Supporting Information

Phosphonic acid mediated practical dehalogenation and benzylation with benzyl halides

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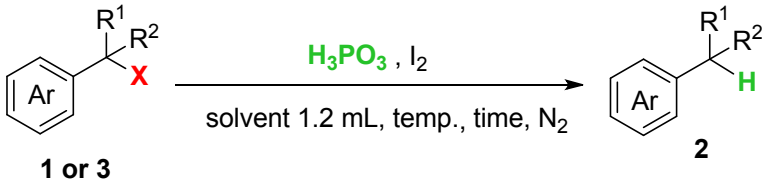
1. General information

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. Unless otherwise noted, all reactions were performed in 10-mL glass vessel tubes carried out under N_2 atmosphere.

Flash column chromatography was performed using 200-300 mesh silica gel or preparation GPC. Visualization on TLC was achieved by the use of UV light (254 nm). ^1H NMR and ^{13}C NMR spectra were measured on a Bruker AV-II 500 MHz NMR spectrometer (^1H 500 MHz, ^{13}C 125 MHz), using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard. Chemical shifts are reported in ppm and referenced to residual solvent peaks ($CHCl_3$ in $CDCl_3$: 7.26 ppm for ^1H and 77.0 ppm for ^{13}C). The coupling constants *J* are given in Hz. Mass spectra were recorded by GCMS-QP 2010 plus spectrometer. FULI GC- 9790 Ⅱ equipped with FID detector was used to analysis the reaction mixture.

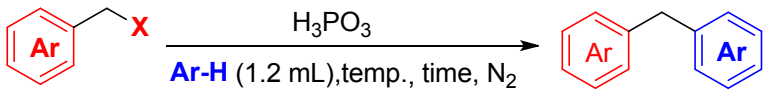
2. Typical procedure for reduction of the benzyl halides with H_3PO_3/I_2.



1 or 3 **2**

A 25 mL sealed Schlenk tube equipped with a magnetic stir bar was charged with H_3PO_3. After the tube was evacuated and backfilled with N_2 (repeated 3 times), benzyl halides 0.6 mmol and I_2 were added with solvent (1.2 mL). The reaction mixture was stirred at indicated temperature for indicated time. After the reaction completed, the mixture was concentrated and the residue was further purified by column chromatography on silica gel to give the analytic pure product **2**.

3. Typical procedure for benzylation of arenes with benzyl halides.

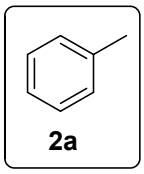


1 or **3** **4**

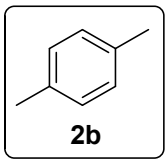
A 25 mL sealed Schlenk tube equipped with a magnetic stir bar was charged with H_3PO_3. After the tube was evacuated and backfilled with N_2 (repeated 3 times), benzyl halides 0.6 mmol and arenes (1.2 mL) were added. The reaction mixture was stirred at indicated temperature for indicated time. After the reaction completed, the mixture was concentrated and the residue was

further purified by column chromatography on silica gel to give the analytic pure product **4**.

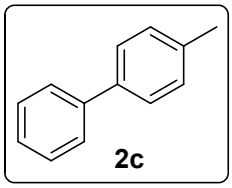
4. Characterization and analytical data of products (*average yields based on three parallel reactions*)



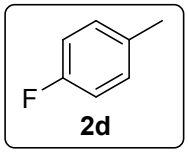
Toluene 2a, 38%, 62.9 mg (Eluent: petroleum ether); ^{1}H NMR (500 MHz $CDCl_3$): δ 7.36–7.33 (m, 2H), 7.27–7.23 (m, 3H), 2.44 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 138.03, 129.22, 128.41, 125.49, 21.63. GC-MS (EI, 70 eV) *m/z* = 92 (M^+). This compound is known.[1]



***p*-Xylene 2b**, 41%, 78.2 mg (Eluent: petroleum ether); ^{1}H NMR (500 MHz $CDCl_3$): δ 6.99 (s, 4H), 2.23 (s, 6H). ^{13}C NMR (125 MHz $CDCl_3$): δ 134.23, 128.46, 20.51. GC-MS (EI, 70 eV) *m/z* = 106 (M^+). This compound is known.[1]

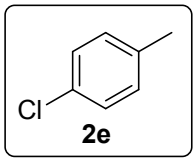


4-Methyl-1,1'-biphenyl 2c, yield 98%, 296.4 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.51–7.50 (m, 2H), 7.43–7.41 (m, 2H), 7.37–7.33 (m, 2H), 7.26–7.23 (m, 1H), 7.17 (d, J = 8.5 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 140.69, 137.89, 136.54, 129.00, 128.23, 126.51, 126.50, 20.62. GC-MS (EI, 70 eV) *m/z* = 168 (M^+). This compound is known.[2]



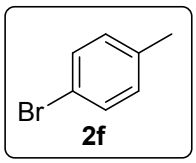
2d

1-Fluoro-4-methylbenzene 2d, yield 32%, 63.4 mg (Eluent: petroleum ether). ^{1}H NMR (400 MHz $CDCl_3$): δ 7.17–7.14 (m, 2H), 7.00–6.96 (m, 2H), 2.36 (s, 3H). ^{13}C NMR (100 MHz $CDCl_3$): δ 161.07 (d, J = 241Hz), 133.35 (d, J = 3.1Hz), 130.30 (d, J = 7.6 Hz), 114.92 (d, J = 241Hz), 20.61. GC-MS (EI, 70 eV) *m/z* = 110 (M^+). This compound is known.[1]



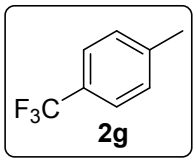
2e

1-Chloro-4-methylbenzene 2e, yield 49%, 111.1 mg (Eluent: petroleum ether); ^{1}H NMR (500 MHz $CDCl_3$): δ 7.27–7.25 (m, 2H), 7.14–7.13 (m, 2H), 2.36 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 135.78, 130.60, 129.92, 127.81, 20.39. GC-MS (EI, 70 eV) *m/z* = 126 (M^+). This compound is known.[1]



2f

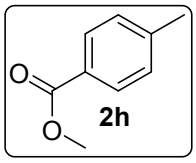
1-Bromo-4-methylbenzene 2f, yield 68%, 209.3 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.41–7.40 (m, 2H), 7.09–7.07 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 13C NMR (126 MHz, CDCl3) δ 136.79, 131.26, 130.84, 119.08, 20.95. GC-MS (EI, 70 eV) *m/z* = 171 (M^+). This compound is known.[1]



2g

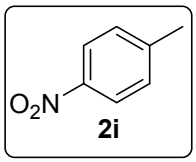
1-Methyl-4-(trifluoromethyl)benzene 2g, yield 26%, 74.9 mg (Eluent: petroleum

ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.52–7.50 (m, 2H), 7.29–7.27 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 141.57, 128.81, 127.35 (d, $J_{C\text{-}F}$ = 32.3 Hz), 124.63 (q, $J_{C\text{-}F}$ = 3.6 Hz), 123.95 (q, $J_{C\text{-}F}$ = 270.0 Hz), 20.89. GC-MS (EI, 70 eV) *m/z* = 160 (M^+). This compound is known.[1]



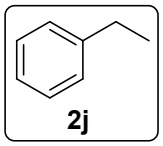
2h

Methyl 4-methylbenzoate 2h, yield 61%, 164.7 mg (Eluent: petroleum ether/ethyl acetate = 10/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.78 (d, J = 8.0 Hz, 2H), 7.08(d, J = 8.0 Hz, 2H), 3.75 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 167.17, 143.54, 129.60, 129.07, 127.44, 51.91, 21.61. GC-MS (EI, 70 eV) *m/z* = 150 (M^+). This compound is known.[1]

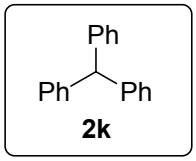


2i

1-Methyl-4-nitrobenzene 2i, yield 52%, 128.2 mg (Eluent: petroleum ether/ethyl acetate = 10/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 8.11 (d, J = 9.0 Hz, 2H), 7.31(d, J = 8.0 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 146.00, 145.44, 129.31, 123.04, 21.12. GC-MS (EI, 70 eV) *m/z* = 137 (M^+). This compound is known.[1]

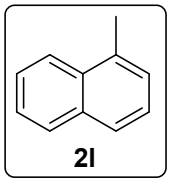

2j

Ethylbenzene 2j, yield 39%, 74.4 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.45–7.42 (m, 2H), 7.36–7.32 (m, 3H), 2.81 (q, J = 7.5 Hz, 2H), 1.40(t, J = 7.5 Hz, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 144.36, 128.44, 127.99, 125.73, 29.03, 15.76. GC-MS (EI, 70 eV) *m/z* = 106 (M^+). This compound is known.[3]

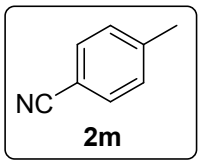


2k

Triphenylmethane 2k, yield 97%, 426.0 mg (Eluent: petroleum ether/ethyl acetate = 50/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.30–7.27 (m, 6H), 7.23–7.20 (m, 3H), 7.13–7.12 (m, 6H), 5.56 (s, 1H). ^{13}C NMR (125 MHz $CDCl_3$): δ 143.91, 129.47, 128.31, 126.31, 56.85. GC-MS (EI, 70 eV) *m/z* = 244 (M^+). This compound is known.[3]

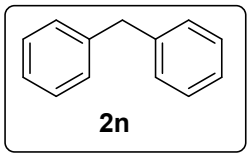

2l

1-Methylnaphthalene 2l, yield 78%, 199.4 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 8.15–8.13 (m, 1H), 8.00–7.99 (m, 1H), 7.87–7.85 (m, 1H), 7.68–7.63 (m, 2H), 7.54–7.46 (m, 2H), 2.84 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 133.91, 133.21, 132.27, 128.19, 126.23, 126.05, 125.38, 125.24, 125.20, 123.78, 19.05. GC-MS (EI, 70 eV) *m/z* = 142 (M^+). This compound is known.[4]

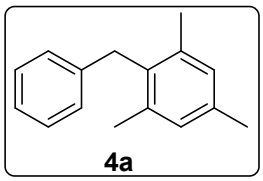


2m

4-Methylbenzonitrile 2m, yield 53%, 111.6 mg (Eluent: petroleum ether/ethyl acetate = 40/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.42–7.41 (m, 2H), 7.15–7.14 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 143.71, 132.07, 129.85, 119.18, 109.33, 21.85. GC-MS (EI, 70 eV) *m/z* = 117 (M^+). This compound is known.[1]

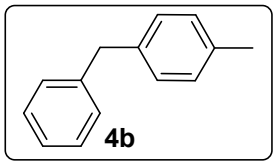

2n

Diphenylmethane 2n, yield 99%, 299.4 mg; 77%, 232.8 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.41–7.39 (m, 4H), 7.32–7.29 (m, 6H), 4.10 (s, 2H). ^{13}C NMR (125 MHz $CDCl_3$): δ 141.24, 129.07, 128.59, 126.20, 42.05. GC-MS (EI, 70 eV) *m/z* = 168 (M^+). This compound is known.[5]



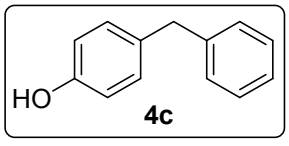
4a

2-Benzyl-1,3,5-trimethylbenzene 4a, for benzyl chloride: yield 95%, 359.1 mg; for benzyl bromide: 96%, 362.9 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.15–7.12 (m, 2H), 7.07–7.04 (m, 1H), 6.93–6.92 (m, 2H), 6.80 （d, J = 7.5 Hz, 2H）, 3.93 (s, 2H), 2.21 (s, 3H), 2.12 (s, 6H). ^{13}C NMR (125 MHz $CDCl_3$): δ 140.18, 137.09, 135.73, 133.86, 128.96, 128.41, 127.92, 125.73, 34.78, 20.99, 20.21. GC-MS (EI, 70 eV) m/z = 210 (M^+). This compound is known.[5]



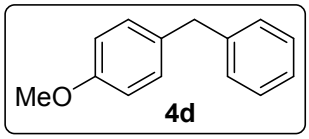
4b

1-Benzyl-4-methylbenzene (isomer) 4b, for benzyl chloride: yield 95%, 311.2 mg; for benzyl bromide: 78%, 255.5 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.35–7.32 (m, 3.15H), 7.29–7.13 (m, 10.74H), 7.07–7.04 (m, 0.39H), 4.05 (s, 1.29H, minor), 4.00 (s, 2H, major), 2.37 (s, 3H, major), 2.30 (s, 1.92H, minor). ^{13}C NMR (125 MHz $CDCl_3$): δ 140.96, 139.94, 138.47, 137.62, 136.18, 135.08, 129.83, 129.49, 128.69, 128.42, 128.36, 128.29, 127.97, 127.93, 125.99, 125.52, 125.46, 41.07 (major), 39.00 (minor), 20.55 (major), 19.21 (minor). GC-MS (EI, 70 eV) m/z = 182 (M^+). This compound is known.[5]



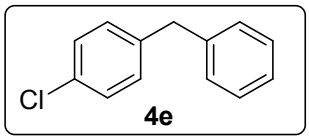
4c

4-benzylphenol 4c, for benzyl chloride: yield 99%, 327.9 mg; for benzyl bromide: 98%, 324.6 mg (Eluent: petroleum ether/ethyl acetate = 10/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.21–7.18 (m, 2H), 7.13–7.09 (m, 3H), 6.99–6.97 (m, 2H), 6.69–6.66 (m, 2H), 3.84 (s, 2H). ^{13}C NMR (125 MHz $CDCl_3$): δ 153.81, 141.53, 133.45, 130.09, 128.84, 128.46, 126.03, 115.30, 41.04. GC-MS (EI, 70 eV) m/z = 184 (M^+). This compound is known.[6]



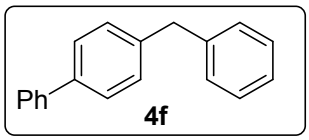
4d

1-Benzyl-4-methoxybenzene (isomer) 4d, for benzyl chloride: yield 94%, 335.0 mg; for benzyl bromide: 92%, 327.9 mg (Eluent: petroleum ether/ethyl acetate = 10/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.31–7.27 (m, 2.48H), 7.24–7.19 (m, 4.02H), 7.13–7.08 (m, 2.23H), 6.90–6.84 (m, 2.58H), 4.00 (s, 0.69H, minor), 3.95 (s, 1.98H, major), 3.83 (s, 1.12H, minor), 3.80 (s, 3H, major). ^{13}C NMR (125 MHz $CDCl_3$): δ 157.99, 141.62, 141.05, 133.28, 130.34, 129.89, 129.69, 128.99, 128.84, 128.46, 128.28, 127.43, 126.01, 125.79, 120.49, 113.90, 110.42, 55.37 (minor), 55.28 (major), 41.06 (major), 35.88 (minor). GC-MS (EI, 70 eV) *m/z* = 198 (M^+). This compound is known.[7]



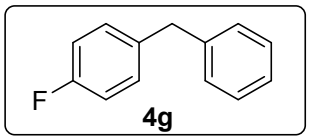
4e

1-Benzyl-4-chlorobenzene 4e, for benzyl chloride: yield 72%, 261.8 mg; 92%, 334.5 mg; for benzyl bromide: 56%, 203.6 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.37–7.25 (m, 5H), 7.22–7.21 (m, 2H), 7.17–7.15 (m, 2H), 4.00 (s, 2H). ^{13}C NMR (125 MHz $CDCl_3$): δ 140.59, 139.63, 131.93, 130.30, 128.90, 128.61, 126.33, 41.28. GC-MS (EI, 70 eV) *m/z* = 202 (M^+). This compound is known.[3]



4f

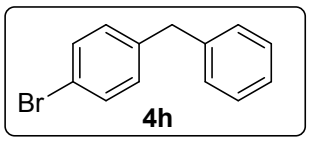
4-Benzyl-1,1'-biphenyl 4f, for benzyl bromide: 59%, 259.1 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.50–7.48 (m, 2H), 7.45–7.43 (m, 2H), 7.36–7.33 (m, 2H), 7.26–7.12 (m, 8H), 3.95 (s, 2H). ^{13}C NMR (125 MHz $CDCl_3$): δ 141.04, 141.03, 140.28, 139.07, 129.35, 129.00, 128.75, 128.56, 127.25, 127.11, 127.04, 126.18, 41.62. GC-MS (EI, 70 eV) *m/z* = 244 (M^+). This compound is known.[8]



4g

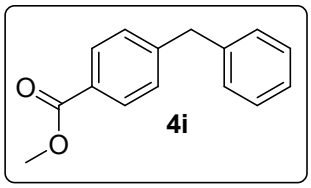
1-Benzyl-4-fluorobenzene 4g, for benzyl chloride: yield 99%, 331.5 mg; for benzyl

bromide: 74%, 247.8 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.36–7.33 (m, 2H), 7.28–7.17 (m, 5H), 7.04–7.00 (m, 2H), 4.00 (s, 2H). ^{13}C NMR (125 MHz $CDCl_3$): δ 161.45 (d, $J_{C\text{-}F}$ = 242.4 Hz), 140.98, 136.80 (d, $J_{C\text{-}F}$ = 3.1 Hz), 130.32 (d, $J_{C\text{-}F}$ = 7.8 Hz), 128.87, 128.57, 126.24, 115.24 (d, $J_{C\text{-}F}$ = 21.0 Hz), 41.11. GC-MS (EI, 70 eV) *m/z* = 186 (M^+). This compound is known.[5]



4h

1-Benzyl-4-bromobenzene 4h, for benzyl chloride: yield 81%, 360.1 mg; for benzyl bromide: 53%, 235.6 mg (Eluent: petroleum ether). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.32 (d, J = 8.5 Hz, 2H), 7.23–7.20 (m, 2H), 7.15–7.07 (m, 3H), 6.98 (d, J = 8.0 Hz, 2H), 3.85 (s, 2H). ^{13}C NMR (125 MHz $CDCl_3$): δ 140.46, 140.12, 131.53, 130.69, 128.88, 128.59, 126.32, 119.95, 41.32. GC-MS (EI, 70 eV) *m/z* = 247 (M^+). This compound is known.[9]



4i

Methyl 4-benzylbenzoate 4i, for benzyl bromide: 35%, 142.4 mg (Eluent: petroleum ether/ethyl acetate = 10/1). ^{1}H NMR (500 MHz $CDCl_3$): δ 7.87 (d, J = 8.0 Hz, 2H), 7.23–7.12 (m, 5H), 7.10–7.08 (m, 2H), 3.94 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$): δ 167.10, 146.55, 140.15, 129.85, 128.98, 128.64, 128.11, 126.40, 52.04, 41.94. GC-MS (EI, 70 eV) *m/z* = 226 (M^+). This compound is known.[10]

5. References

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(8) C.-B. Kim, H. Jo, B.-K. Ahn, C. K. Kim and K. Park, *J. Org. Chem.,* 2009, 74, 9566-9569.
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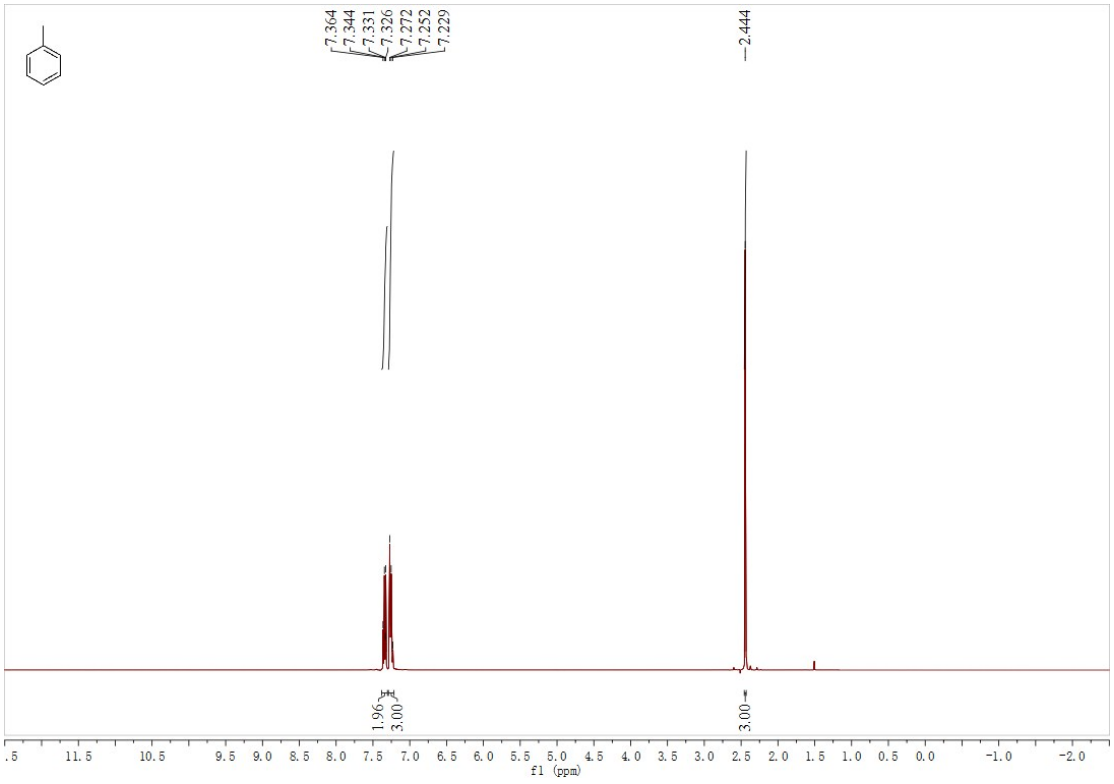
6. Copies of ^{1}H NMR and ^{13}C NMR spectra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7.252
7.229
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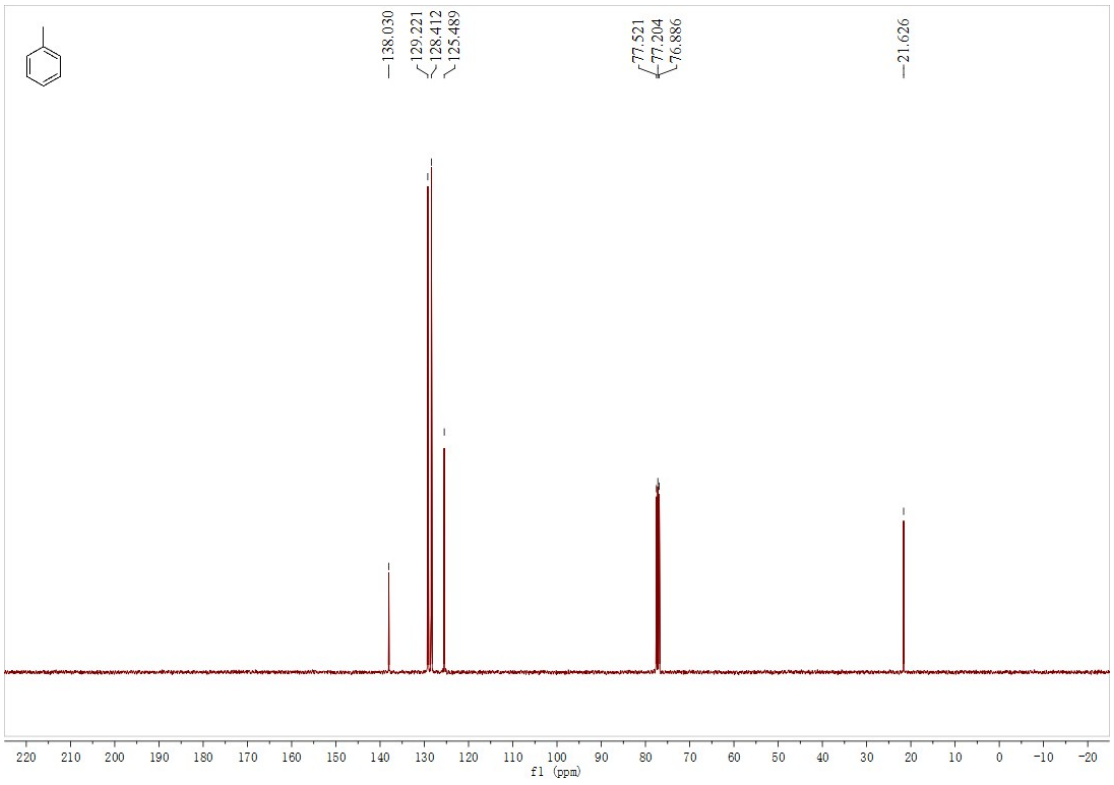
3.00
f1 (ppm)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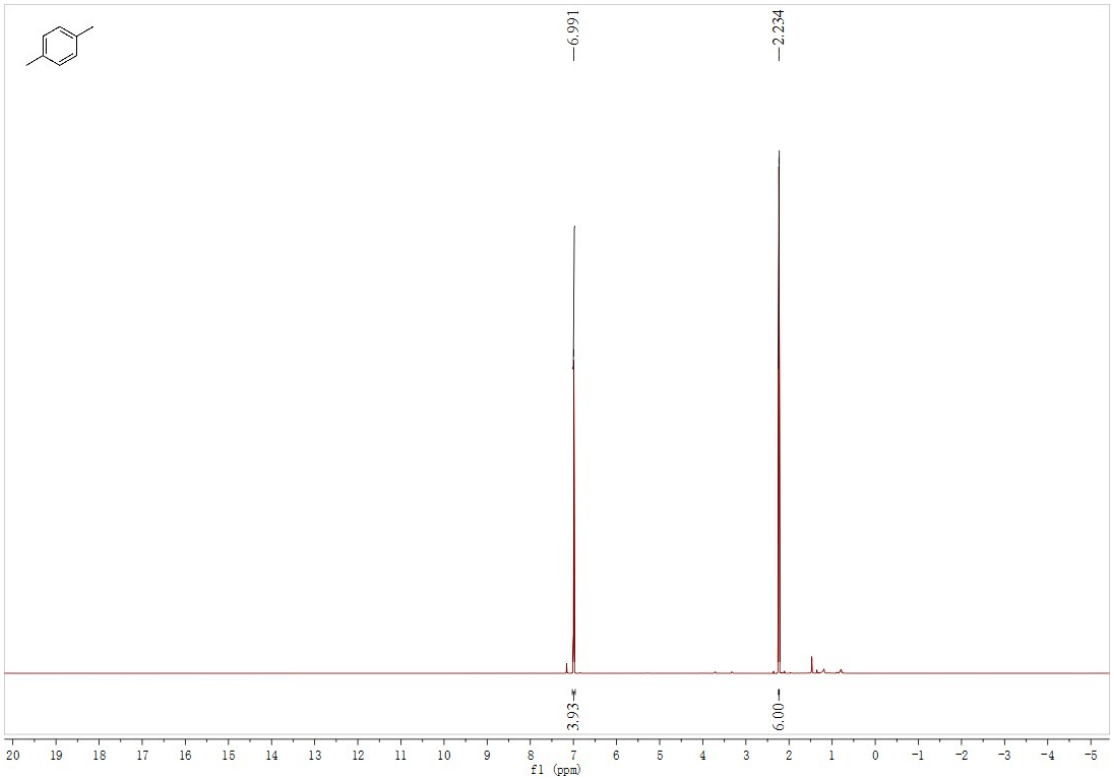
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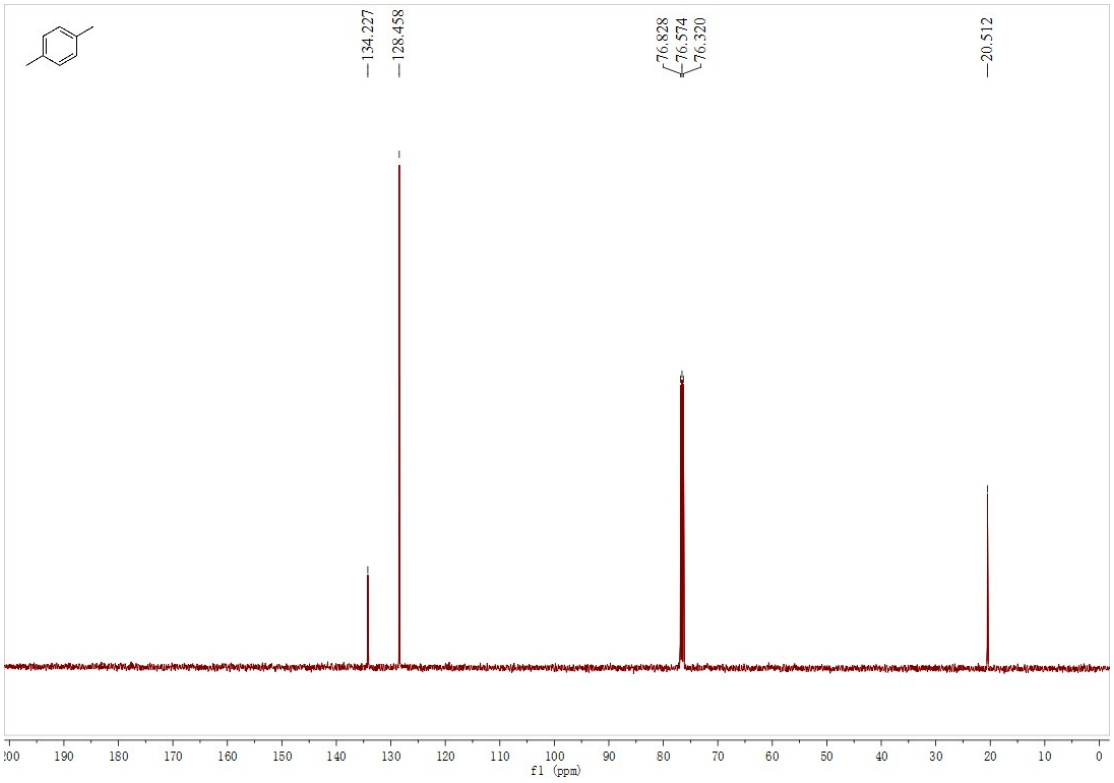
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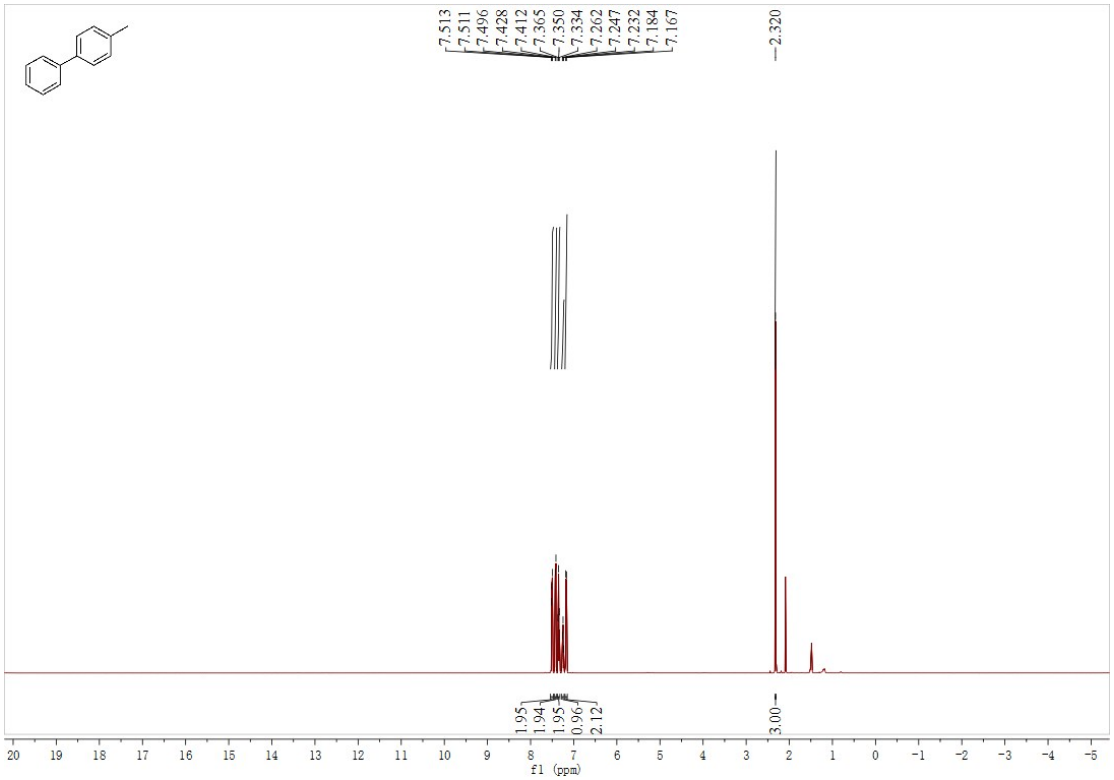
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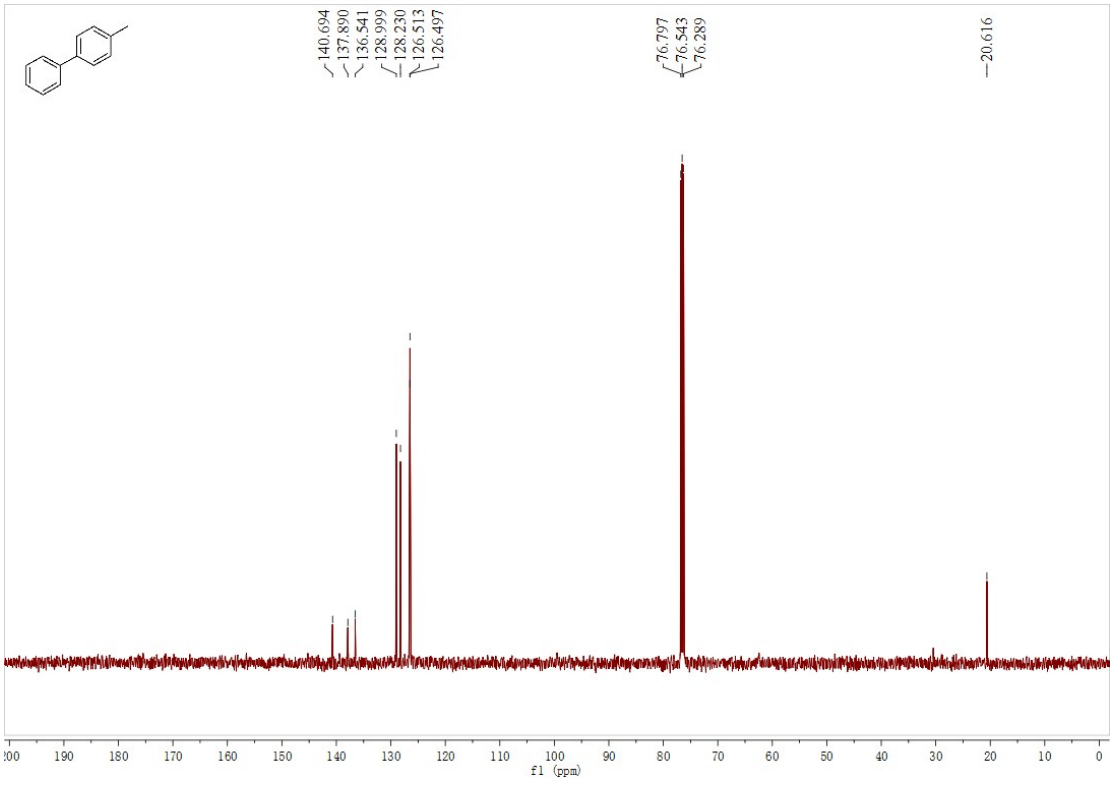
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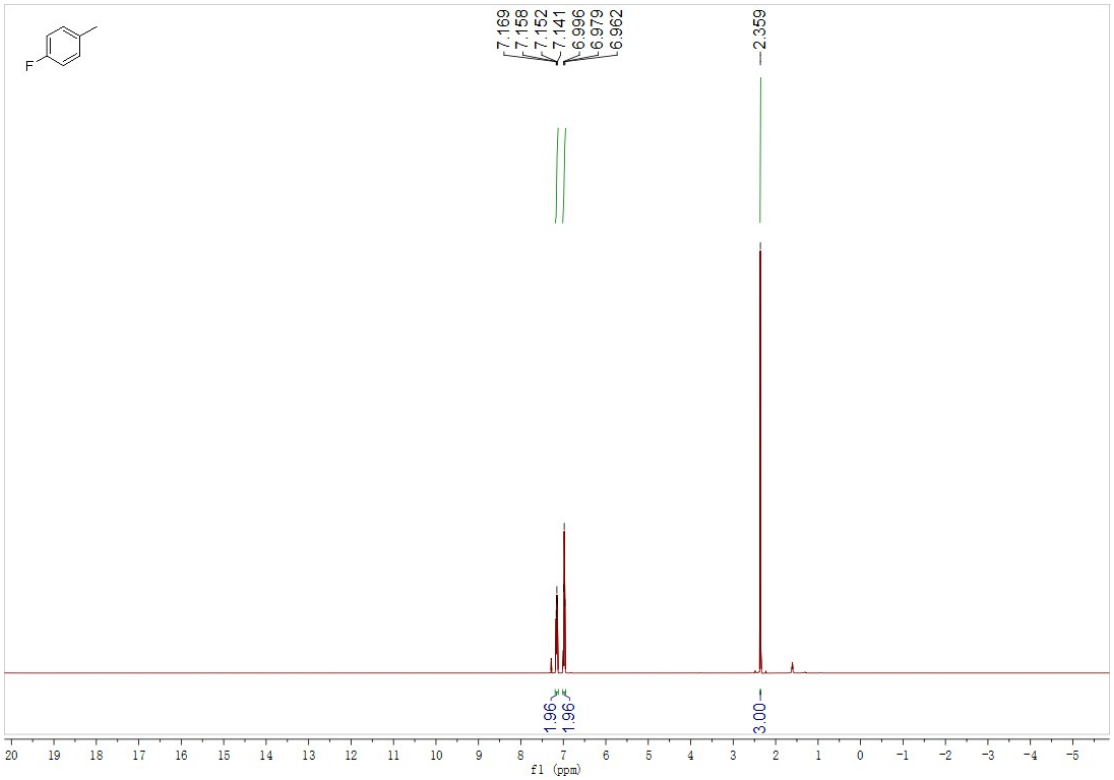
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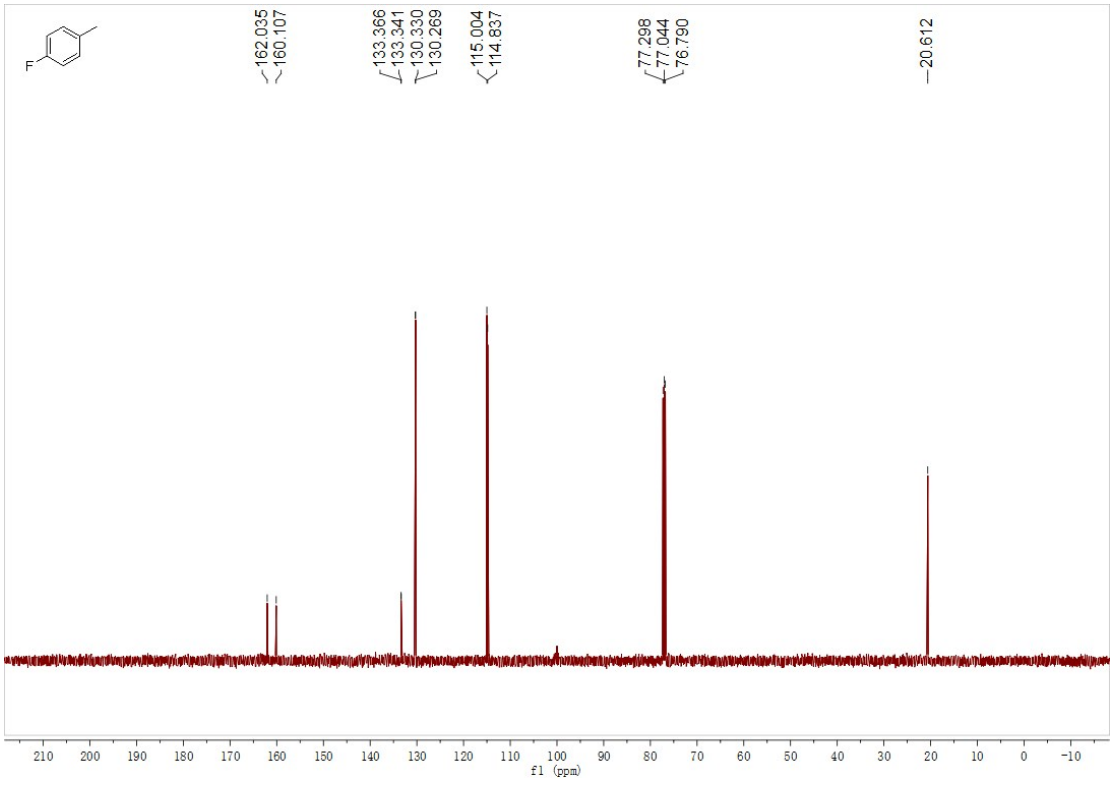
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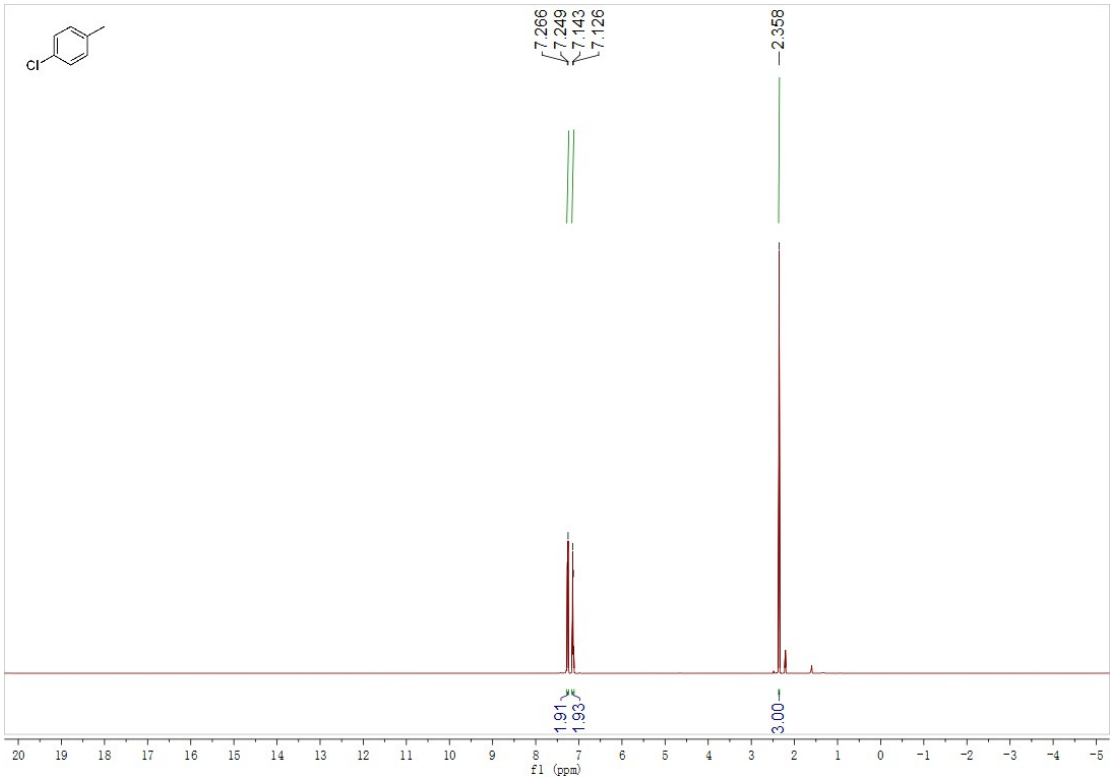
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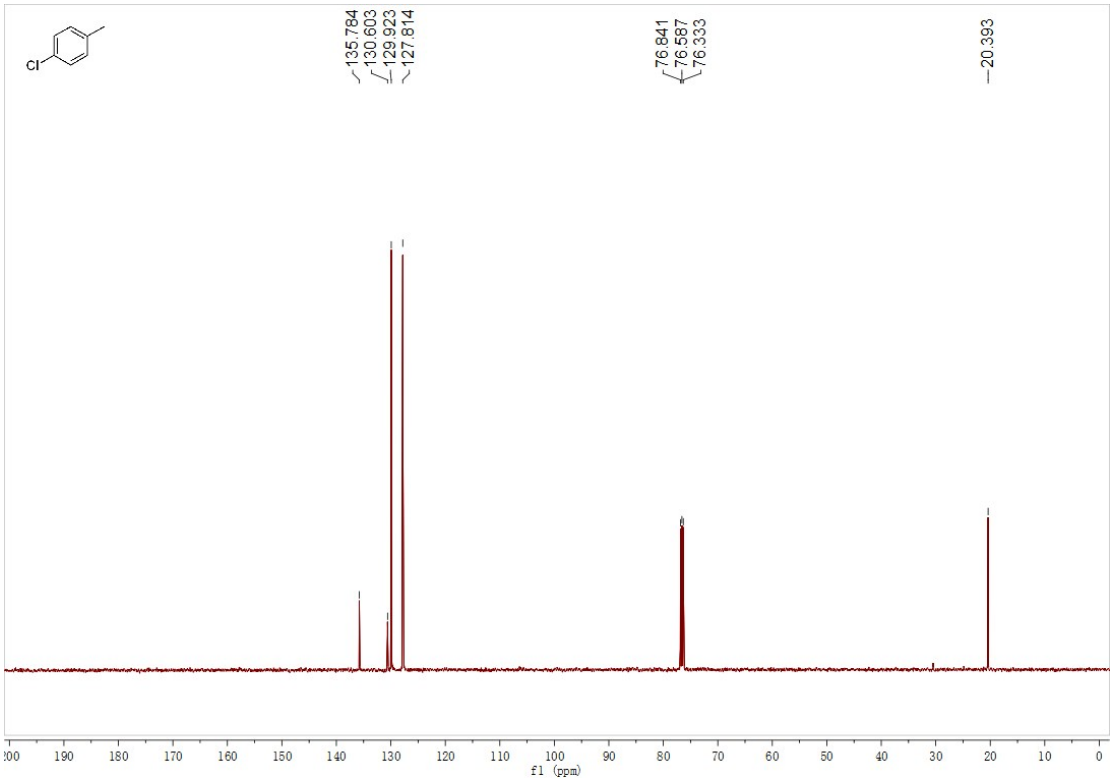
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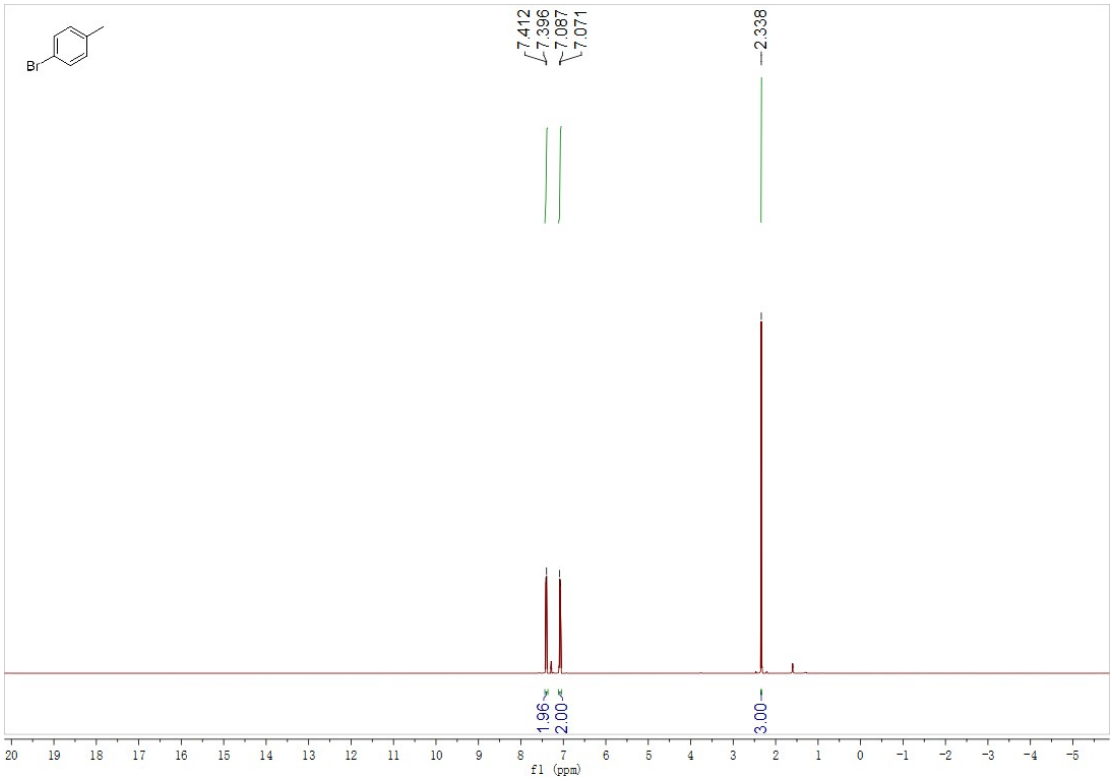
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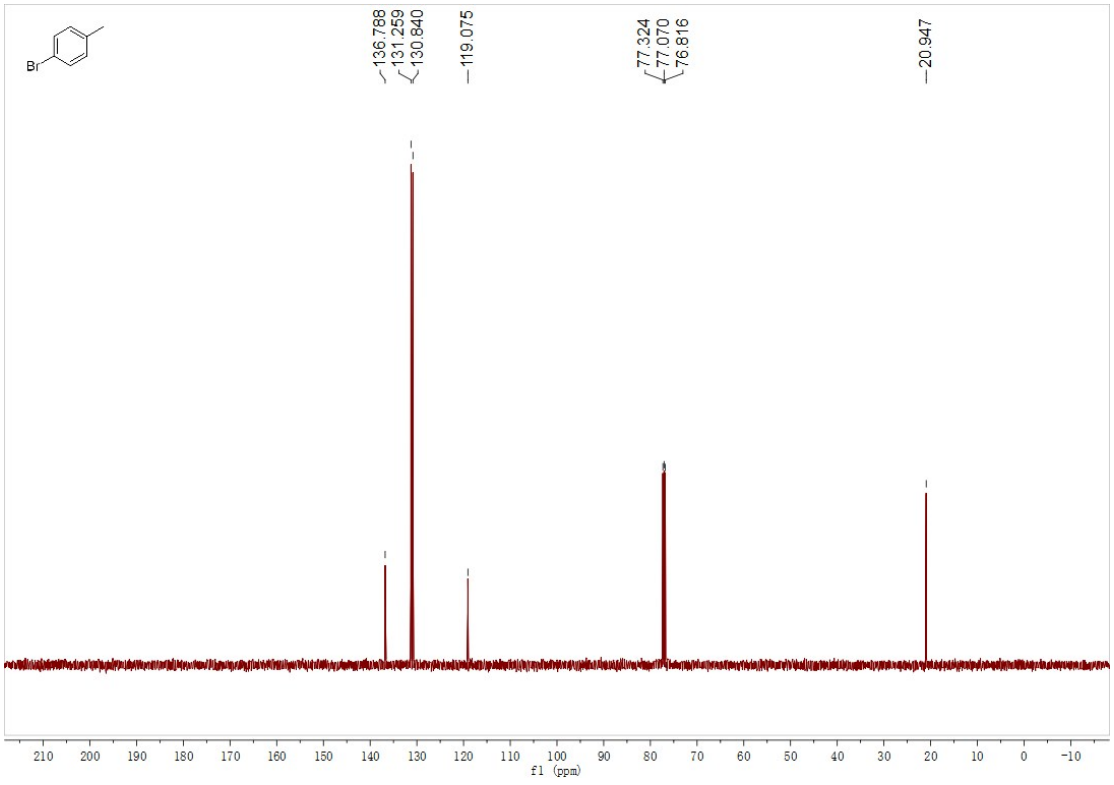
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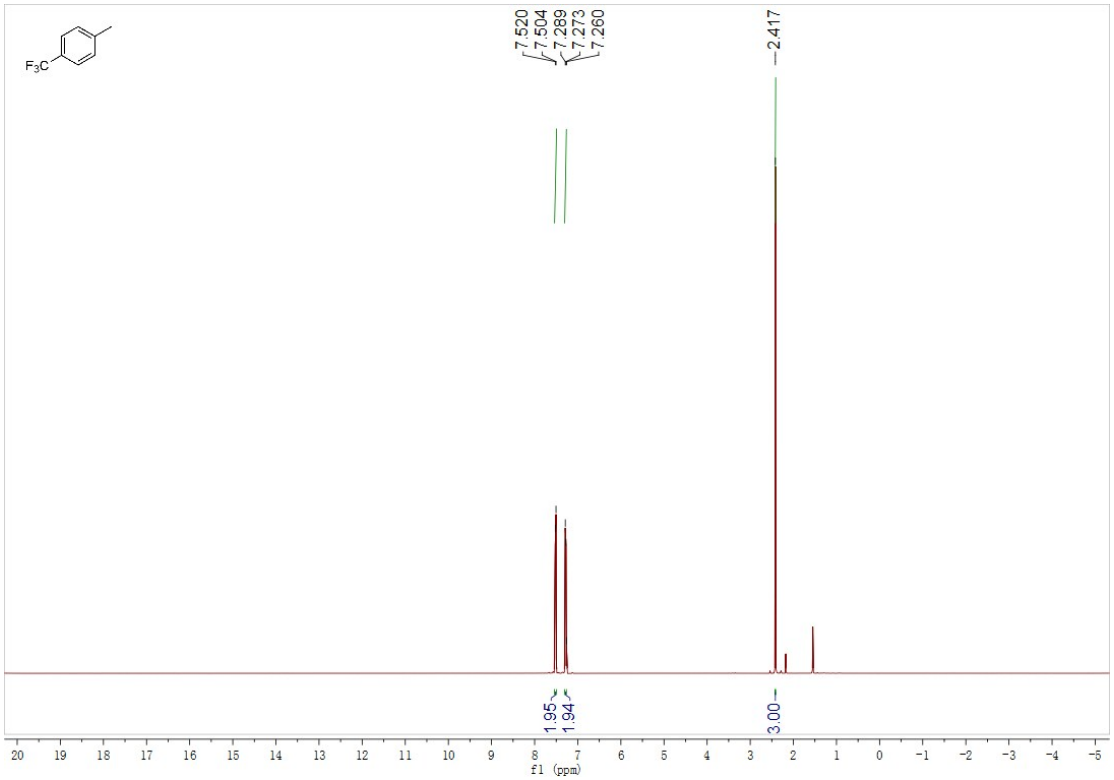
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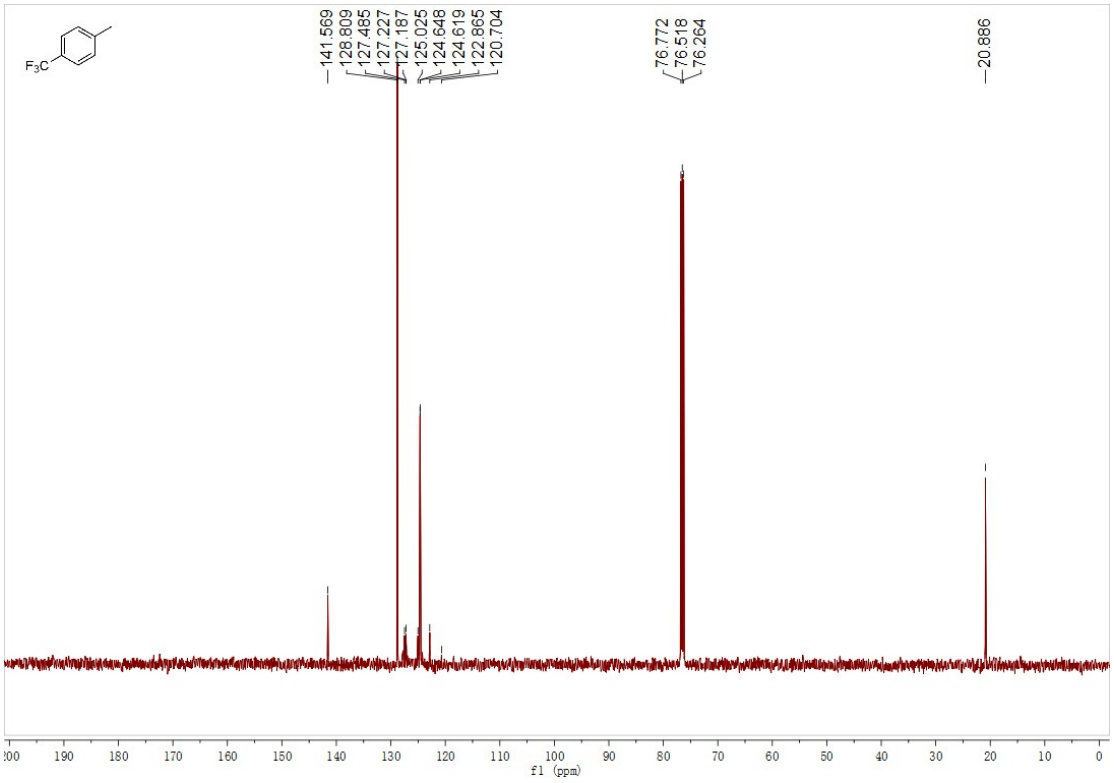
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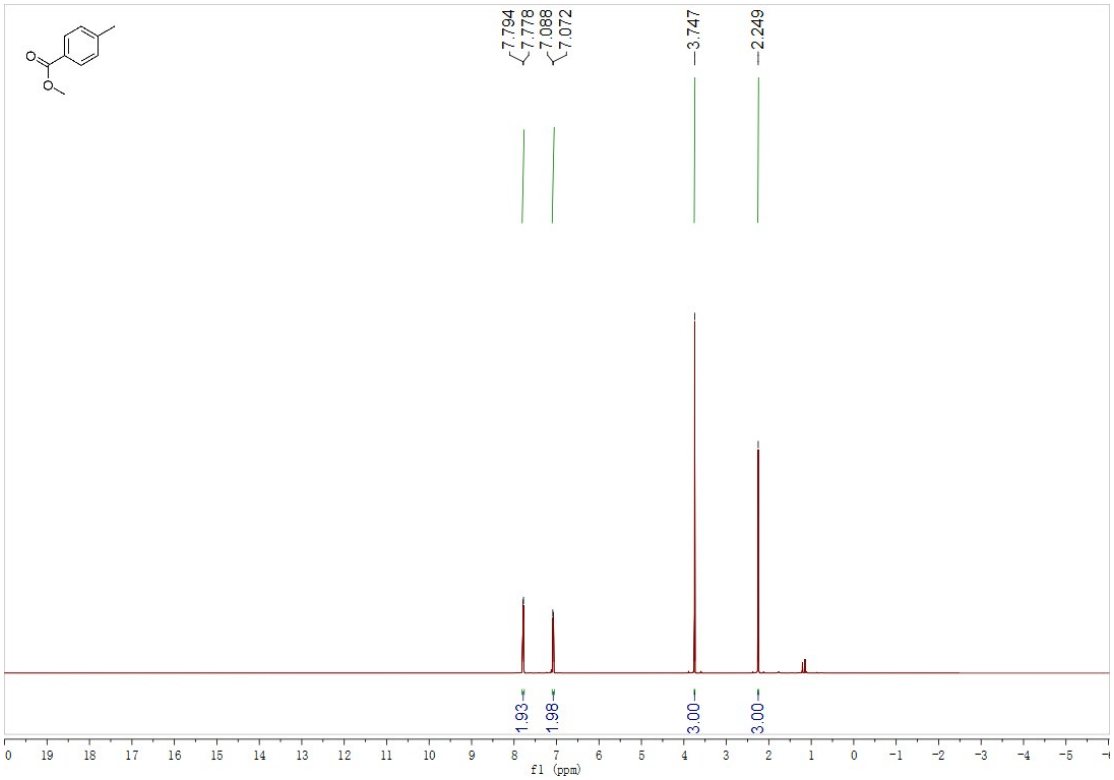
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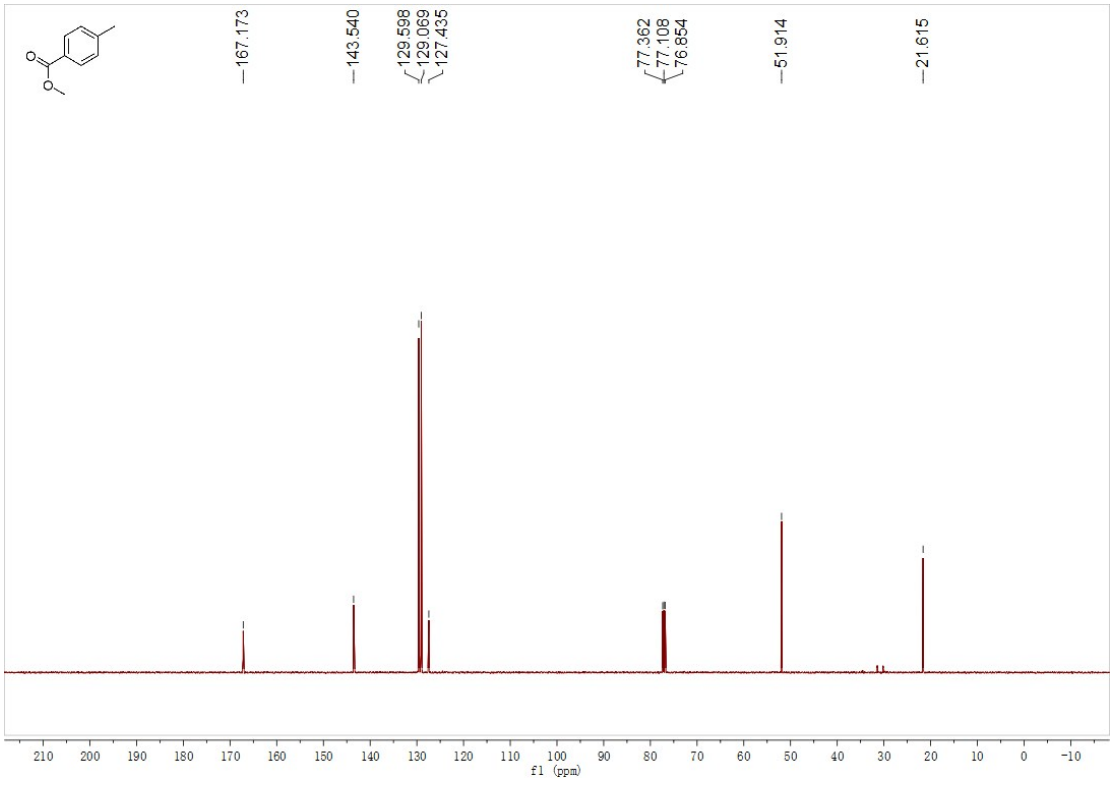
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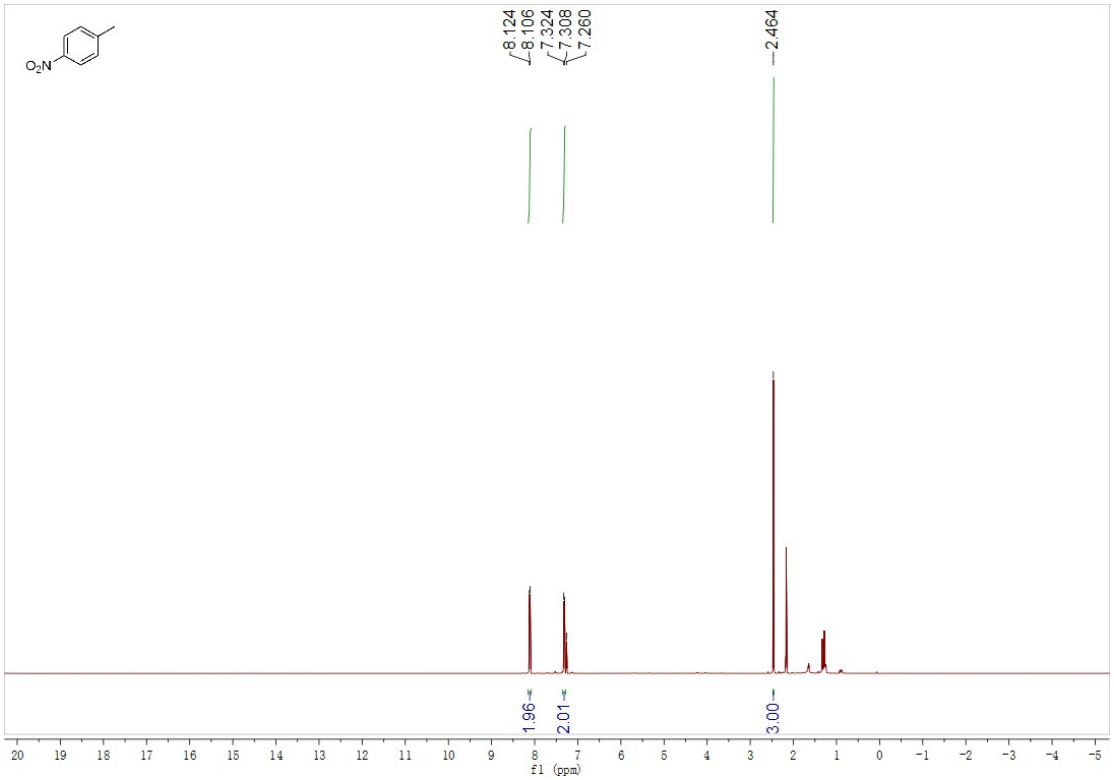
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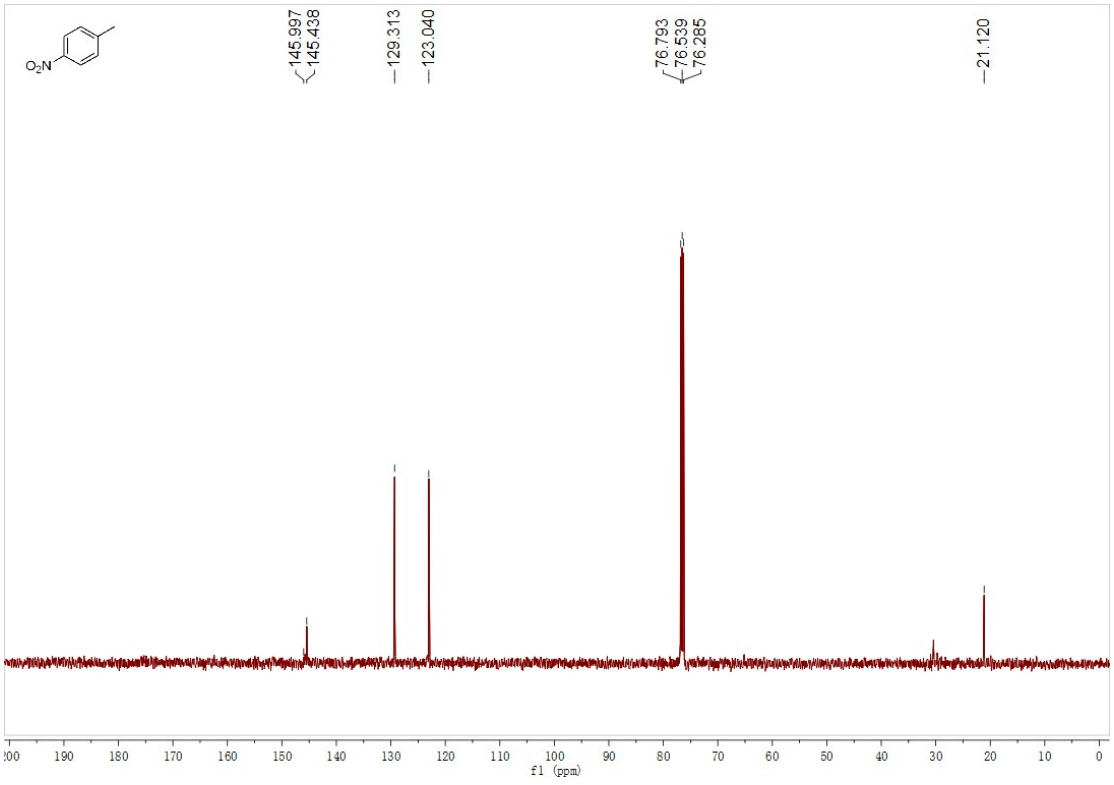
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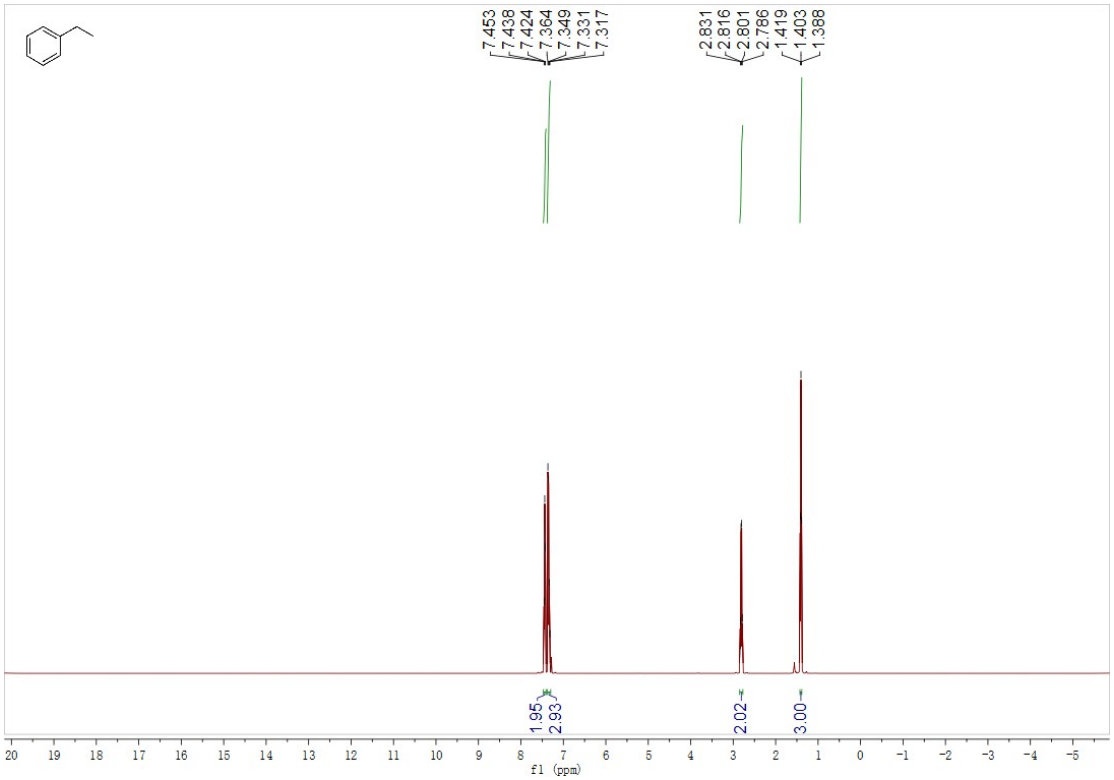
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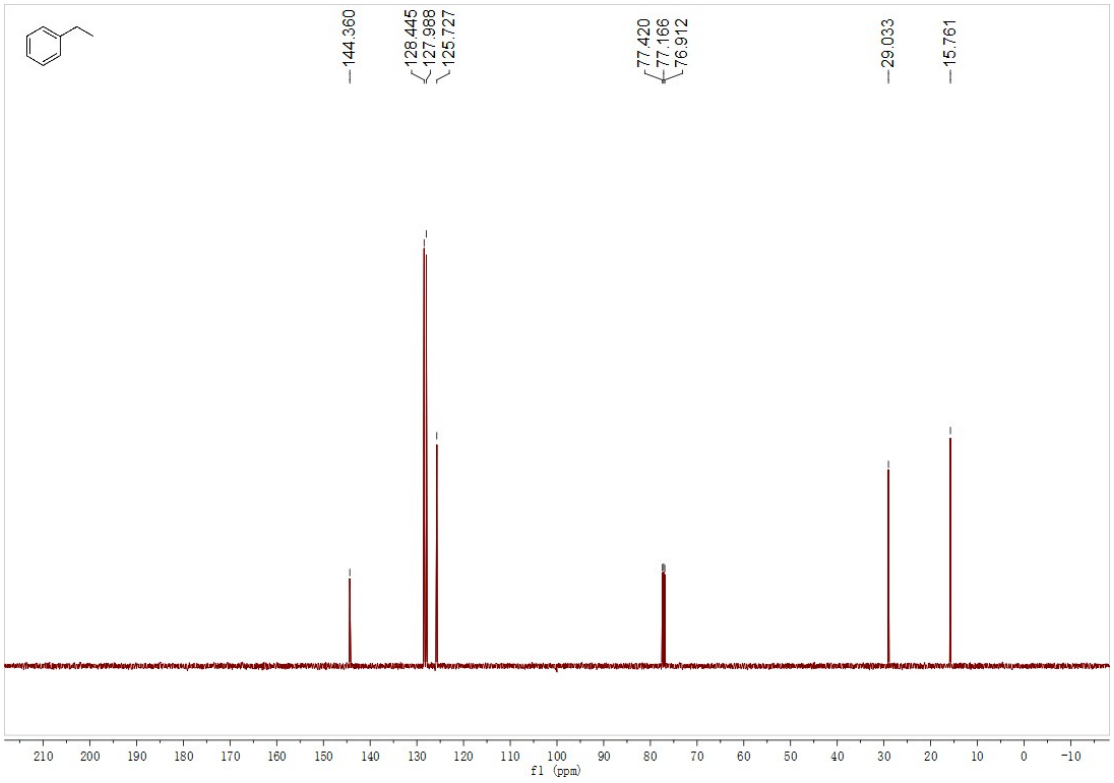
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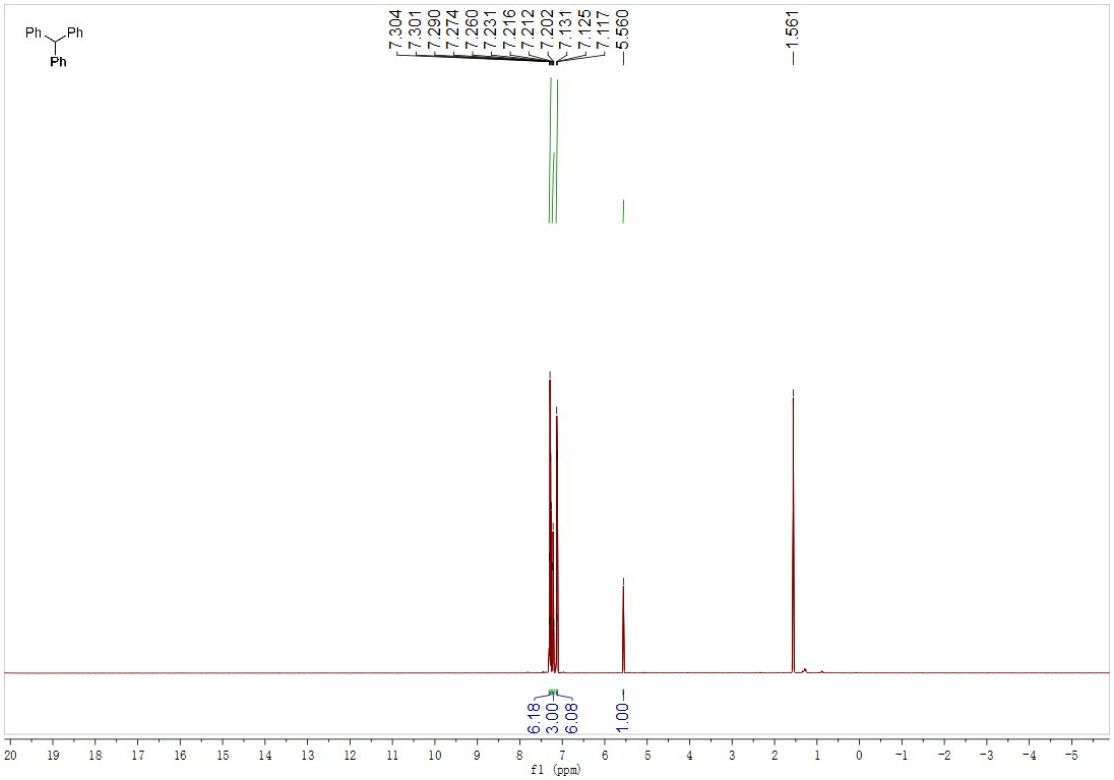
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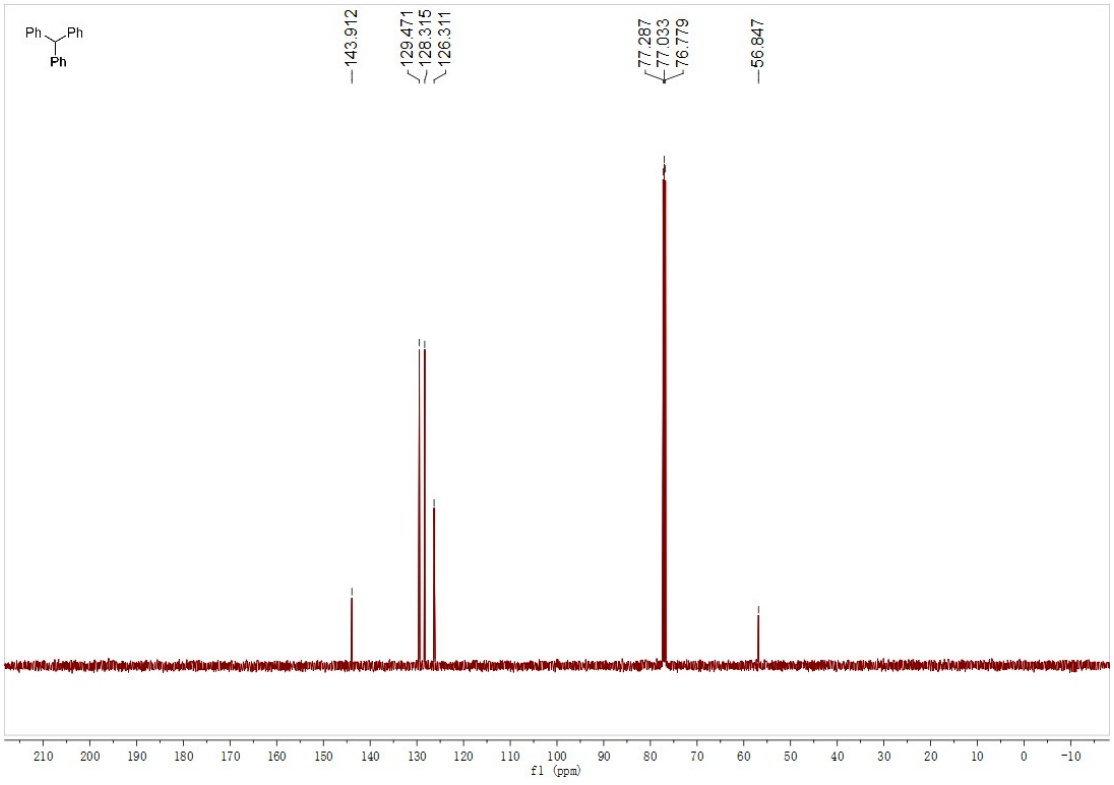
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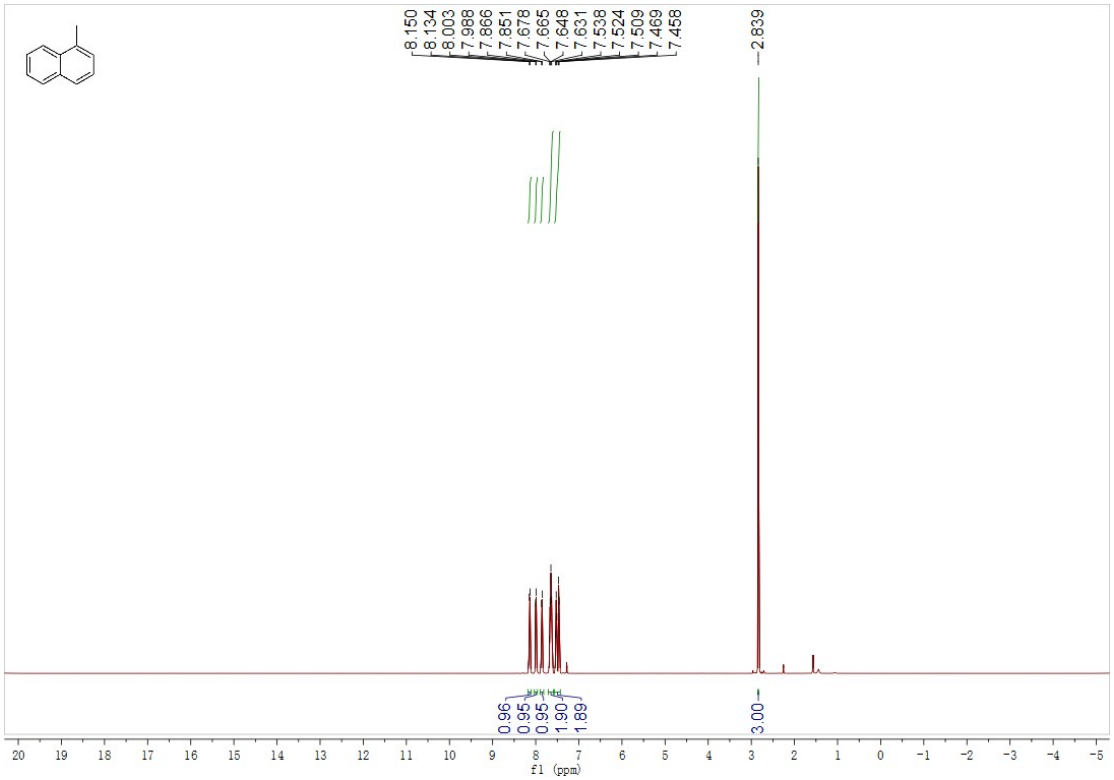
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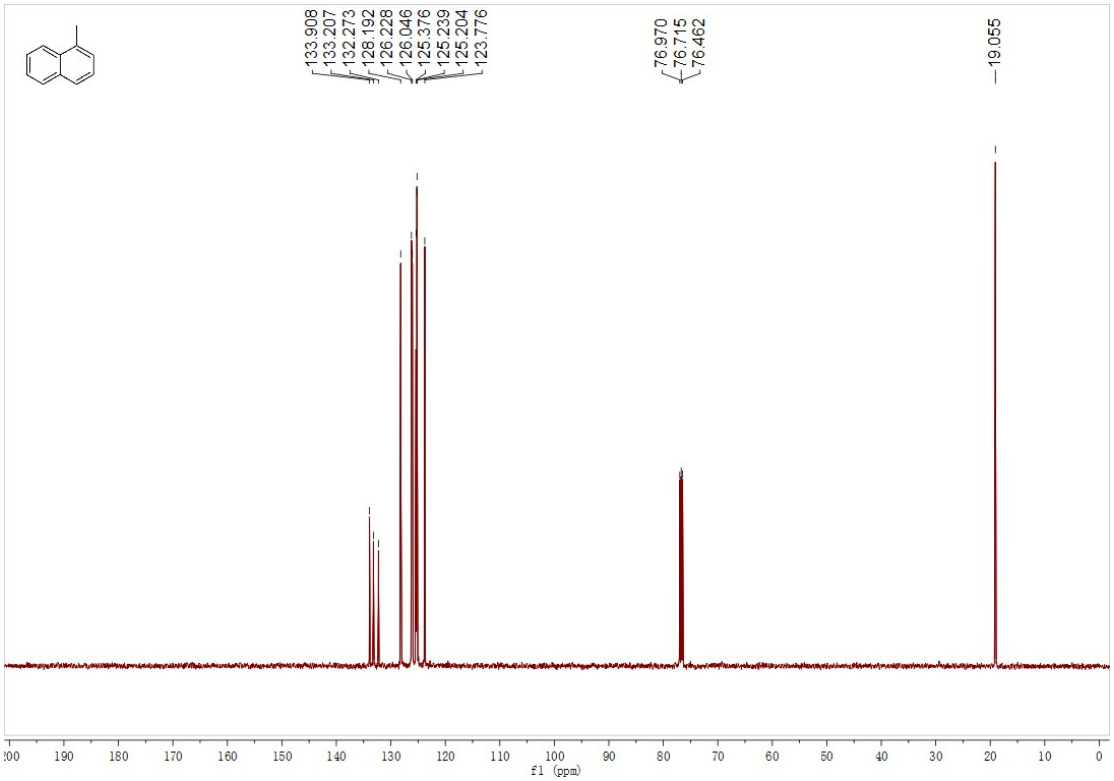
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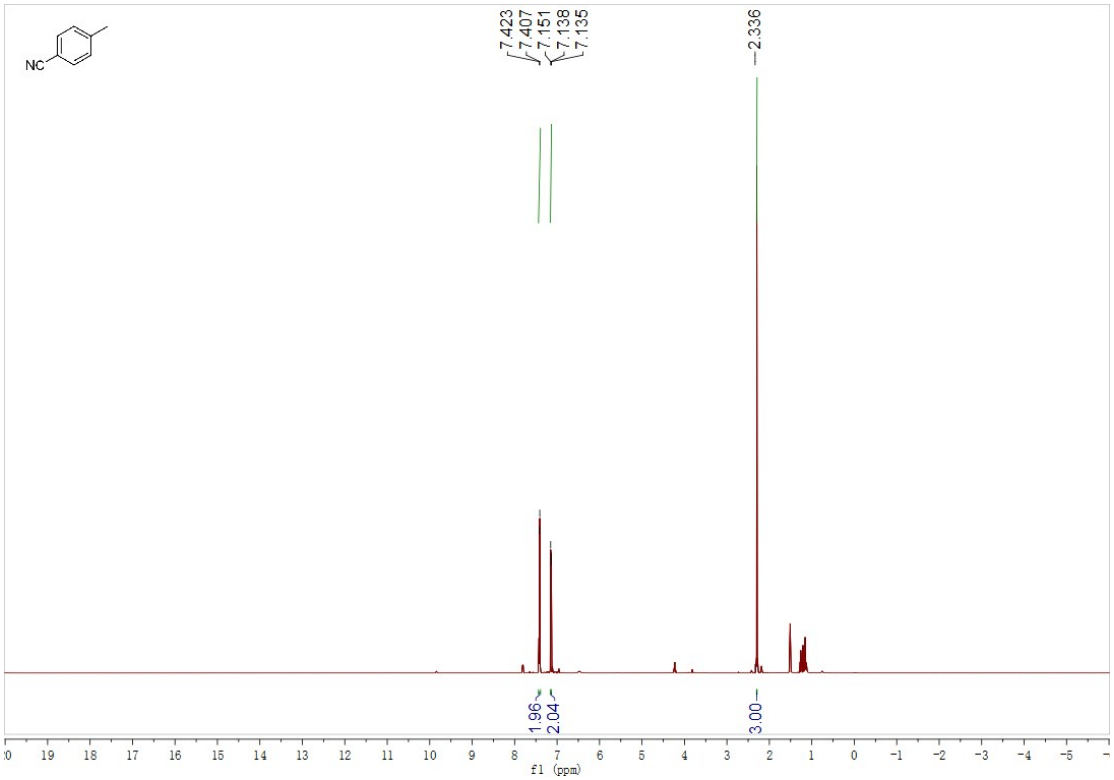
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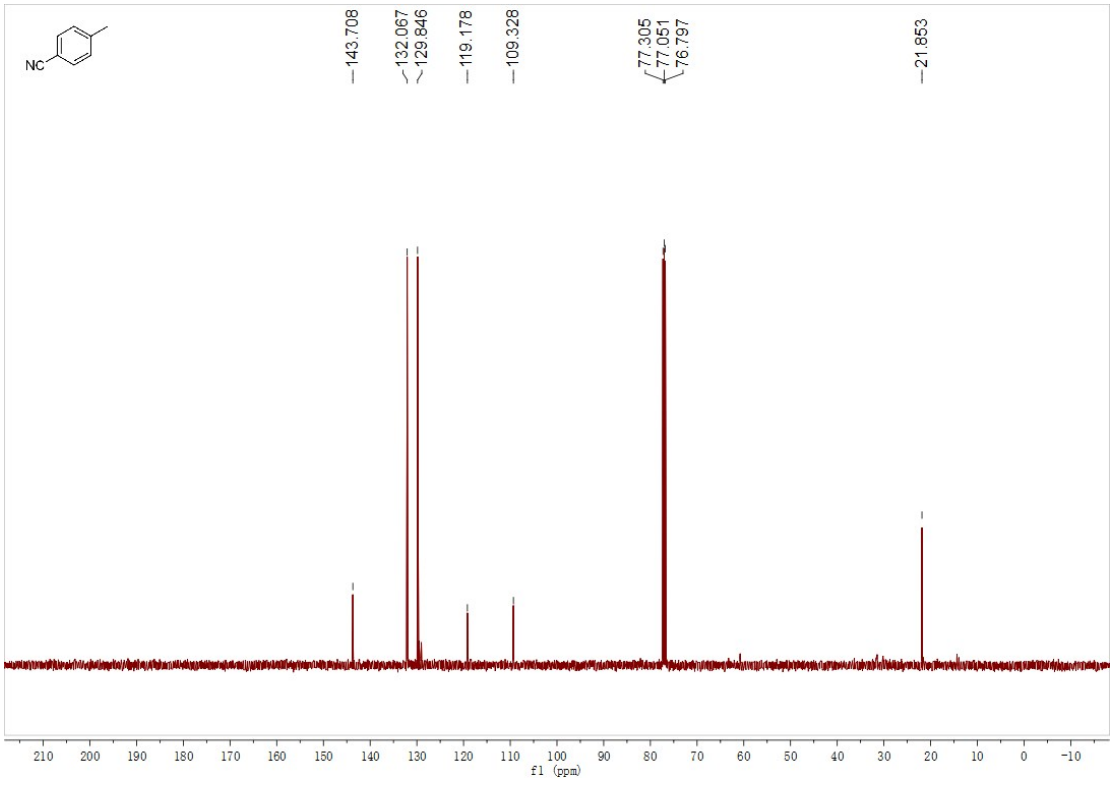
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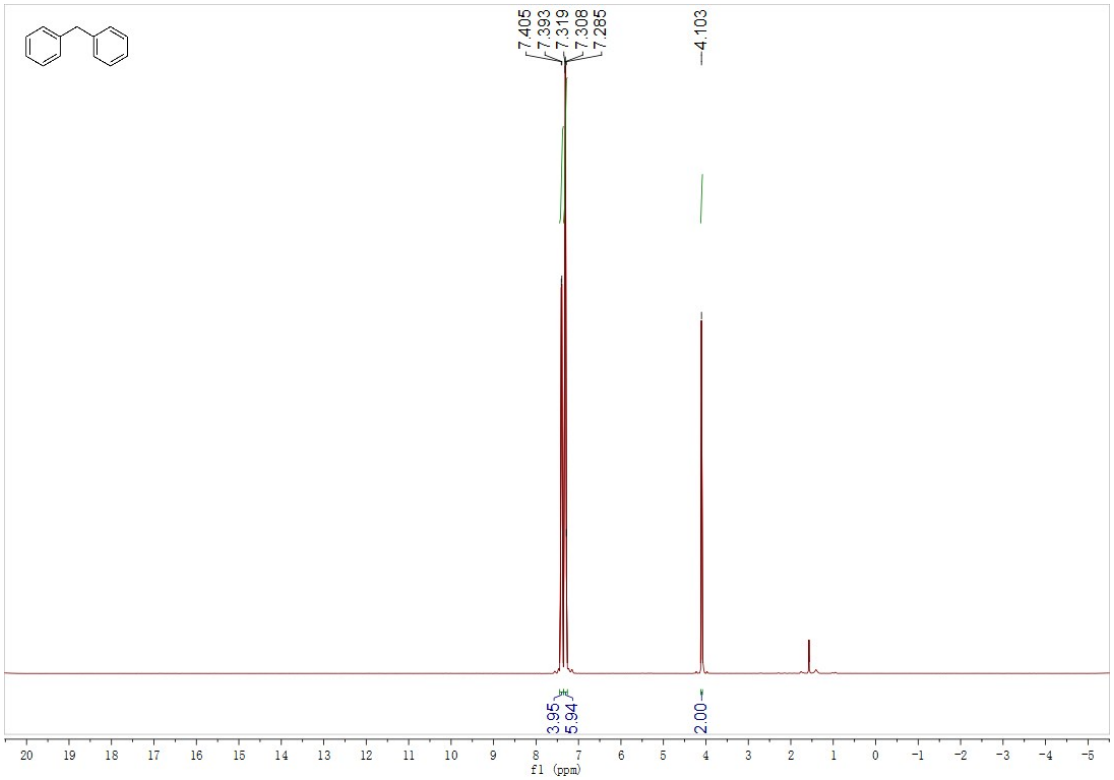
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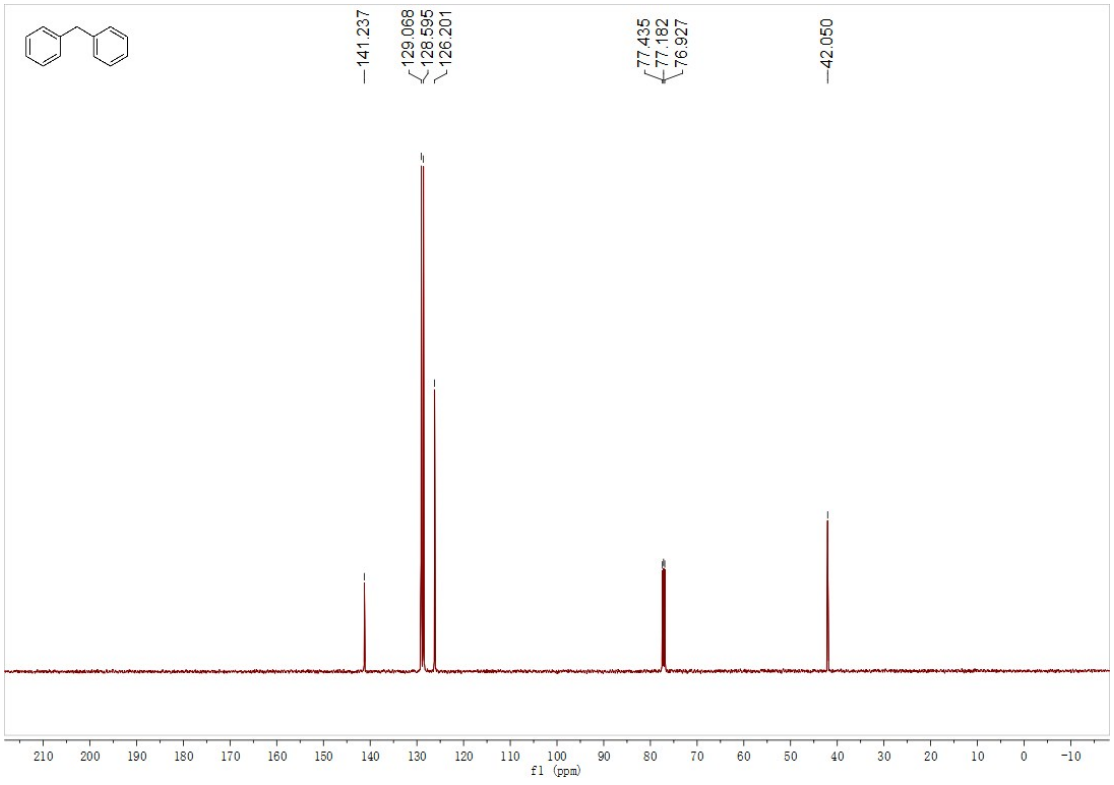
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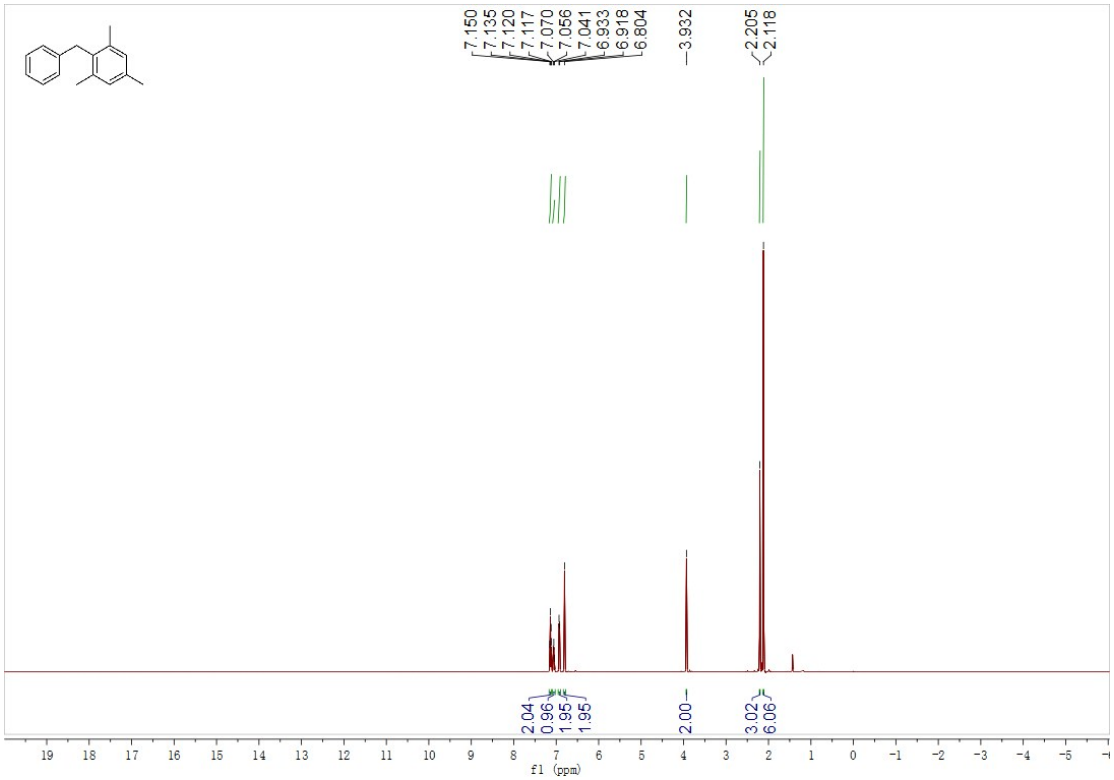
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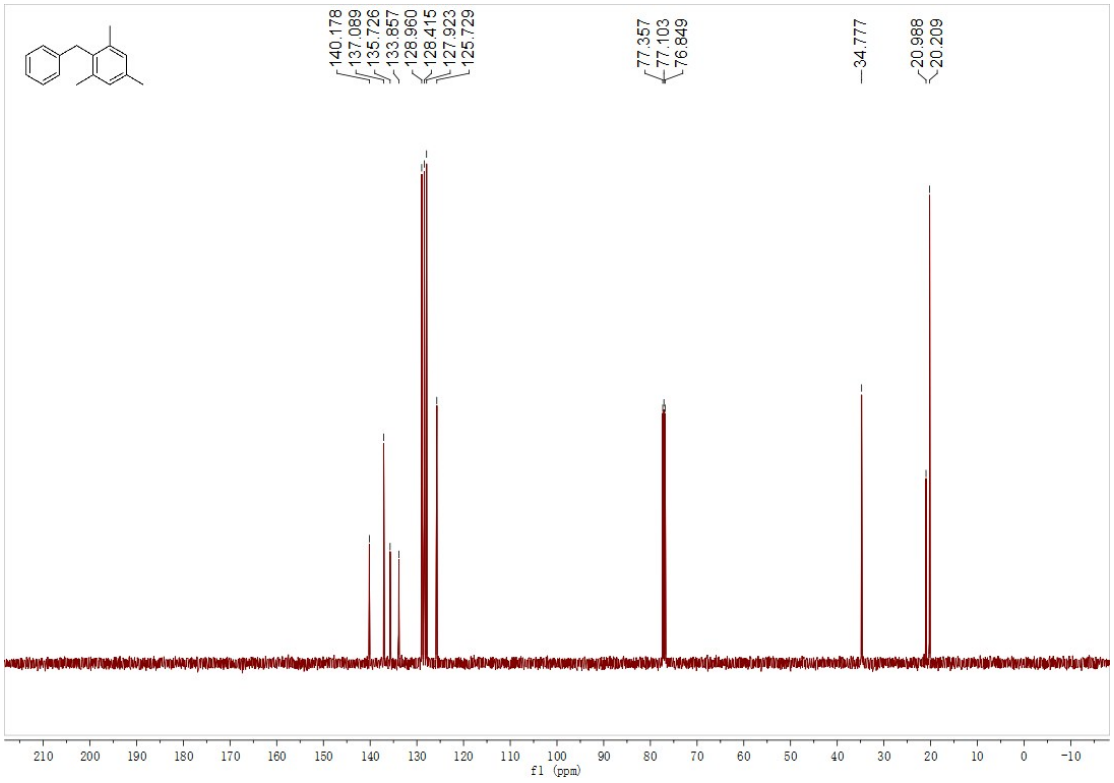
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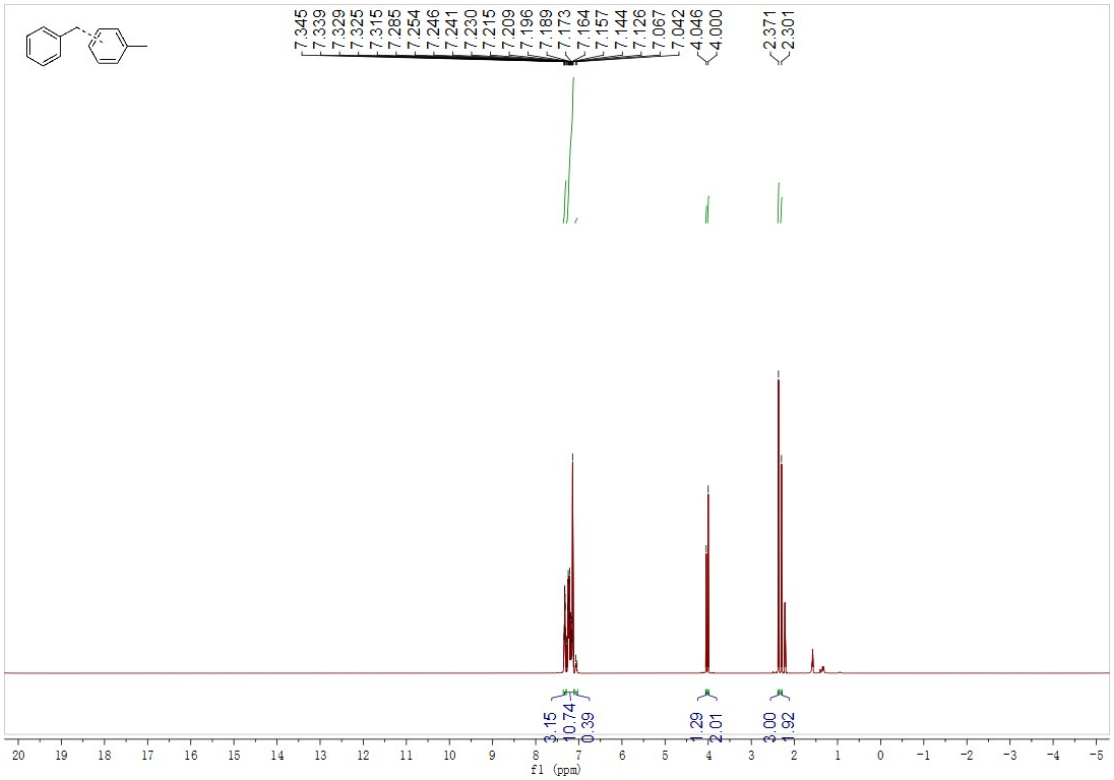
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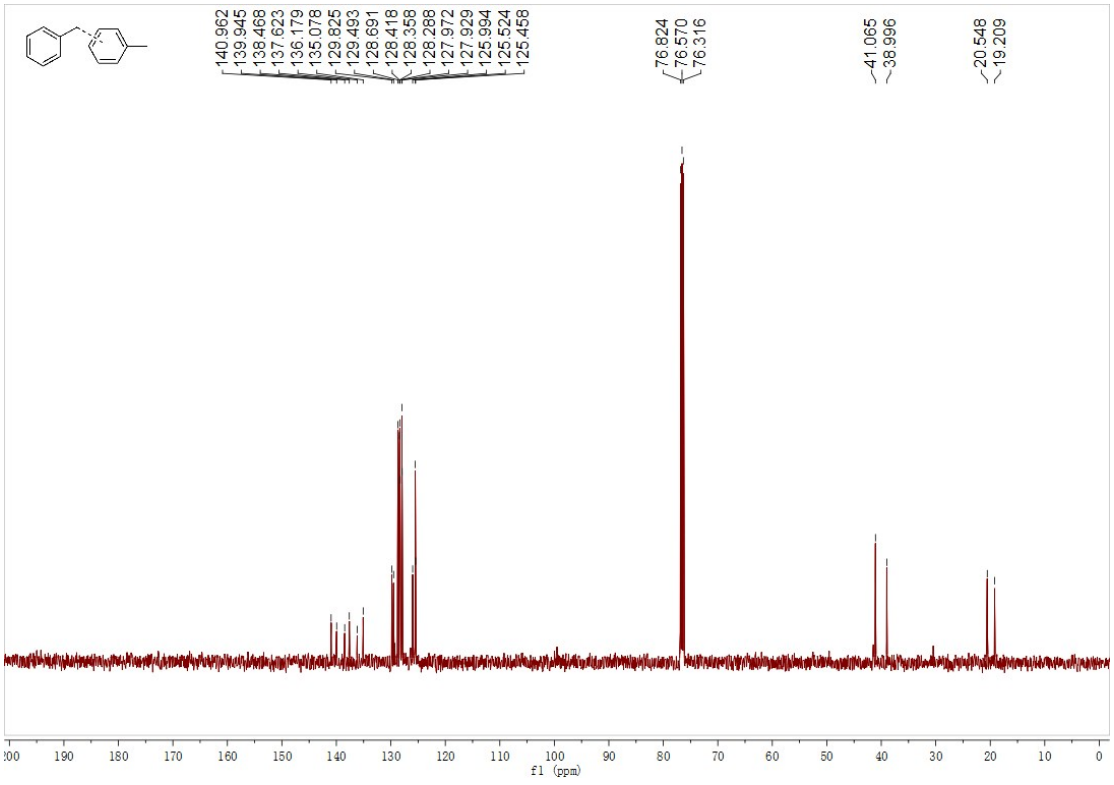
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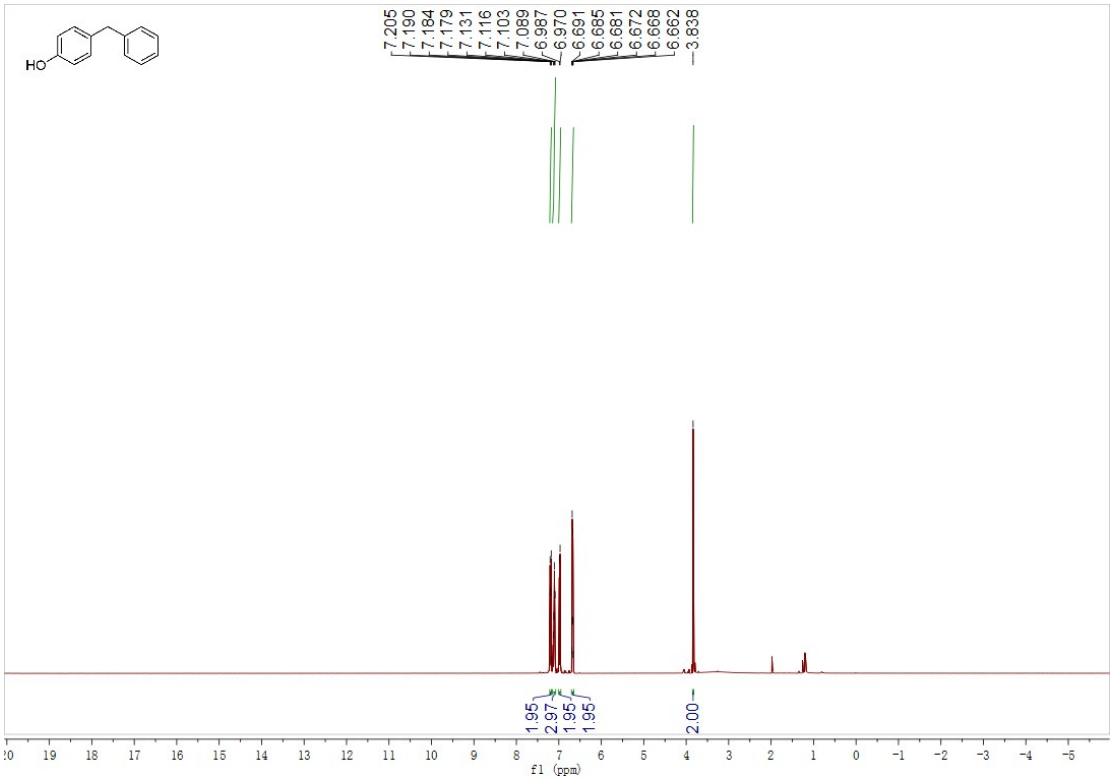
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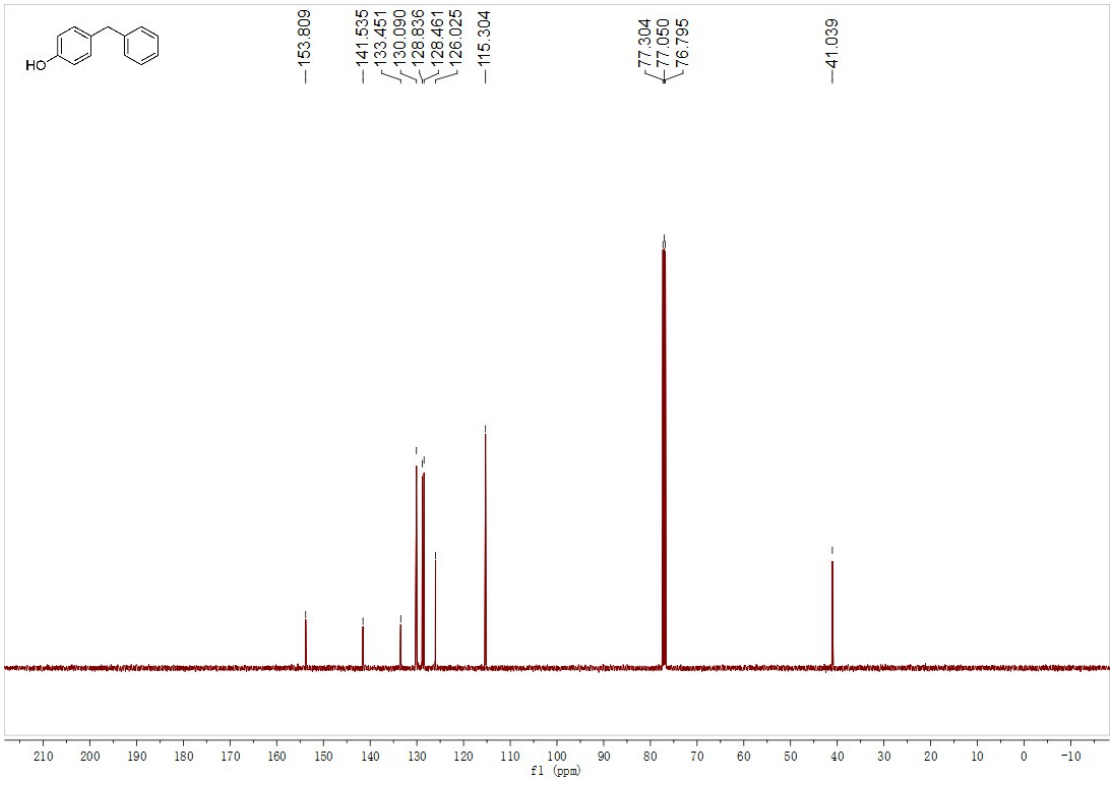
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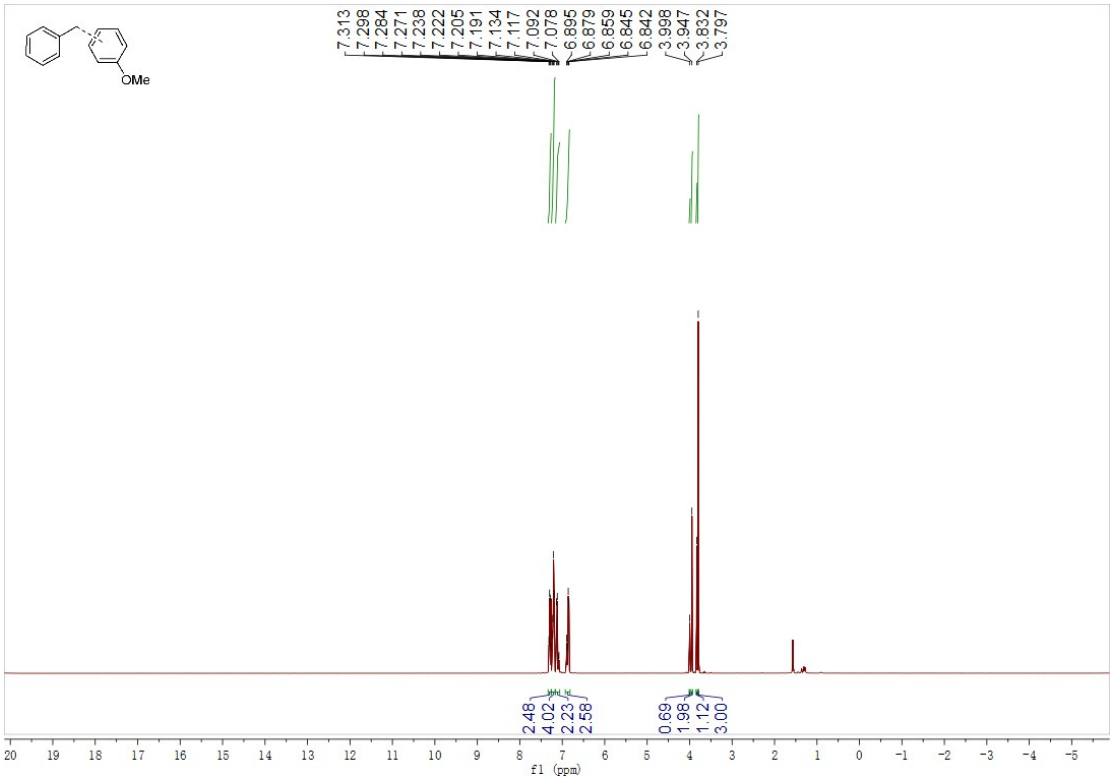
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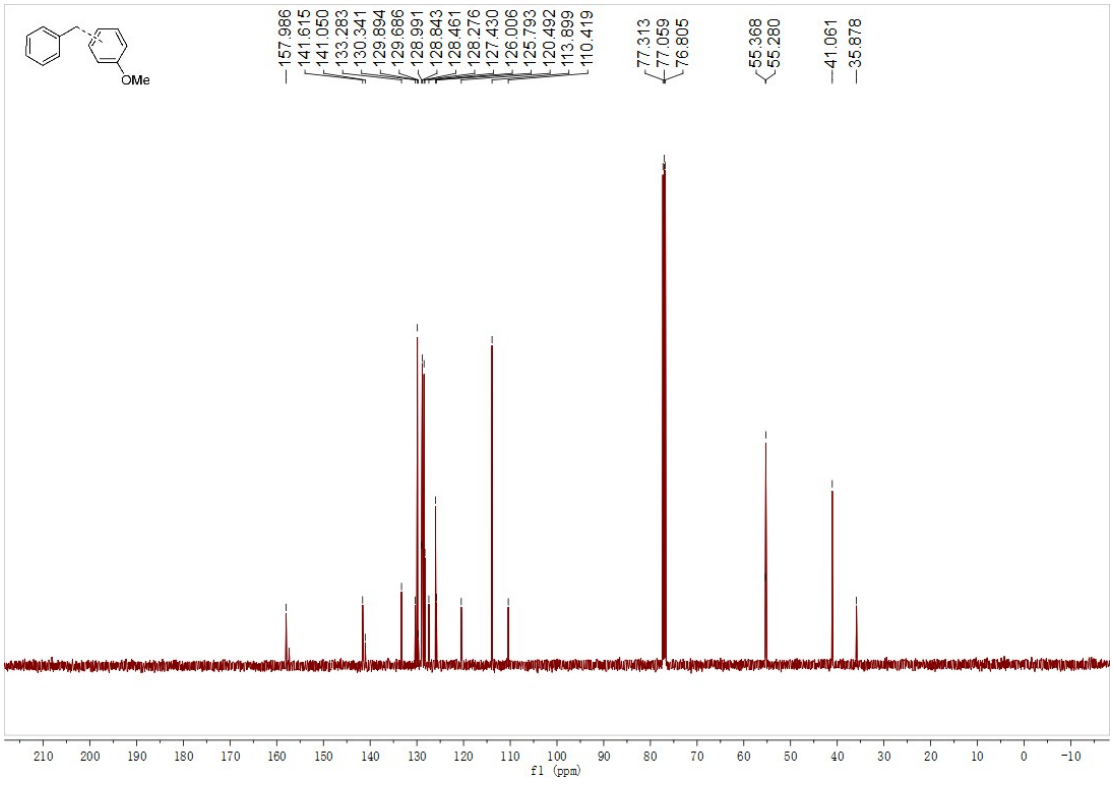
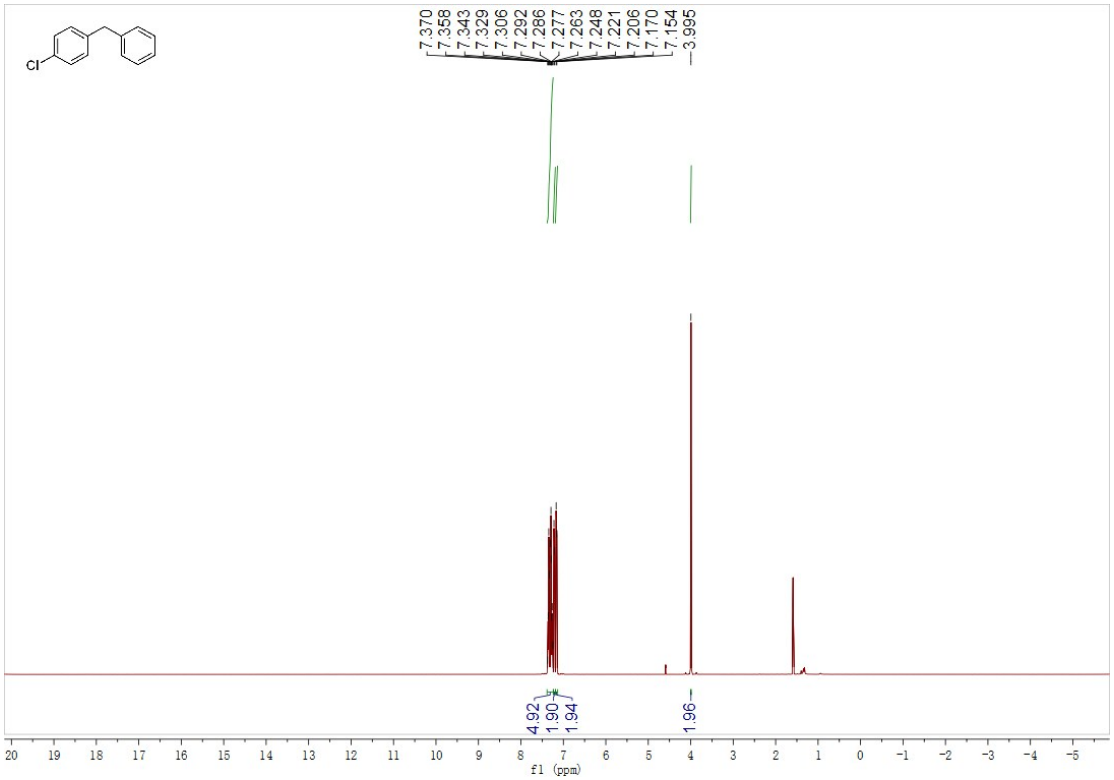
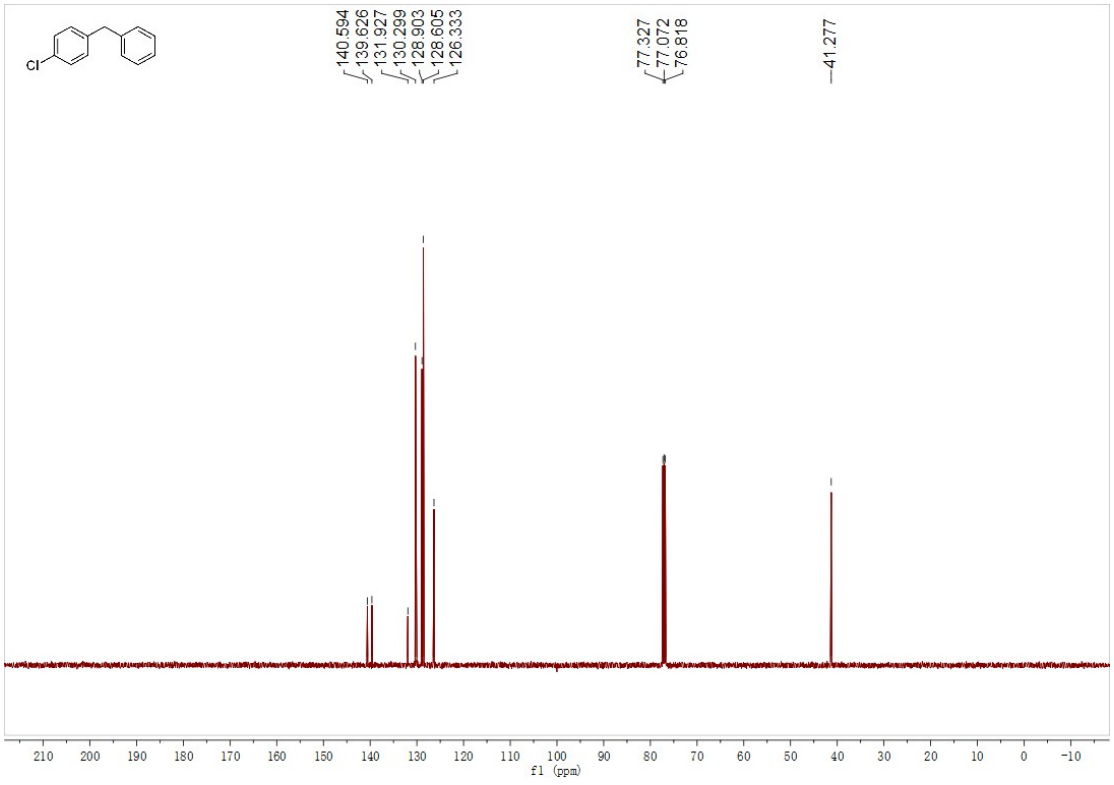
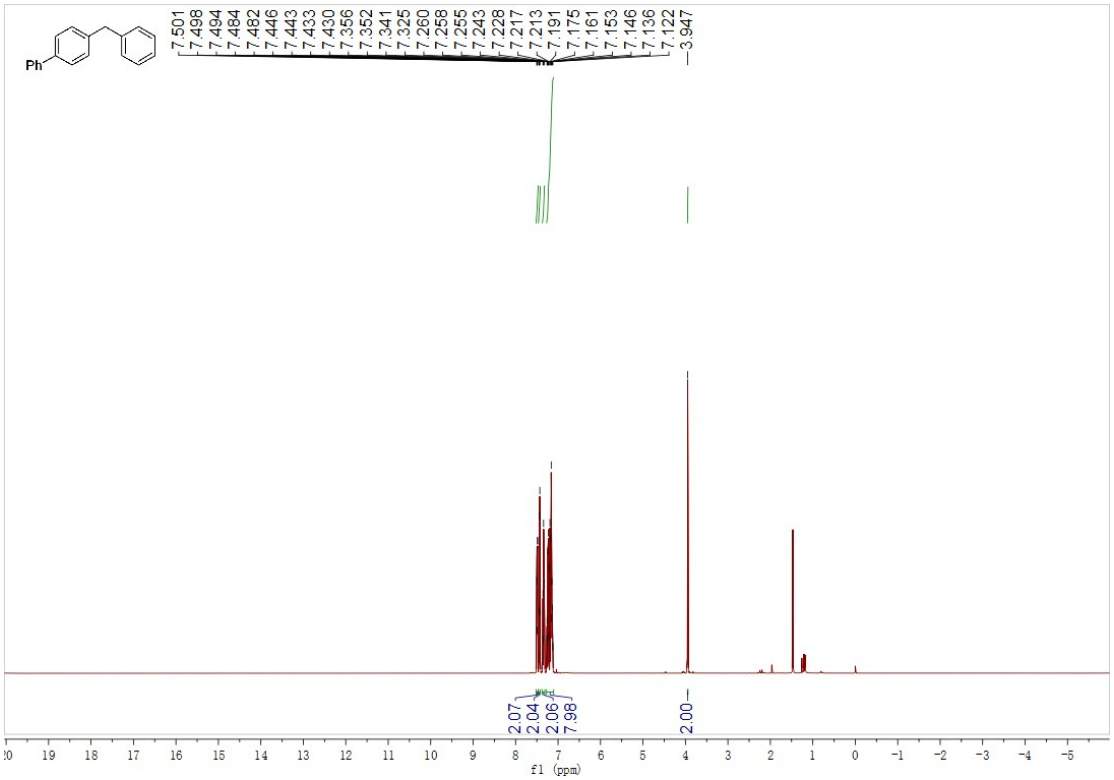
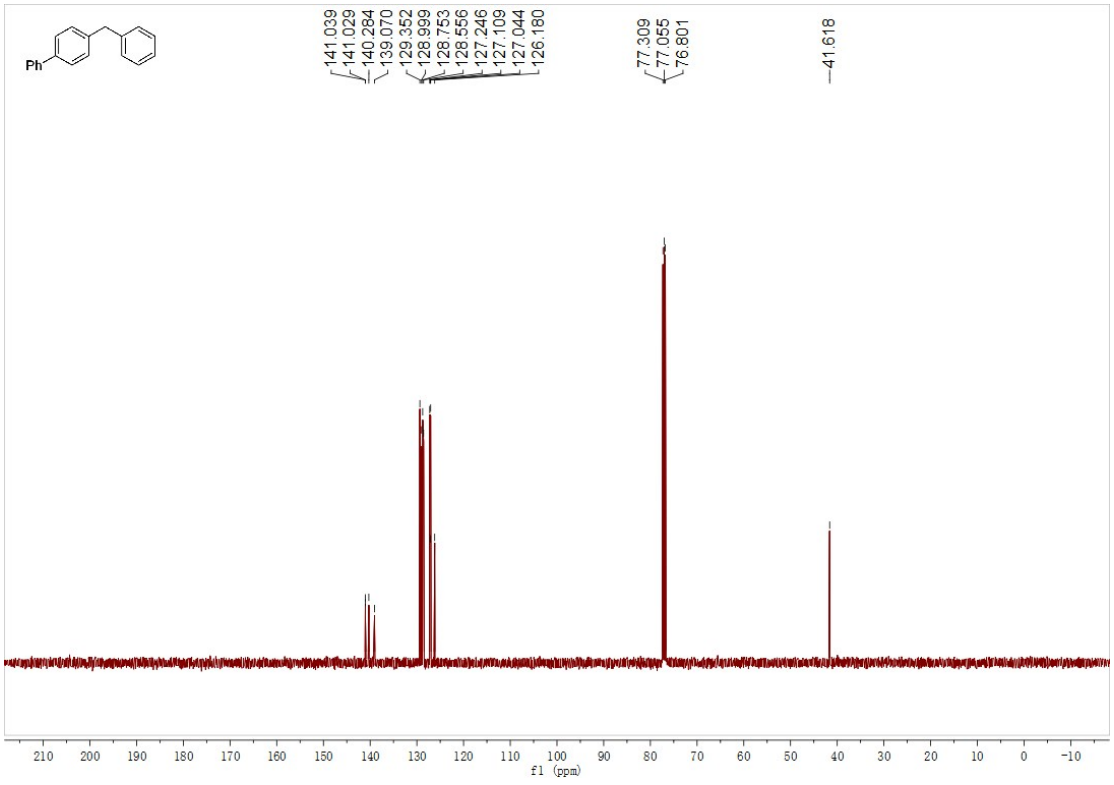
7.092
7.078
6.895
6.879
6.859
6.845
6.842
3.998
3.947
3.832
3.797
2.48
4.02
2.23
2.58
0.69
1.98
1.12
3.00
f1 (ppm)

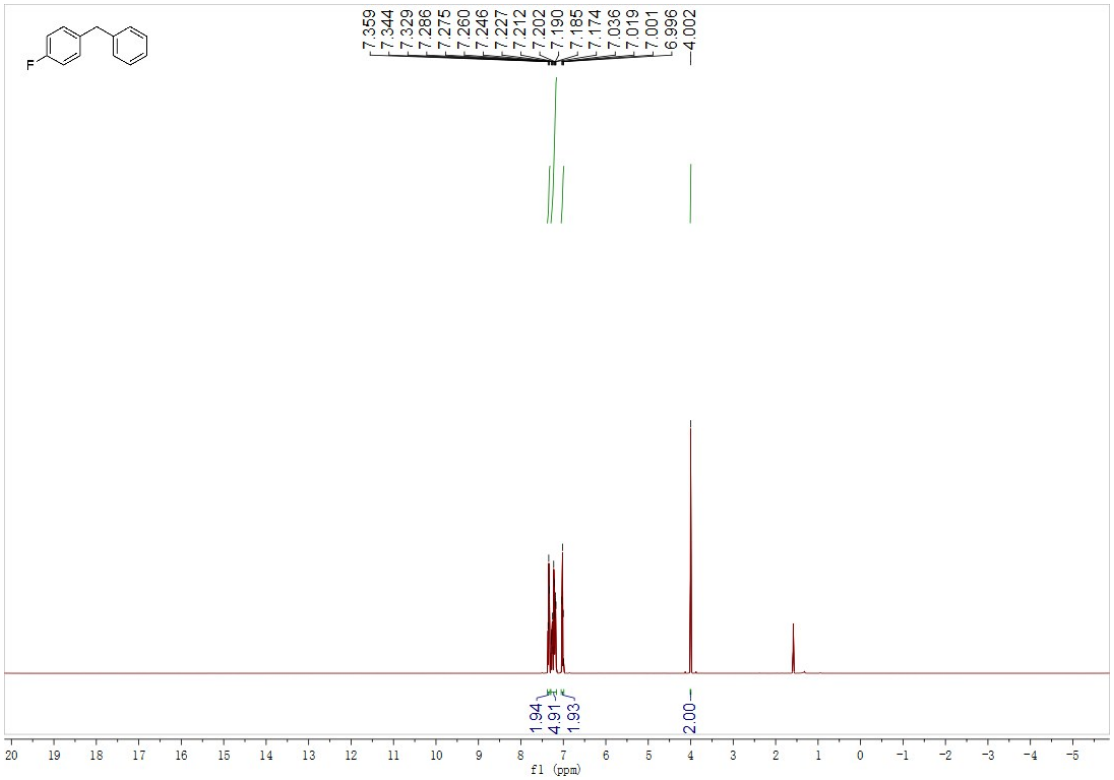

OMe
157.986
141.615
141.050
133.283
130.341
129.894
129.686
128.991
128.843
128.461
128.276
127.430
126.006
125.793
120.492
113.899
110.419
77.313
77.059
76.805
55.368
55.280
41.061
35.878
f1 (ppm)

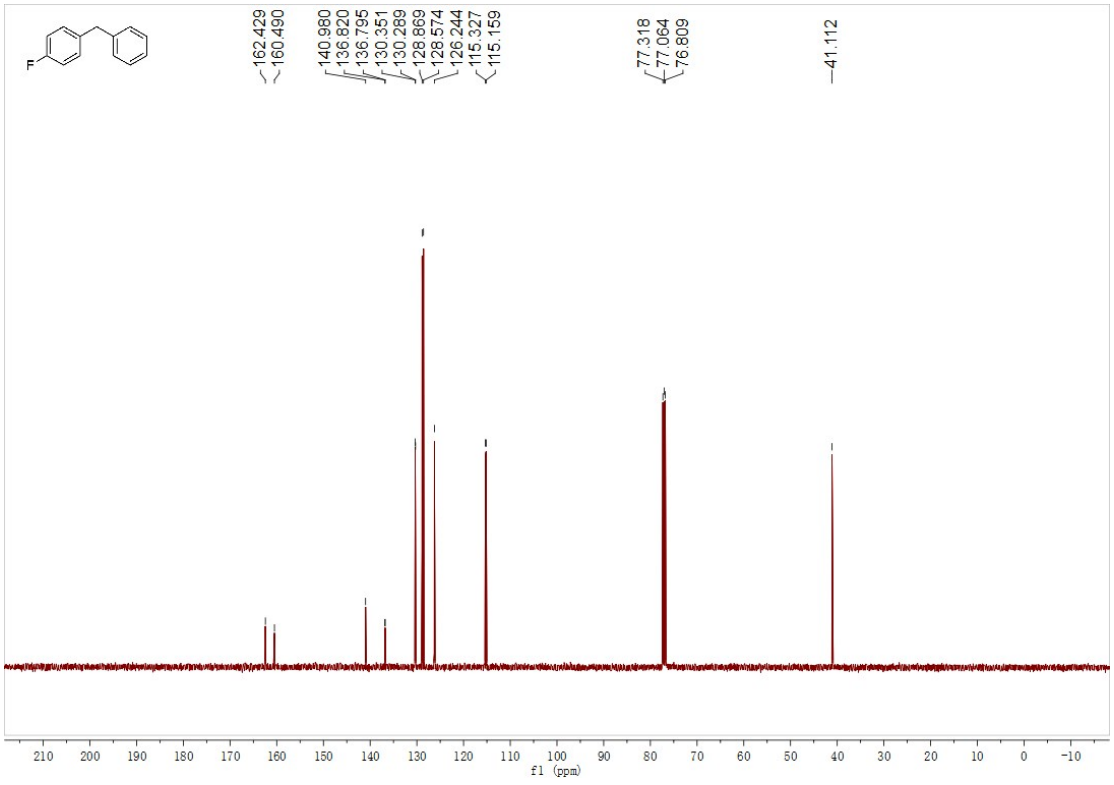

Cl
7.370
7.358
7.343
7.329
7.306
7.292
7.286
7.277
7.263
7.248
7.221
7.206
7.170
7.154
3.995
4.92
1.90
1.94
1.96
f1 (ppm)

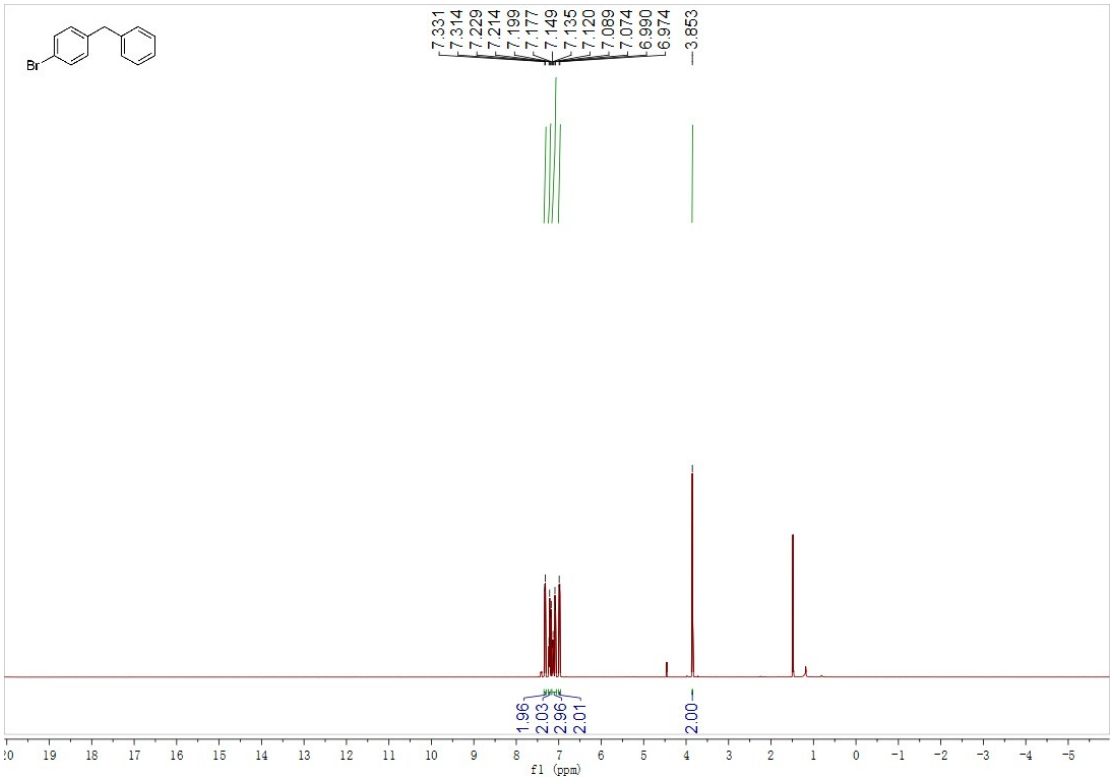

Cl
140.594
139.626
131.927
130.299
128.903
128.605
126.333
77.327
77.072
76.818
41.277
f1 (ppm)

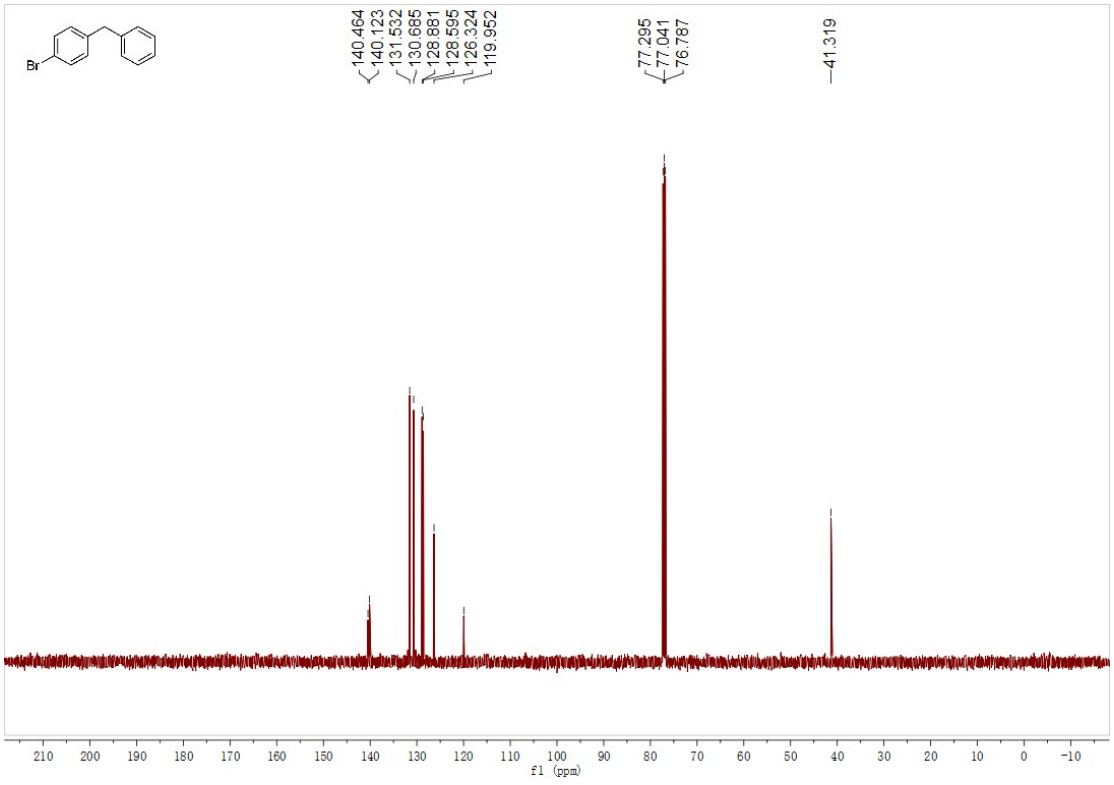

Ph
7.501
7.498
7.494
7.484
7.482
7.446
7.443
7.433
7.430
7.356
7.352
7.341
7.325
7.260
7.258
7.255
7.243
7.228
7.217
7.213
7.191
7.175
7.161
7.153
7.146
7.136
7.122
3.947
2.07
2.04
2.06
7.98
2.00
f1 (ppm)

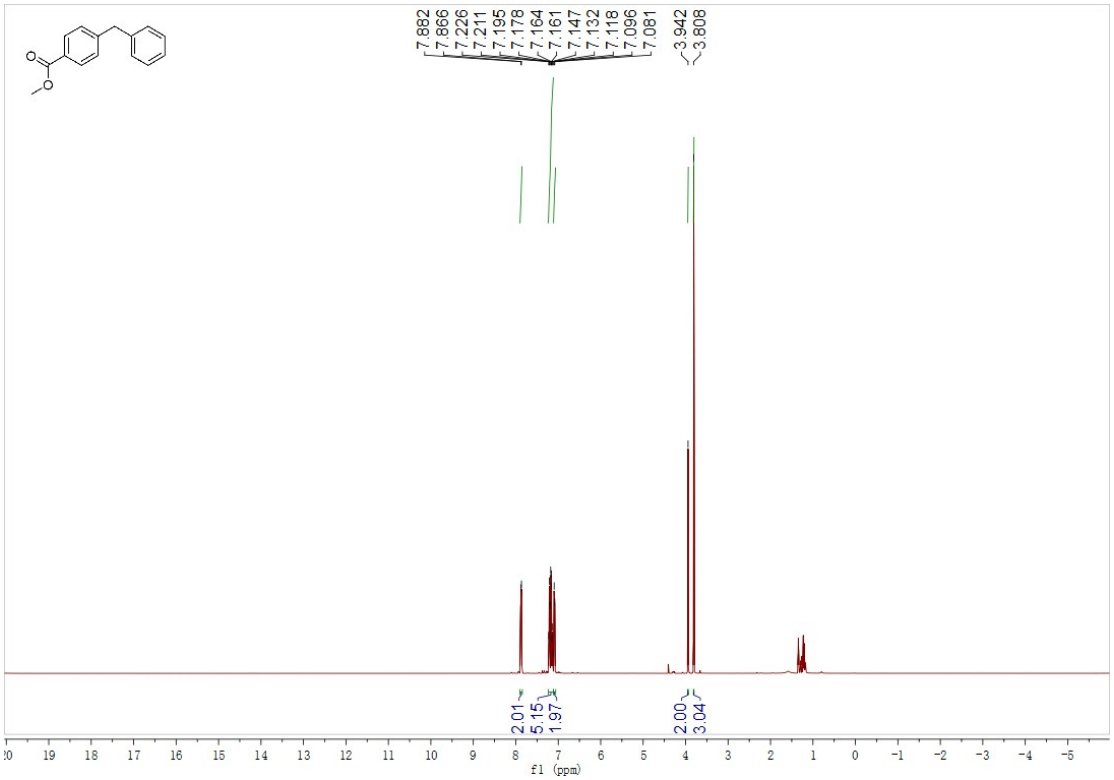

Ph
141.039
141.029
140.284
139.070
129.352
128.999
128.753
128.556
127.246
127.109
127.044
126.180
77.309
77.055
76.801
41.618
f1 (ppm)

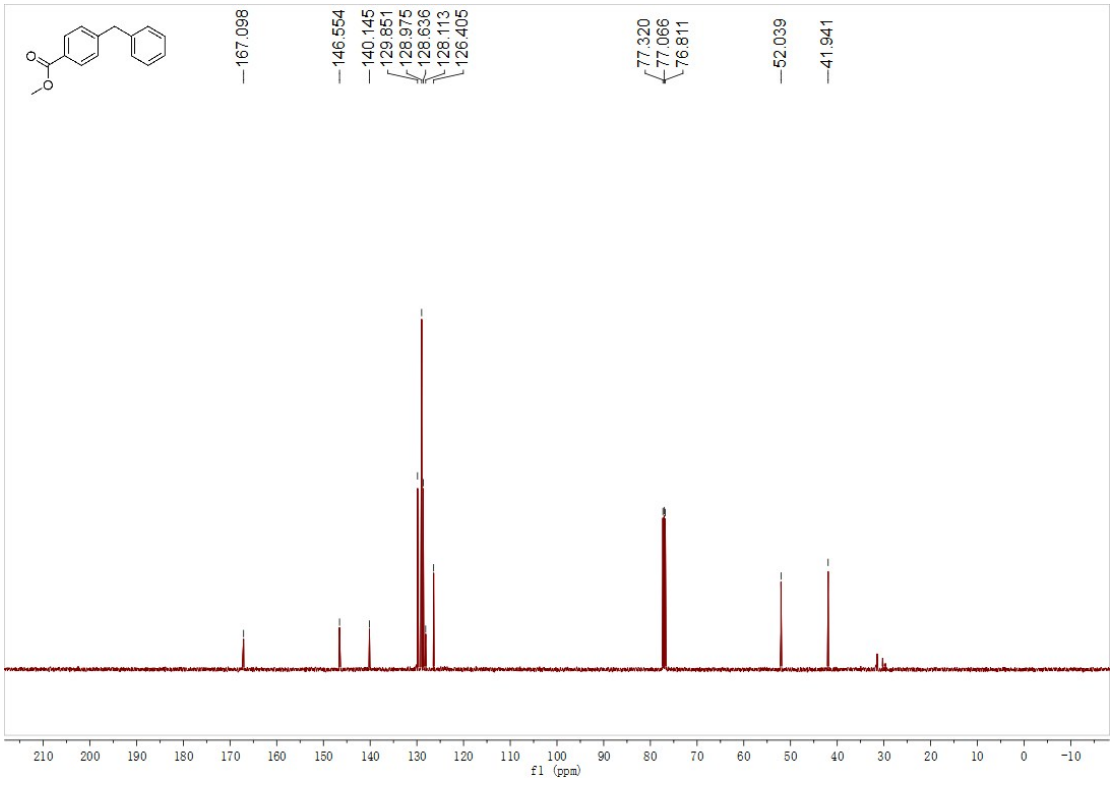

F
7.359
7.344
7.329
7.286
7.275
7.260
7.246
7.227
7.212
7.202
7.190
7.185
7.174
7.036
7.019
7.001
6.996
4.002
1.94
4.91
1.93
2.00
f1 (ppm)


F
162.429
160.490
140.980
136.820
136.795
130.351
130.289
128.869
128.574
126.244
115.327
115.159
77.318
77.064
76.809
41.112
f1 (ppm)


Br
7.331
7.314
7.229
7.214
7.199
7.177
7.149
7.135
7.120
7.089
7.074
6.990
6.974
3.853
1.96
2.03
2.96
2.01
2.00
f1 (ppm)


Br
140.464
140.123
131.532
130.685
128.881
128.595
126.324
119.952
77.295
77.041
76.787
41.319
f1 (ppm)


7.882
7.866
7.226
7.211
7.195
7.178
7.164
7.161
7.147
7.132
7.118
7.096
7.081
3.942
3.808
2.01
5.15
1.97
2.00
3.04
f1 (ppm)


167.098
146.554
140.145
129.851
128.975
128.636
128.113
126.405
77.320
77.066
76.811
52.039
41.941
f1 (ppm)