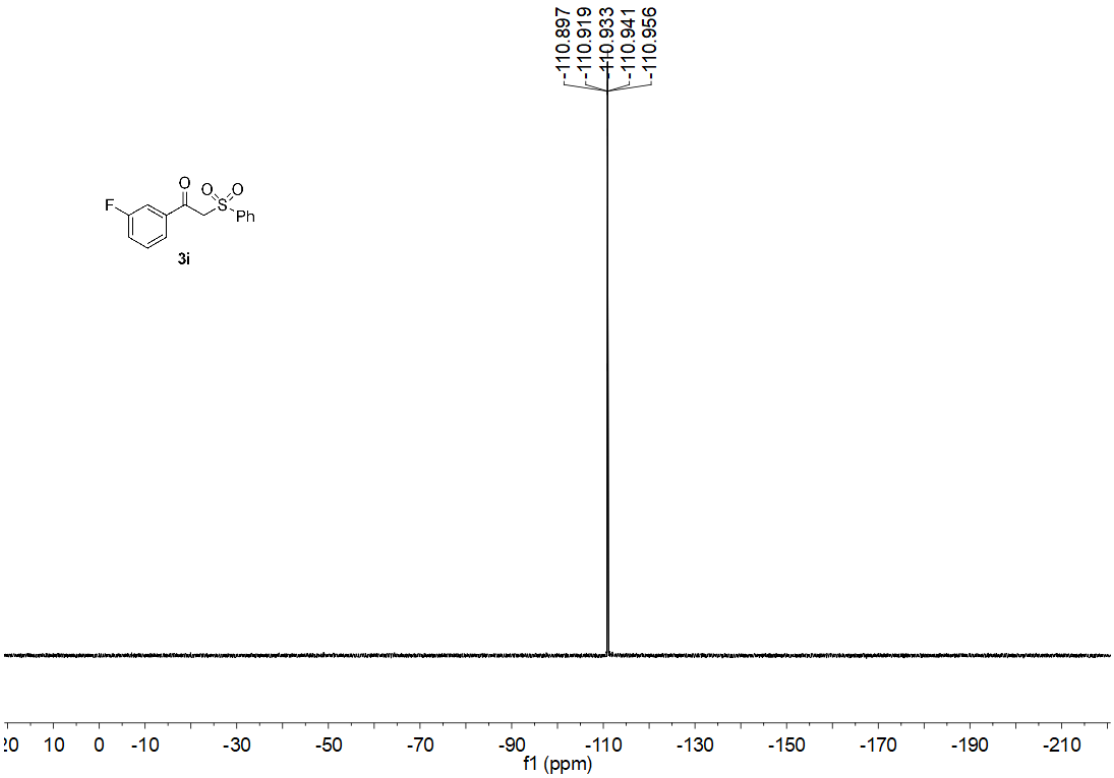
f1 (ppm)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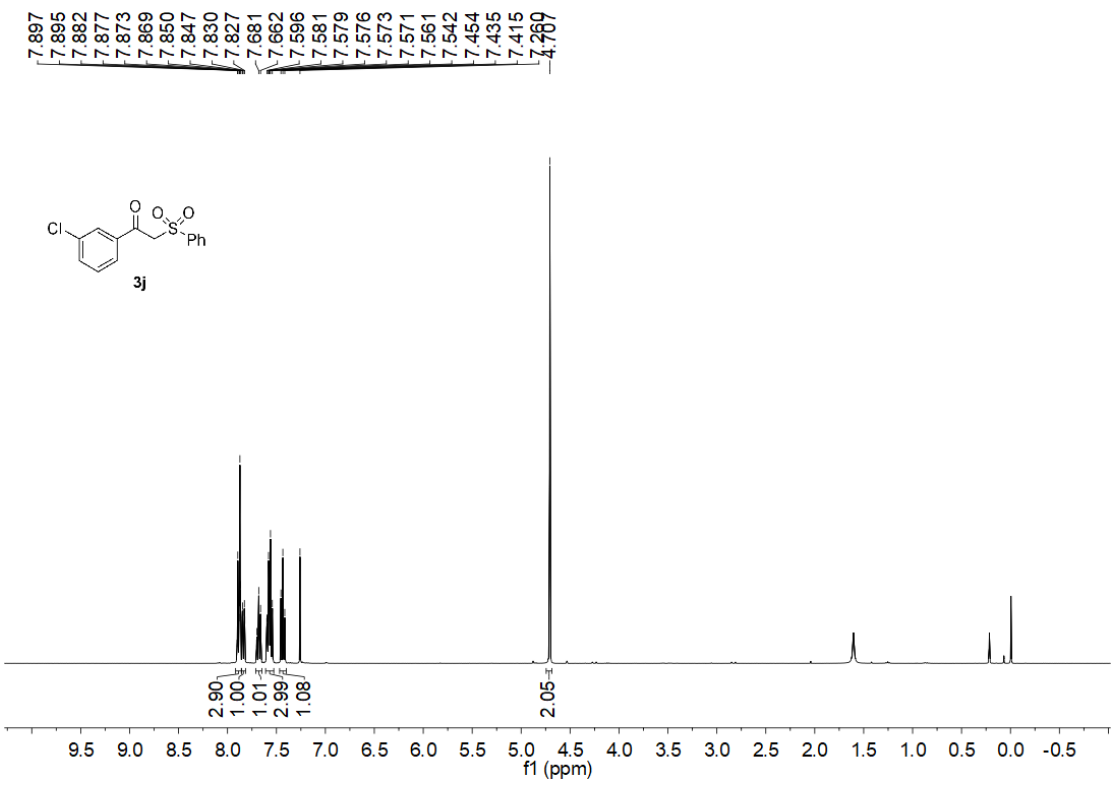
O
O
S
O
Ph
3i
f1 (ppm)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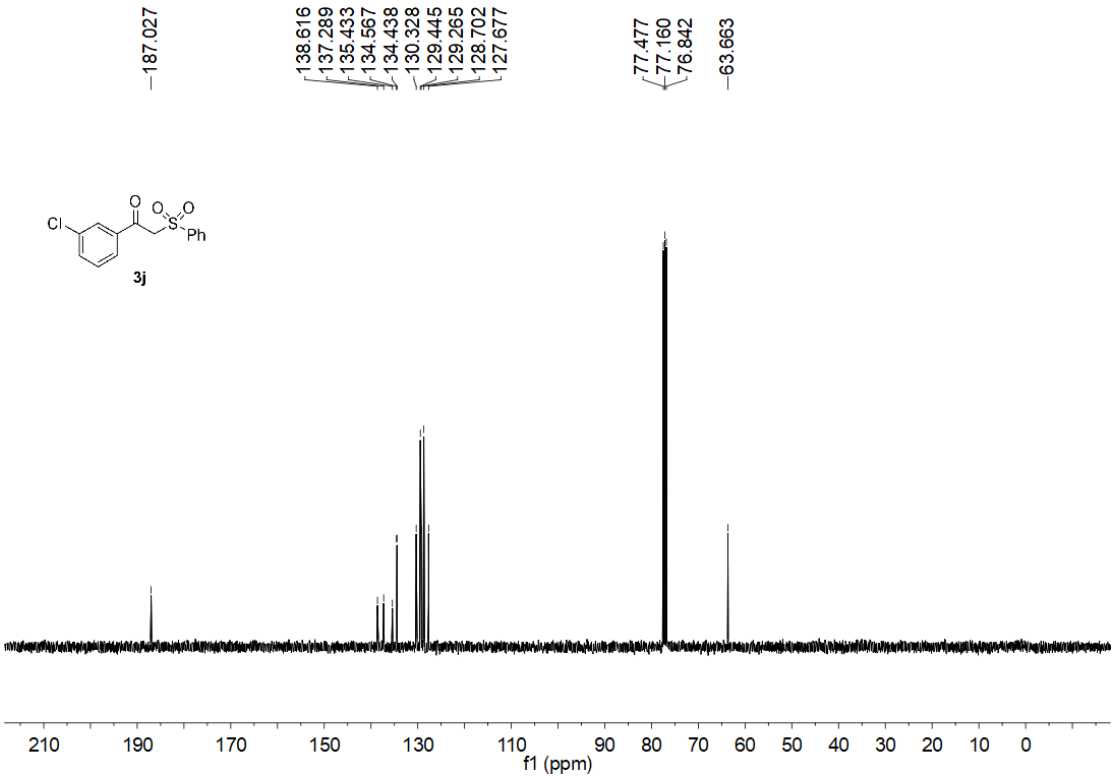
2.99
1.08
2.05
f1 (ppm)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128.702
127.677
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77.160
76.842
63.663
Cl
O
O
S
Ph
3j
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170
150
130
110
90
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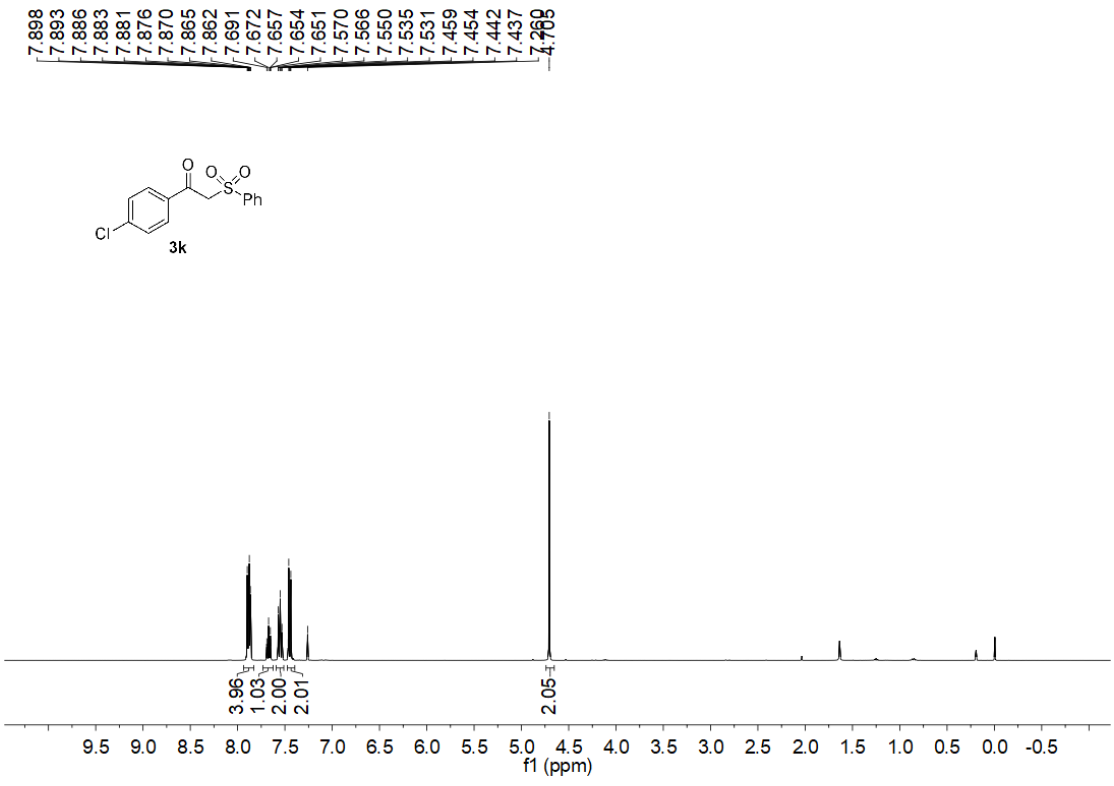
70
60
50
40
30
20
10
0
f1 (ppm)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7.876
7.870
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7.691
7.672
7.657
7.654
7.651
7.570
7.566
7.550
7.535
7.531
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7.454
7.442
7.437
Cl
O
O
S
Ph
3k
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2.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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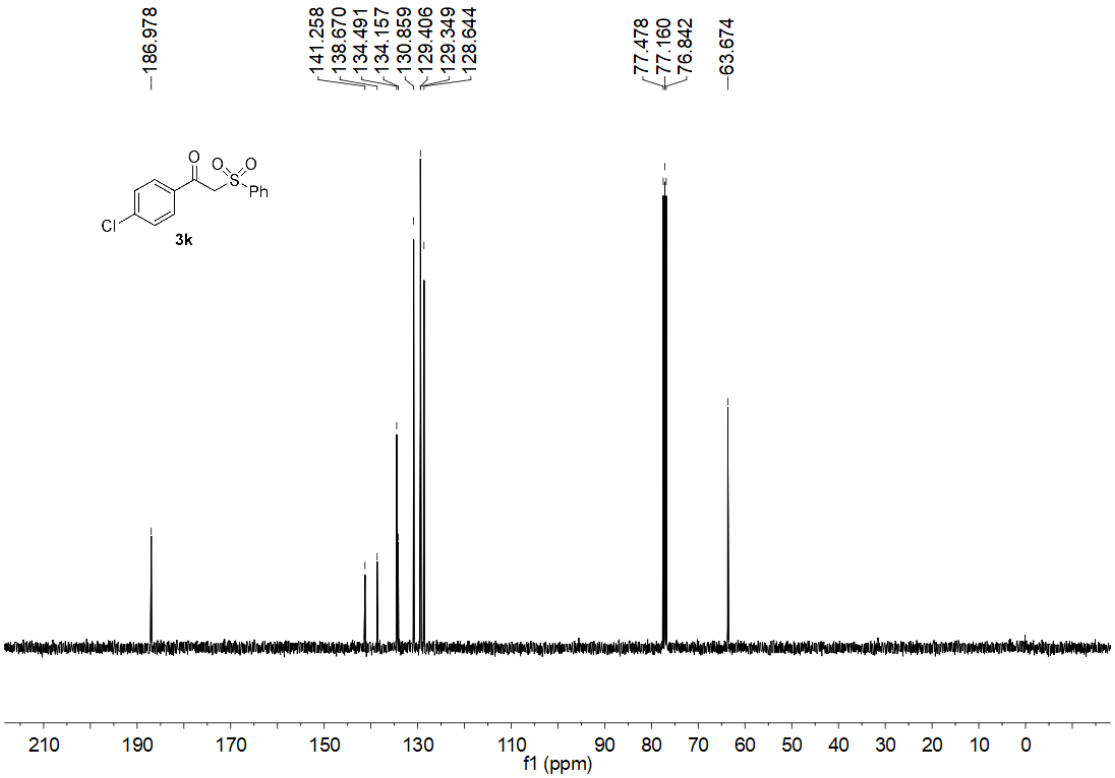
-0.5
f1 (ppm)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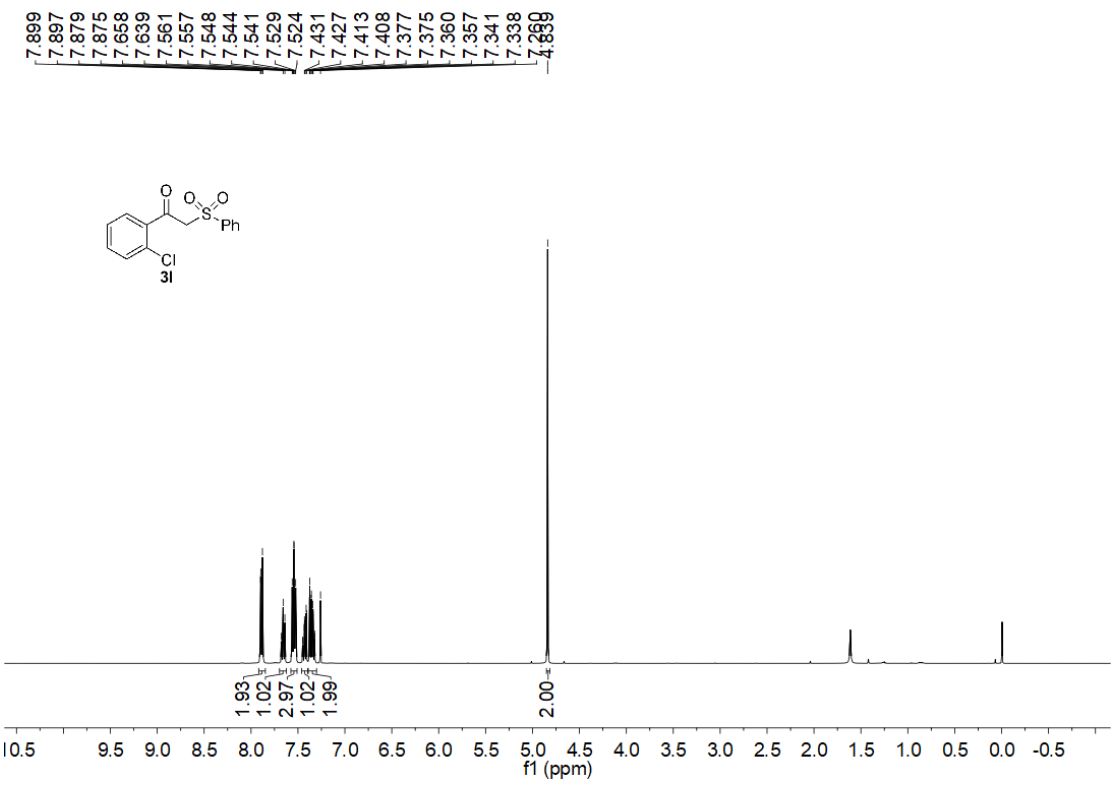
138.670
134.491
134.157
130.859
129.406
129.349
128.644
77.478
77.160
76.842
63.674
O
O
S
O
Ph
Cl
3k
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.879
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7.561
7.557
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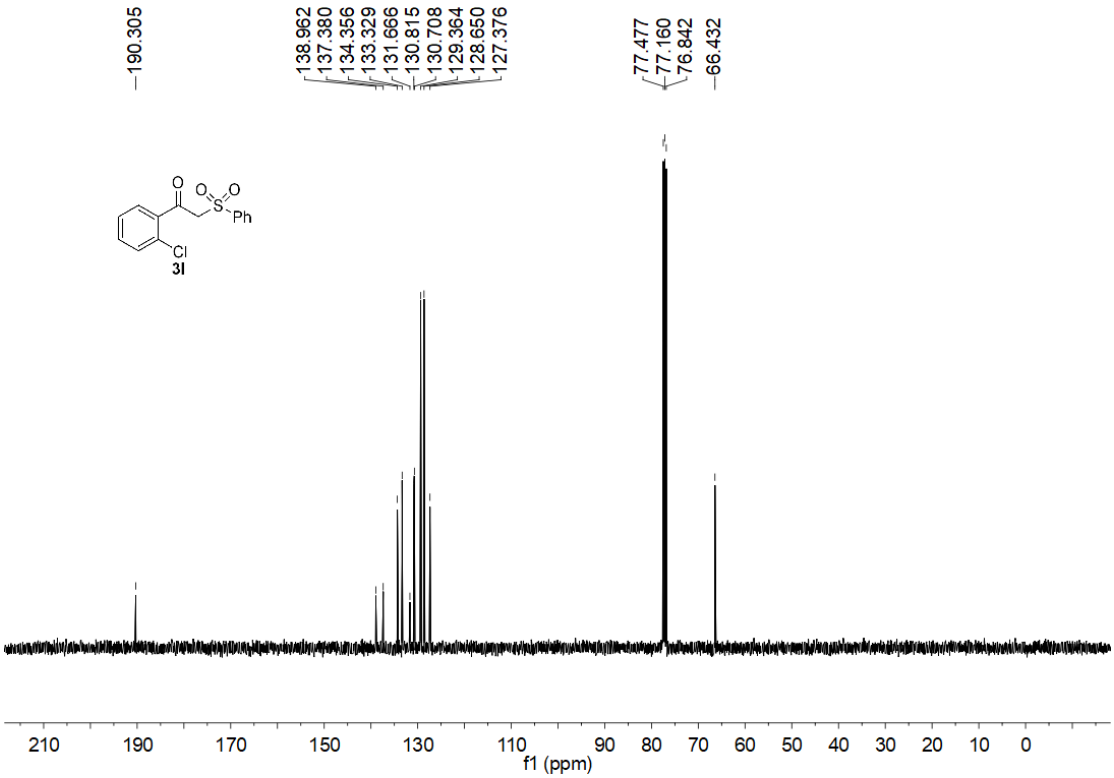
7.544
7.541
7.529
7.524
7.431
7.427
7.413
7.408
7.377
7.375
7.360
7.357
7.341
7.338
O
O
S
O
Ph
Cl
3l
1.93
1.02
2.97
1.02
1.99
2.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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137.380
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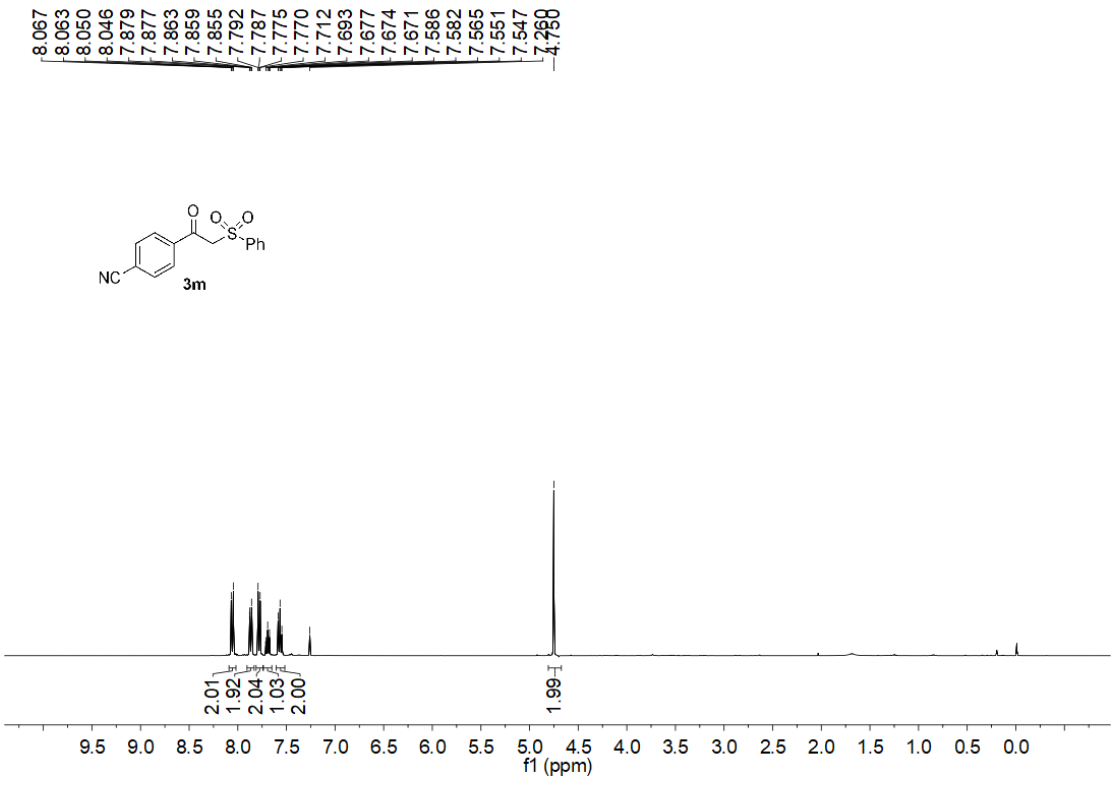
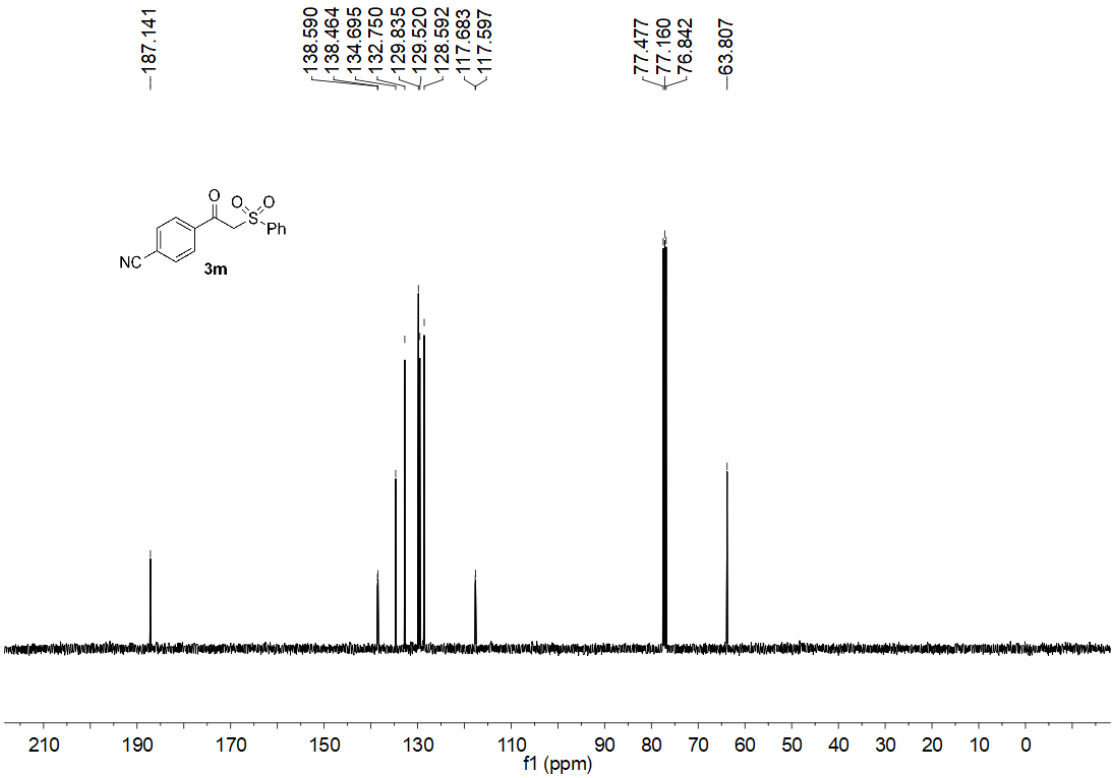
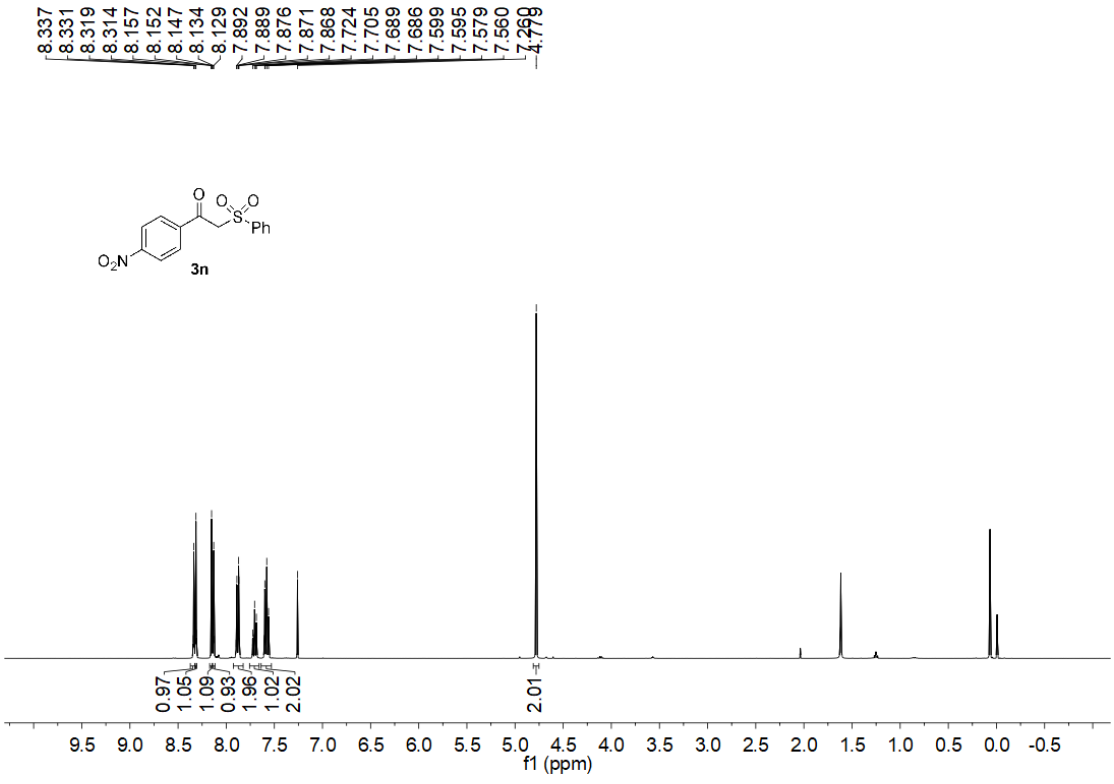
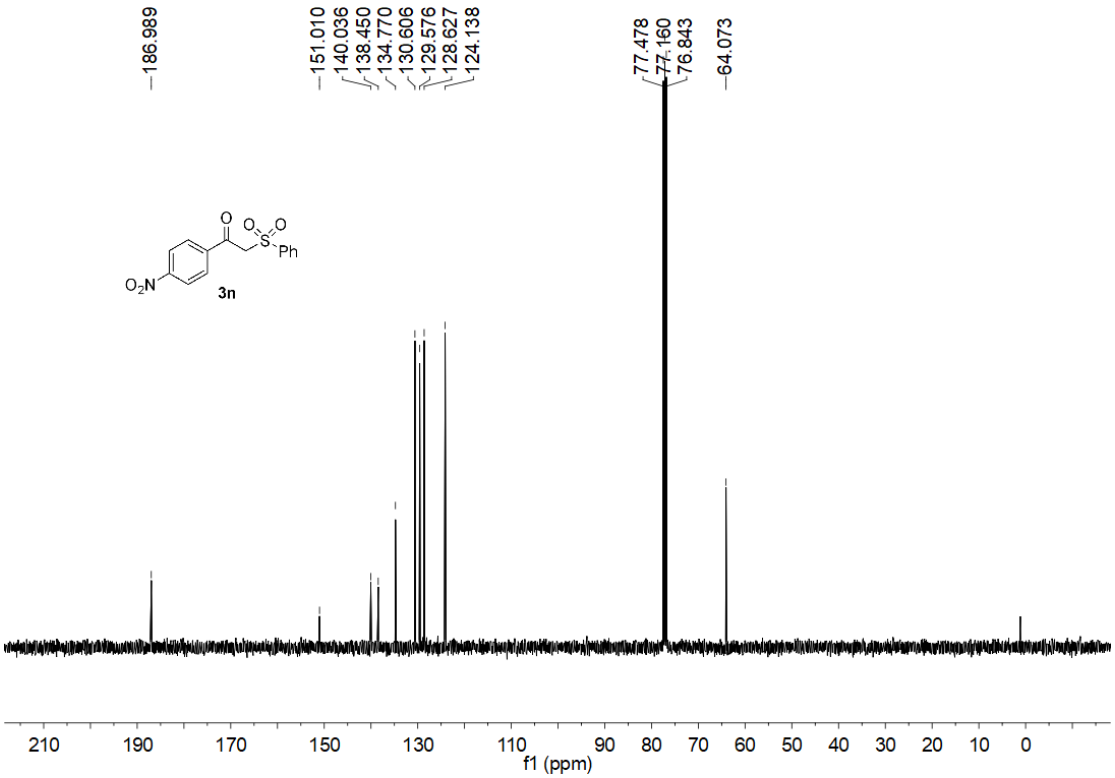
131.666
130.815
130.708
129.364
128.650
127.376
77.477
77.160
76.842
66.432
O
O
S
O
Ph
Cl
3l
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.067
8.063
8.050
8.046
7.879
7.877
7.863
7.859
7.855
7.792
7.787
7.775
7.770
7.712
7.693
7.677
7.674
7.671
7.586
7.582
7.565
7.551
7.547
7.260
4.750
O
O
S
O
Ph
NC
3m
2.01
1.92
2.04
1.03
2.00
1.99
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)


187.141
138.590
138.464
134.695
132.750
129.835
129.520
128.592
117.683
117.597
77.477
77.160
76.842
63.807
NC
O
O
S
O
Ph
3m
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.337
8.331
8.319
8.314
8.157
8.152
8.147
8.134
8.129
7.892
7.889
7.876
7.871
7.868
7.724
7.705
7.689
7.686
7.599
7.595
7.579
7.560
4.779
O
O
S
O
Ph
O2N
3n
0.97
1.05
1.09
0.93
1.96
1.02
2.02
2.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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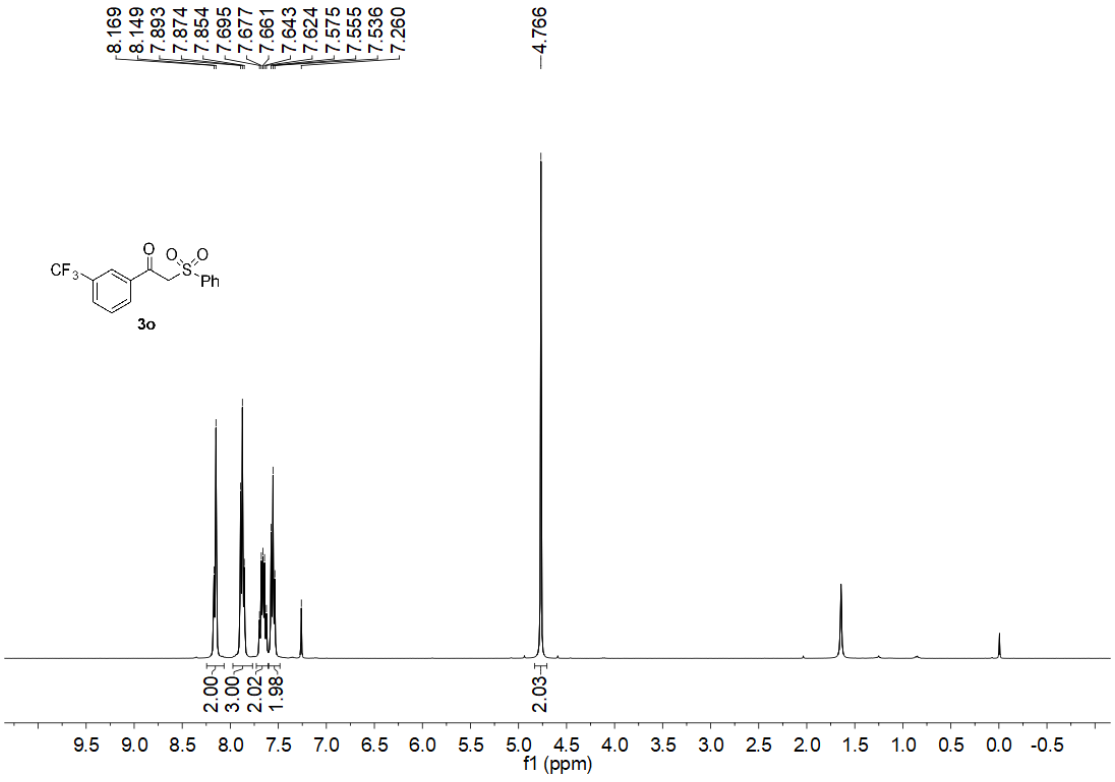
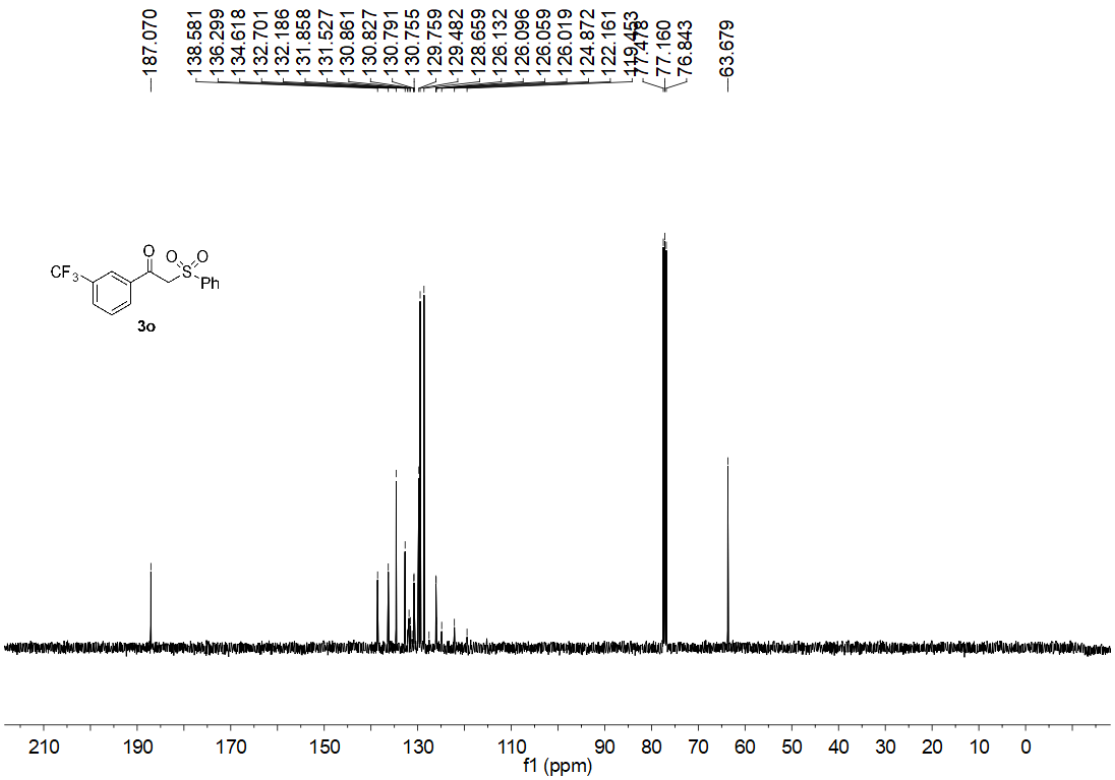
151.010
140.036
138.450
134.770
130.606
129.576
128.627
124.138
77.478
77.160
76.843
64.073
O
O
S
O
Ph
O2N
3n
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.169
8.149
7.893
7.874
7.854
7.695
7.677
7.661
7.643
7.624
7.575
7.555
7.536
7.260
4.766
CF3
O
O
S
O
Ph
3o
2.00
3.00
2.02
1.98
2.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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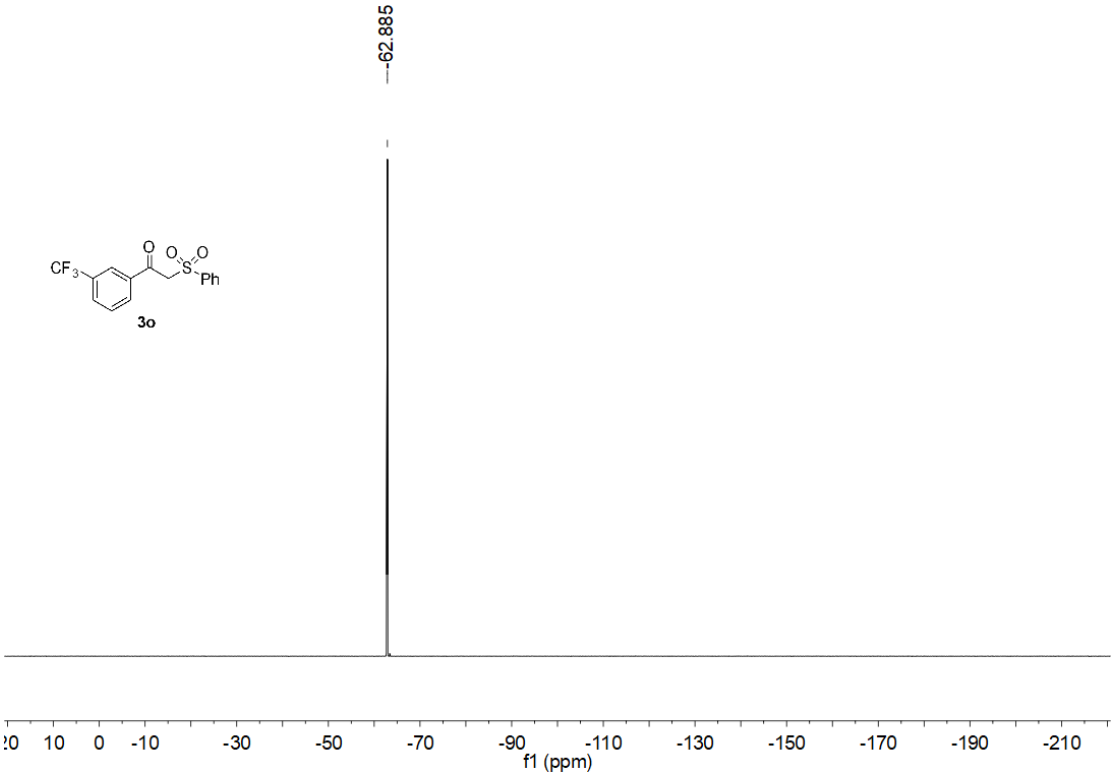
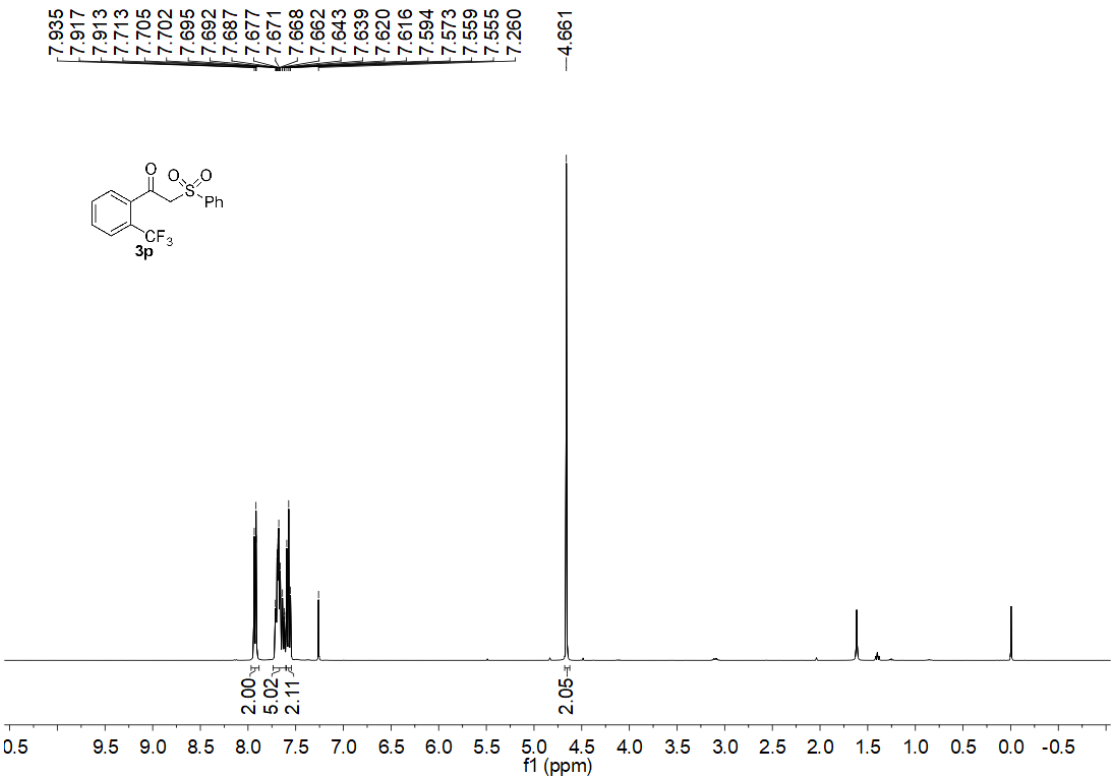
138.581
136.299
134.618
132.701
132.186
131.858
131.527
130.861
130.827
130.791
130.755
129.759
129.482
128.659
126.132
126.096
126.059
126.019
124.872
122.161
119.453
77.478
77.160
76.843
63.679
CF3
O
O
S
O
Ph
3o
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


62.885
CF3
O
O
S
O
Ph
3o
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)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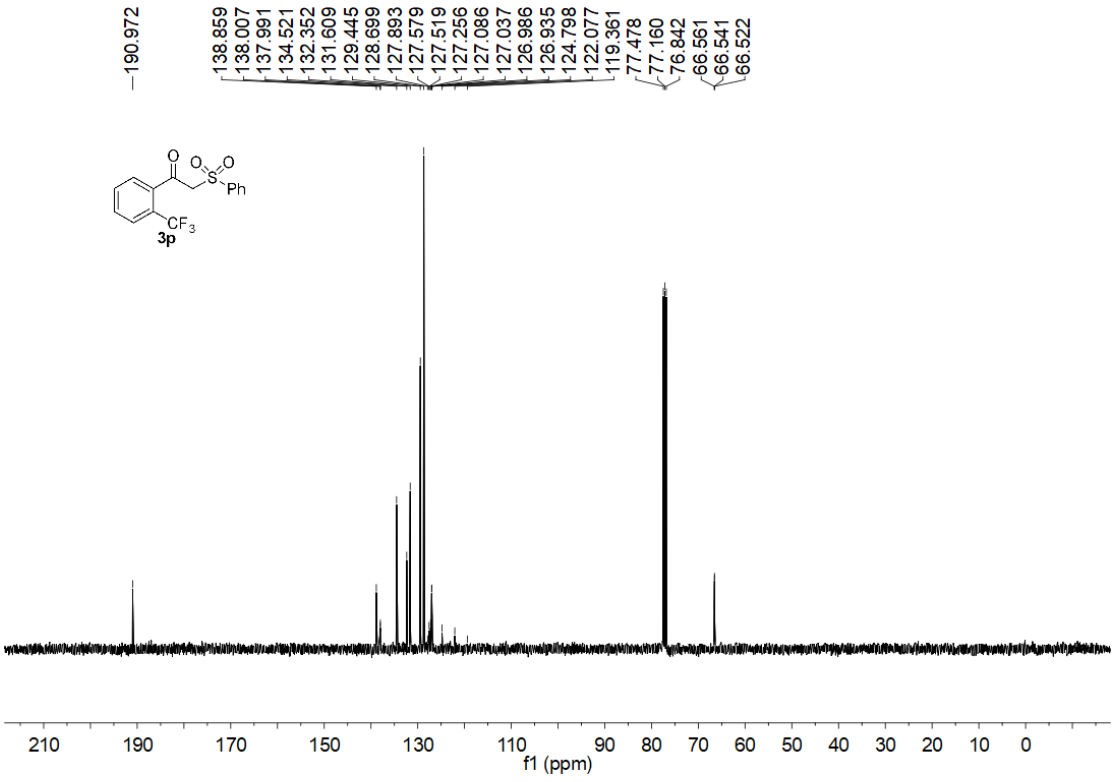
7.913
7.713
7.705
7.702
7.695
7.692
7.687
7.677
7.671
7.668
7.662
7.643
7.639
7.620
7.616
7.594
7.573
7.559
7.555
7.260
4.661
O
O
S
O
Ph
CF3
3p
2.00
5.02
2.11
2.05
f1 (ppm)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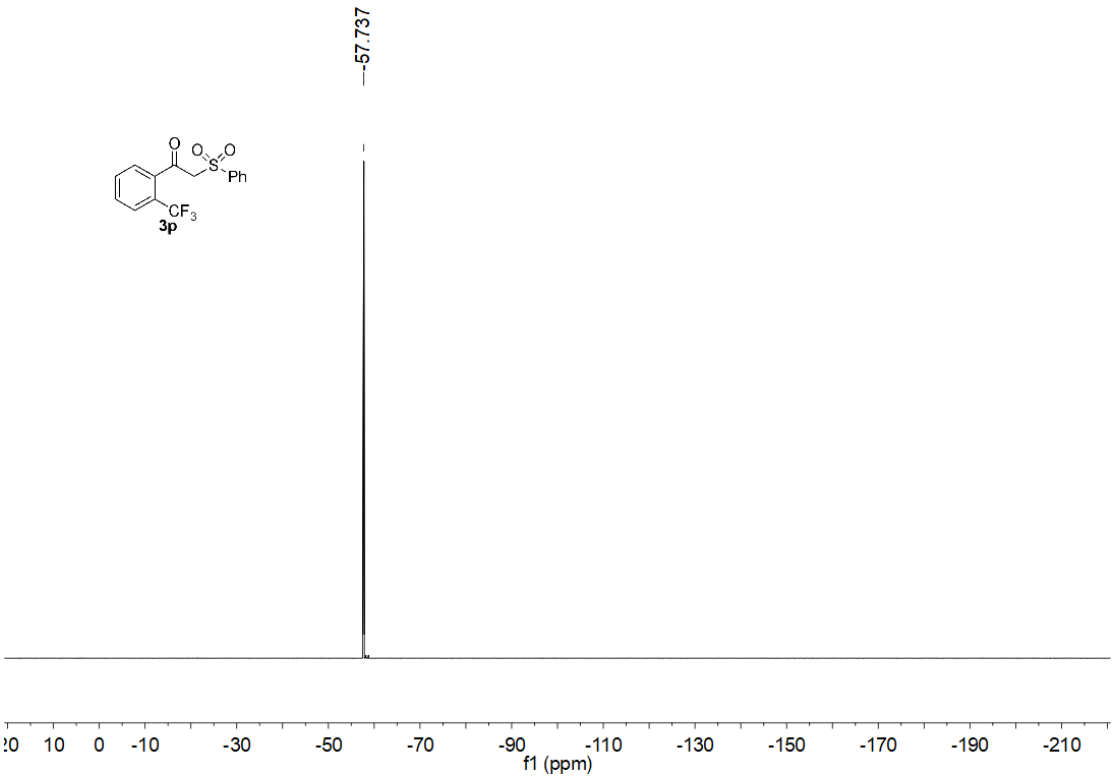
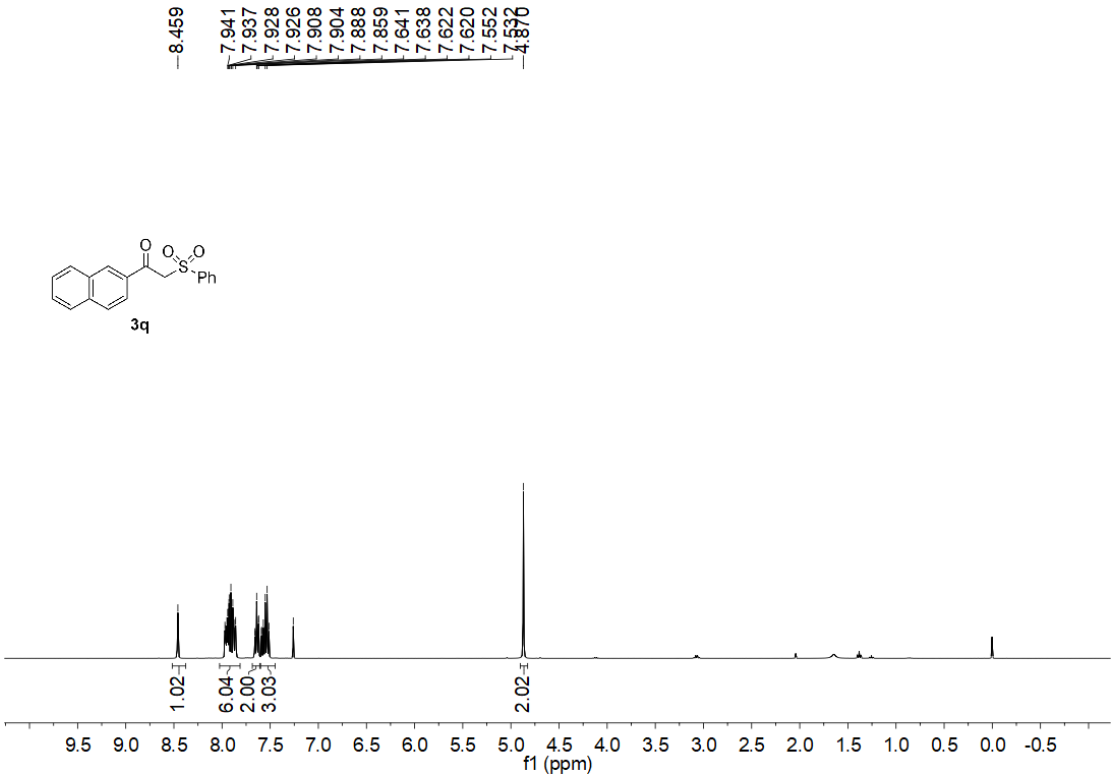
138.007
137.991
134.521
132.352
131.609
129.445
128.699
127.893
127.579
127.519
127.256
127.086
127.037
126.986
126.935
124.798
122.077
119.361
77.478
77.160
76.842
66.561
66.541
66.522
O
O
S
O
Ph
CF3
3p
f1 (ppm)


-57.737
Ph
CF3
3p
f1 (ppm)


8.459
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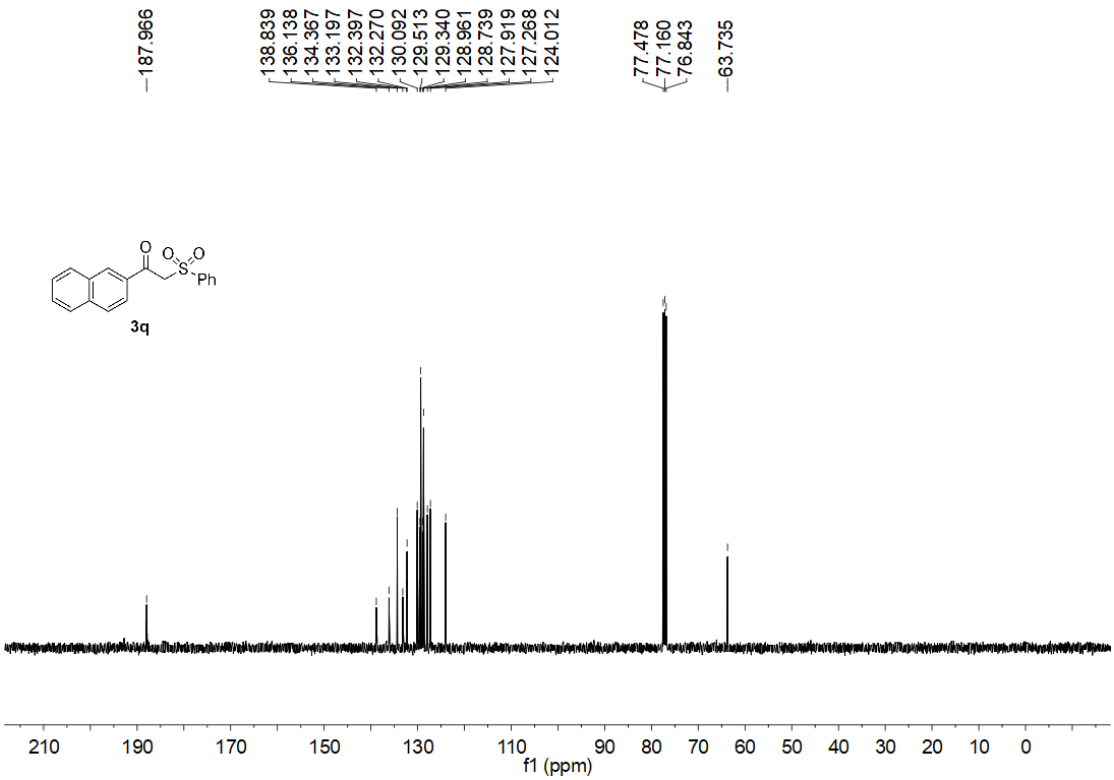
7.937
7.928
7.926
7.908
7.904
7.888
7.859
7.641
7.638
7.622
7.620
7.552
4.870
Ph
3q
1.02
6.04
2.00
3.03
2.02
f1 (ppm)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134.367
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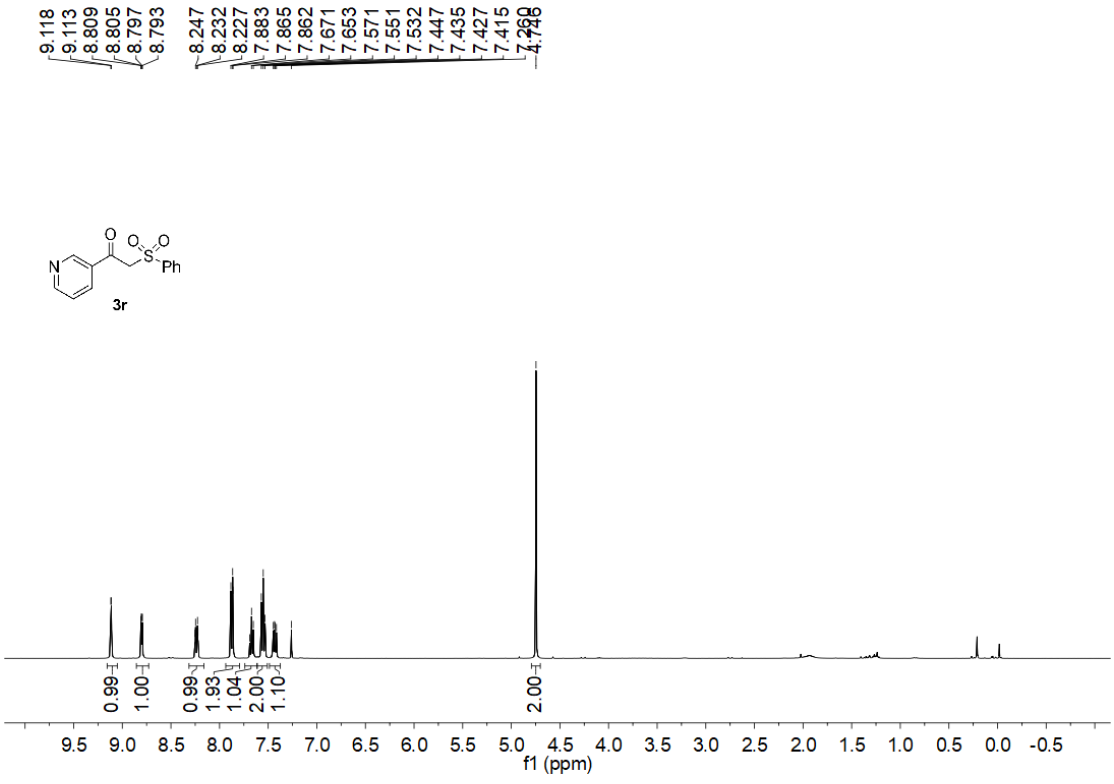
132.270
130.092
129.513
129.340
128.961
128.739
127.919
127.268
124.012
77.478
77.160
76.843
63.735
O
O
S
O
Ph
3q
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.793
8.247
8.232
8.227
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7.865
7.862
7.671
7.653
7.571
7.551
7.532
7.447
7.435
7.427
7.415
4.748
O
O
S
O
Ph
N
3r
0.99
1.00
0.99
1.93
1.04
2.00
1.10
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.5
2.0
1.5
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0.5
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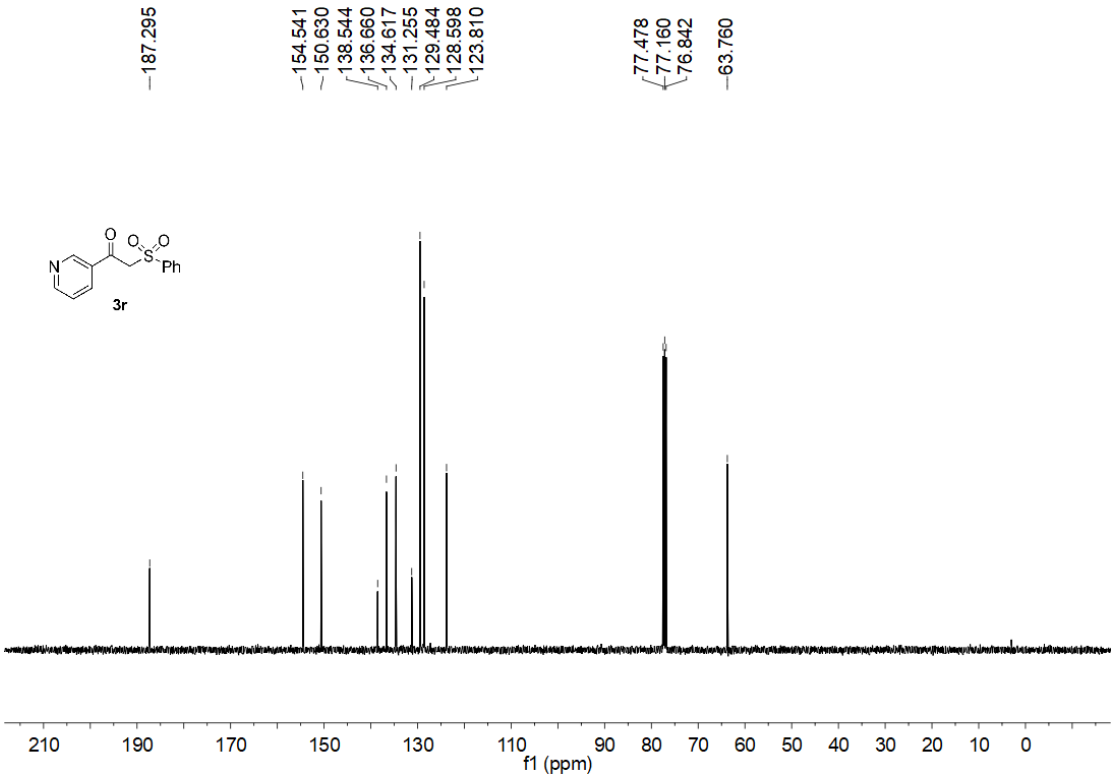
f1 (ppm)


187.295
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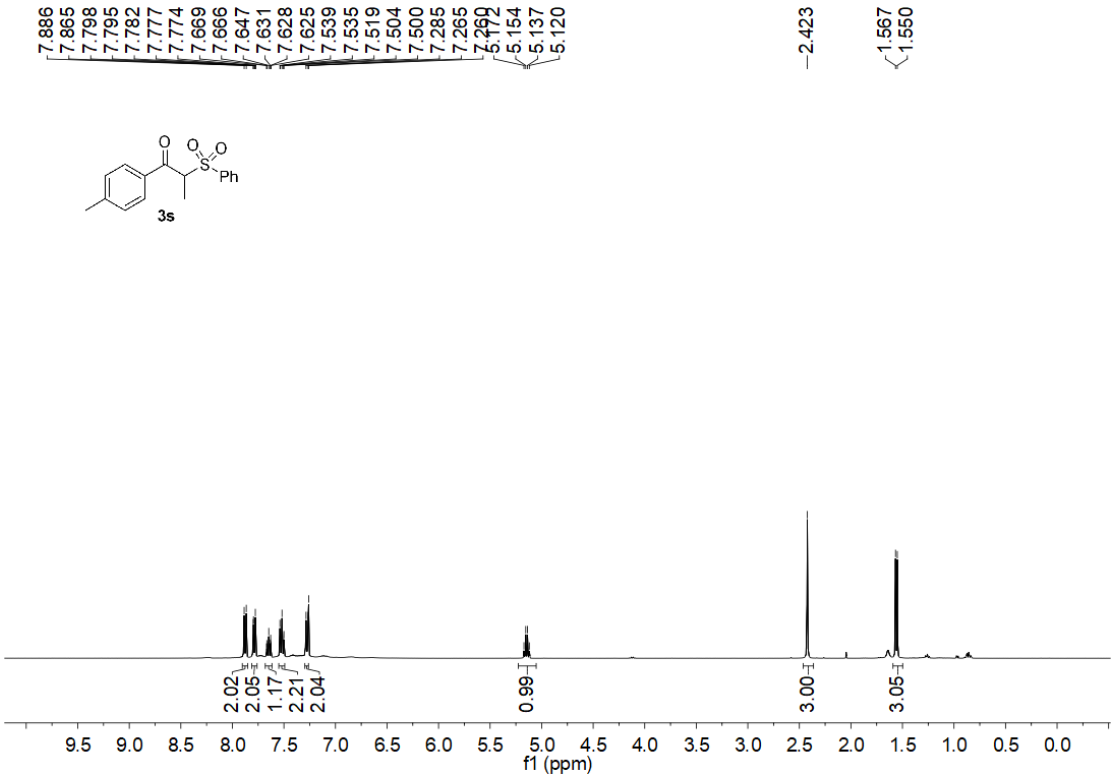
138.544
136.660
134.617
131.255
129.484
128.598
123.810
77.478
77.160
76.842
63.760
3r
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.777
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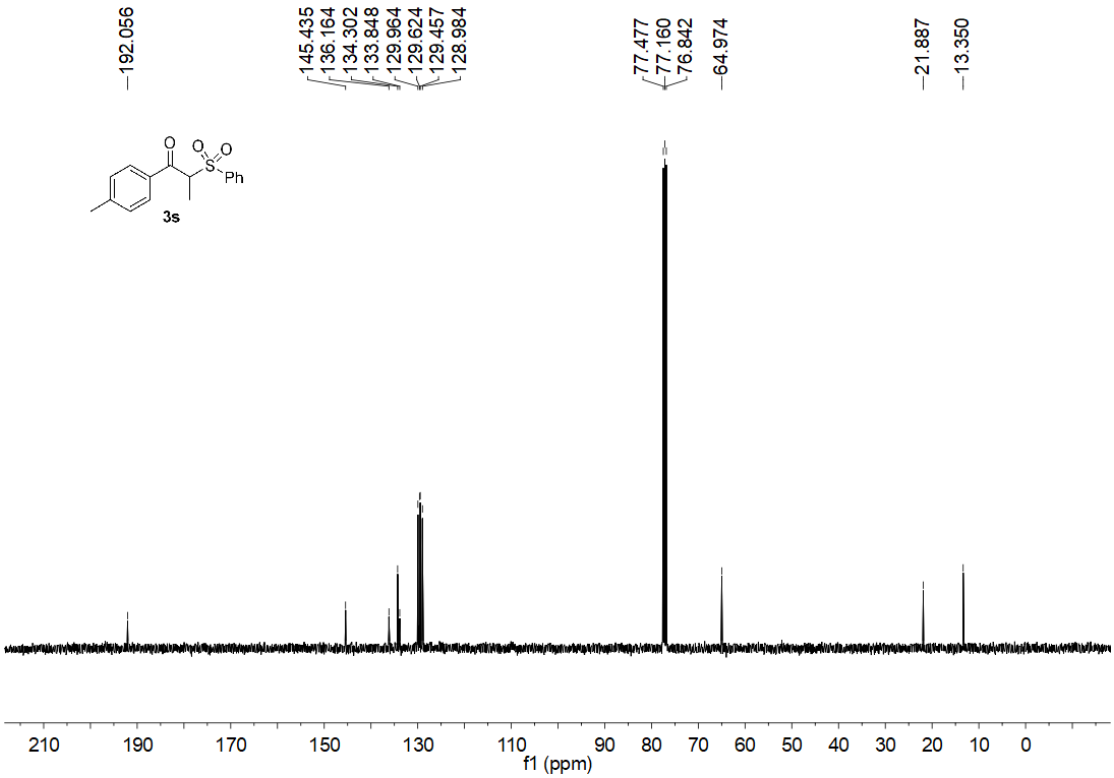
7.669
7.666
7.647
7.631
7.628
7.625
7.539
7.535
7.519
7.504
7.500
7.285
7.265
5.154
5.137
5.120
2.423
1.567
1.550
3s
2.02
2.05
1.17
2.21
2.04
0.99
3.00
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


192.056
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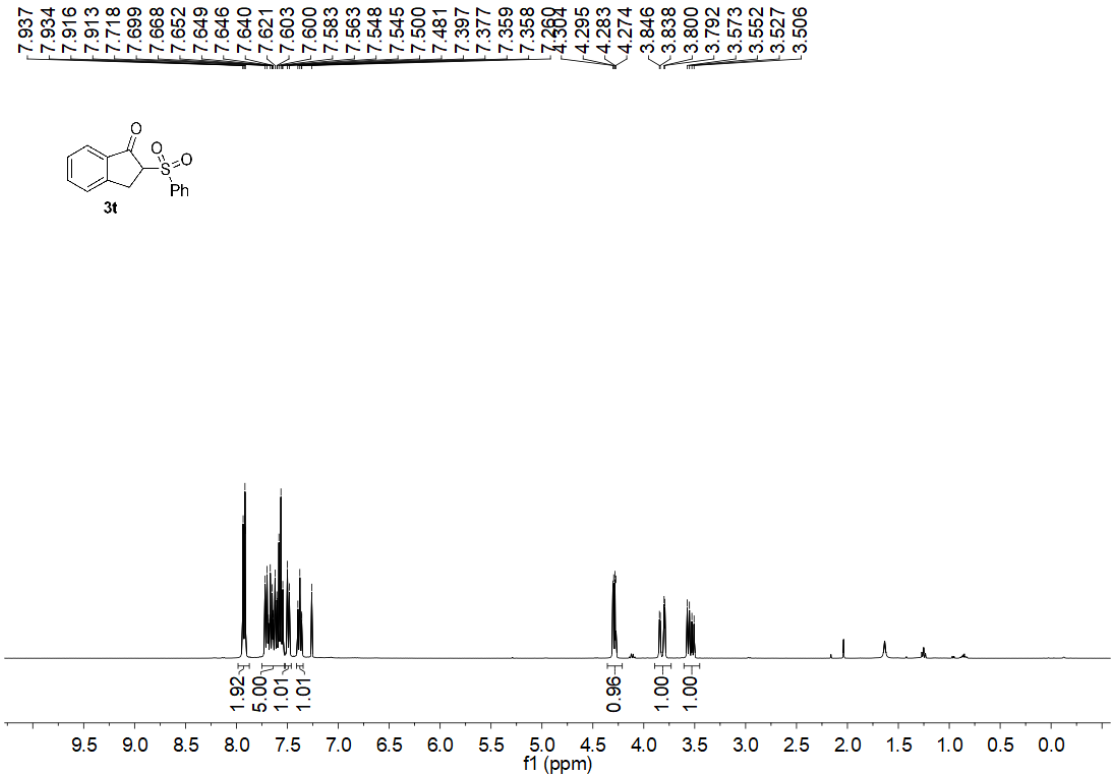
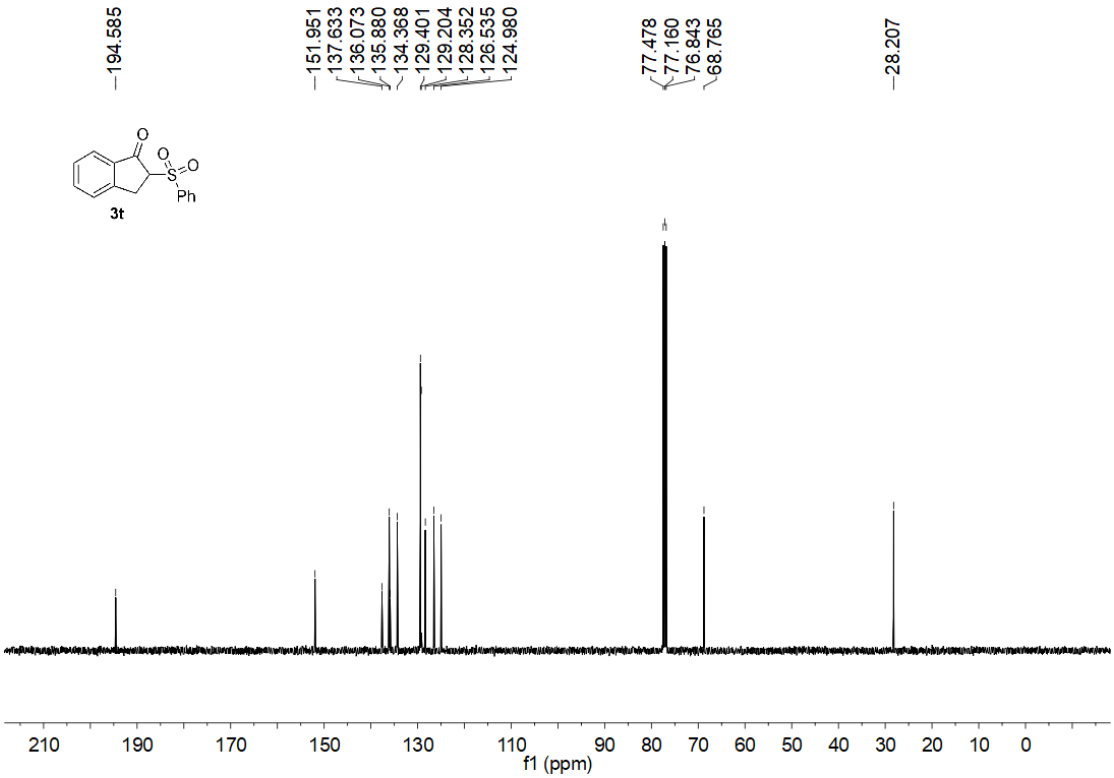
136.164
134.302
133.848
129.964
129.624
129.457
128.984
77.477
77.160
76.842
64.974
21.887
13.350
3s
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.937
7.934
7.916
7.913
7.718
7.699
7.668
7.652
7.649
7.646
7.640
7.621
7.603
7.600
7.583
7.563
7.548
7.545
7.500
7.481
7.397
7.377
7.359
7.358
4.295
4.283
4.274
3.846
3.838
3.800
3.792
3.573
3.552
3.527
3.506
3t
1.92
5.00
1.01
1.01
0.96
1.00
1.00
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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137.633
136.073
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134.368
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129.204
128.352
126.535
124.980
77.478
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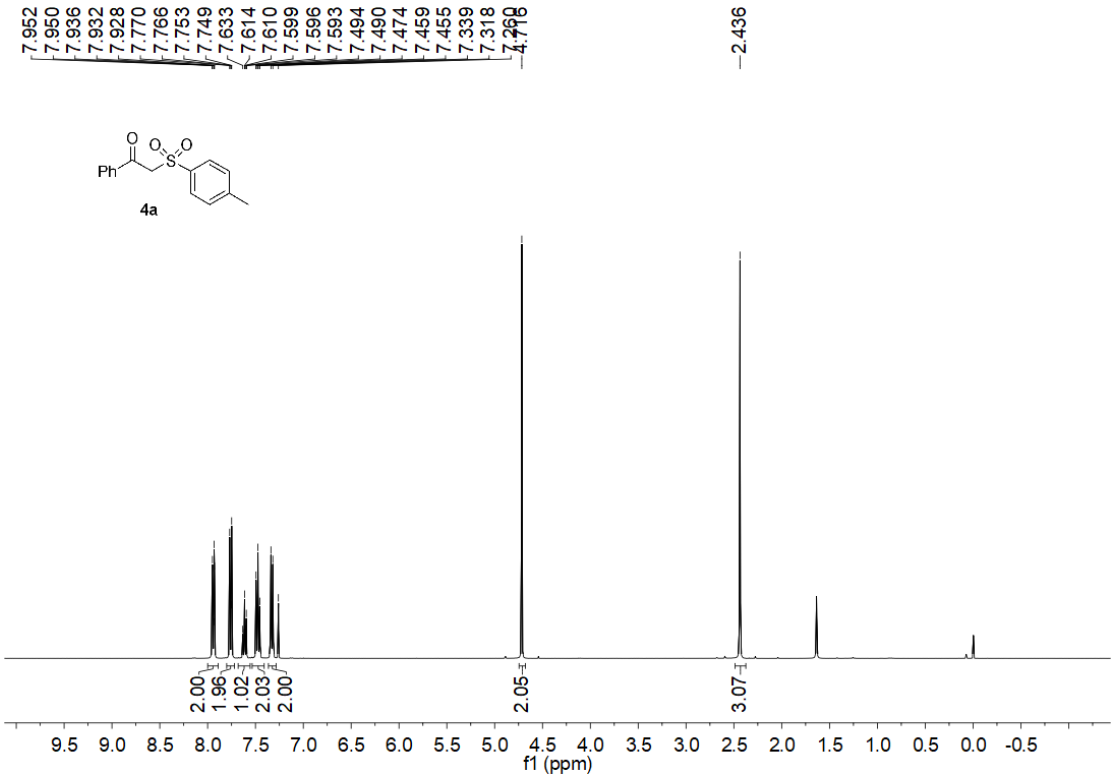
76.843
68.765
28.207
3t
f1 (ppm)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7.950
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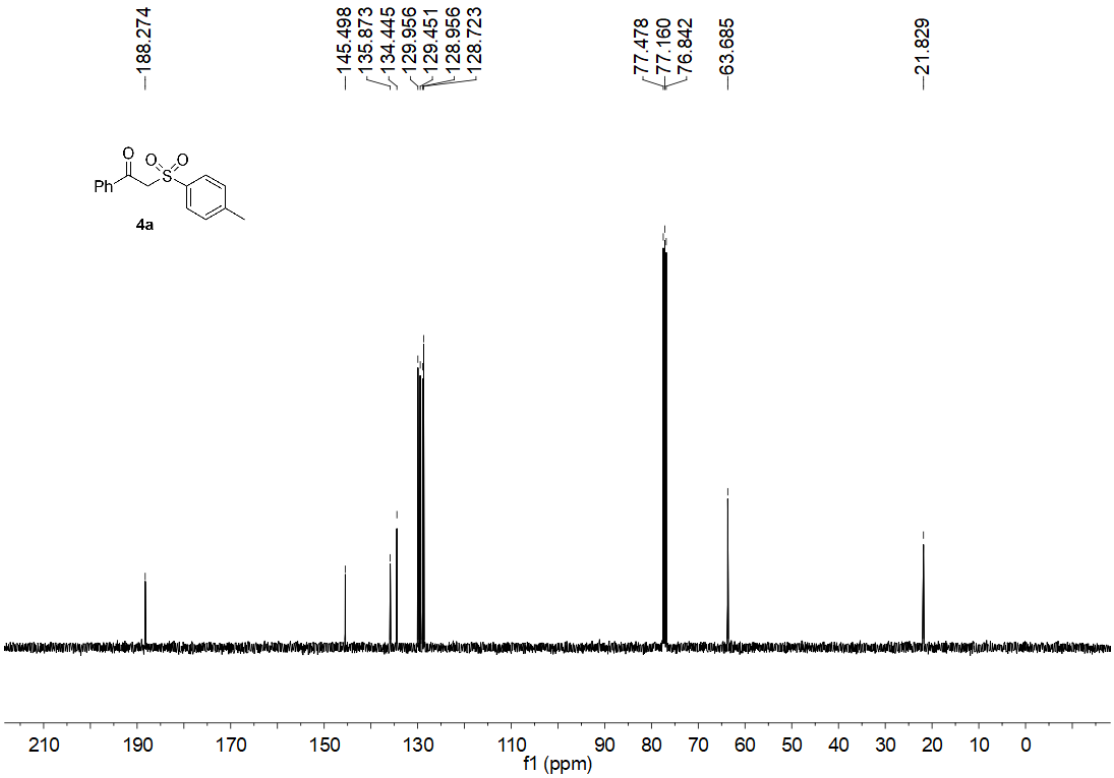
7.932
7.928
7.770
7.766
7.753
7.749
7.633
7.614
7.610
7.599
7.596
7.593
7.494
7.490
7.474
7.459
7.455
7.339
7.318
4.718
2.436
4a
2.00
1.96
1.02
2.03
2.00
2.05
3.07
f1 (ppm)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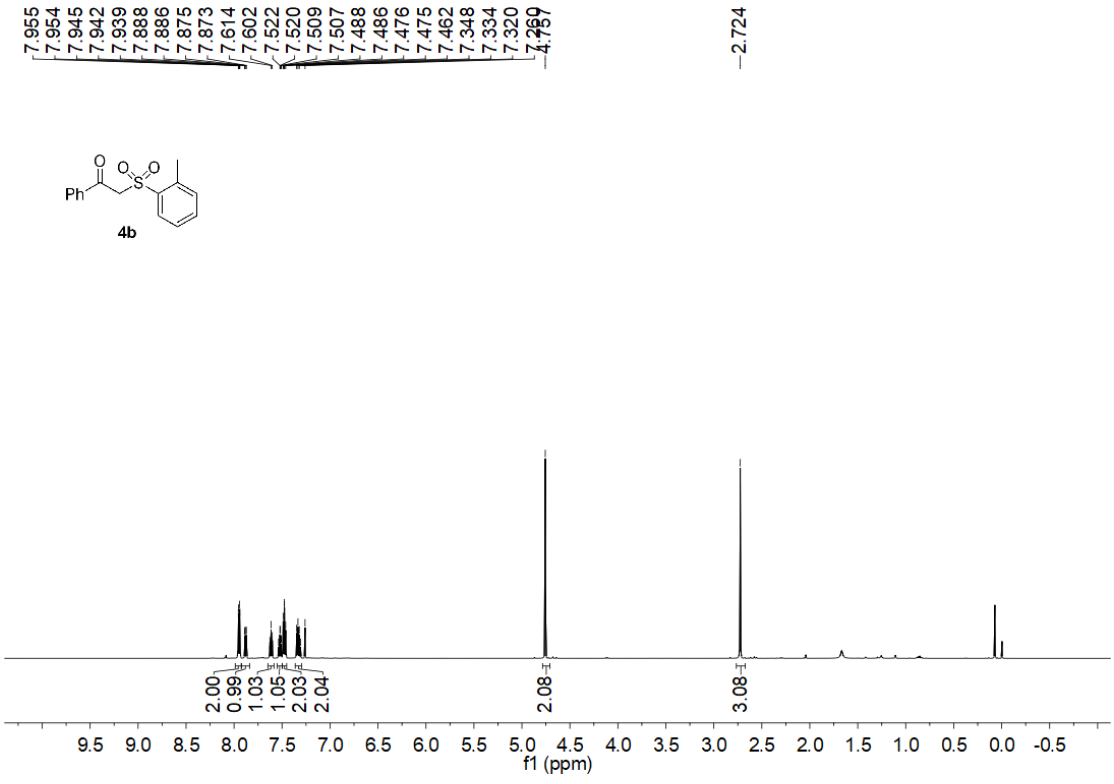
128.956
128.723
77.478
77.160
76.842
63.685
21.829
Ph
4a
f1 (ppm)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7.954
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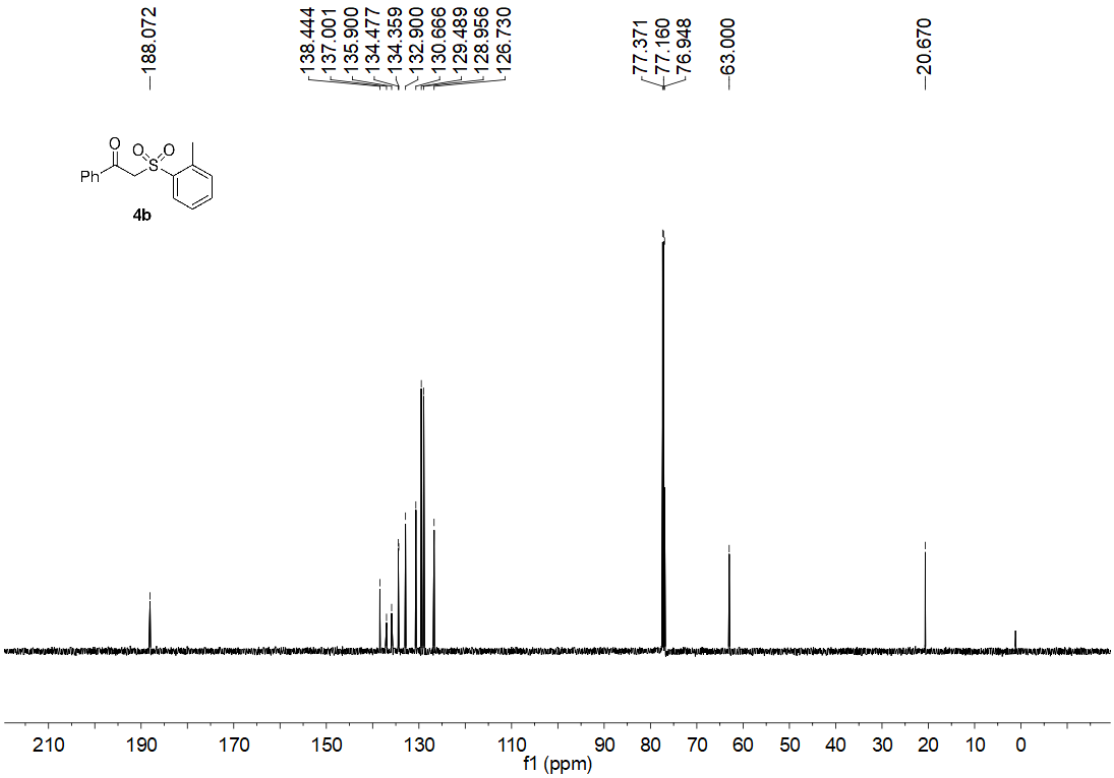
7.942
7.939
7.888
7.886
7.875
7.873
7.614
7.602
7.522
7.520
7.509
7.507
7.488
7.486
7.476
7.475
7.462
7.348
7.334
7.320
7.260
4.757
2.724
Ph
4b
2.00
0.99
1.03
1.05
2.03
2.04
2.08
3.08
f1 (ppm)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126.730
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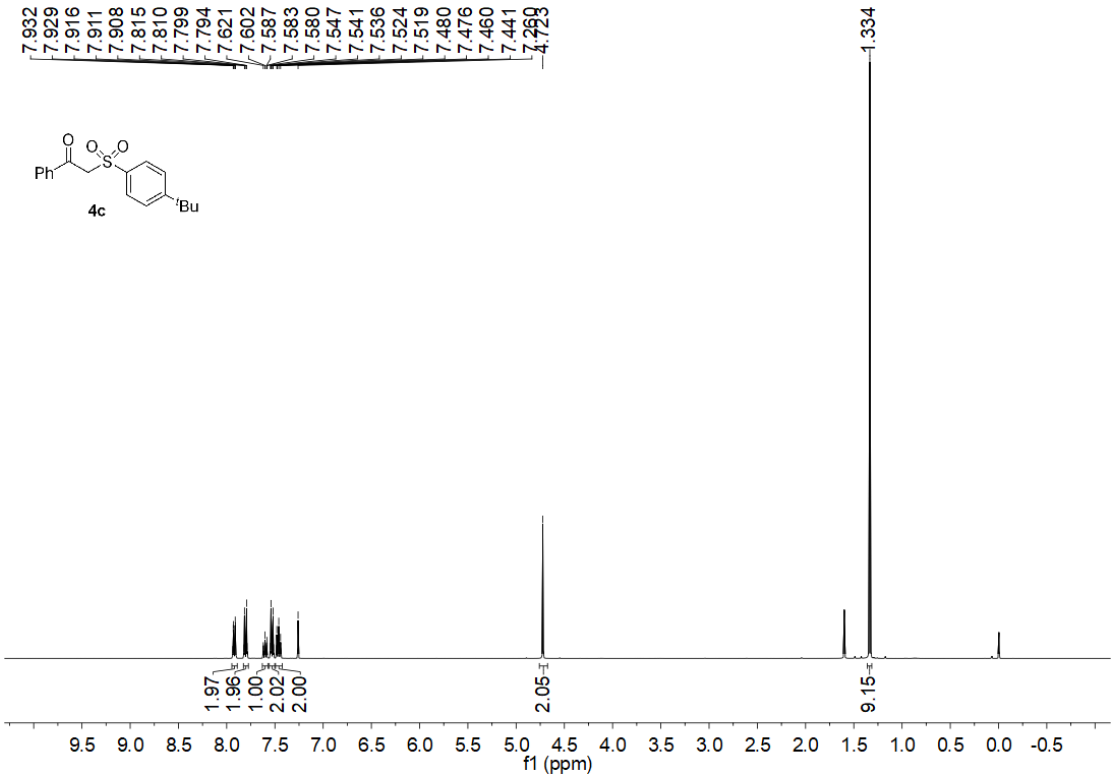
77.160
76.948
63.000
20.670
Ph
4b
f1 (ppm)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7.916
7.911
7.908
7.815
7.810
7.799
7.794
7.621
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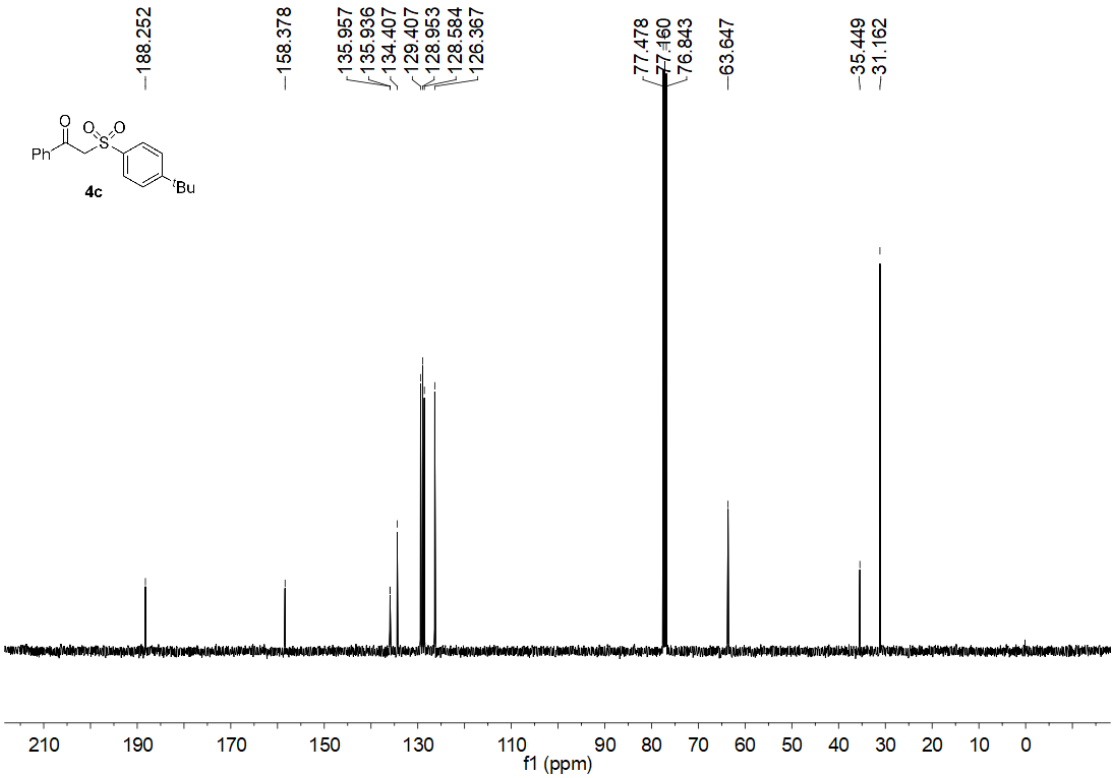
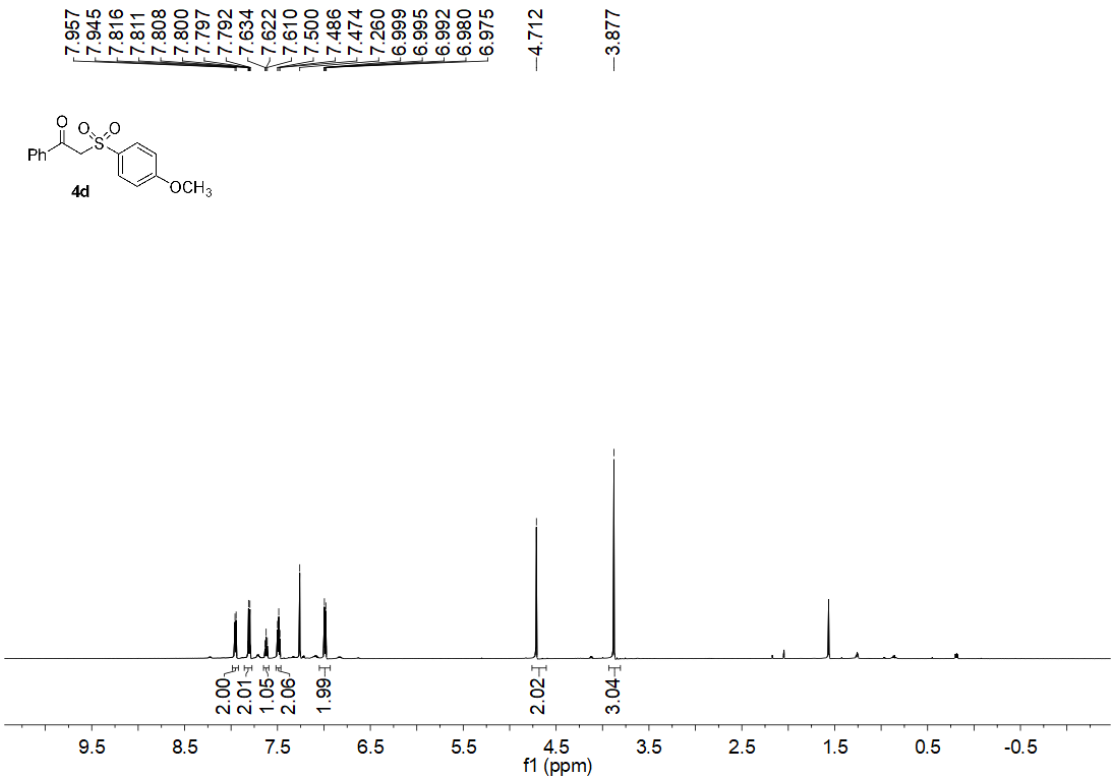
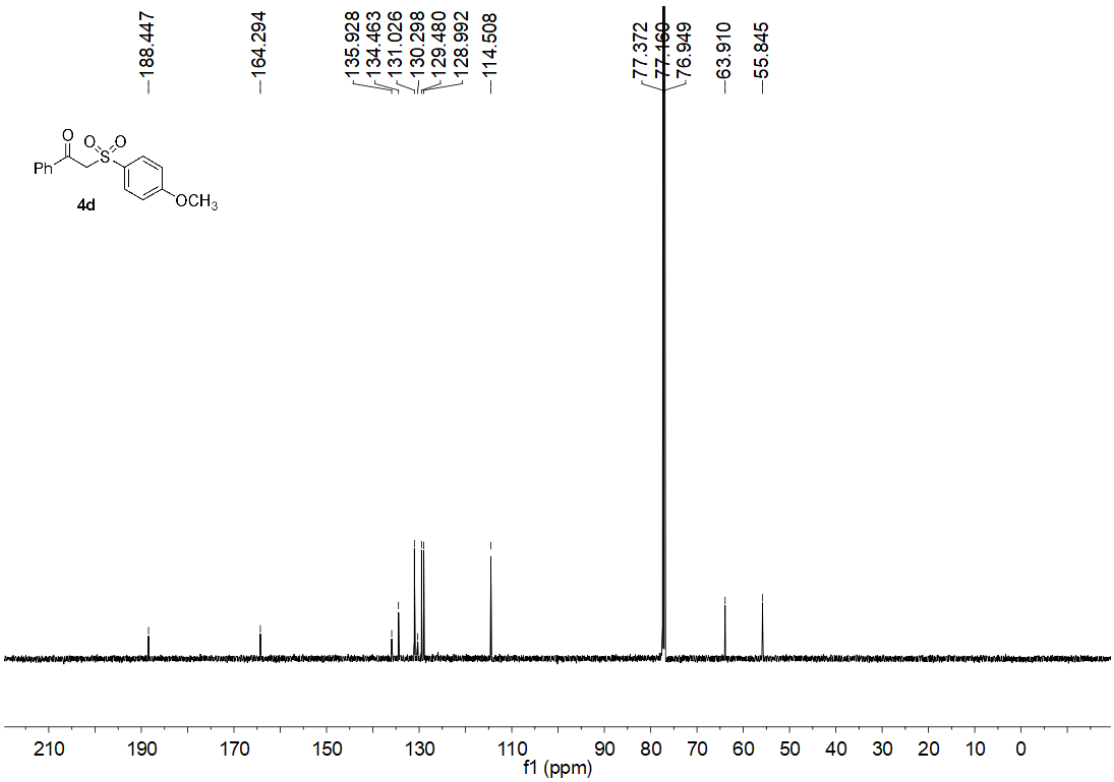
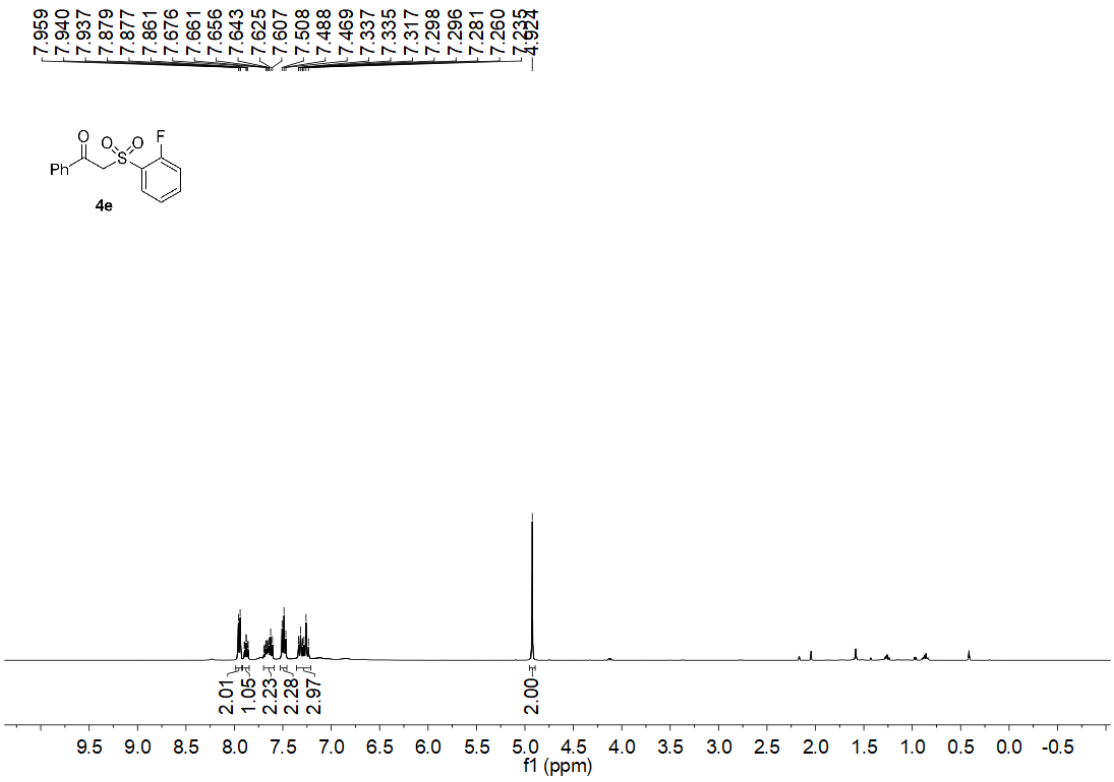
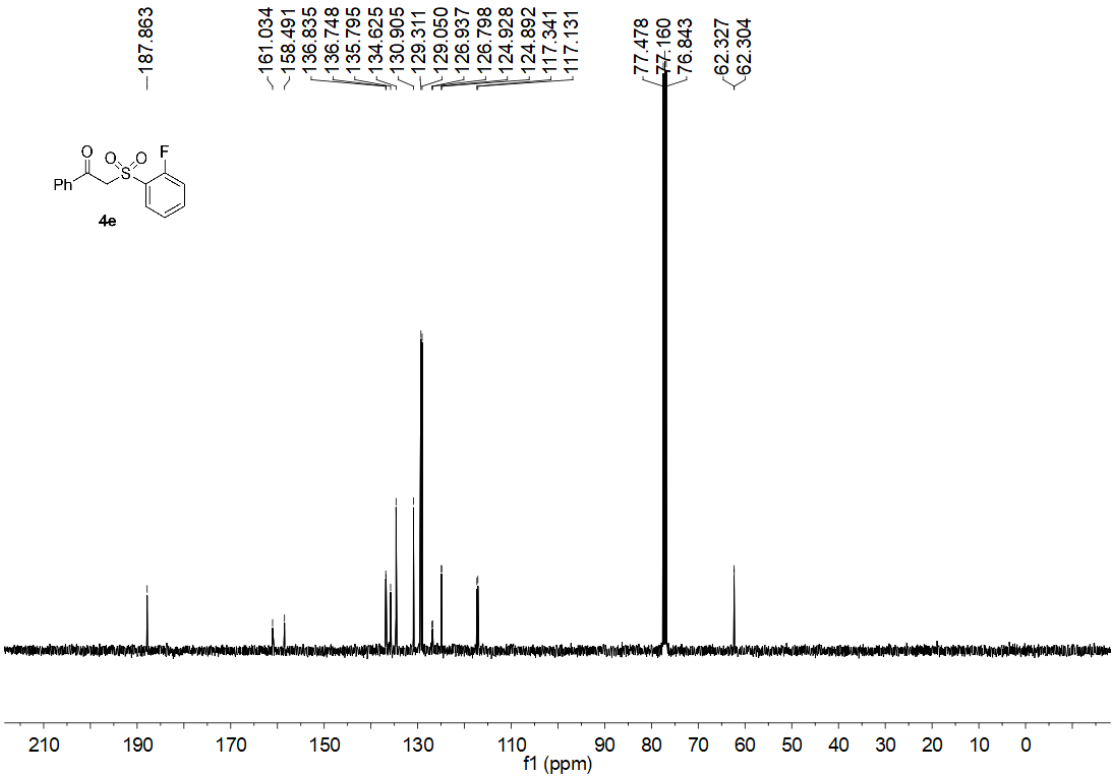
7.587
7.583
7.580
7.547
7.541
7.536
7.524
7.519
7.480
7.476
7.460
7.441
7.260
4.723
1.334
Ph
tBu
4c
1.97
1.96
1.00
2.02
2.00
2.05
9.15
f1 (ppm)

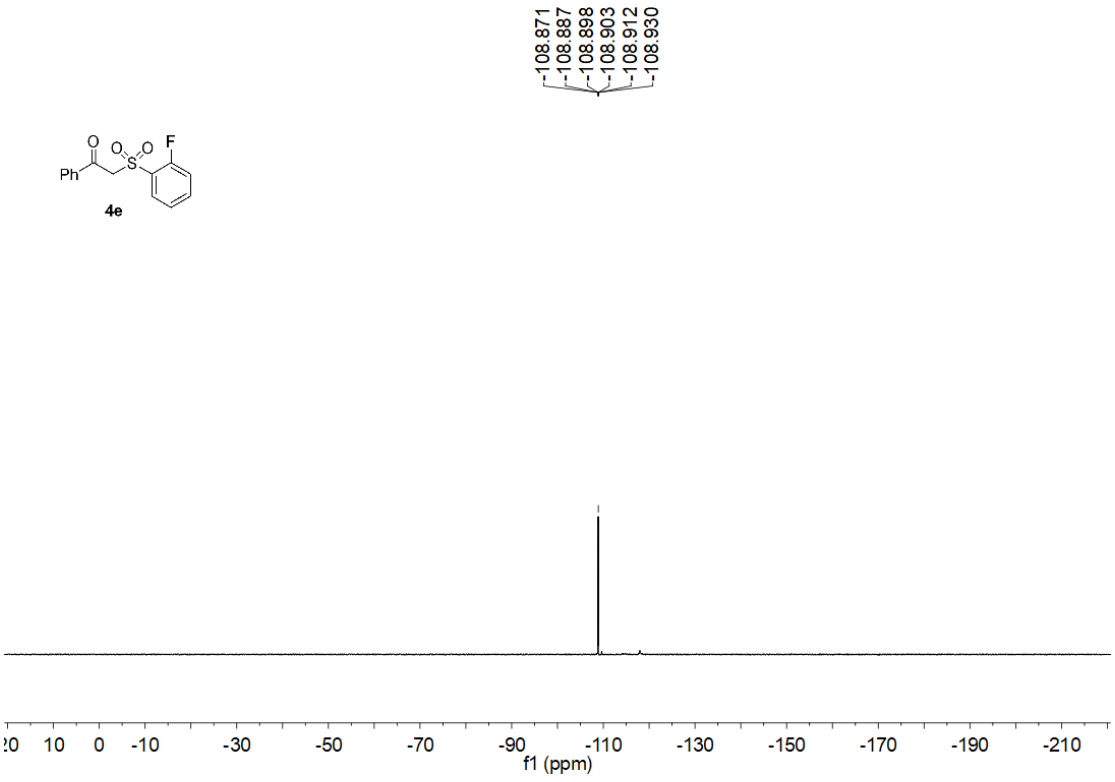

188.252
158.378
135.957
135.936
134.407
129.407
128.953
128.584
126.367
77.478
77.460
76.843
63.647
35.449
31.162
Ph
O
O
S
O
tBu
4c
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

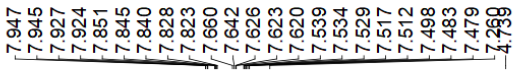

7.957
7.945
7.816
7.811
7.808
7.800
7.797
7.792
7.634
7.622
7.610
7.500
7.486
7.474
7.260
6.999
6.995
6.992
6.980
6.975
4.712
3.877
Ph
O
O
S
O
OCH3
4d
2.00
2.01
1.05
2.06
1.99
2.02
3.04
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

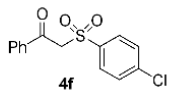

188.447
164.294
135.928
134.463
131.026
130.298
129.480
128.992
114.508
77.372
77.160
76.949
63.910
55.845
Ph
O
O
O
S
OCH3
4d
f1 (ppm)


7.959
7.940
7.937
7.879
7.877
7.861
7.676
7.661
7.656
7.643
7.625
7.607
7.508
7.488
7.469
7.337
7.335
7.317
7.298
7.296
7.281
7.260
4.924
Ph
O
O
O
S
F
4e
2.01
1.05
2.23
2.28
2.97
2.00
f1 (ppm)

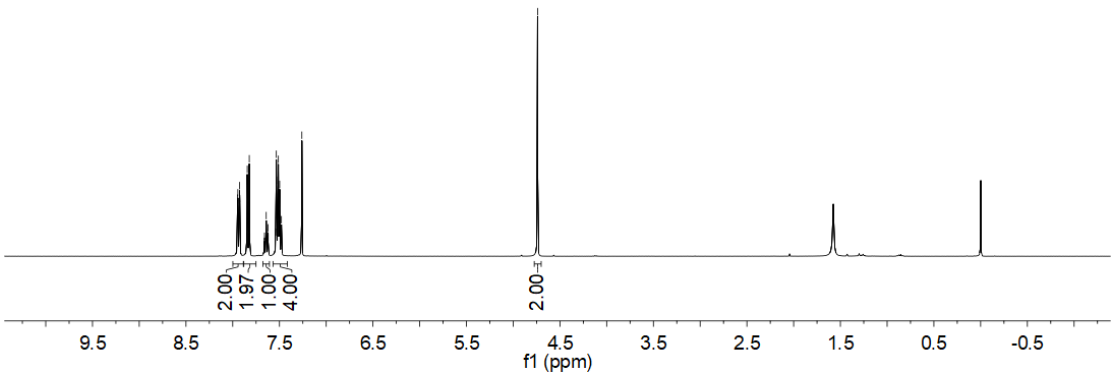

187.863
161.034
158.491
136.835
136.748
135.795
134.625
130.905
129.311
129.050
126.937
126.798
124.928
124.892
117.341
117.131
77.478
77.160
76.843
62.327
62.304
Ph
O
O
S
O
F
4e
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

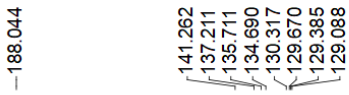

108.871
108.887
108.898
108.903
108.912
108.930
Ph
O
O
S
O
F
4e
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

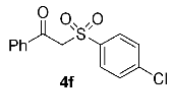

7.947
7.945
7.927
7.924
7.851
7.845
7.840
7.828
7.823
7.660
7.642
7.626
7.623
7.620
7.539
7.534
7.529
7.517
7.512
7.498
7.483
7.479
7.260
4.739


O
O
S
O
Ph
Cl

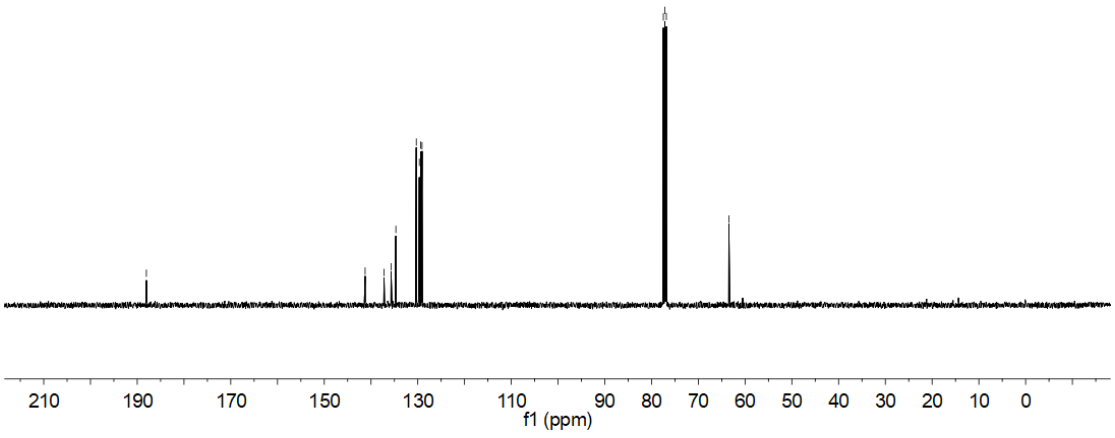
4f

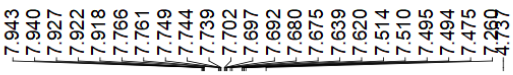

2.00
1.97
1.00
4.00
2.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

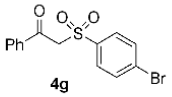

188.044
141.262
137.211
135.711
134.690
130.317
129.670
129.385
129.088
77.478
77.160
76.843
63.464


O
O
S
O
Ph
Cl

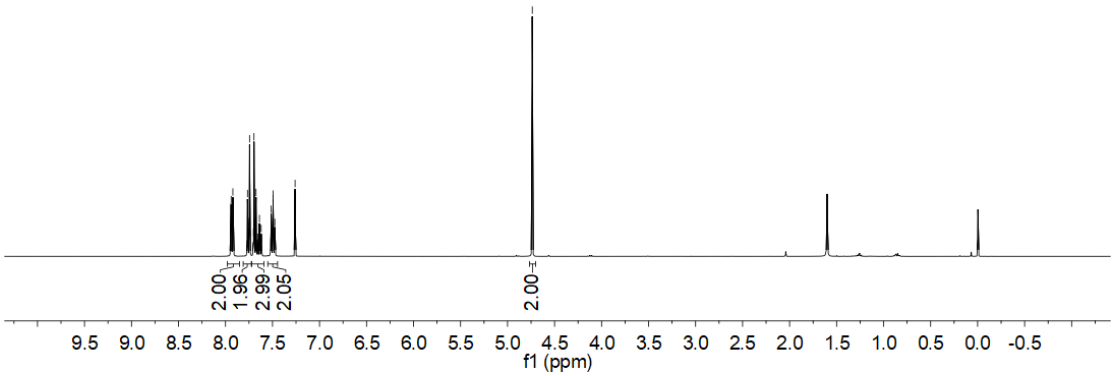
4f

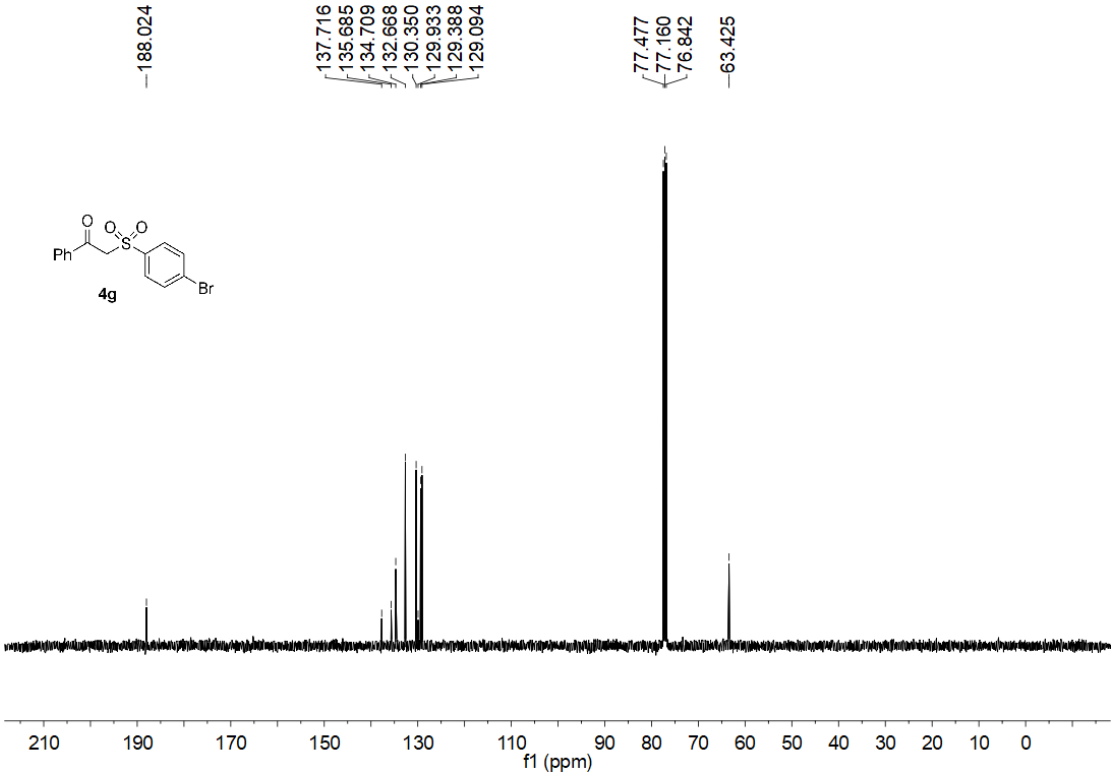

210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.943
7.940
7.927
7.922
7.918
7.766
7.761
7.749
7.744
7.739
7.702
7.697
7.692
7.680
7.675
7.639
7.620
7.514
7.510
7.495
7.494
7.475


O
O
S
O
Ph
Br

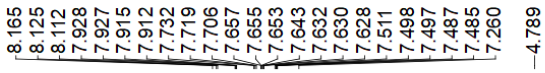
4g

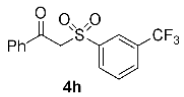

2.00
1.96
2.99
2.05
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


188.024
137.716
135.685
134.709
132.668
130.350
129.933
129.388
129.094
77.477
77.160
76.842
63.425
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

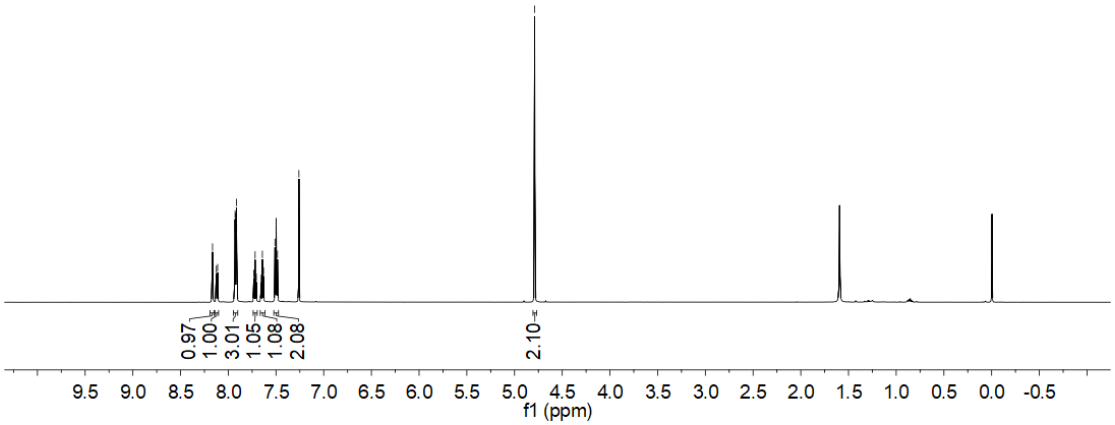

O
O
S
O
Ph
Br

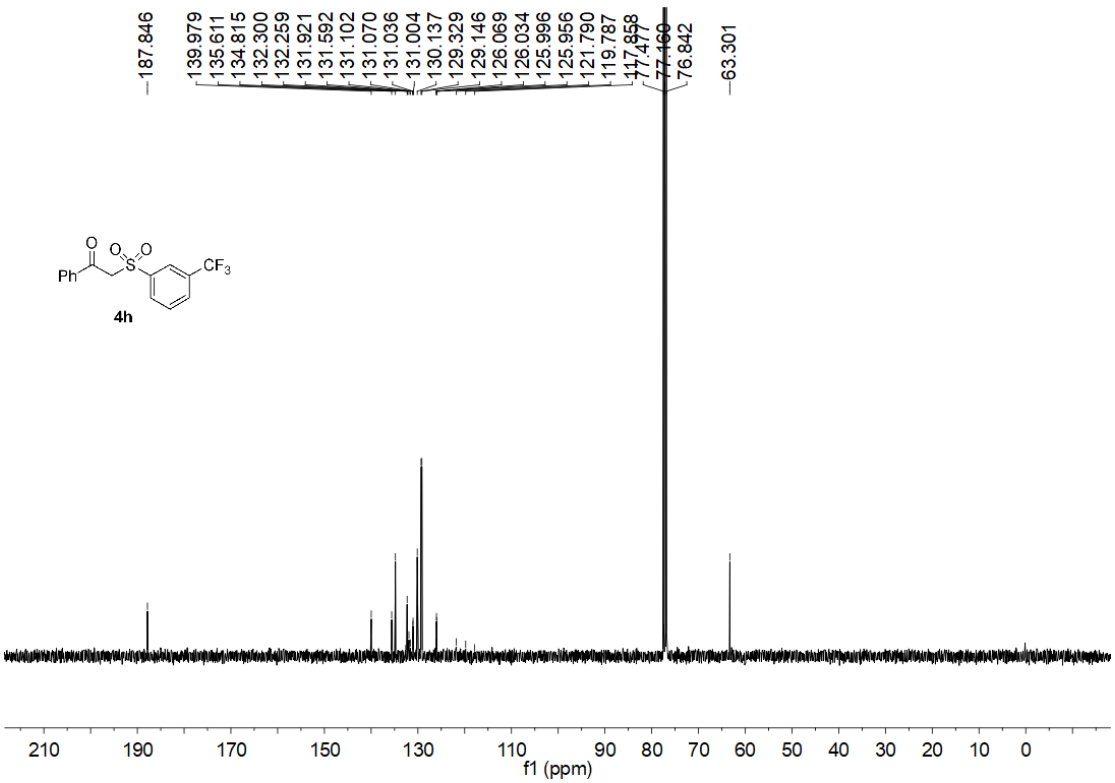
4g


8.165
8.125
8.112
7.928
7.927
7.915
7.912
7.732
7.719
7.706
7.657
7.655
7.653
7.643
7.632
7.630
7.628
7.511
7.498
7.497
7.487
7.485
7.260
4.789


O
O
S
O
Ph
CF3

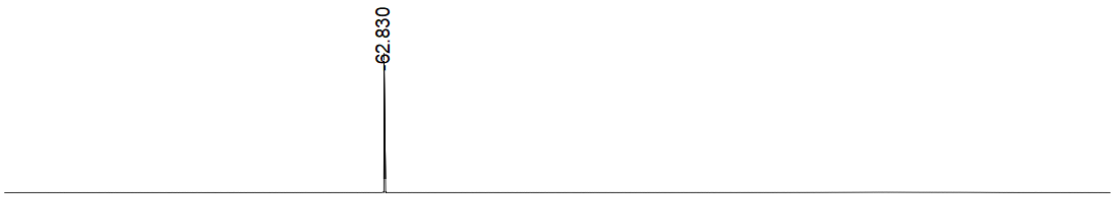
4h

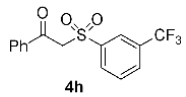

0.97
1.00
3.01
1.05
1.08
2.08
2.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


187.846
139.979
135.611
134.815
132.300
132.259
131.921
131.592
131.102
131.070
131.036
131.004
130.137
129.329
129.146
126.069
126.034
125.996
125.956
121.790
119.787
117.858
117.477
77.160
76.842
63.301
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

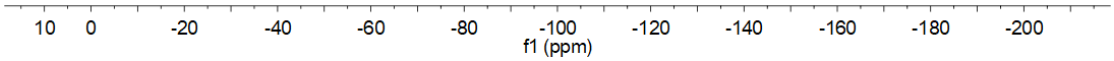

O
O
S
O
Ph
CF3

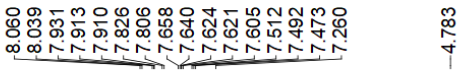
4h

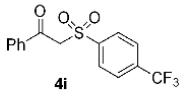

62.830



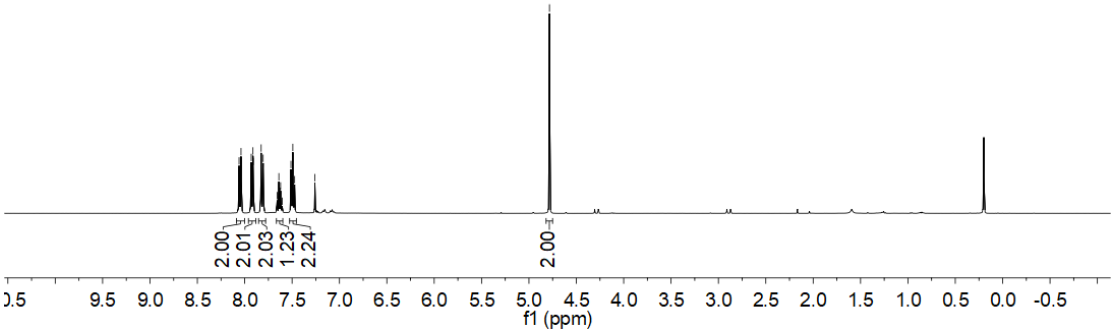
4h

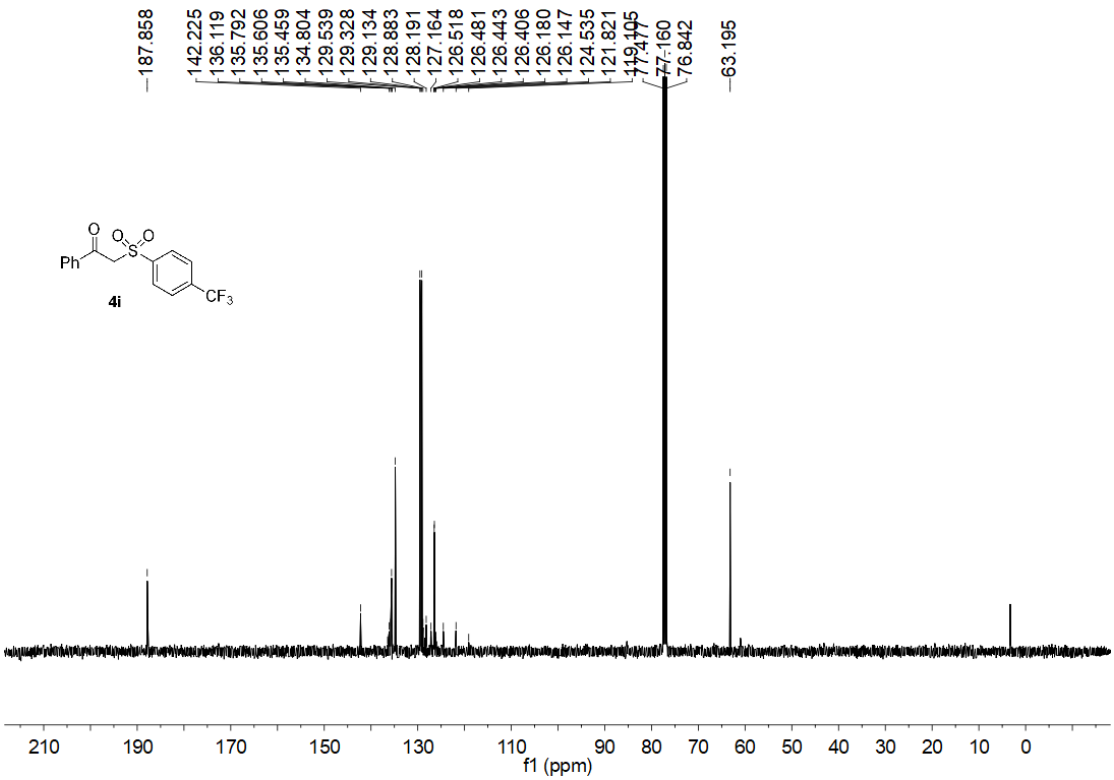

10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)

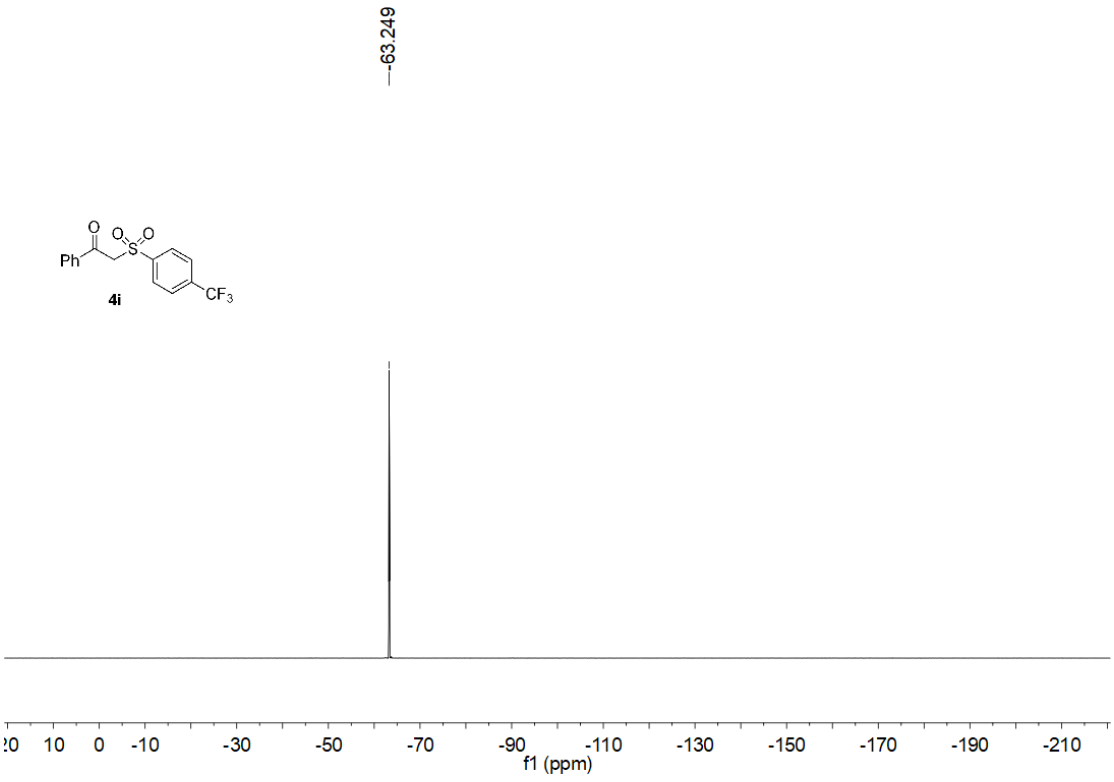

8.060
8.039
7.931
7.913
7.910
7.826
7.806
7.658
7.640
7.624
7.621
7.605
7.512
7.492
7.473
7.260
4.783

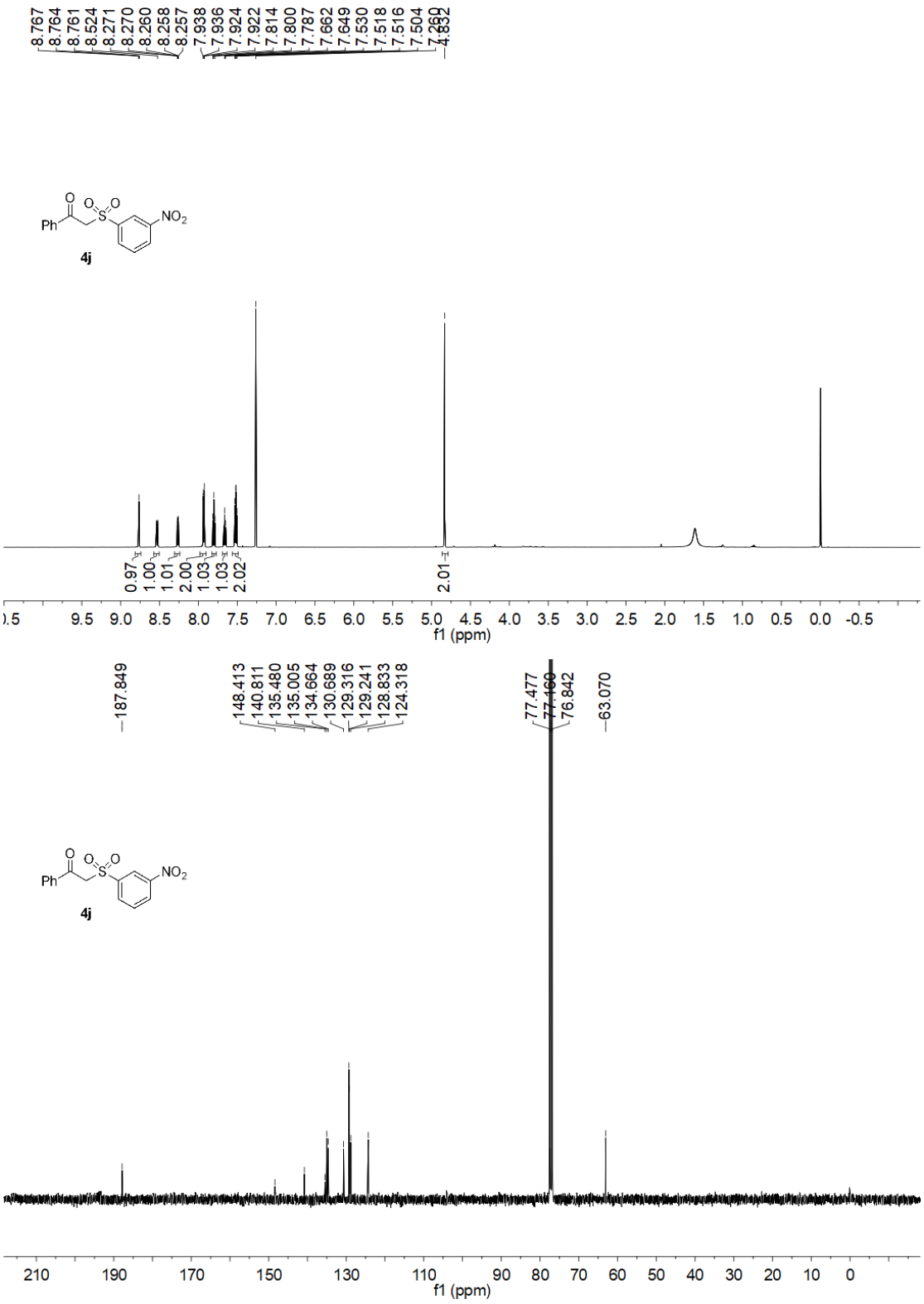


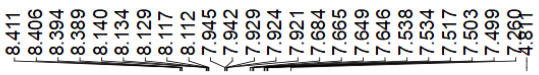
4i


2.00
2.01
2.03
1.23
2.24
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


187.858
142.225
136.119
135.792
135.606
135.459
134.804
129.539
129.328
129.134
128.883
128.191
127.164
126.518
126.481
126.443
126.406
126.180
126.147
124.535
121.821
119.105
77.417
77.160
76.842
63.195
Ph
O
O
S
O
CF3
4i
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


63.249
Ph
O
O
S
O
CF3
4i
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


8.767
8.764
8.761
8.524
8.271
8.270
8.260
8.258
8.257
7.938
7.936
7.924
7.922
7.814
7.800
7.787
7.662
7.649
7.530
7.518
7.516
7.504
4j
0.97
1.00
1.01
2.00
1.03
1.03
2.02
2.01
f1 (ppm)
187.849
148.413
140.811
135.480
135.005
134.664
130.689
129.316
129.241
128.833
124.318
77.477
77.160
76.842
63.070
4j
f1 (ppm)


8.411
8.406
8.394
8.389
8.140
8.134
8.129
8.117
8.112
7.945
7.942
7.929
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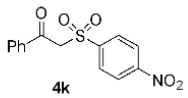
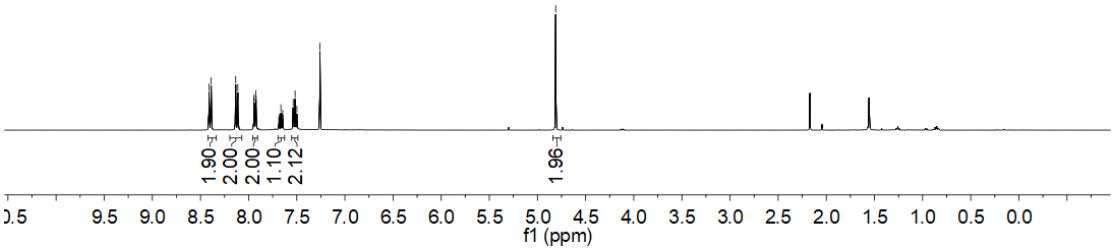
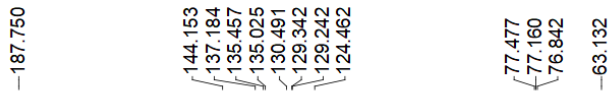
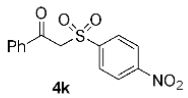
7.538
7.534
7.517
7.503
7.499
7.260


Ph
O
O
S
O
NO2

4k


1.90
2.00
2.00
1.10
2.12
1.96
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)


187.750
144.153
137.184
135.457
135.025
130.491
129.342
129.242
124.462
77.477
77.160
76.842
63.132


Ph
O
O
S
O
NO2

4k


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