Supplemental Material for

An Improved Method for the Synthesis of Phenylacetic Acid Derivatives via Carbonylation

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I. Analytical Data of Compounds

2-Chlorophenylacetic acid (**2b**): a white solid; mp 91-95 °C (lit.[1] 91-93 °C), IR (KBr) 735, 768, 931, 1059, 1201, 1245, 1301, 1348, 1406, 1480, 1713, 2920 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.50 (s, 1H), 7.51 - 7.36 (m, 1H), 7.40 - 7.25 (m, 3H), 3.71 (s, 2H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 171.98, 134.18, 133.81, 132.65, 129.45, 129.20, 127.57, 39.15 ppm.

3-Chlorophenylacetic acid (**3b**): a white solid; mp 76-78 °C (lit.[2] 76 °C), IR (KBr) 690, 726, 791, 891, 1080, 1250, 1411, 1480, 1705, 3054 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.46 (s, 1H), 7.39 - 7.19 (m, 4H), 3.62 (s, 2H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 172.73, 137.96, 133.17, 130.47, 129.83, 128.72, 127.03, 40.8 ppm.

4-Chlorophenylacetic acid (**4b**): a white solid; mp 101-103 °C (lit.[3] 104-106 °C), IR (KBr) 733, 806, 856, 926, 1020, 1090, 1170, 1200, 1260, 1300, 1340, 1410, 1490, 1700, 2970 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.40 (s, 1H), 7.41 - 7.33 (d, J = 8.6 Hz, 2H), 7.33 - 7.24 (d, J = 8.5 Hz, 2H), 3.59 (s, 2H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 172.88, 134.55, 131.80, 131.75, 128.59, 39.96 ppm.

2,6-Dichlorophenylacetic acid (**5b**): a white solid; mp 159-162 °C (lit.[4] 154-156 °C), IR (KBr) 671, 764, 787, 937, 1090, 1170, 1240, 1330, 1430, 1560, 1590, 1720, 2640, 2940 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.74 (s, 1H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.34 (t, J = 8.3 Hz, 1H), 3.89 (s, 2H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 170.71, 135.73, 132.07, 130.03, 128.65, 37.00 ppm.

3,5-Dichlorophenylacetic acid (**6b**): a white solid; mp 110-113 °C (lit.[5] 112-115 °C), IR (KBr) 733, 802, 852, 933, 1170, 1250, 1330, 1420, 1570, 1590, 1710, 2920 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.60 - 12.55 (m, 1H), 7.49 (t, *J* = 1.9 Hz, 1H), 7.36 (d, *J* = 1.9 Hz, 2H), 3.66 (s, 2H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 172.31, 139.70, 134.06, 128.97, 126.72, 39.82 ppm.

2-Methylphenylacetic acid (**7b**): a white solid; mp 88-90 °C (lit.[6] 86-89 °C), IR (KBr) 674, 718, 741, 910, 1211, 1236, 1283, 1331, 1412, 1455, 1493, 1693, 3020 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.31 (s, 1H), 7.15 (m, 4H), 3.57 (s, 2H), 2.23 (s, 3H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 173.00, 137.08, 134.27, 130.32, 127.31, 126.23, 39.20, 19.56 ppm.

3-Methylphenylacetic acid (**8b**): a white crystal; mp 63-65 °C (lit.[7] 62 °C), IR (KBr) 704, 753, 914, 1095, 1202, 1405, 1701, 3015 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.29 (s, 1H), 7.19 (m, 4H), 3.35 (s, 2H), 2.47 (s, 3H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 173.19, 137.74, 135.33, 130.43, 128.61, 127.67, 126.87, 41.12, 21.41 ppm.

4-Methylphenylacetic acid (**9b**): a white crystal; mp 92-94 ºC (lit.[7] 92 ºC), IR (KBr) 679, 714, 768, 806, 922, 1040, 1114, 1170, 1208, 1250, 1340, 1420, 1517, 1690, 3030 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 7.13 (m, 4H), 3.49 (s, 2H), 2.27 (s, 3H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 173.36, 135.97, 132.57, 129.66, 129.23, 40.93, 21.12 ppm.

2,4-Dimethylphenylacetic acid (**10b**): a white powder; mp 102-103 ºC (lit.[8] 100-101 ºC), IR (KBr) 798, 841, 891, 1180, 1220, 1380, 1500, 1660, 1690, 3120 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.24 (s, 1H), 7.04 (d, J = 7.9 Hz, 1H), 7.01-6.89 (m, 2H), 3.35 (s, 2H), 2.21 (s, 6H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 173.15, 136.80, 136.22, 131.22, 131.02, 130.61, 126.75, 38.81, 21.04, 19.51 ppm.

3,5-Dimethylphenylacetic acid (**11b**): a white solid; mp 98-100 ºC (lit.[9] 96-98 ºC), IR (KBr) 687, 779, 845, 926, 1040, 1150, 1270, 1300, 1410, 1600, 1710, 2910 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.24 (s, 1H), 6.87 (s, 1H), 6.85 (s, 2H), 3.46 (s, 2H), 2.24 (s, 6H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 173.22, 137.61, 135.19, 128.44, 127.53, 41.10, 21.31 ppm.

2-Fluorophenylacetic acid (**12b**): a white solid; mp 62-65 ºC (lit.[10] 59-60 ºC), IR (KBr) 671, 744, 779, 879, 930, 1030, 1100, 1230, 1290, 1340, 1430, 1450, 1500, 1590, 1700, 3050 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.47 (s, 1H), 7.38 - 7.26 (m, 2H), 7.16 (m, 2H), 3.74 (s, 1H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 172.19, 162.36 (d, J_{C-F} = 244 Hz), 159.94, 132.52 (d, J_{C-F} = 4.61 Hz), 129.46 (d, J_{C-F} = 8.1 Hz), 124.70 (d, J_{C-F} = 3.8 Hz), 122.71 (d, J_{C-F} = 16 Hz), 115.56 (d, J_{C-F} = 22 Hz), 34.68 (d, J_{C-F} = 2.7 Hz) ppm.

3-Fluorophenylacetic acid (**13b**): a white solid; mp 43-45 ºC (lit.[11] 43 ºC), IR (KBr) 698, 764, 791, 914, 960, 1140, 1270, 1350, 1410, 1450, 1490, 1590, 1620, 1690, 3040 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.49 - 12.43 (m, 1H), 7.35 (t, J = 8.0 Hz, 2H), 7.18 - 7.02 (m, 2H), 3.62 (s, 2H), ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 172.73, 163.66, 138.17, 130.51, 126.06 (d, J_{C-F} = 21.1 Hz), 116.61 (d, J_{C-F} = 22.1 Hz), 113.94, 40.11 ppm.

4-Fluorophenylacetic acid (**14b**): a white solid; mp 81-84 ºC (lit.[3] 82-85 ºC), IR (KBr) 717, 783, 825, 1100, 1230, 1350, 1410, 1520, 1620, 1690, 3040 cm^{-1}; ^{1}H NMR (400 MHz; DMSO-d_6) δ: 12.37 (s, 1H), 7.34 - 7.24 (m, 2H), 7.22 - 7.07 (t, J = 8.78 Hz, 2H), 3.57 (s, 2H) ppm; ^{13}C NMR (100 MHz; DMSO-d_6) δ: 173.12, 162.75 (d, J_{C-F} = 250.6 Hz), 131.70 (d, J_{C-F} = 9.5 Hz), 115.26 (d, J_{C-F} = 22.1 Hz), 40.09 ppm.

References

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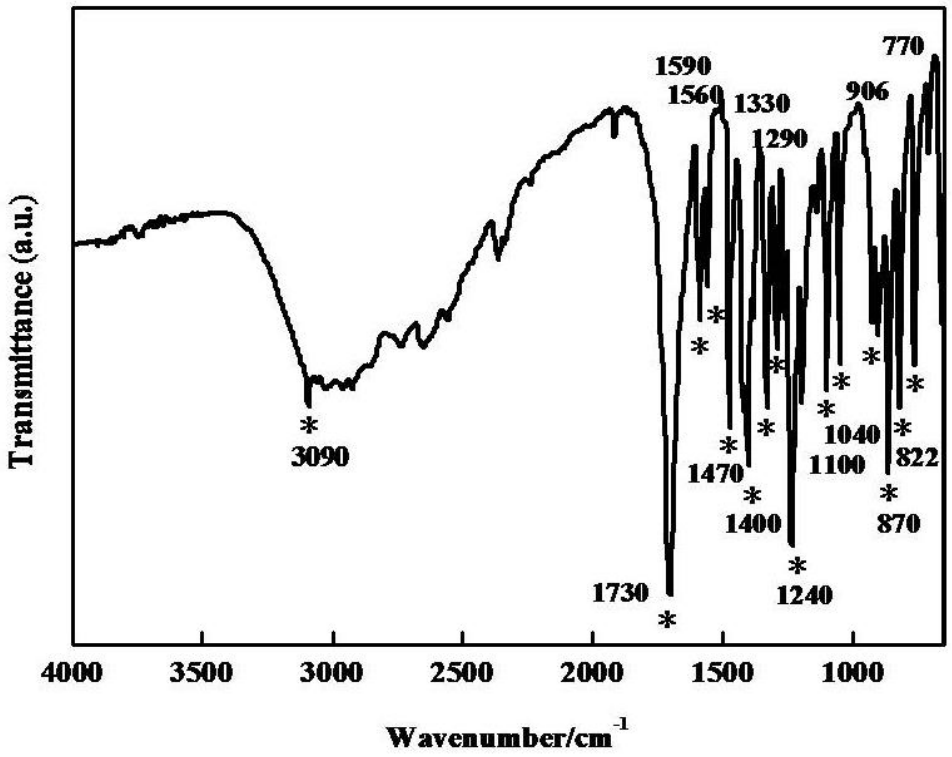
II. FT-IR Spectra

2,4-Dichlorophenylacetic acid (1b)



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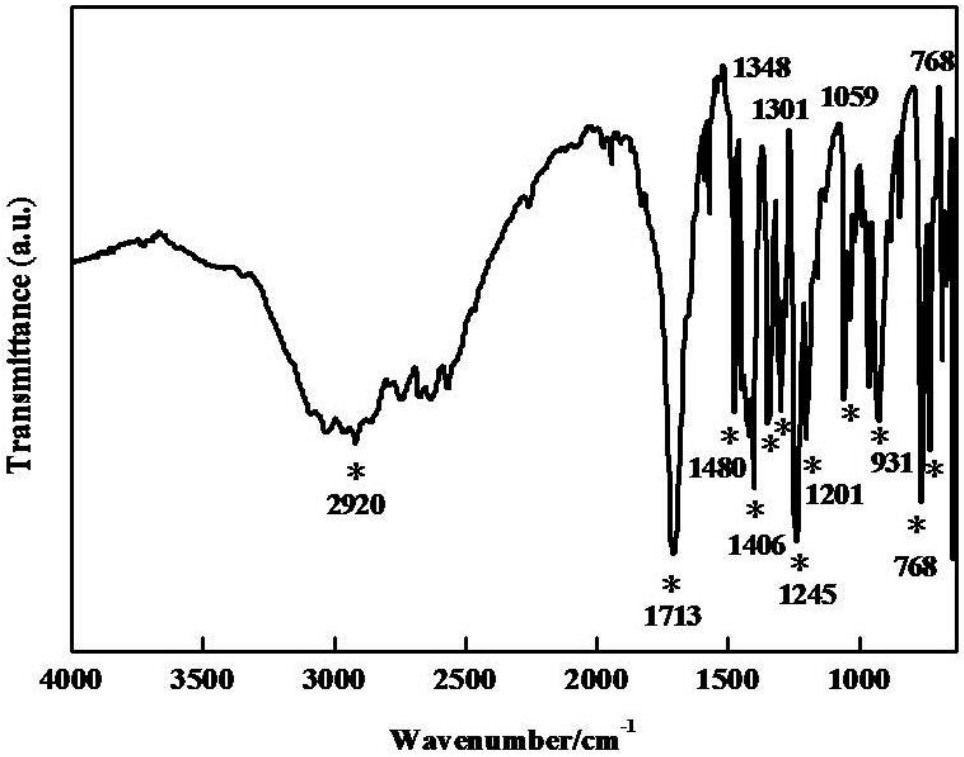

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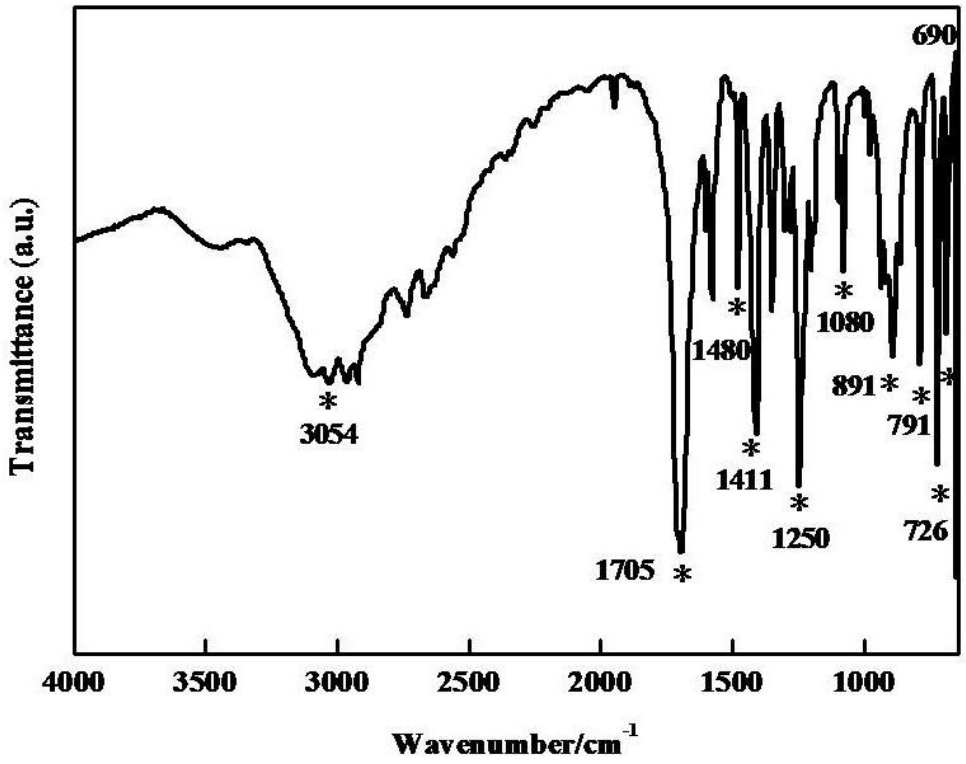
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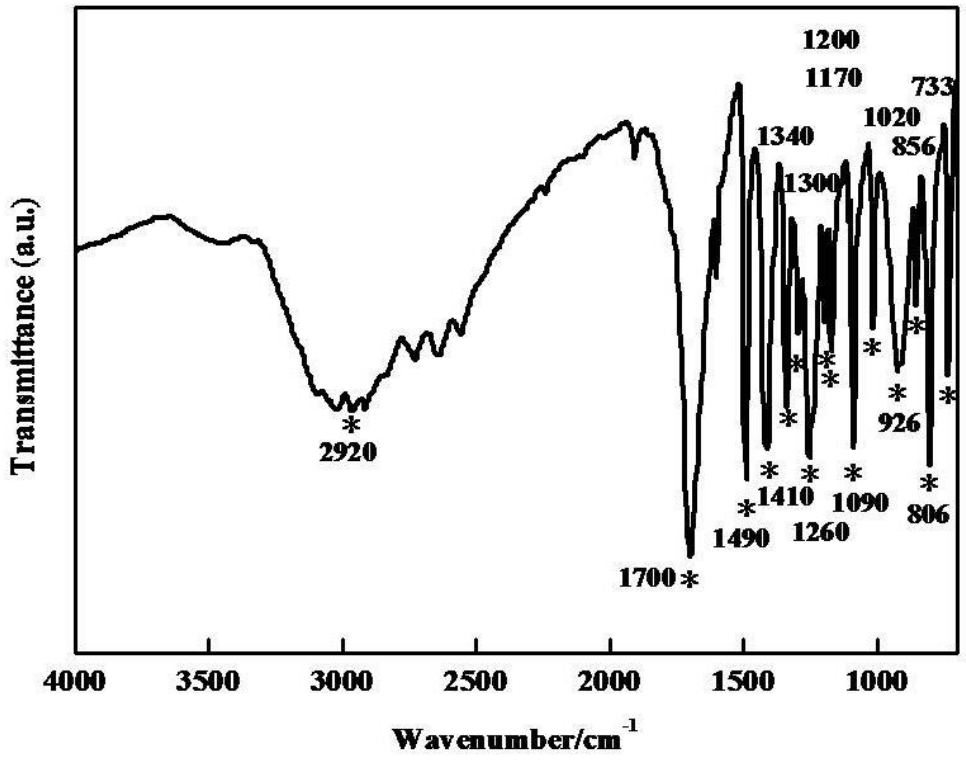
1500
1000
Wavenumber/cm-1

4b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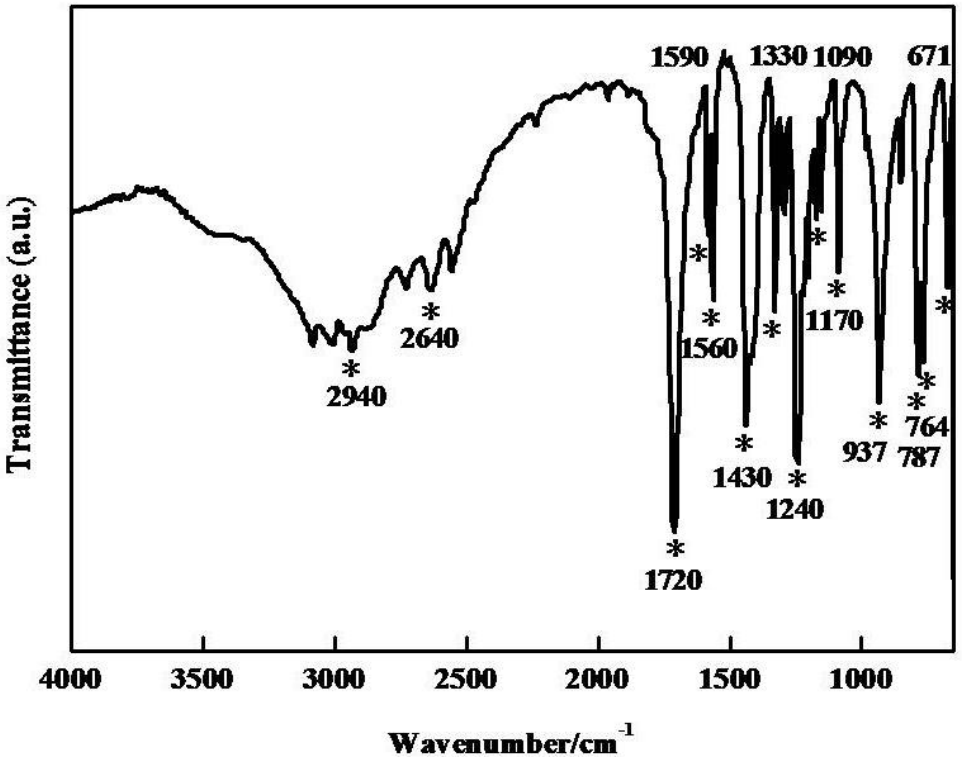
1500
1000
Wavenumber/cm-1

5b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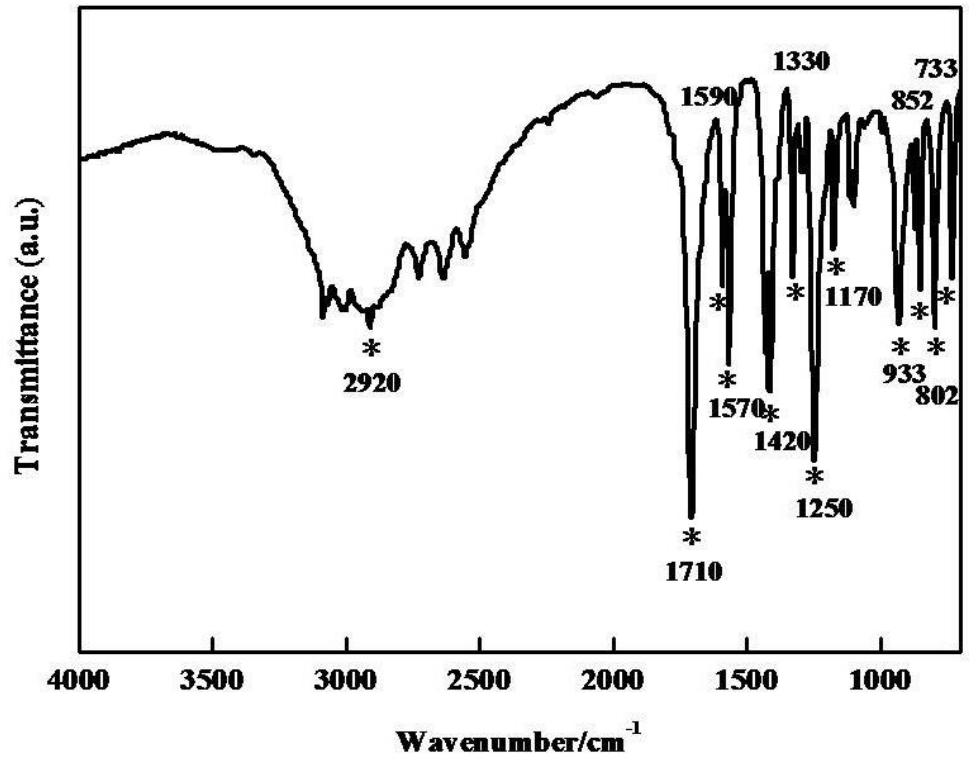
6b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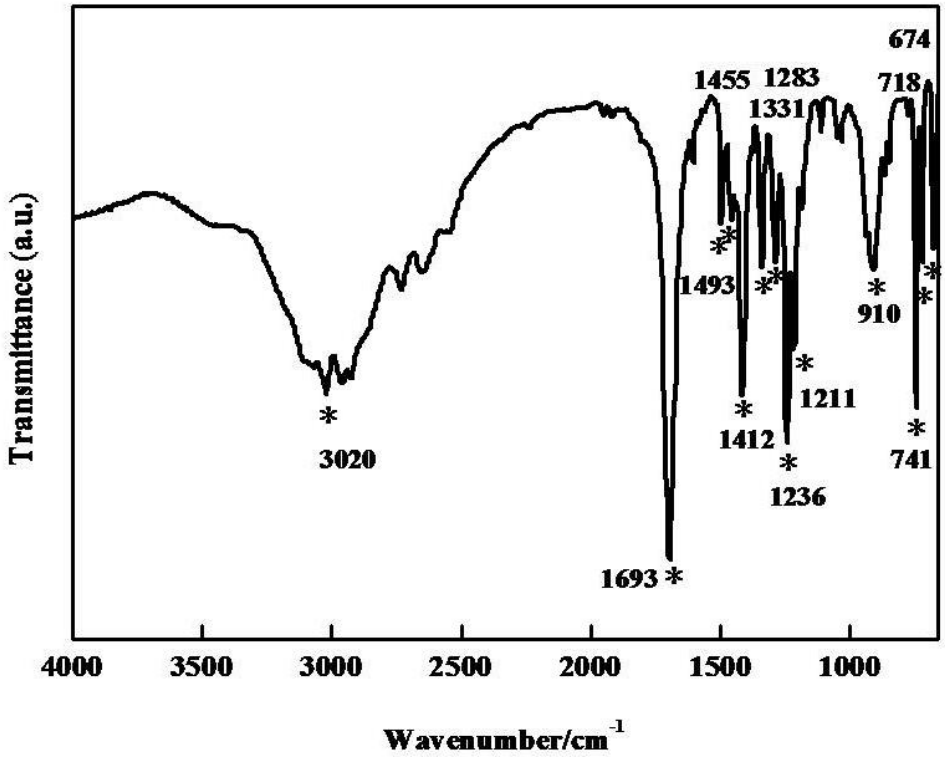
Wavenumber/cm-1

7b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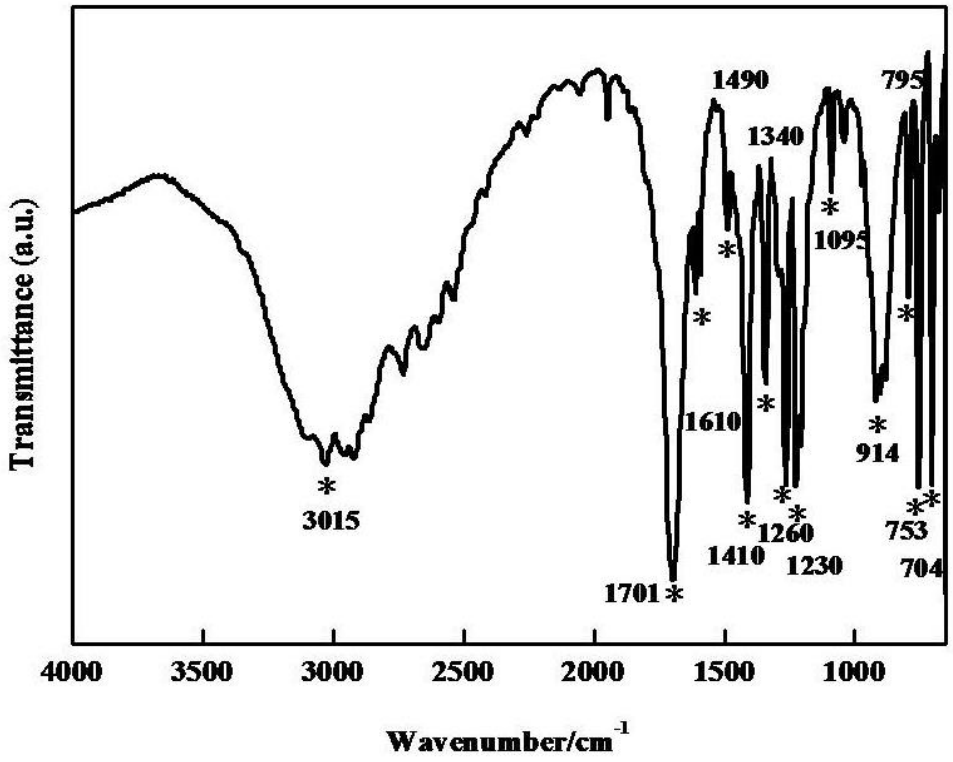
Wavenumber/cm-1

8b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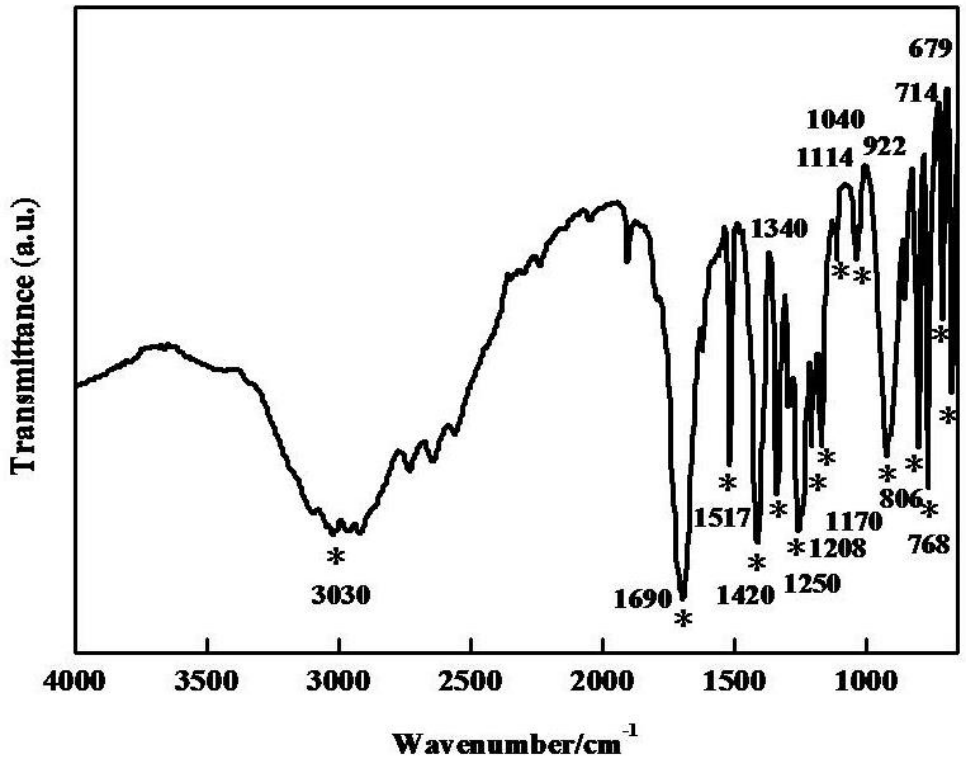
Wavenumber/cm-1

9b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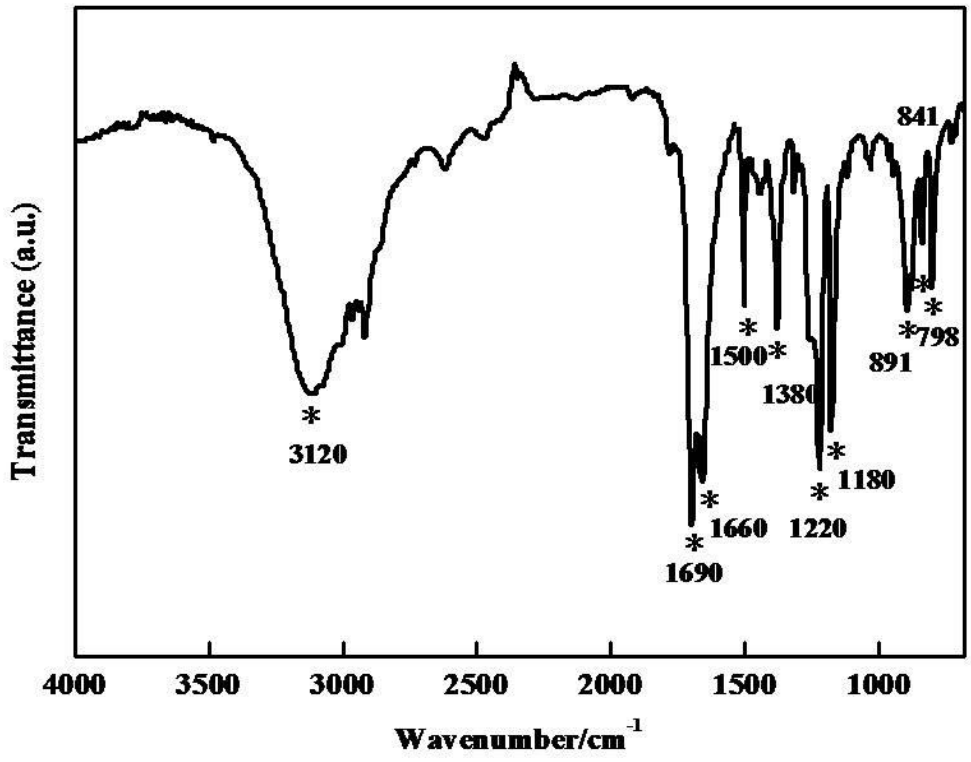
1500
1000
Wavenumber/cm-1

10b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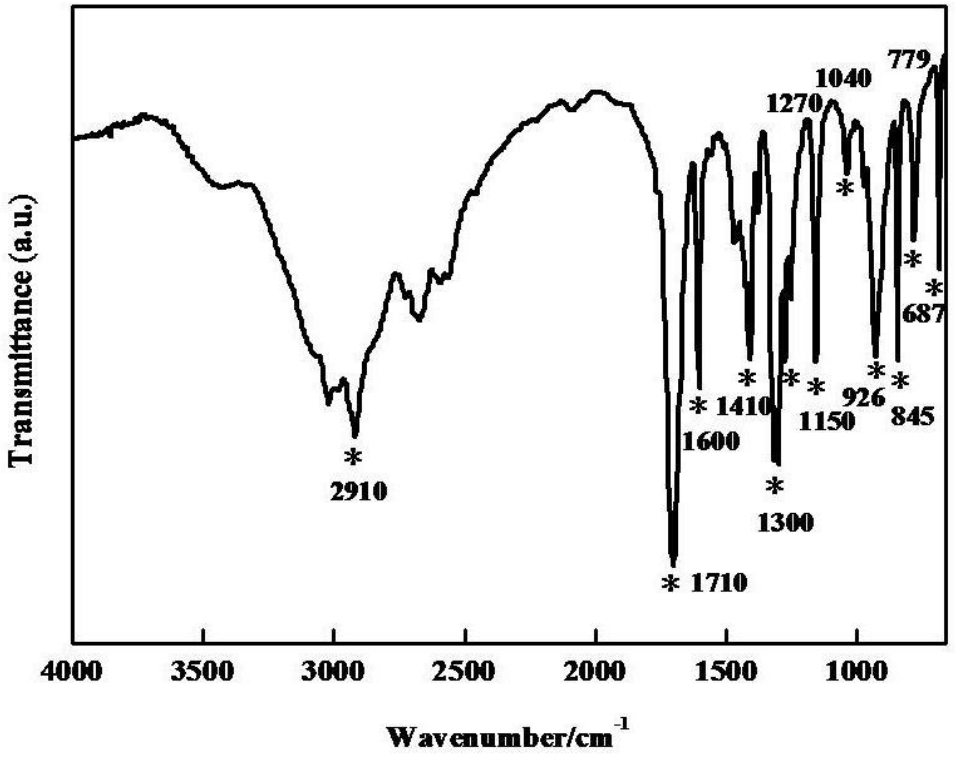
Wavenumber/cm-1

11b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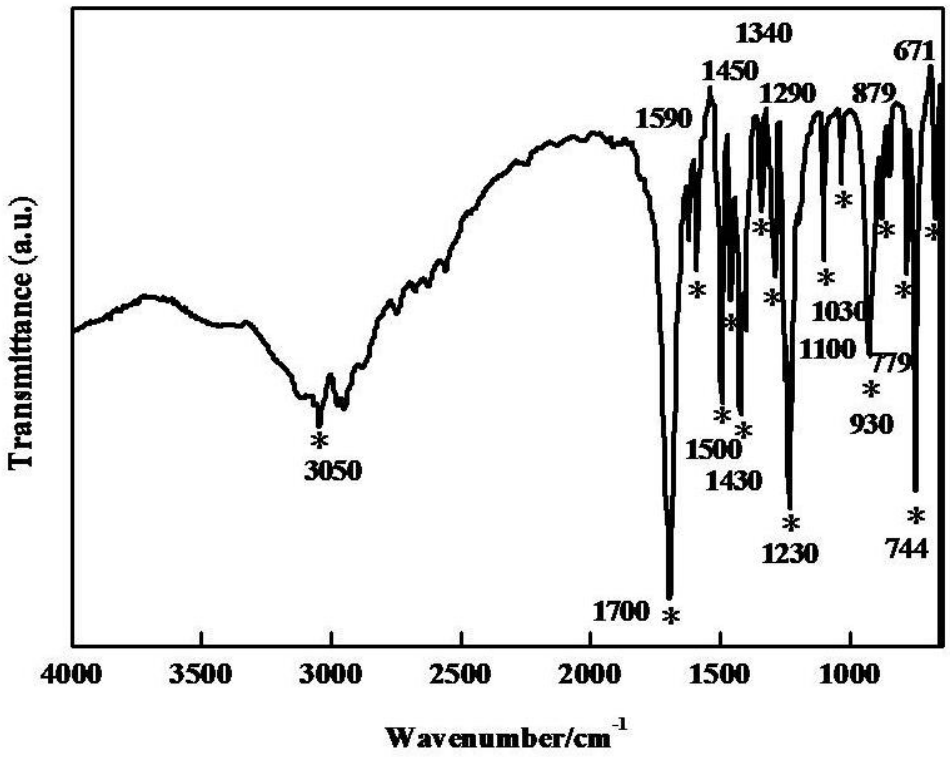
12b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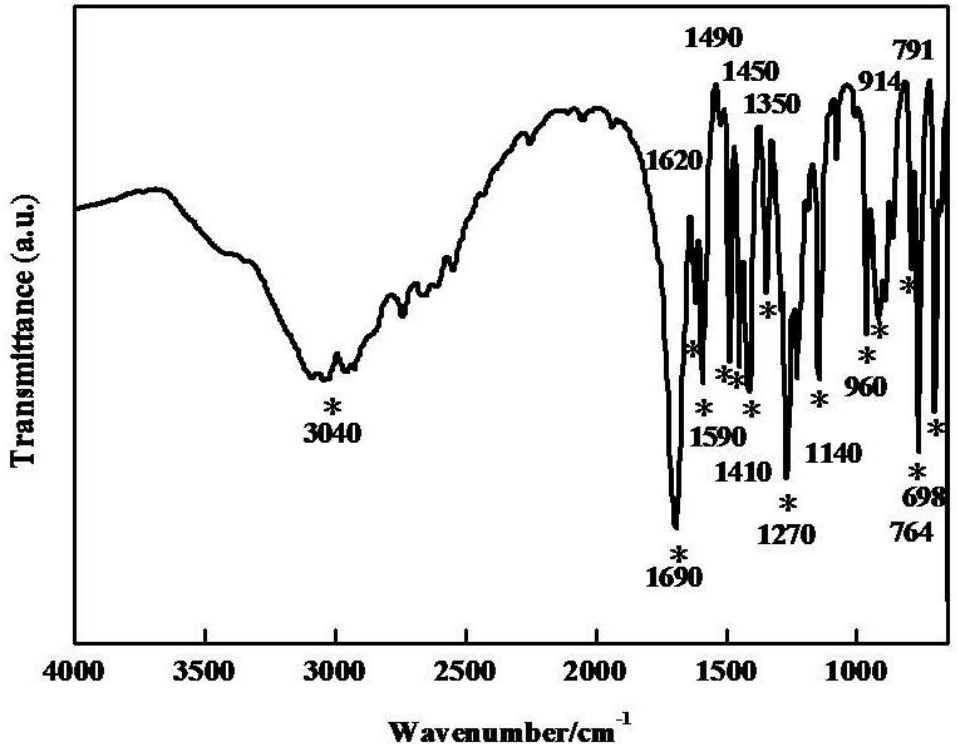
13b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764
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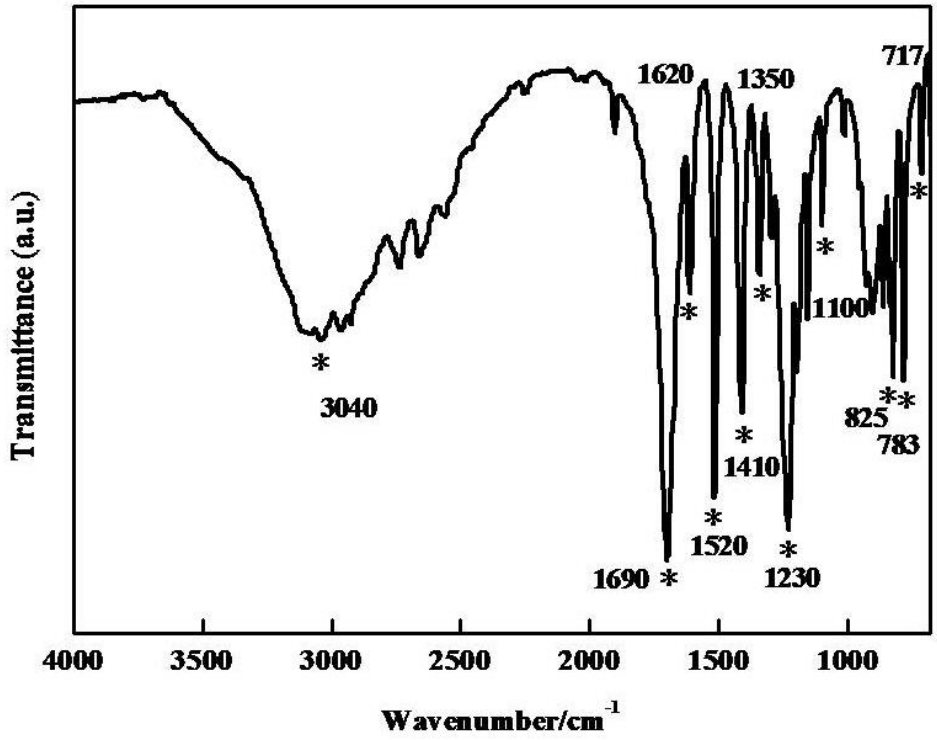
14b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Wavenumber/cm-1
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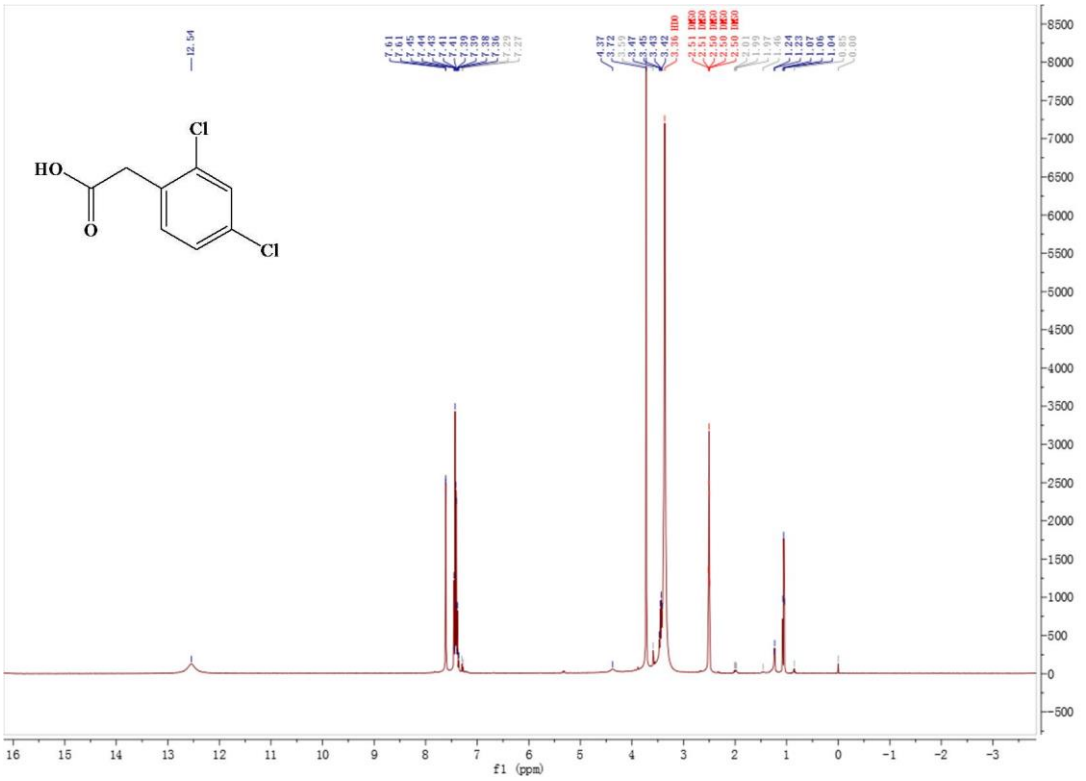
783
717

III. NMR Spectra

^{1}H NMR of 1b



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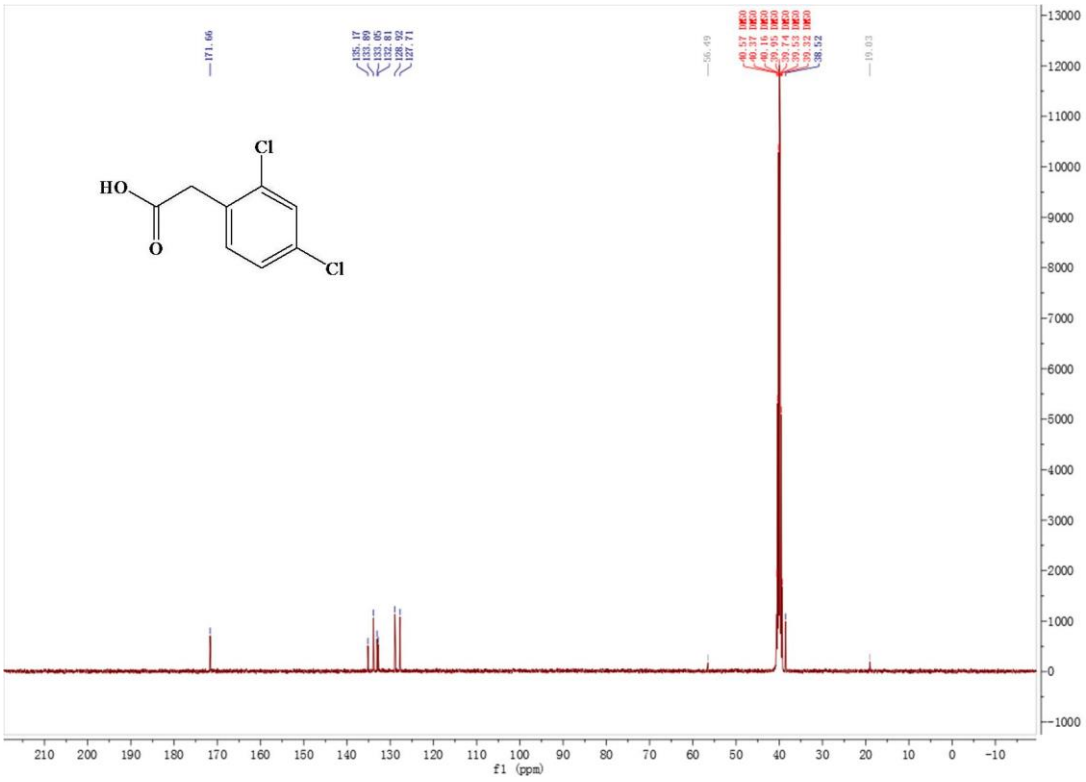

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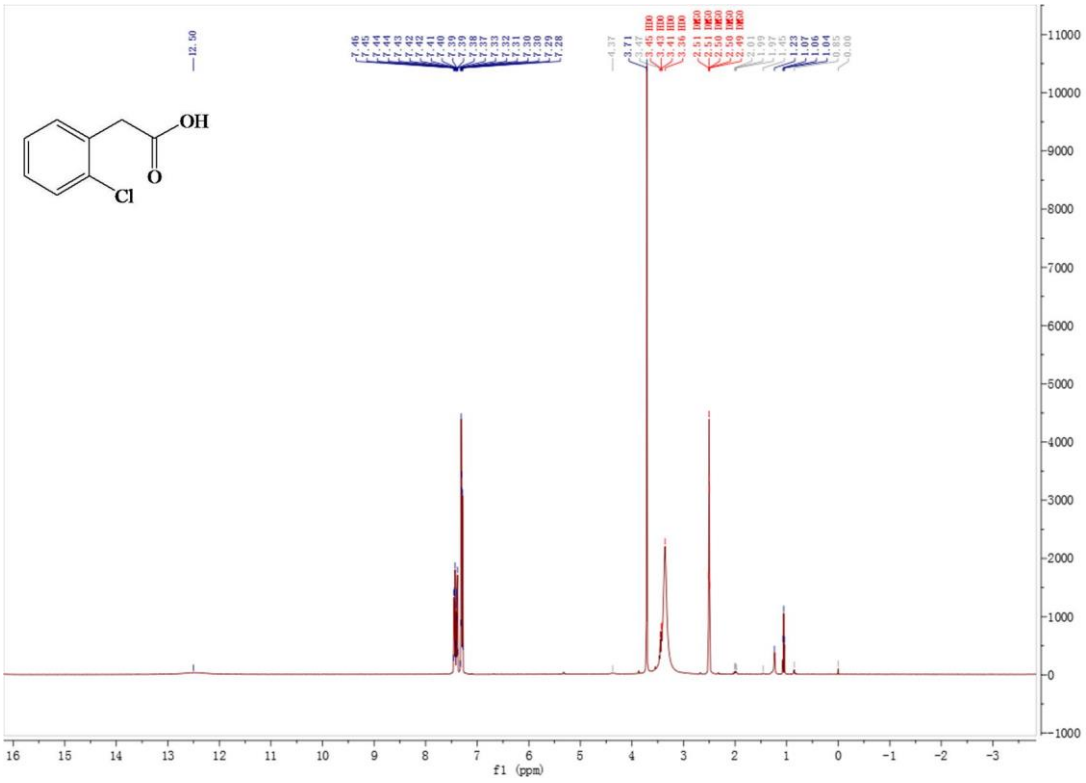

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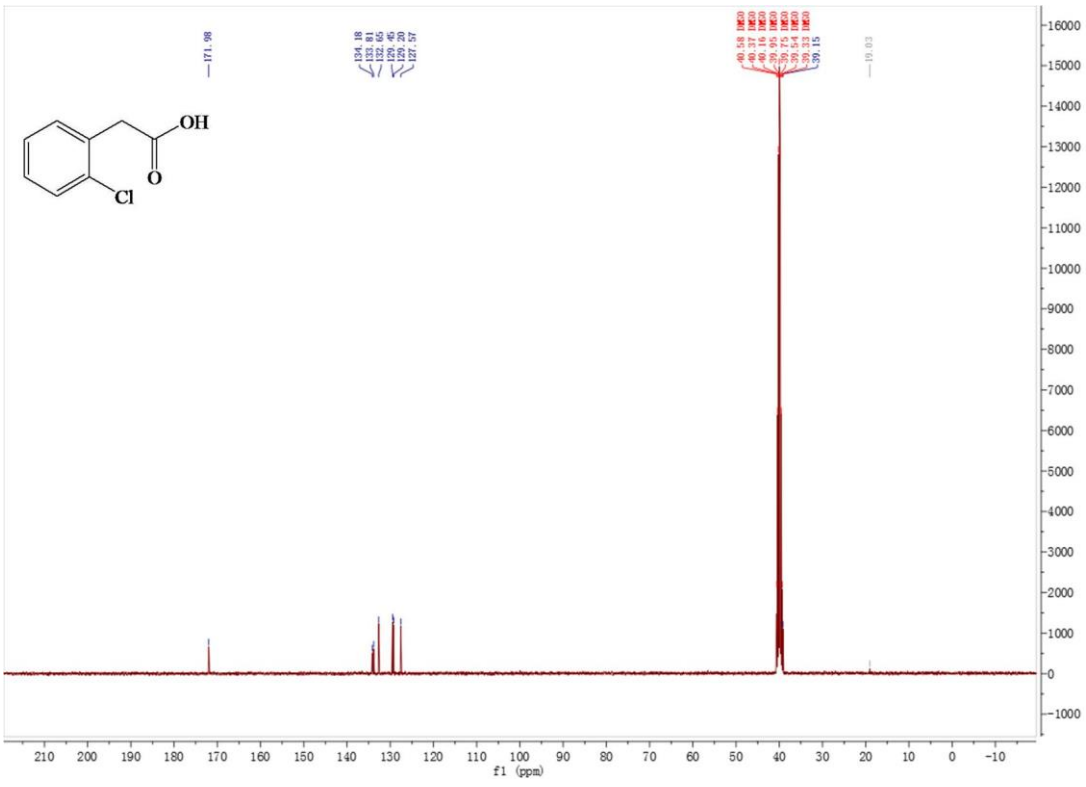

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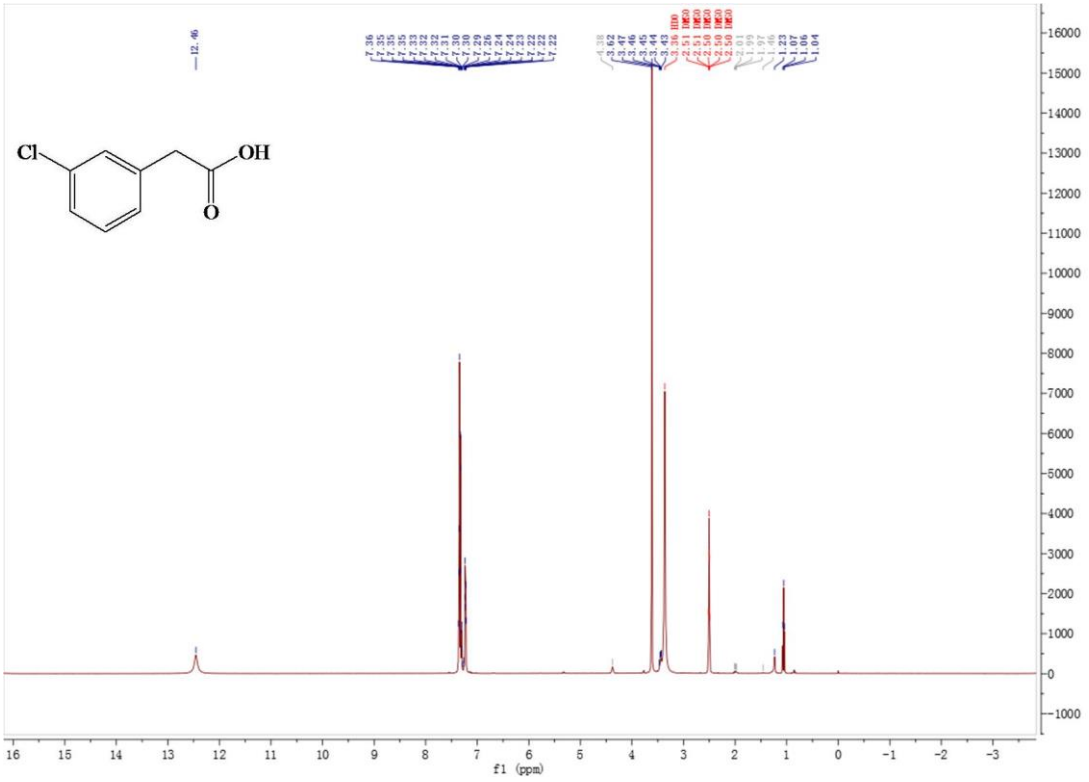

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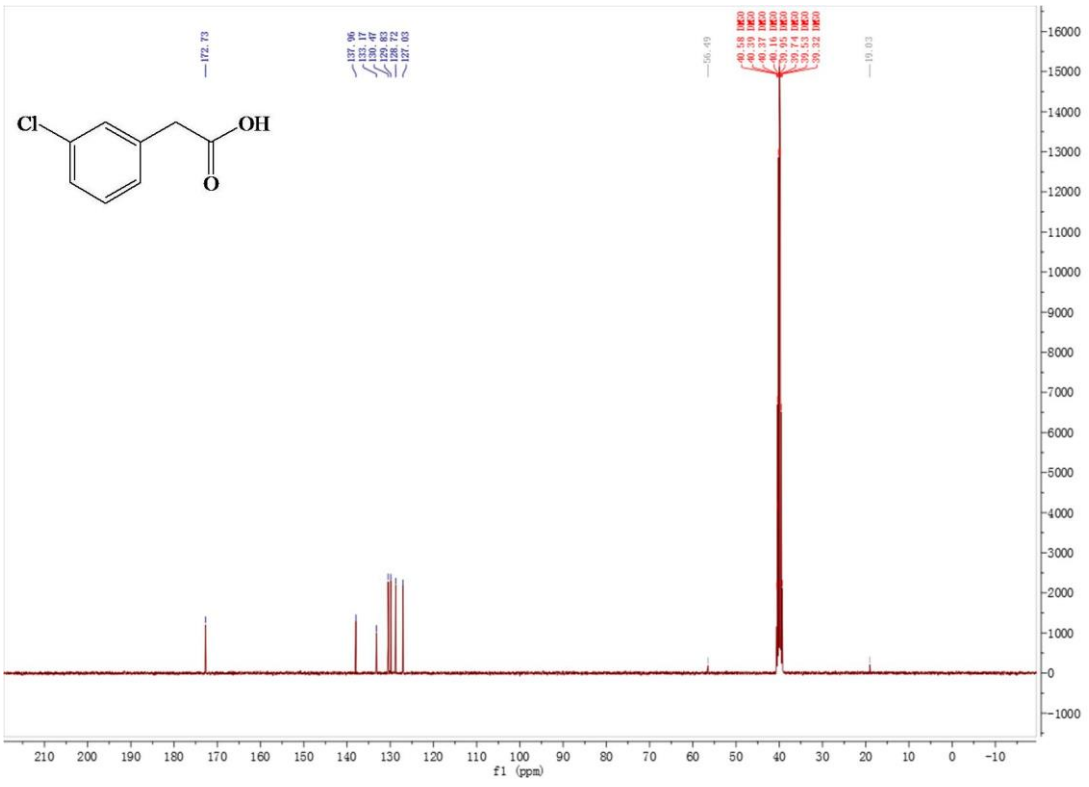

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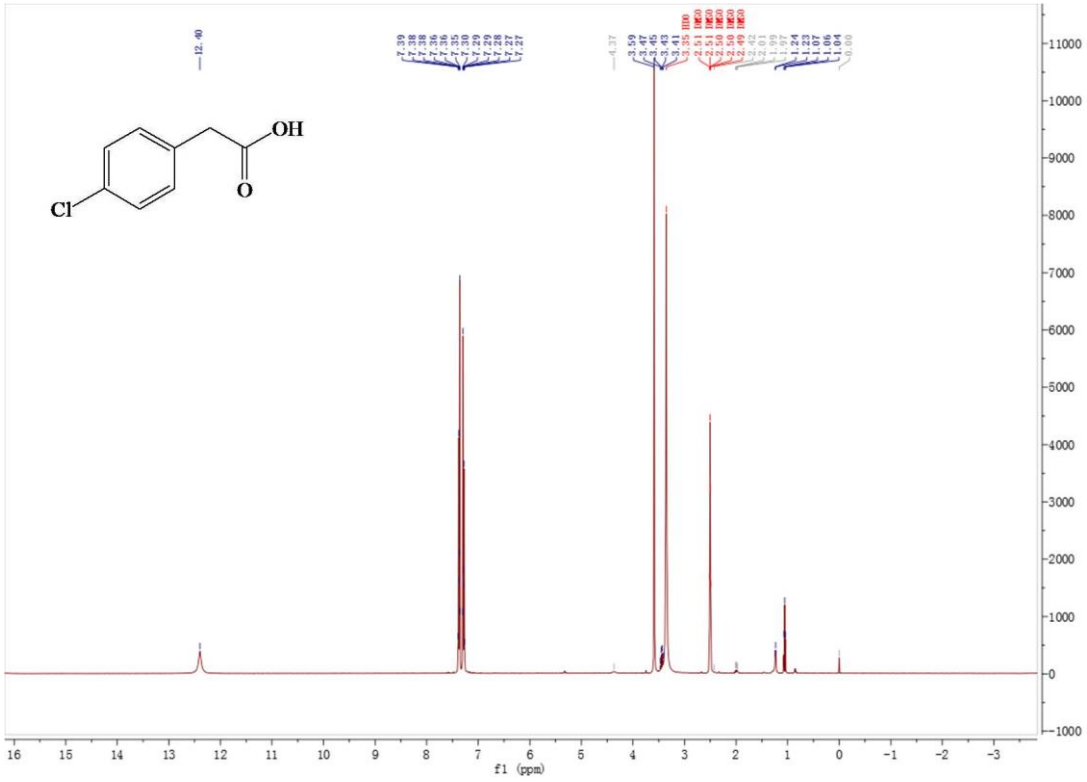

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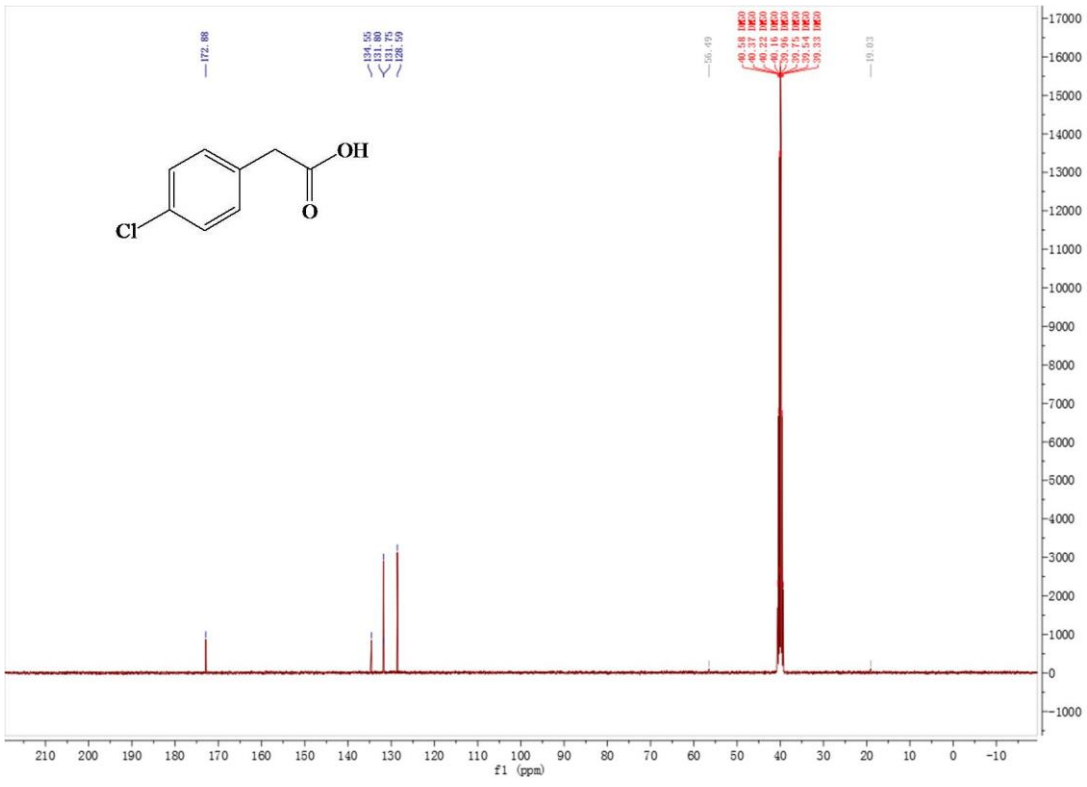

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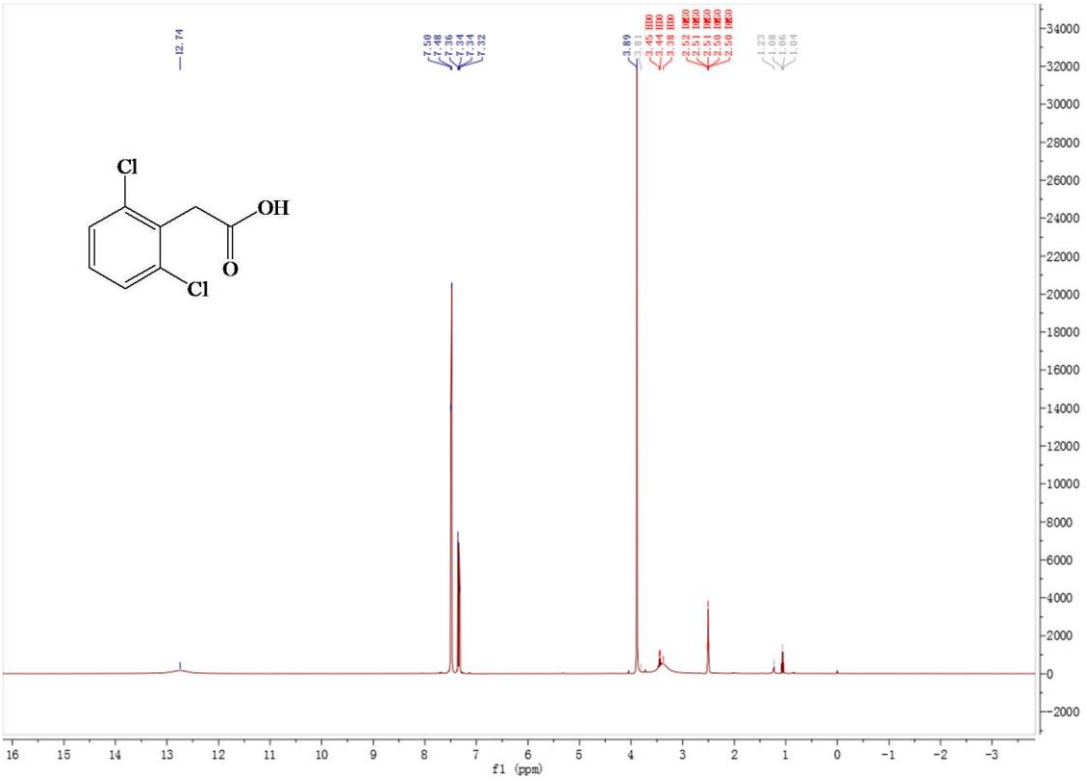

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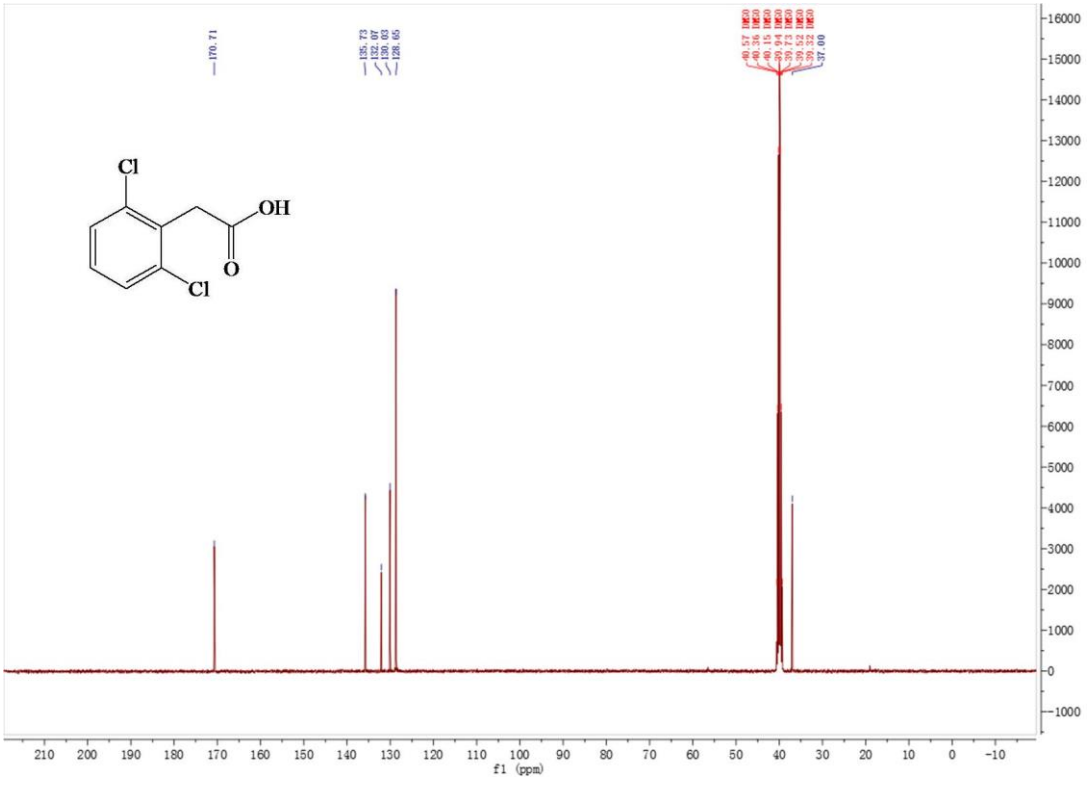

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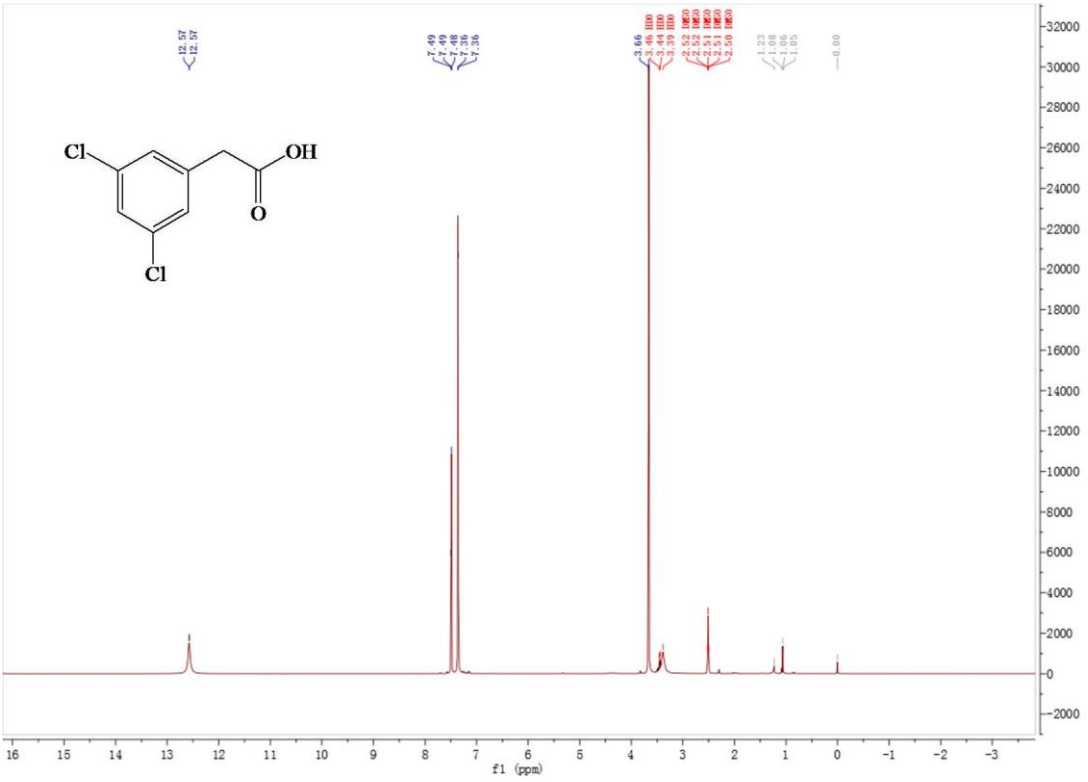

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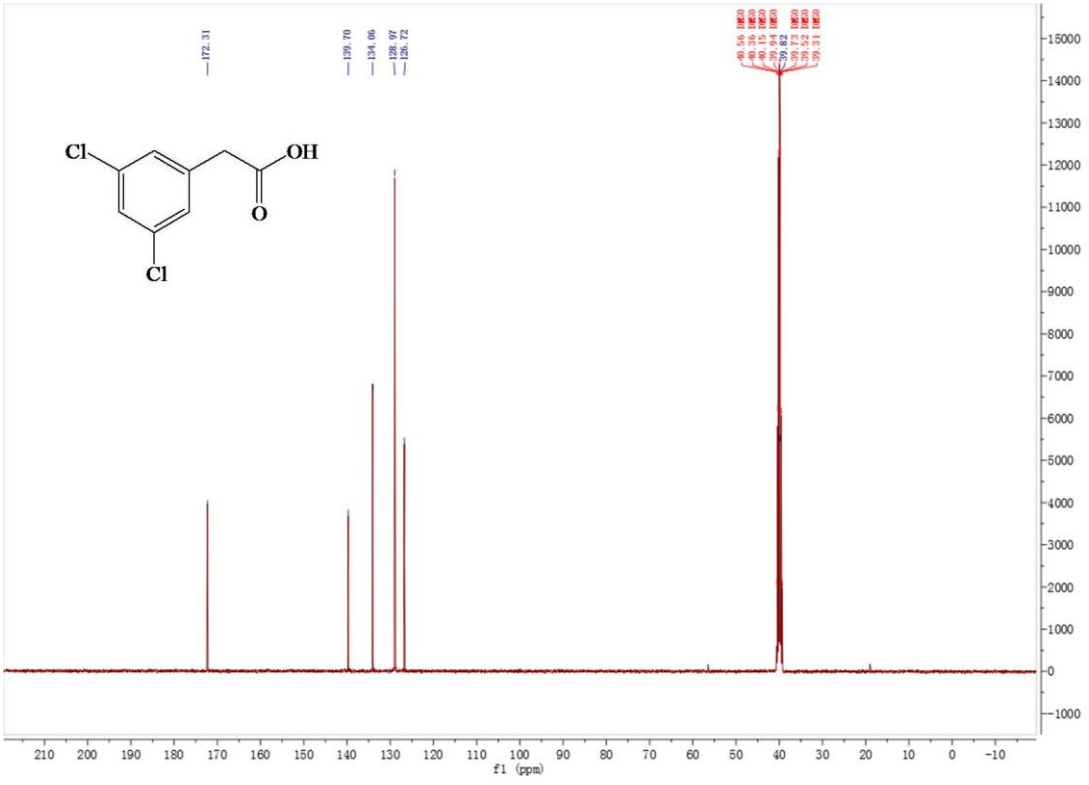

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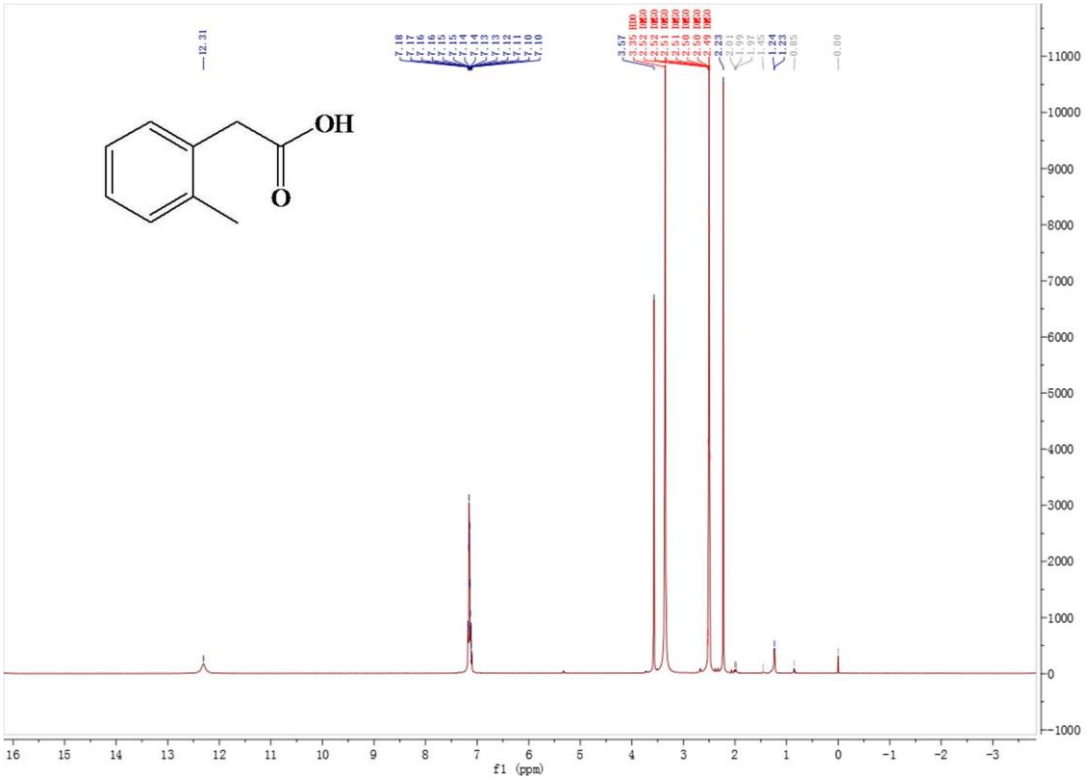
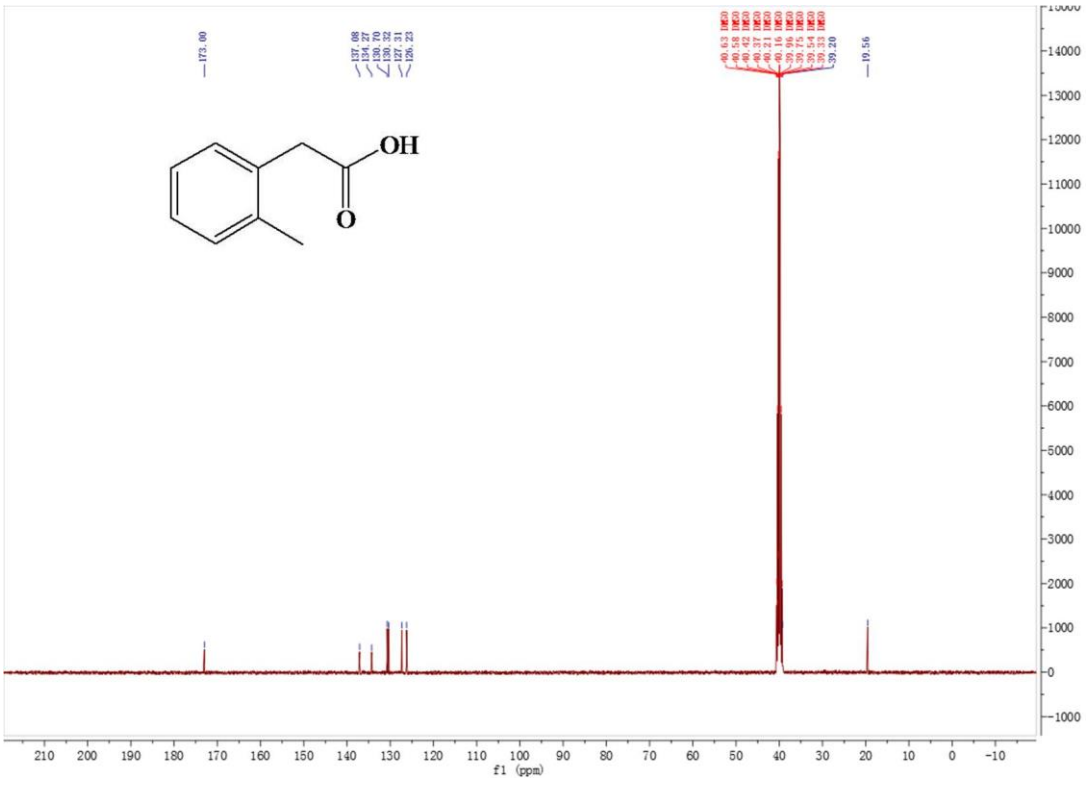
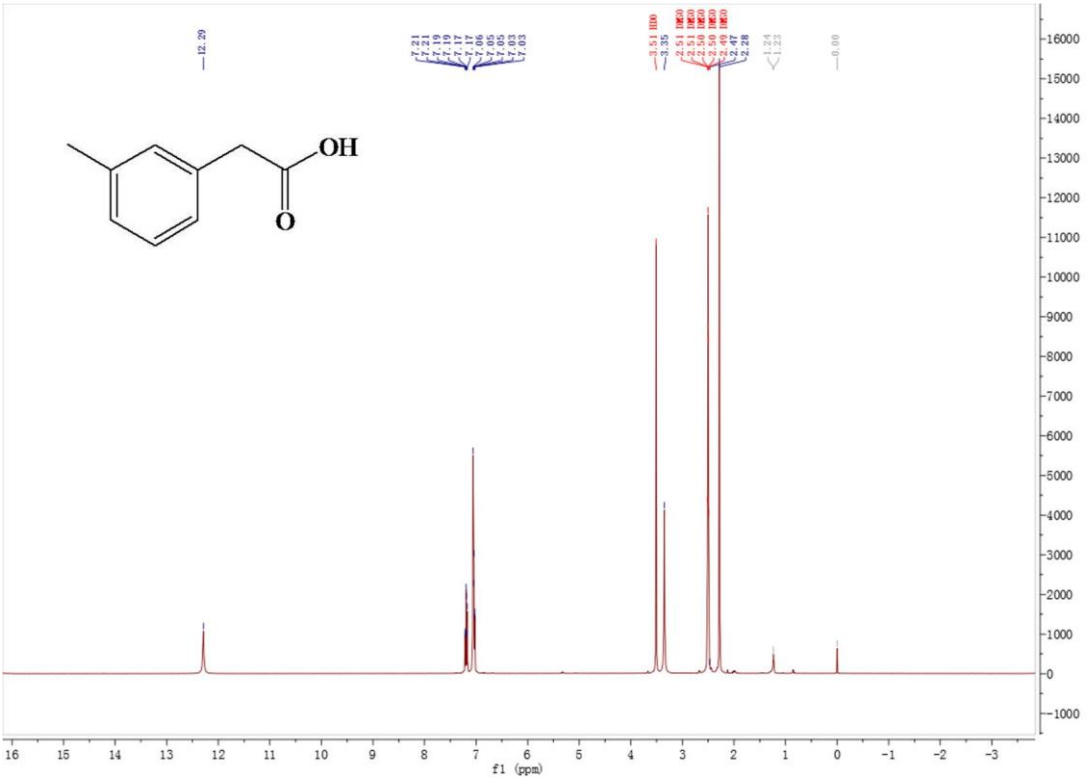


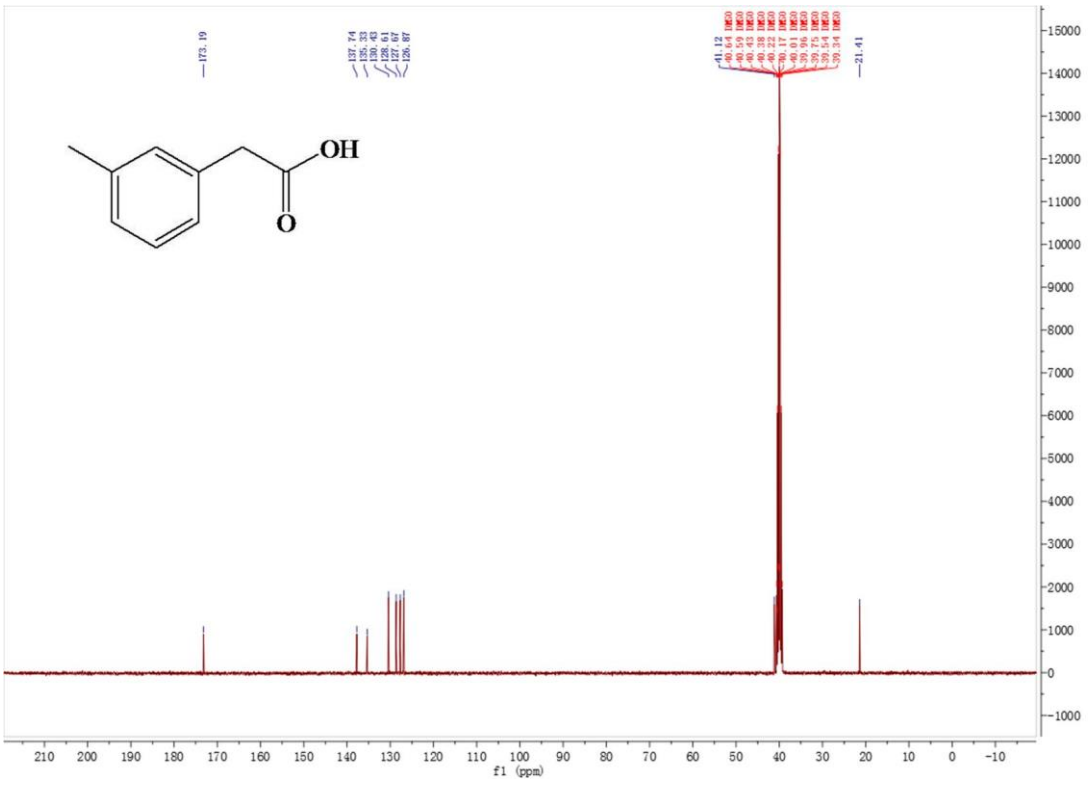
^{13}C NMR of 7b



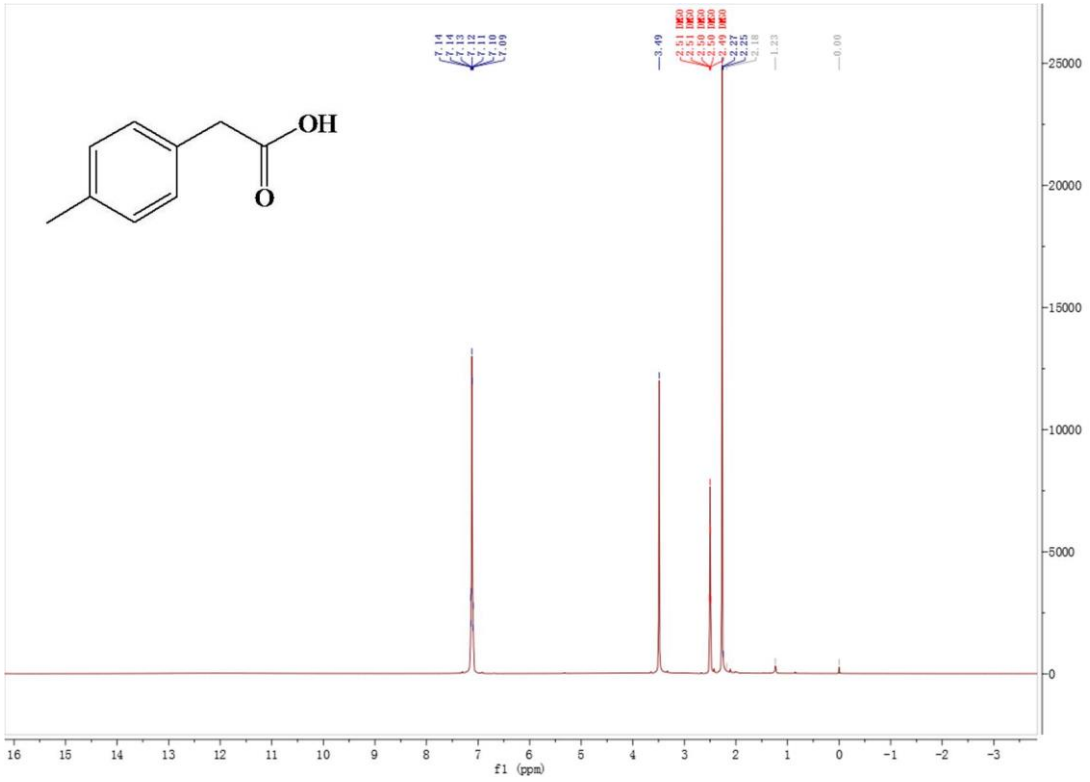
^{1}H NMR of 8b



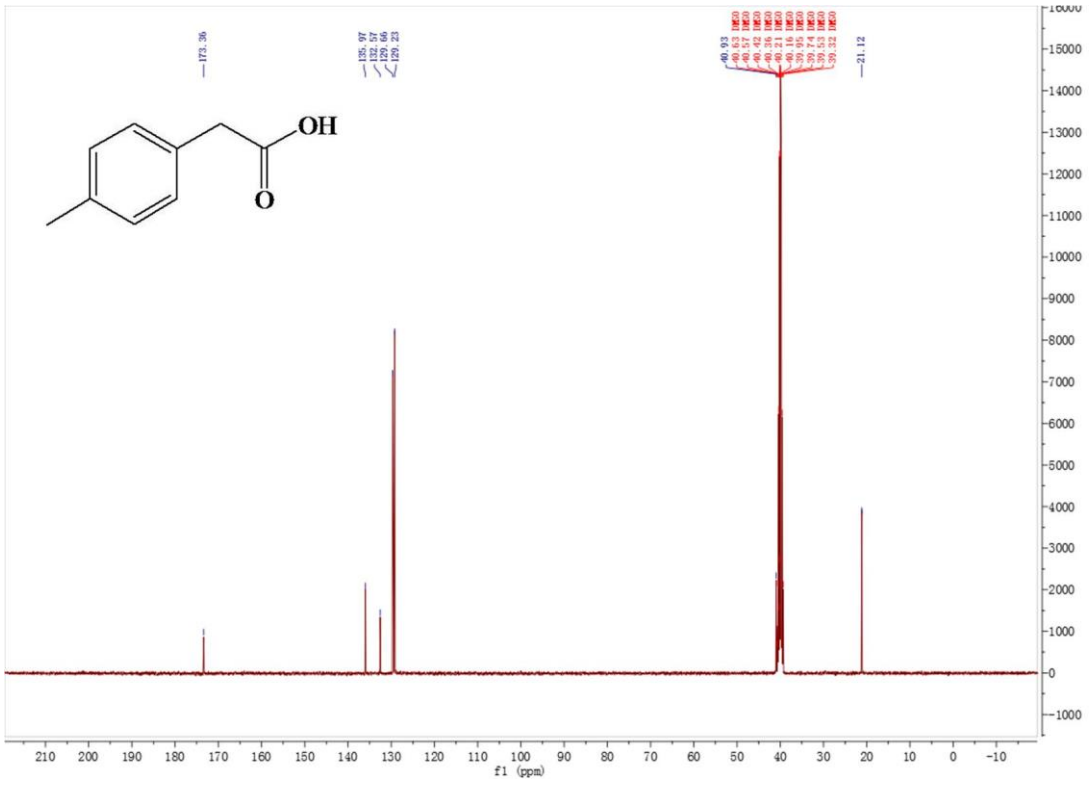
^{13}C NMR of 8b



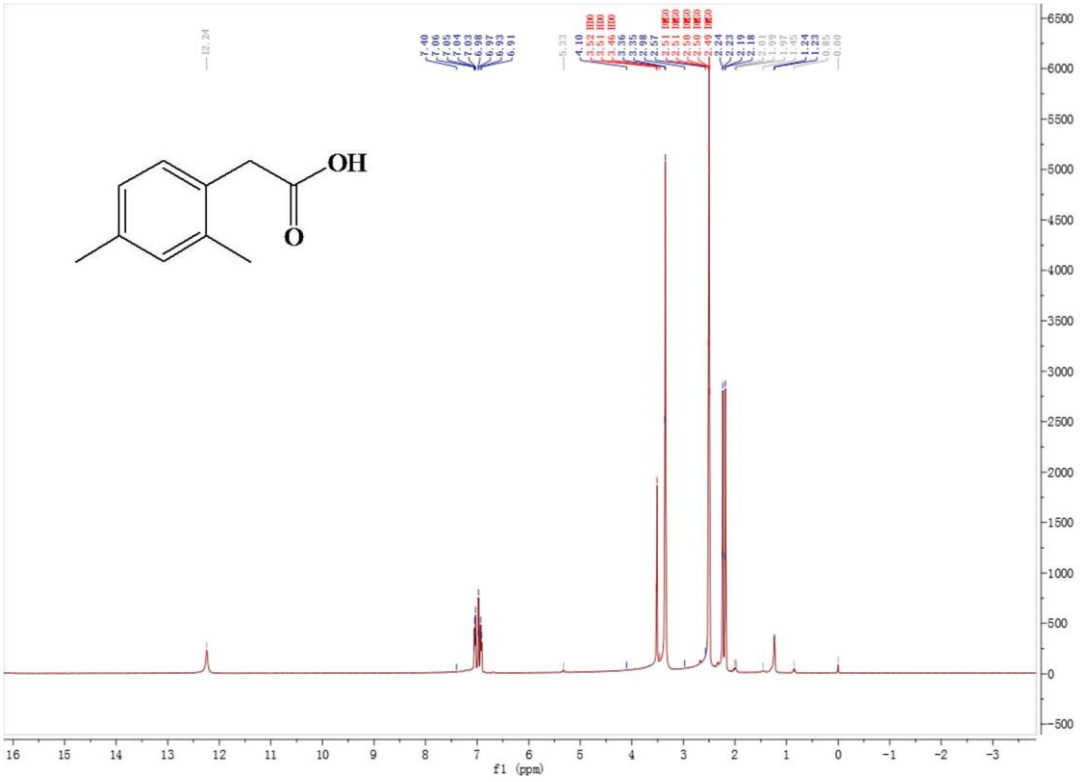
^{1}H NMR of 9b



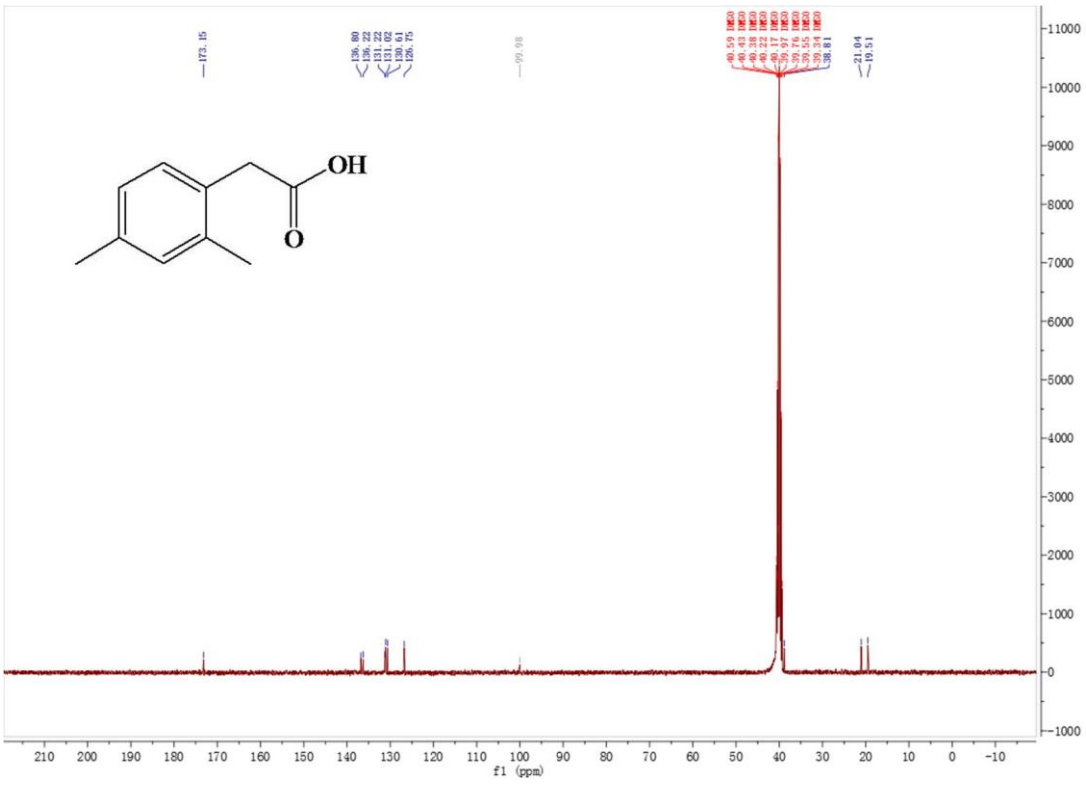
^{13}C NMR of 9b



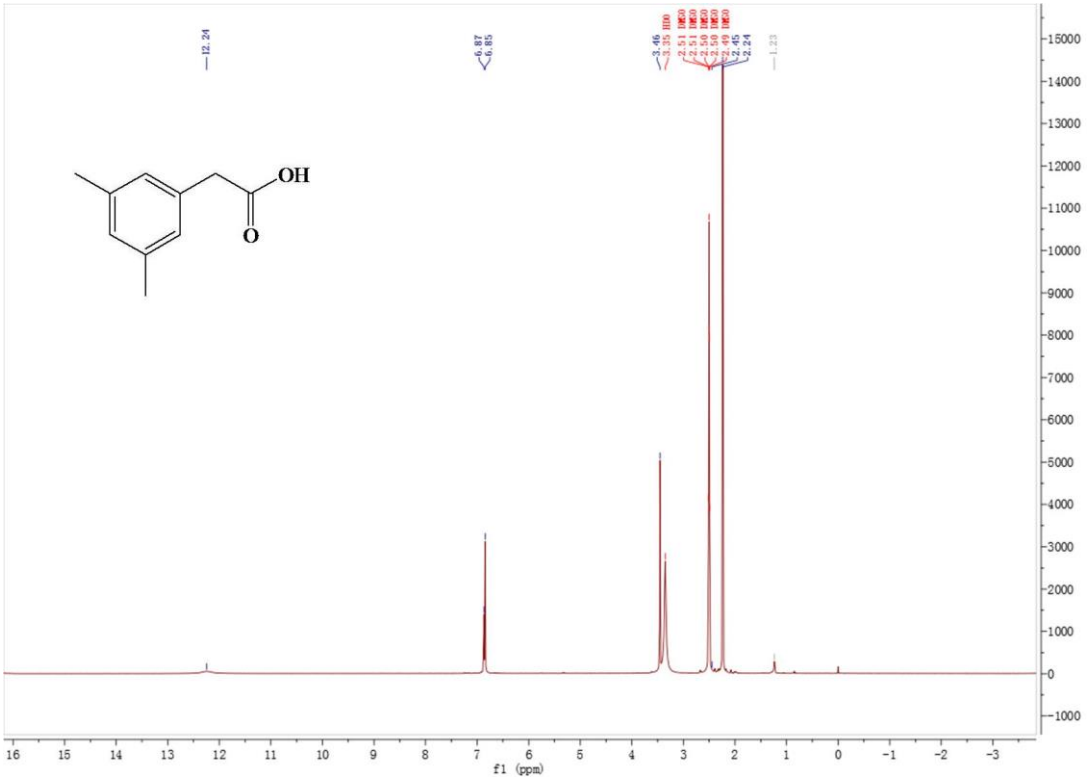
^{1}H NMR of 10b



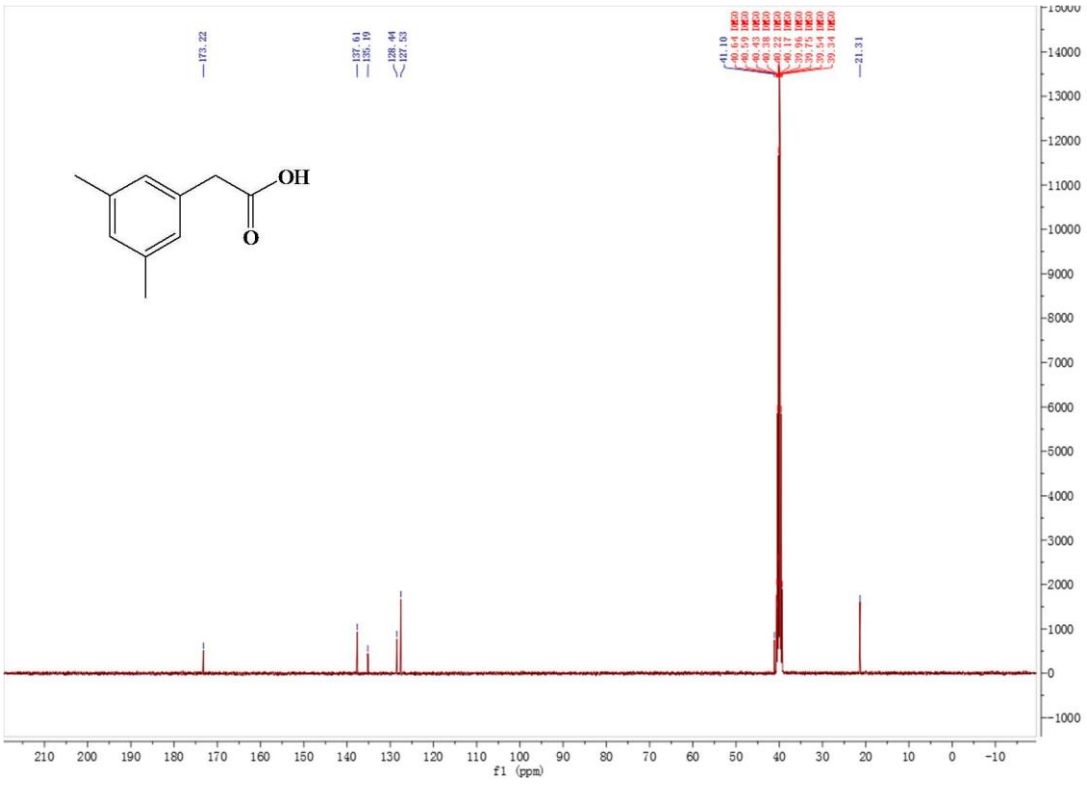
^{13}C NMR of 10b



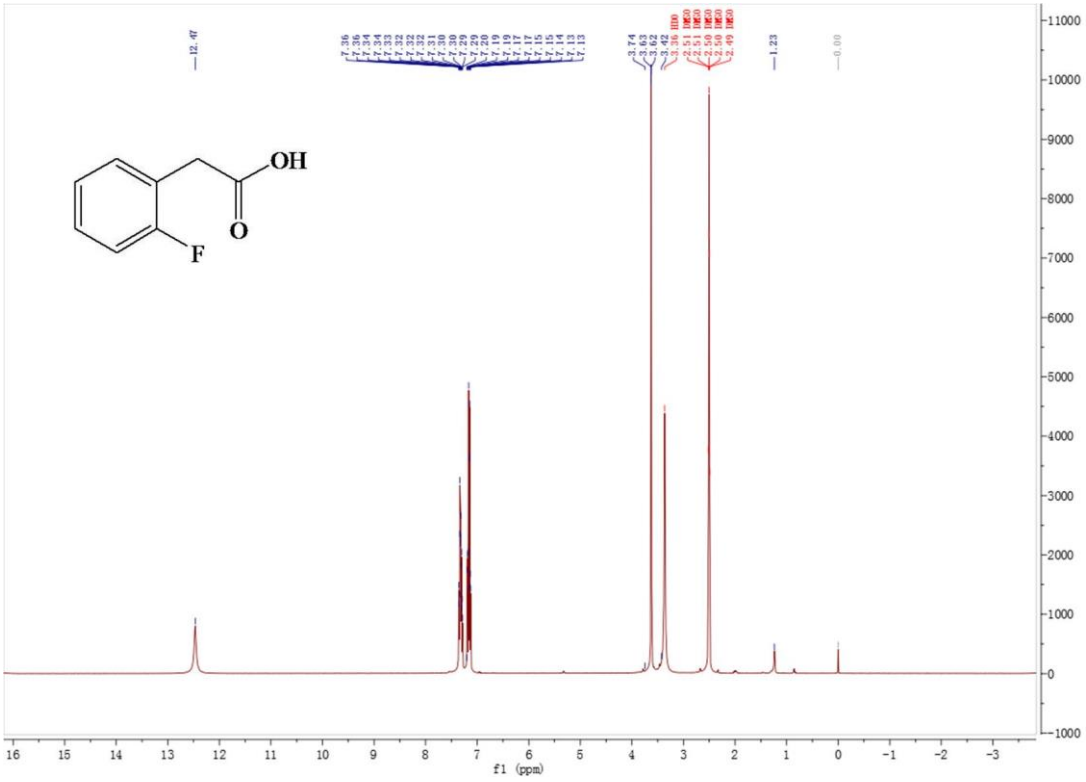
^{1}H NMR of 11b



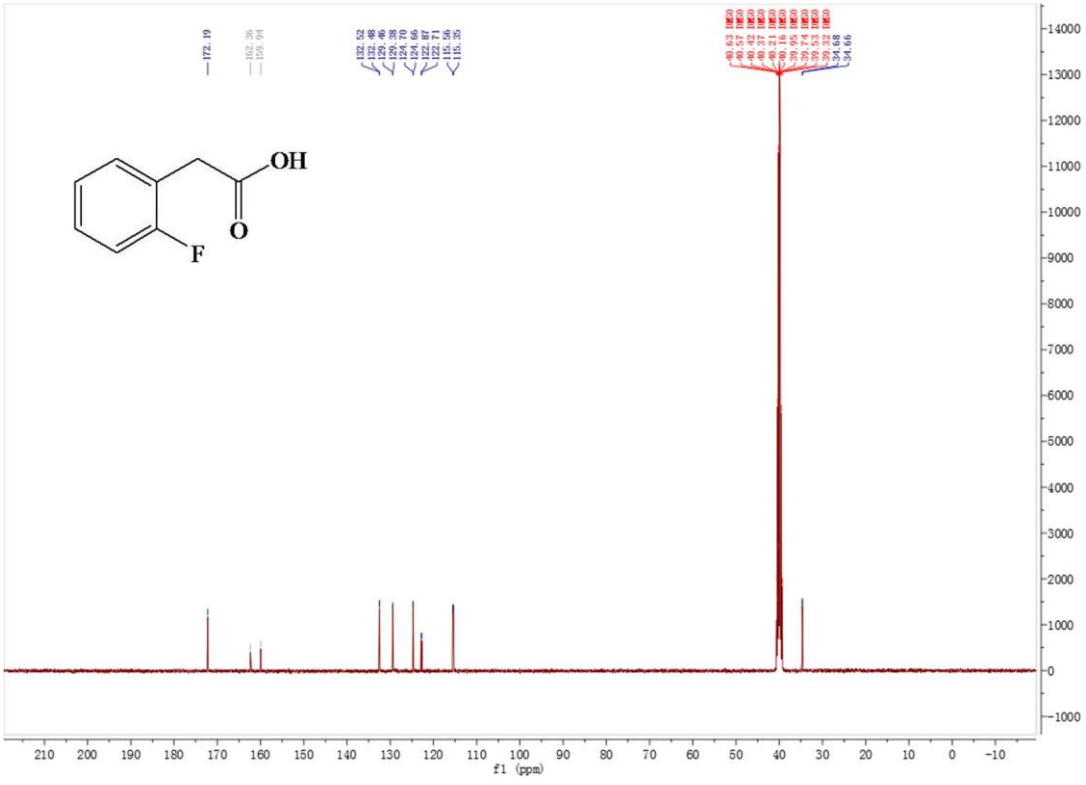
^{13}C NMR of 11b



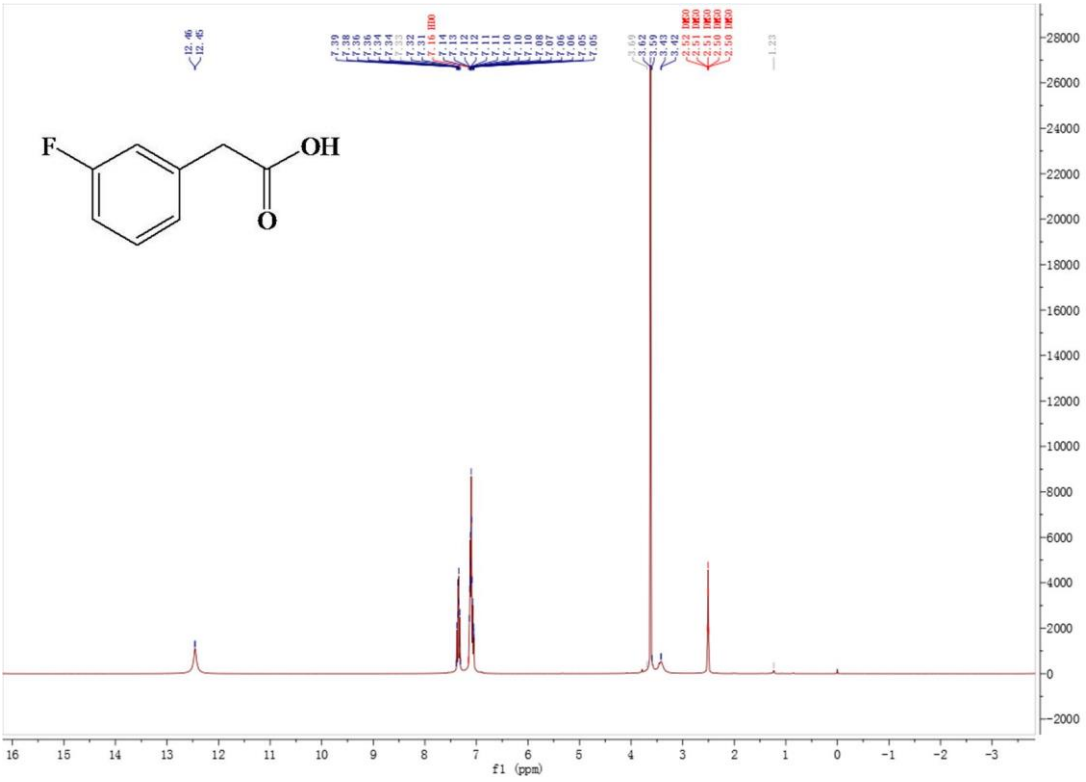
^{1}H NMR of 12b



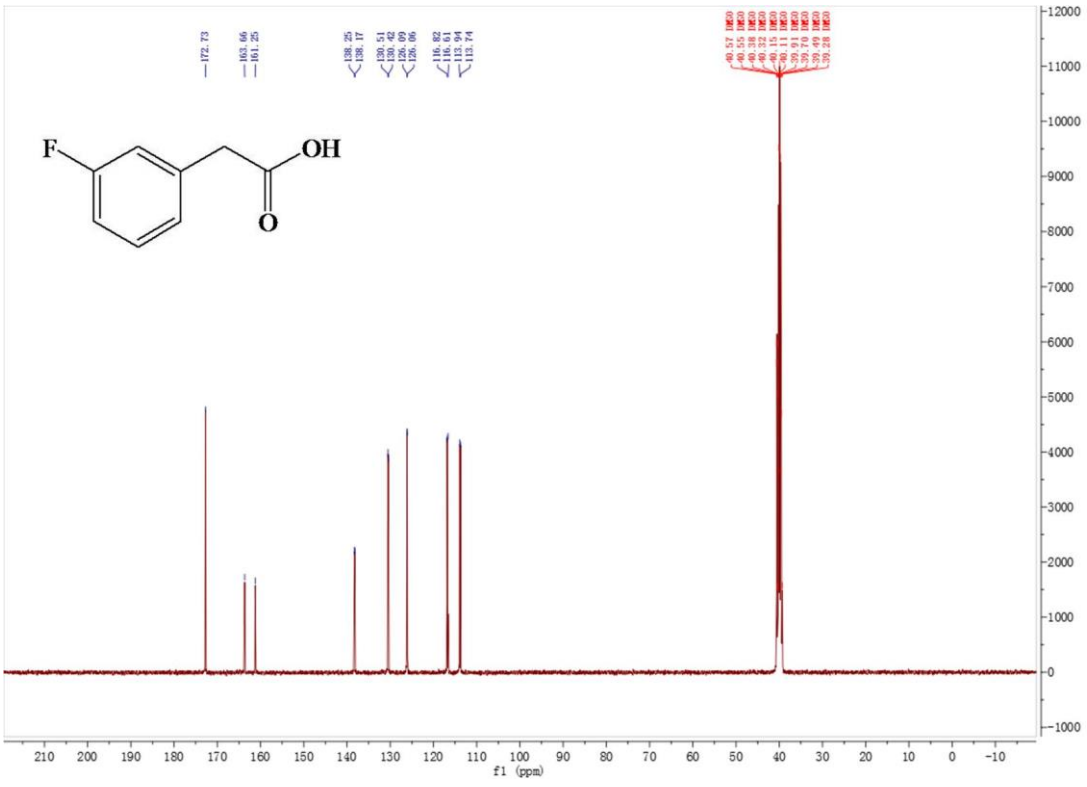
^{13}C NMR of 12b



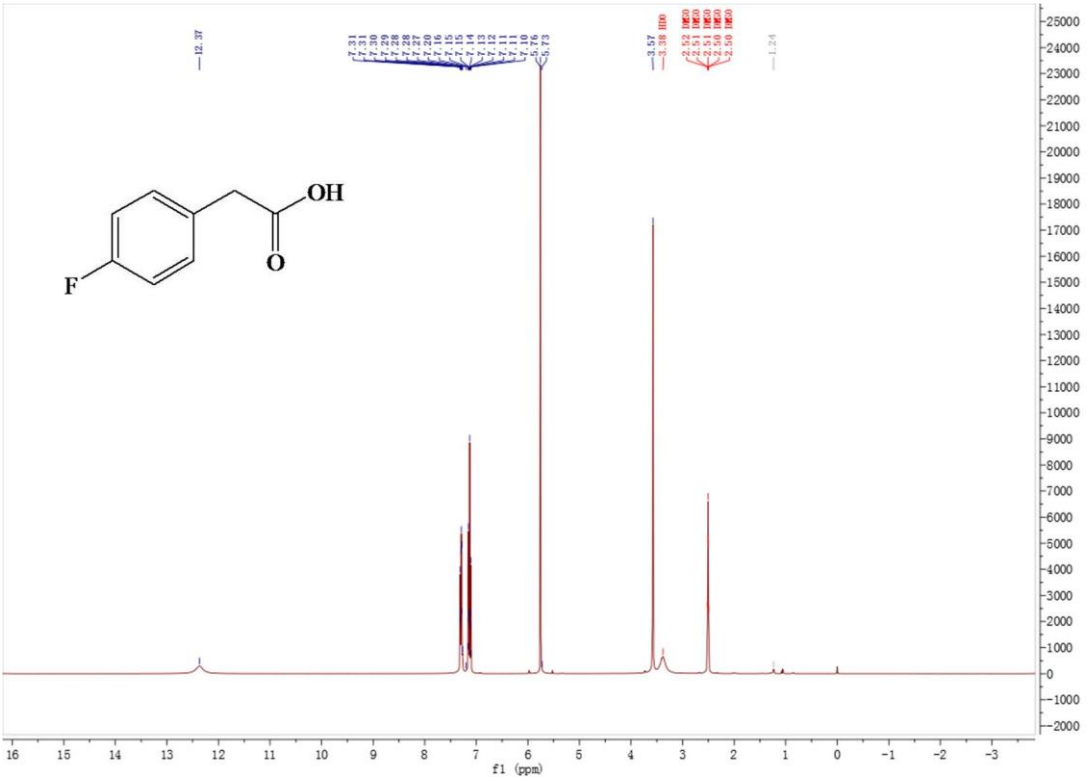
^{1}H NMR of 13b



^{13}C NMR of 13b



^{1}H NMR of 14b



^{13}C NMR of 14b