Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Nickel-Catalyzed Product-Controllable Amidation and Imidation of sp^3 C-H bond in Substituted Toluenes with Sulfonamides

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1.General information

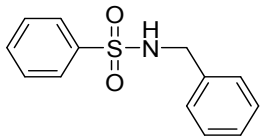
All chemical reagents are obtained from commercial suppliers and used without further purification. All compounds are characterized by ^{1}H NMR, ^{13}C NMR, MS and elemental analyses.Analytical thin-layer chromatography is performed on glass plates precoated with silica gel impregnated with a fluorescent indicator (254 nm), and the plates are visualized by exposure to ultraviolet light. ^{1}H NMR and ^{13}C NMR spectra are recorded on an AVANCE 500 Bruker spectrometer operating at 500 MHz and 125 MHz in $CDCl_3$, respectively, and chemical shifts are reported in ppm.GC analyses are performed on an Agilent 7890A instrument (Column: Agilent 19091J-413:30 m × 320 μm × 0.25 μm, H, FID detection). GC-MS data was recorded on a 5975C Mass Selective Detector,coupled with a 7890A Gas Chromatograph (Agilent Technologies).

2.General procedure

General procedure for the amidation of sulfonamides with toluene : A 50 mL Schlenk tube was added sulfonamides **1** (0.5 mmol), toluenes **2** (1.5 mL), $Ni(OAc)_2$ (10 mol %) and DTBP (2 equiv). The tube was then sealed and exchanged with N_2 for 3 times, and was stirred at 120°C for 24 h. The reaction mixture was then cooled to room temperature, extracted with ethyl acetate (3×5ml), washed with brine (10 mL) and then dried, filtered, concentrated in vacuo. The resulting mixture was purified by silica gel column chromatography to afford the desired products **3.**

.**General procedure for the imidation of sulfonamides with toluene :** A 50 mL Schlenk tube was added sulfonamides **1** (0.5 mmol), toluenes **2** (1.5 mL), $Ni(OAc)_2$ (10 mol %) and DTBP (2 equiv). The tube was then charged with O_2 for 3 times, and was stirred at 120°C for 24 h. The reaction mixture was then cooled to room temperature. 10 mL ethyl acetate was added to dissolve the reaction mixture, filtered by celite and then concentrated in vacuo. The resulting mixture was purified by silica gel column chromatography to afford the desired products **4.**

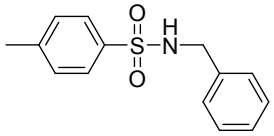
3.Characterization data



Formula:$C_{13}H_{13}NO_2S$

Mass:247

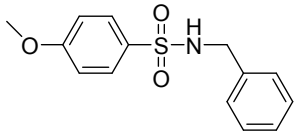
***N*-benzylbenzenesulfonamide(3a):** The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3a** as white solid (92.6mg, 75%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.29 – 7.22 (m, 3H), 7.21 – 7.13 (m, 2H), 4.96 (t, *J* = 5.7 Hz, 1H), 4.14 (d, *J* = 6.2 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 140.1, 136.3, 132.8, 129.3, 128.8, 128.1, 128.0, 127.2, 47.4. GC-MS (EI) *m/z*: 247.



Formula: $C_{14}H_{15}NO_2S$

Mass: 261

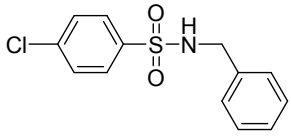
***N*-benzyl-4-methylbenzenesulfonamide(3b)**: The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3b** as white solid (91.4 mg, 70%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.17 (m, 5H), 7.13 – 7.09 (m, 2H), 4.64 (t, *J* = 5.7 Hz, 1H), 4.04 (d, *J* = 6.2 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 142.6, 135.9, 135.3, 128.8, 127.7, 126.9, 126.5, 126.2, 46.5, 20.6. GC-MS (EI) *m/z*: 261.



Formula: $C_{14}H_{15}NO_3S$

Mass:277

***N*-benzyl-4-methoxybenzenesulfonamide(3c)**: The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3c** as white solid (99.7 mg, 72%).^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.9 Hz, 2H), 7.20 – 7.14 (m, 3H), 7.12 – 7.06 (m, 2H), 6.85 (d, *J* = 8.9 Hz, 2H), 4.65 (t, *J* = 6.2 Hz, 1H), 3.99 (d, *J* = 6.2 Hz, 2H), 3.76 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 162.0, 135.3, 130.5, 128.4, 127.7, 127.2, 126.9, 113.3, 54.7, 46.3. GC-MS (EI) *m/z*: 277.

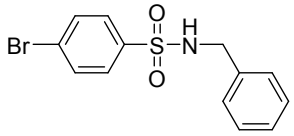


Formula: $C_{13}H_{12}ClNO_2S$

Mass:281

***N*-benzyl-4-chlorobenzenesulfonamide(3d)**: The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3d**

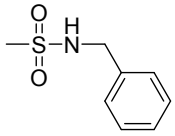
as white solid (91.3 mg, 65%).[1]H NMR (500 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.20 – 7.06 (m, 5H), 4.85 (t, *J* = 5.7 Hz, 1H), 4.06 (d, *J* = 6.1 Hz, 2H). [13]C NMR (126 MHz, Chloroform-*d*) δ 138.3, 137.6, 134.9, 128.4, 127.8, 127.6, 127.1, 126.9, 46.3. GC-MS (EI) *m/z*: 281.



Formula: $C_{13}H_{12}BrNO_2S$

Mass:325

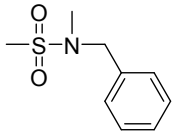
***N*-benzyl-4-bromobenzenesulfonamide(3e)**: The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give **3e** as white solid (102.4mg, 63%).[1]H NMR (500 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.21 – 7.08 (m, 5H), 4.66 (t, *J* = 5.3 Hz, 1H), 4.08 (d, *J* = 6.1 Hz, 2H).[13]C NMR (126 MHz, DMSO-d_6) δ 140.6, 137.9, 132.7, 129.1, 128.8, 128.2, 127.7,126.6, 46.7. GC-MS (EI) *m/z*: 325.



Formula: $C_8H_{11}NO_2S$

Mass:185

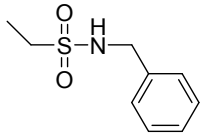
***N*-benzylmethanesulfonamides(3f)**: The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =15:1) to give **3f** as white solid (72.1mg, 78%). [1]H NMR (500 MHz, Chloroform-*d*) δ 7.32 – 7.19 (m, 5H), 5.60 (t, *J* = 5.3 Hz, 1H), 4.17 (d, *J* = 6.6 Hz, 2H), 2.70 (s, 3H). [13]C NMR (126 MHz, Chloroform-*d*) δ 136.2, 127.8, 127.0, 126.9, 46.0, 39.6. GC-MS (EI) *m/z*: 185.



Formula: $C_9H_{13}NO_2S$

Mass:199

N-benzyl-N-methylmethanesulfonamide(3g): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =15:1) to give **3g** as white solid (59.7mg, 60%). [1]H NMR (500 MHz, Chloroform-*d*) δ 7.45 – 7.24 (m, 5H), 4.31 (s, 2H), 2.80 (d, *J* = 30.7 Hz, 6H).[13]C NMR (126 MHz, Chloroform-*d*) δ 134.6, 127.8, 127.4, 127.1, 53.0, 35.1, 33.4. GC-MS (EI) *m/z*: 199.

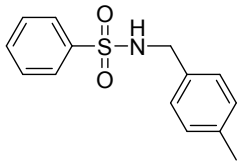


Formula: $C_9H_{13}NO_2S$

Mass: 199

N-benzylethanesulfonamide(3h): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =15:1) to give **3h** as white solid (85.2mg, 80%). [1]H NMR (500 MHz, Chloroform-*d*) δ 7.27 – 7.05 (m, 5H), 5.57 (t, *J* = 6.3 Hz, 1H), 4.09 (d, *J* = 6.6 Hz, 2H), 2.72 (q, *J* = 7.4 Hz, 2H), 1.08 (t, *J* =

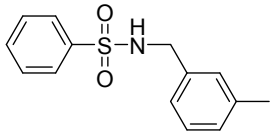
7.5 Hz, 3H).^{13}C NMR (126 MHz, Chloroform-*d*) δ 136.6, 127.7, 126.9, 126.8, 46.2, 45.8, 7.1. GC-MS (EI) *m/z*: 199.



Formula: $C_{14}H_{15}NO_2S$

Mass:261

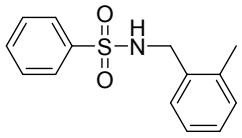
N-(4-methylbenzyl)benzenesulfonamide(3i): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3i** as white solid (100.5mg, 77%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.91 – 7.83 (m, 2H), 7.65 – 7.46 (m, 3H), 7.07 (s, 4H), 4.77 (t, *J* = 6.1 Hz, 1H), 4.10 (d, *J* = 6.1 Hz, 2H), 2.31 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 136.8, 132.2, 131.7, 128.4, 128.2, 126.9, 126.2, 46.1, 20.1. GC-MS (EI) *m/z*: 261.



Formula: $C_{14}H_{15}NO_2S$

Mass:261

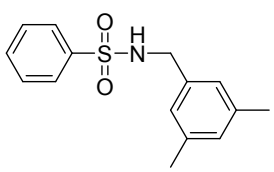
N-(3-methylbenzyl)benzenesulfonamide(3j): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3j** as white solid(90.0mg, 69%).^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.97 (d, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 7.1 Hz, 2H), 4.71 (t, *J* = 6.2 Hz, 1H), 4.03 (d, *J* = 6.1 Hz, 2H), 2.19 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.0, 137.4, 135.2, 133.5, 131.7, 128.1, 127.6, 126.3, 126.2, 123.9, 46.3, 20.3. GC-MS (EI) *m/z*: 261.



Formula: $C_{14}H_{15}NO_2S$

Mass:261

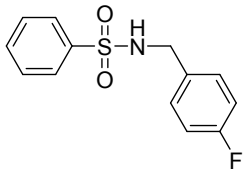
N-(2-methylbenzyl)benzenesulfonamide(3k): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3k** as white solid (86.1mg, 66%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 7.8 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.11 – 6.98 (m, 4H), 4.59 (t, *J* = 5.1 Hz, 1H), 4.03 (d, *J* = 5.9 Hz, 2H), 2.15 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.7, 140.3, 139.4, 136.6, 134.2, 133.4, 132.9, 131.7, 130.8, 129.9, 48.5, 22.7. GC-MS (EI) *m/z*: 261.



Formula: $C_{15}H_{17}NO_2S$

Mass:275

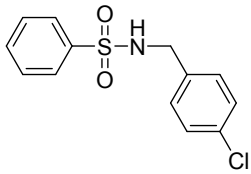
N-(3,5-dimethylbenzyl)benzenesulfonamide(**3l**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3l** as white solid (99.0mg, 72%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.7 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 6.87 (s, 1H), 6.76 (s, 2H), 4.82 (t, *J* = 5.7 Hz, 1H), 4.07 (d, *J* = 6.1 Hz, 2H), 2.23 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.0, 137.4, 135.2, 131.7, 128.1, 127.6, 126.2, 123.9, 46.3, 20.3. GC-MS (EI) *m/z*: 275.



Formula: $C_{13}H_{12}FNO_2S$

Mass:265

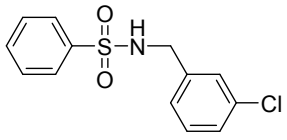
N-(4-fluorobenzyl)benzenesulfonamide(**3m**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3m** as white solid (76.9mg, 58%).^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.11 – 7.04 (m, 2H), 6.86 (t, *J* = 8.5 Hz, 2H), 4.78 (t, *J* = 5.2 Hz, 1H), 4.04 (d, *J* = 6.2 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 160.4, 138.9, 131.8, 131.1, 128.7, 128.2, 126.1, 114.5, 45.6. GC-MS (EI) *m/z*: 265.



Formula: $C_{13}H_{12}ClNO_2S$

Mass:281

N-(4-chlorobenzyl)benzenesulfonamide(**3n**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3n** as white solid (101.2mg, 72%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 4.91 (t, *J* = 5.5 Hz, 1H), 4.03 (d, *J* = 6.3 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 133.5, 131.9, 129.0, 128.2, 127.1, 127.0, 126.1, 125.0, 45.7. GC-MS (EI) *m/z*: 281.

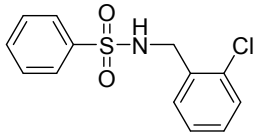


Formula: $C_{13}H_{12}ClNO_2S$

Mass:281

N-(3-chlorobenzyl)benzenesulfonamide(**3o**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3o** as white solid (88.5mg, 63%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.4 Hz, 2H), 7.54 (dt, *J* = 42.0, 7.5 Hz, 3H), 7.22 – 7.06 (m, 4H), 5.28 – 5.12 (t, *J* = 7.5

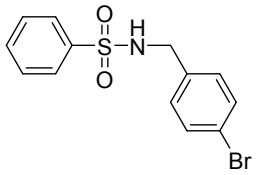
Hz, 1H), 4.12 (d, *J* = 6.3 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.8, 137.3, 133.5, 131.9, 129.0, 128.2, 127.1, 127.0, 126.1, 125.0, 45.7. GC-MS (EI) *m/z*: 281.



Formula:$C_{13}H_{12}ClNO_2S$

Mass: 281

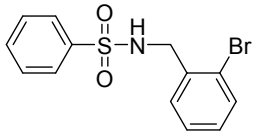
N-(2-chlorobenzyl)benzenesulfonamide(**3p**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3p** as white solid (106.8mg, 76%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.70 (d, *J* = 7.3 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.17 (d, *J* = 9.2 Hz, 1H), 7.12 (d, *J* = 7.3 Hz, 1H), 7.06 – 6.99 (m, 2H), 5.24 (t, *J* = 6.3 Hz, 1H), 4.14 (d, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 139.0, 132.8, 132.4, 131.7, 129.3, 128.5, 128.3, 128.1, 127.8, 126.0, 44.2. GC-MS (EI) *m/z*: 281.



Formula: $C_{13}H_{12}BrNO_2S$

Mass:325

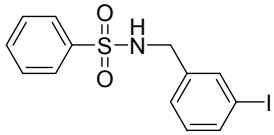
N-(4-bromobenzyl)benzenesulfonamide(**3q**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3q** as white solid(125.1mg, 77%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93 – 7.77 (m, 2H), 7.63 – 7.46 (m, 3H), 7.28 – 6.87 (m, 4H), 5.07 – 5.04 (t, *J* = 7.5 Hz, 1H), 4.15 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.9, 133.8, 132.9, 132.0, 131.9, 128.2, 127. , 126.1, 45.6. GC-MS (EI) *m/z*: 325.



Formula: $C_{13}H_{12}BrNO_2S$

Mass:325

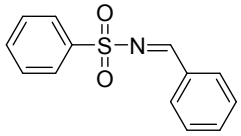
N-(2-bromobenzyl)benzenesulfonamide(**3r**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3r** as white solid(105.6mg, 65%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 – 7.78 (m, 2H), 7.49 (dt, *J* = 42.7, 7.7 Hz, 4H), 7.29 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.09 (td, *J* = 7.7, 1.6 Hz, 1H), 5.16 (t, *J* = 6.5 Hz, 1H), 4.25 (d, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.9, 134.4, 131.8, 131.7, 129.5, 128.6, 128.1, 126.7, 126.1,122.5, 46.5. GC-MS (EI) *m/z*: 325.



Formula: $C_{13}H_{12}INO_2S$

Mass:373

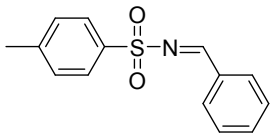
N-(3-iodobenzyl)benzenesulfonamide(**3s**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =5:1) to give **3s** as white solid(112.1mg, 69%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.4 Hz, 2H), 7.62 – 7.47 (m, 5H), 7.17 (d, *J* = 7.2 Hz, 1H), 6.99 (t, *J* = 7.7 Hz, 1H), 5.04 (t, *J* = 6.0 Hz, 1H), 4.15– 4.04 (d, *J* = 3.5 Hz, 2H).^{13}C NMR (126 MHz, Chloroform-*d*) δ 138.8, 137.6, 136.0, 135.8, 132.3, 131.9, 129.4, 128.3, 126.1, 93.5, 45.5. GC-MS (EI) *m/z*: 373.



Formula: $C_{13}H_{11}NO_2S$

Mass:245

N-benzylidenebenzenesulfonamide(**4a**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =15:1) to give **4a** as white solid (88.2mg, 72%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.07 (s, 1H), 8.04 – 7.94 (m, 4H), 7.66 – 7.61 (m, 2H), 7.57 (d, *J* = 7.7 Hz, 2H), 7.52 – 7.48 (m, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.8, 135.1, 133.7, 132.8, 132.4, 131.5, 129.3, 128.2, 126.5. GC-MS (EI) *m/z*: 245.

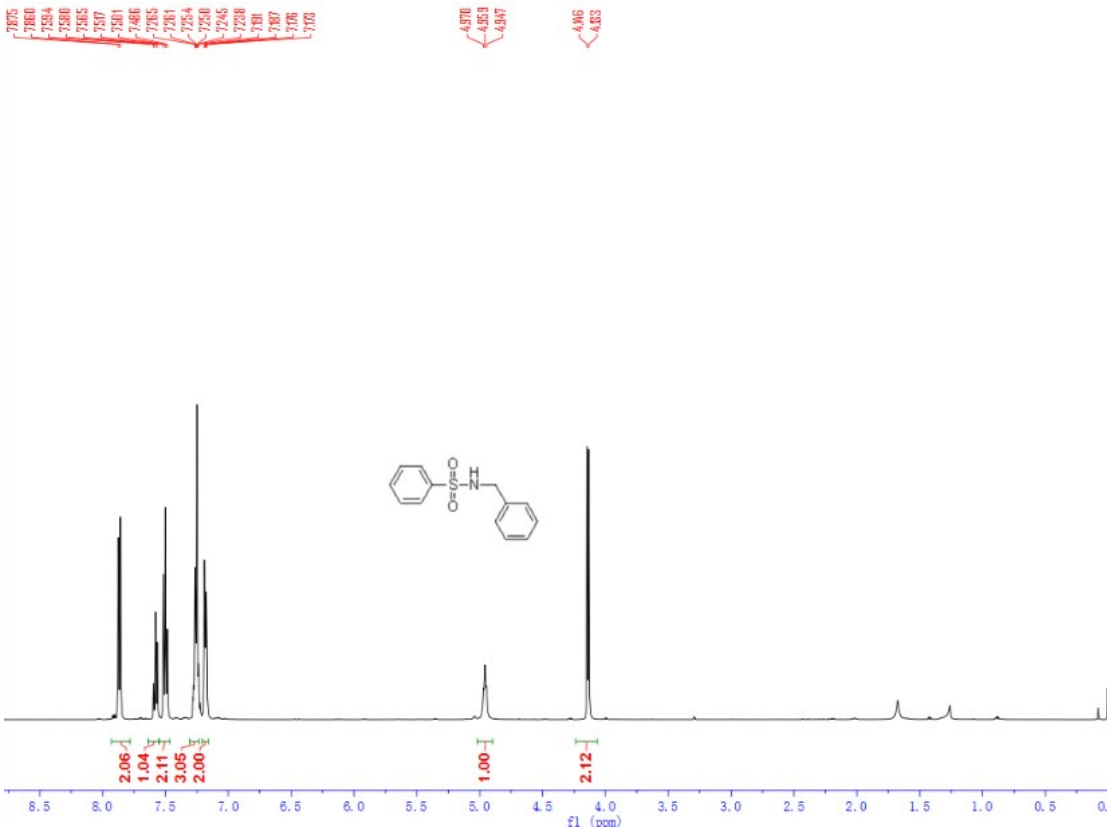


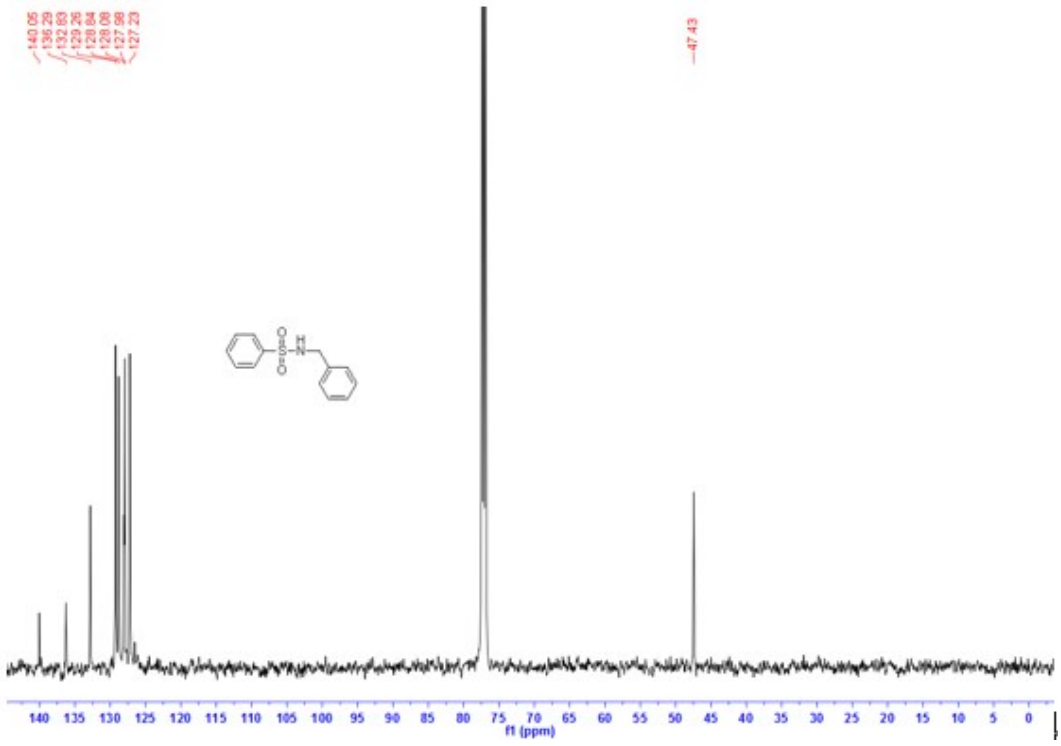
Formula: $C_{14}H_{13}NO_2S$

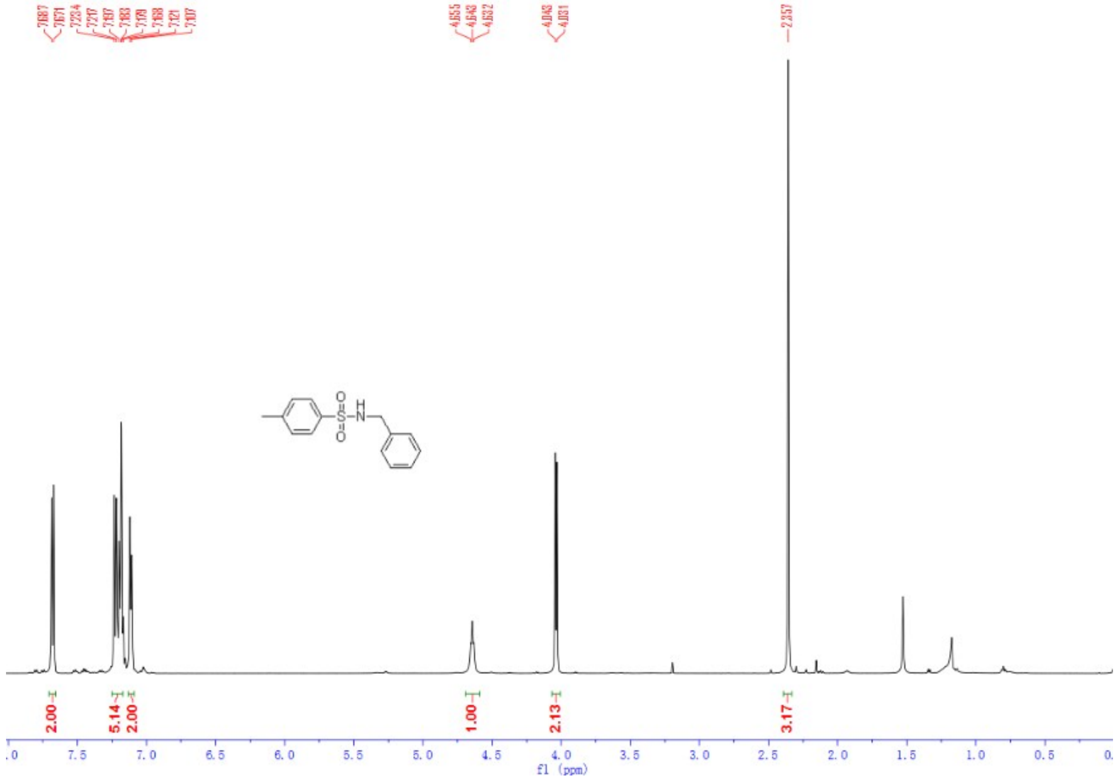
Mass:259

N-benzylidene-4-methylbenzenesulfonamide(**4b**): The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =15:1) to give **4b** as white solid (77.7mg, 60%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.32 (s, 1H), 7.99 – 7.94 (m, 3H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.53 – 7.41 (m, 3H), 7.24 – 7.20 (m, 2H), 2.56 (s, 3H).^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.1, 143.6, 134.2, 134.0 , 130.3 , 128.8 , 128.2 , 127.6 , 127.1, 20.6. GC-MS (EI) *m/z*: 259.

4. NMR spectra



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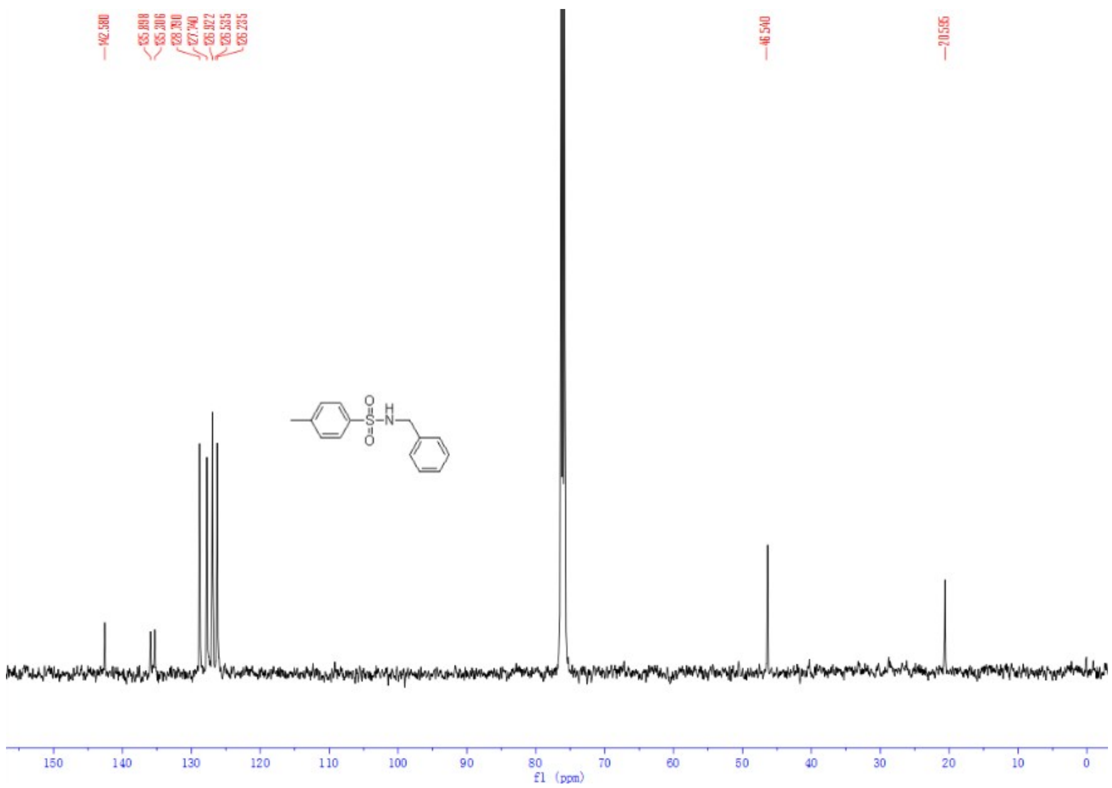
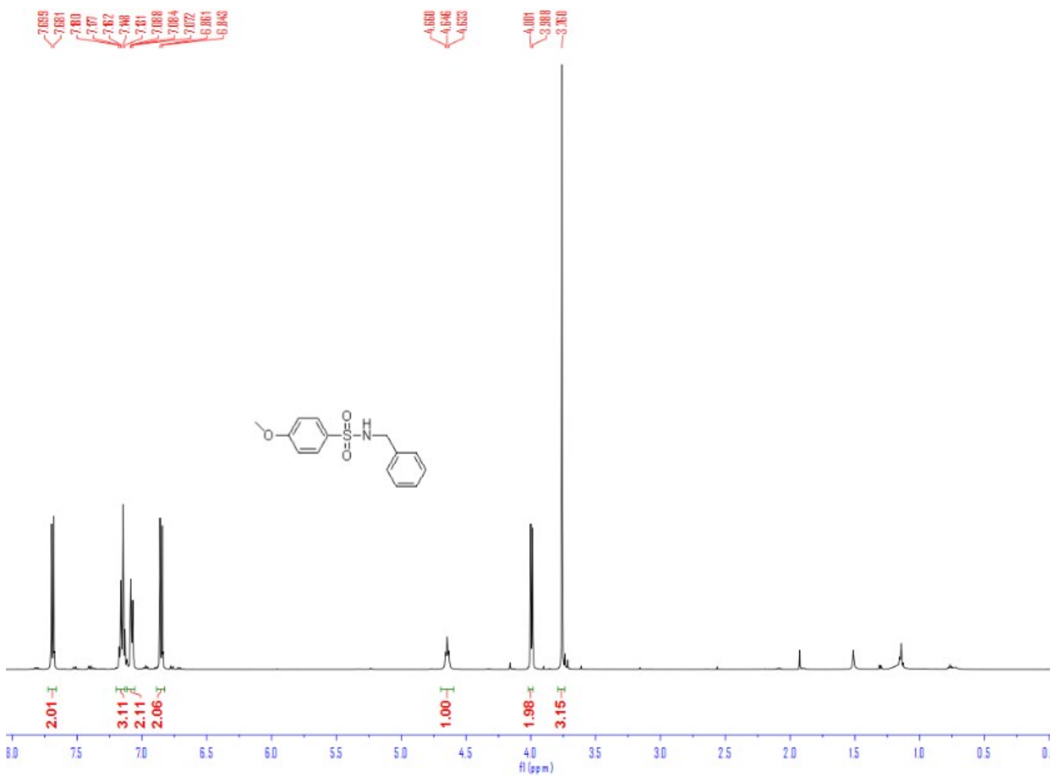
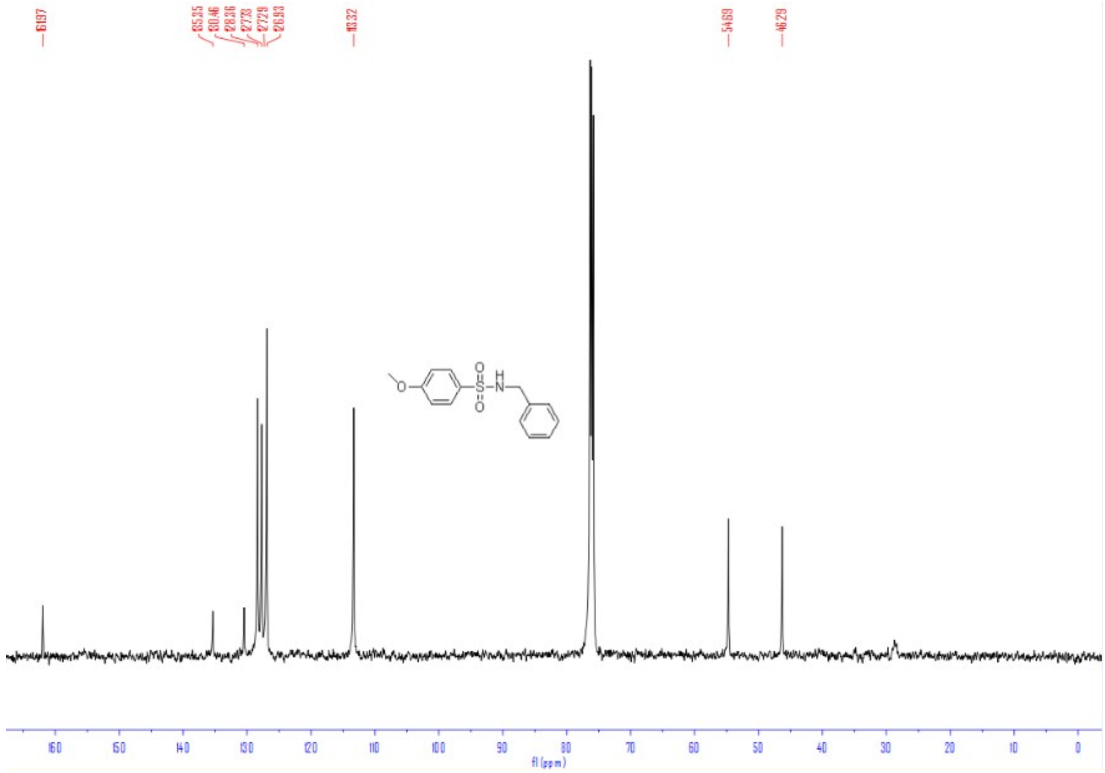
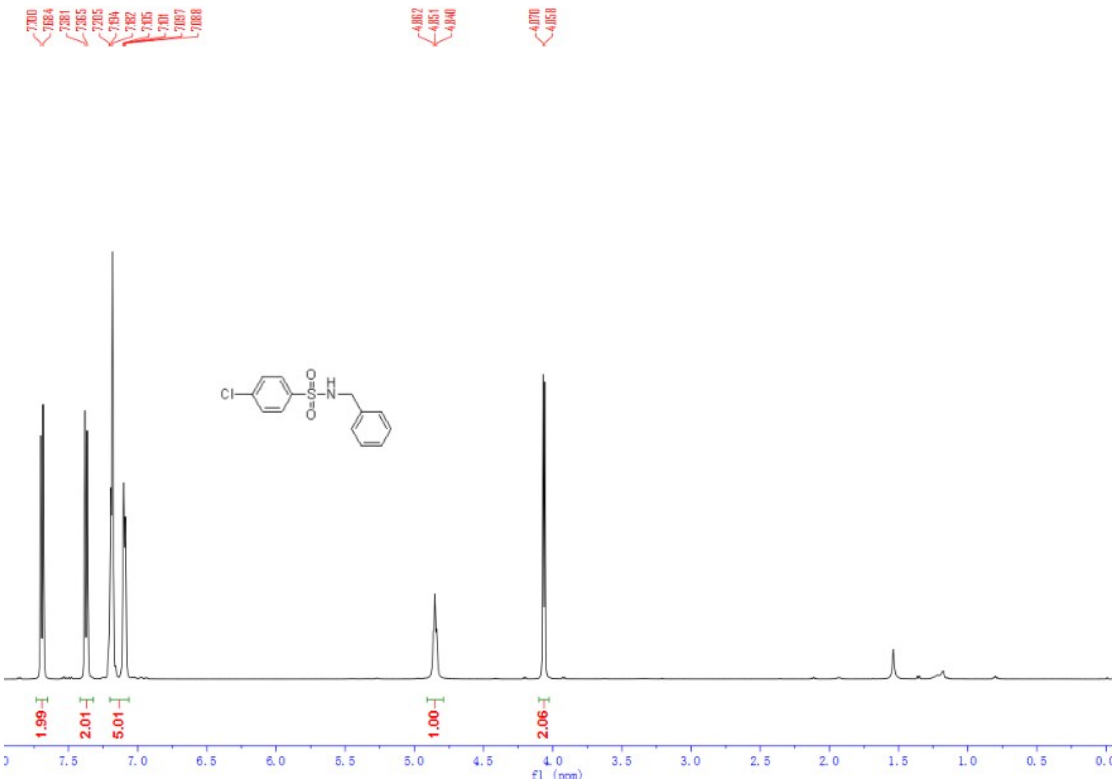
2.00
5.14
2.00
1.00
2.13
3.17
f1 (ppm)


142.580
46.540
20.595
f1 (ppm)



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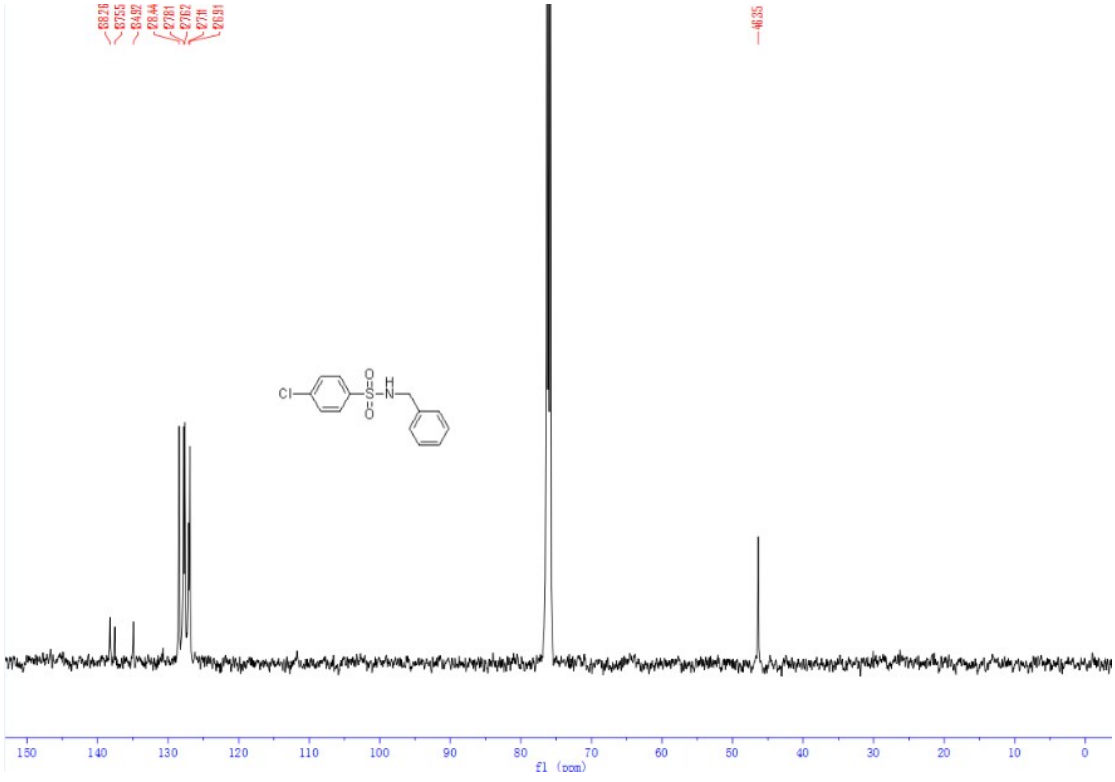
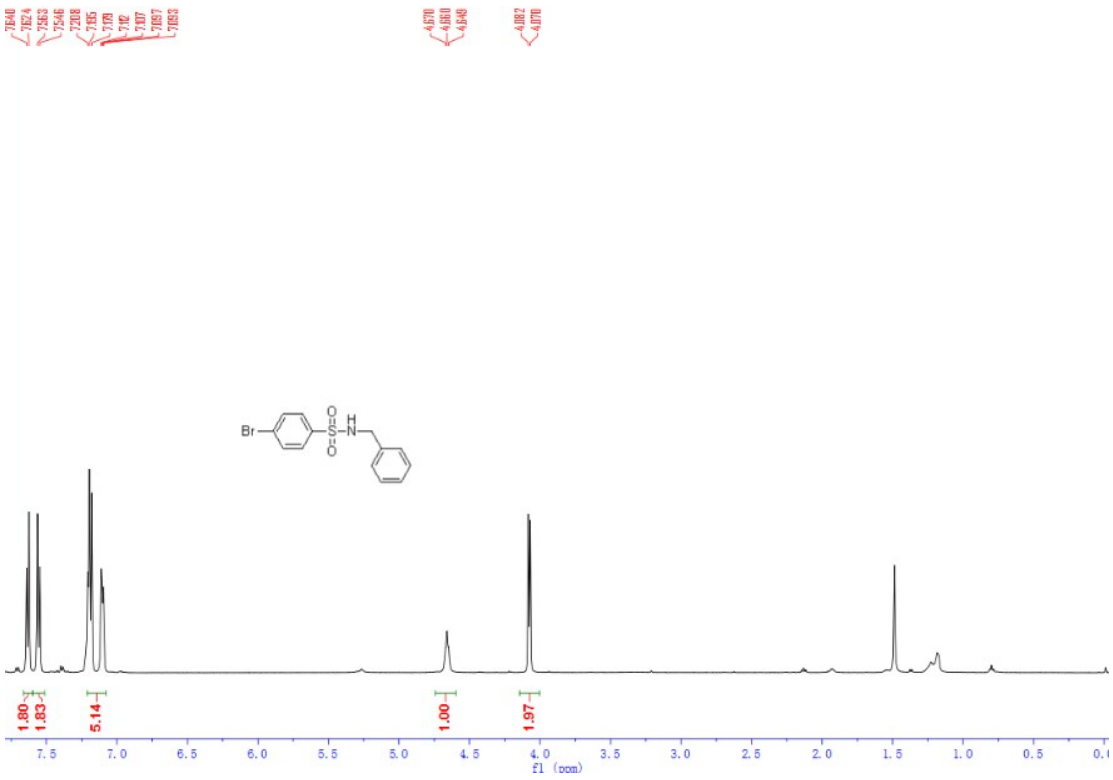
7.281
7.265
7.205
7.194
7.182
7.165
7.101
7.097
7.088
4.062
4.053
4.040
4.070
4.058
Cl
1.99
2.01
5.01
1.00
2.06
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


138.26
137.55
134.92
129.44
127.81
127.62
127.11
126.91
46.35
Cl
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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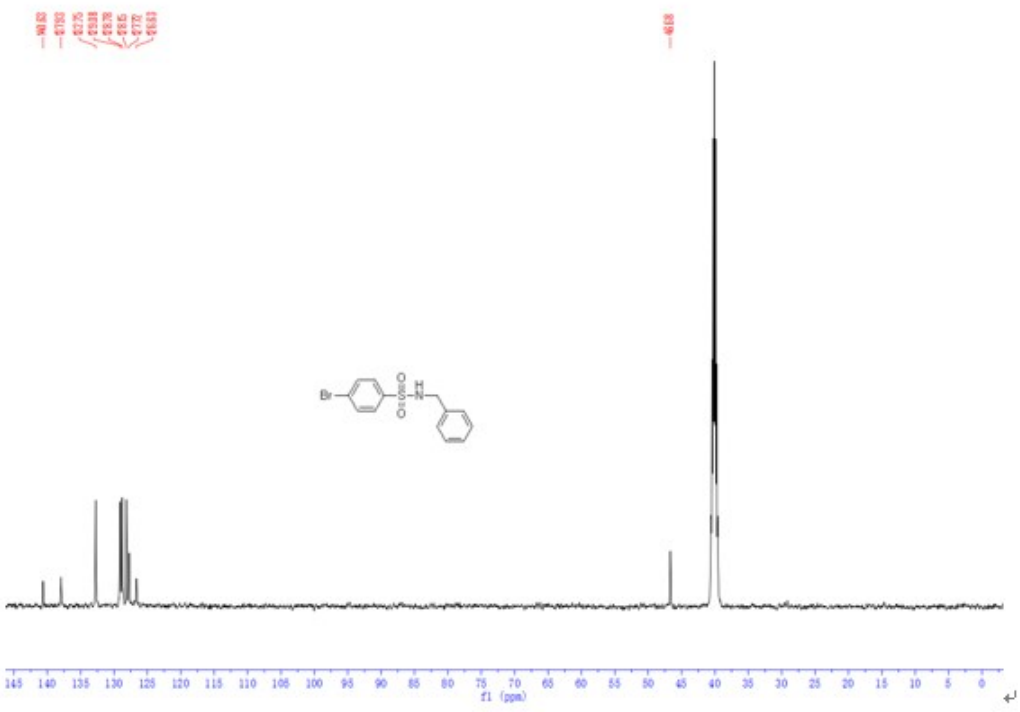
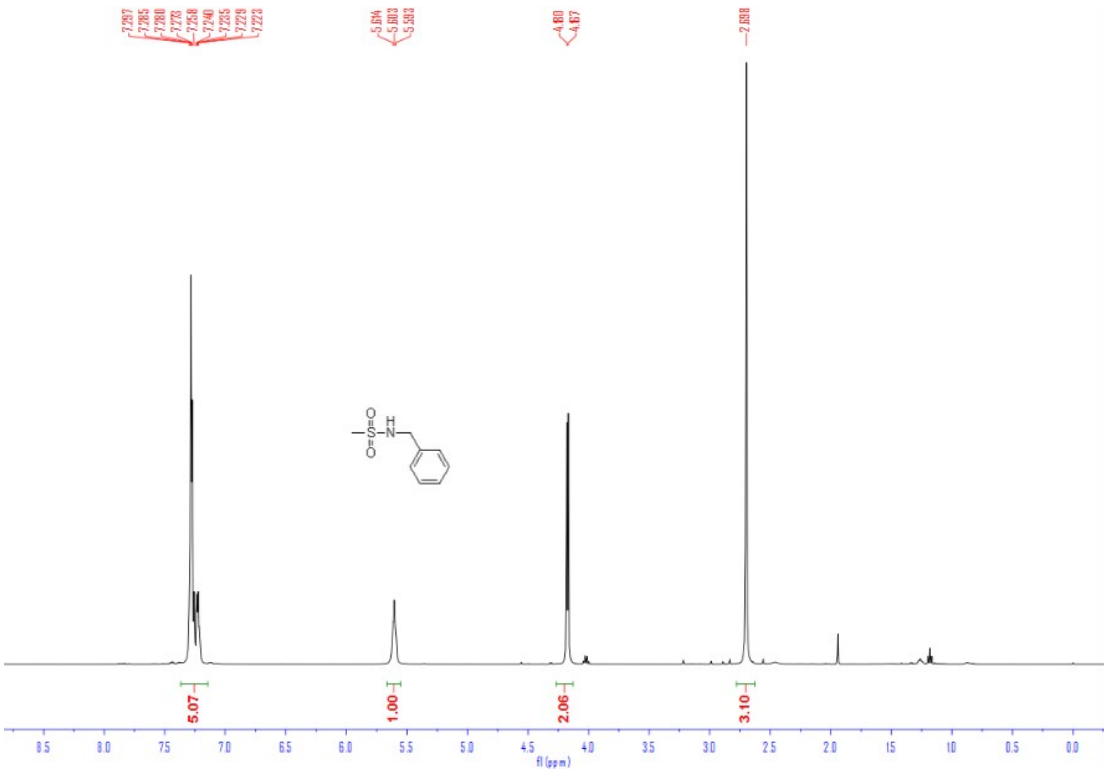
5.14
1.00
1.97
f1 (ppm)


Br
f1 (ppm)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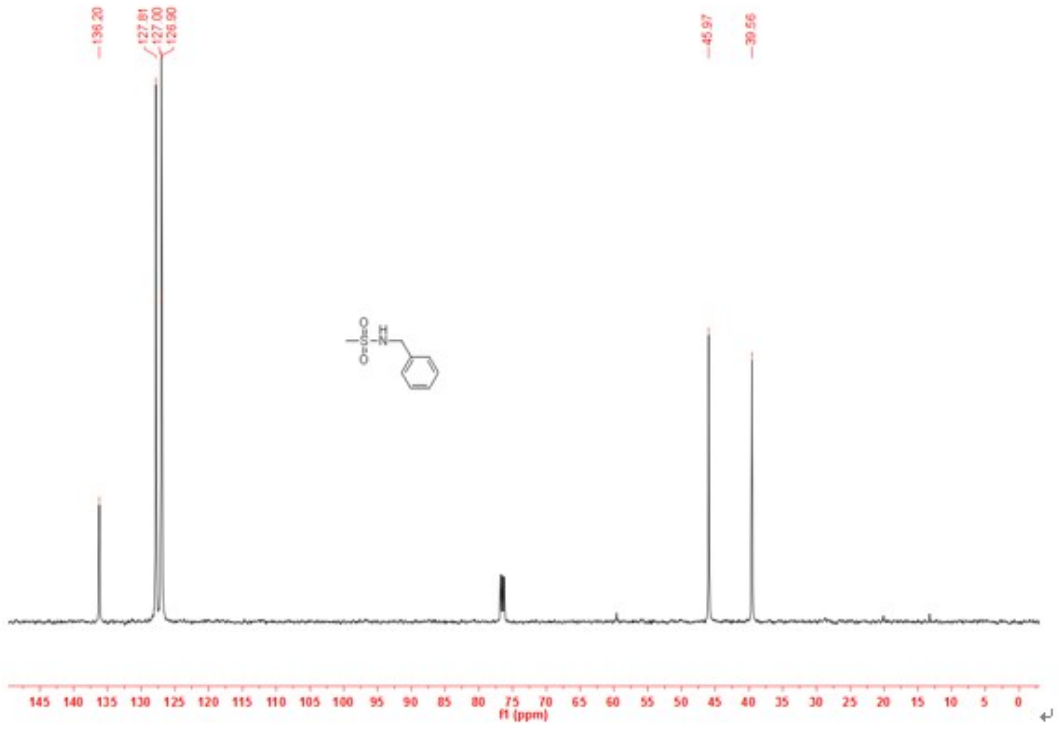
7.285
7.280
7.278
7.258
7.240
7.225
7.220
7.223
5.594
5.593
5.593
4.681
4.667
2.888
5.07
1.00
2.06
3.10
f1 (ppm)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127.00
126.90
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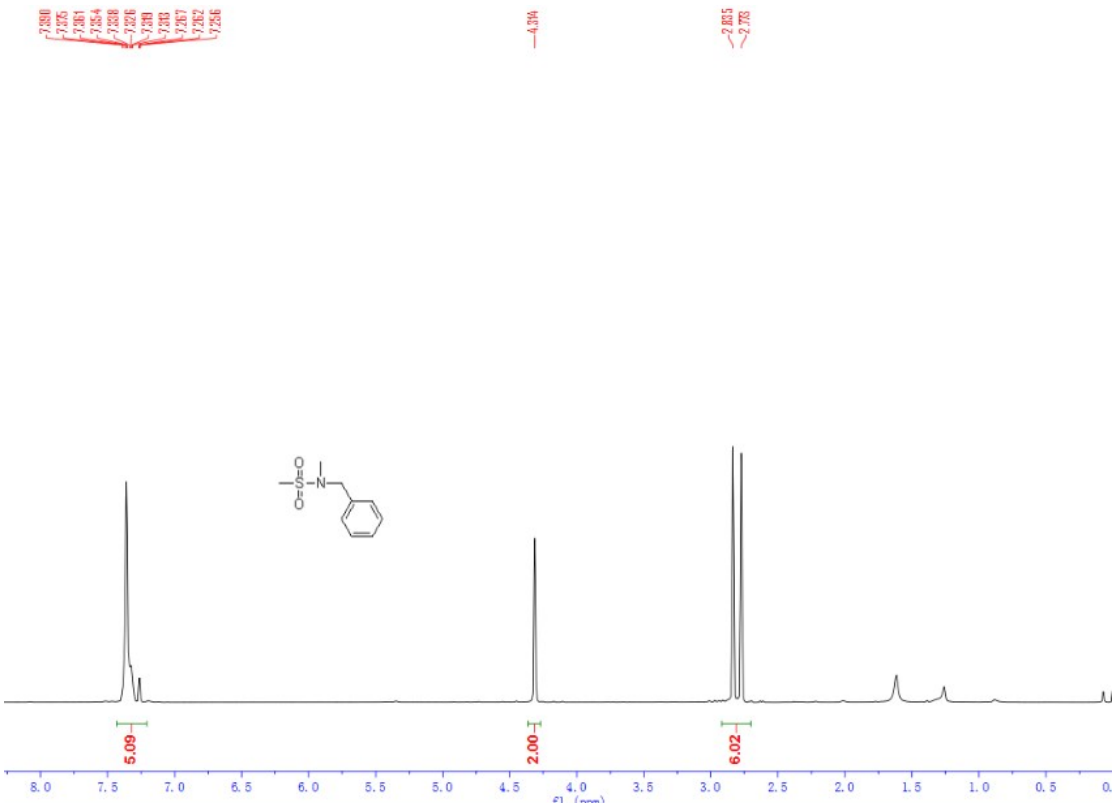
39.56
f1 (ppm)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7.361
7.354
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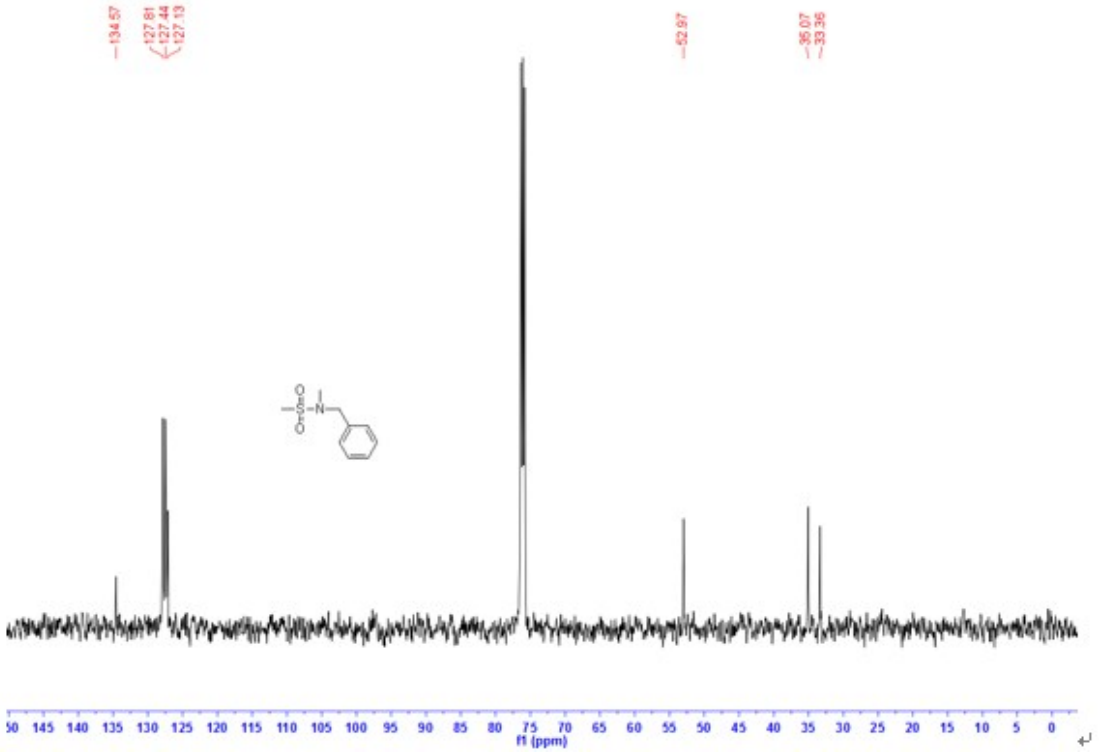
7.326
7.319
7.313
7.267
7.262
7.256
4.314
2.805
2.793
5.09
2.00
6.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5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127.81
127.44
127.13
52.97
35.07
33.36
50
145
140
135
130
125
120
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105
100
95
90
85
80
75
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65
60
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50
45
40
35
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25
20
15
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5
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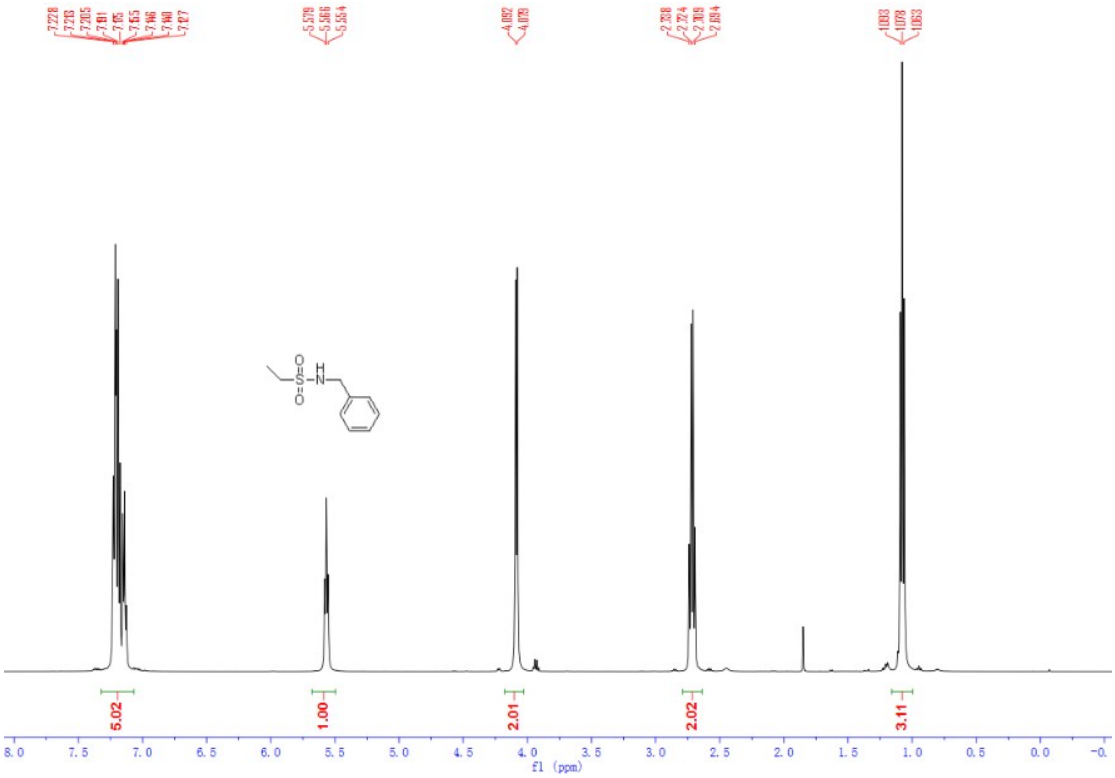
f1 (ppm)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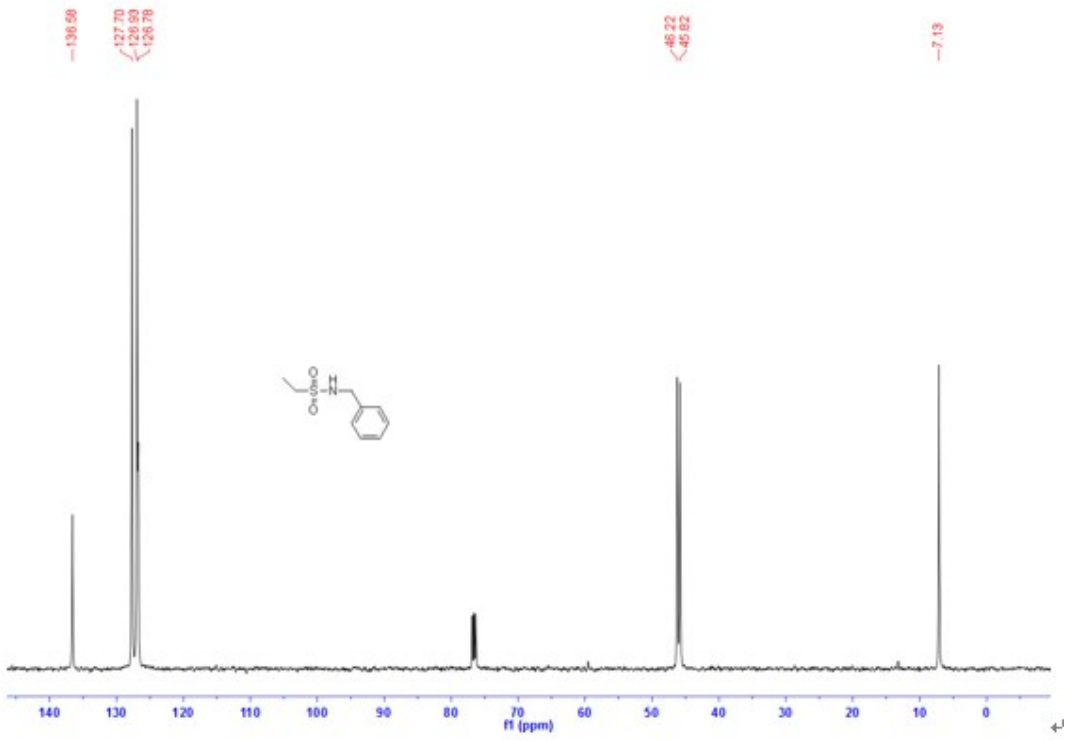
7.205
7.191
7.165
7.155
7.146
7.140
7.127
5.578
5.566
5.554
4.082
4.078
2.338
2.274
2.209
2.184
1.083
1.079
1.063
5.02
1.00
2.01
2.02
3.11
f1 (ppm)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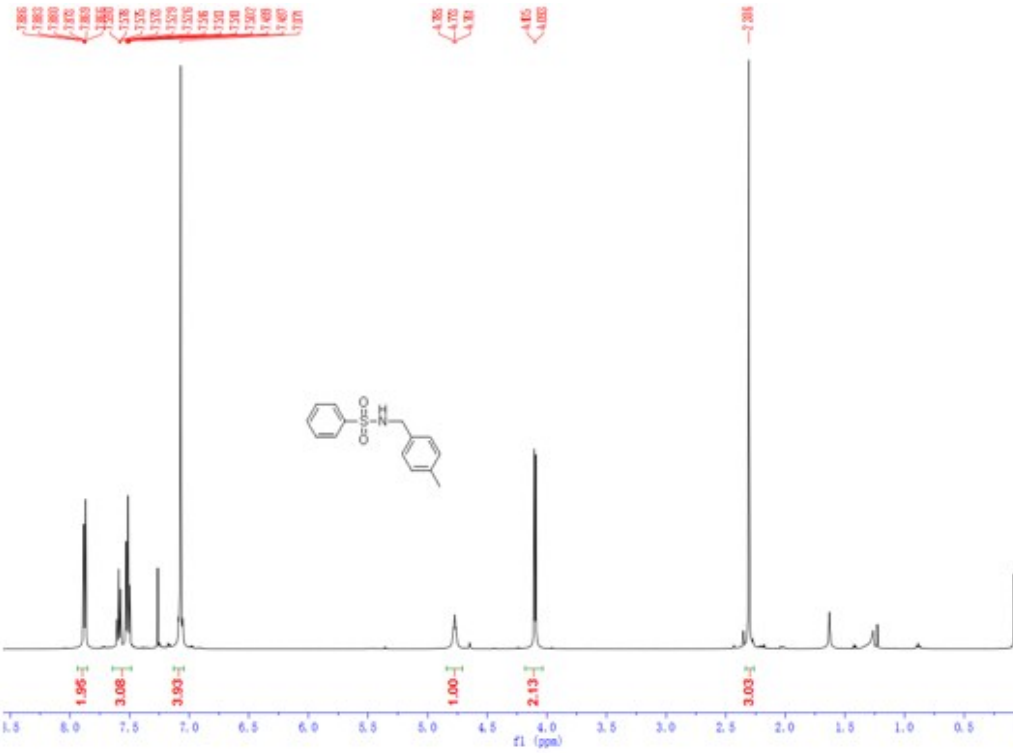
126.69
126.78
46.22
45.82
7.13
f1 (ppm)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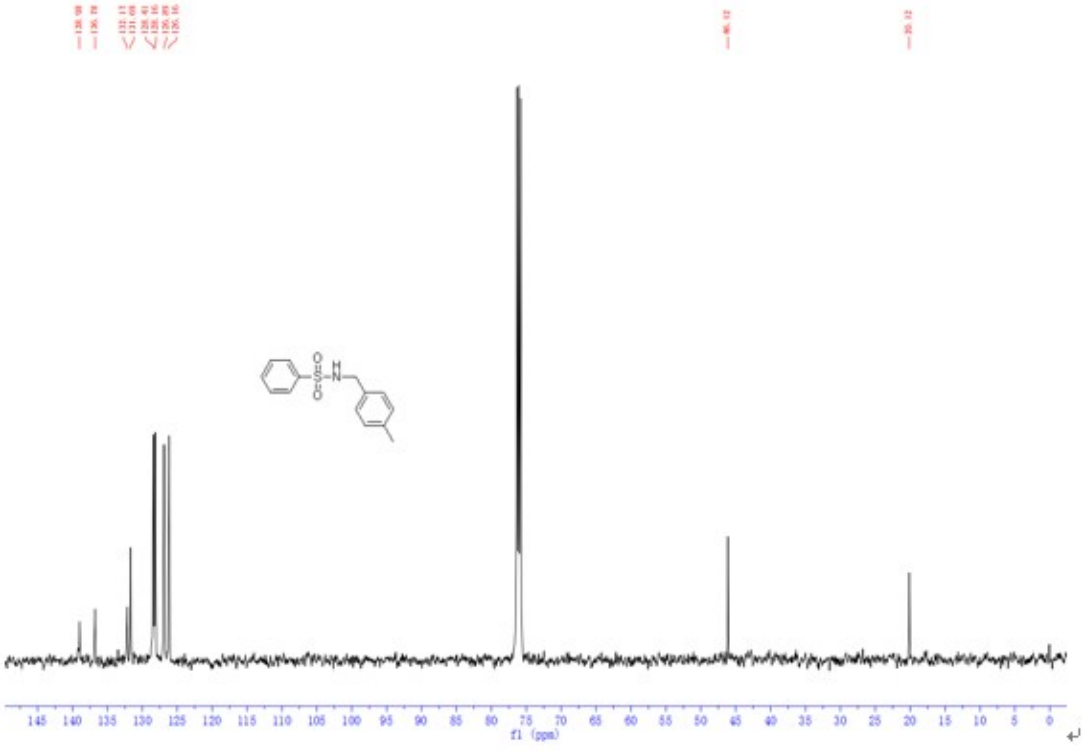
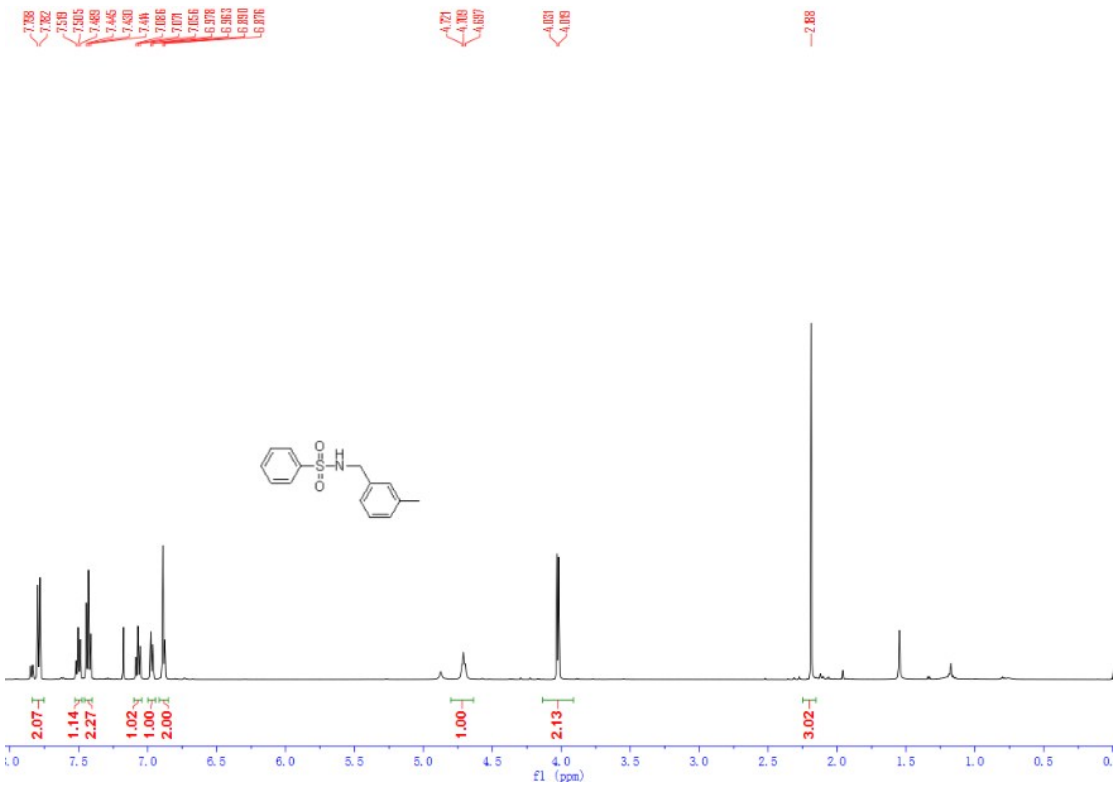
3.93
1.00
2.13
3.03
f1 (ppm)


f1 (ppm)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7.469
7.445
7.430
7.414
7.066
7.061
7.056
6.978
6.963
6.950
6.876
4.721
4.709
4.697
4.031
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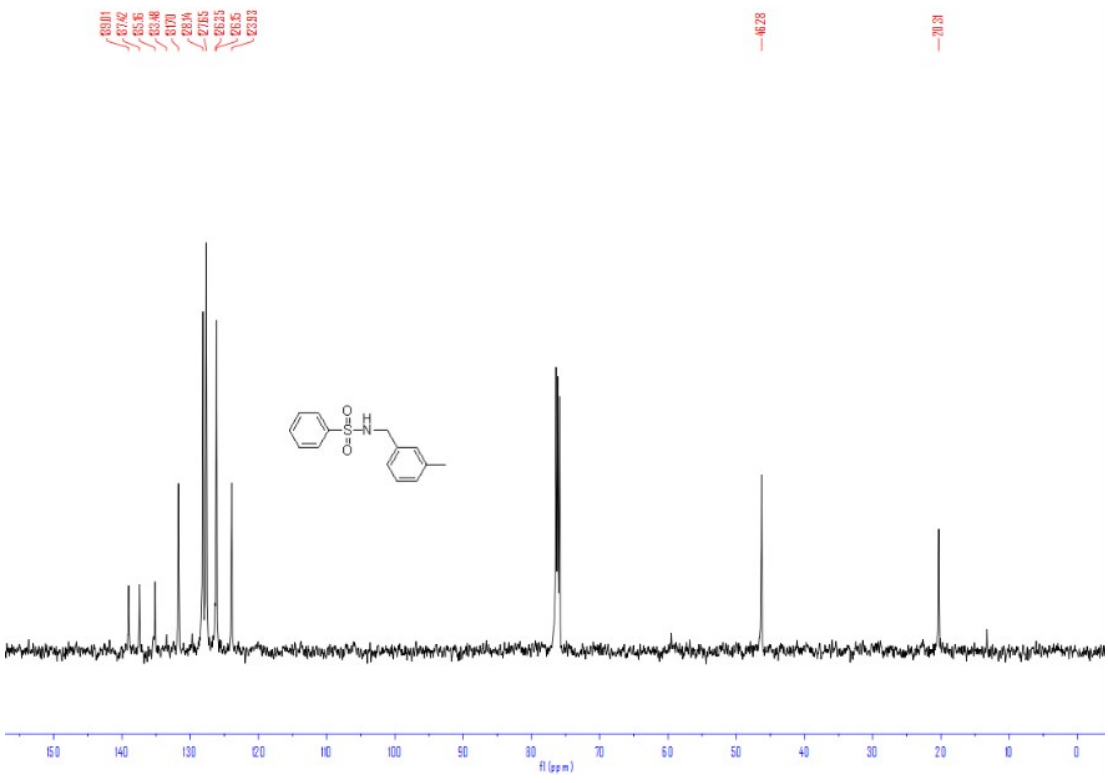
1.02
1.00
2.00
1.00
2.13
3.02
f1 (ppm)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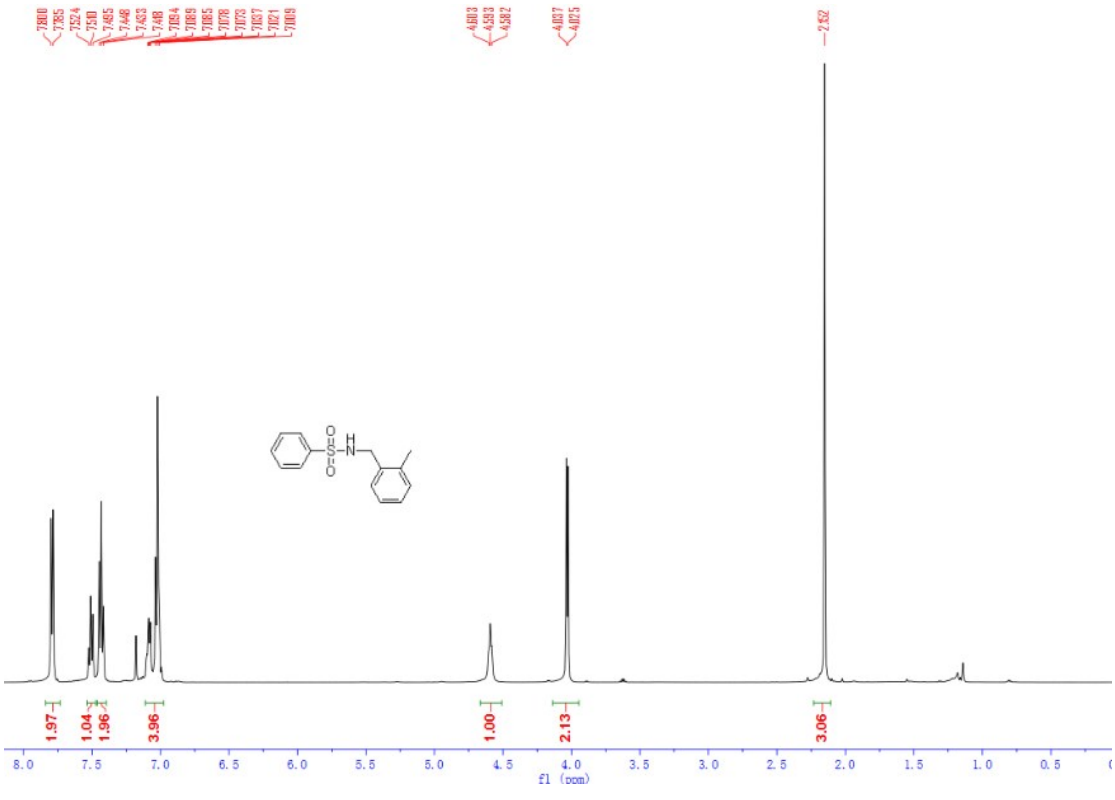
135.35
133.48
131.70
128.34
127.65
126.25
126.15
123.83
46.28
20.31
f1 (ppm)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7.448
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7.418
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7.069
7.065
7.078
7.073
7.037
7.021
7.009
4.593
4.583
4.582
4.037
4.025
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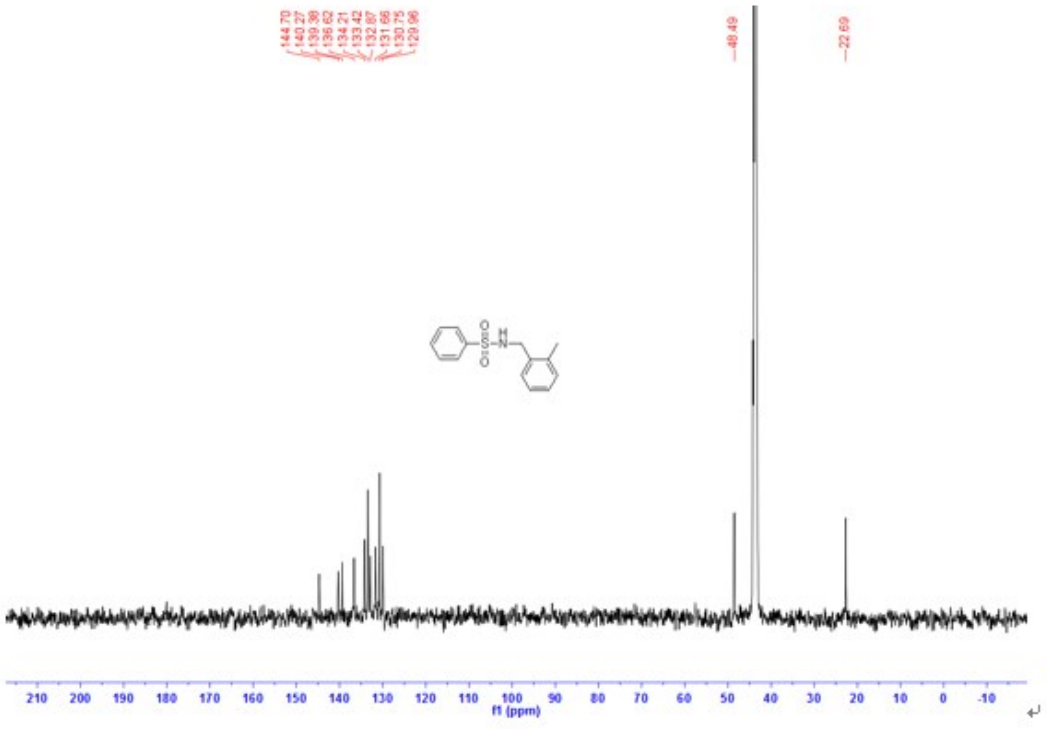
1.04
1.96
3.96
1.00
2.13
3.06
f1 (ppm)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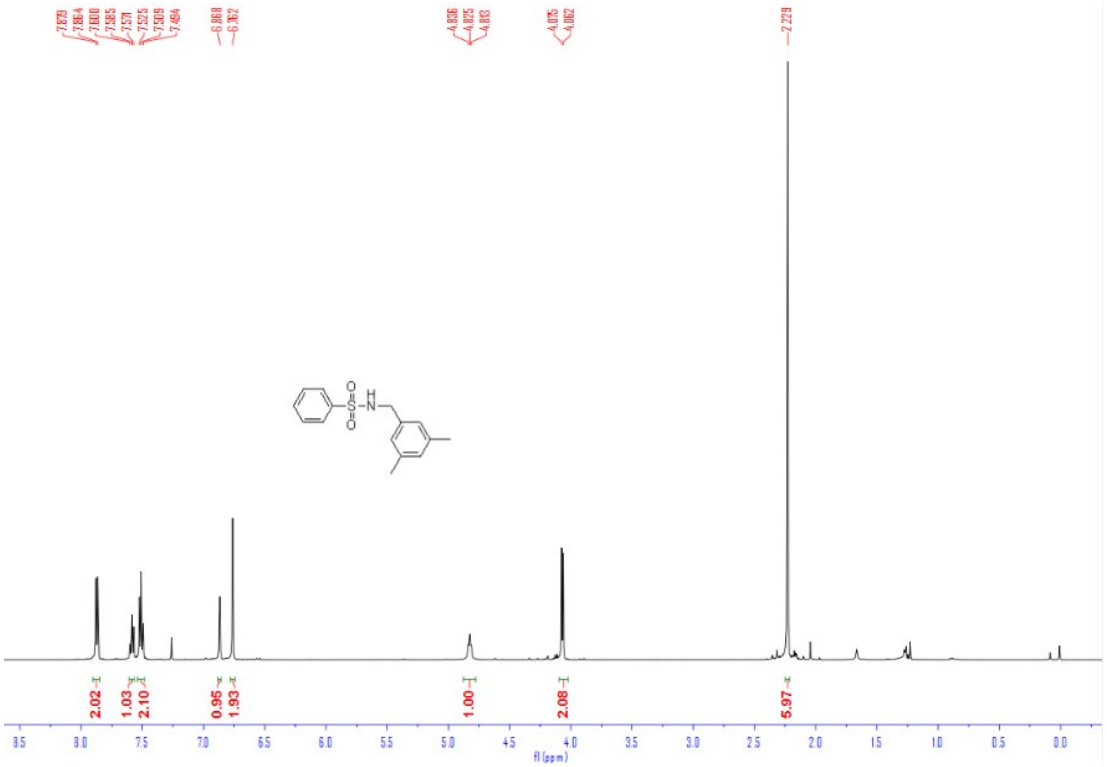
22.69
f1 (ppm)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6.852
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4.825
4.813
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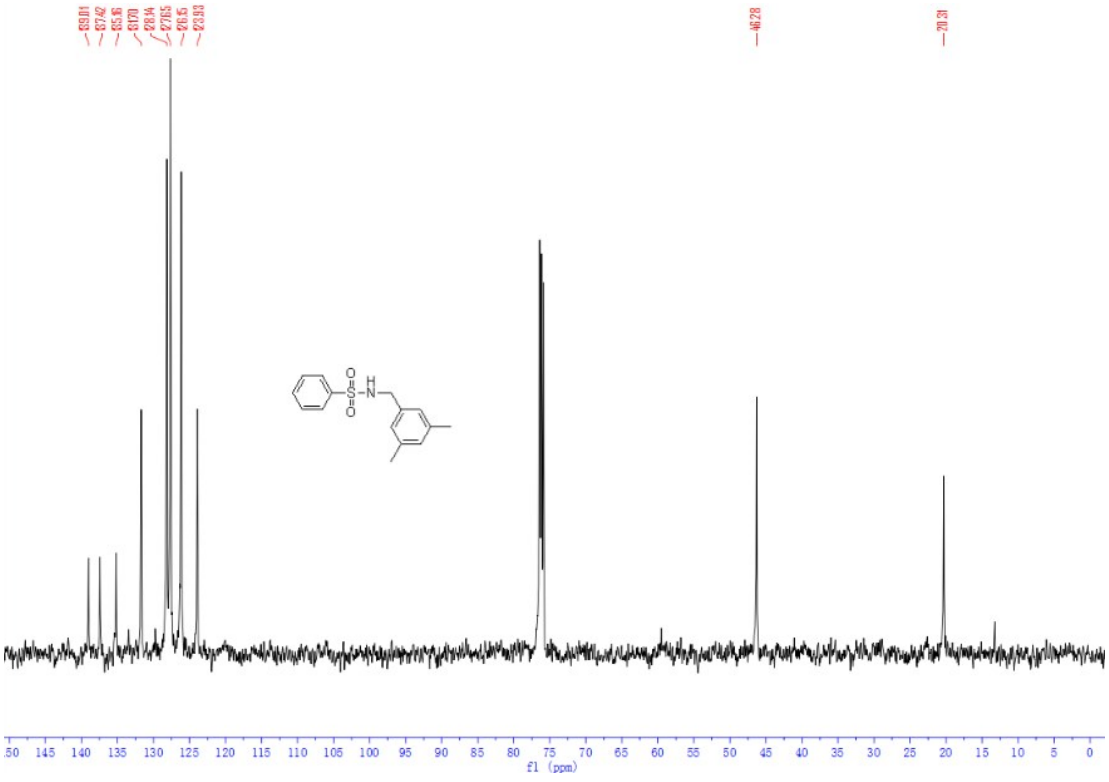
5.97
f1 (ppm)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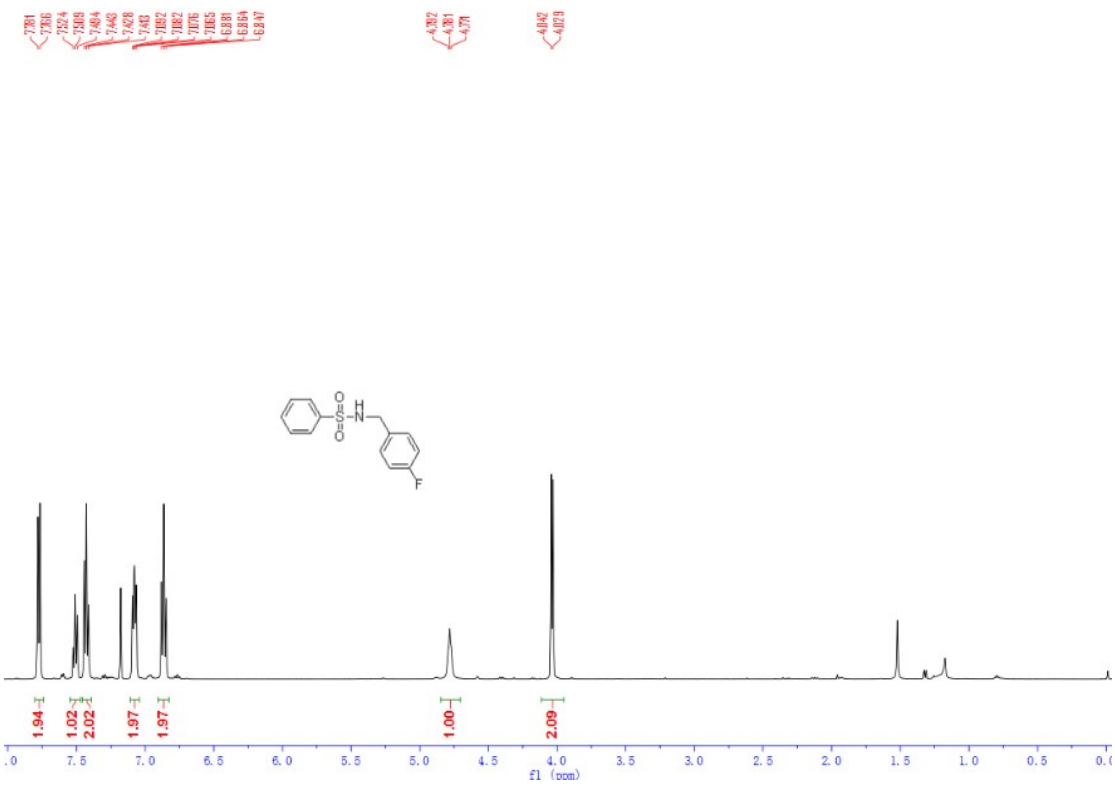
20.31
f1 (ppm)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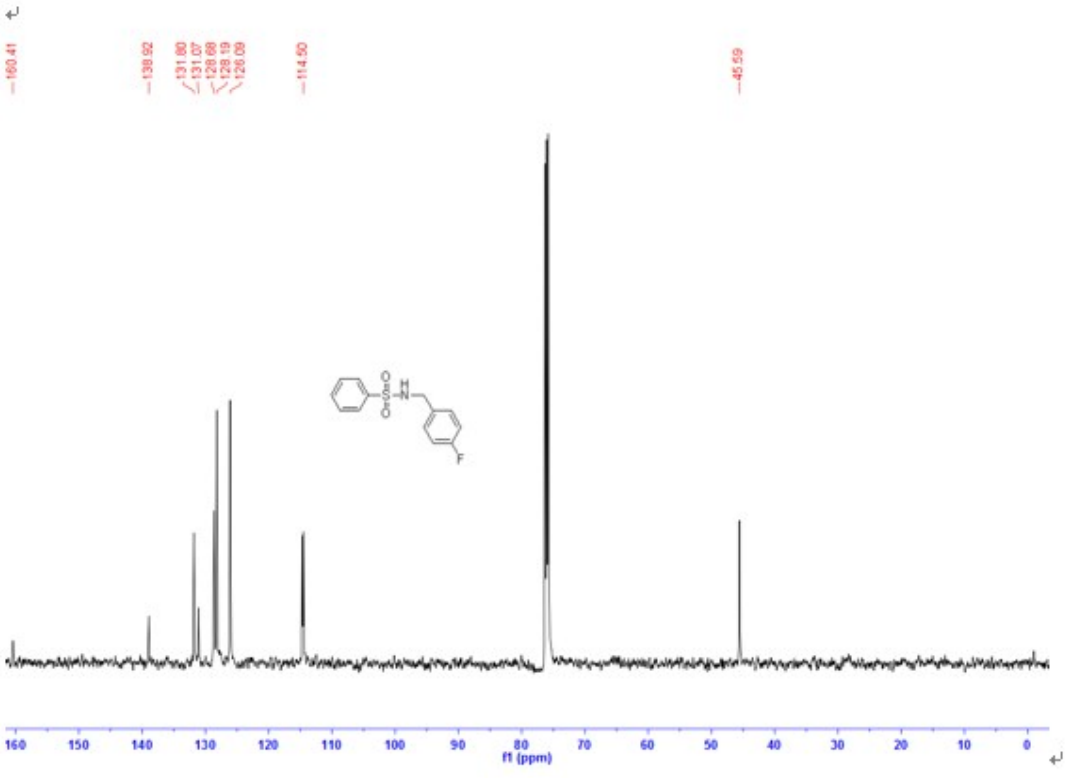
f1 (ppm)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128.19
126.09
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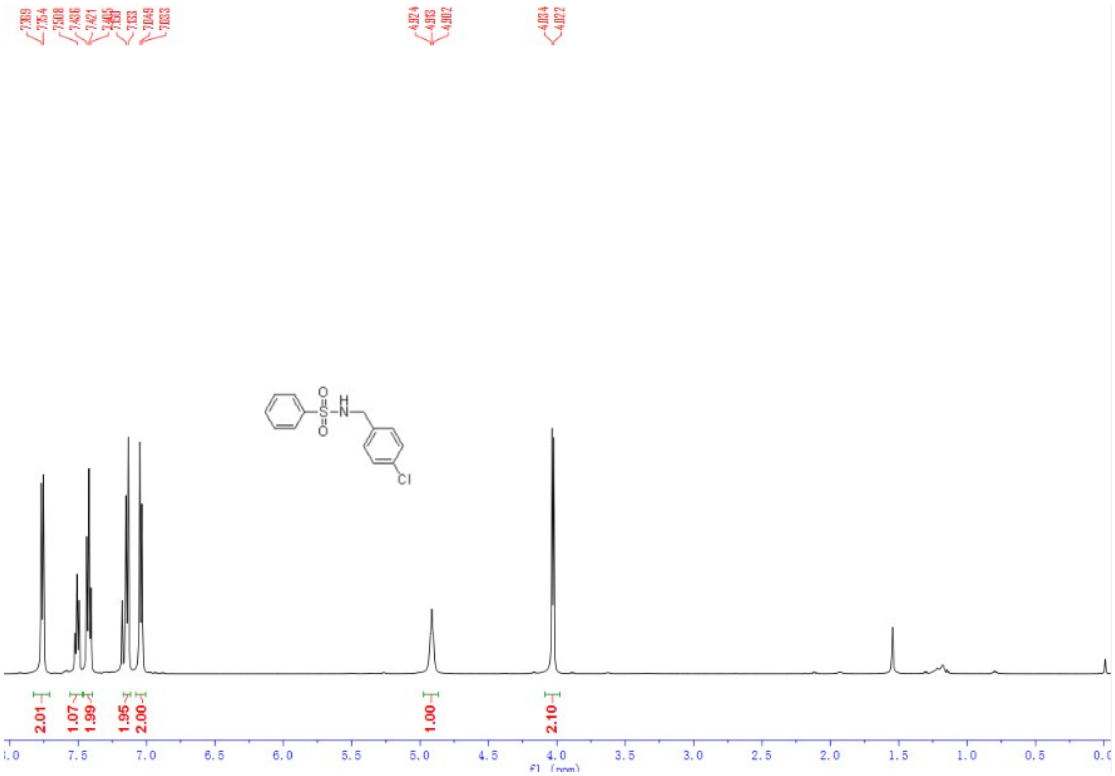
45.59
f1 (ppm)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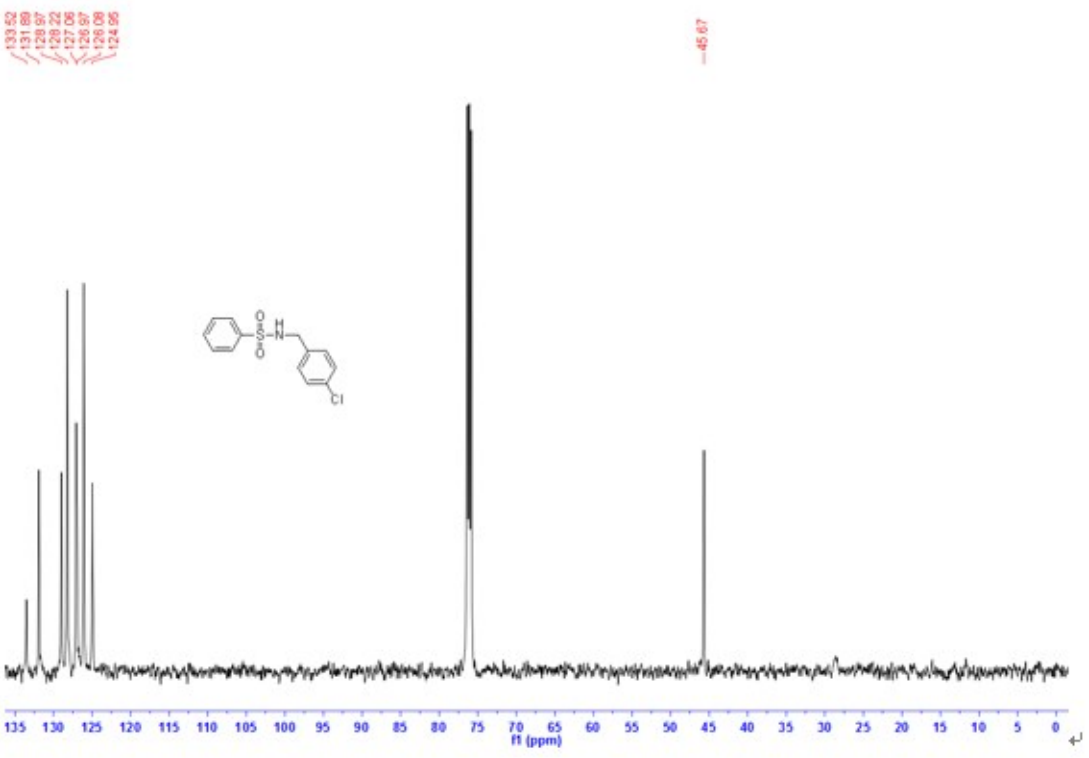
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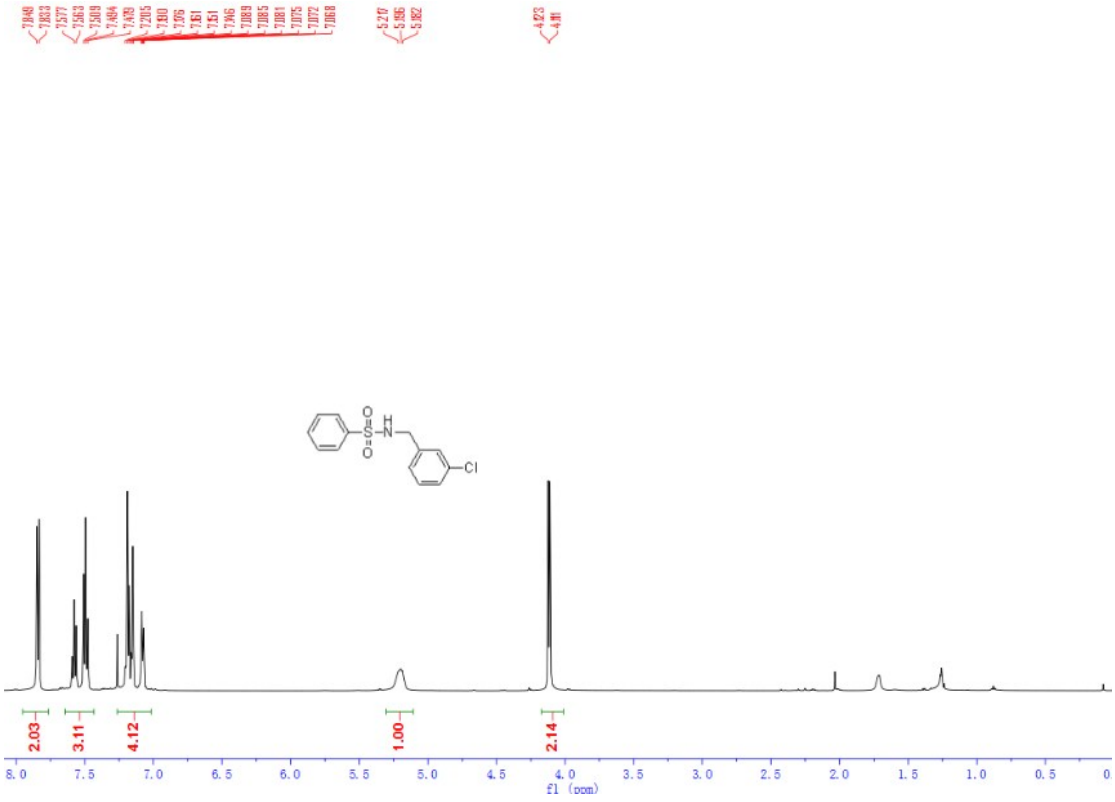
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7.7081
7.7075
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4.12
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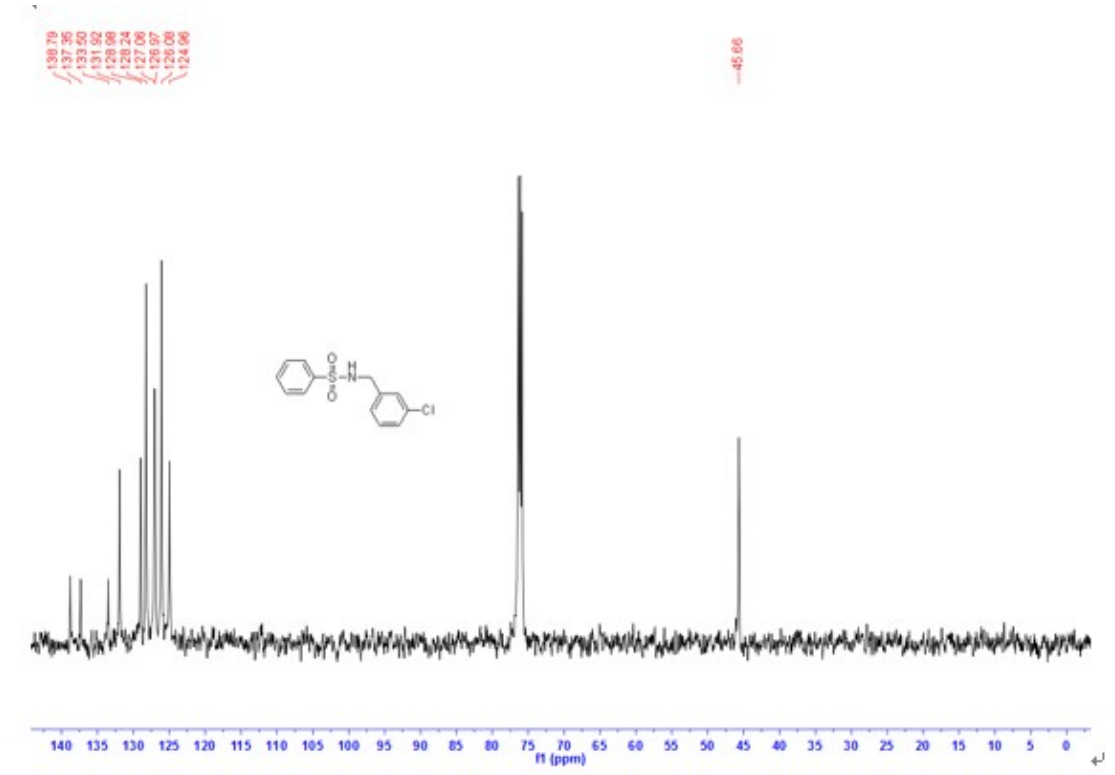
2.14
f1 (ppm)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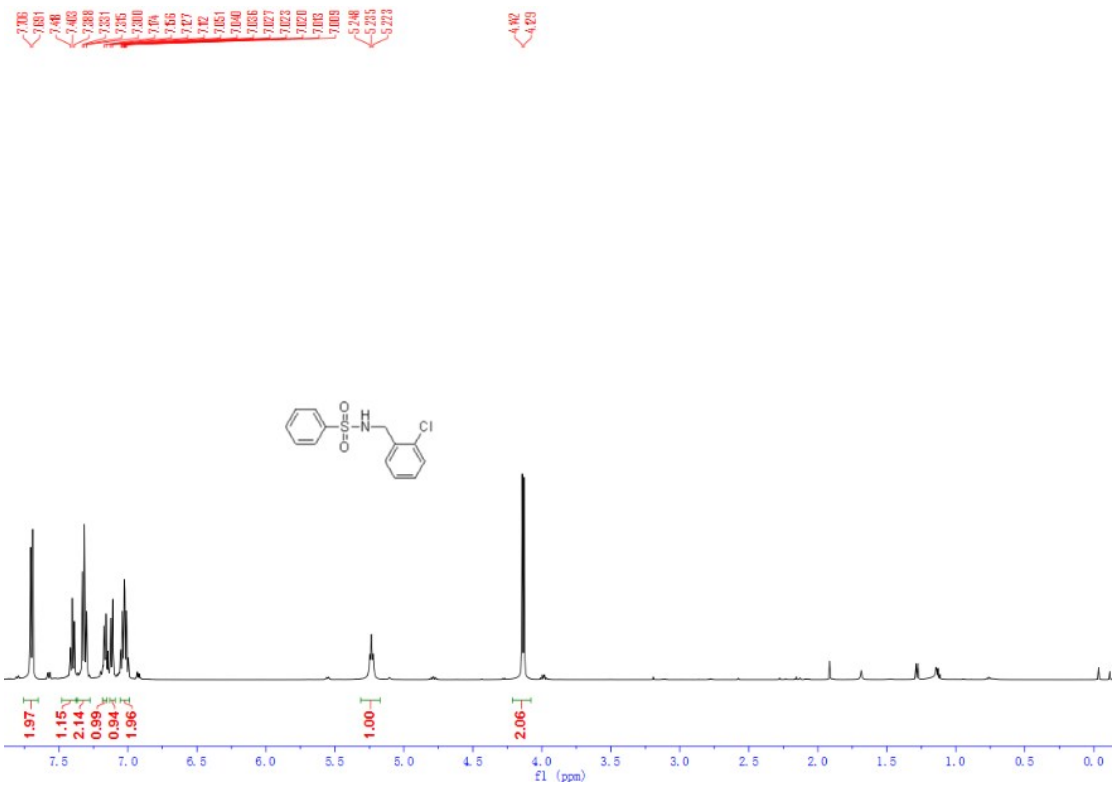
124.96
45.66
Cl
f1 (ppm)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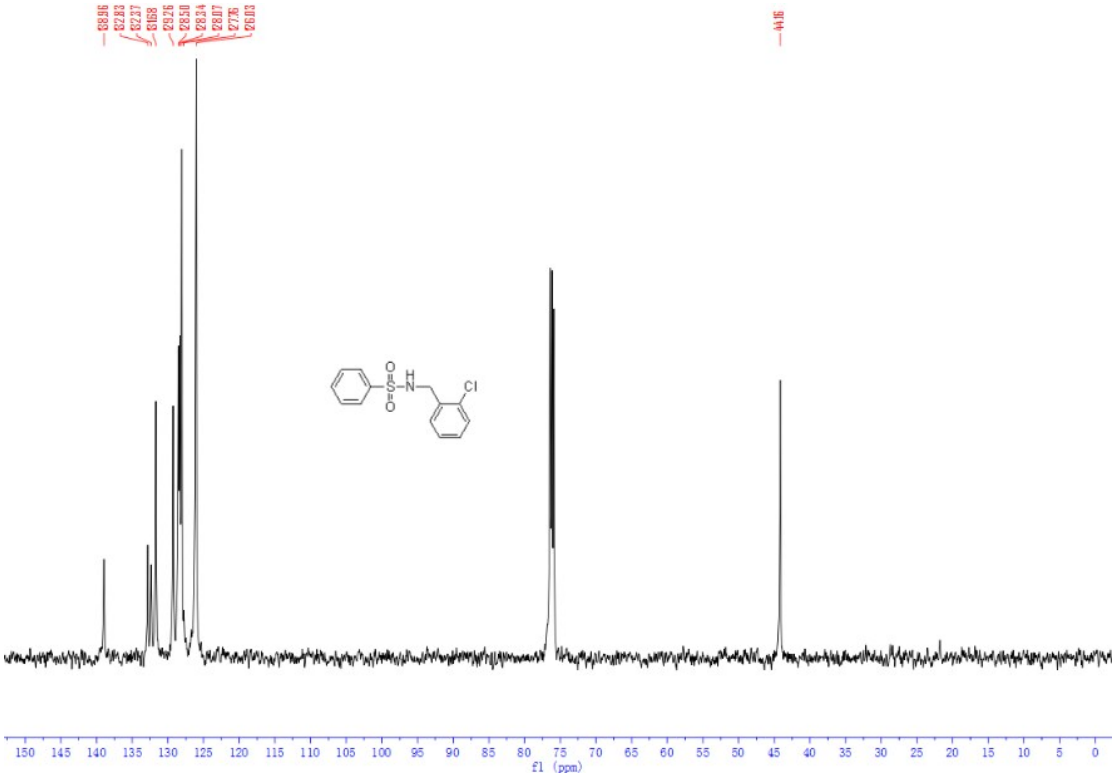
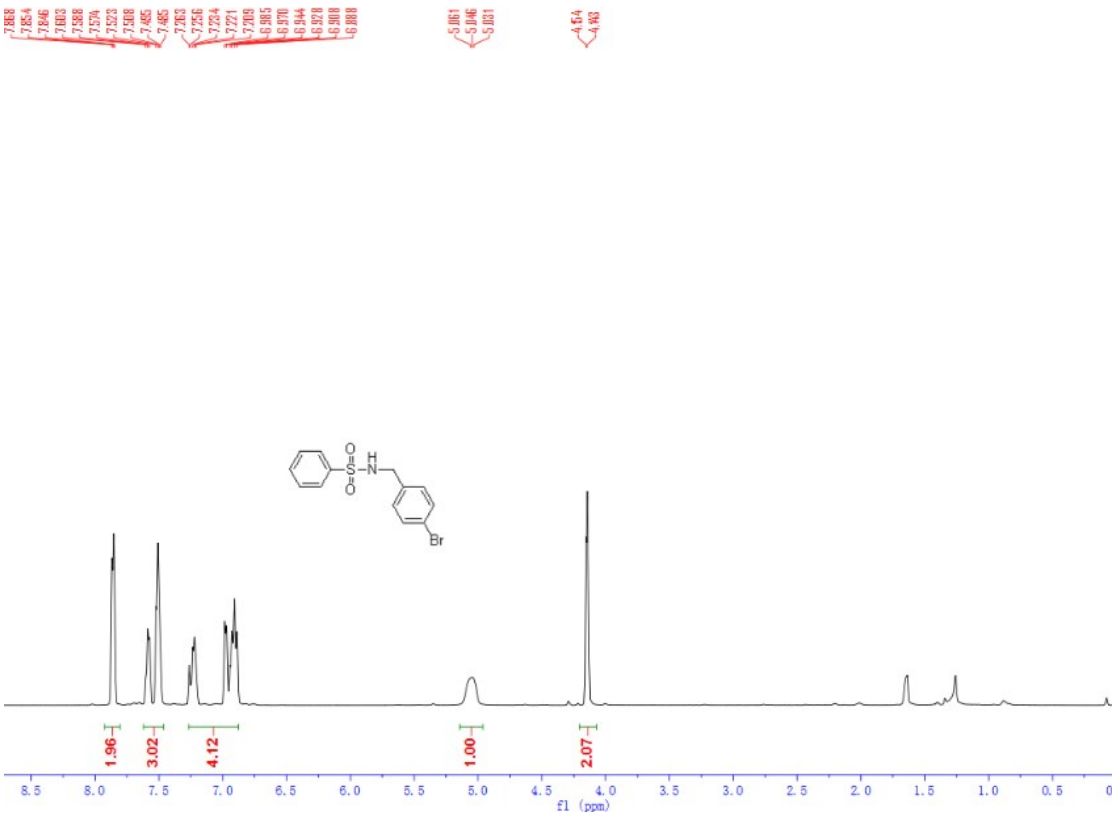
0.94
1.96
1.00
2.06
f1 (ppm)


f1 (ppm)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7.209
6.985
6.970
6.944
6.928
6.908
6.888
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Br
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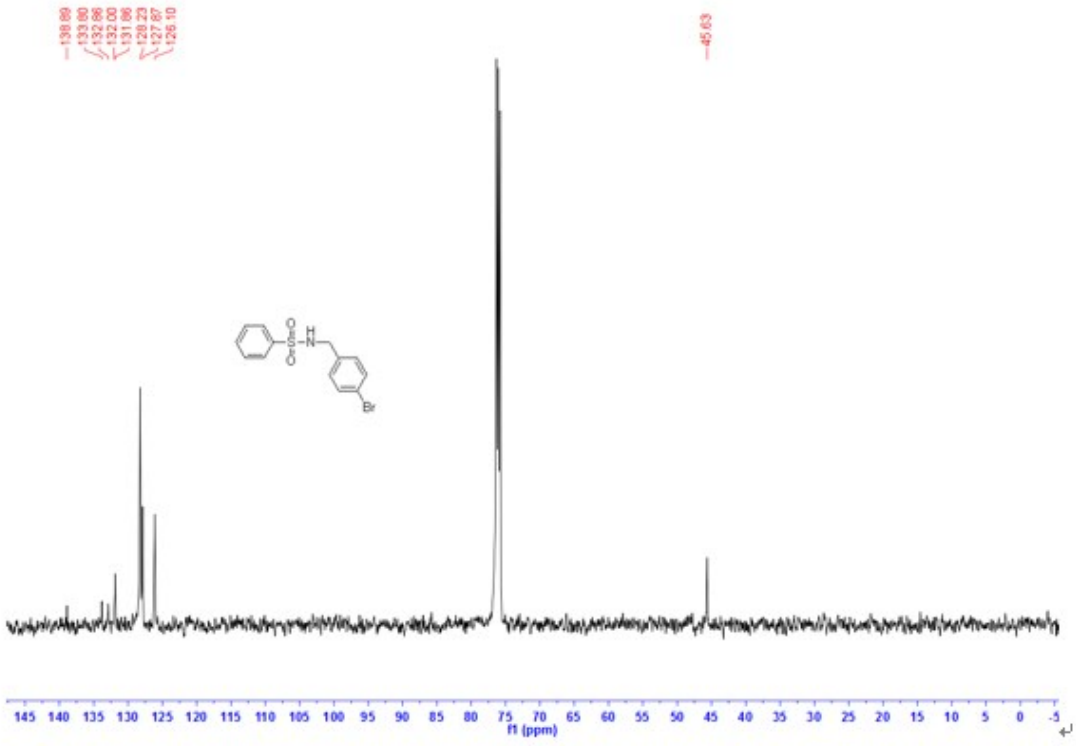
f1 (ppm)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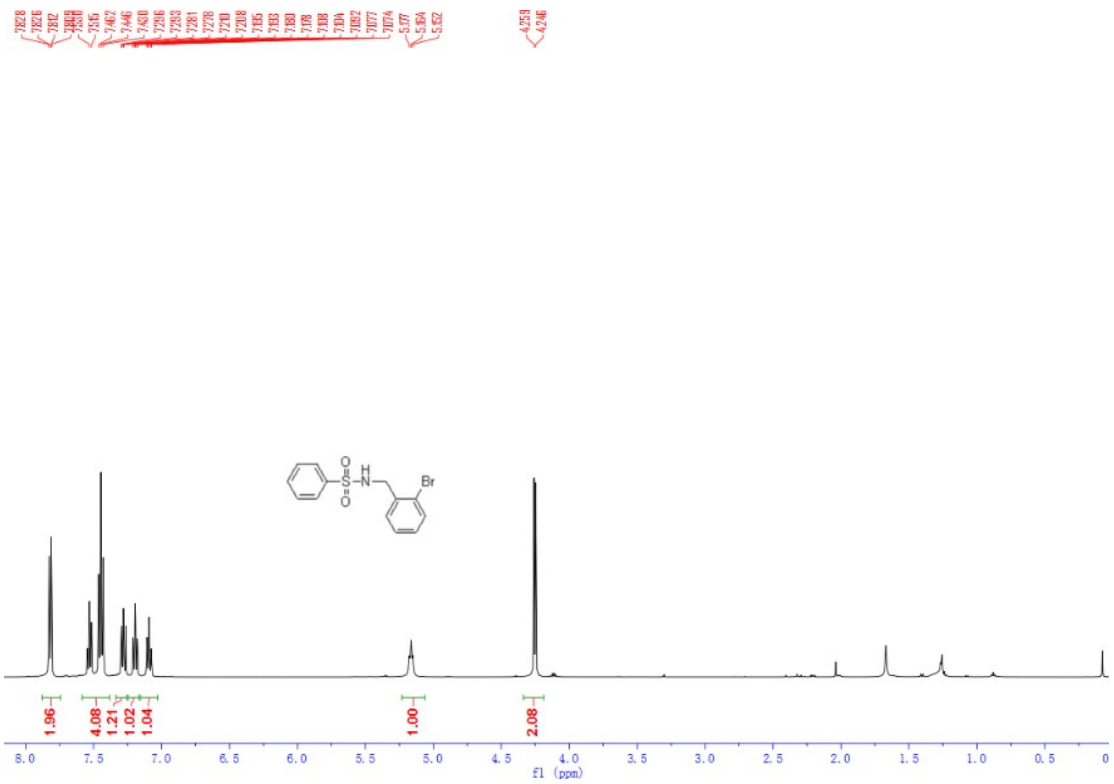
45.63
Br
f1 (ppm)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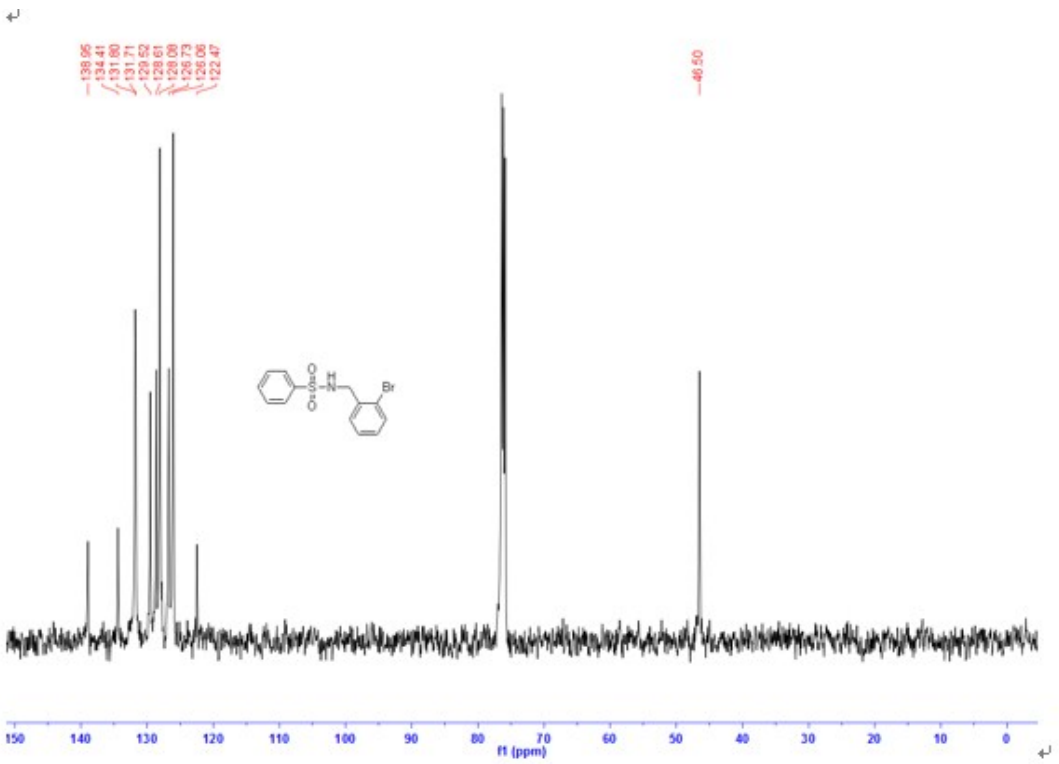
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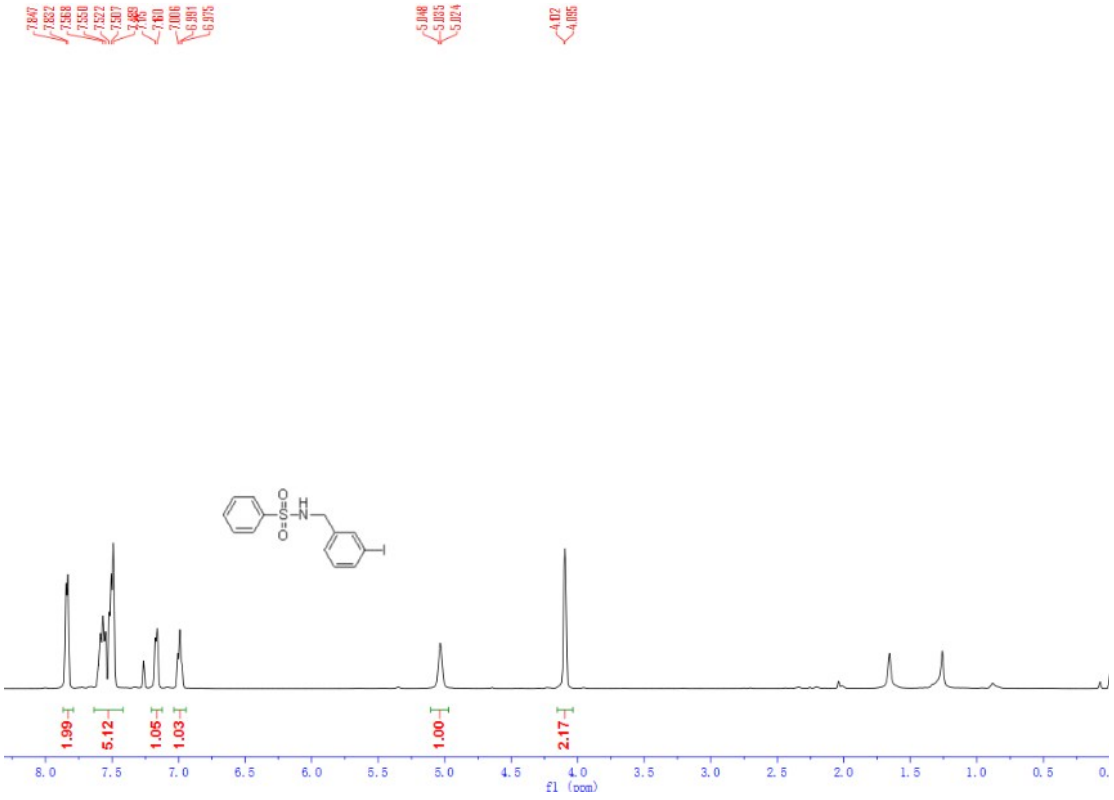
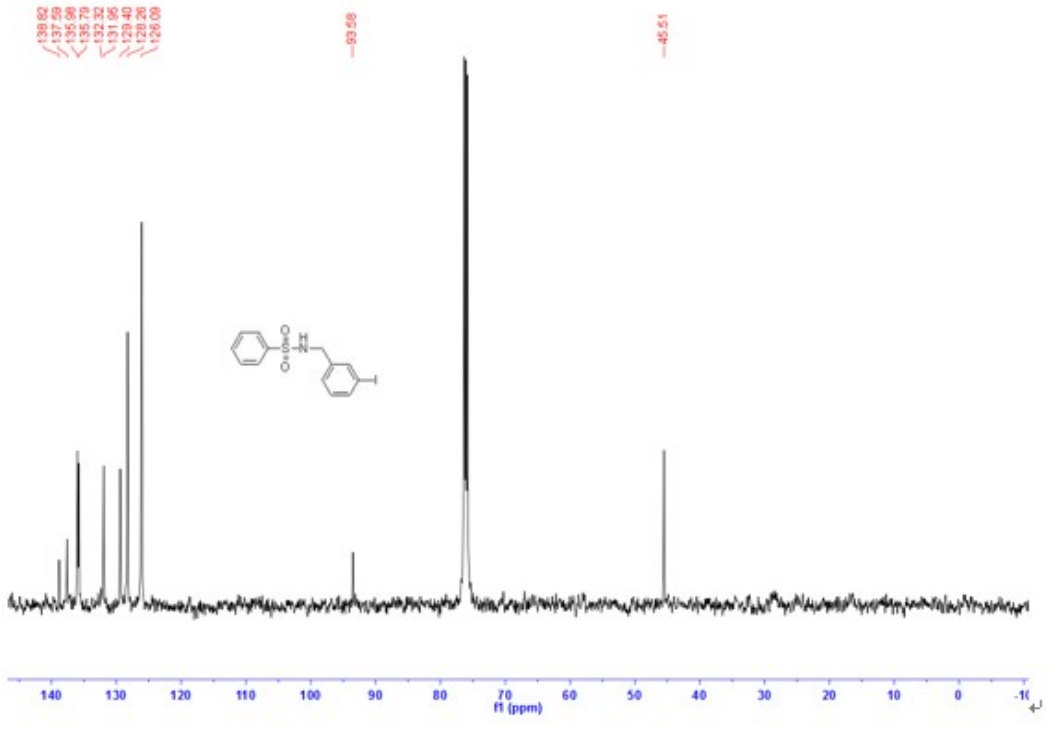
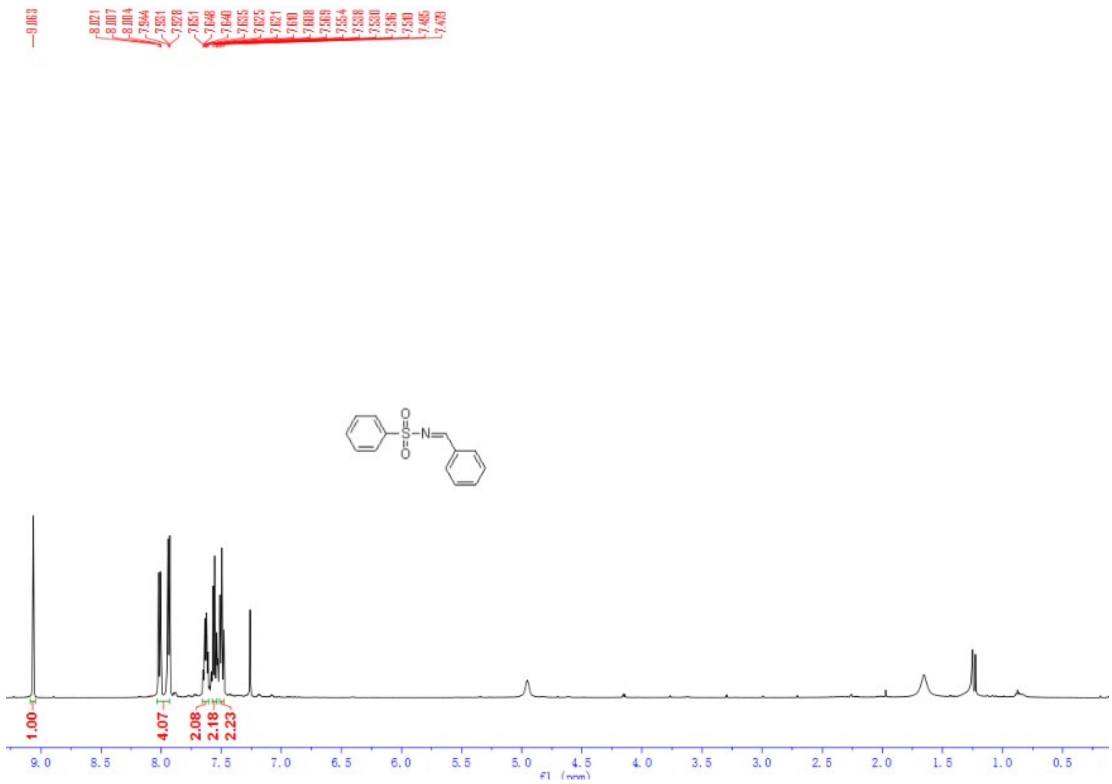
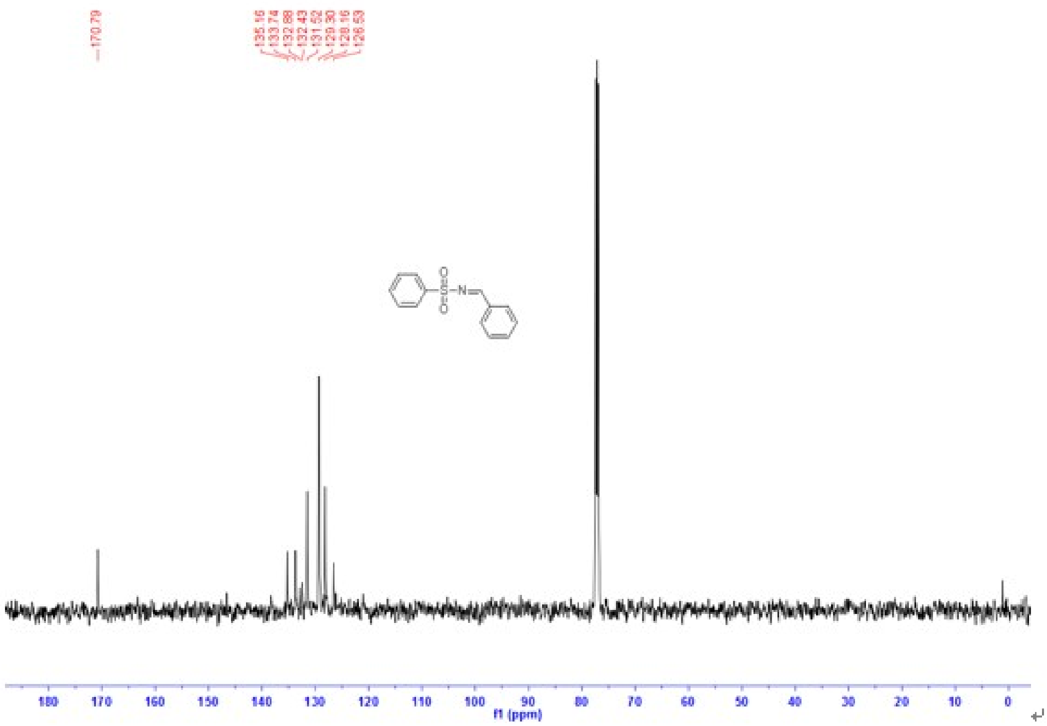
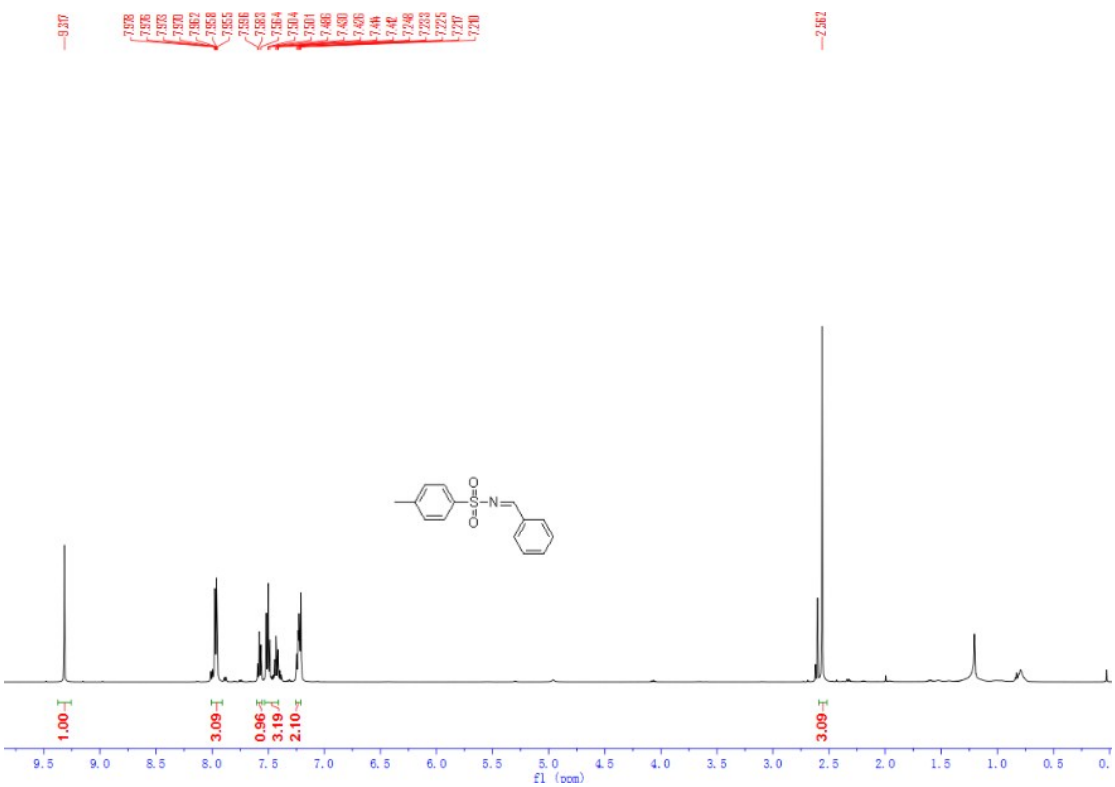
131.71
129.52
128.61
128.09
126.73
126.06
122.47
46.50
f1 (ppm)


7.847
7.822
7.548
7.550
7.522
7.507
7.488
7.476
7.451
7.006
6.991
6.975
5.048
5.035
5.024
4.072
4.055
1.99
5.12
1.05
1.03
1.00
2.17
f1 (ppm)


138.62
137.59
135.98
135.79
132.32
131.95
129.40
128.26
126.09
93.58
45.51
f1 (ppm)


1.00
4.07
2.08
2.18
2.23
f1 (ppm)


170.79
135.16
133.74
132.88
132.43
131.52
129.30
128.16
126.53
f1 (ppm)


1.00
3.09
0.96
3.19
2.10
3.09
f1 (ppm)