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An efficient and atom-economical route to *N*-aryl amino alcohols from primary amines

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Experimental Section

Instrumentation and chemicals

^{1}H NMR, ^{13}C NMR spectra were recorded on a Bruker DPX-400 spectrometer with $CDCl_3$ as the solvent and TMS as an internal standard, operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR. Melting points were measured by SGW X-4A microscopic apparatus. The X-ray crystallography was measured on Bruker D8 VENTURE PHOTON instrument. HRMS-ESI were measured by Q Exactive LC/HRMS spectrometer. Ethyl acetate and hexane were used for column chromatography without further purification. All solvents and chemicals were obtained from commercial sources and used as received unless otherwise noted. All the substrates **2** were prepared through the coupling between corresponding picolinamides and cyclic ethers according to our previous work. [1]

General Procedure for the Reduction/Ring-opening Reaction of 2. A mixture of the picolinamide **2** (0.2 mmol), NaBH4 (5 equiv, 1.0 mmol) were added into a vial containing a stirring bar and sealed with a Teflon-lined cap. Then ethanol and water (1mL, v:v=100:1) was introduced. The resulting mixture was stirred at 60 °C for 12 h. Then it was added into H2O (15 mL) and extracted with EtOAc (10 mL) for three times. The combined organic layer was dried over anhydrous MgSO4 and filtered. After removal of the solvent *in vacuo*, the product was obtained through column chromatography with EtOAc/hexane (1/10).

Synthesis of picolinamide 1f. A mixture of 2-picolinic acid (1.48 g, 12 mmol), 4-methoxyaniline (1.23 g, 10 mmol) and triethylamine (2.0 equiv) were dissolved in dichloromethane (10 mL) in a 50 mL round-bottom flask. Dropwise POCl3 (2.0 equiv) was added under stirring in ice-bath. The reaction solution was allowed to warm to room temperature for 2 hour. Then reaction mixture was diluted with CH2Cl2 (20 mL) and 1 M NaOH solution (5mL) and extracted with CH2Cl2 for 3 times. The crude organic layers were collected and washed by water (15 mL).Then it was dried over anhydrous MgSO4, filtered and concentrated *in vacuo*. The product was obtained throughcolumn chromatography with EtOAc/hexane (1/20).

Synthesis of 2f. A mixture of *N*-(4-methoxyphenyl)-*N*-(2-tetrahydrofuranyl)picolinamide (9.47

mmol), $Cu(OAc)_2$ (5 mol%), 1,10-phenanthroline (5 mol%) and TBHP (3.5 equiv, 70% aqueous solution) were added into a vial containing a stirring bar and sealed with a Teflon-lined cap. Then ether (20 mL) was introduced. The resulting mixture was stirred at 25 °C for 8 h. After reaction the mixture was added into H_2O (25 mL) and extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over anhydrous $MgSO_4$ and filtered. After removal of the solvent in vacuo, the residue was purified by column chromatography (EtOAc/hexane=1:5) to afford the pure product.

Synthesis of 3f. A mixture of the **2f** (8.89 mmol), NaBH4 (5 equiv, 44.45 mmol) were added into a vial containing a stirring bar and sealed with a Teflon-lined cap. Then ethanol and water (v:v=100:1) was introduced. The resulting mixture was stirred at 60 °C for 12 h. Then the mixture was added into H2O (25 mL) and extracted with EtOAc (20 mL) for three times. The combined organic layer was dried over anhydrous MgSO4 and filtered. After removal of the solvent *in vacuo*, the product was obtained through column chromatography with EtOAc/hexane (1/10).

Synthesis of 4. To a solution of alcohol (1 equiv) in toluene (0.1 Malcohol) was added the benzhydrol (1 equiv) and dry *p*-TsOH (1 equiv). This mixture was refluxed using a Dean–Stark trap for 6 h. The reaction was diluted with ethyl acetate and extracted two times with saturated $NaHCO_3$. The organic layer was dried over Na_2SO_4, concentrated under reduced pressure, and purified by flash chromatography. Note: Dry *p*-TsOH was obtained by refluxing *p*-TsOH monohydrate in toluene under Dean–Stark conditions for 6 h. This mixture was then concentrated under reduced pressure and placed under vacuum to afford brown solid. Place under vacuum for 30 min before each use.

Characterization Data

Characterization data of all substrates **2** are reported[1] except **2s** and **2t** whose data are in the following.

N-(1,3-dihydroisobenzofuran-1-yl)-*N*-phenylpicolinamide (**2s**)

Yellow Oil, ^1H NMR (400 MHz, $CDCl_3$): δ 4.51–4.55 (m, 1H), 4.80–4.82 (m, 1H), 6.91–7.23 (m,

9H), 7.45–7.83 (m, 4H), 8.27 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 73.1, 89.9, 120.8, 123.4, 124.0, 127.5, 127.7, 128.2, 128.9, 130.5, 136.4, 137.8, 139.8, 148.6, 154.9, 169.3; HRMS-ESI (m/z): calcd for $C20H17N_2O_2$ (M+H): 317.1285, found 317.1284.

N-(isochroman-1-yl)-*N*-phenylpicolinamide (**2t**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.50–2.69 (m, 2H), 3.87–3.97 (m, 2H), 6.97–7.23 (m, 9H), 7.45–7.52 (m, 4H), 8.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.5, 63.8, 123.6, 123.9, 124.0, 126.5, 126.9, 127.2, 127.5, 128.1, 128.4, 128.9, 130.2, 133.2, 135.8, 136.2, 148.6, 154.3, 170.0; HRMS-ESI (m/z): calcd for $C_{21}H19N_2O_2$ (M+H): 331.1441, found 331.1444.

4-(phenylamino)butan-1-ol (**3a**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.65–1.66 (m, 4H), 2.90 (br, 2H), 3.10–3.13 (m, 2H), 3.62-3.65 (m, 2H), 6.60–6.62 (m, 2H), 6.68–6.72 (m, 1H), 7.15-7.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.1, 30.3, 44.0, 62.5, 113.1, 117.5, 129.3, 148.4; HRMS-ESI (m/z): calcd for C10H16NO (M+H): 166.1226, found 166.1229.

4-(o-tolylamino)butan-1-ol (**3b**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.68–1.77 (m, 4H), 2.13 (s, 3H), 2.69 (br, 2H),3.17–3.20 (m, 2H), 3.67-3.70 (m, 2H), 6.61–6.68 (m, 2H), 7.05–7.06 (m, 1H), 7.11-7.15 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 17.6, 26.1, 30.4, 43.8, 62.6, 109.9, 117.0, 122.1, 127.2, 130.1, 146.2; HRMS-ESI (m/z): calcd for C11H18NO (M+H): 180.1383, found 180.1382.

4-(m-tolylamino)butan-1-ol (**3c**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.66–1.71 (m, 4H), 2.27 (s, 3H), 2.48 (br, 2H), 3.12–3.15 (m, 2H), 3.66-3.69 (m, 2H), 6.42–6.44 (m, 2H), 6.52–6.54 (m, 1H), 7.04-7.08 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 26.2, 30.4, 44.0, 62.6, 110.2, 113.8, 118.5, 129.1, 139.0, 148.4; HRMS-ESI (m/z): calcd for C11H18NO (M+H): 180.1383, found 180.1380.

4-(p-tolylamino)butan-1-ol (**3d**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.68–1.70 (m, 4H), 2.24 (s, 3H), 2.51 (br, 2H), 3.11-

3.15 (m, 2H), 3.66–3.70 (m, 2H), 6.55–6.57 (m, 2H), 6.98–7.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.4, 26.2, 30.5, 44.4, 62.7, 113.3, 126.9, 129.8, 146.0; HRMS-ESI (m/z): calcd for C11H18NO (M+H): 180.1383, found 180.1385.

4-((4-ethylphenyl)amino)butan-1-ol (**3e**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.17–1.20 (m, 3H), 1.68-1.70 (m, 4H), 2.44 (br, 2H), 2.54 (dd, J_1= 7.60Hz, J_2=15.16Hz), 3.12–3.15 (m, 2H), 3.67-3.70 (m, 2H), 6.57–6.59 (m, 2H), 7.01-7.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 16.0, 26.2, 30.5, 44.3, 62.6, 113.2, 128.6, 133.5, 146.2; HRMS-ESI (m/z): calcd for C12H20NO (M+H): 194.1539, found 194.1535.

4-((4-methoxyphenyl)amino)butan-1-ol (**3f**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.69–1.70 (m, 4H), 2.59 (br, 2H), 3.09–3.13 (m, 2H), 3.66-3.69 (m, 2H), 3.75 (s, 3H), 6.61–6.63 (m, 2H), 6.77–6.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.4, 30.6, 45.2, 55.8, 62.6, 114.7, 114.9, 142.3, 152.4; HRMS-ESI (m/z): calcd for C11H18NO_2 (M+H): 196.1332, found 196.1333.

4-((4-fluorophenyl)amino)butan-1-ol (**3g**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.69–1.71 (m, 4H), 2.20-2.34 (m, 2H), 3.10–3.13 (m, 2H), 3.69-3.71 (m, 2H), 6.54–6.58 (m, 2H), 6.87–6.91 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.1, 30.4, 44.7, 62.6, 113.9 (d, *J*=7.37Hz), 115.7 (d, *J*=22.15Hz), 144.6, 155.9 (d, *J*=233.55Hz); HRMS-ESI (m/z): calcd for C10H15FNO (M+H): 184.1132, found 184.1130.

4-((4-chlorophenyl)amino)butan-1-ol (**3h**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.67–1.70 (m, 4H), 2.63 (br, 2H), 3.09–3.12 (m, 2H), 3.66-3.69 (m, 2H), 6.51–6.53 (m, 2H), 7.10–7.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.9, 30.2, 44.0, 62.5, 113.9, 121.8, 129.1, 147.0；HRMS-ESI (m/z): calcd for C10H15ClNO (M+H): 200.0837, found 200.0839.

4-((4-bromophenyl)amino)butan-1-ol (**3i**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.67–1.69 (m, 4H), 2.59 (br, 2H), 3.09–3.12 (m, 2H),

3.67-3.70 (m, 2H), 6.47–6.49 (m, 2H), 7.22–7.23 (m, 1H), 7.24-7.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.9, 30.2, 43.8, 62.5, 108.8, 114.4, 131.9, 147.3; HRMS-ESI (m/z): calcd for C10H15BrNO (M+H): 244.0332, found 244.0330.

4-((3,4-dimethylphenyl)amino)butan-1-ol (**3j**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.67–1.70 (m, 4H), 2.15 (s, 3H), 2.19 (s, 3H), 2.51 (br, 2H), 3.11–3.14 (m, 2H), 3.66-3.69 (m, 2H), 6.39–6.42 (m, 1H), 6.46–6.47 (m, 1H), 6.93-6.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.7, 20.1, 26.3, 30.5, 44.4, 62.7, 110.6, 115.1, 125.7, 130.3, 137.3, 146.4; HRMS-ESI (m/z): calcd for C12H20NO (M+H): 194.1539, found 194.1543.

4-((3-methoxy-4-methylphenyl)amino)butan-1-ol (**3k**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.69–1.70 (m, 4H), 2.10 (s, 3H), 2.49 (br, 2H), 3.12–3.15 (m, 2H), 3.67-3.70 (m, 2H), 3.79 (s, 3H), 6.14–6.16 (m, 2H), 6.91-6.93 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.3, 26.2, 30.5, 44.4, 55.2, 62.7, 96.8, 104.5, 115.7, 131.0, 147.8, 158.5; HRMS-ESI (m/z): calcd for $C12H20NO_2$ (M+H): 210.1489, found 210.1491.

4-((3-fluoro-4-methylphenyl)amino)butan-1-ol (**3l**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.67–1.69 (m, 4H), 2.14 (d, *J*=1.56Hz), 2.65 (br, 2H), 3.09–3.12 (m, 2H), 3.67-3.69 (m, 2H), 6.27–6.31 (m, 2H), 6.91–6.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.6 (d, *J*=3.25Hz), 26.0, 30.3, 44.1, 62.6, 99.7 (d, *J*=25.95Hz), 108.7 (d, *J*=2.66Hz), 112.8 (d, *J*=17.62Hz), 131.6 (d, *J*=7.11Hz), 148.0 (d, *J*=10.42Hz), 162.13 (d, *J*=240.58Hz); HRMS-ESI (m/z): calcd for C11H17FNO (M+H): 198.1289, found 198.1285.

4-((3-chloro-4-methylphenyl)amino)butan-1-ol (**3m**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.66–1.69 (m, 4H), 2.24 (s, 3H), 2.59 (br, 2H), 3.09–3.10 (m, 2H), 3.67-3.70 (m, 2H), 6.41–6.44 (m, 1H), 6.61–6.62 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.8, 25.9, 30.2, 43.9, 62.5, 111.7, 113.0, 124.1, 131.2, 134.7, 147.4; HRMS-ESI (m/z): calcd for C11H17ClNO (M+H): 214.0993, found 214.0994.

4-((3-bromo-4-methylphenyl)amino)butan-1-ol (**3n**)

Yellow solid, mp 65–68 °C; ^{1}H NMR (400 MHz, CDCl3): δ 1.67–1.69 (m, 4H), 2.27 (s, 3H), 2.57 (br, 2H), 3.09–3.12 (m, 2H), 3.67-3.70 (m, 2H), 6.46–6.48 (m, 1H), 6.80–6.81 (m, 1H), 6.99-7.00 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.7, 25.9, 30.2, 43.9, 62.6, 112.4, 116.2, 125.4, 126.0, 131.0, 147.4; HRMS-ESI (m/z): calcd for C11H17BrNO (M+H): 258.0488, found 258.0486.

5-(phenylamino)pentan-2-ol (**3o**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.21 (d, *J*=6.20Hz, 3H), 1.53–1.58 (m, 2H), 1.64-1.76 (m, 2H), 3.12–3.15 (m, 2H), 3.51 (br, 2H), 3.82–3.87 (m, 1H), 6.61–6.63 (m, 2H), 6.69–6.73 (m, 1H), 7.15–7.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.6, 25.9, 36.8, 44.2, 67.9, 113.1, 117.6, 129.3, 148.3; HRMS-ESI (m/z): calcd for C11H18NO (M+H): 180.1383, found 180.1386.

5-(phenylamino)pentan-1-ol (**3p**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.46–1.52 (m, 2H), 1.59–1.67 (m, 4H), 2.32 (br, 2H), 3.11-3.14 (m, 2H), 3.65–3.68 (m, 2H), 6.59–6.62 (m, 2H), 6.67–6.71 (m, 1H), 7.15–7.19 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.3, 29.3, 32.4, 43.8, 62.8, 112.7, 117.2, 129.2, 148.4; HRMS-ESI (m/z): calcd for C11H18NO (M+H): 180.1383, found 180.1384.

2-(2-(phenylamino)ethoxy)ethan-1-ol (**3q**)

Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.83 (br, 2H), 3.31–3.33 (m, 2H), 3.58–3.60 (m, 2H), 3.70-3.76 (m, 4H), 6.64–6.74 (m, 3H), 7.16–7.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.7, 61.8, 69.7, 72.2, 113.2, 117.8, 129.3, 148.1; HRMS-ESI (m/z): calcd for C10H16NO_2 (M+H): 182.1176, found 182.1178.

4-(phenylamino)butane-1-thiol (**3r**)

Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.80–0.90 (m, 1H), 1.96–2.02 (m, 1H), 2.07-2.16 (m, 2H), 2.23–2.31 (m, 1H), 2.90–2.96 (m, 1H), 3.02–3.08 (m, 1H), 5.32–5.35 (m, 1H), 6.64–6.66 (m, 2H), 6.76–6.80 (m, 1H), 7.18–7.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 29.2, 32.3, 38.1, 64.2, 114.1, 118.8, 129.4, 146.2; HRMS-ESI (m/z): calcd for C10H16NS (M+H): 182.0998, found 182.0995.

(2-((phenylamino)methyl)phenyl)methanol (**3s**)

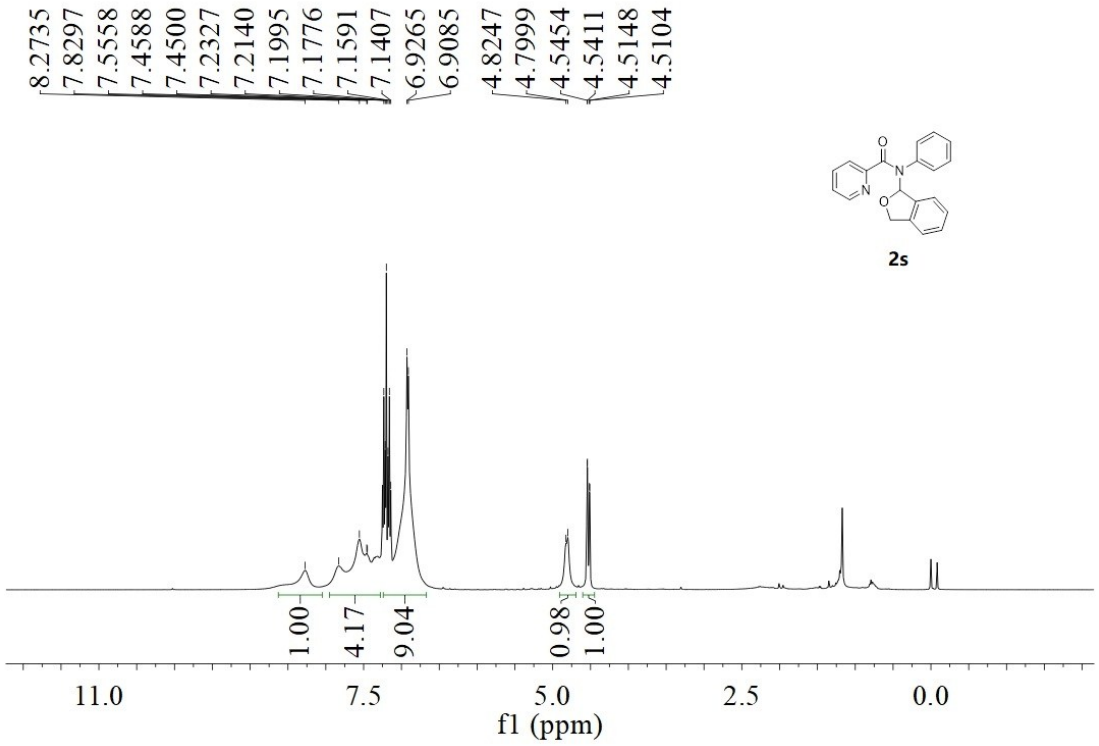
Yellow Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.68 (br, 2H), 4.30 (s, 1H), 4.66 (s, 2H), 6.69–6.71 (m, 2H), 6.78–6.82 (m, 1H), 7.17–7.21 (m, 2H), 7.28–7.31 (m, 2H), 7.34–7.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 47.4, 63.7, 114.3, 119.1, 128.3, 128.4, 129.4, 129.5, 129.8, 137.2, 139.8, 147.8; HRMS-ESI (m/z): calcd for C14H16NO (M+H): 214.1226, found 214.1230.

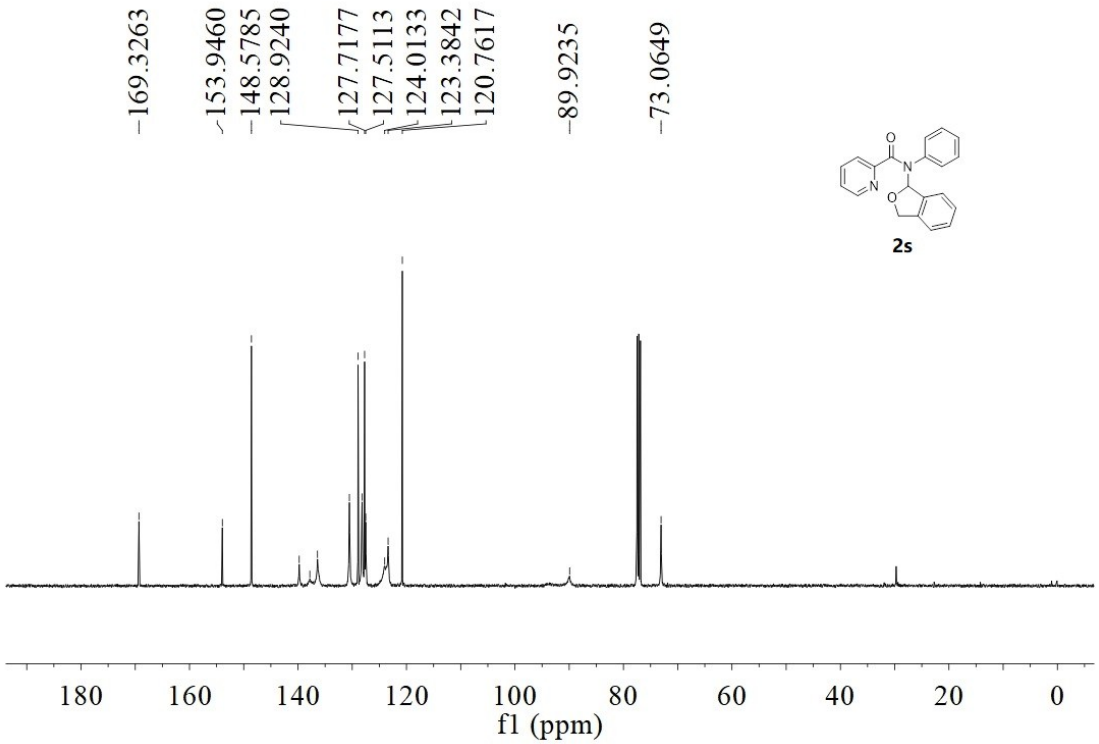
2-(2-((phenylamino)methyl)phenyl)ethan-1-ol (**3t**)

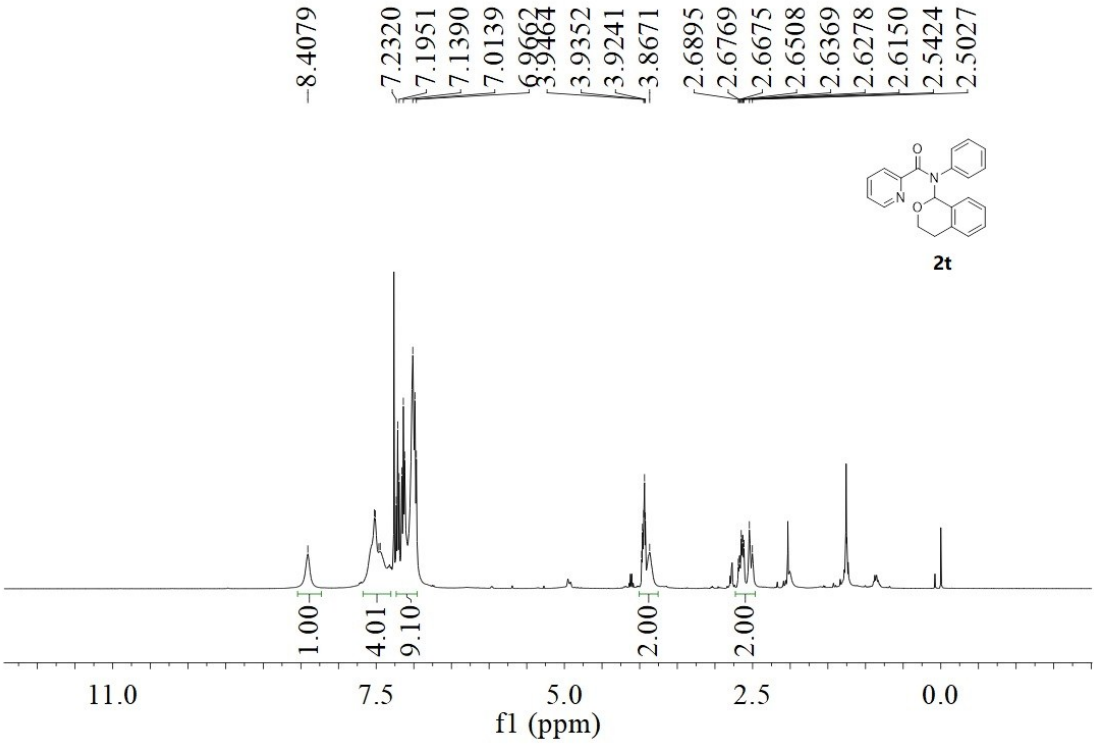
Brown Oil, ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.79–2.82 (m, 2H), 2.93–3.02 (m, 2H), 3.88 (t, *J*=6.36Hz, 2H), 4.28 (s, 2H), 6.60–6.77 (m, 3H), 7.14–7.31 (m, 5H), 7.34–7.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.4, 46.6, 63.5, 113.3, 118.1, 126.9, 128.0, 129.3, 129.6, 130.2, 137.3, 137.7, 148.1; HRMS-ESI (m/z): calcd for C15H18NO (M+H): 228.1383, found 228.1381.

[1] Q. Yue, Z. Xiao, Z. Kuang, Z. Su, Q. Zhang and D. Li, *Adv. Synth. Catal.*, 2018, **360**, 1193.

Copies of ^{1}H and ^{13}C NMR spectra



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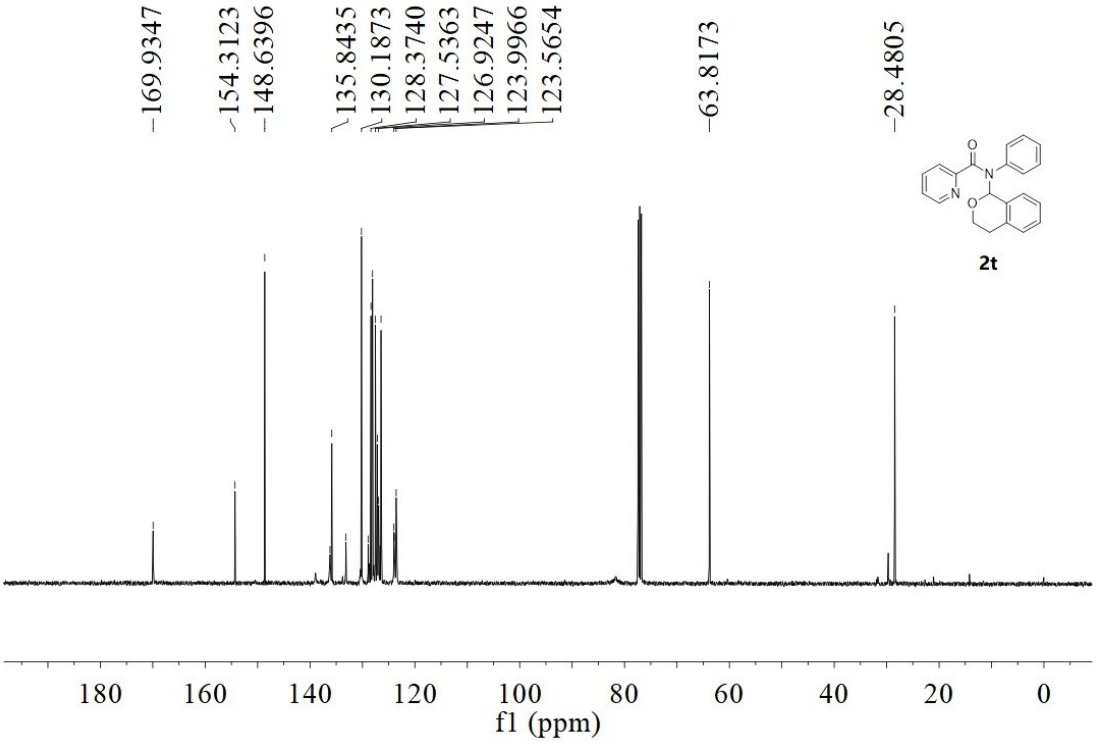
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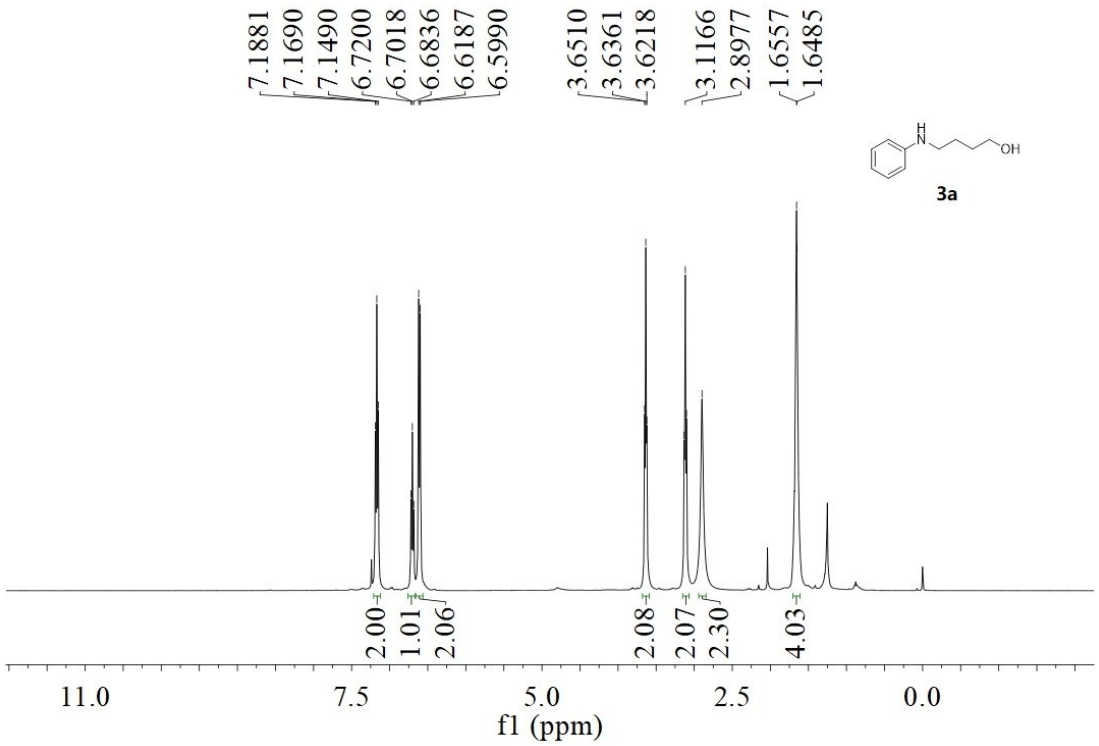
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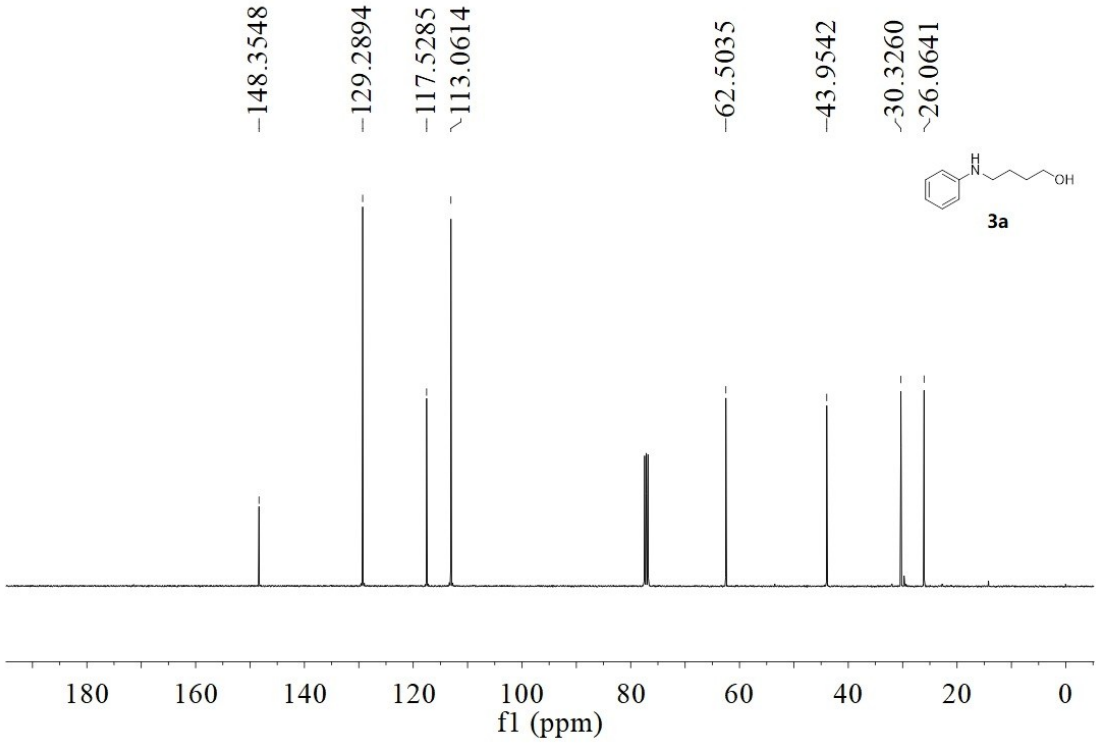
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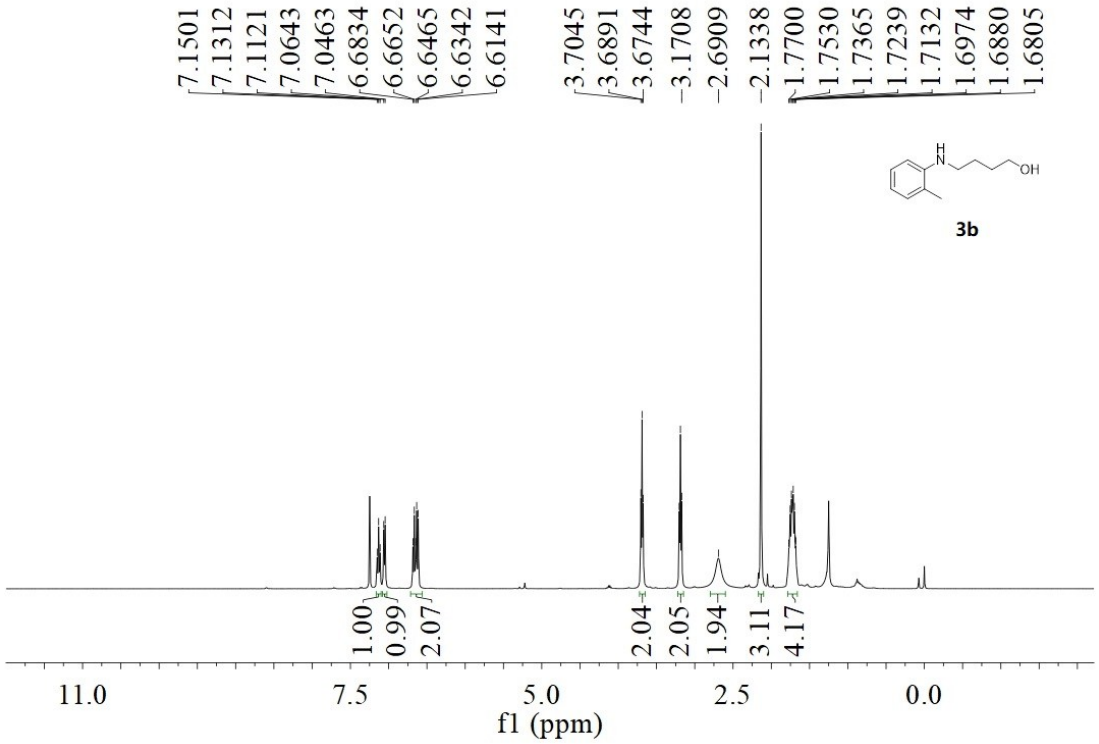
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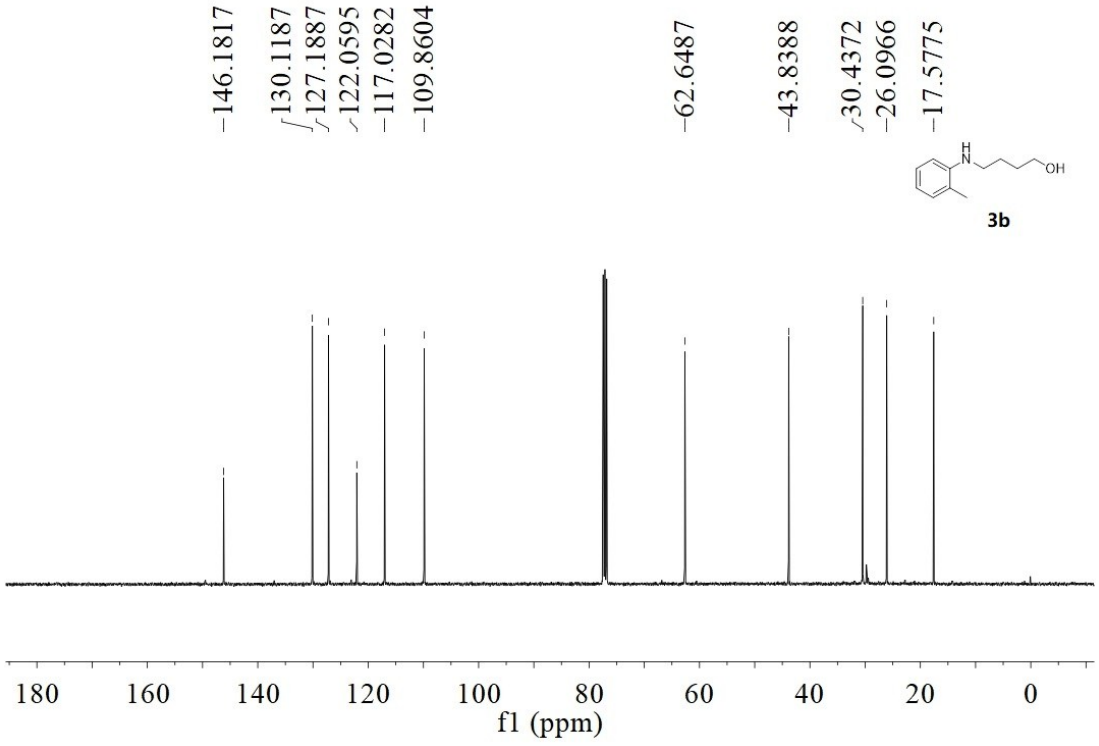
11.0
7.5
5.0
2.5
0.0
f1 (ppm)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127.1887
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117.0282
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62.6487
43.8388
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17.5775
OH
3b
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20
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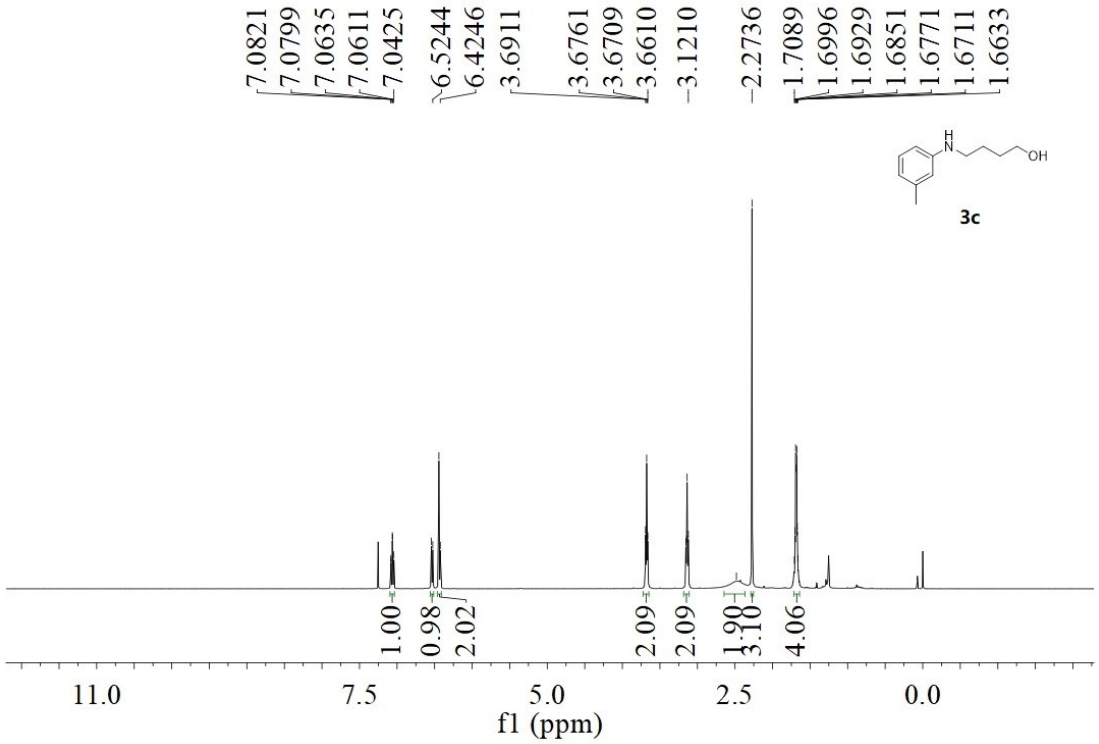
f1 (ppm)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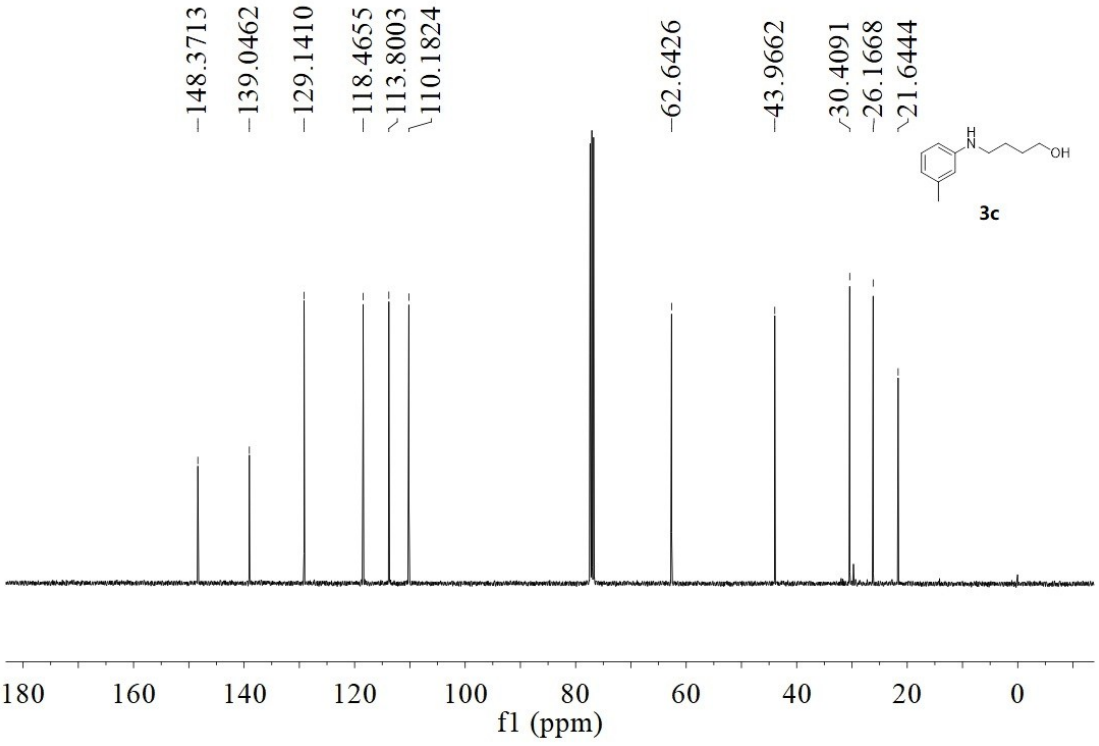
7.0425
6.5244
6.4246
3.6911
3.6761
3.6709
3.6610
3.1210
2.2736
1.7089
1.6996
1.6929
1.6851
1.6771
1.6711
1.6633
3c
1.00
0.98
2.02
2.09
2.09
1.90
3.10
4.06
11.0
7.5
5.0
2.5
0.0
f1 (ppm)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62.6426
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21.6444
3c
180
160
140
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100
80
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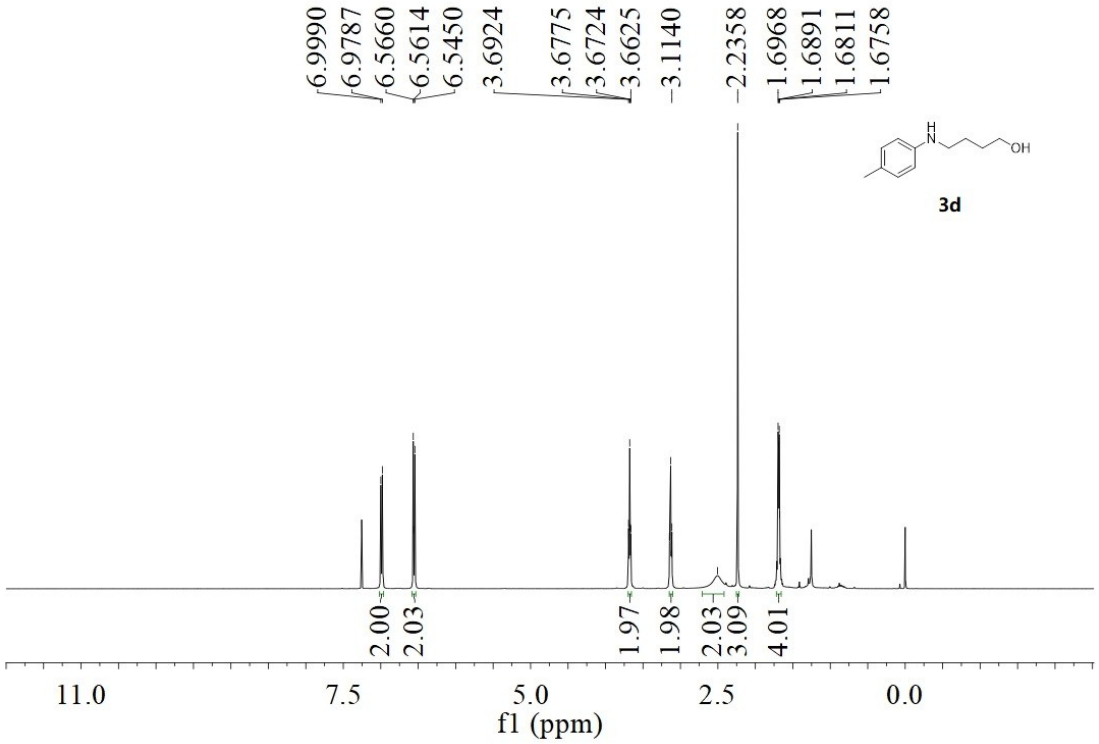
40
20
0
f1 (ppm)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6.5450
3.6924
3.6775
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3.6625
3.1140
2.2358
1.6968
1.6891
1.6811
1.6758
OH
3d
2.00
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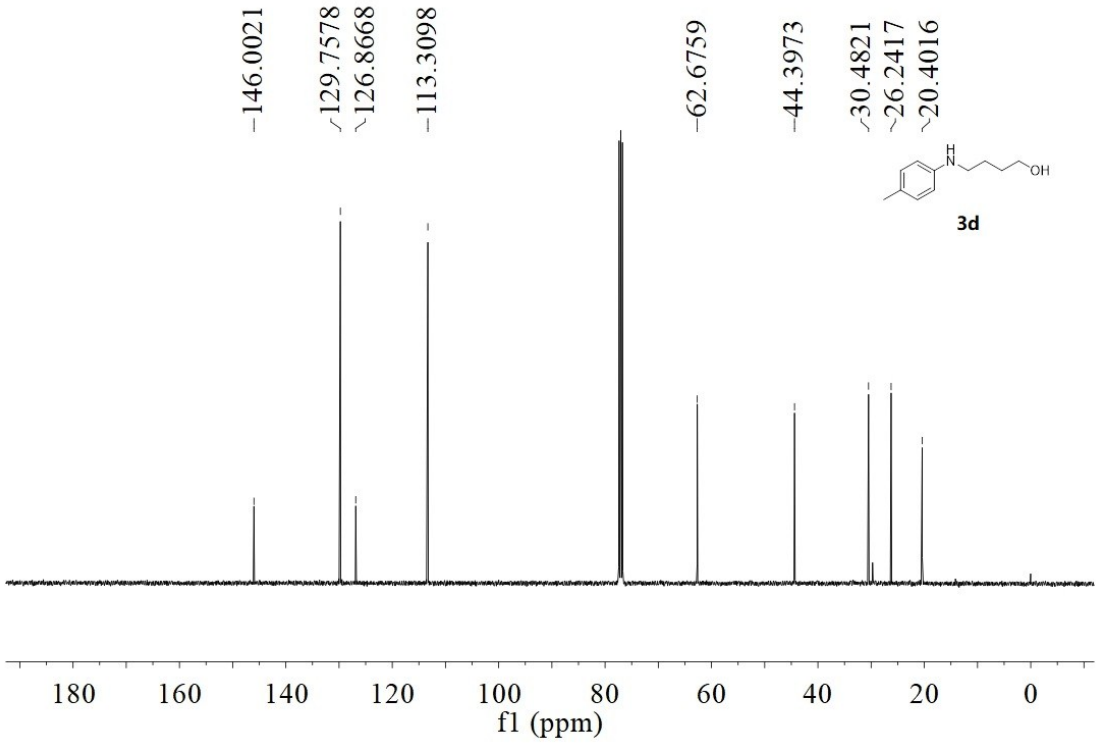
1.97
1.98
2.03
3.09
4.01
11.0
7.5
5.0
2.5
0.0
f1 (ppm)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OH
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100
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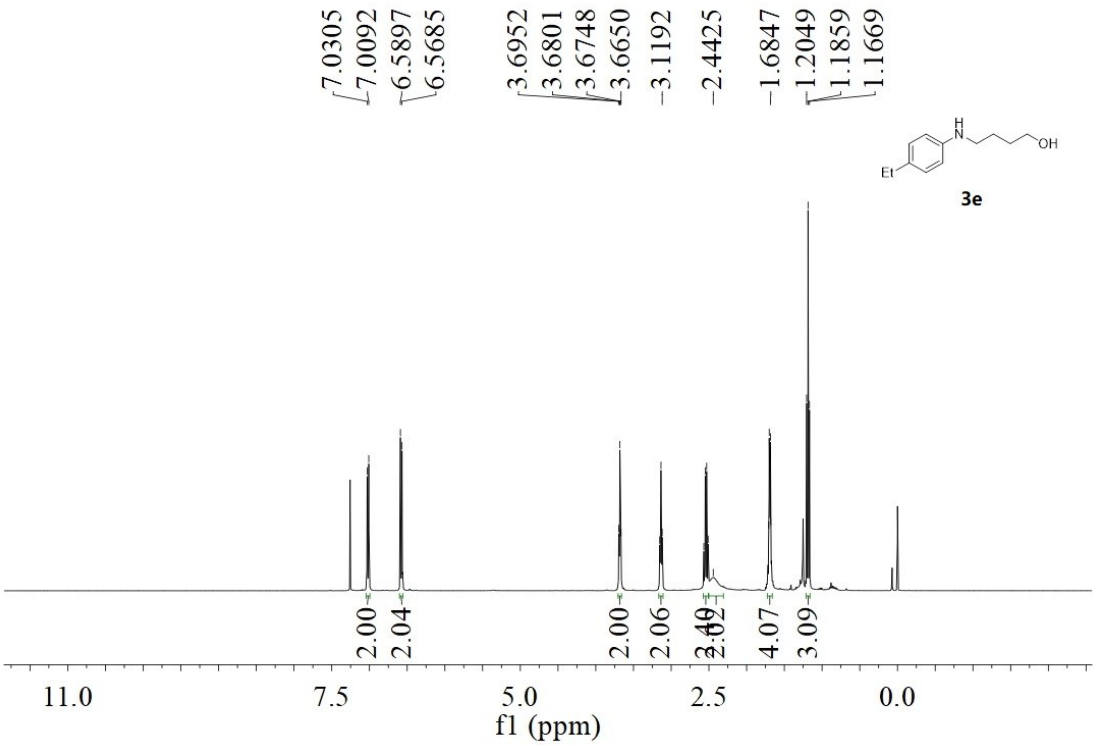
20
0
f1 (ppm)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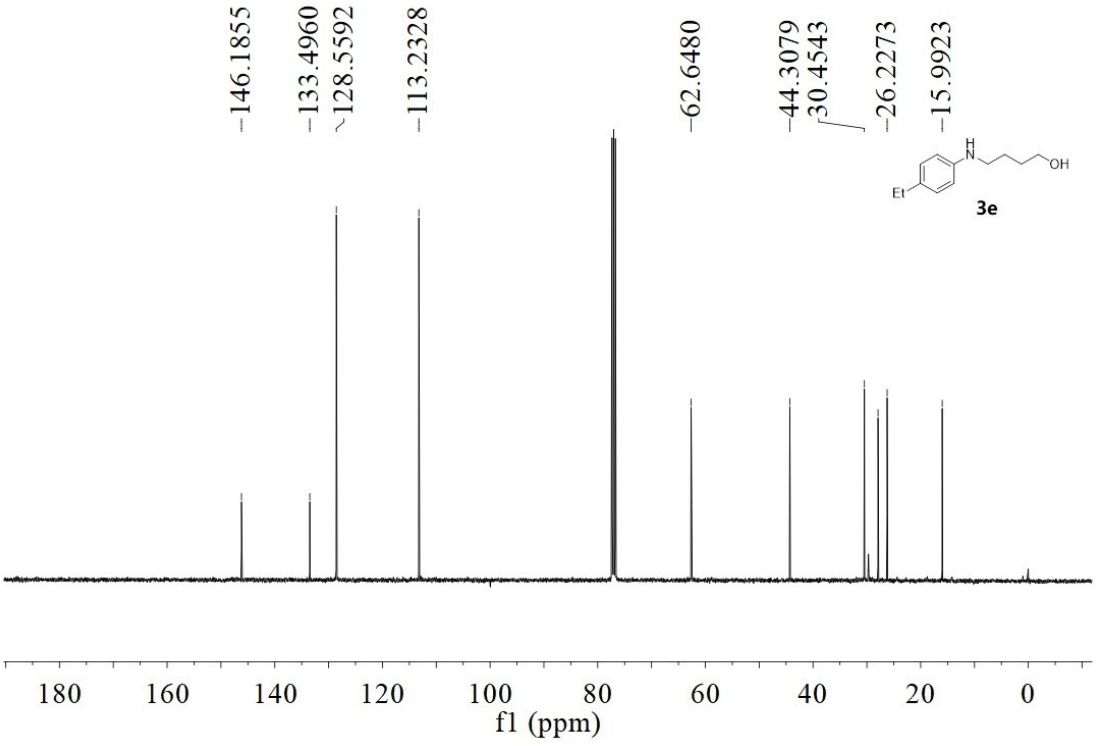
6.5897
6.5685
3.6952
3.6801
3.6748
3.6650
3.1192
2.4425
1.6847
1.2049
1.1859
1.1669
3e
2.00
2.04
2.00
2.06
3.40
2.02
4.07
3.09
11.0
7.5
5.0
2.5
0.0
f1 (ppm)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133.4960
128.5592
113.2328
62.6480
44.3079
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15.9923
3e
180
160
140
120
100
80
60
40
20
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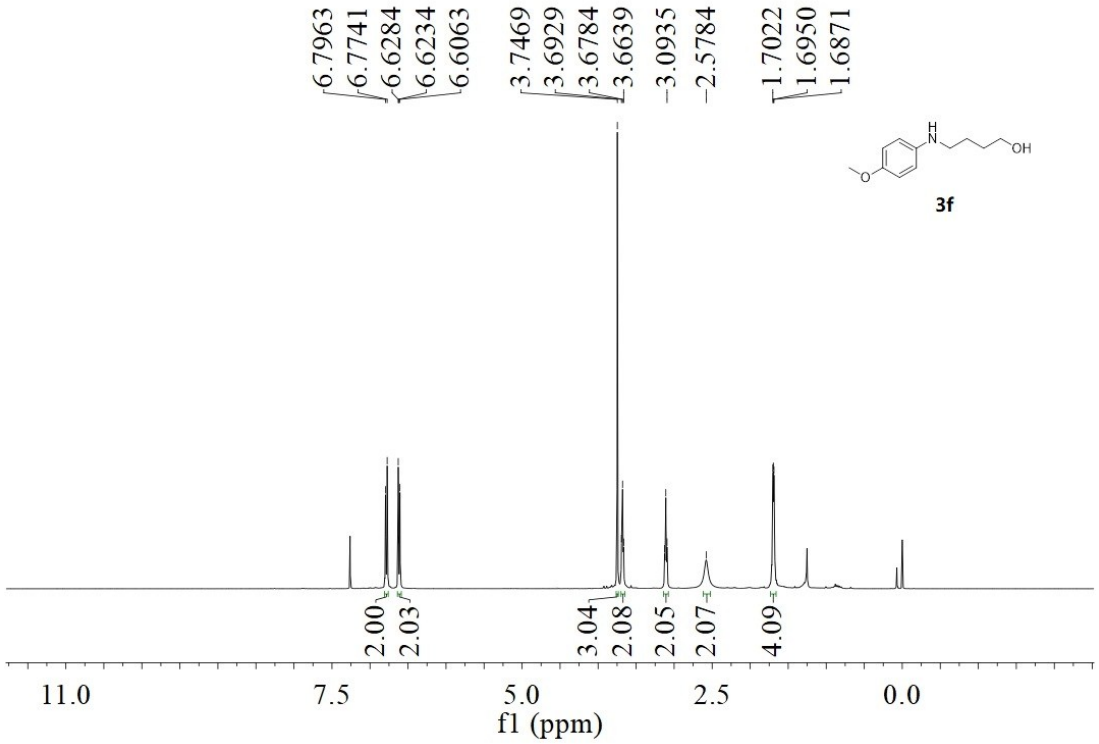
f1 (ppm)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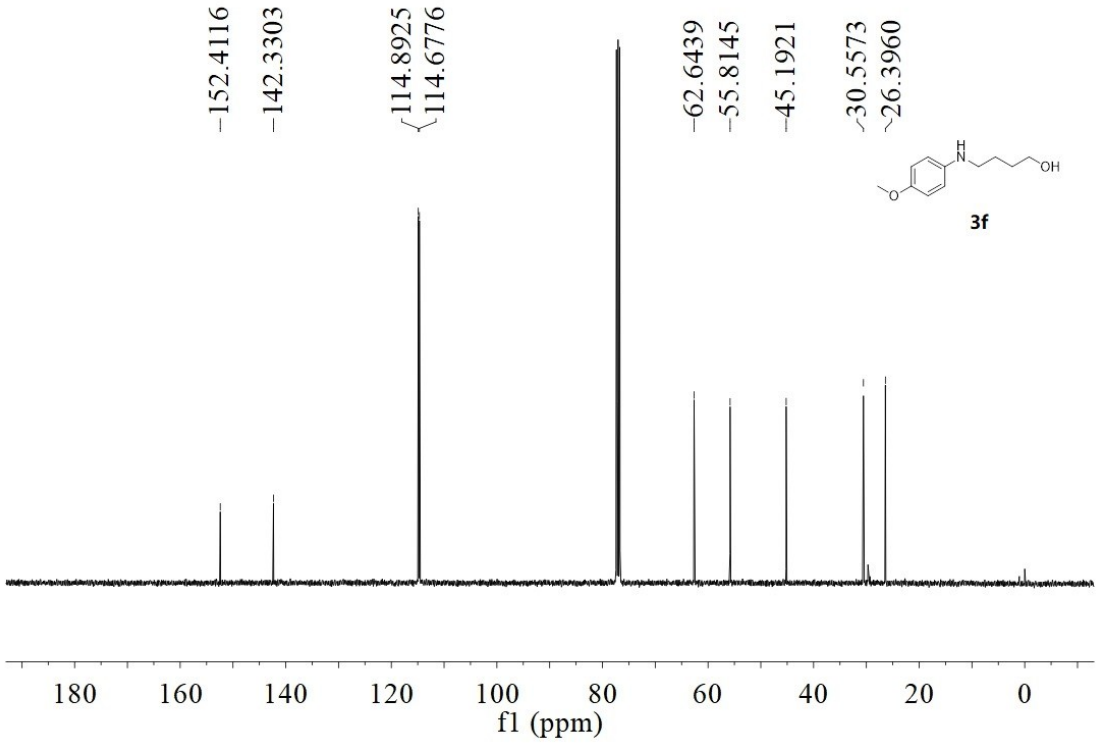
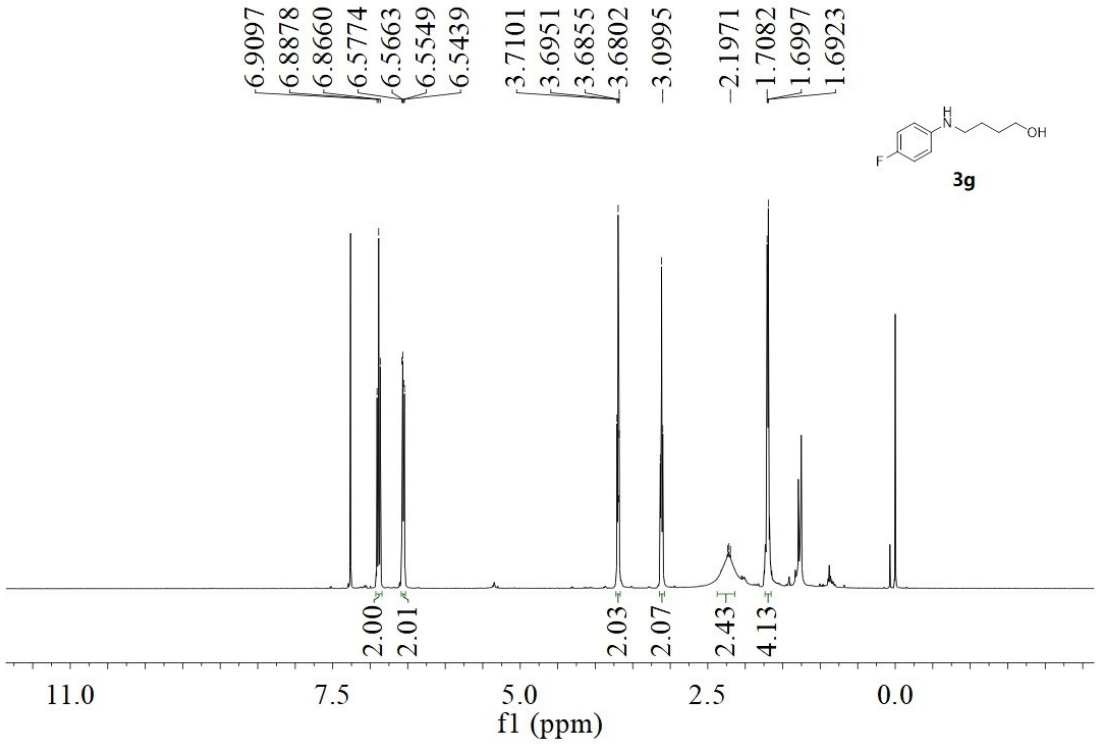
6.6284
6.6234
6.6063
3.7469
3.6929
3.6784
3.6639
3.0935
2.5784
1.7022
1.6950
1.6871
OH
3f
2.00
2.03
3.04
2.08
2.05
2.07
4.09
11.0
7.5
5.0
2.5
0.0
f1 (ppm)


152.4116
142.3303
114.8925
114.6776
62.6439
55.8145
45.1921
30.5573
26.3960
OH
3f
180
160
140
120
100
80
60
40
20
0
f1 (ppm)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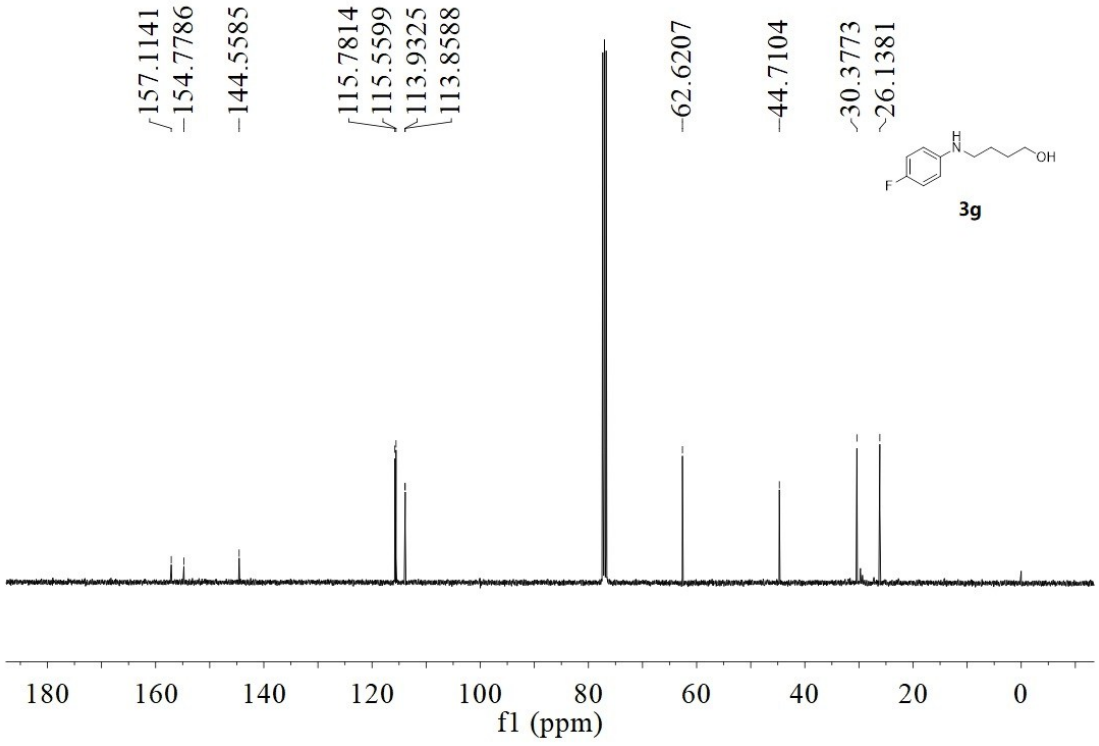
6.8660
6.5774
6.5663
6.5549
6.5439
3.7101
3.6951
3.6855
3.6802
3.0995
2.1971
1.7082
1.6997
1.6923
3g
2.00
2.01
2.03
2.07
2.43
4.13
11.0
7.5
5.0
2.5
0.0
f1 (ppm)


157.1141
154.7786
144.5585
115.7814
115.5599
113.9325
113.8588
62.6207
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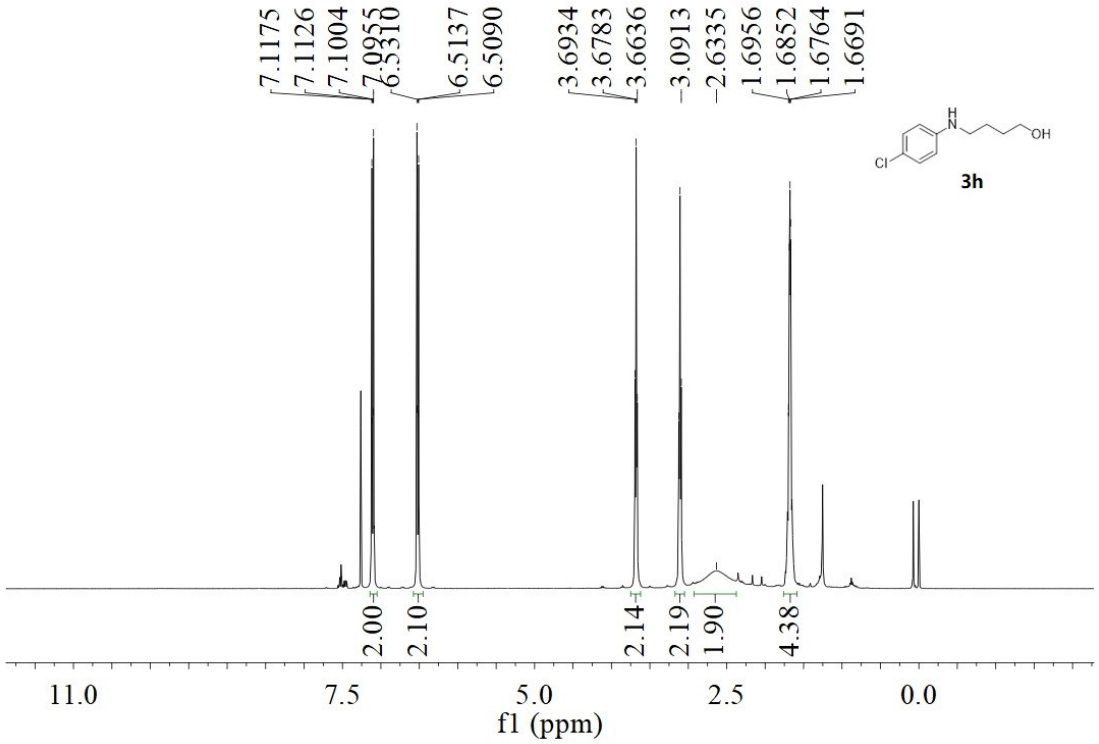
26.1381
3g
180
160
140
120
100
80
60
40
20
0
f1 (ppm)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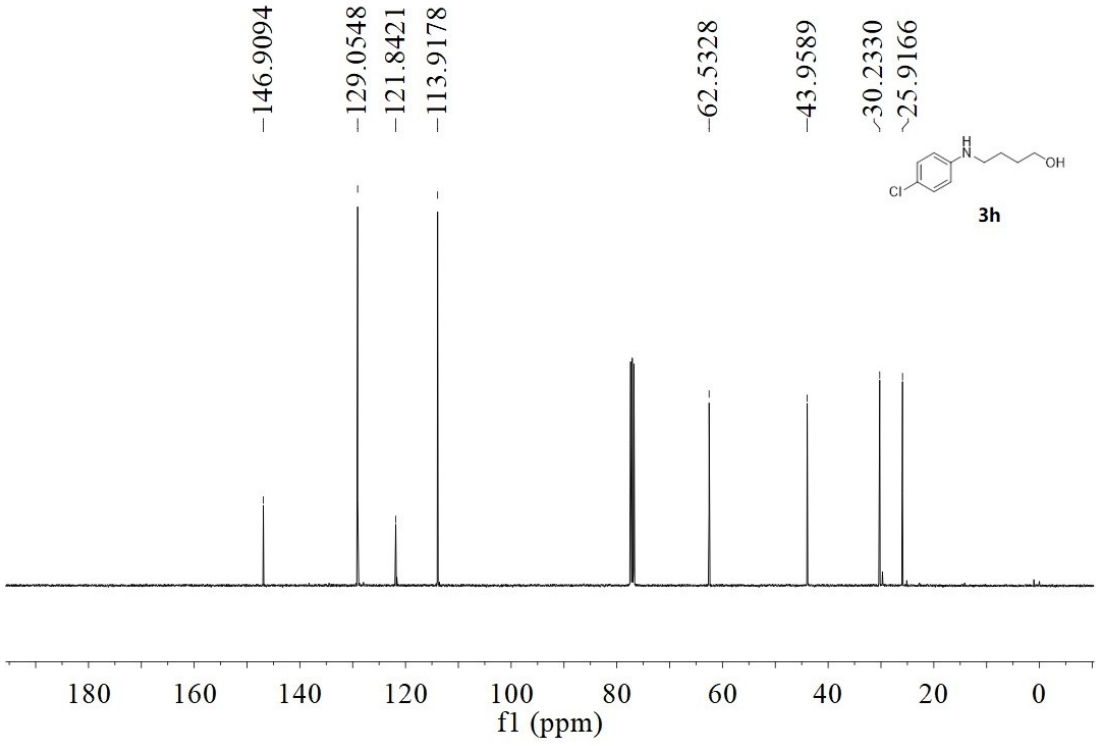
7.1004
7.0955
6.5310
6.5137
6.5090
3.6934
3.6783
3.6636
3.0913
2.6335
1.6956
1.6852
1.6764
1.6691
2.00
2.10
2.14
2.19
1.90
4.38
11.0
7.5
5.0
2.5
0.0
f1 (ppm)
3h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121.8421
113.9178
62.5328
43.9589
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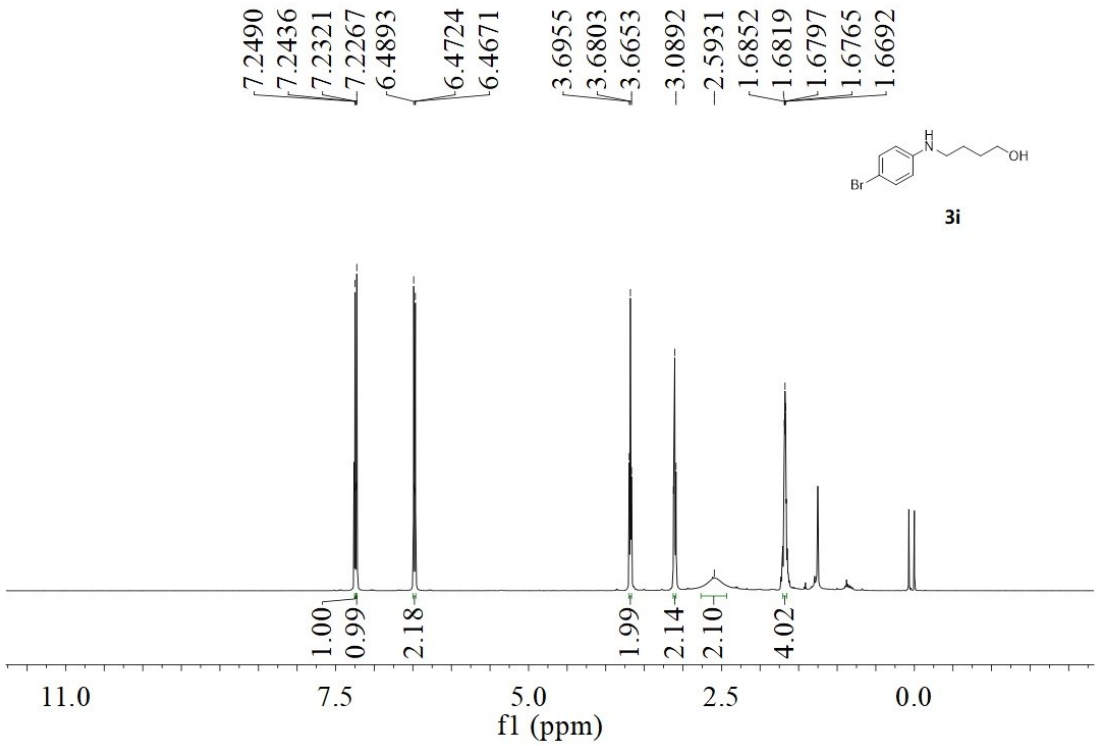
25.9166
180
160
140
120
100
80
60
40
20
0
f1 (ppm)
3h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7.2321
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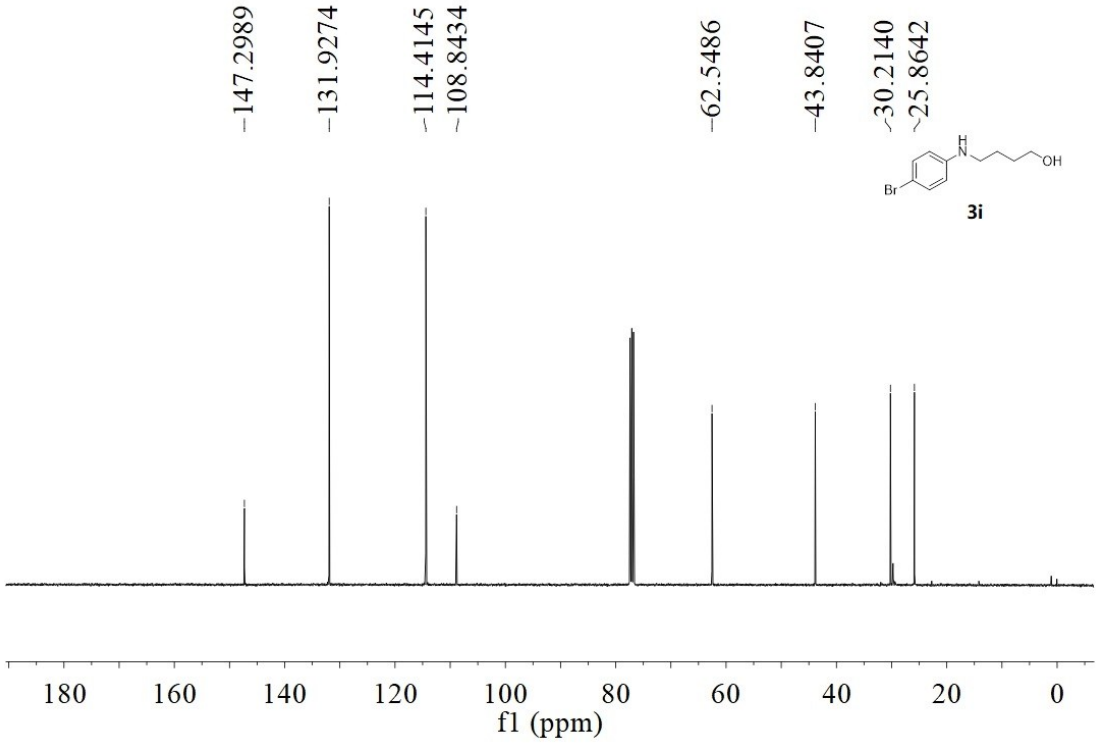
6.4893
6.4724
6.4671
3.6955
3.6803
3.6653
3.0892
2.5931
1.6852
1.6819
1.6797
1.6765
1.6692
H
N
OH
Br
3i
1.00
0.99
2.18
1.99
2.14
2.10
4.02
11.0
7.5
5.0
2.5
0.0
f1 (ppm)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43.8407
30.2140
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N
OH
Br
3i
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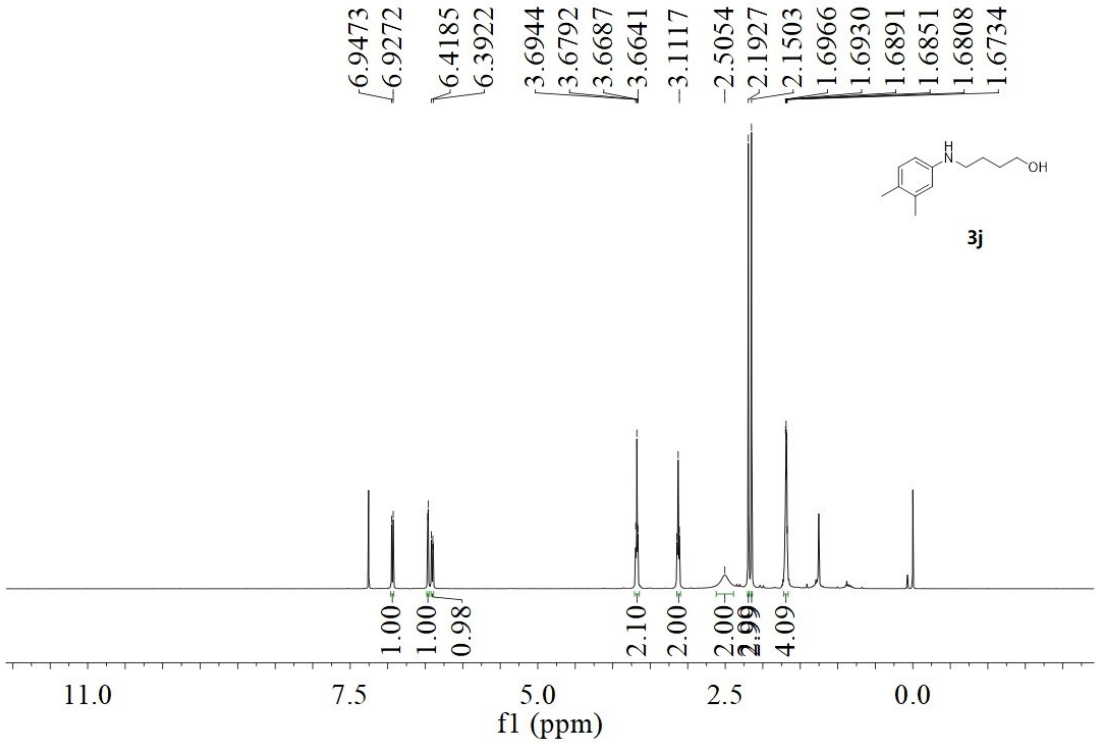
140
120
100
80
60
40
20
0
f1 (ppm)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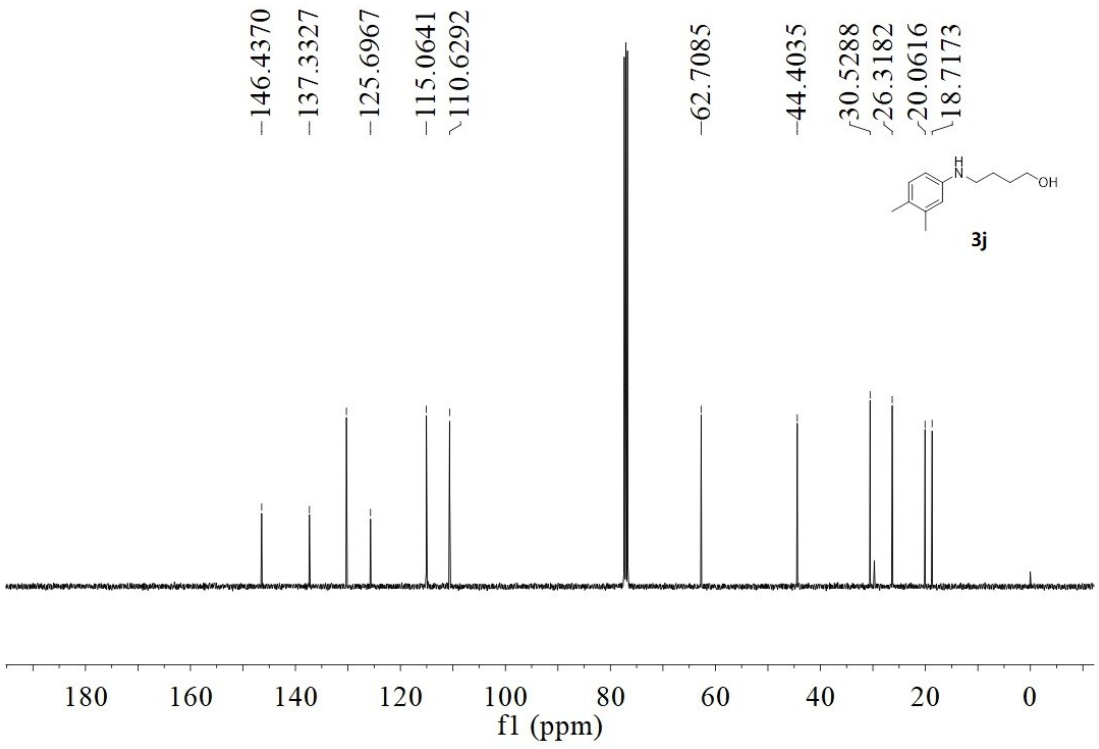
6.4185
6.3922
3.6944
3.6792
3.6687
3.6641
3.1117
2.5054
2.1927
2.1503
1.6966
1.6930
1.6891
1.6851
1.6808
1.6734
1.00
1.00
0.98
2.10
2.00
2.00
4.09
11.0
7.5
5.0
2.5
0.0
f1 (ppm)
3j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110.6292
62.7085
44.4035
30.5288
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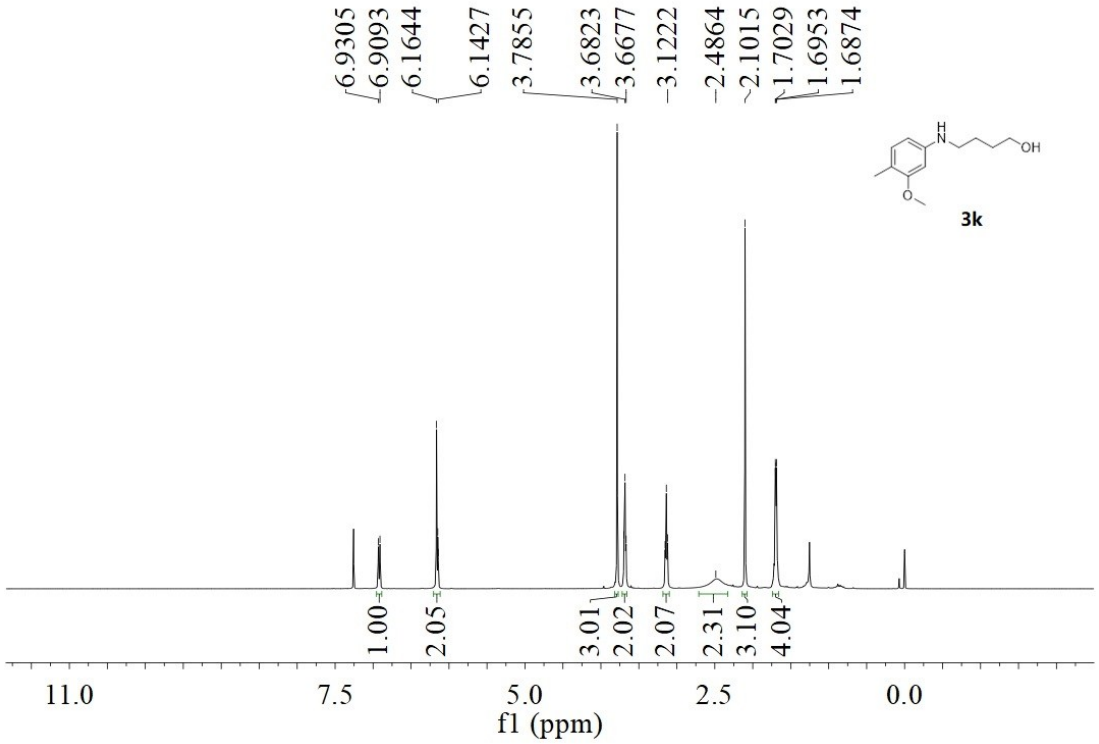
18.7173
180
160
140
120
100
80
60
40
20
0
f1 (ppm)
3j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6.1427
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2.4864
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1.7029
1.6953
1.6874
1.00
2.05
3.01
2.02
2.07
2.31
3.10
4.04
11.0
7.5
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2.5
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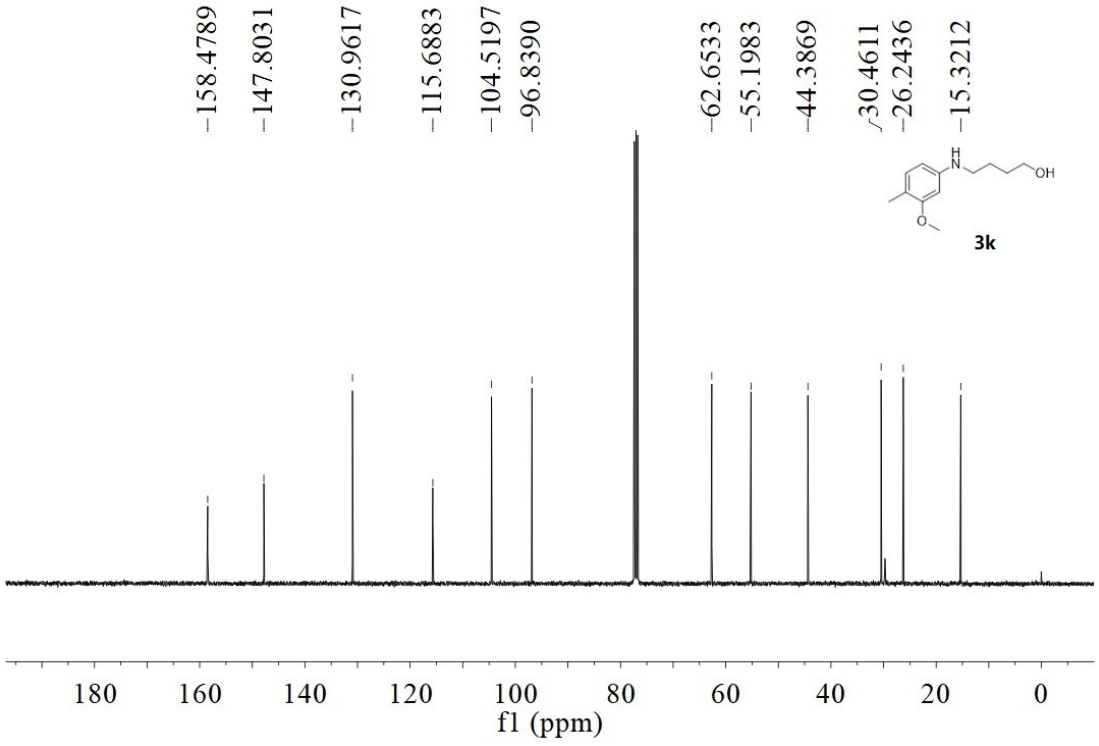
f1 (ppm)
3k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96.8390
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55.1983
44.3869
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15.3212
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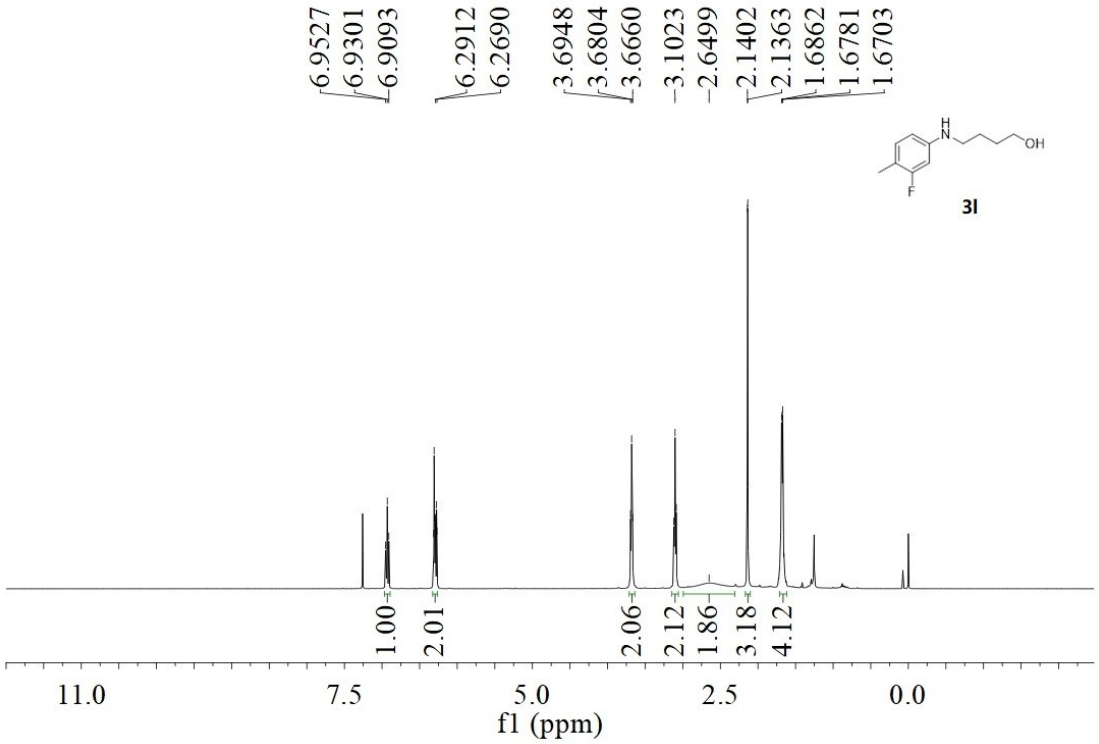
140
120
100
80
60
40
20
0
f1 (ppm)
3k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6.2690
3.6948
3.6804
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3.1023
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2.1402
2.1363
1.6862
1.6781
1.6703
OH
3l
1.00
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1.86
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11.0
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5.0
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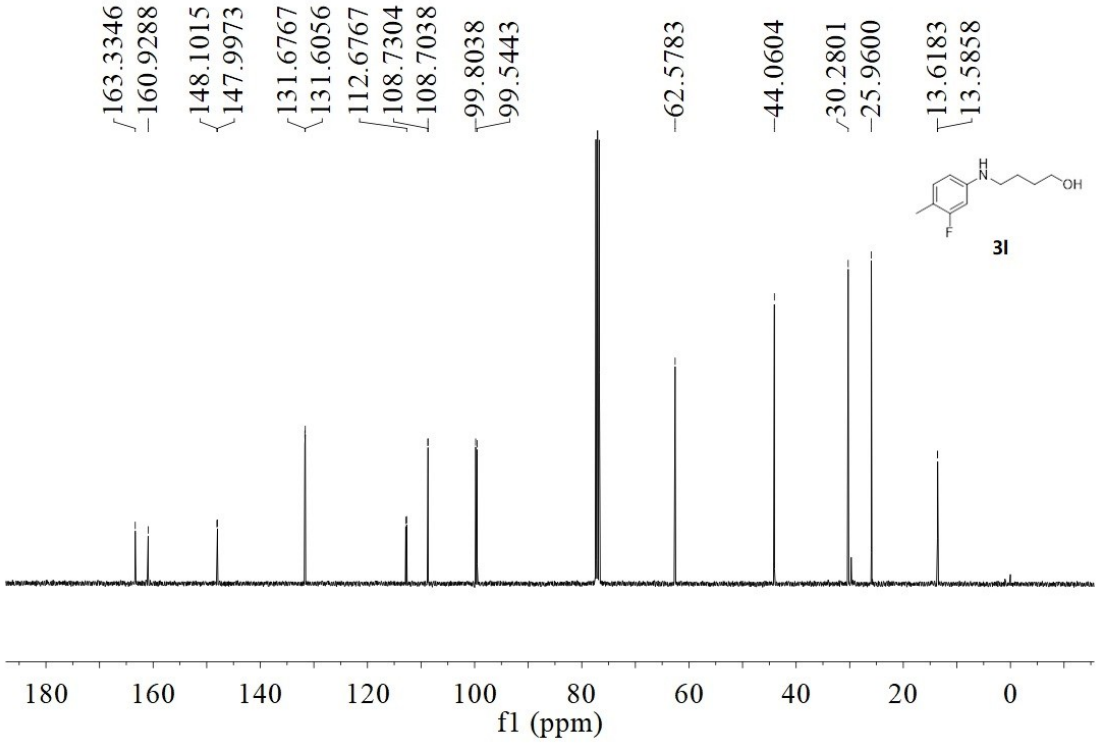
f1 (ppm)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148.1015
147.9973
131.6767
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112.6767
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108.7038
99.8038
99.5443
62.5783
44.0604
30.2801
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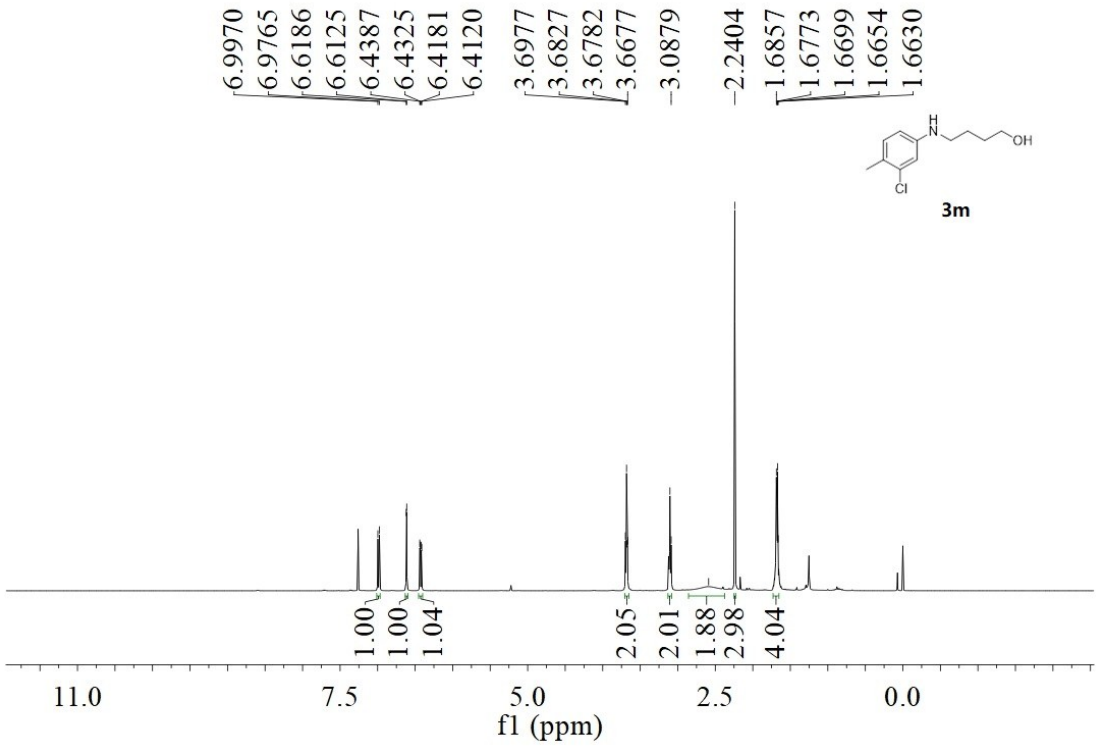
13.6183
13.5858
OH
3l
180
160
140
120
100
80
60
40
20
0
f1 (ppm)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6.4181
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3.6827
3.6782
3.6677
3.0879
2.2404
1.6857
1.6773
1.6699
1.6654
1.6630
OH
Cl
3m
1.00
1.00
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2.05
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2.98
4.04
11.0
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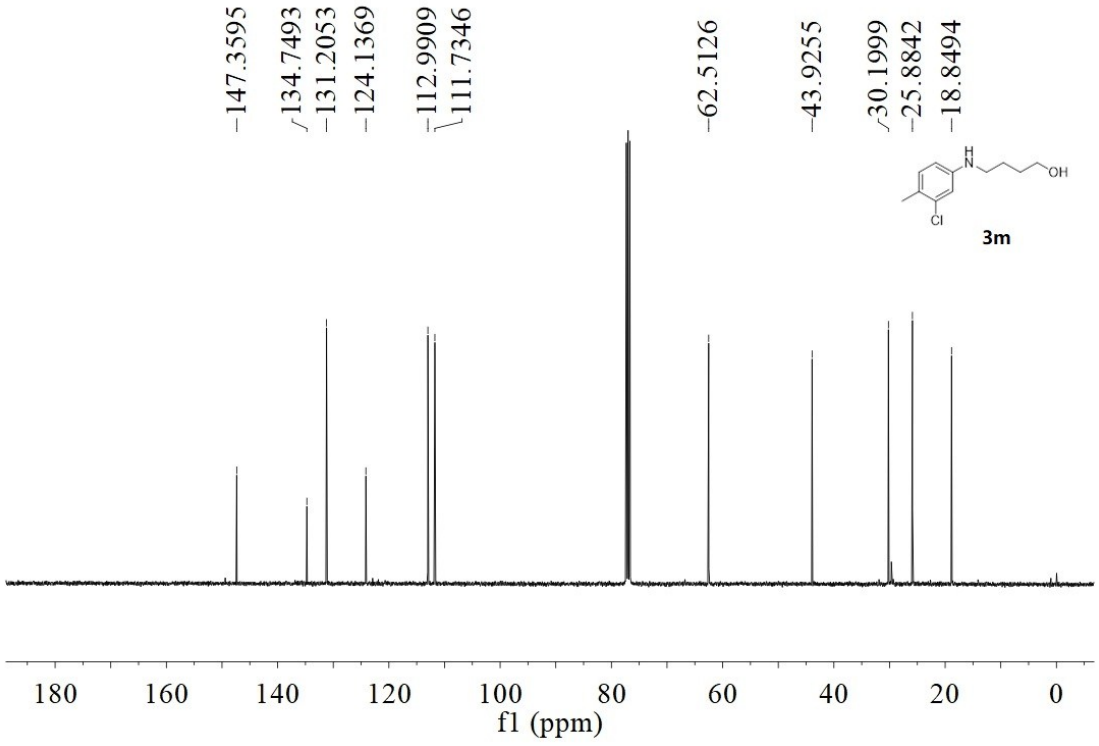
5.0
2.5
0.0
f1 (ppm)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30.1999
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Cl
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100
80
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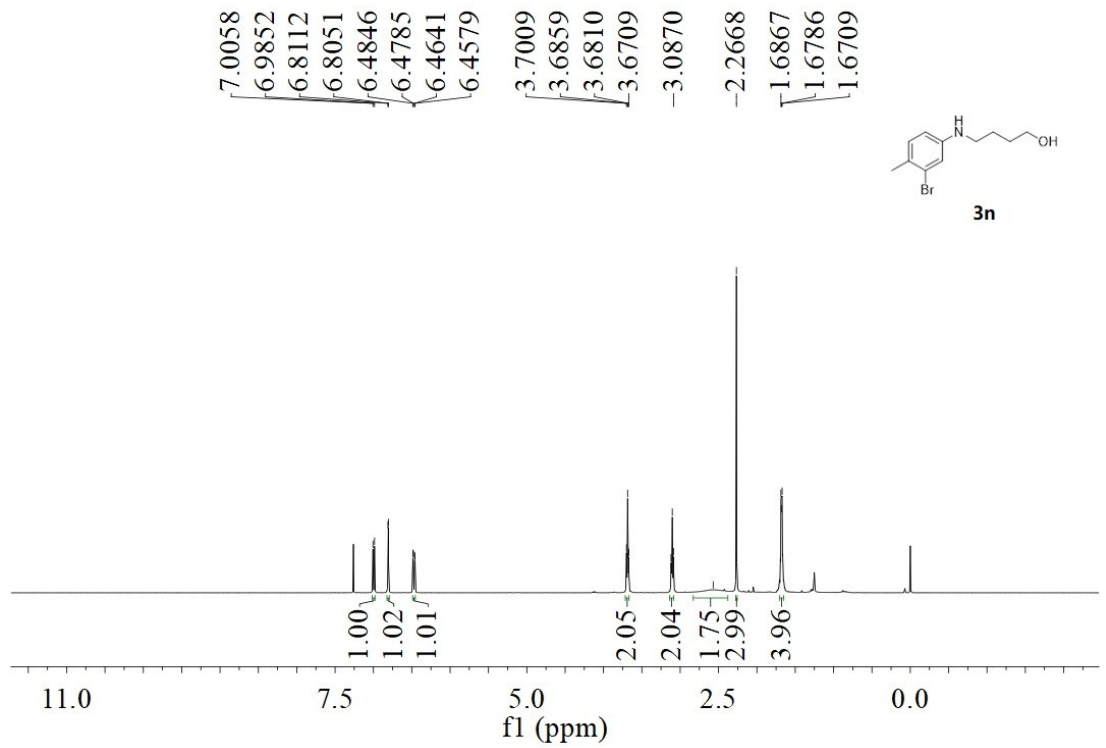
40
20
0
f1 (ppm)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6.4785
6.4641
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3.7009
3.6859
3.6810
3.6709
3.0870
2.2668
1.6867
1.6786
1.6709
H
N
OH
Br
3n
1.00
1.02
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2.99
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5.0
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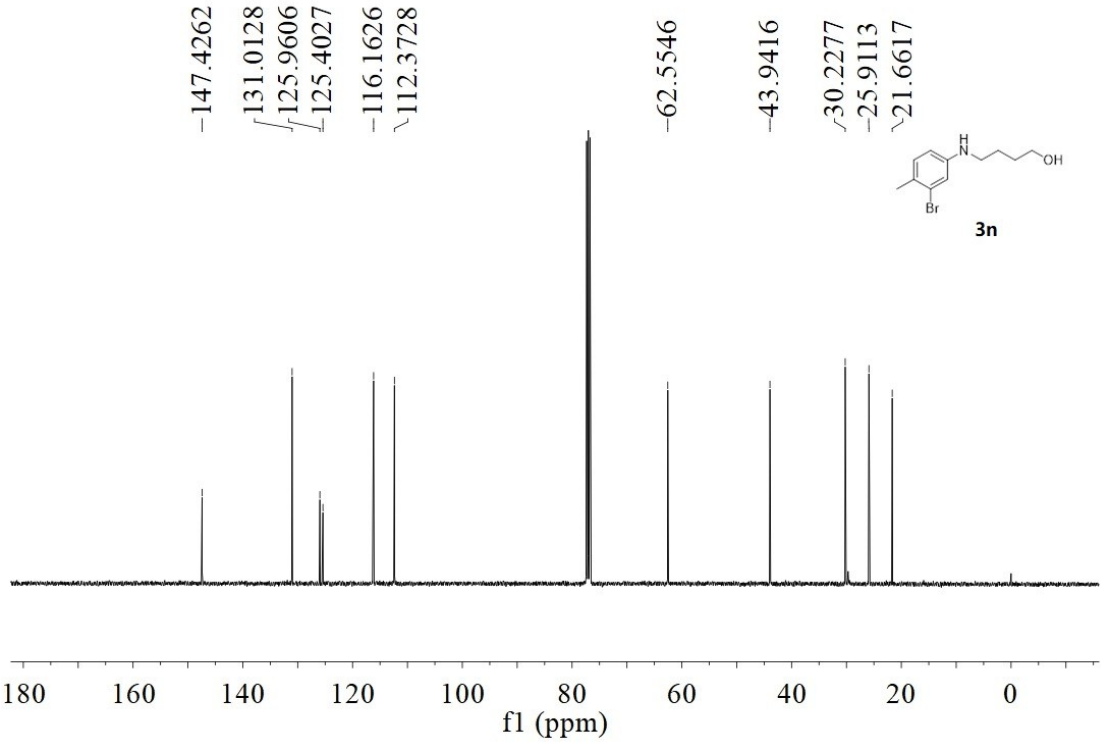
f1 (ppm)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30.2277
25.9113
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N
OH
Br
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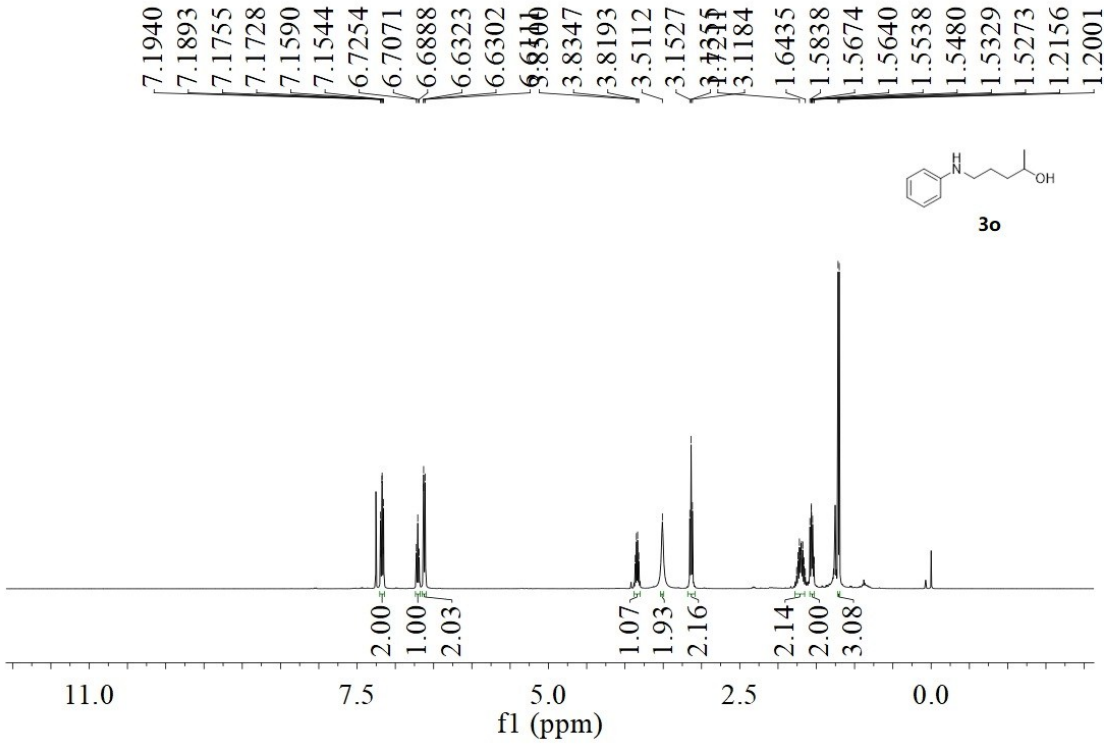
160
140
120
100
80
60
40
20
0
f1 (ppm)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3.8347
3.8193
3.5112
3.1527
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1.6435
1.5838
1.5674
1.5640
1.5538
1.5480
1.5329
1.5273
1.2156
1.2001
3o
2.00
1.00
2.03
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2.14
2.00
3.08
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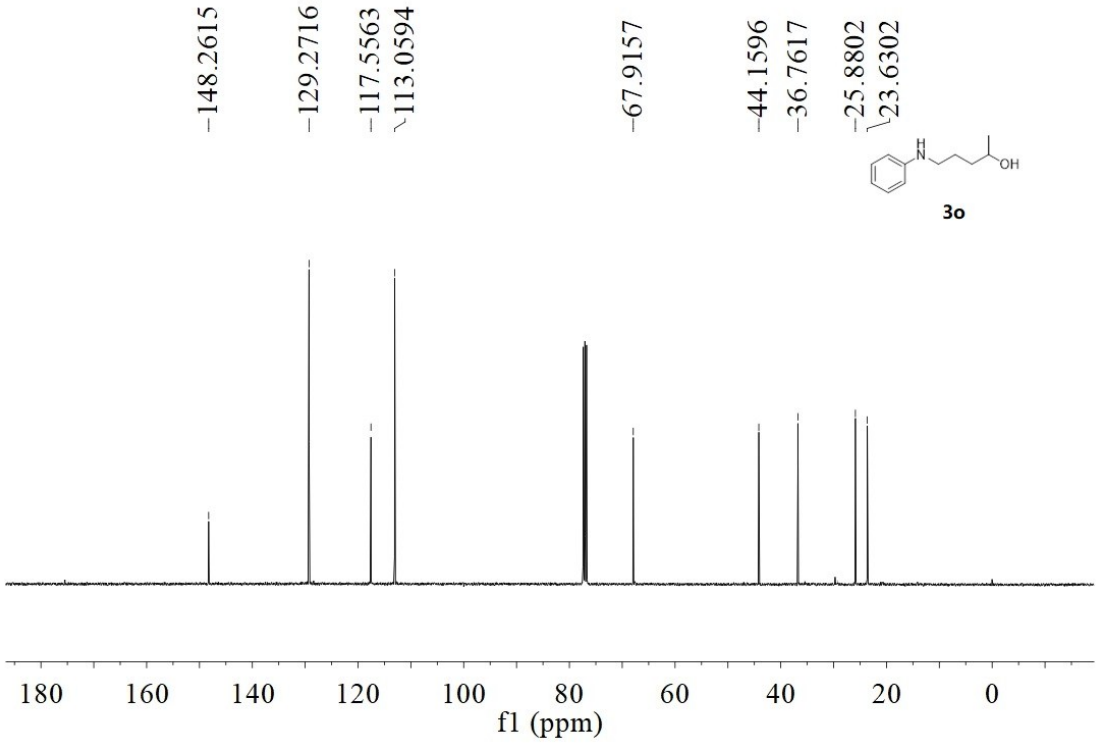
0.0
f1 (ppm)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67.9157
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140
120
100
80
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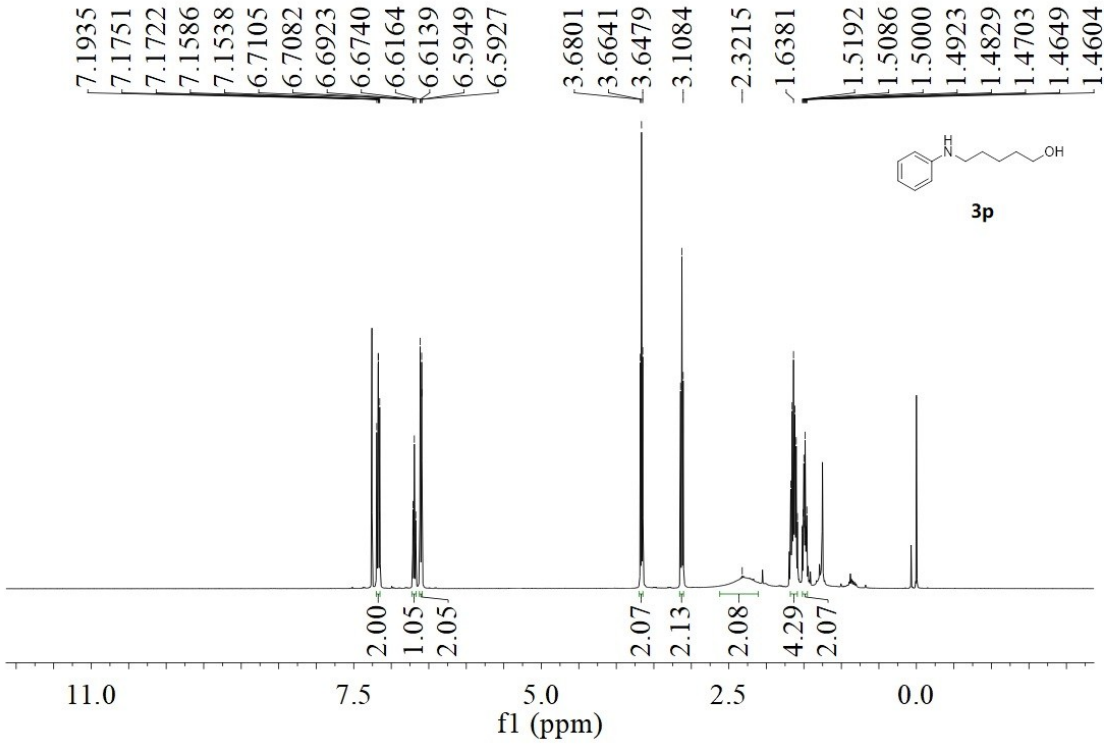
40
20
0
f1 (ppm)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6.5927
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1.5192
1.5086
1.5000
1.4923
1.4829
1.4703
1.4649
1.4604
3p
2.00
1.05
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2.13
2.08
4.29
2.07
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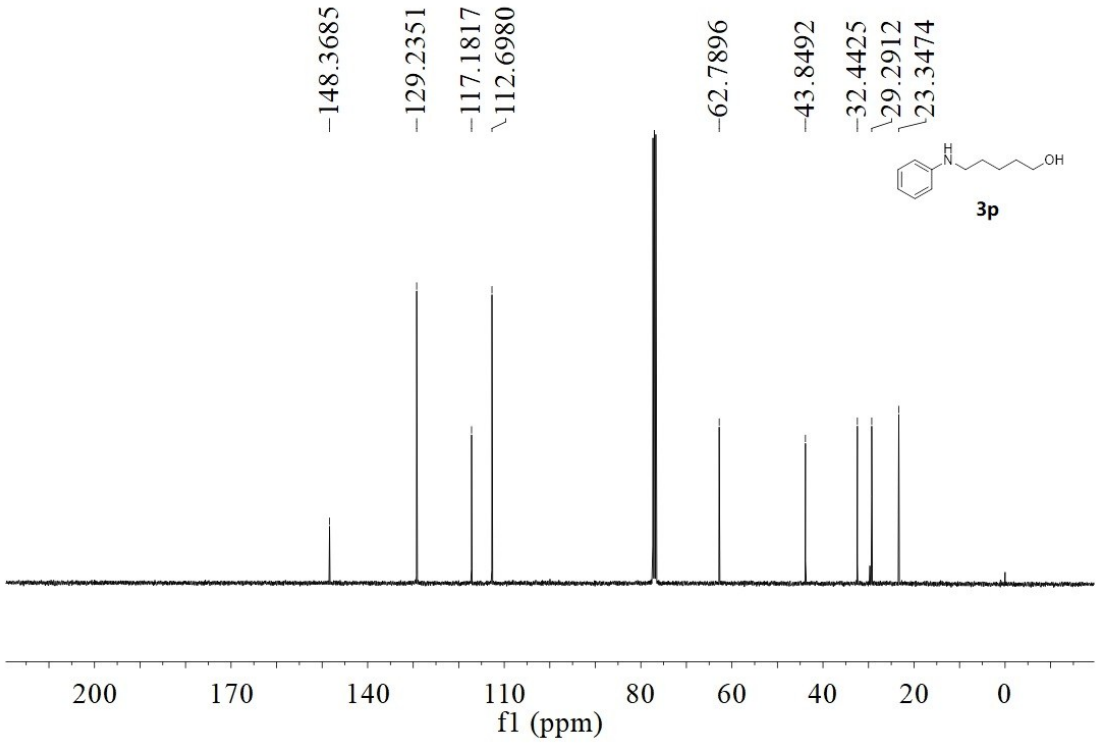
5.0
2.5
0.0
f1 (ppm)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112.6980
62.7896
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23.3474
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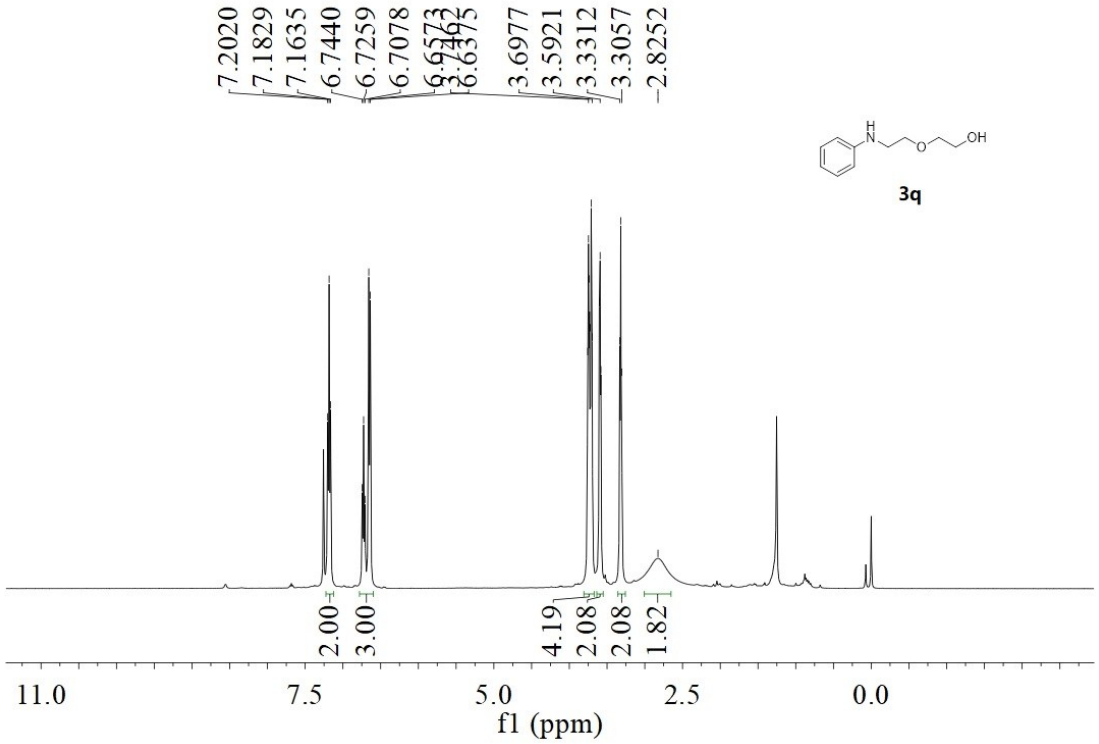
110
80
60
40
20
0
f1 (ppm)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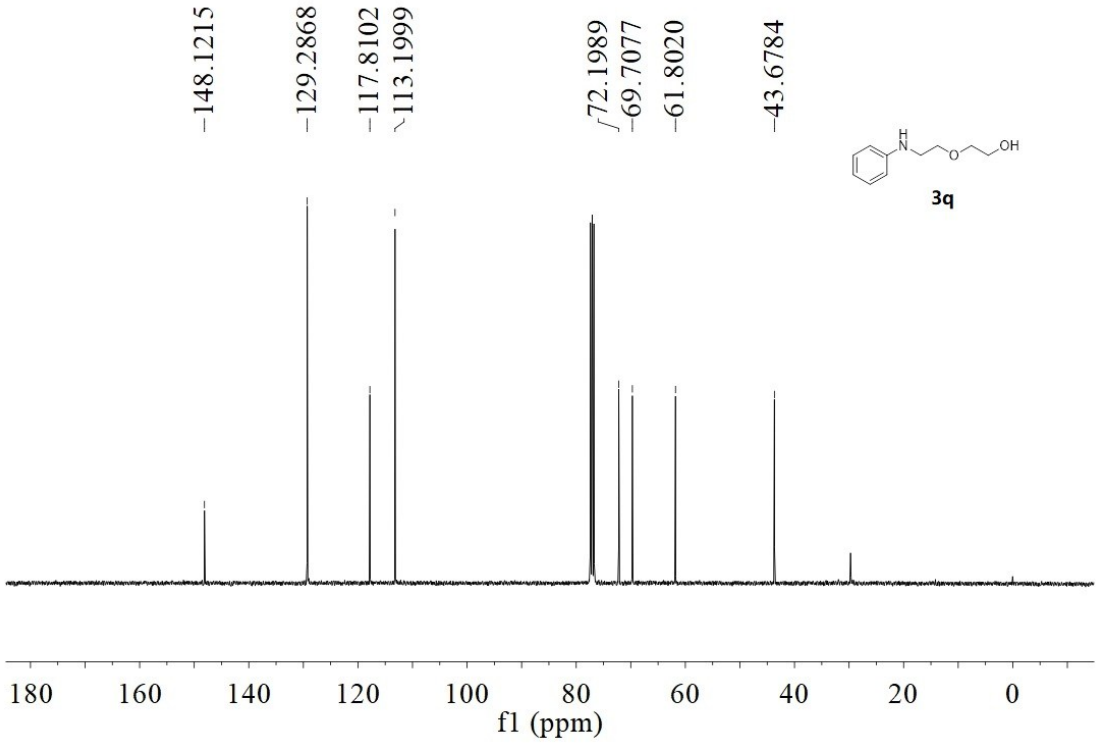
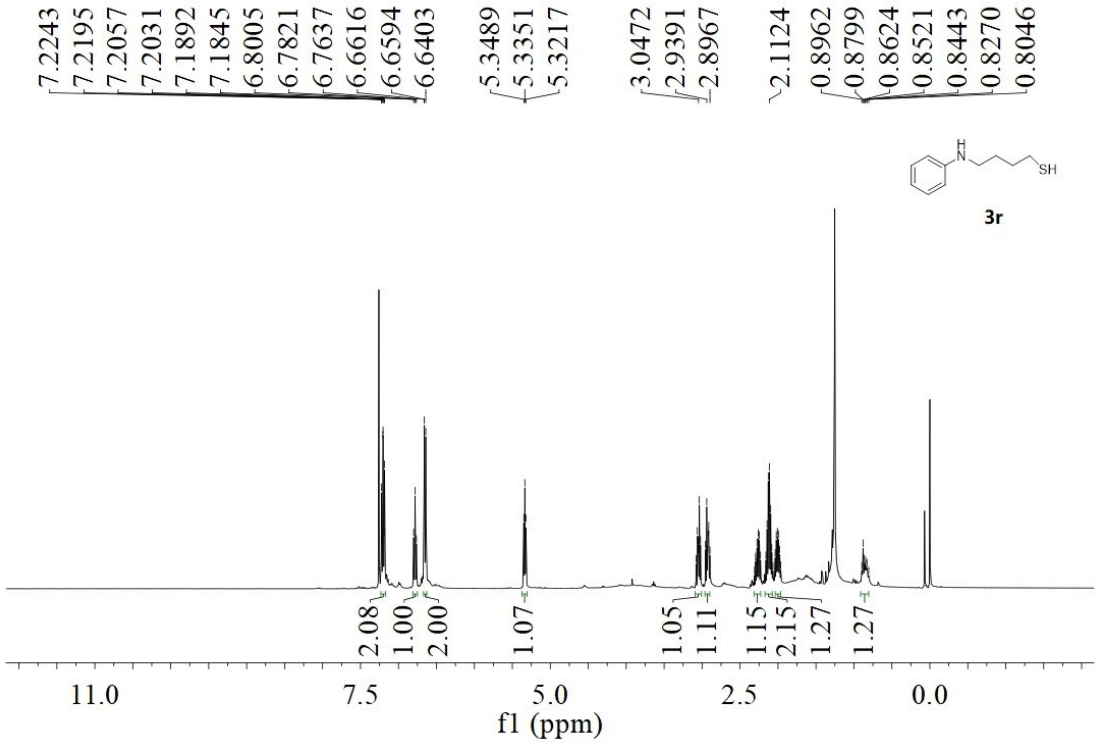
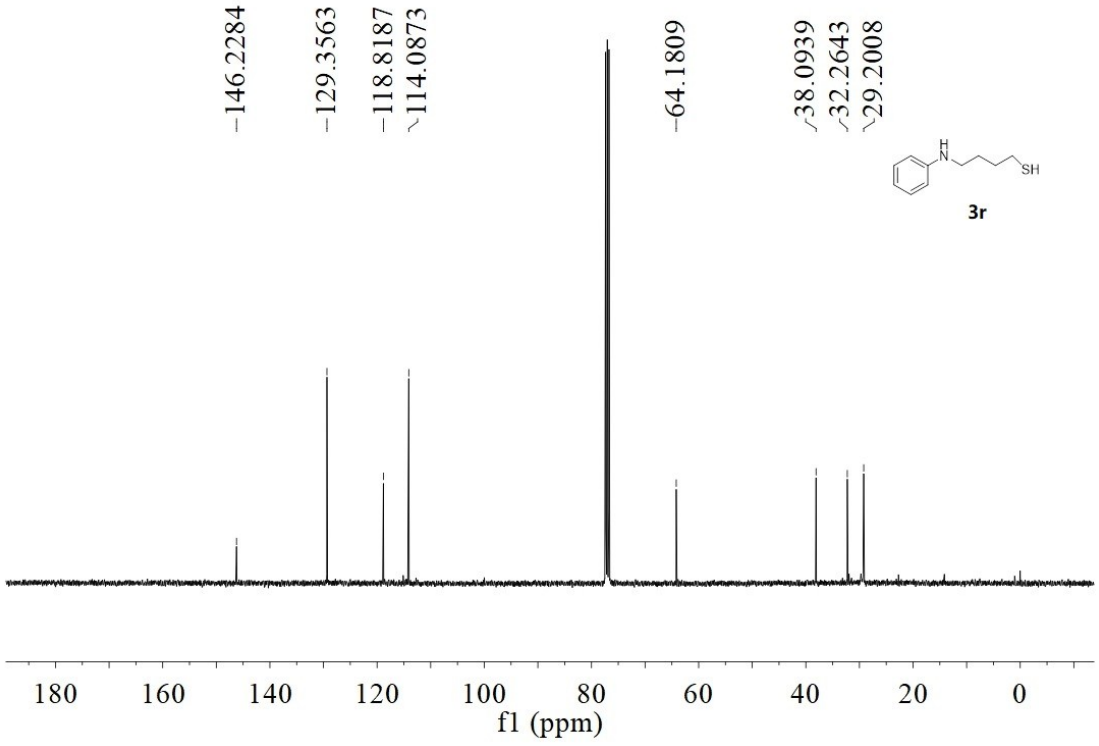
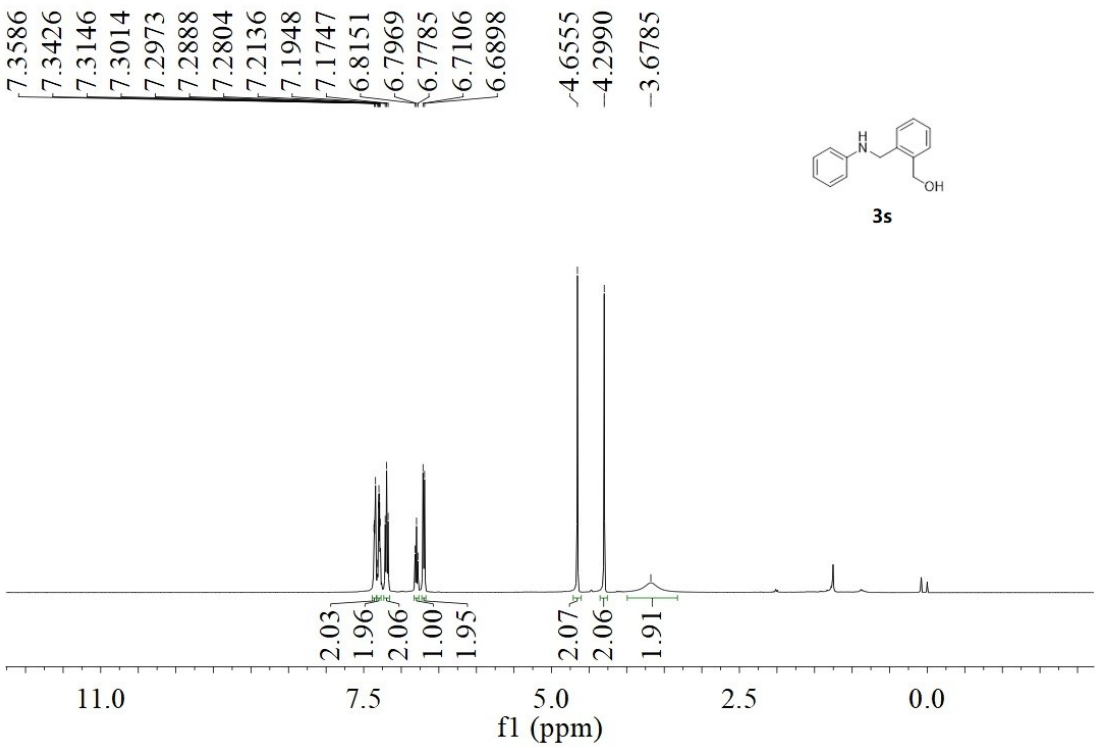
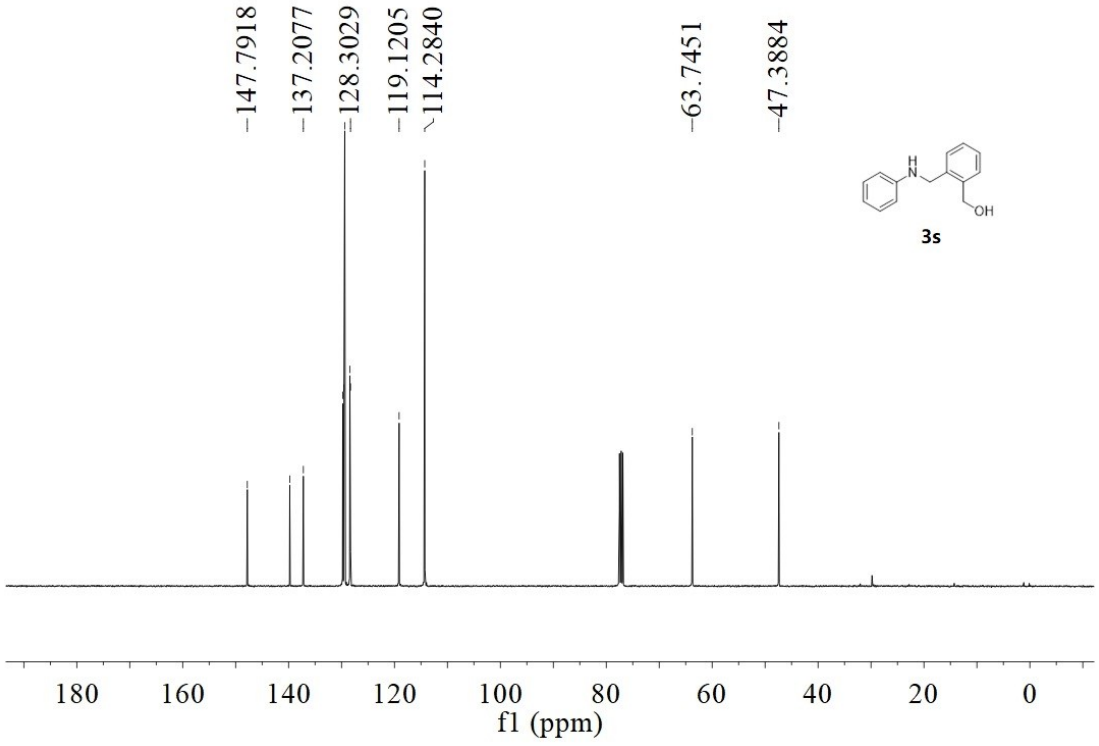
2.8252
3q
2.00
3.00
4.19
2.08
2.08
1.82
11.0
7.5
5.0
2.5
0.0
f1 (ppm)

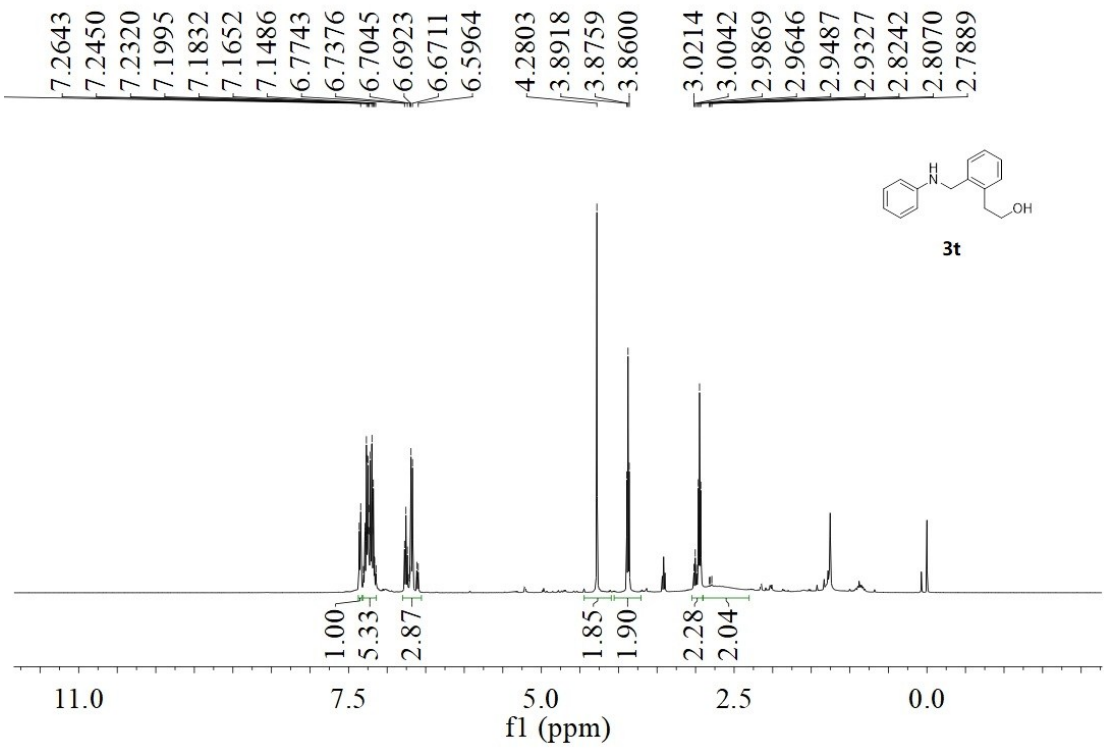

148.1215
129.2868
117.8102
113.1999
72.1989
69.7077
61.8020
43.6784
3q
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

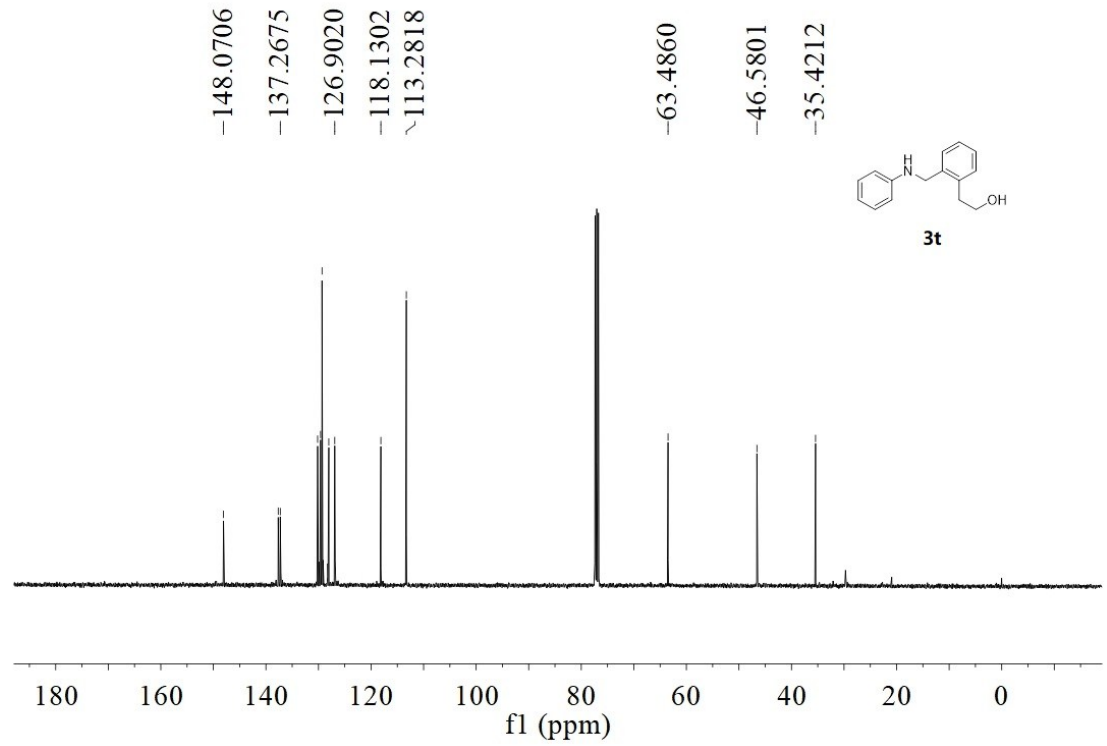

7.2243
7.2195
7.2057
7.2031
7.1892
7.1845
6.8005
6.7821
6.7637
6.6616
6.6594
6.6403
5.3489
5.3351
5.3217
3.0472
2.9391
2.8967
2.1124
0.8962
0.8799
0.8624
0.8521
0.8443
0.8270
0.8046
3r
2.08
1.00
2.00
1.07
1.05
1.11
1.15
2.15
1.27
1.27
11.0
7.5
5.0
2.5
0.0
f1 (ppm)


146.2284
129.3563
118.8187
114.0873
64.1809
38.0939
32.2643
29.2008
3r
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


7.3586
7.3426
7.3146
7.3014
7.2973
7.2888
7.2804
7.2136
7.1948
7.1747
6.8151
6.7969
6.7785
6.7106
6.6898
4.6555
4.2990
3.6785
3s
2.03
1.96
2.06
1.00
1.95
2.07
2.06
1.91
11.0
7.5
5.0
2.5
0.0
f1 (ppm)


147.7918
137.2077
128.3029
119.1205
114.2840
63.7451
47.3884
3s
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


7.2643
7.2450
7.2320
7.1995
7.1832
7.1652
7.1486
6.7743
6.7376
6.7045
6.6923
6.6711
6.5964
4.2803
3.8918
3.8759
3.8600
3.0214
3.0042
2.9869
2.9646
2.9487
2.9327
2.8242
2.8070
2.7889
3t
1.00
5.33
2.87
1.85
1.90
2.28
2.04
11.0
7.5
5.0
2.5
0.0
f1 (ppm)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137.2675
126.9020
118.1302
113.2818
63.4860
46.5801
35.4212
3t
180
160
140
120
100
80
60
40
20
0
f1 (ppm)