Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## Iodine-induced synthesis of sulfonate esters from sodium sulfinates and phenols under mild conditions

Jian Gao, Xiaojun Pan, Juan Liu, Junyi Lai, Liming Chang, and Gaoqing Yuan*

*School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China*

*E-mail: gqyuan@scut.edu.cn*

## 1. General Information.

Unless otherwise noted, all of solvents and reagents were used as received. $^{1}H$ and $^{13}C$ NMR spectra were recorded on a Brüker Advance 400 spectrometer ($^{1}H$: 400 MHz, $^{13}C$: 100 MHz).The chemical shifts were referenced to signals at 7.26 and 77.0 ppm, respectively. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Mass spectra were recorded on a Shimadzu GCMS-QP5050A spectrometer at an ionization voltage of 70 eV equipped with a DB-WAX capillary column. GC-MS was obtained using electron ionization (EI). High-resolution mass spectra (ESI) were obtained with a LCMS-IT-TOF mass spectrometer.

## 2. General Procedure for the Synthesis of Sodium Sulfinates (2w-2y).[1]

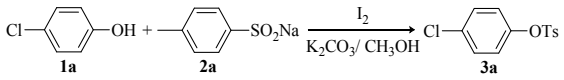
Sodium 4-ethylbenzenesulfinate (**2w)** was prepared by heating 2.04 g of 4-ethylbenzenesulphonyl chloride, 2.5 g of sodium sulfite and 1.68 g of sodium bicarbonate in 10 mL of water at 70-80°C for 4 h. After cooling to room temperature, water was removed under vacuum. The residue was extracted by ethanol. The pure product (white solid) was obtained via recrystallization, and the yield was 71% (1.36 g). Similarly, sodium 4-methoxybenzenesulfinate (**2x**) and sodium phenylmethanesulfinate (**2y**) were prepared from the corresponding sulphonyl chlorides.

## 3. General Procedure for the Synthesis of Sulfonate Esters

4-Chlorophenol **1a** (0.5 mmol), sodium p-tolylsulfanolate **2a** (0.6 mmol), $I_2$ (0.5 mmol), $K_2CO_3$ (1 equiv) and $CH_3OH$ (2 mL) were added to a 10 mL glass tube at room temperature under continuously stirring for 5 h and monitored periodically by TLC. The reaction mixture was decolorized by adding $Na_2S_2O_3$ aqueous solution and washed with water (20 mL). Then the aqueous solution was extracted with diethyl ether (3 × 5 mL) and dried by anhydrous $MgSO_4$. The solvent was removed under reduced pressure by an aspirator, and the crude product was purified by silica gel column chromatography using petroleum ether and ethyl acetate (20:1–8:1) as eluent to give the pure product **3a**.

## 4. Optimization of Reaction Conditions.

**Table S1** Optimization of reaction conditions [a]




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

| Entry | $I_2$ (mmol) | $K_2CO_3$ (mmol) | Time (h) | Yield [b] (%) |
|---|---|---|---|---|
| 1 | 0.10 | 0.50 | 5 | 20 |
| 2 | 0.20 | 0.50 | 5 | 38 |
| 3 | 0.30 | 0.50 | 5 | 57 |
| 4 | 0.40 | 0.50 | 5 | 79 |
| 5 | 0.50 | 0.50 | 5 | 98 |
| 6 | 0.50 | 0.25 | 5 | 86 |
| 7 | 0.50 | 0.80 | 5 | 97 |
| 8 | 0.50 | 1.00 | 5 | 95 |

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (0.6 mmol), $CH_3OH$ (2 mL) and room temperature. [b] GC yield based on **1a**.

## 5. Analytical Data for All Products

**4-Chlorophenyl 4-methylbenzenesulfonate** (**3a**).[2] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.6 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 2.45 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 148.07, 145.65, 132.78, 132.07, 129.87, 129.72, 128.53, 123.78, 21.72.

**Phenyl 4-methylbenzenesulfonate** (**3b**).[2] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J*= 8.1 Hz, 2H), 7.40–7.17 (m, 5H), 6.98 (d, *J* = 7.4 Hz, 2H), 2.44 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.69, 145.33, 132.48, 129.74, 129.60, 128.52, 127.07, 122.39, 21.70.

***p*-Tolyl 4-methylbenzenesulfonate** (**3c**).[3] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.84 (d, *J* = 8.2 Hz, 2H), 2.43 (s, 3H), 2.29 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 147.51, 145.26, 136.94, 132.52, 130.09, 129.72, 128.52, 122.05, 21.69, 20.86.

**4-Bromophenyl 4-methylbenzenesulfonate** (**3d**).[4] $^1$H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 2.45 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 148.63, 145.68, 132.73, 132.04, 129.89, 128.53, 124.17, 120.58,

21.74.

**4-Iodophenyl 4-methylbenzenesulfonate** (**3e**). Yellow solid; $^1$H NMR (400 MHz, CDCl3) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* =7.9 Hz, 2H), 6.73 (d, *J* = 8.5 Hz, 2H), 2.43 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.47, 145.73, 138.76, 132.01, 129.94, 128.51, 124.51, 91.80, 21.78. ESI-HRMS calcd for $C_{13}H_{11}INaO_3S$ $[M+Na]^+$ 396.9366, found396.9373.

**4-Nitrophenyl 4-methylbenzenesulfonate** (**3f**).[2] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.6 Hz, 2H), 7.73 (d, *J* = 7.8 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.6 Hz, 2H), 2.47 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.93, 146.26, 146.21, 131.75, 130.12, 128.48, 125.40, 123.22, 21.76.

**4-Isopropylphenyl 4-methylbenzenesulfonate** (**3g**). Colorless oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.7 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 2H), 6.88 (d, *J* = 7.9 Hz, 2H), 2.86 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.44 (s, 3H), 1.20 (d, *J* = 6.9 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 147.79, 147.59, 145.20, 132.70, 129.70, 128.49, 127.48, 122.06, 33.58, 23.91, 21.69. ESI-HRMS calcd for $C_{16}H_{18}NaO_3S$ $[M+Na]^+$ 313.0876, found 313.0869.

***o*-Tolyl 4-methylbenzenesulfonate** (**3h**).[4] Colorless oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.12 (dd, *J* = 9.7, 4.5 Hz, 3H), 6.99 (d, *J* = 7.6 Hz, 1H), 2.44 (s, 3H), 2.07 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 148.38, 145.35, 133.24, 131.59, 129.81, 128.39, 126.98, 126.91, 122.30, 21.70, 16.29.

**2-Chlorophenyl 4-methylbenzenesulfonate** (**3i**).[2] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 8.4 Hz, 4H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 2.44 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 145.74, 145.63, 132.65, 130.76, 129.80, 128.63, 127.92, 127.82, 127.62, 124.22, 21.75.

**2-Iodophenyl 4-methylbenzenesulfonate** (**3j**). Yellow solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 12.5 Hz, 4H), 7.05 – 6.87 (m, 1H), 2.43 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.01, 145.84, 140.11, 132.79, 129.87, 129.57, 128.85, 128.44, 122.98, 90.31, 21.81. ESI-HRMS calcd for $C_{13}H_{11}INaO_3S$ $[M+Na]^+$ 396.9364, found 396.9366.

**2-Cyanophenyl 4-methylbenzenesulfonate** (**3k**). Colorless oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 1H),

7.37 (dd, *J* = 12.7, 7.8 Hz, 3H), 2.45 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.24, 146.46, 134.38, 133.79, 131.50, 130.13, 128.78, 127.50, 123.71, 114.50, 107.77, 21.79.

***m*-Tolyl 4-methylbenzenesulfonate** (**3l**). Colorless oil; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.13 (t, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.86 (s, 1H), 6.72 (d, *J* = 8.1 Hz, 1H), 2.44 (s, 3H), 2.29 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.61, 145.24, 139.97, 132.62, 129.69, 129.20, 128.51, 127.84, 123.00, 119.13, 21.70, 21.23. ESI-HRMS calcd for $C_{14}H_{14}NaO_3S$ $[M+Na]^+$ 282.0559, found 282.0556.

**Naphthalen-1-yl 4-methylbenzenesulfonate** (**3m**).[2] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.1 Hz, 1H), 7.77 (t, *J* = 8.2 Hz, 3H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.48–7.37 (m, 2H), 7.34 (t, *J* = 7.9 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.20 (d, *J* = 7.6 Hz, 1H), 2.38 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 145.82, 145.45, 134.75, 132.83, 129.81, 128.49, 127.71, 127.33, 127.10, 126.73, 126.71, 125.13, 121.81, 118.40, 21.67.

**Naphthalen-2-yl 4-methylbenzenesulfonate** (**3n**).[7] White needles; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 5.2 Hz, 1H), 7.73 (t, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 7.4 Hz, 3H), 7.29 (d, *J* = 8.0 Hz, 4H), 7.09 (d, *J* = 8.9 Hz, 1H), 2.43 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 147.22, 145.40, 133.46, 132.47, 131.90, 129.80, 129.76, 128.58, 127.89, 127.77, 126.86, 126.39, 121.19, 119.97, 21.73.

**Quinolin-8-yl 4-methylbenzenesulfonate** (**3o**).[2] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 1.5 Hz, 1H), 8.08 (d, *J*= 8.2 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 2H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.34 (dd, *J* = 7.4, 3.3 Hz, 1H), 7.21 (d, *J* = 7.8 Hz, 2H), 2.35 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.77, 145.51, 145.12, 141.52, 135.76, 133.12, 129.62, 129.45, 128.71, 127.06, 125.95, 122.35, 121.88, 21.61.

**4-Chlorophenyl benzenesulfonate** (**3p**).[6] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.7 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 2H), 7.25 (d, *J* = 8.6 Hz, 2H), 6.92 (d, *J* = 8.5 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 147.99, 135.08, 134.44, 132.89, 129.76, 129.26, 128.50, 123.74.

**phenethyl 4-methylbenzenesulfonate (3q)**.[8] Colorless oil ; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.6 Hz, 2H), 7.28 – 7.19 (m, 5H), 7.10 (d, *J* = 7.1 Hz, 2H), 4.21 (t, *J* = 7.0 Hz, 2H), 2.95 (t, *J* = 7.0 Hz, 2H), 2.42 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 144.66, 136.24, 133.04, 129.80, 128.91, 128.60, 127.83, 126.88, 70.61, 35.37, 21.62.

**propyl 4-methylbenzenesulfonate (3r)**.[8] Yellow liquid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 7.7 Hz, 2H), 3.99 (t, *J* = 6.5 Hz, 2H), 2.45 (s, 3H), 1.70 – 1.65 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 144.64, 133.27, 129.81, 127.88, 72.15, 22.32, 21.63, 9.97.

**hexyl 4-methylbenzenesulfonate (3s)**.[8] $^1$H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 2H), 4.02 (t, *J* = 6.5 Hz, 2H), 2.45 (s, 3H), 1.65 – 1.60 (m, 2H), 1.26 (dt, *J* = 24.8, 9.1 Hz, 6H), 0.85 (t, *J* = 6.7 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 144.62, 133.28, 129.80, 127.90, 70.71, 31.09, 28.78, 25.00, 22.41, 21.63, 13.91.

**4-Chlorophenyl 4-fluorobenzenesulfonate** (**3t**). White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.79 (m, 2H), 7.27 (d, *J* = 8.7 Hz, 2H), 7.22 (t, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 167.42, 164.86, 147.86, 133.07, 131.47, 131.38, 131.02, 129.87, 123.70, 116.82, 116.60. ESI-HRMS calcd for $C_{12}H_8ClFNaO_3S$ $[M+Na]^+$ 308.9764, found 308.9759.

**4-Chlorophenyl 4-chlorobenzenesulfonate** (**3u**).[6] White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 147.82, 141.30, 133.52, 133.14, 130.28, 129.91, 129.65, 123.66.

**4-Chlorophenyl 4-bromobenzenesulfonate** (**3v**). White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 4H), 7.27 (d, *J* = 8.5 Hz, 2H), 6.94 (d, *J* = 8.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 147.81, 134.05, 133.12, 132.66, 129.93, 129.92, 129.89, 123.67. ESI-HRMS calcd for $C_{12}H_8BrClNaO_3S$ $[M+Na]^+$ 368.8958, found 368.8957.

**4-Chlorophenyl 4-ethylbenzenesulfonate** (**3w**). White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 2.74 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 151.74, 148.06, 132.82, 132.76, 132.20, 129.72, 128.73, 128.63, 123.80, 28.92, 14.94. ESI-HRMS calcd for $C_{14}H_{13}ClNaO_3S$ $[M+Na]^+$ 319.0172, found 319.0166.

**4-Chlorophenyl 4-methoxybenzenesulfonate** (**3x**). White solid; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 8.9 Hz, 2H), 6.95 (dd, *J* = 19.5, 8.8 Hz, 4H), 3.89 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.26, 148.10, 132.74, 130.80, 129.70, 126.30, 123.85, 114.42, 55.75.

ESI-HRMS calcd for $C_{13}H_{11}ClNaO_4S$ $[M+Na]^+$ 320.9960, found 320.9959.

**4-Chlorophenylphenylmethanesulfonate** (**3y**). White solid; $^1H$ NMR (400 MHz, CDCl3) δ 7.41 (s, 5H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 4.50 (s, 2H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 147.57, 132.79, 130.90, 129.95, 129.44, 129.09, 127.06, 123.43, 56.97. ESI-HRMS calcd for $C_{13}H_{11}ClNaO_3S$ $[M+Na]^+$ 305.0005, found 305.0010.

**Reference**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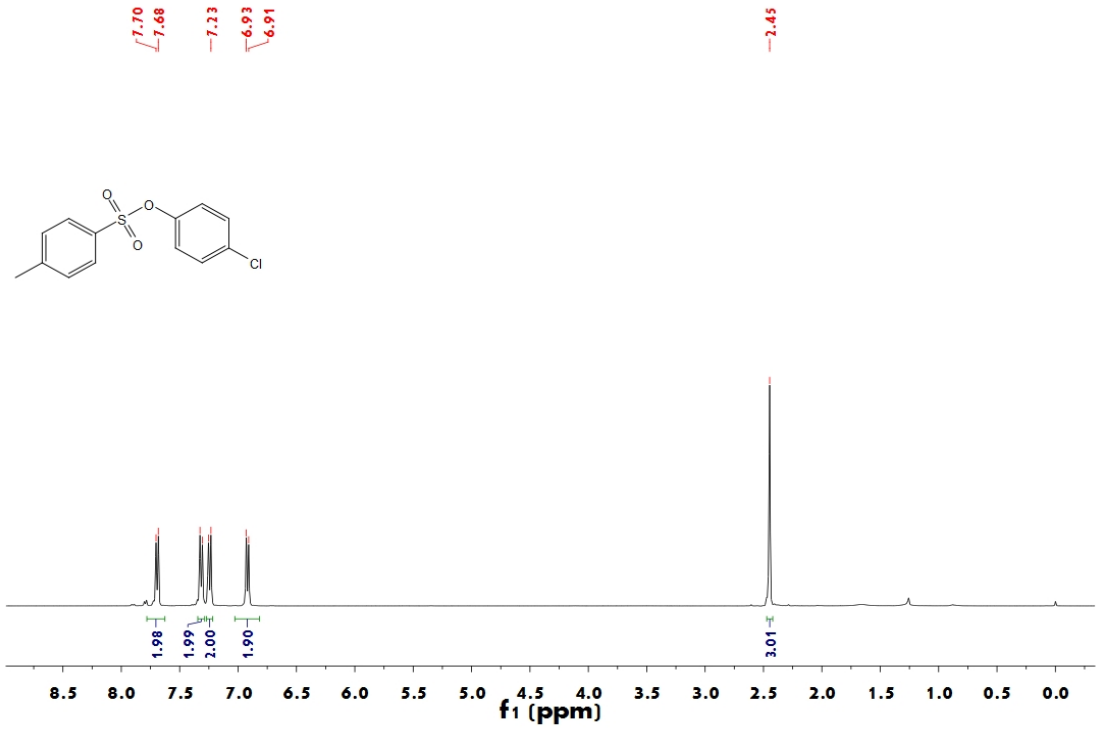
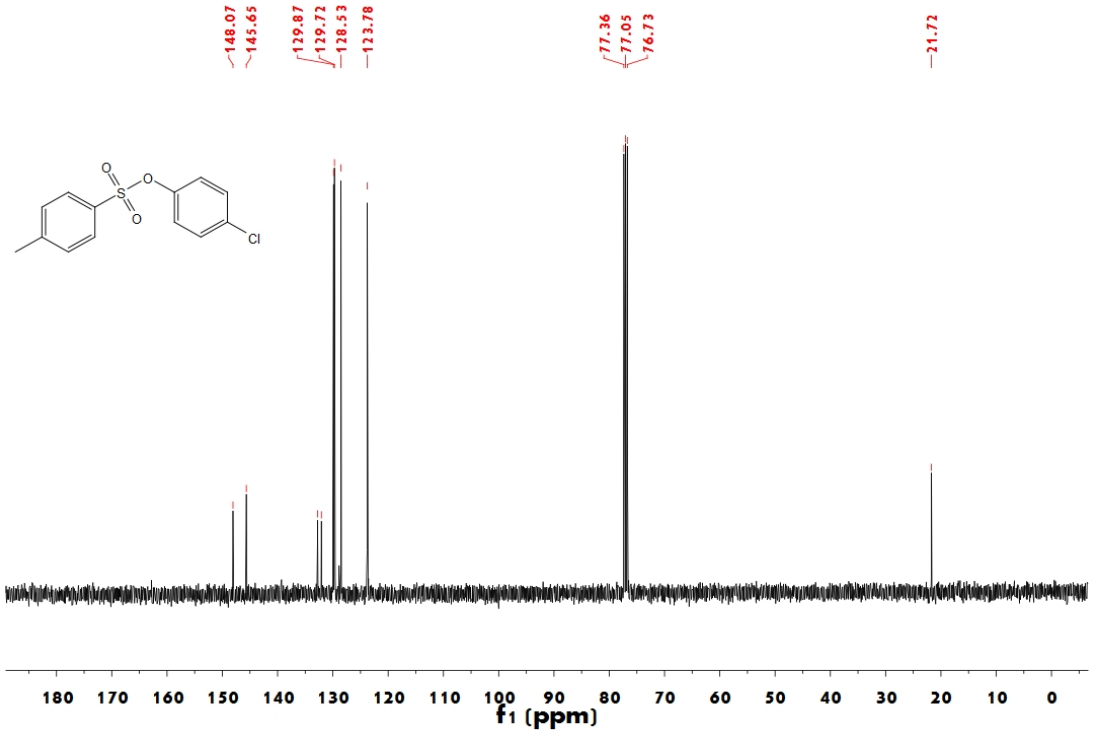
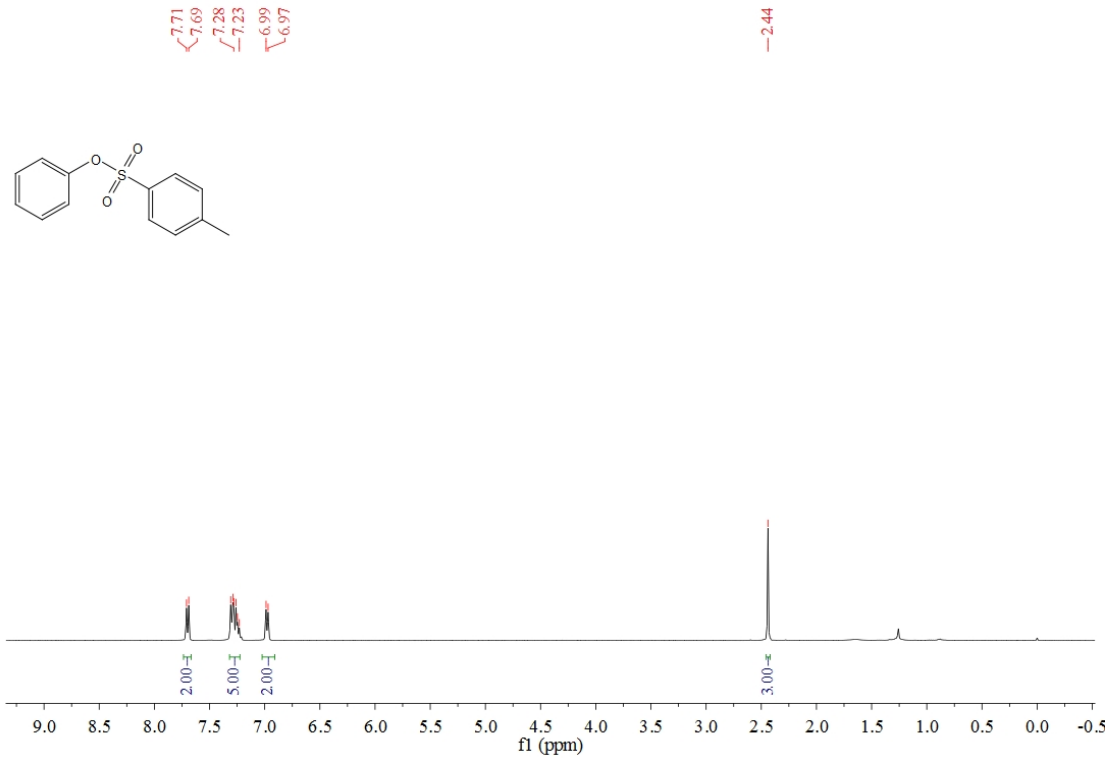
## 6. NMR Spectra

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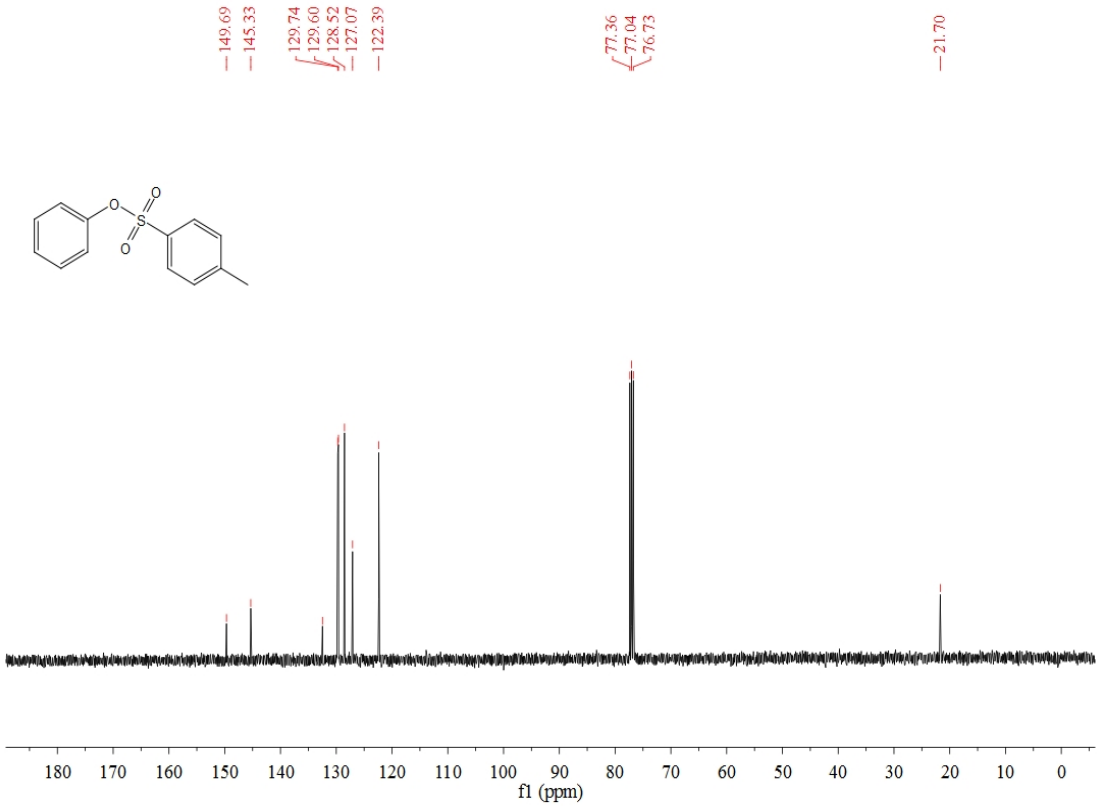
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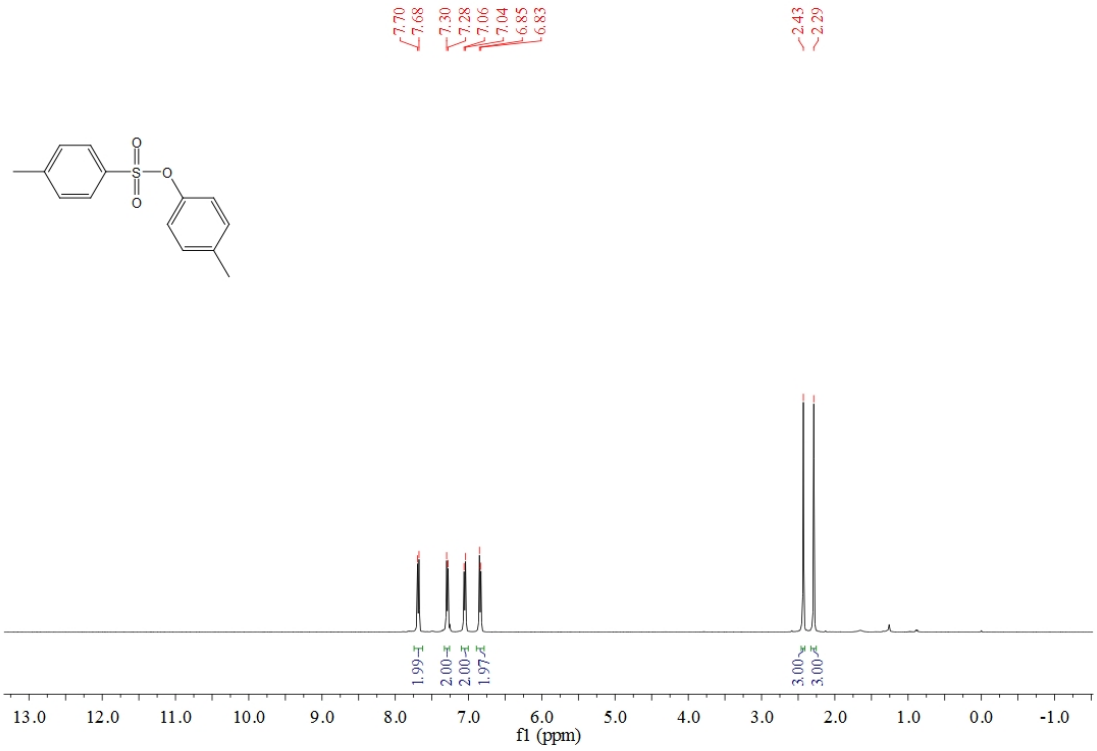
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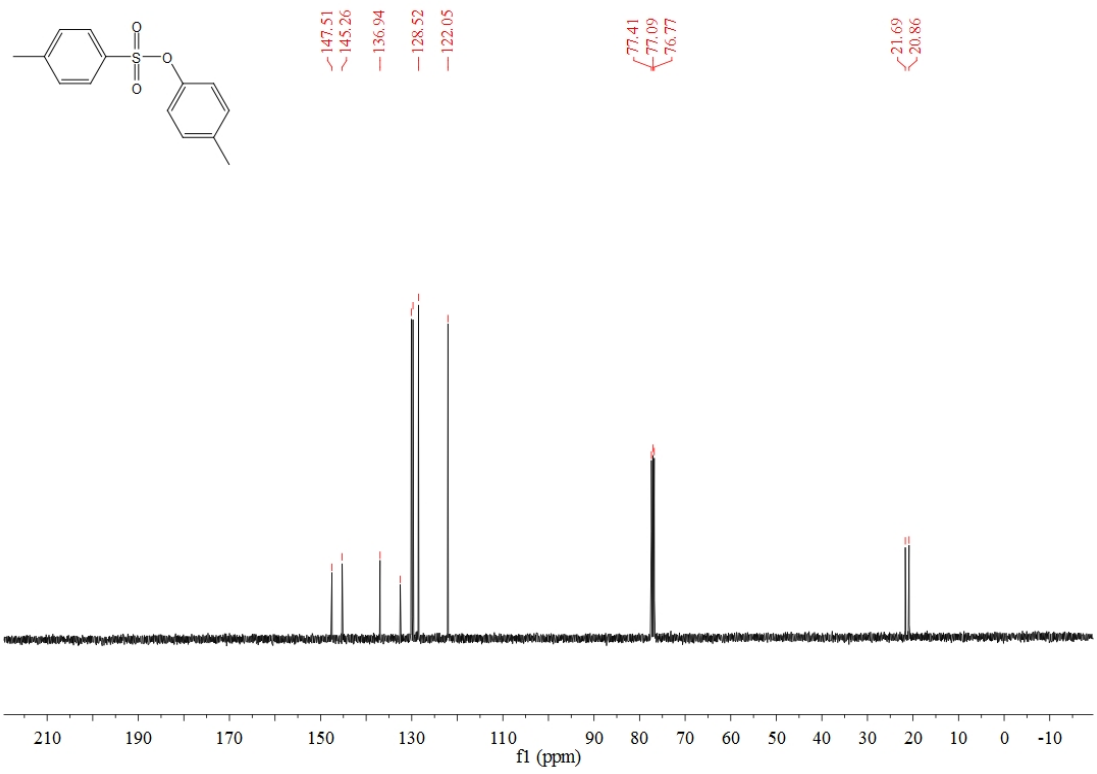
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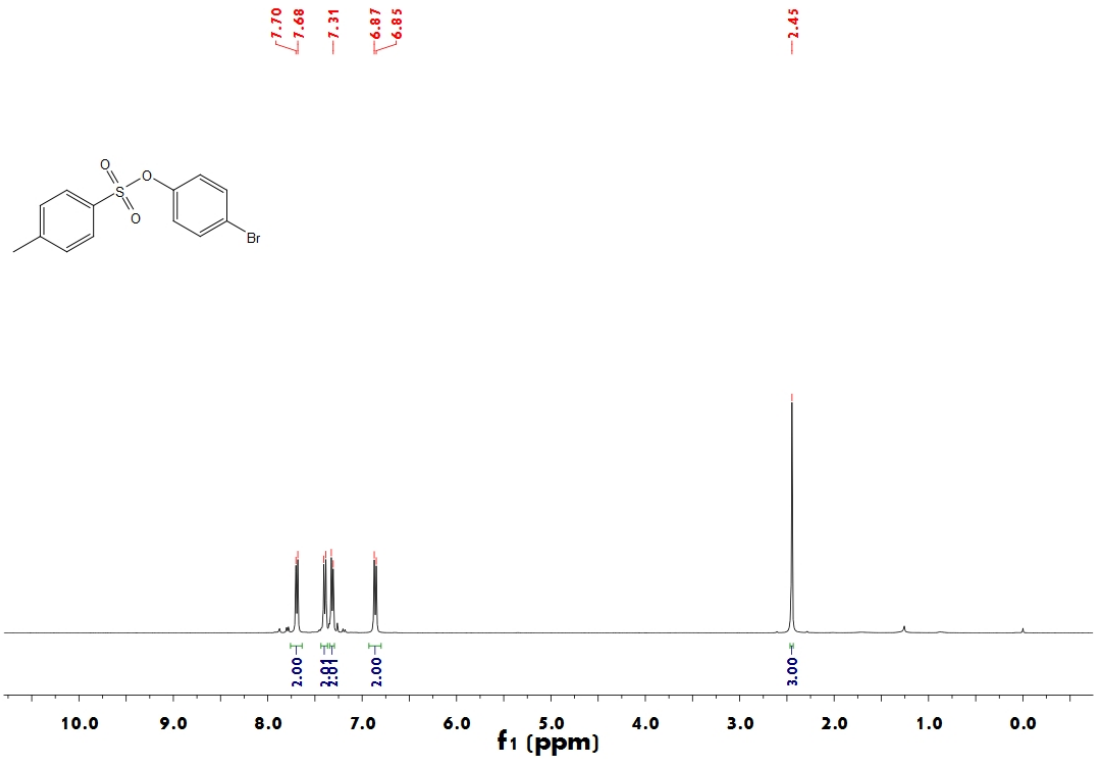
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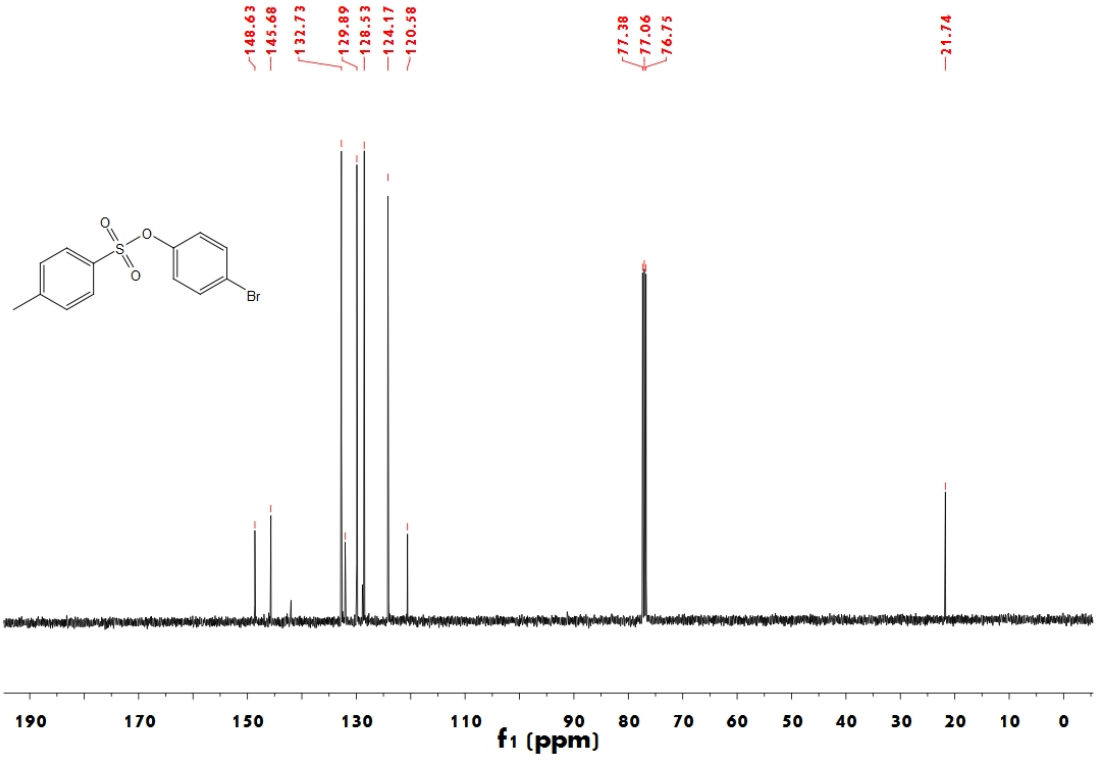
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128.53
124.17
120.58
77.38
77.06
76.75
21.74
O
S
O
O
Br
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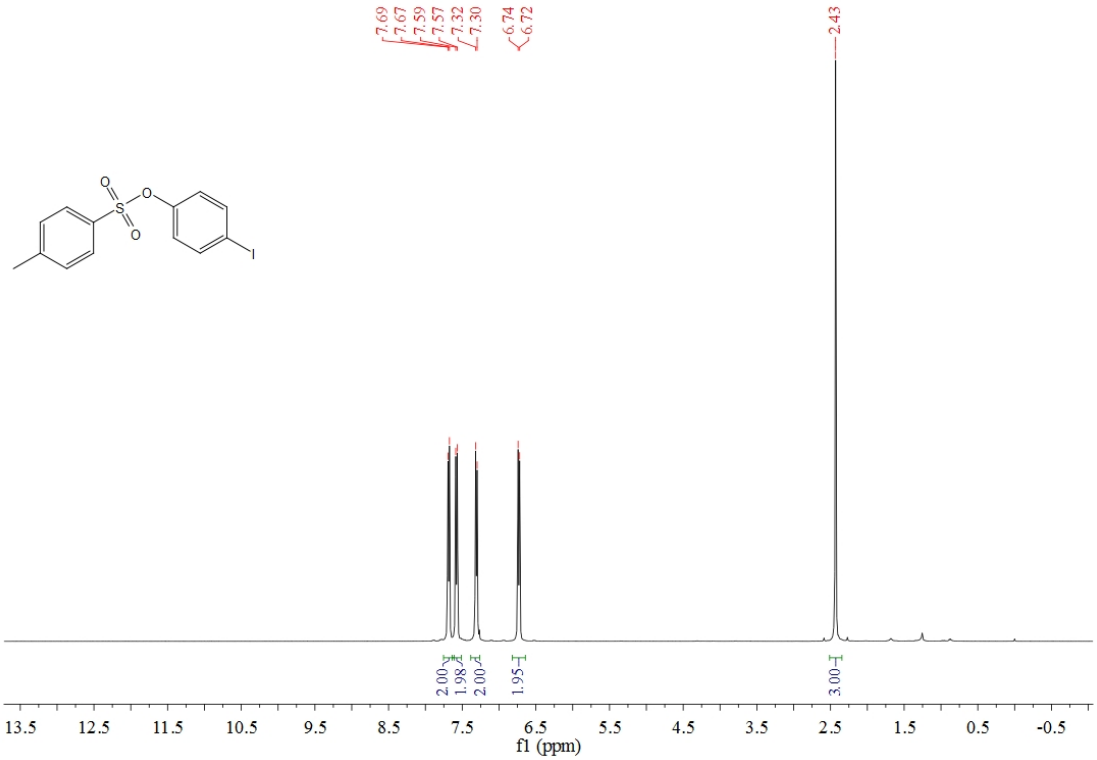
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.67
7.59
7.57
7.32
7.30
6.74
6.72
2.43
2.00
1.98
2.00
1.95
3.00
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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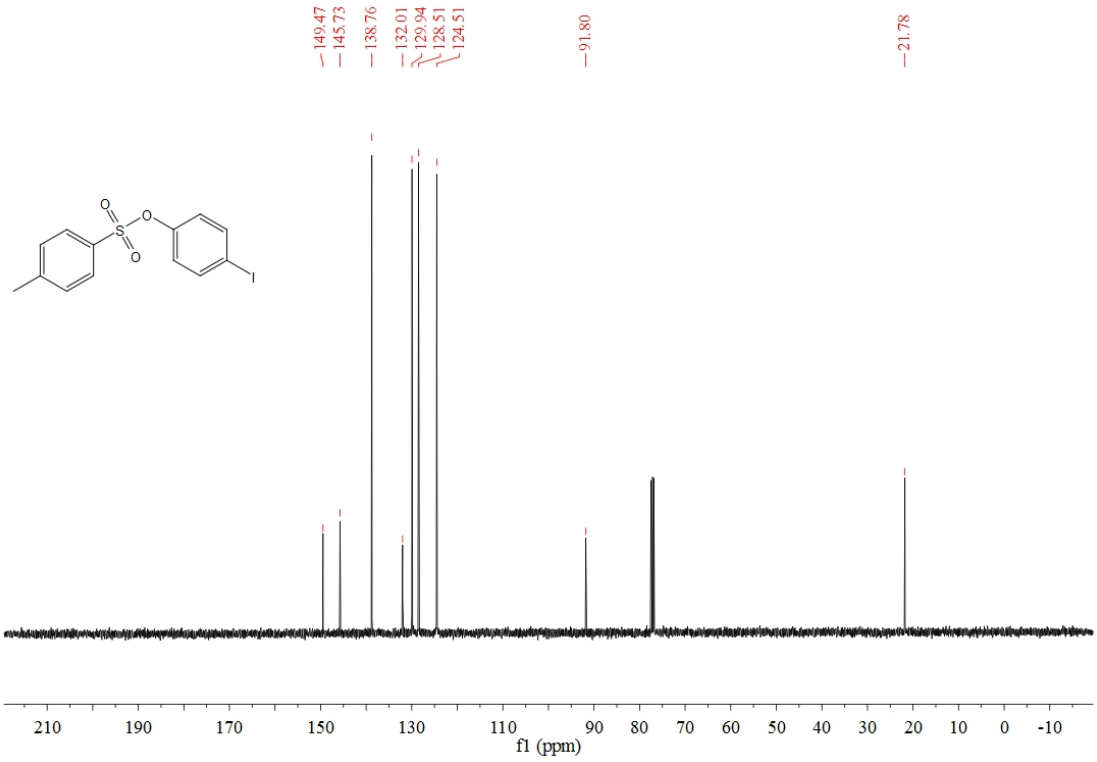
-0.5
f1 (ppm)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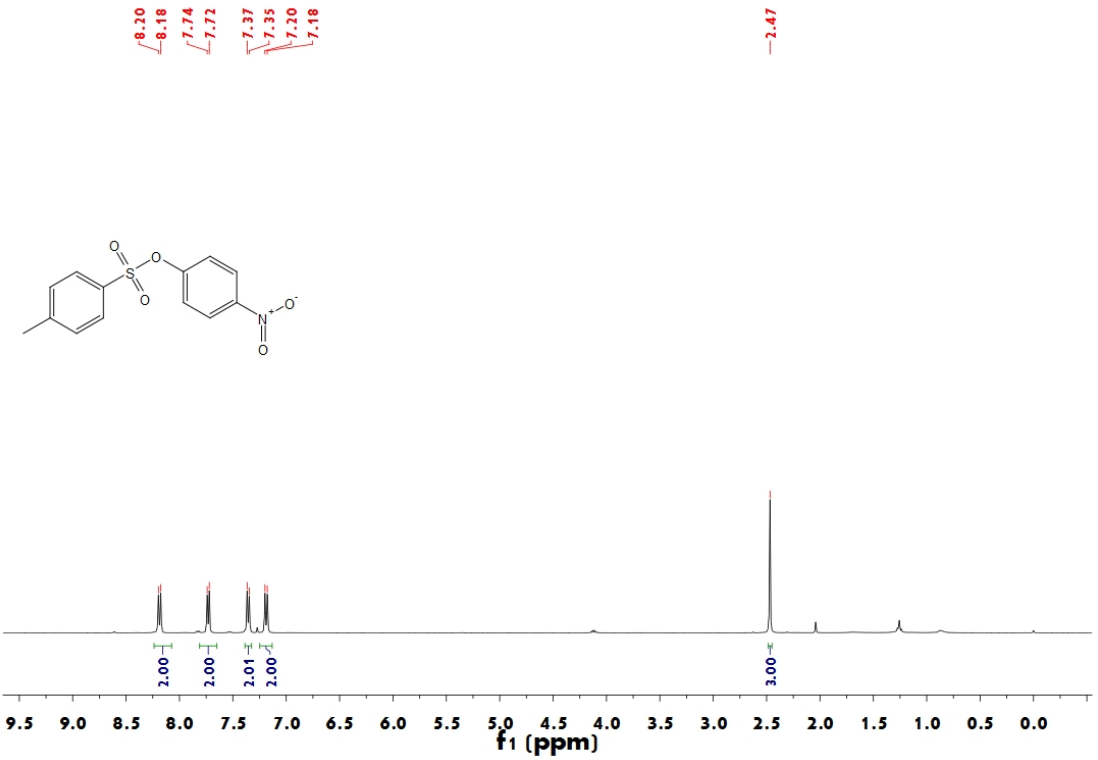
132.01
129.94
128.51
124.51
91.80
21.78
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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8.18
7.74
7.72
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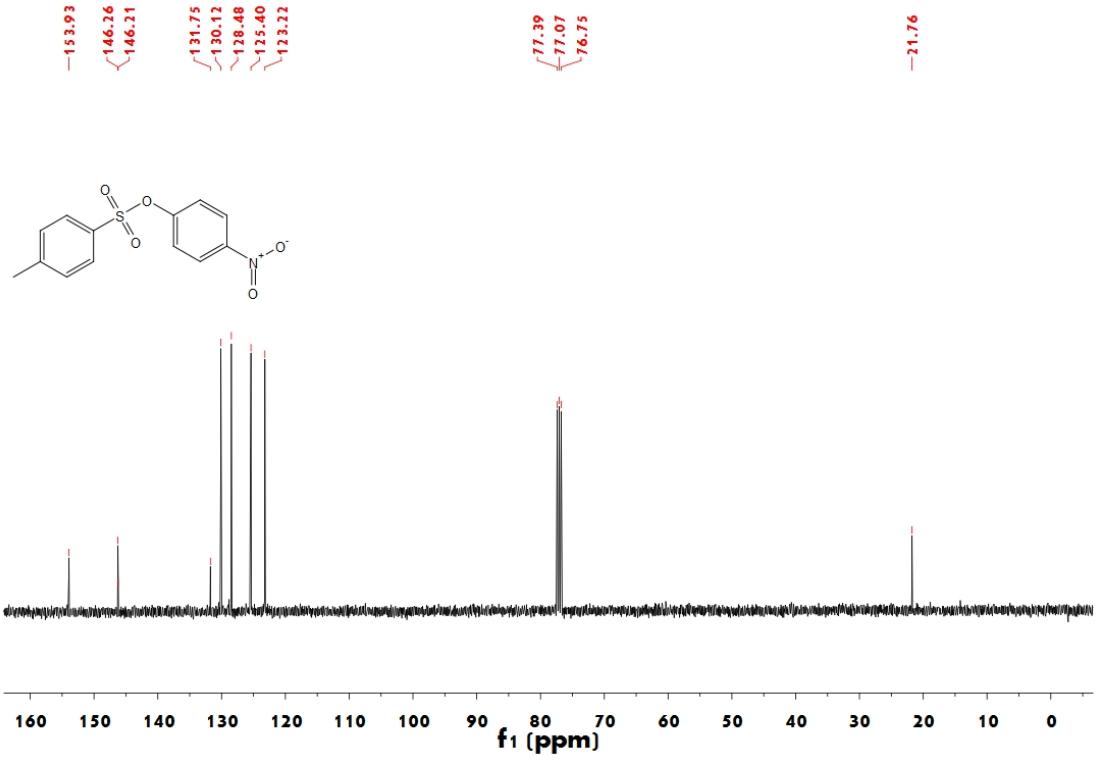
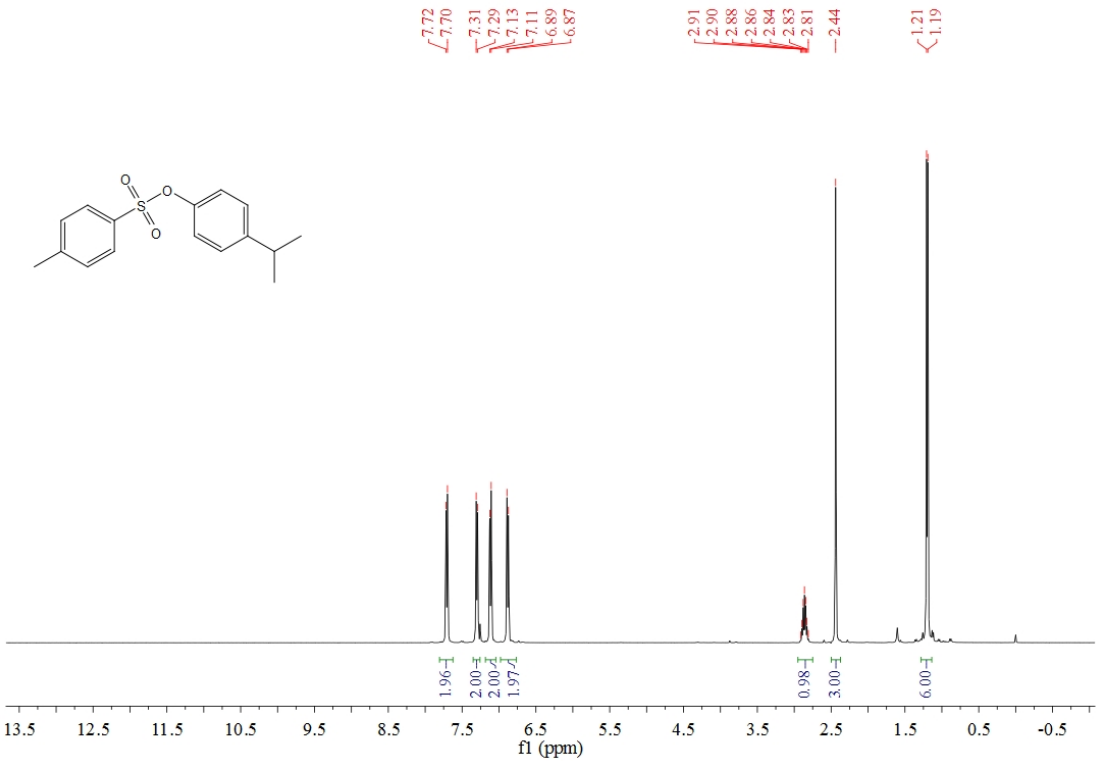
7.35
7.20
7.18
2.47
2.00
2.00
2.01
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


153.93
146.26
146.21
131.75
130.12
128.48
125.40
123.22
77.39
77.07
76.75
21.76
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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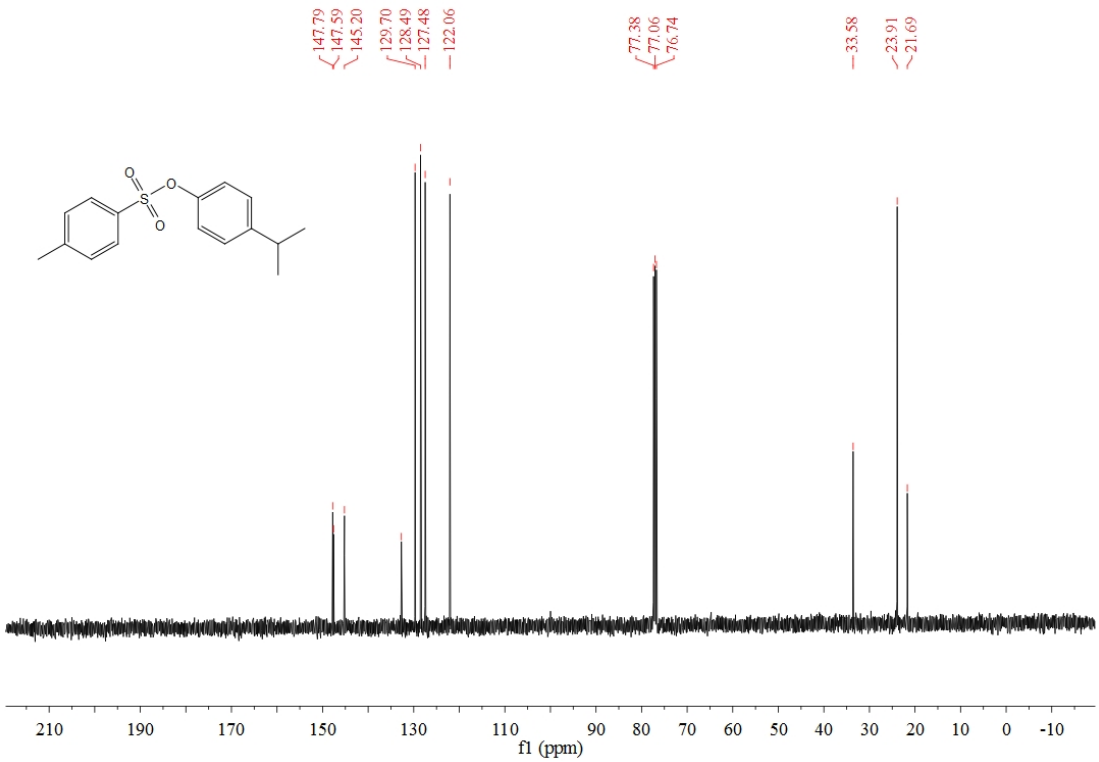
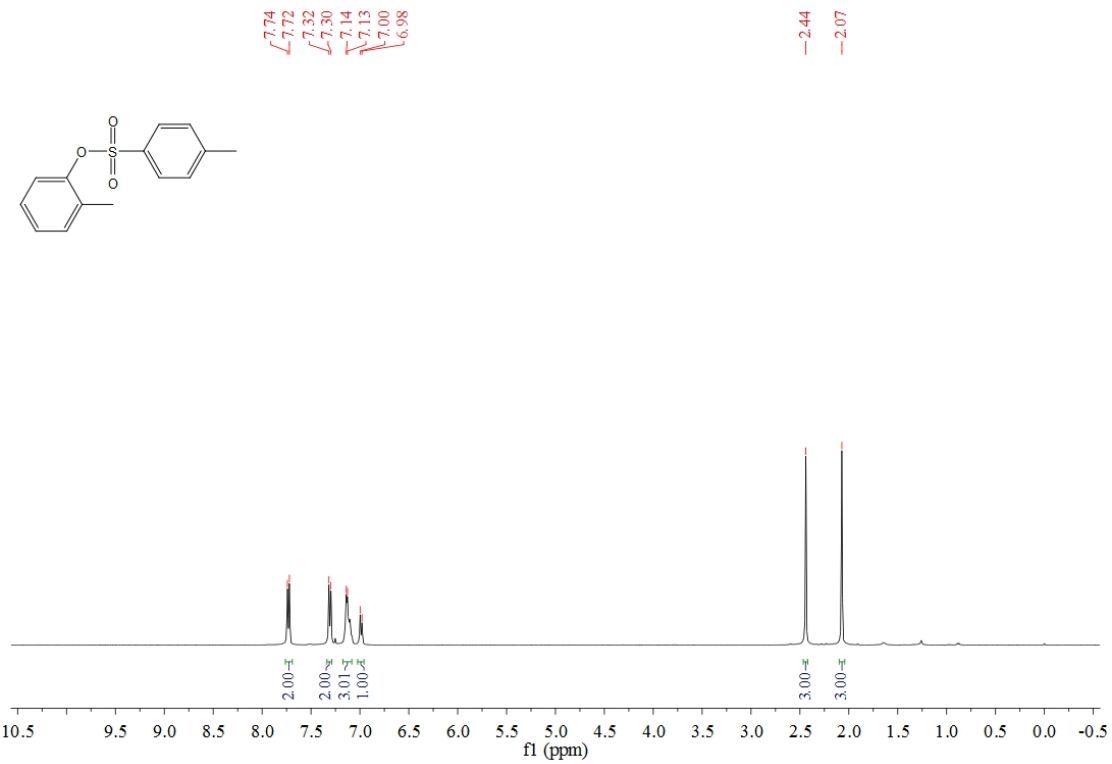
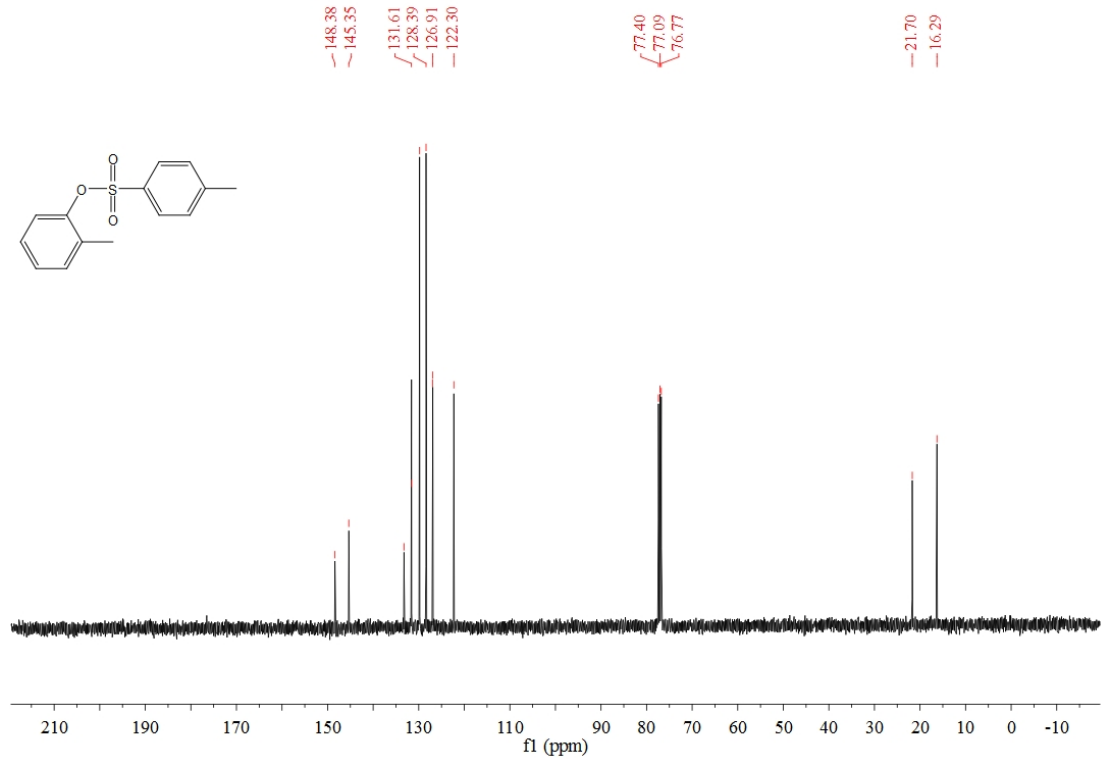
7.70
7.31
7.29
7.13
7.11
6.89
6.87
2.91
2.90
2.88
2.86
2.84
2.83
2.81
2.44
1.21
1.19
1.96
2.00
2.00
1.97
0.98
3.00
6.00
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


147.79
147.59
145.20
129.70
128.49
127.48
122.06
77.38
77.06
76.74
33.58
23.91
21.69
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.74
7.72
7.32
7.30
7.14
7.13
7.00
6.98
2.44
2.07
2.00
2.00
3.01
1.00
3.00
3.00
f1 (ppm)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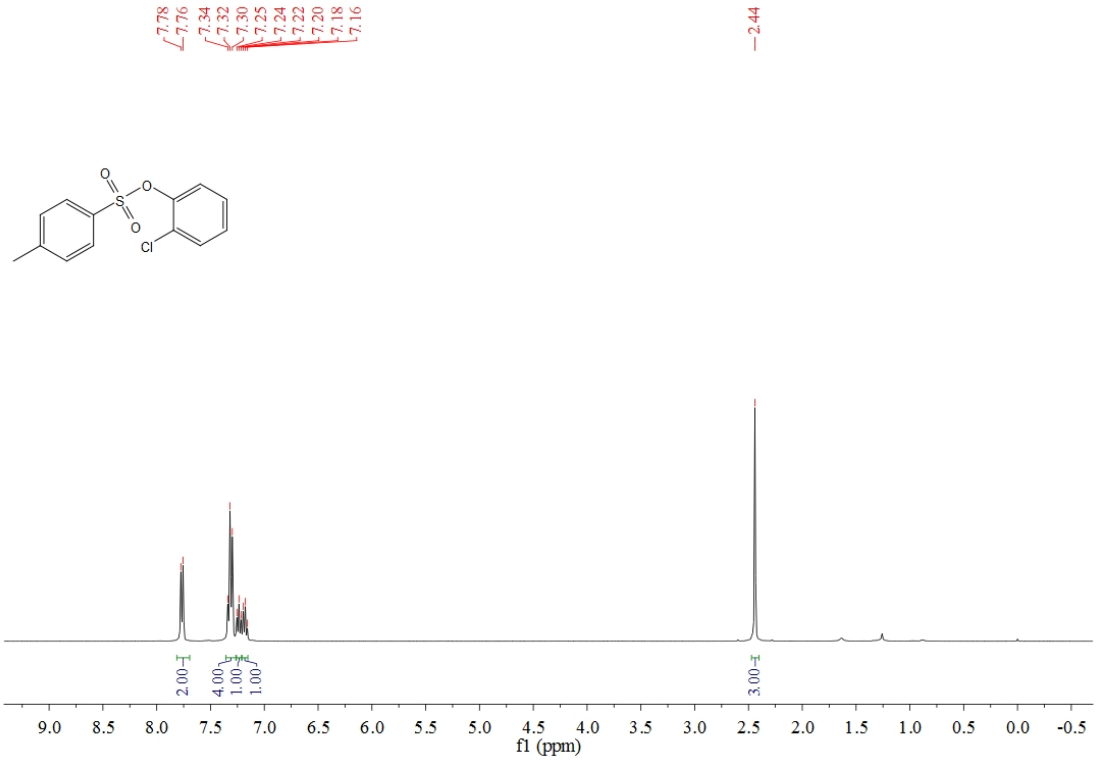
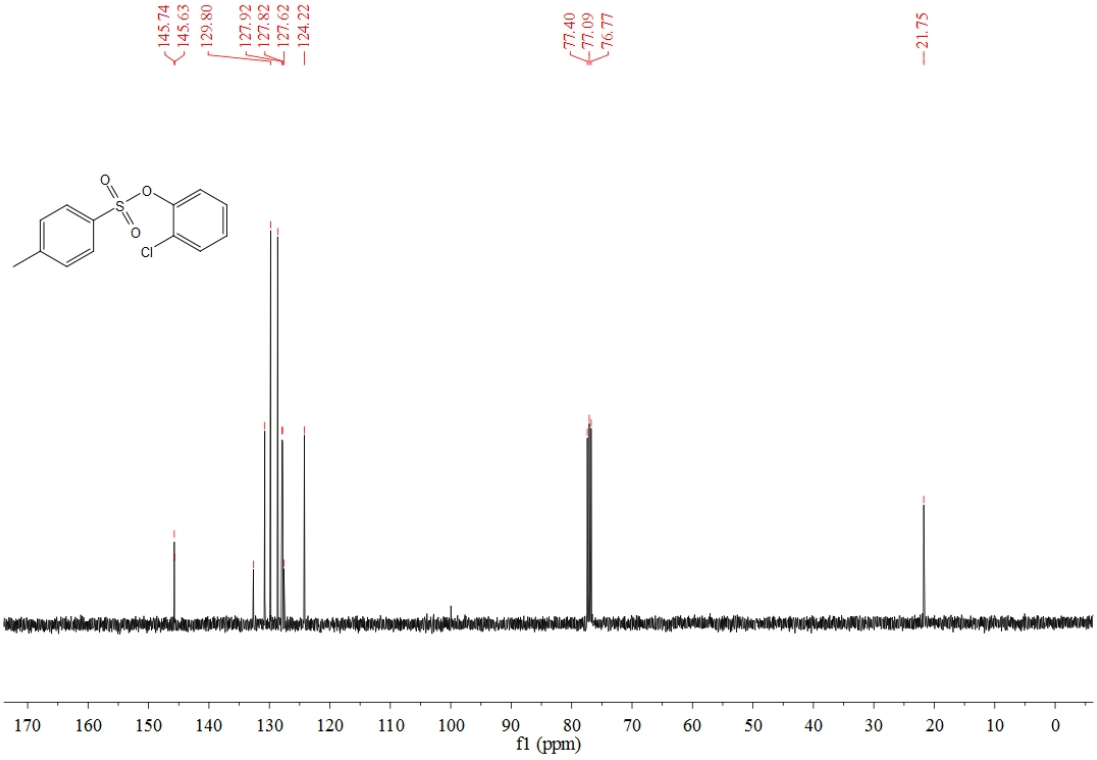
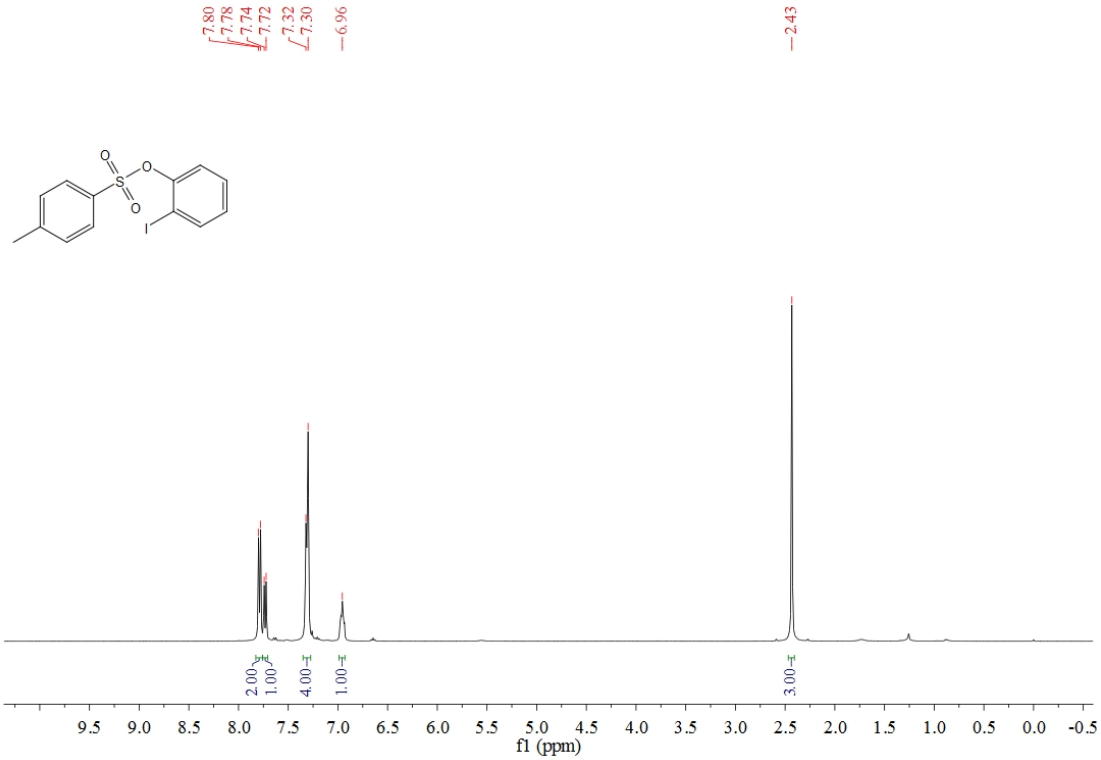
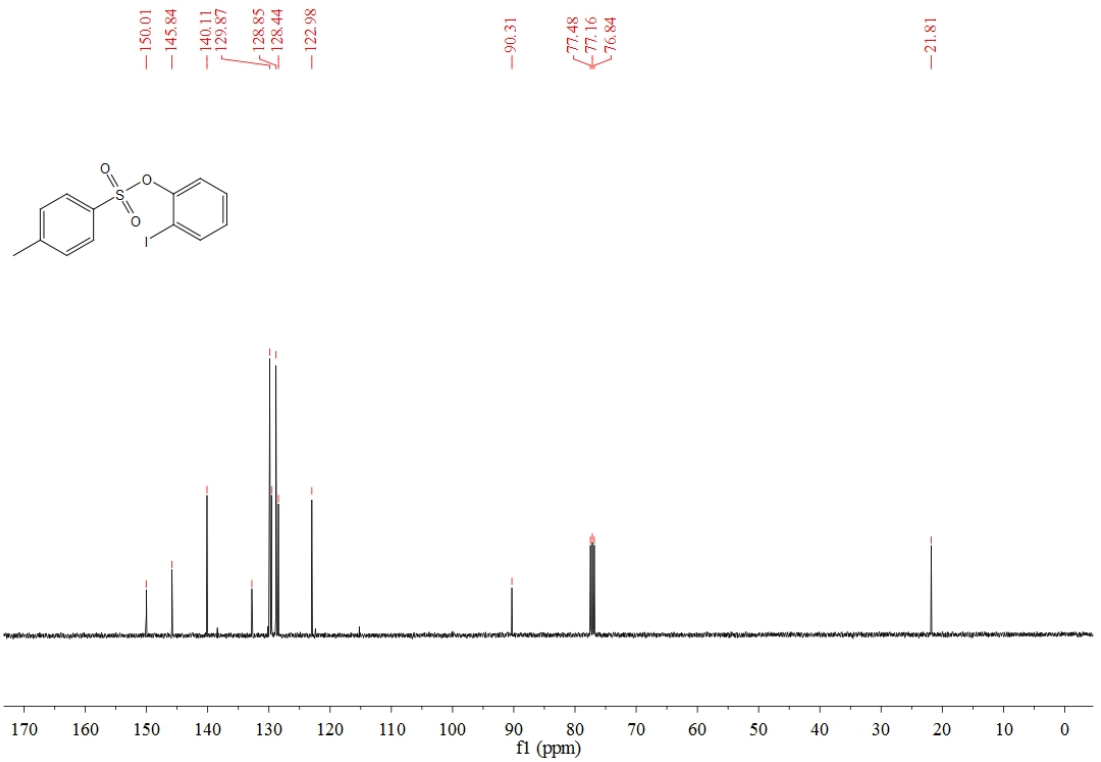
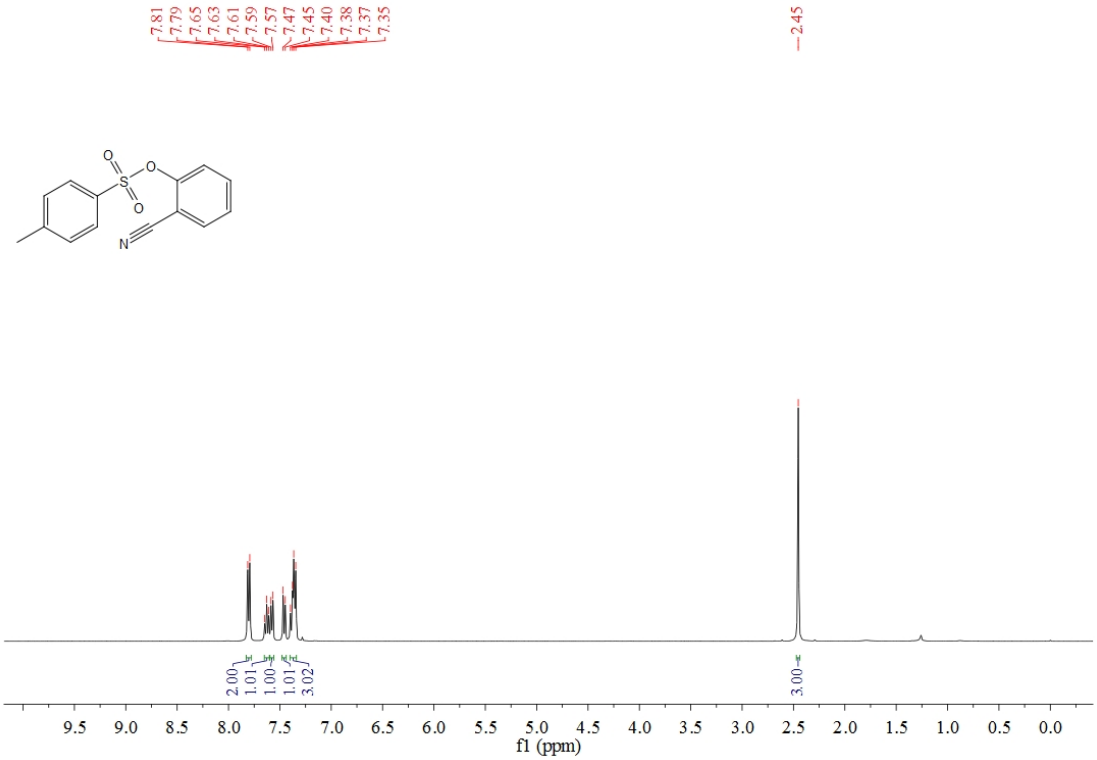
128.39
126.91
122.30
77.40
77.09
76.77
21.70
16.29
f1 (ppm)

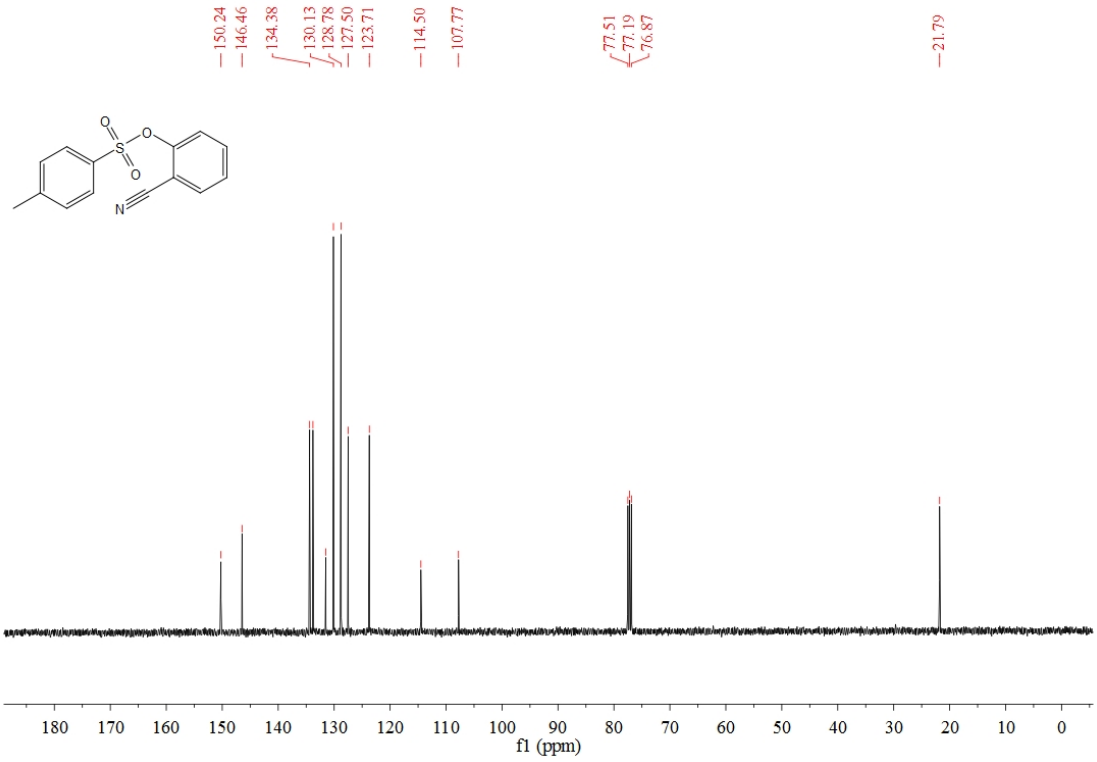

7.78
7.76
7.34
7.32
7.30
7.25
7.24
7.22
7.20
7.18
7.16
2.44
O
S
O
O
Cl
2.00
4.00
1.00
1.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


145.74
145.63
129.80
127.92
127.82
127.62
124.22
77.40
77.09
76.77
21.75
O
S
O
O
Cl
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.80
7.78
7.74
7.72
7.32
7.30
6.96
2.43
2.00
1.00
4.00
1.00
3.00
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)


150.01
145.84
140.11
129.87
128.85
128.44
122.98
90.31
77.48
77.16
76.84
21.81
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.81
7.79
7.65
7.63
7.61
7.59
7.57
7.47
7.45
7.40
7.38
7.37
7.35
2.45
O
S
O
O
N
2.00
1.01
1.00
1.01
3.02
3.00
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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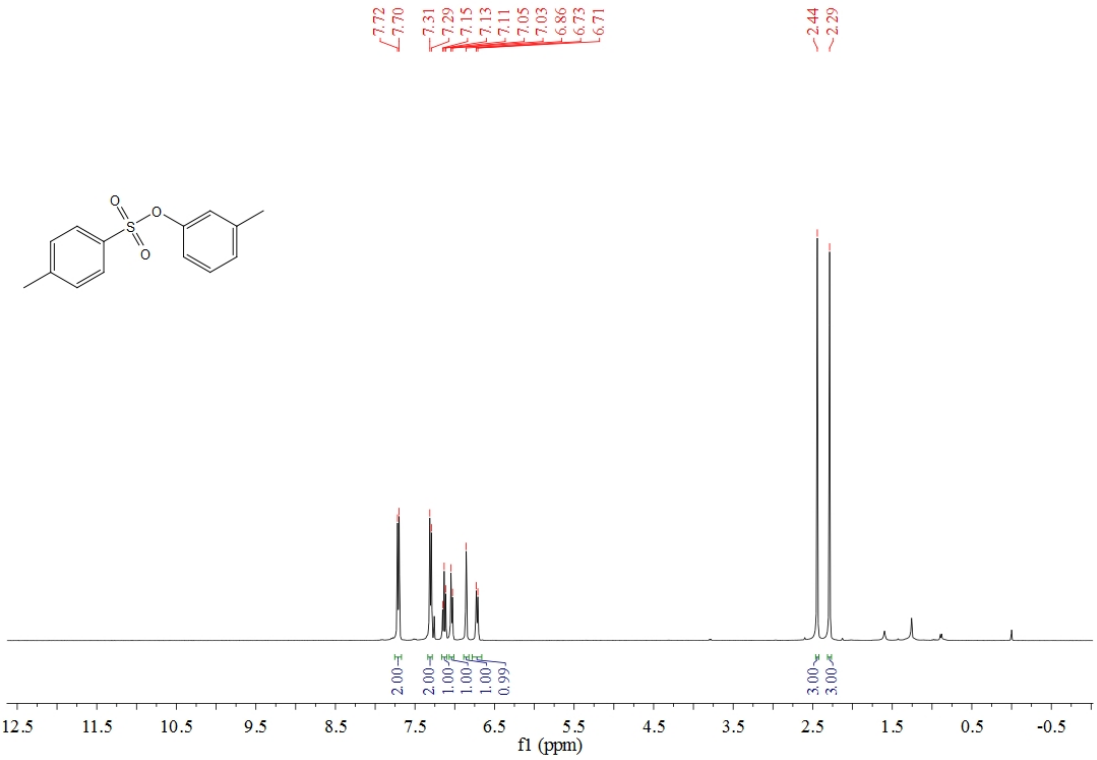
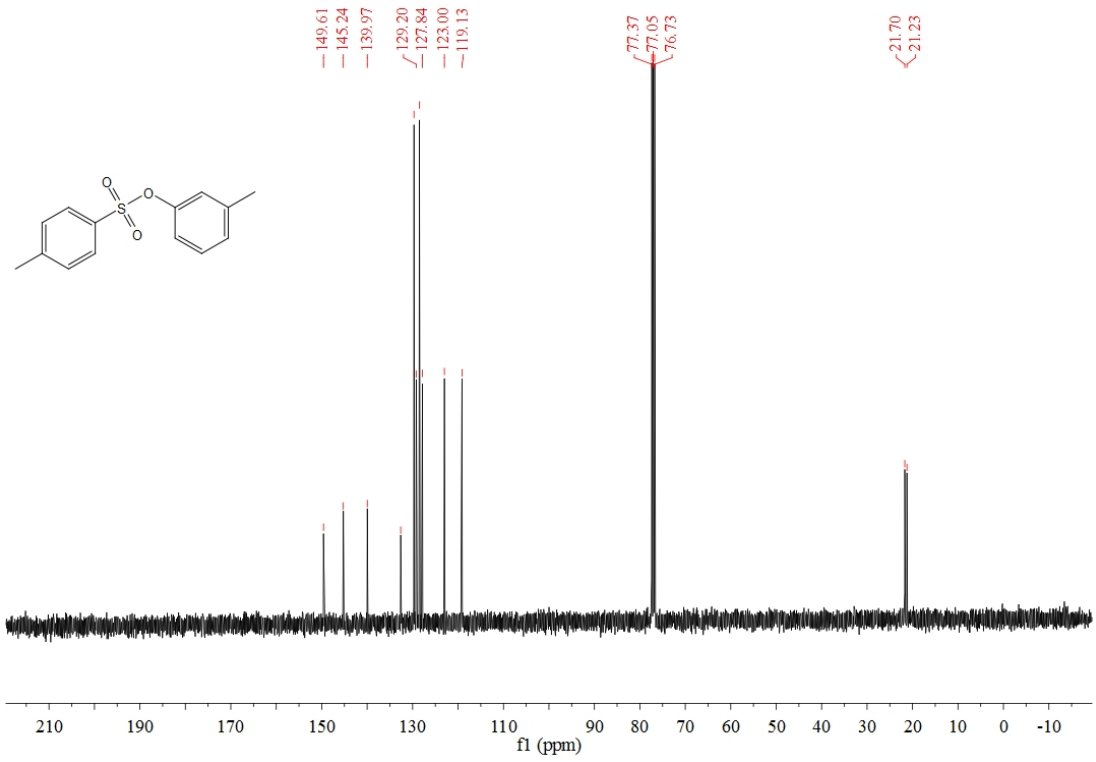
146.46
134.38
130.13
128.78
127.50
123.71
114.50
107.77
77.51
77.19
76.87
21.79
O
S
O
O
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.72
7.70
7.31
7.29
7.15
7.13
7.11
7.05
7.03
6.86
6.73
6.71
2.44
2.29
2.00
2.00
1.00
1.00
1.00
0.99
3.00
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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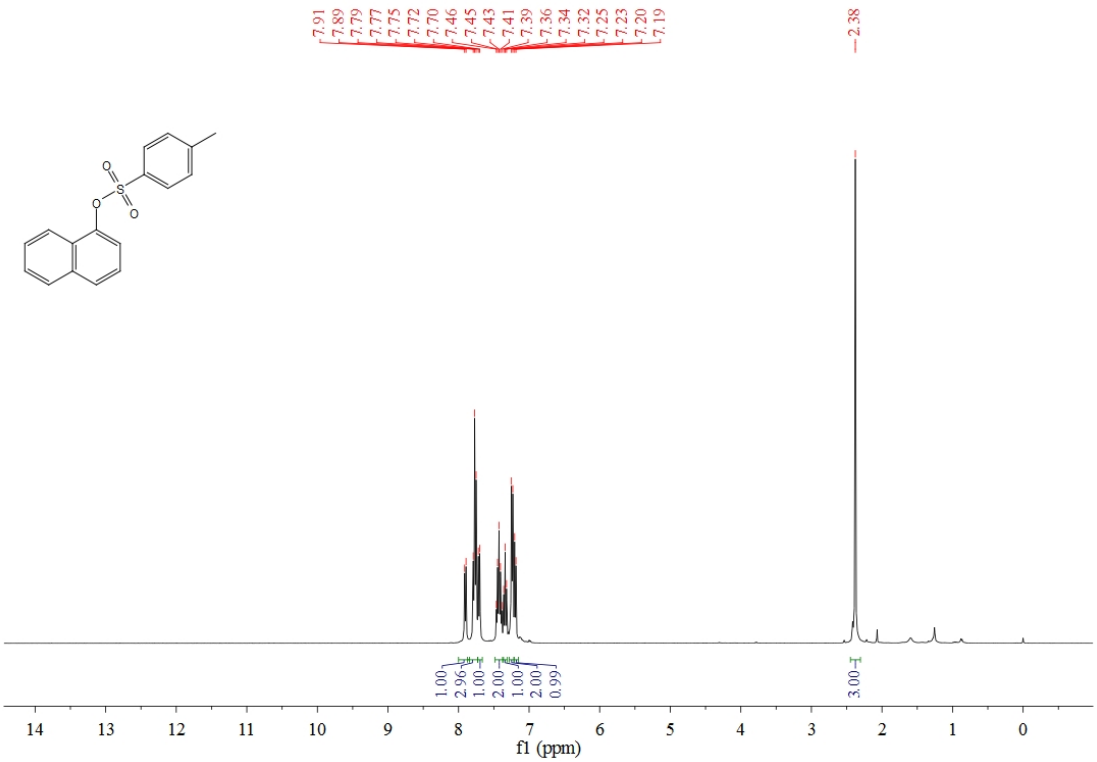
145.24
139.97
129.20
127.84
123.00
119.13
77.37
77.05
76.73
21.70
21.23
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.89
7.79
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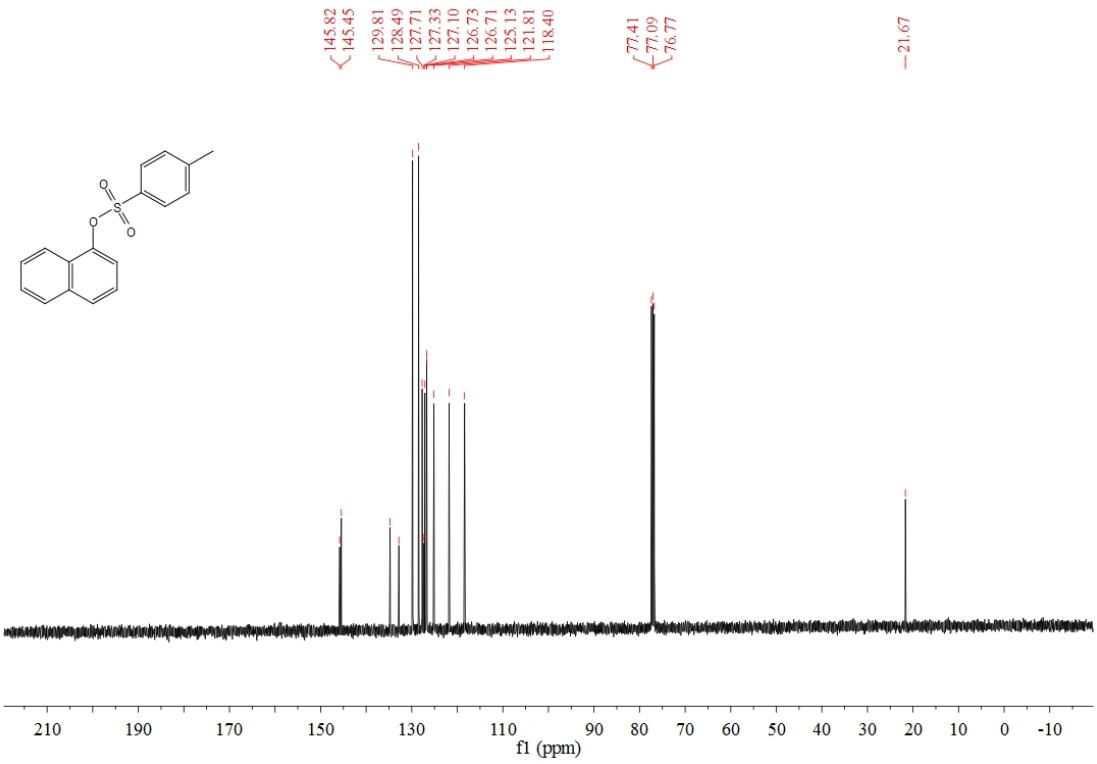
7.72
7.70
7.46
7.45
7.43
7.41
7.39
7.36
7.34
7.32
7.25
7.23
7.20
7.19
2.38
1.00
2.96
1.00
2.00
1.00
2.00
0.99
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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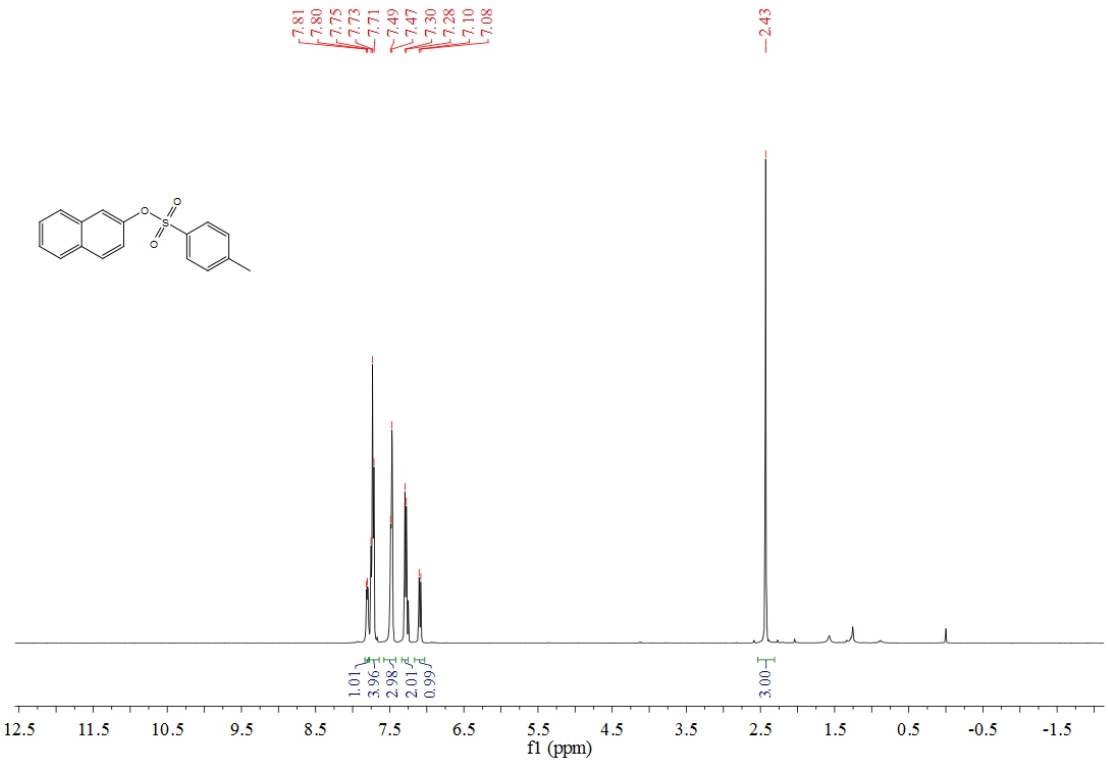
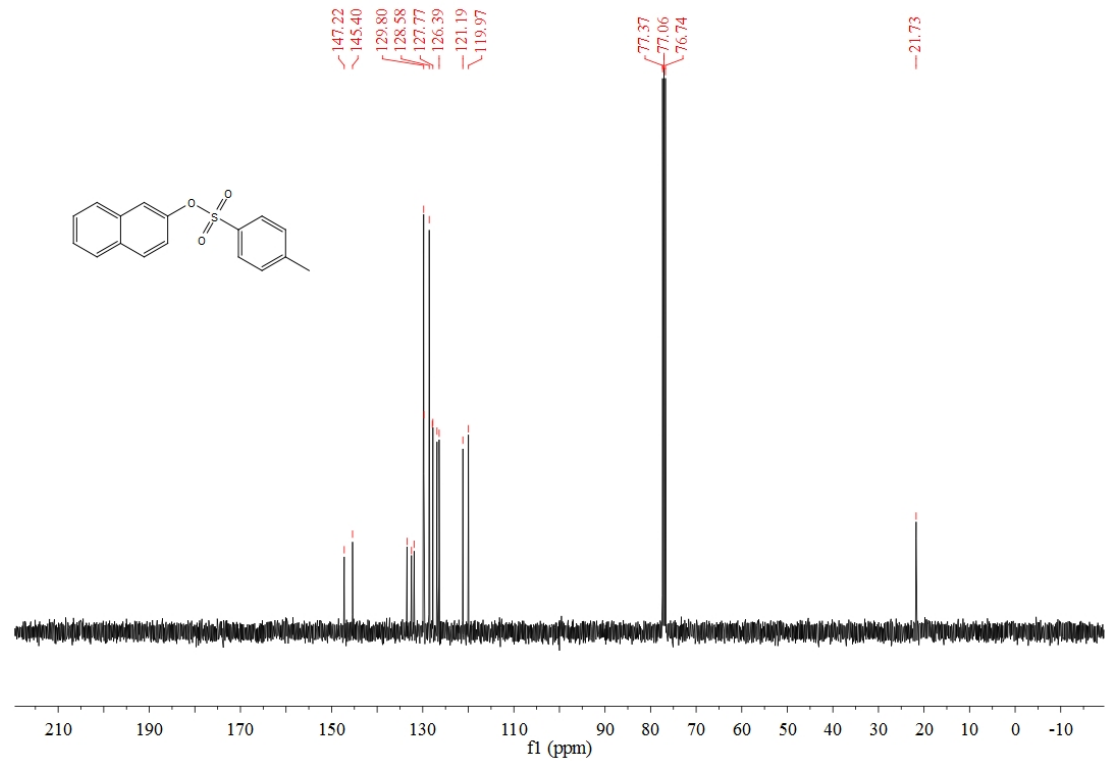
145.45
129.81
128.49
127.71
127.33
127.10
126.73
126.71
125.13
121.81
118.40
77.41
77.09
76.77
21.67
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.81
7.80
7.75
7.73
7.71
7.49
7.47
7.30
7.28
7.10
7.08
2.43
1.01
3.96
2.98
2.01
0.99
3.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)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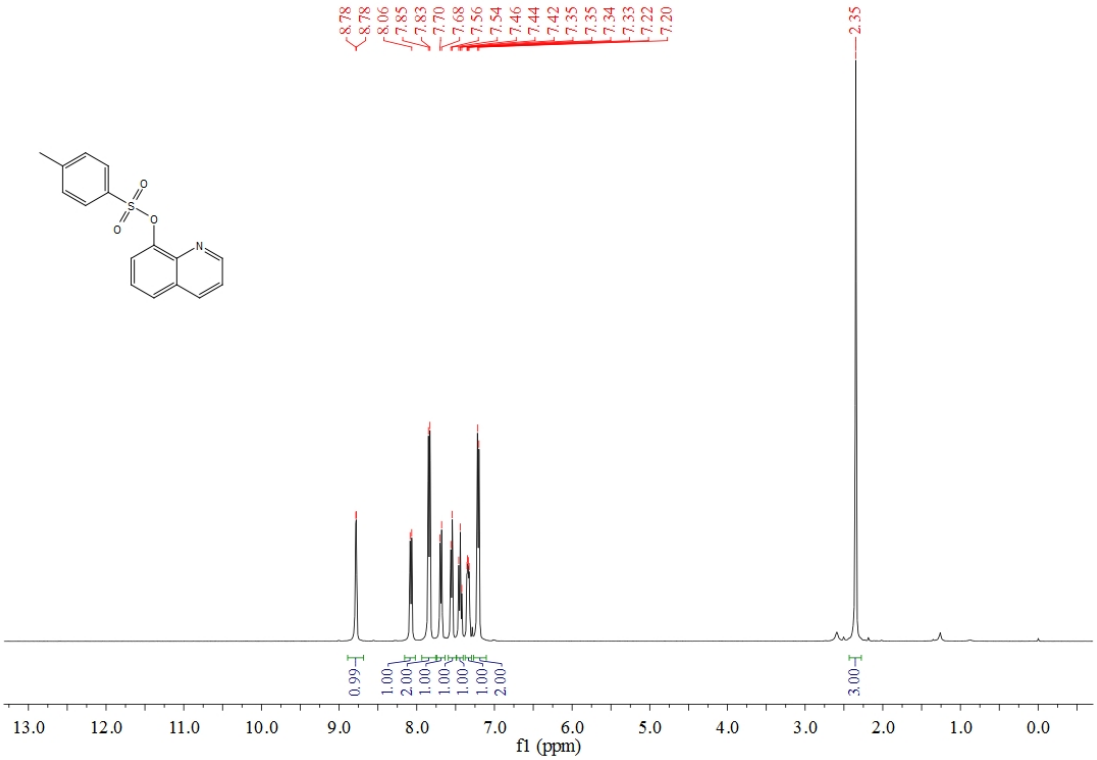
128.58
127.77
126.39
121.19
119.97
77.37
77.06
76.74
21.73
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.78
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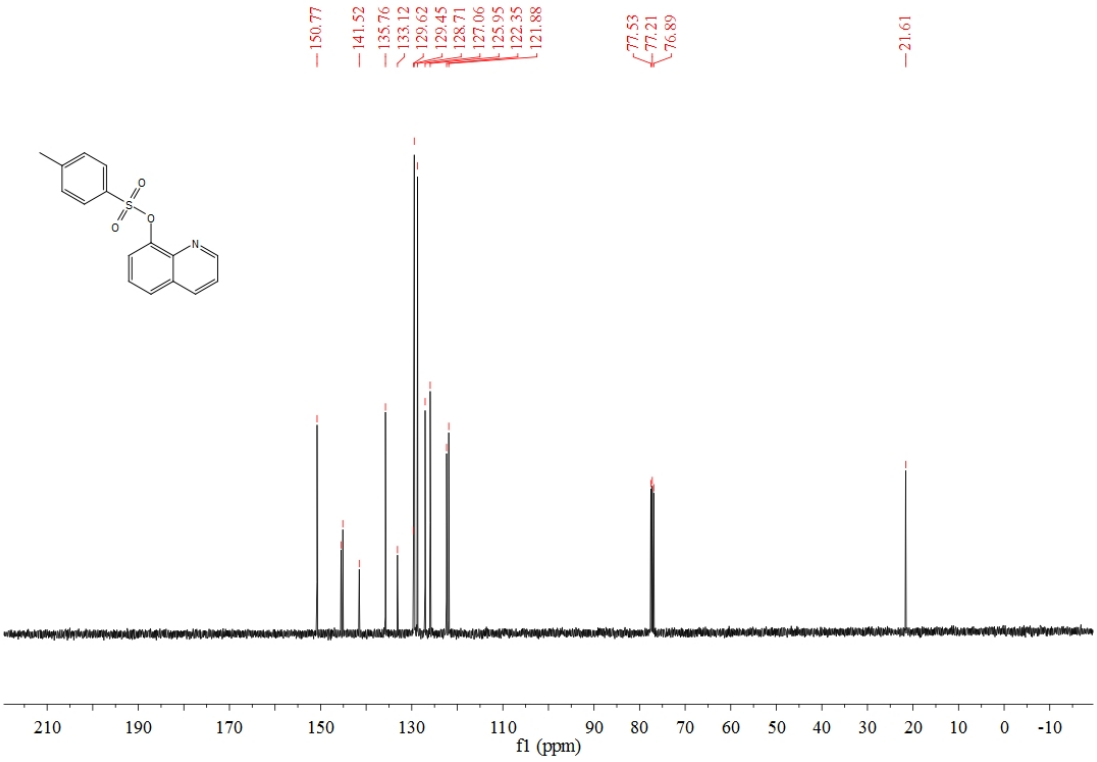
7.83
7.70
7.68
7.56
7.54
7.46
7.44
7.42
7.35
7.35
7.34
7.33
7.22
7.20
2.35
0.99
1.00
2.00
1.00
1.00
1.00
1.00
2.00
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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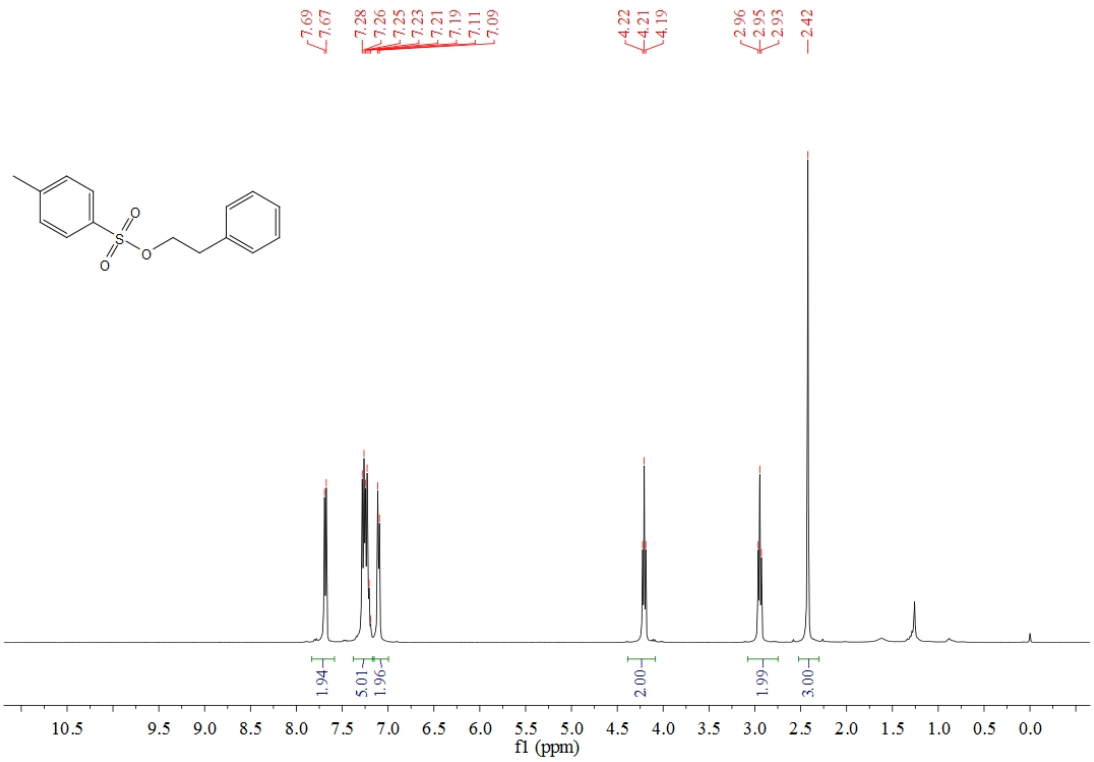
133.12
129.62
129.45
128.71
127.06
125.95
122.35
121.88
77.53
77.21
76.89
21.61
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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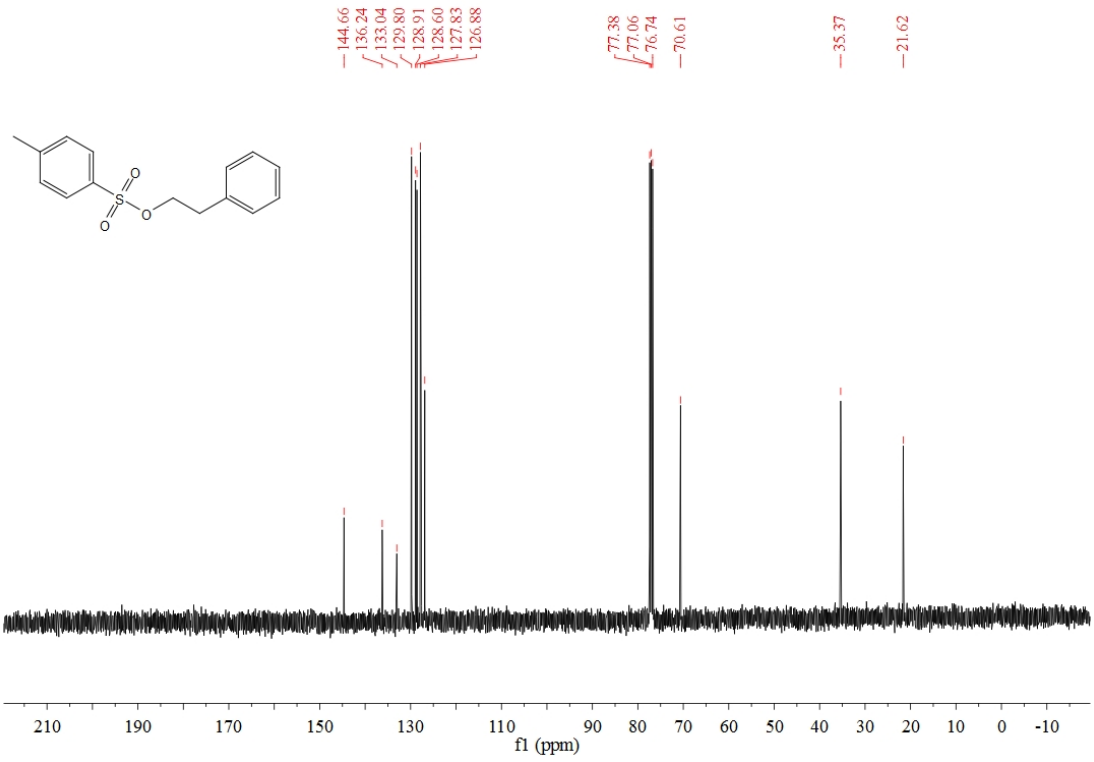
7.67
7.28
7.26
7.25
7.23
7.21
7.19
7.11
7.09
4.22
4.21
4.19
2.96
2.95
2.93
2.42
1.94
5.01
1.96
2.00
1.99
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


144.66
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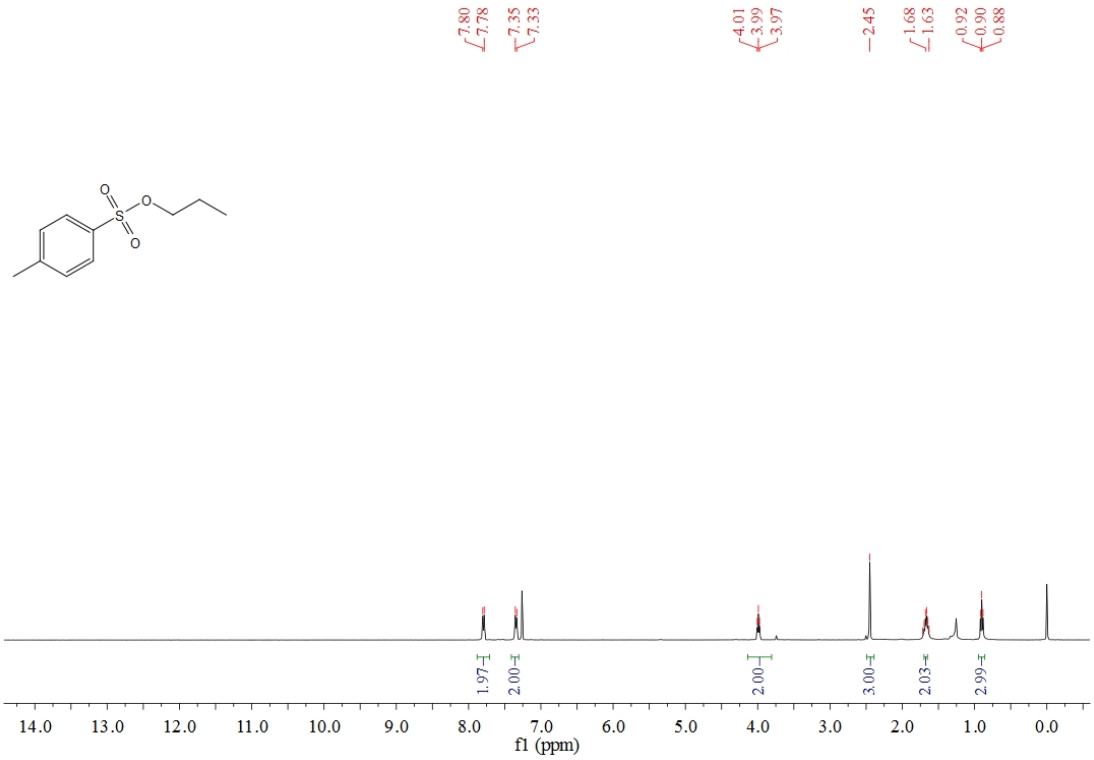
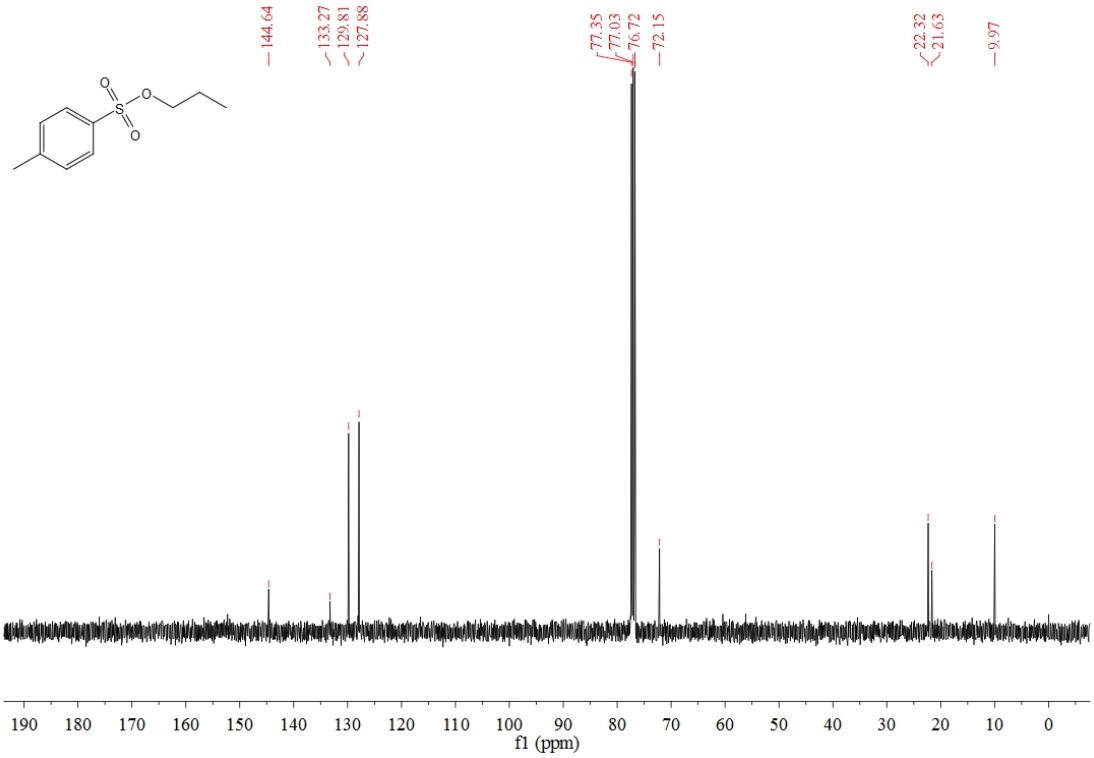
128.91
128.60
127.83
126.88
77.38
77.06
76.74
70.61
35.37
21.62
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.80
7.78
7.35
7.33
4.01
3.99
3.97
2.45
1.68
1.63
0.92
0.90
0.88
1.97
2.00
2.00
3.00
2.03
2.99
14.0 13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


144.64
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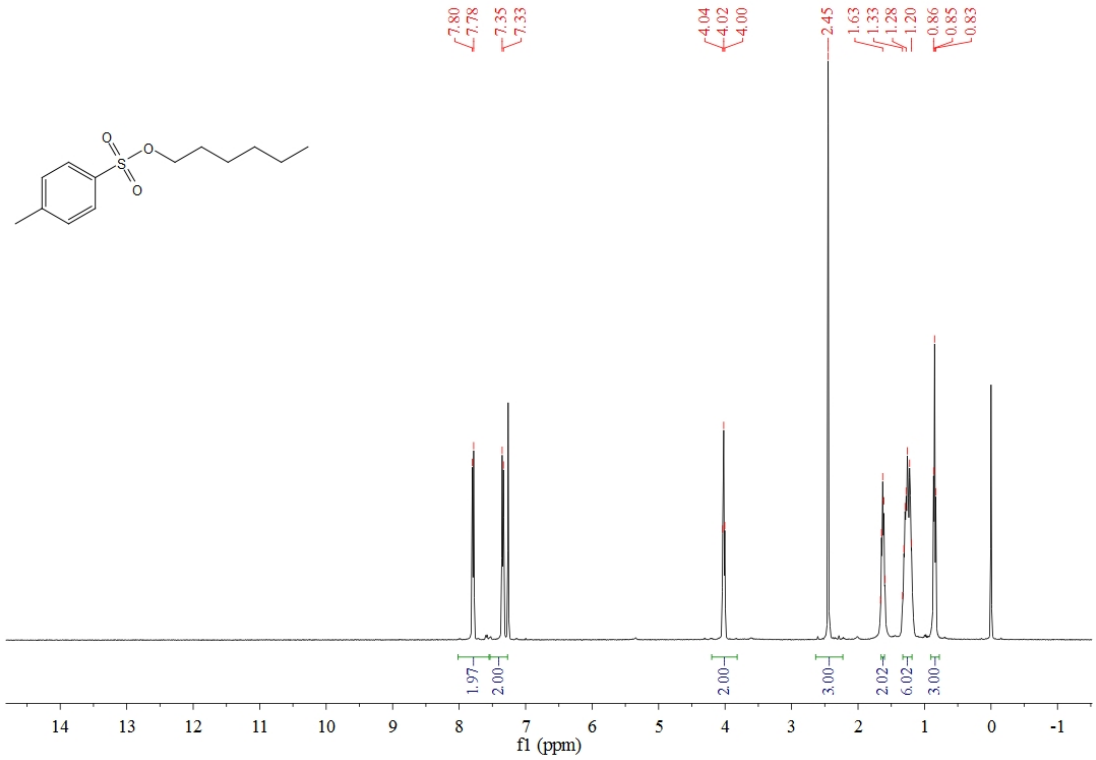
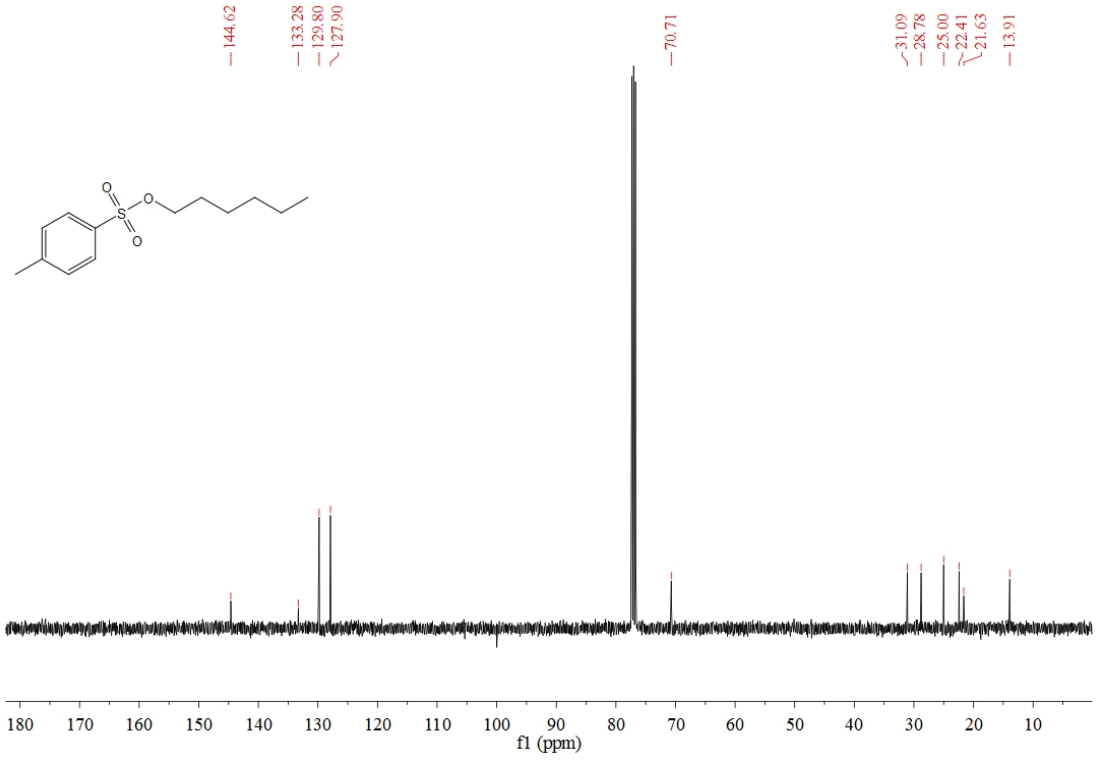
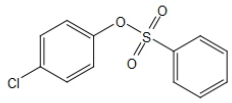
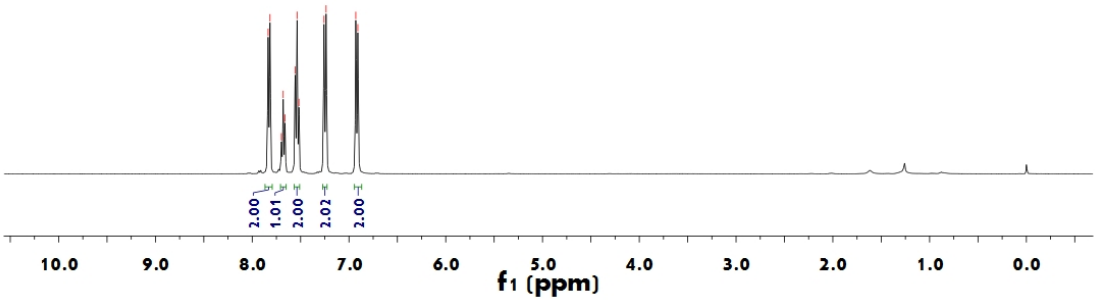
127.88
77.35
77.03
76.72
72.15
22.32
21.63
9.97
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.80
7.78
7.35
7.33
4.04
4.02
4.00
2.45
1.63
1.33
1.28
1.20
0.86
0.85
0.83
1.97
2.00
2.00
3.00
2.02
6.02
3.00
f1 (ppm)

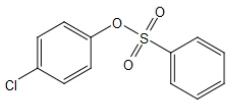

144.62
133.28
129.80
127.90
70.71
31.09
28.78
25.00
22.41
21.63
13.91
f1 (ppm)

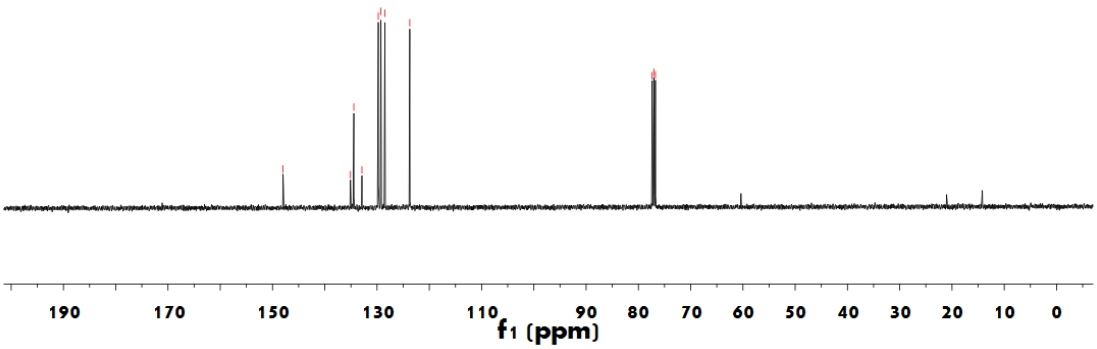

7.84
7.82
7.70
7.68
7.66
7.56
7.54
7.52
7.24
6.93
6.91

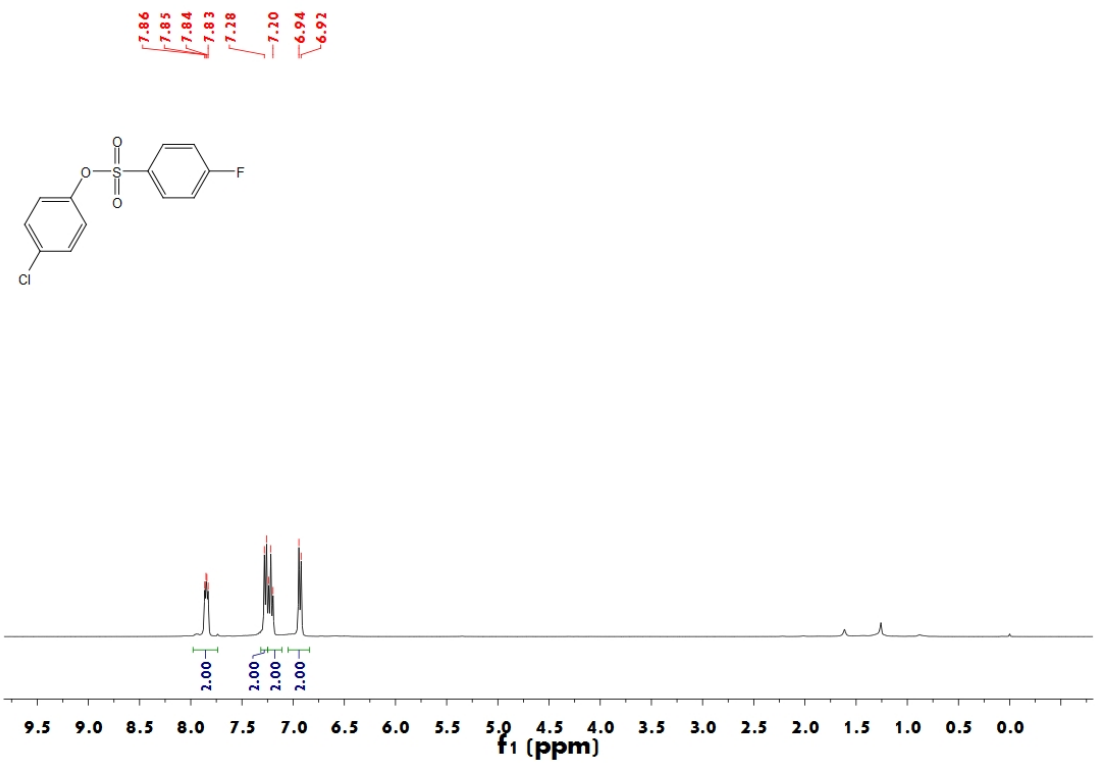

O
O
S
O
Cl

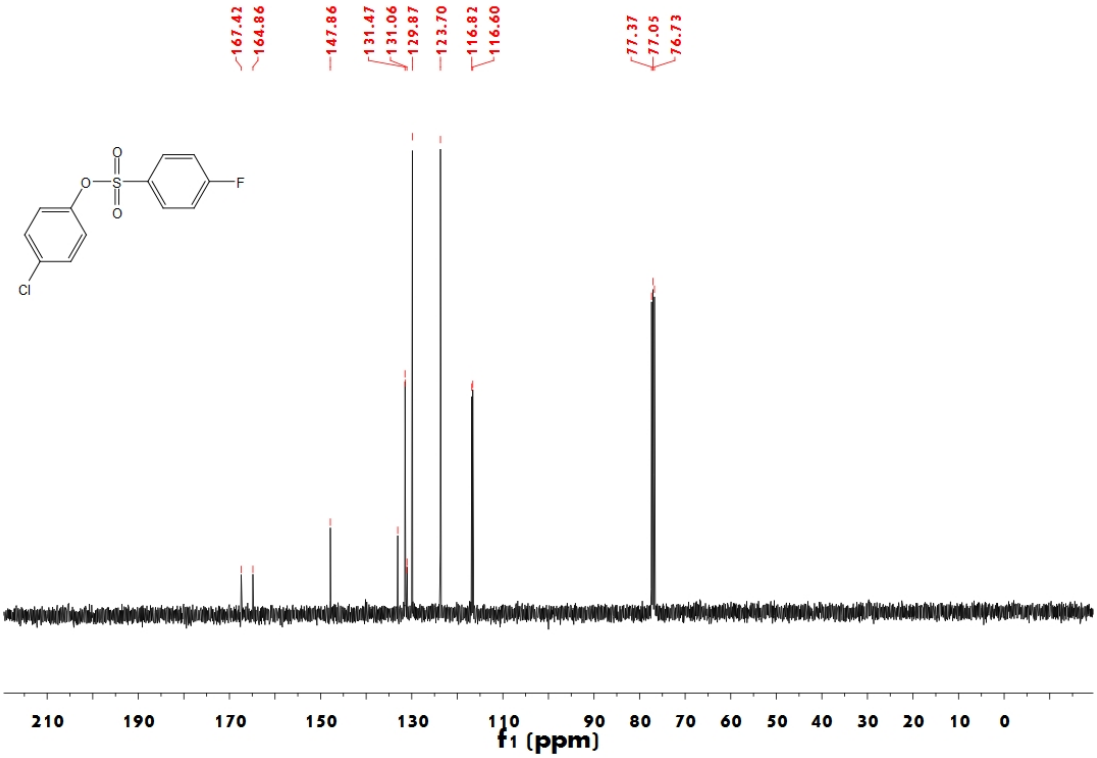

2.00
1.01
2.00
2.02
2.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

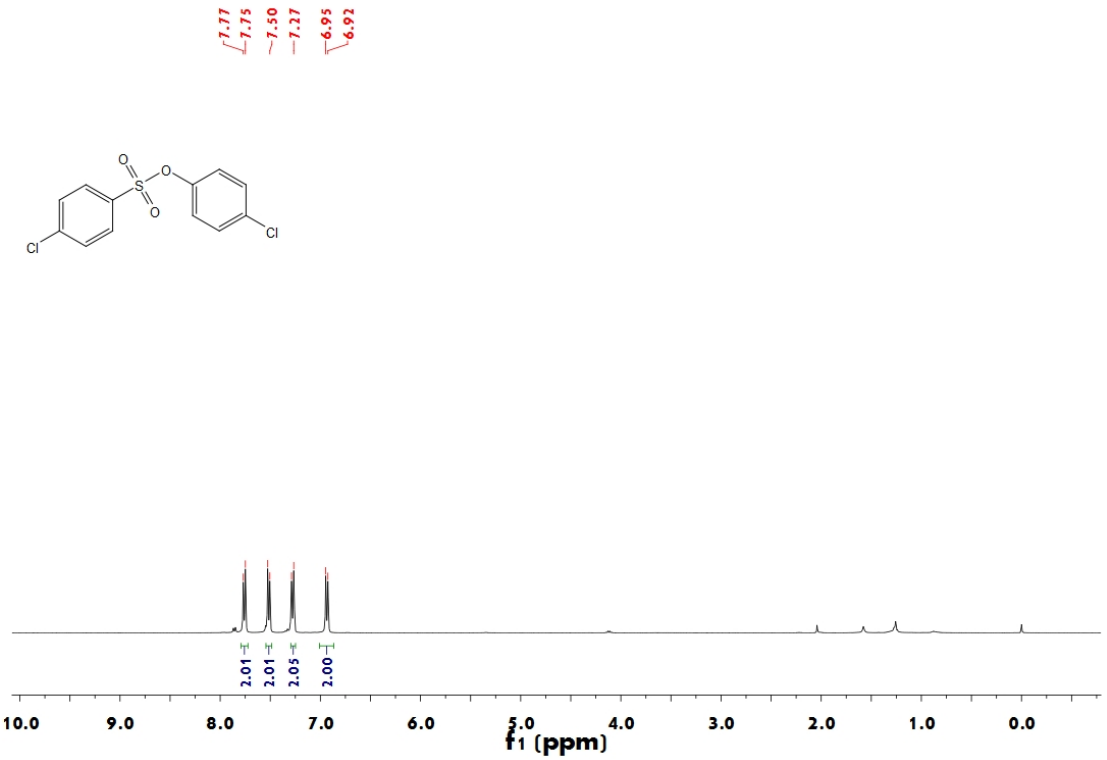

147.99
134.44
129.76
129.26
128.50
123.74
77.37
77.05
76.74

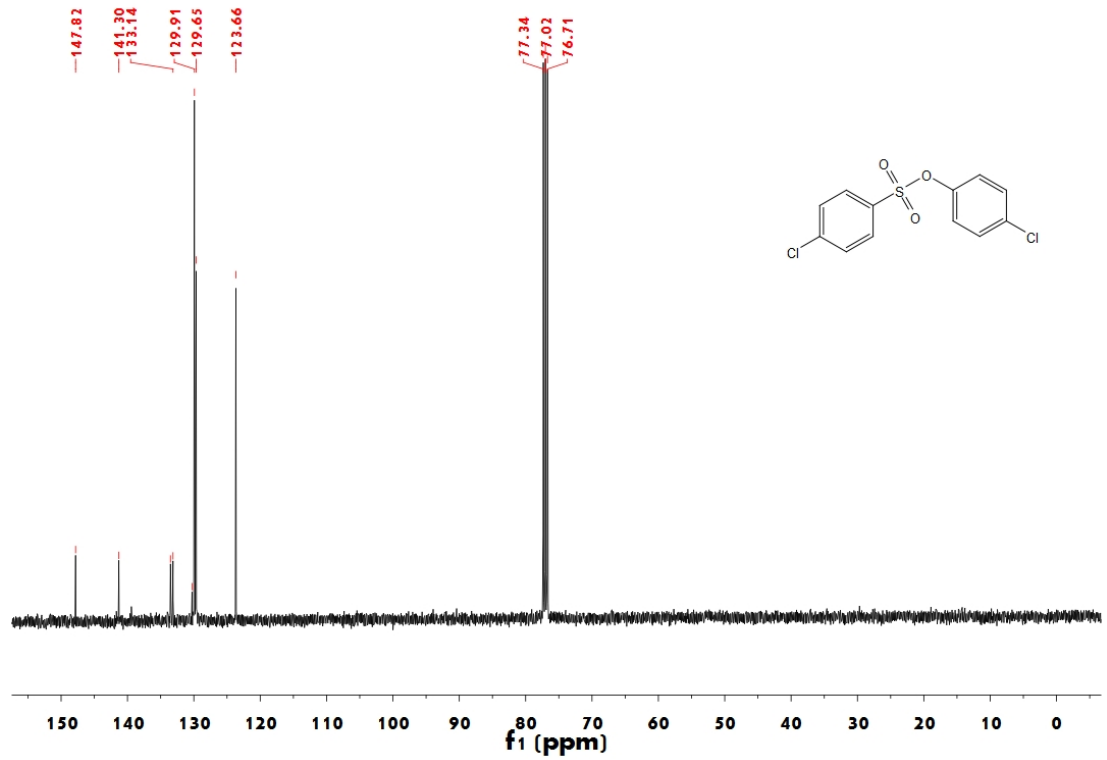

O
O
S
O
Cl

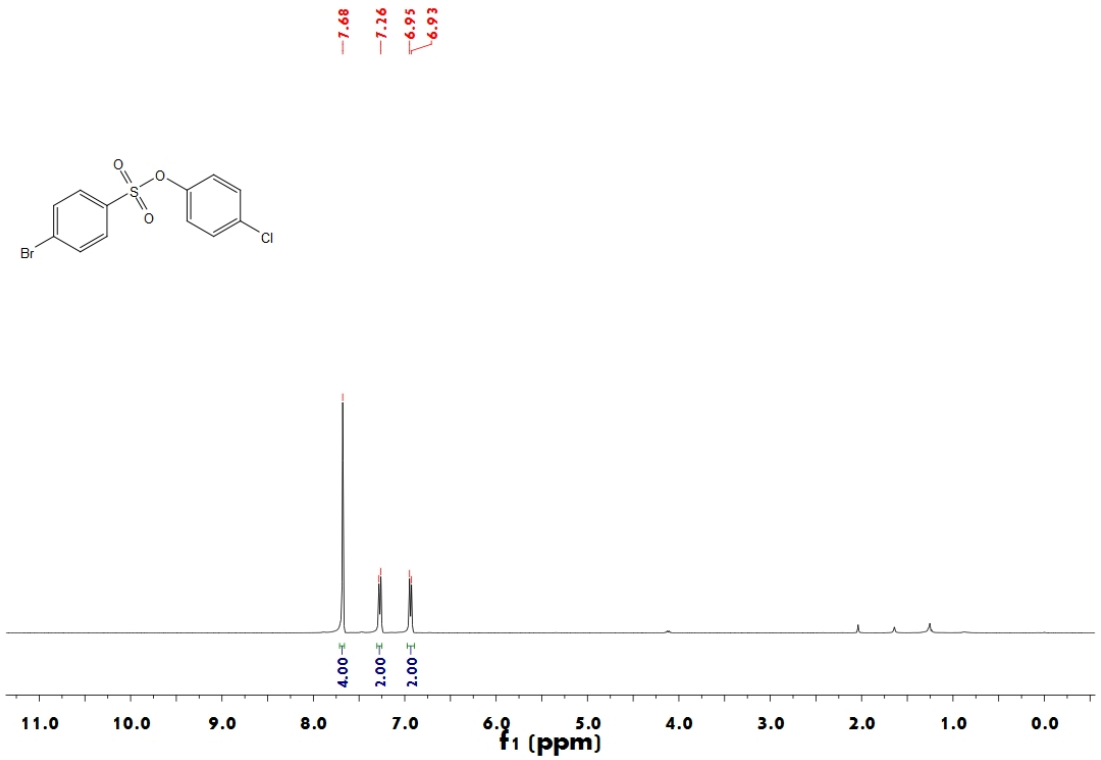

190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

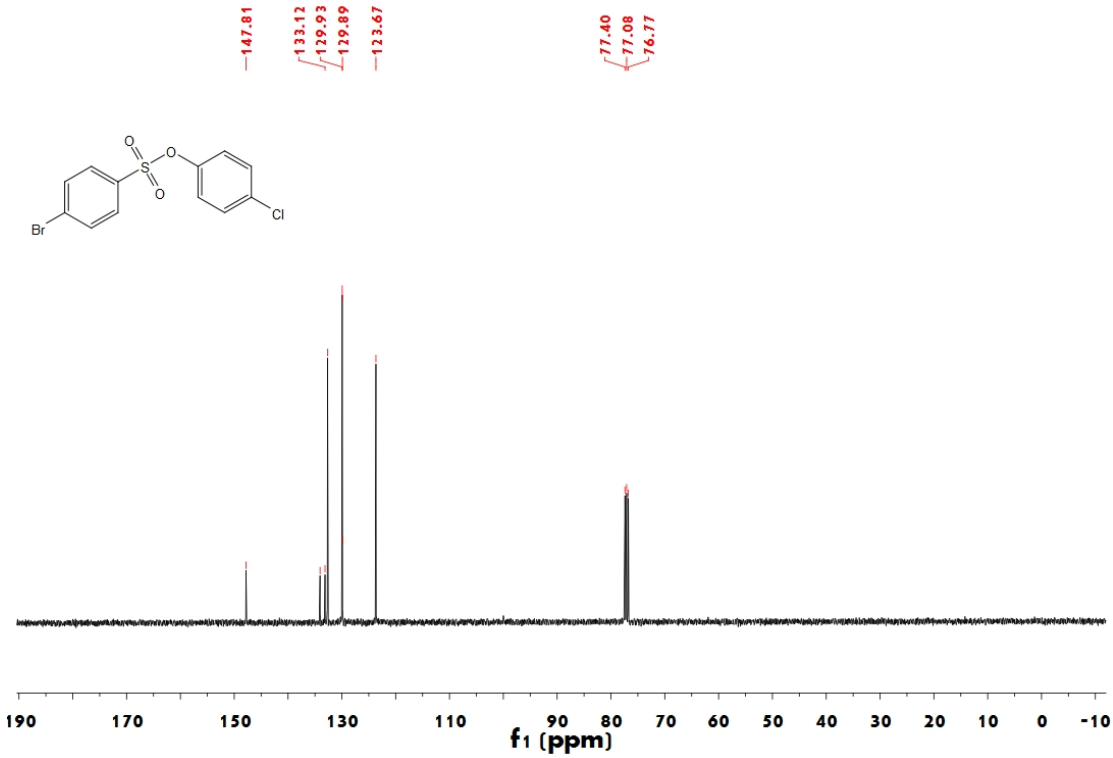

7.86
7.85
7.84
7.83
7.28
7.20
6.94
6.92
O
S
O
O
F
Cl
2.00
2.00
2.00
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

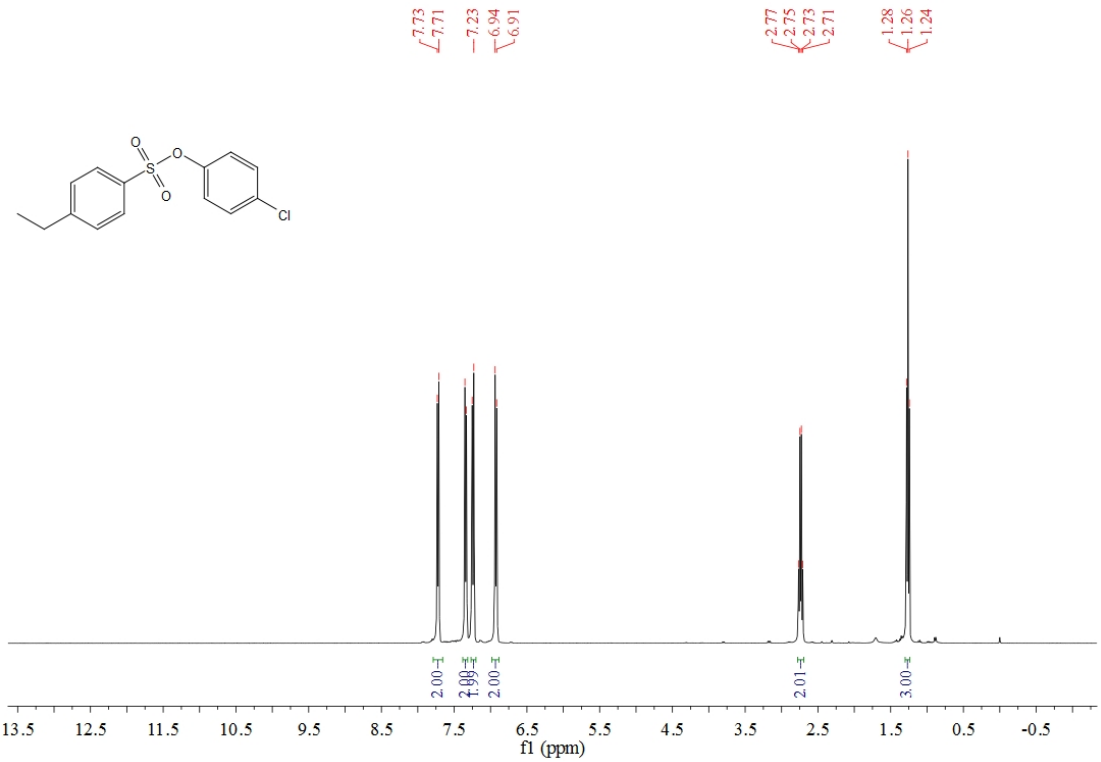

167.42
164.86
147.86
131.47
131.06
129.87
123.70
116.82
116.60
77.37
77.05
76.73
O
S
O
O
F
Cl
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

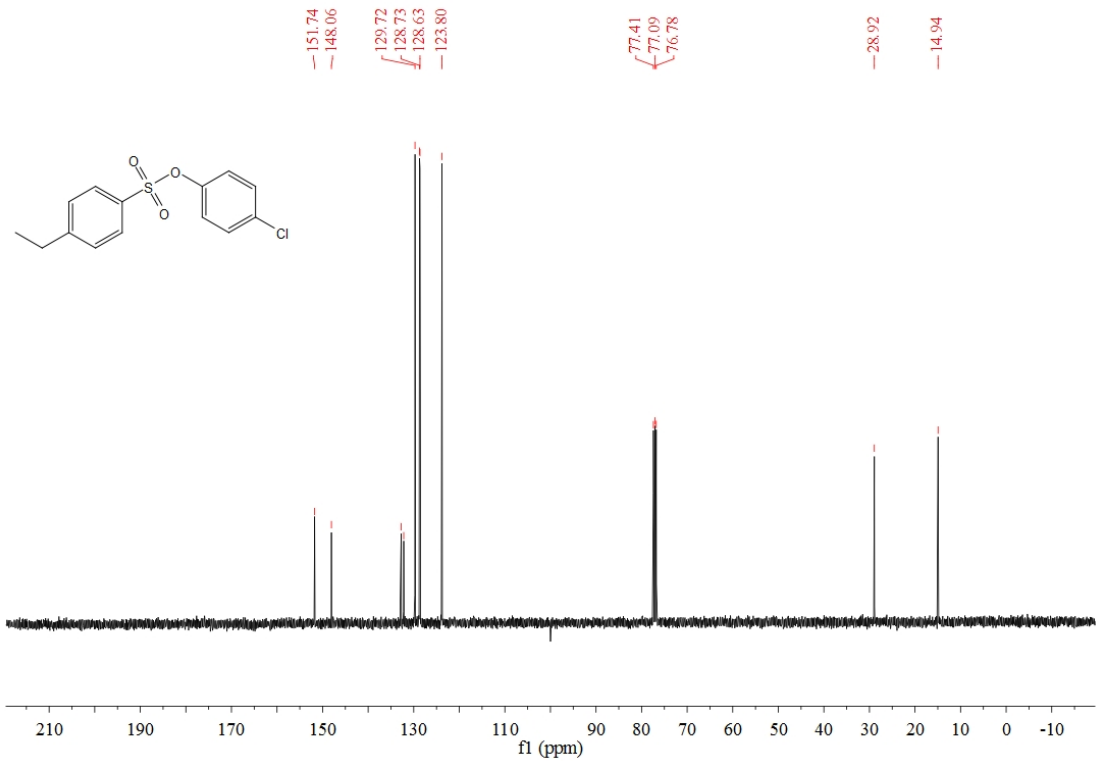

7.77
7.75
7.50
7.27
6.95
6.92
O
S
O
O
Cl
Cl
2.01
2.01
2.05
2.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

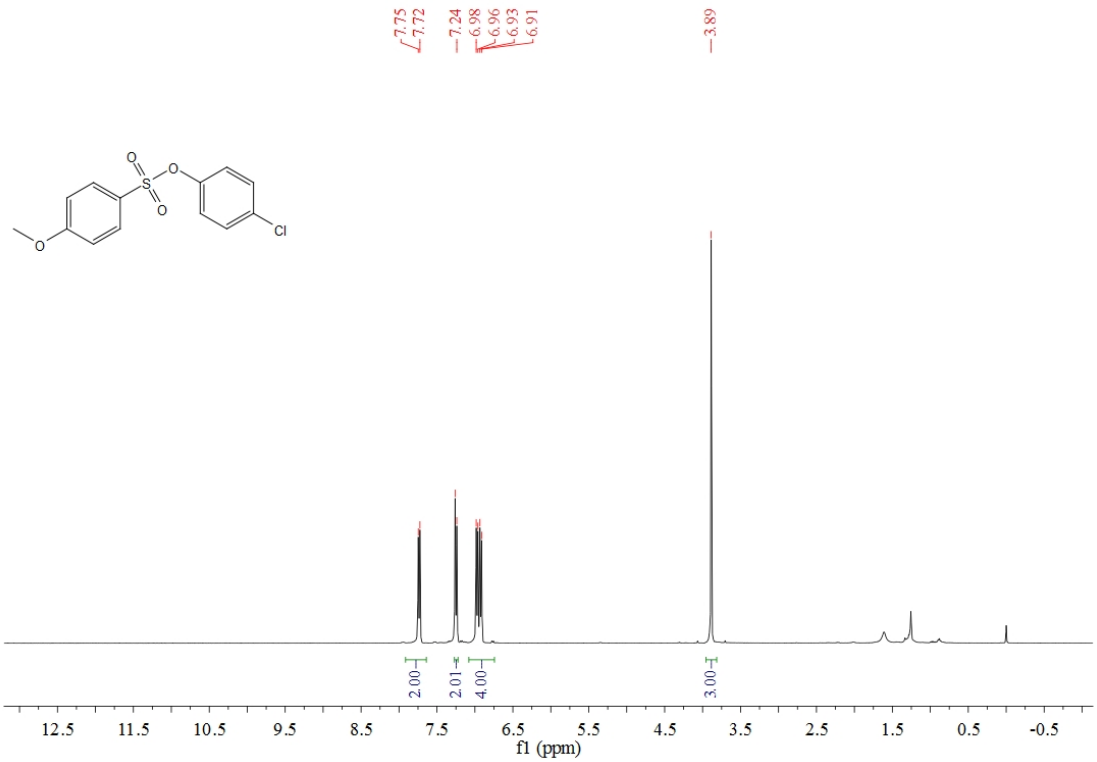

147.82
141.30
133.14
129.91
129.65
123.66
77.34
77.02
76.71
O
S
O
O
Cl
Cl
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

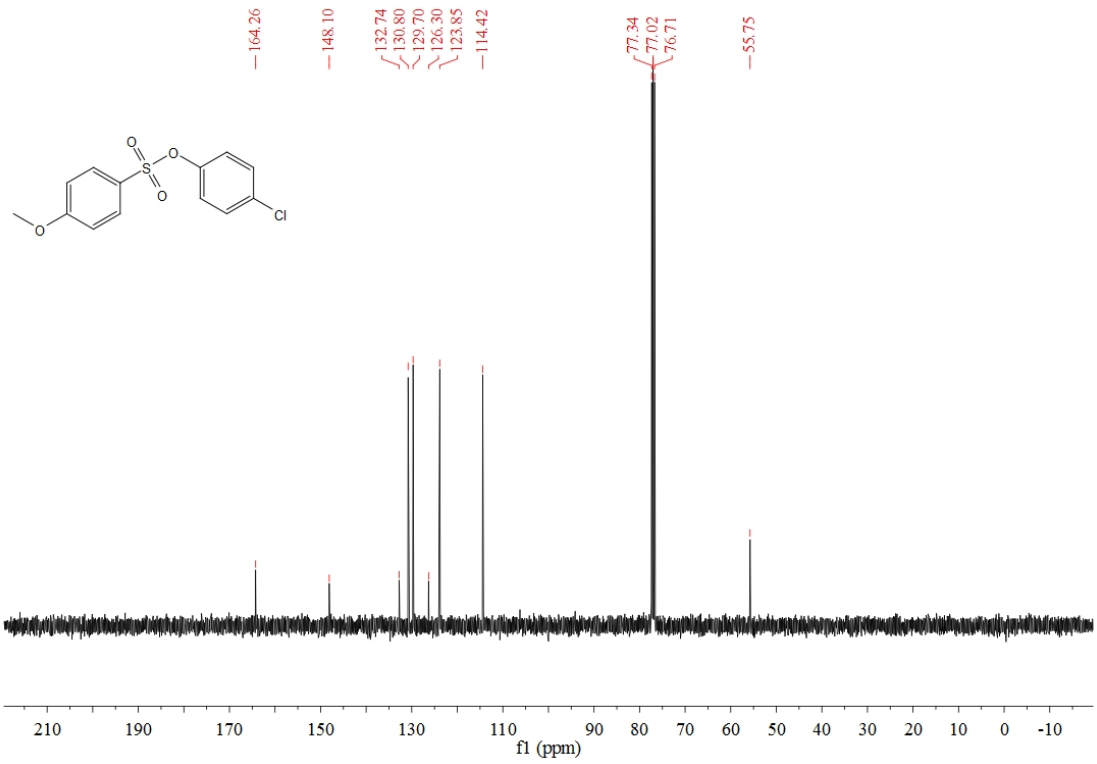

7.68
7.26
6.95
6.93
Br
Cl
4.00
2.00
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

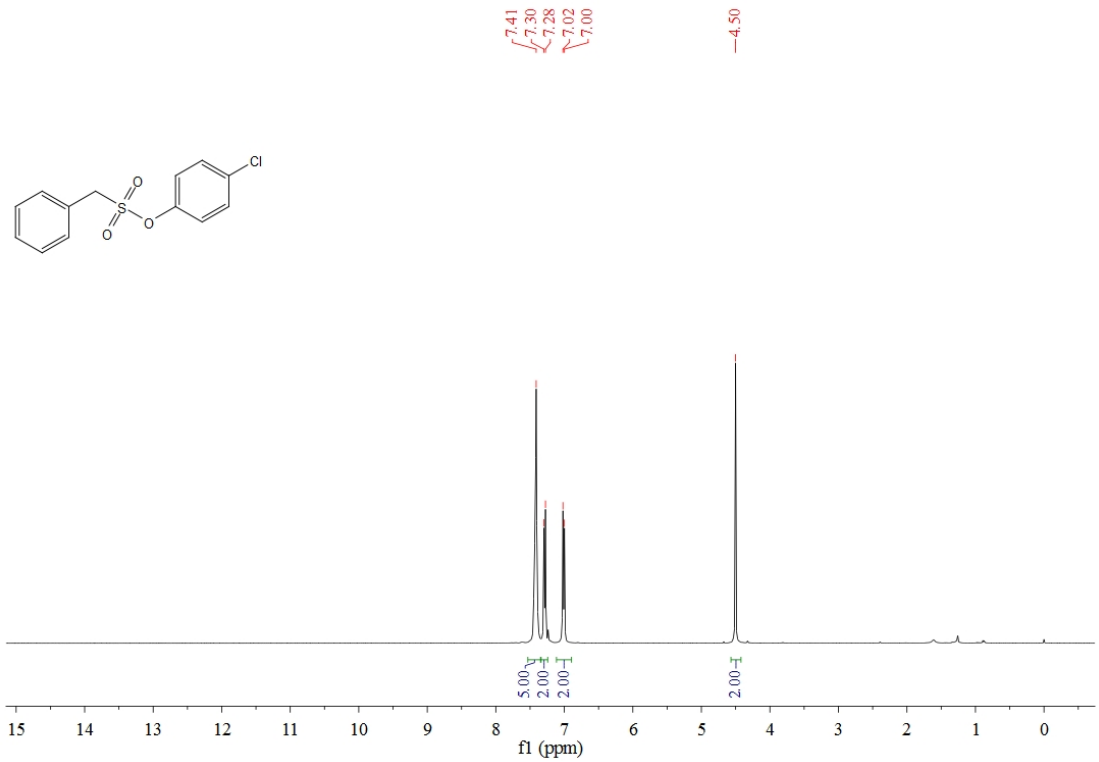

147.81
133.12
129.93
129.89
123.67
77.40
77.08
76.77
Br
Cl
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

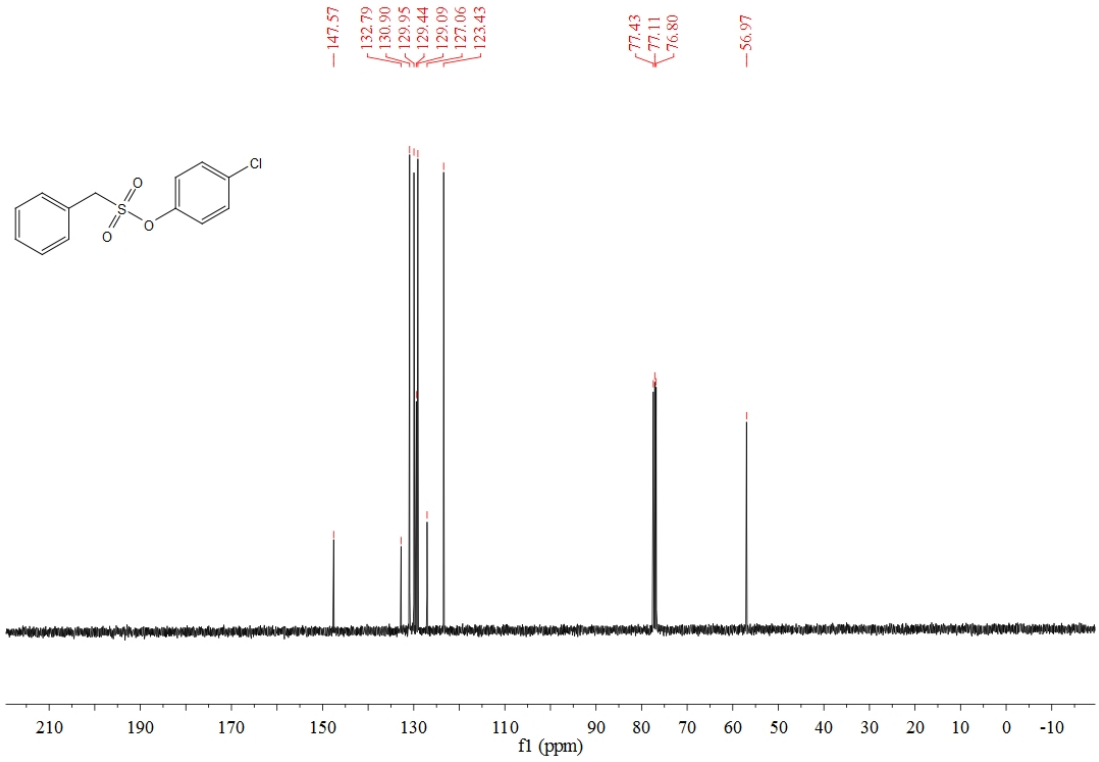

7.73
7.71
7.23
6.94
6.91
2.77
2.75
2.73
2.71
1.28
1.26
1.24
2.00
1.98
2.00
2.01
3.00
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)
O
S
O
O
Cl


151.74
148.06
129.72
128.73
128.63
123.80
77.41
77.09
76.78
28.92
14.94
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
O
S
O
O
Cl


7.75
7.72
7.24
6.98
6.96
6.93
6.91
3.89
O
S
O
O
O
Cl
O
2.00
2.01
4.00
3.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


164.26
148.10
132.74
130.80
129.70
126.30
123.85
114.42
77.34
77.02
76.71
55.75
O
S
O
O
O
Cl
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.41
7.30
7.28
7.02
7.00
4.50
Cl
O
S
O
O
5.00
2.00
2.00
2.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


147.57
132.79
130.90
129.95
129.44
129.09
127.06
123.43
77.43
77.11
76.80
56.97
Cl
O
S
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)