

**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; ¹H NMR (400 MHz; DMSO-d₆) δ: 12.50 (s, 1H), 7.51 - 7.36 (m, 1H), 7.40 - 7.25 (m, 3H), 3.71 (s, 2H) ppm; ¹³C NMR (100 MHz; DMSO-d₆) 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; ¹H NMR (400 MHz; DMSO-d₆) δ: 12.46 (s, 1H), 7.39 - 7.19 (m, 4H), 3.62 (s, 2H) ppm; ¹³C NMR (100 MHz; DMSO-d₆) 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; ¹H NMR (400 MHz; DMSO-d₆) 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; ¹³C NMR (100 MHz; DMSO-d₆) 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; ¹H NMR (400 MHz; DMSO-d₆) 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; ¹³C NMR (100 MHz; DMSO-d₆) 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; ¹H NMR (400 MHz; DMSO-d₆) 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; ¹³C NMR (100 MHz; DMSO-d₆) 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; ¹H NMR (400 MHz; DMSO-d₆) δ: 12.31 (s, 1H), 7.15 (m, 4H), 3.57 (s, 2H), 2.23 (s, 3H) ppm; ¹³C NMR (100 MHz; DMSO-d₆) 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; ¹H NMR (400 MHz; DMSO-d₆) δ: 12.29 (s, 1H), 7.19 (m, 4H), 3.35 (s, 2H), 2.47 (s, 3H) ppm; ¹³C NMR (100 MHz; DMSO-d₆) 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 °C (lit.⁷ 92 °C), IR (KBr) 679, 714, 768, 806, 922, 1040, 1114, 1170, 1208, 1250, 1340, 1420, 1517, 1690, 3030 cm⁻¹; ¹H NMR (400 MHz; DMSO-*d*₆) δ: 7.13 (m, 4H), 3.49 (s, 2H), 2.27 (s, 3H) ppm; ¹³C 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 °C (lit.⁸ 100-101 °C), IR (KBr) 798, 841, 891, 1180, 1220, 1380, 1500, 1660, 1690, 3120 cm⁻¹; ¹H 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; ¹³C 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 °C (lit.⁹ 96-98 °C), IR (KBr) 687, 779, 845, 926, 1040, 1150, 1270, 1300, 1410, 1600, 1710, 2910 cm⁻¹; ¹H 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; ¹³C 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 °C (lit.¹⁰ 59-60 °C), IR (KBr) 671, 744, 779, 879, 930, 1030, 1100, 1230, 1290, 1340, 1430, 1450, 1500, 1590, 1700, 3050 cm⁻¹; ¹H 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; ¹³C 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 °C (lit.¹¹ 43 °C), IR (KBr) 698, 764, 791, 914, 960, 1140, 1270, 1350, 1410, 1450, 1490, 1590, 1620, 1690, 3040 cm⁻¹; ¹H 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; ¹³C 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.

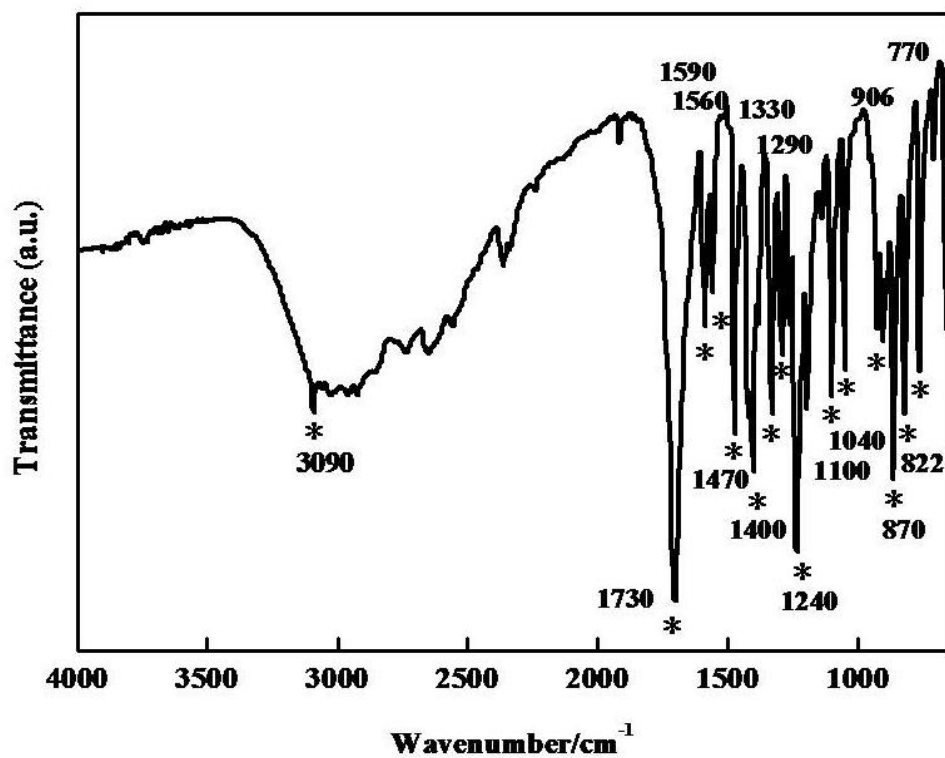
4-Fluorophenylacetic acid (**14b**): a white solid; mp 81-84 °C (lit.³ 82-85 °C), IR (KBr) 717, 783, 825, 1100, 1230, 1350, 1410, 1520, 1620, 1690, 3040 cm⁻¹; ¹H NMR (400 MHz; DMSO-*d*₆) δ: 12.37 (s, 1H), 7.34 - 7.24 (m, 2H), 7.22 - 7.07 (t, *J* = 8.78 Hz, 2H), 3.57 (s, 2H) ppm; ¹³C NMR (100 MHz; DMSO-*d*₆) 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

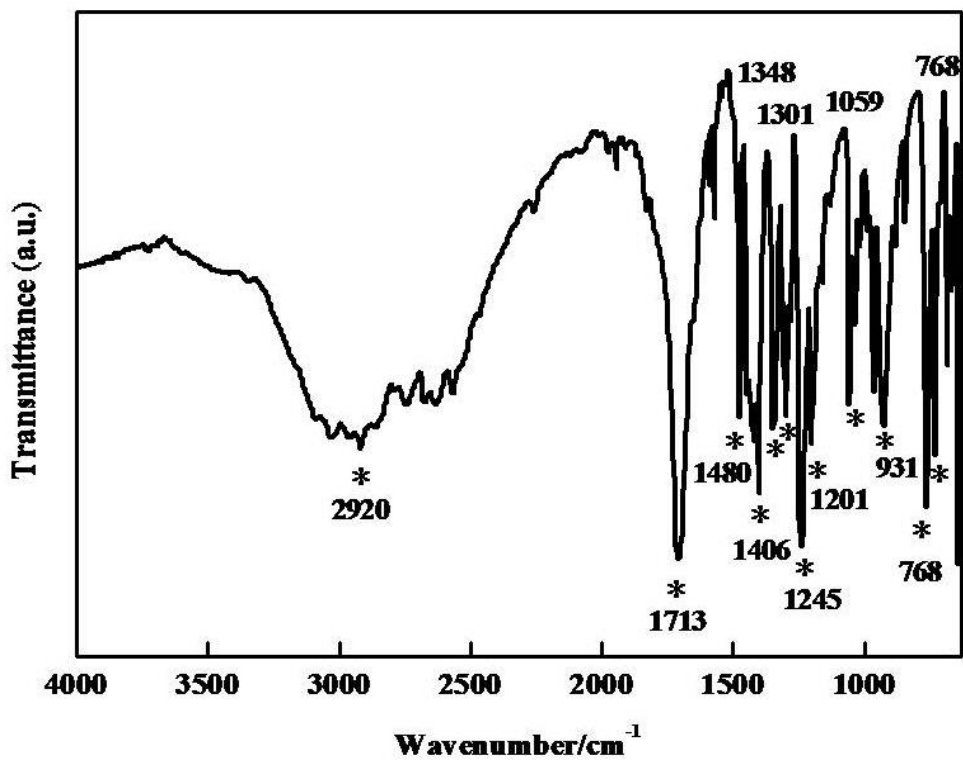
1. Leon T, Correa A and Martin R. *J Am Chem Soc* 2013; **4**: 1221.
2. Silva M, Ferreira A, Lima s, Sousa S. *J Chem Thermodyn* 2008; **40**: 137.
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7. Jayamani M, Pant N, Ananthan S, Narayanan K and Pillai CN. *Tetrahedron* 1986; **42**: 4325.
8. Bost JJ, Kepner RE and Webb AD. *J Org Chem* 1957; **22**: 51.
9. Screttas CG and Micha-Screttas M. *J Organomet Chem* 1985; **290**: 1.
10. Metzger A, Bernhardt S, Manolikakes G and Knochel P. *Angew Chem Int Edi* 2010; **27**: 4665.
11. Hrciar P. *Chem Pap* 1960; **14**: 119.

II. FT-IR Spectra

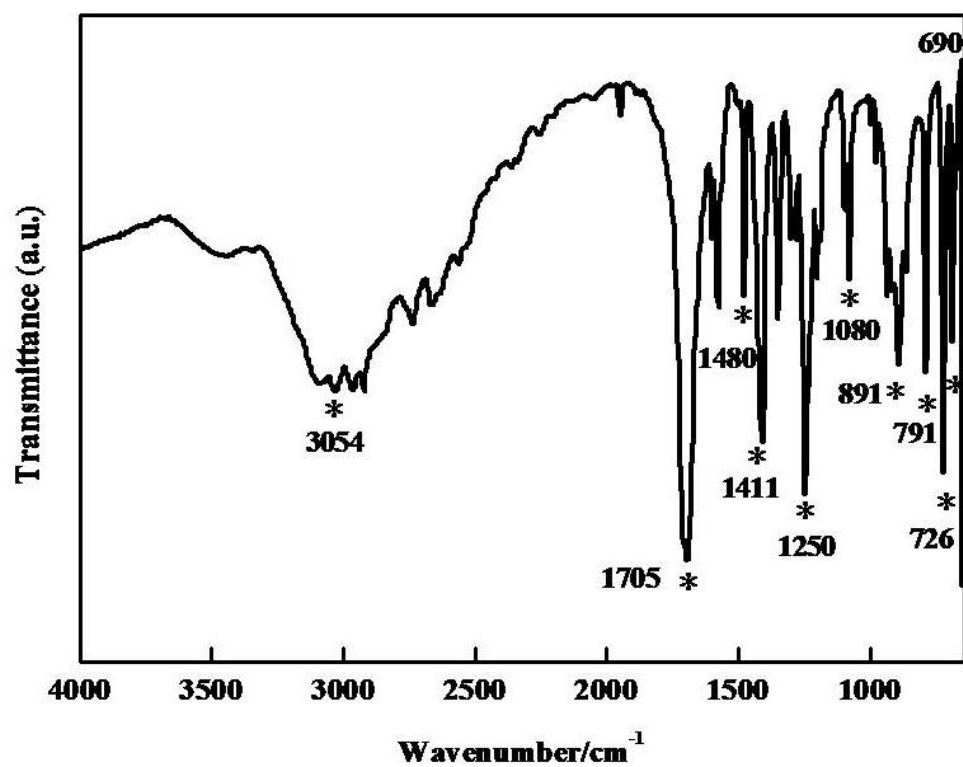
2,4-Dichlorophenylacetic acid (1b)



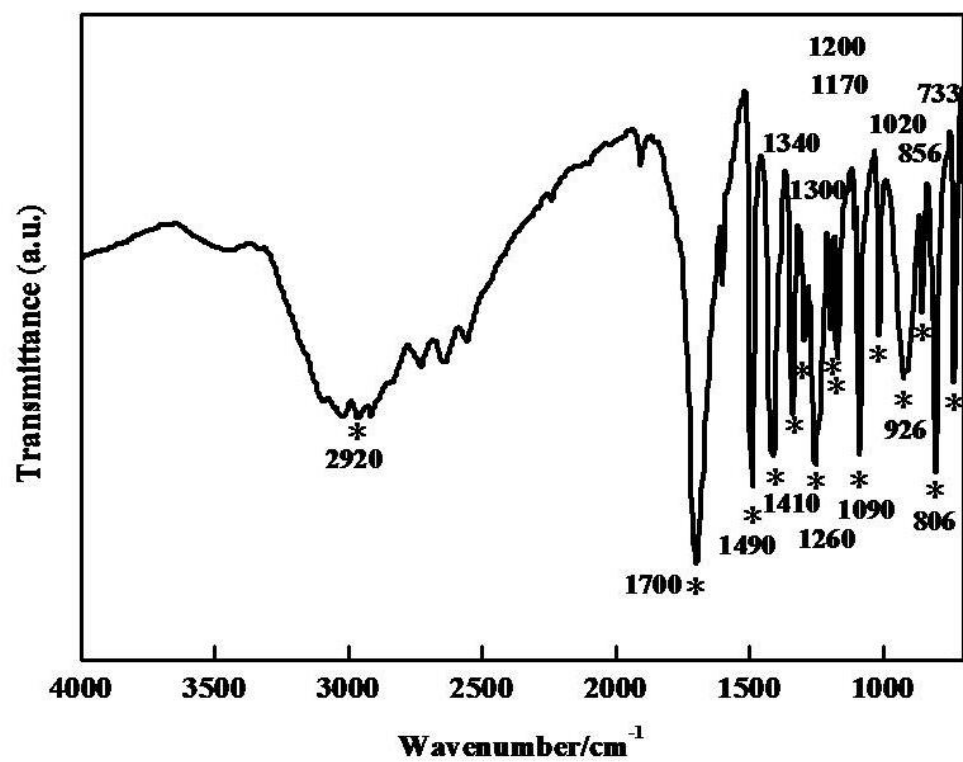
2b



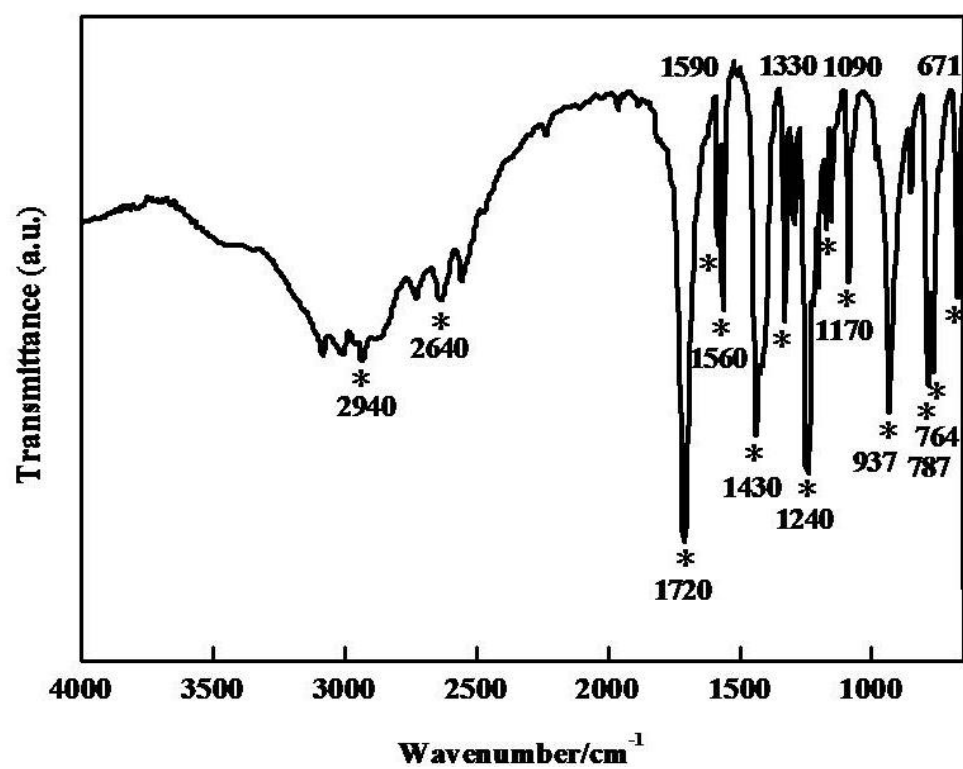
3b



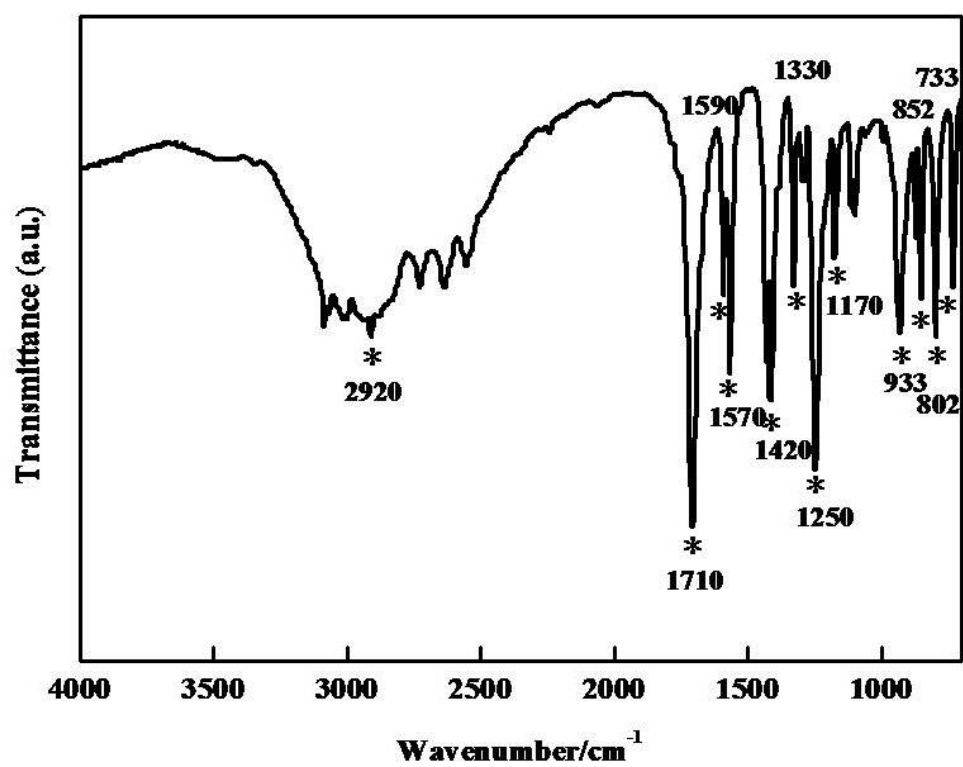
4b



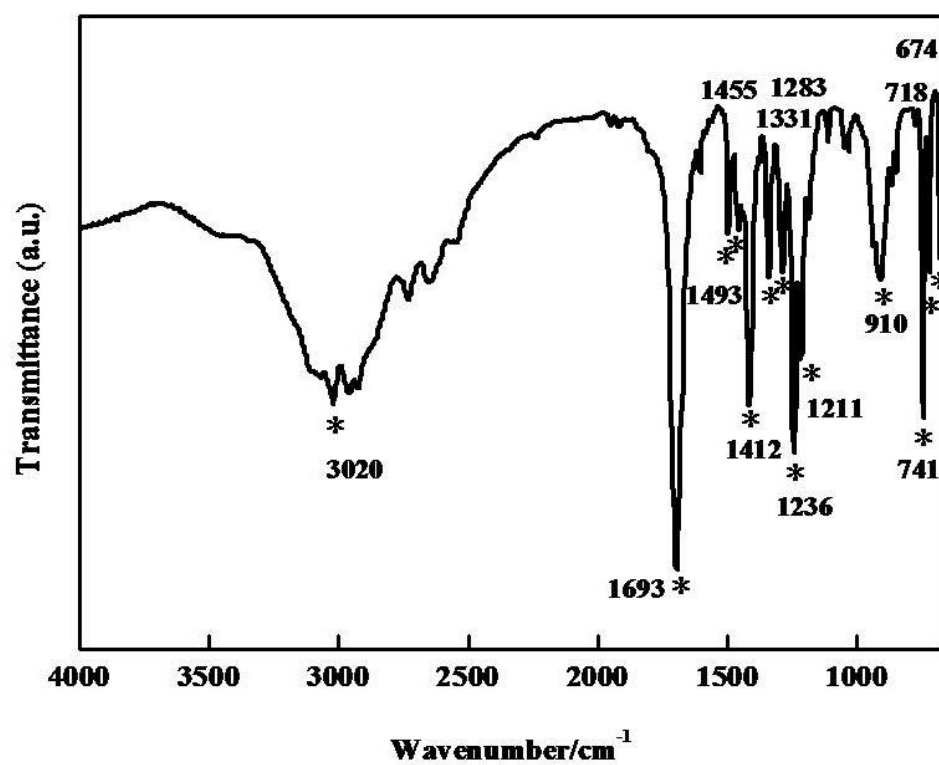
5b



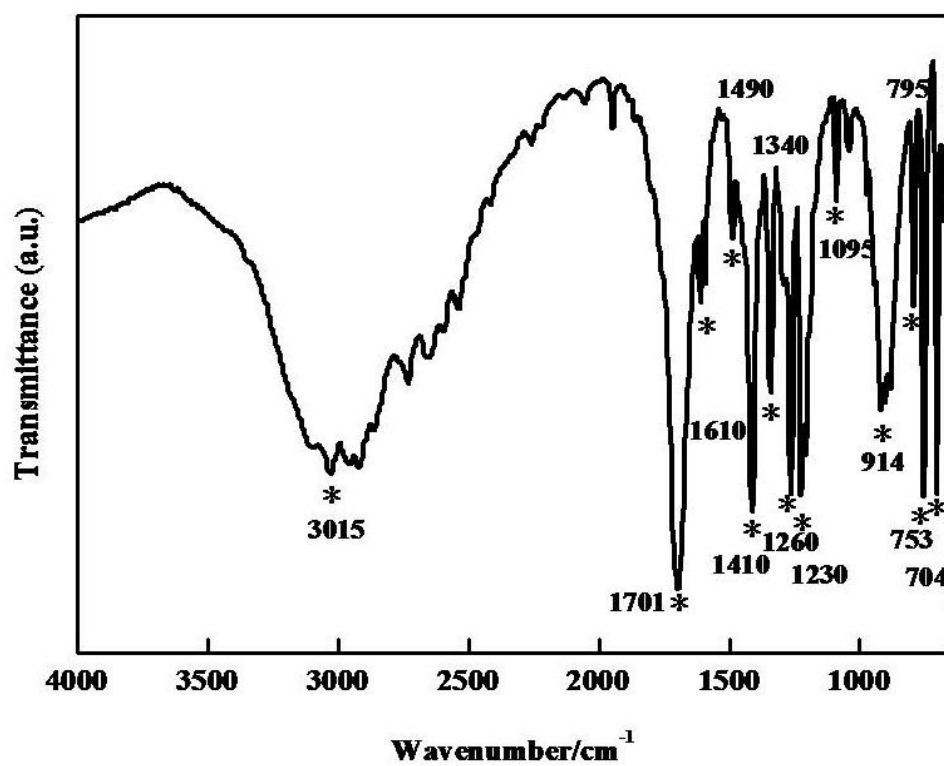
6b



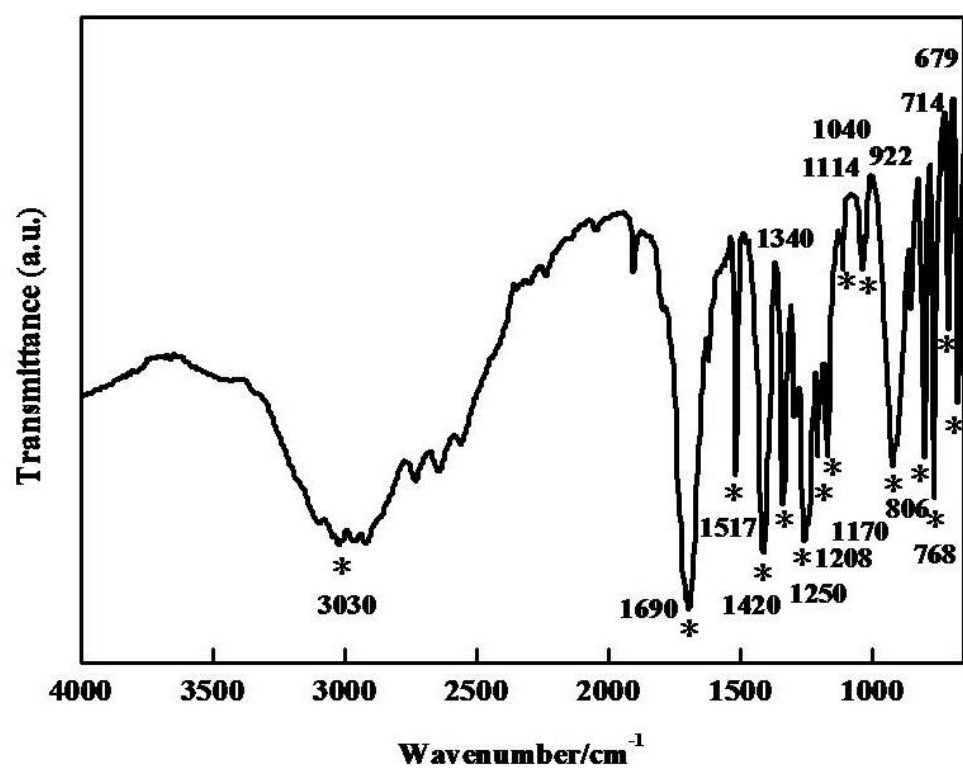
7b



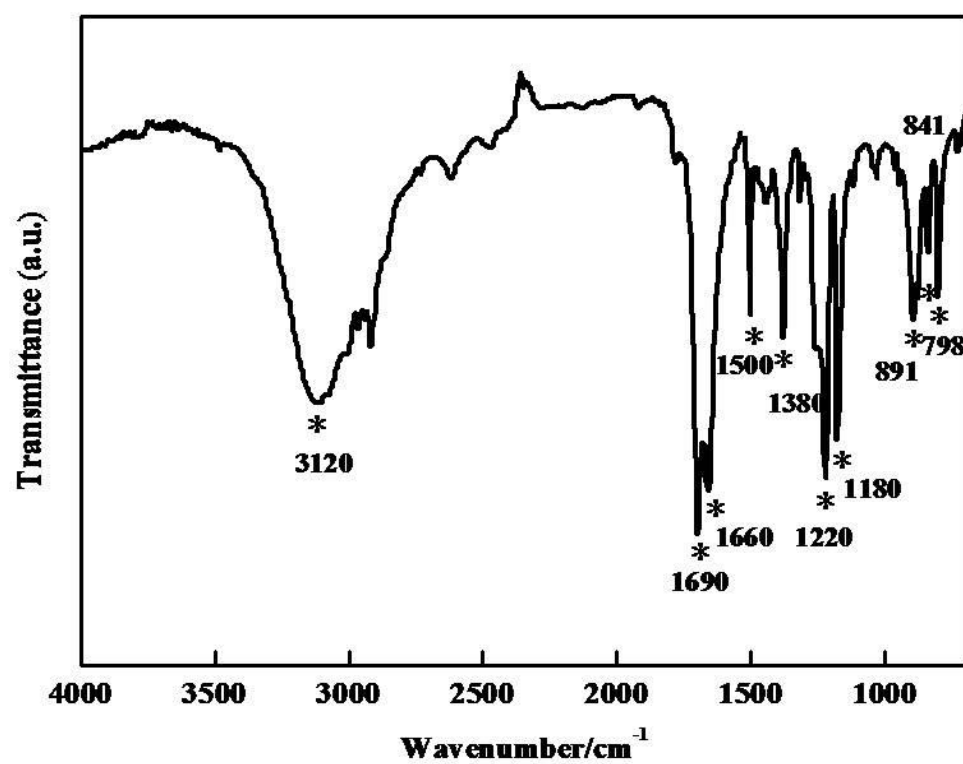
8b



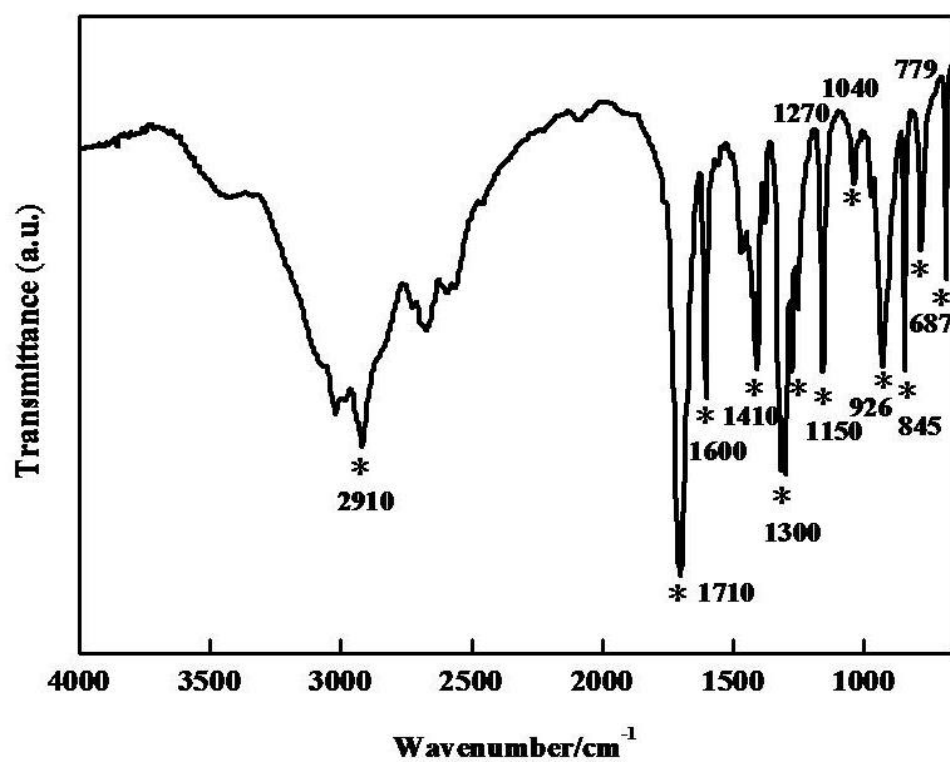
9b



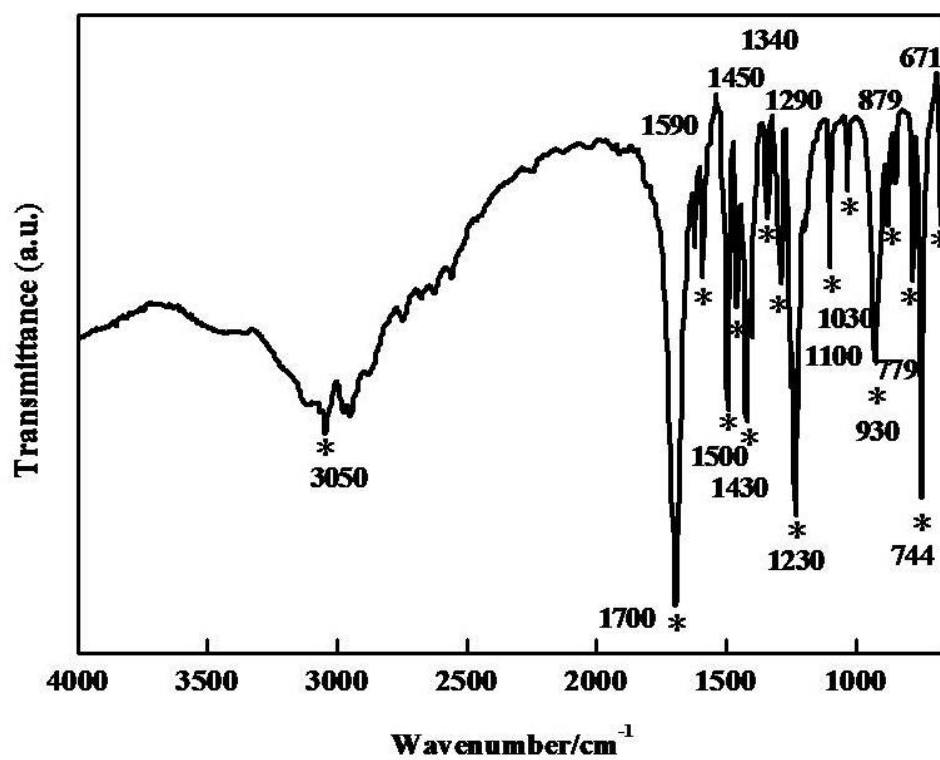
10b



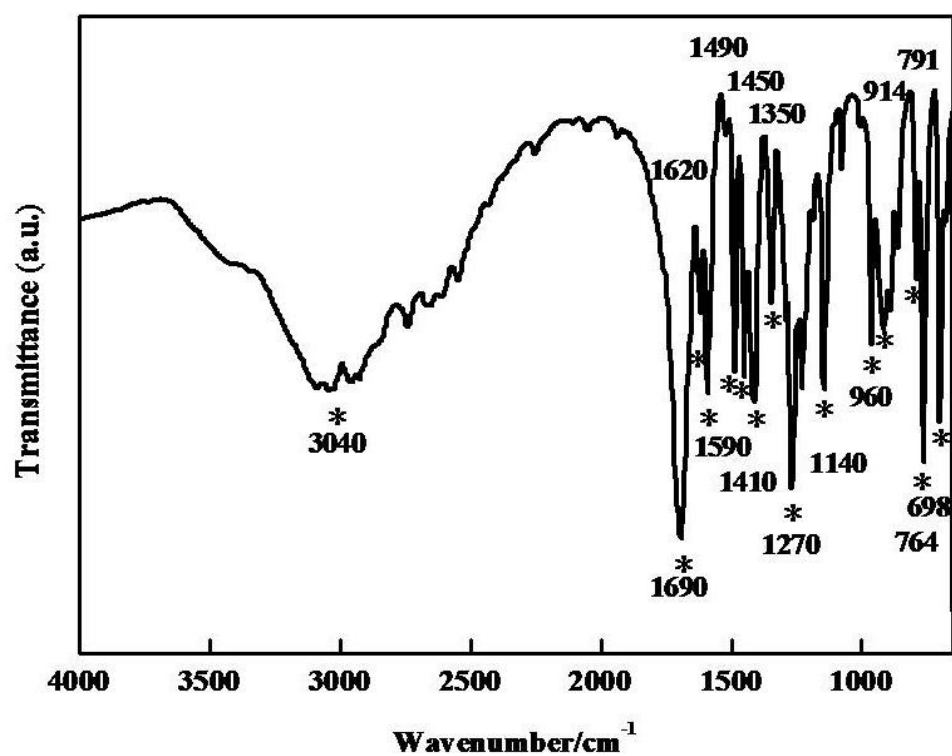
11b



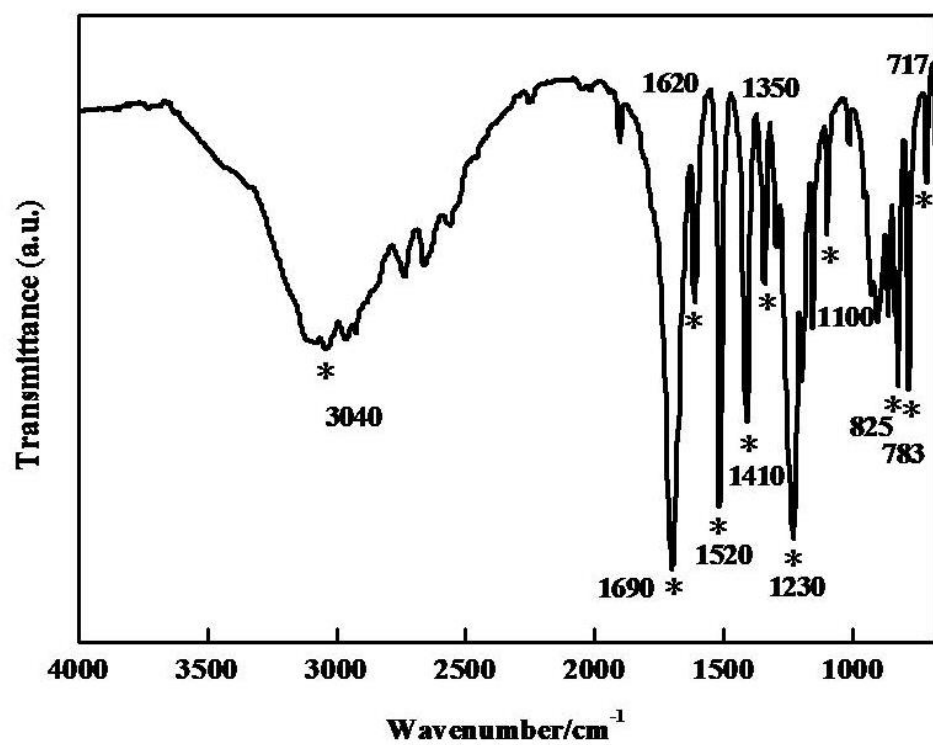
12b



13b

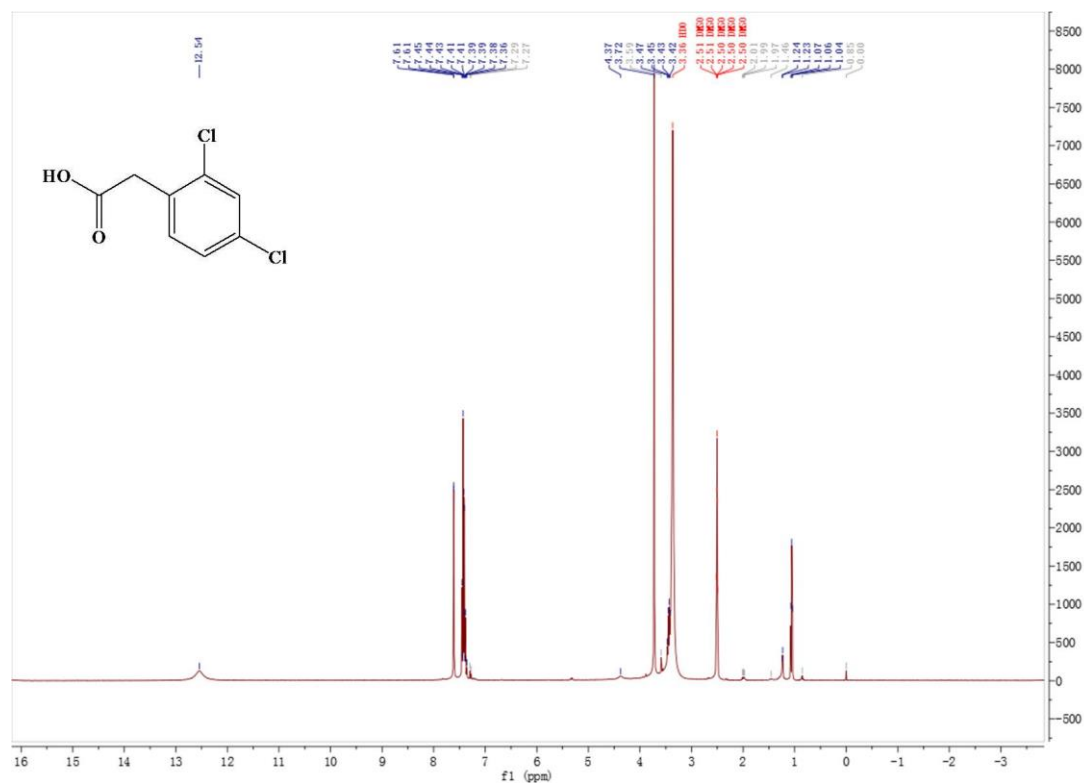


14b

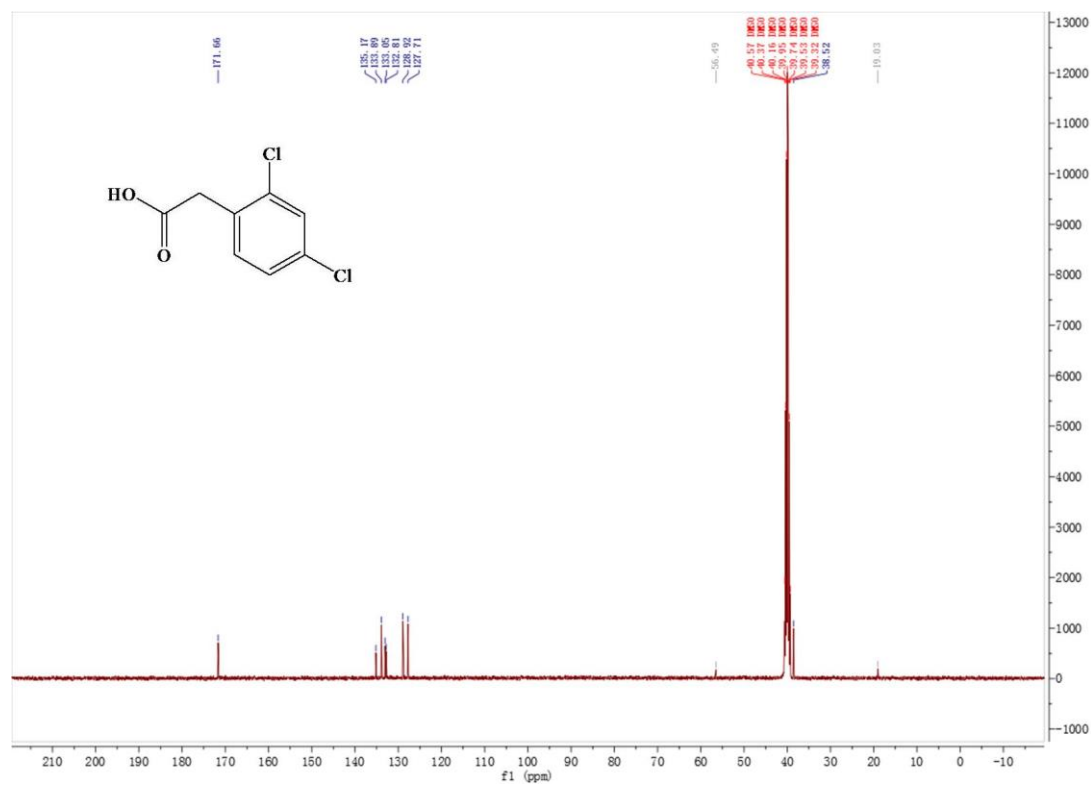


III. NMR Spectra

^1H NMR of 1b



^{13}C NMR of 1b



Chemical structure: O=C(O)C(c1ccccc1)Cl

¹H NMR spectrum (ppm):

- Aromatic protons (7.23-7.46 ppm): Integration 1.00
- Methine proton (3.71 ppm): Integration 1.00
- Methoxy singlet (3.41 ppm): Integration 3.00
- Methine doublet (2.51 ppm): Integration 2.00
- Aliphatic protons (1.07, 1.06, 0.85 ppm): Integration 3.00

Chemical structure: O=C(O)C(c1ccccc1)Cl

¹³C NMR peaks (ppm):

- 171.98 (C=O)
- 134.18, 133.81, 132.75, 129.46, 129.20, 127.57 (aromatic)
- 40.58, 40.37, 39.95, 39.75, 39.65, 39.33, 39.15 (CH-OH)
- 19.03 (CH₃)

Chemical structure: Clc1ccc(cc1)CC(=O)O

¹H NMR spectrum (ppm):

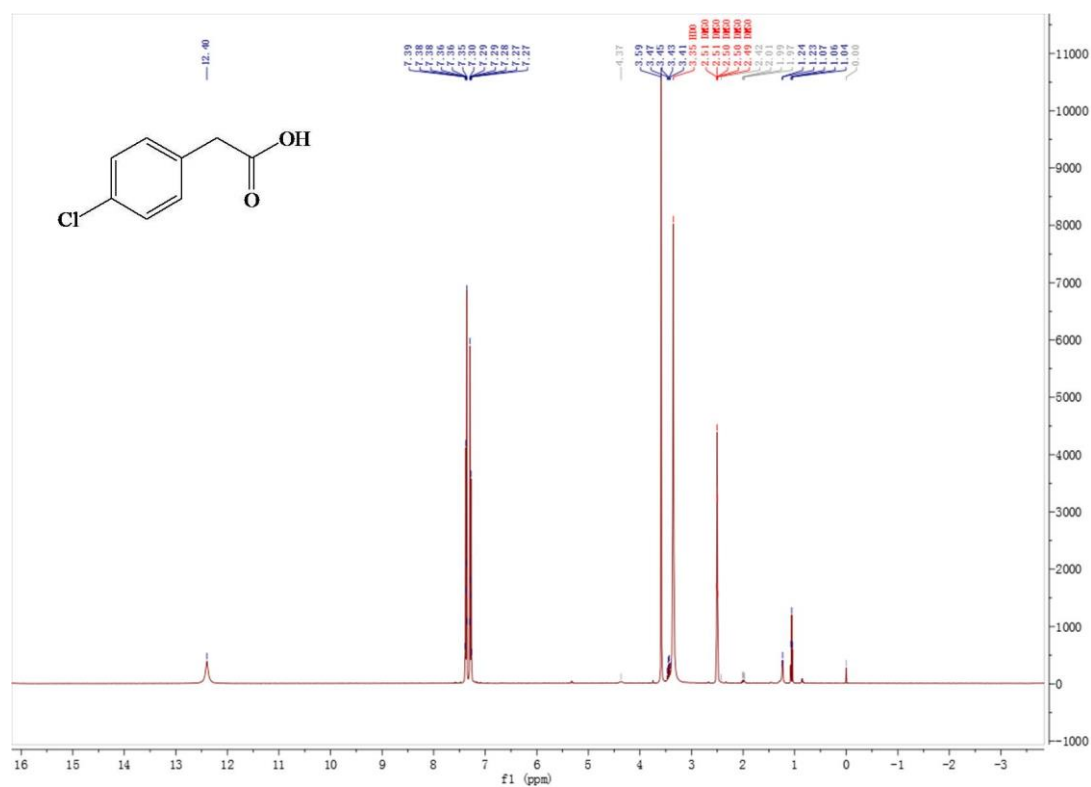
- 12.46 (broad singlet, 1H, integration 1.00)
- 7.36, 7.35, 7.35, 7.35, 7.33, 7.32, 7.32, 7.31, 7.30, 7.29, 7.24, 7.22, 7.22 (multiplet, 5H, integration 1.00)
- 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00 (doublet, 2H, integration 1.00)

Chemical structure: O=Cc1ccc(Cl)cc1

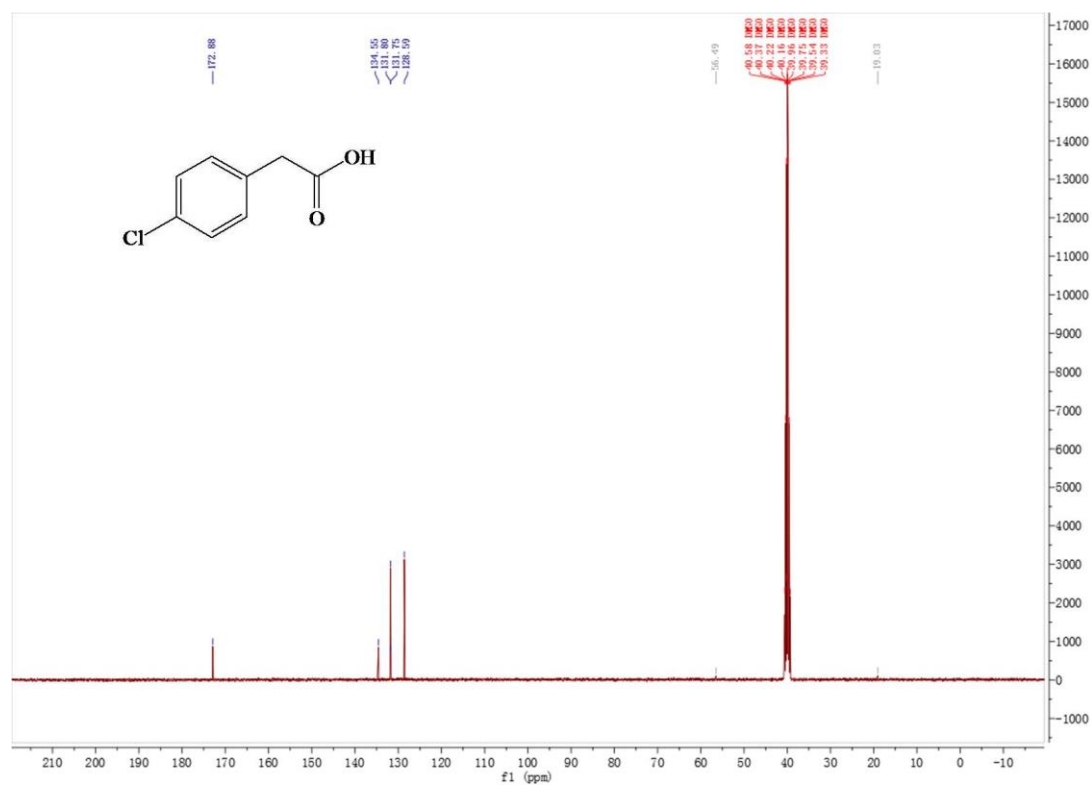
¹³C NMR peaks (ppm):

- 172.73
- 137.96
- 137.17
- 133.47
- 129.83
- 129.52
- 127.03
- 56.49
- 40.58, 40.39, 40.30, 40.16, 39.95, 39.78, 39.53, 39.32 (solvent)
- 0 (TMS)

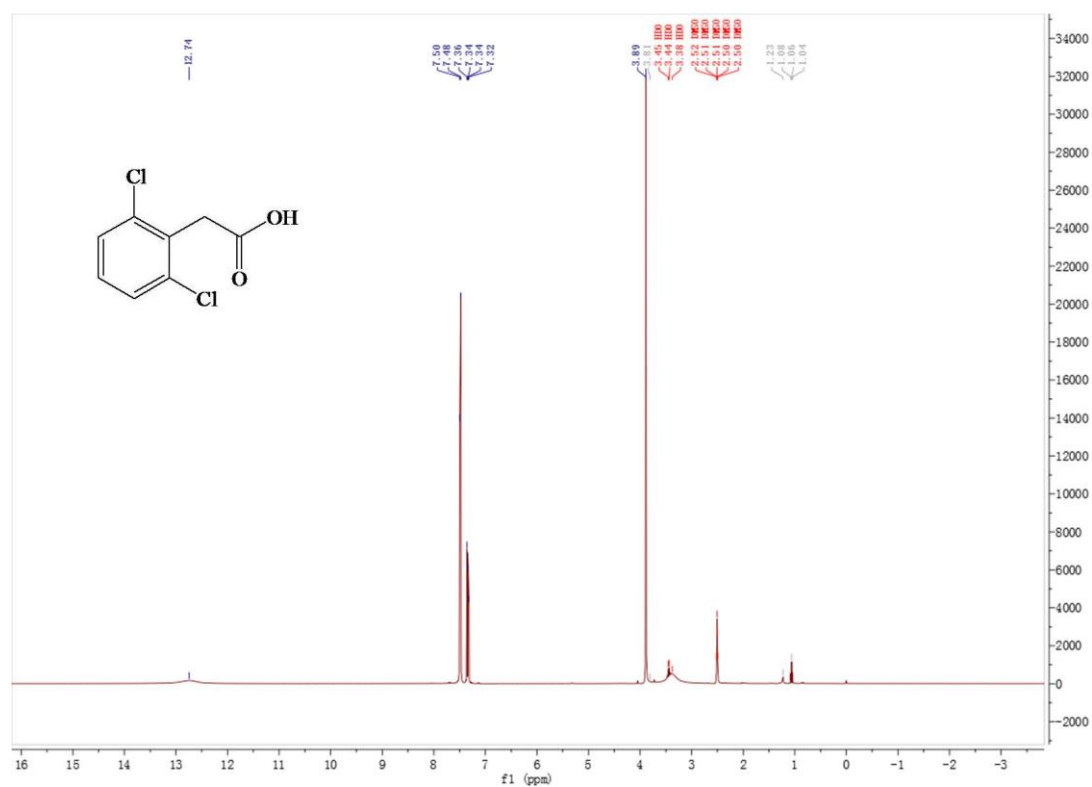
¹H NMR of 4b



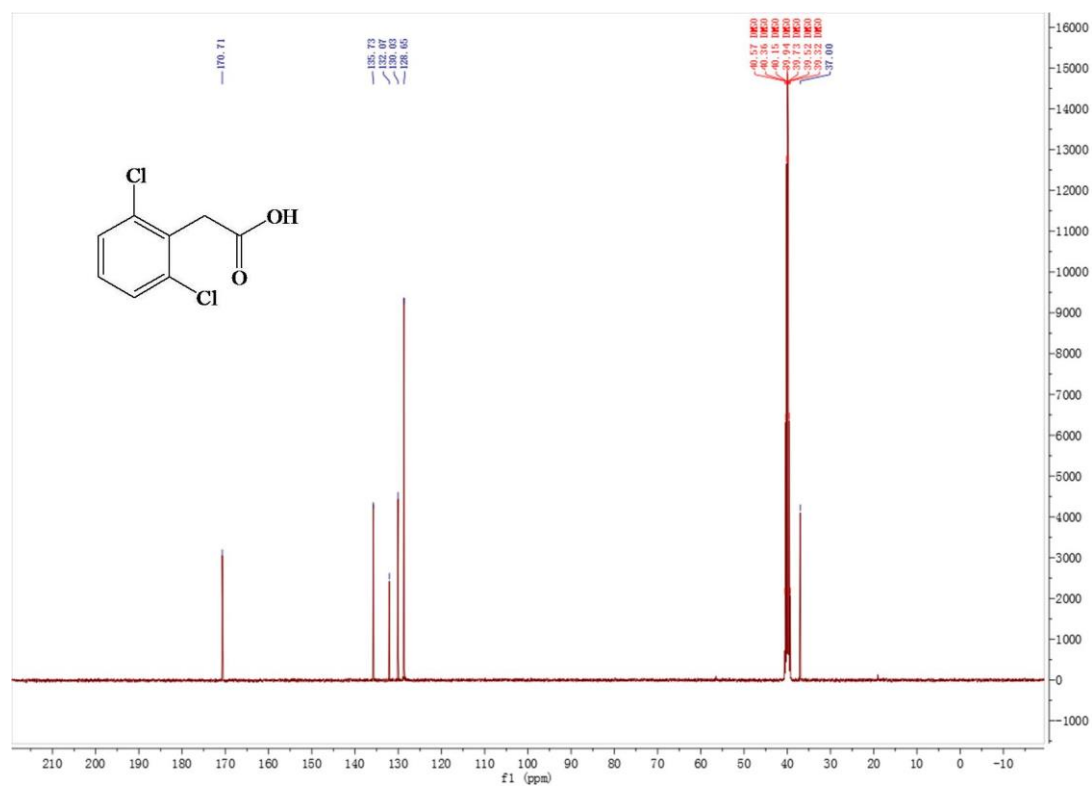
¹³C NMR of 4b



¹H NMR of 5b



¹³C NMR of 5b



Chemical structure: OC(=O)Cc1cc(Cl)cc(Cl)c1

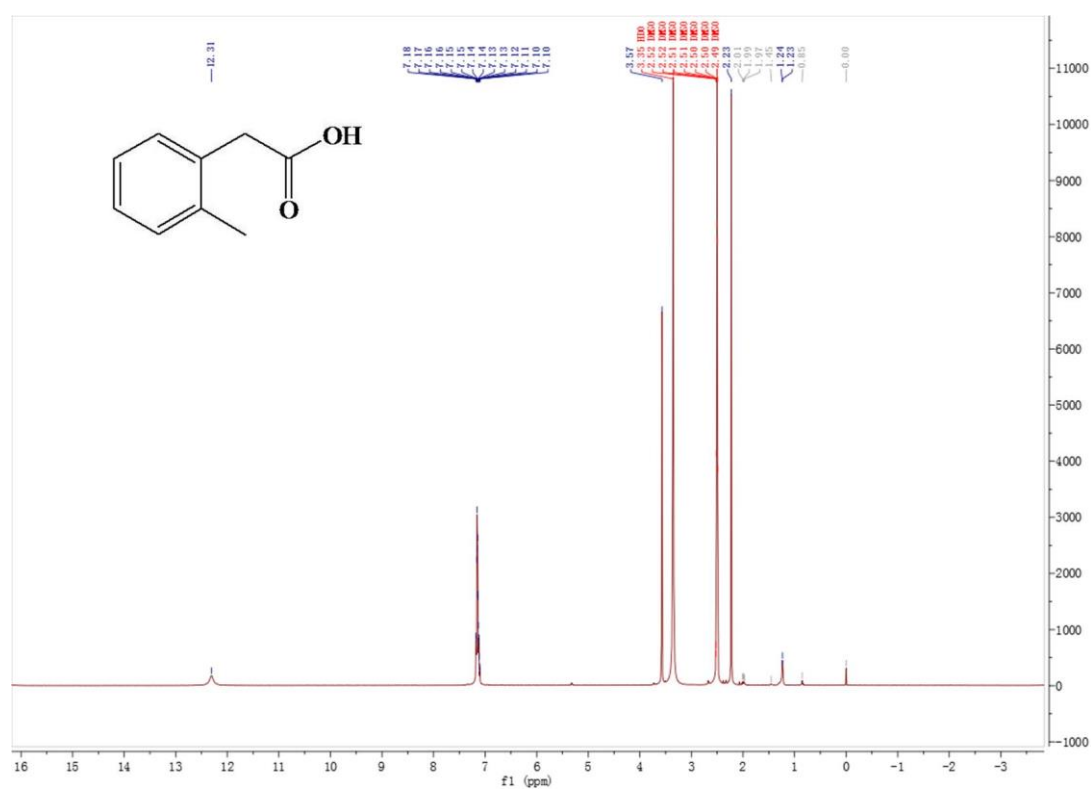
¹H NMR spectrum (ppm):

- 12.57 (s, 1H, integration 0.00)
- 7.40 (d, 1H, integration 1.00)
- 7.36 (d, 1H, integration 1.00)
- 7.34 (d, 1H, integration 1.00)
- 7.28 (d, 1H, integration 1.00)
- 3.96 (s, 2H, integration 2.00)
- 1.08 (s, 3H, integration 3.00)
- 1.05 (s, 3H, integration 3.00)

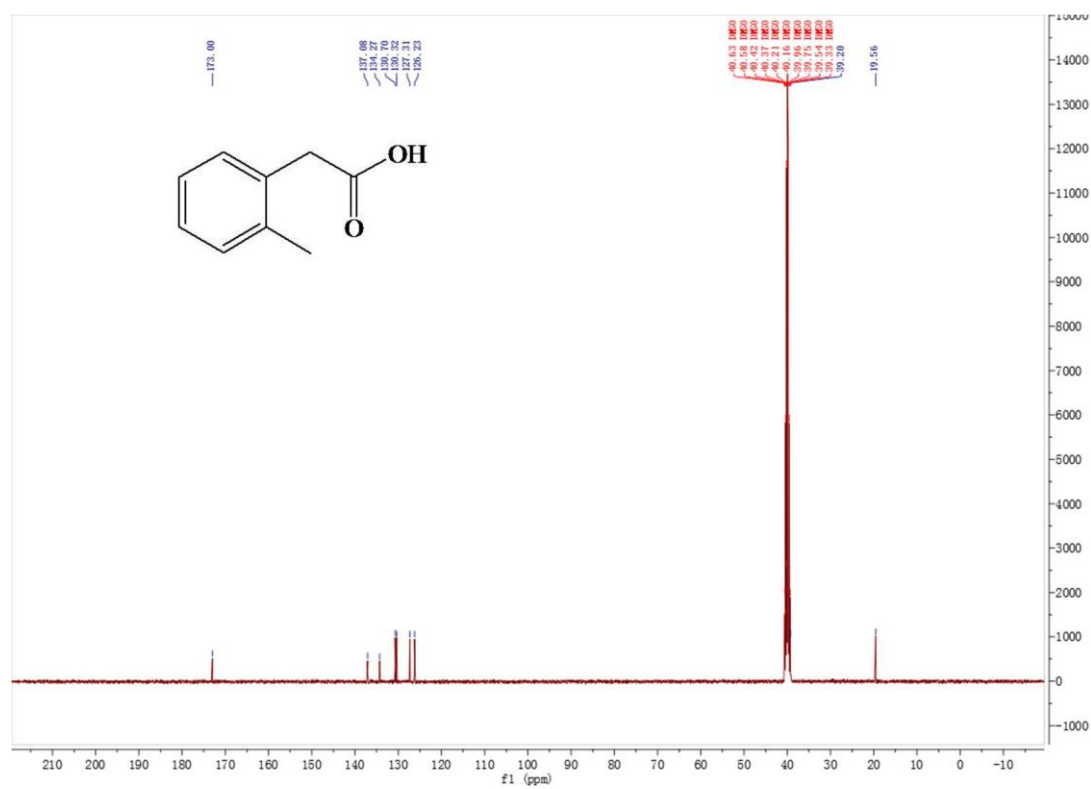
Chemical structure: O=C(O)C=Cc1ccc(Cl)cc1

¹³C NMR peaks (ppm): 172.31, 139.70, 134.06, 128.97, 126.72, 40.56, 39.82, 39.04, 38.26, 37.52, 36.80, 36.08, 35.36, 34.64, 33.92, 33.20, 32.48, 31.76, 31.04, 30.32, 29.60, 28.88, 28.16, 27.44, 26.72, 26.00, 25.28, 24.56, 23.84, 23.12, 22.40, 21.68, 20.96, 20.24, 19.52, 18.80, 18.08, 17.36, 16.64, 15.92, 15.20, 14.48, 13.76, 13.04, 12.32, 11.60, 10.88, 10.16, 9.44, 8.72, 8.00, 7.28, 6.56, 5.84, 5.12, 4.40, 3.68, 2.96, 2.24, 1.52, 0.80, 0.08, -0.64, -1.36, -2.08, -2.80, -3.52, -4.24, -4.96, -5.68, -6.40, -7.12, -7.84, -8.56, -9.28, -10.00.

¹H NMR of 7b



¹³C NMR of 7b



Chemical structure: CC1=CC=C(C(=O)O)C=C1

¹H NMR spectrum (ppm):

- 12.29 (s, 1H, integration 1.00)
- 7.21 (m, 4H, integration 4.00)
- 2.35 (s, 3H, integration 3.00)
- 1.24 (s, 3H, integration 3.00)
- 0.00 (s, 3H, integration 3.00)

Chemical structure: 4-methylbenzoic acid (Cc1ccc(cc1)C(=O)O)

¹H NMR spectrum (DMSO-d₆) showing peaks and integration values:

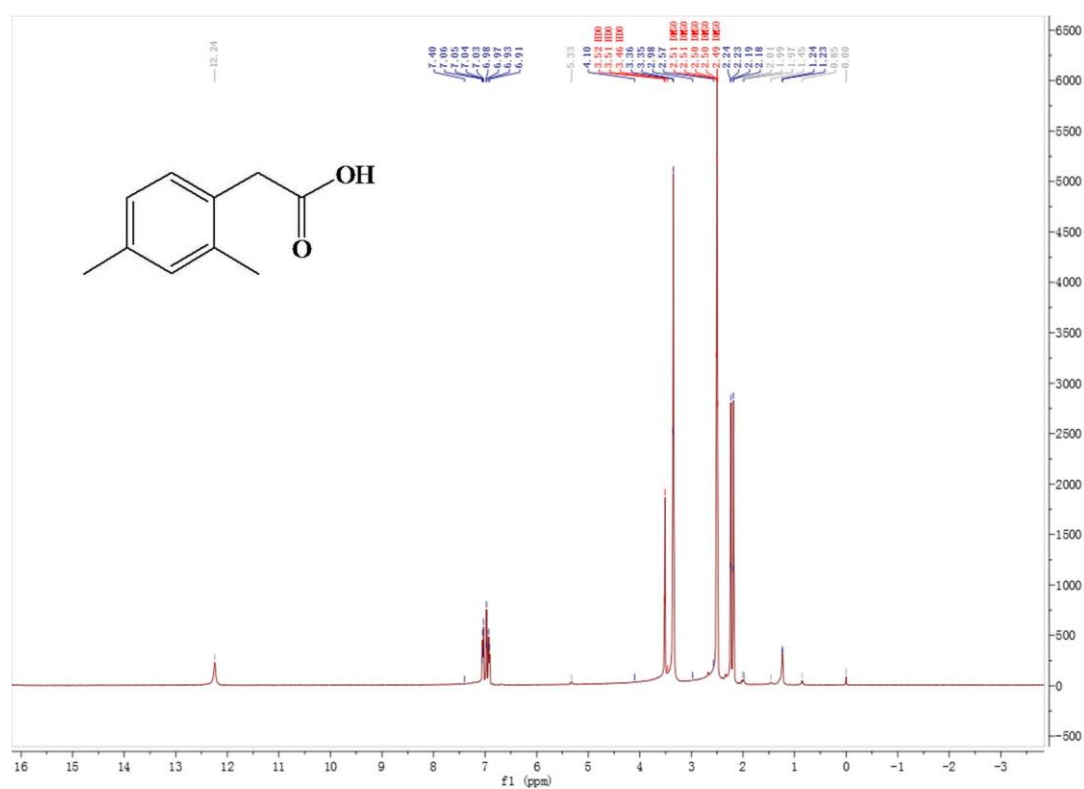
Chemical Shift (ppm)	Integration
7.14, 7.14, 7.12, 7.12, 7.11, 7.11, 7.09, 7.09	1.00
3.40	2.51
2.51, 2.51, 2.51, 2.51, 2.50, 2.50, 2.49, 2.49, 2.48, 2.48	1.00
1.23	2.18
0.00	0.00

Chemical structure: 4-methylbenzoic acid (CC1=CC=C(C(=O)O)C=C1)

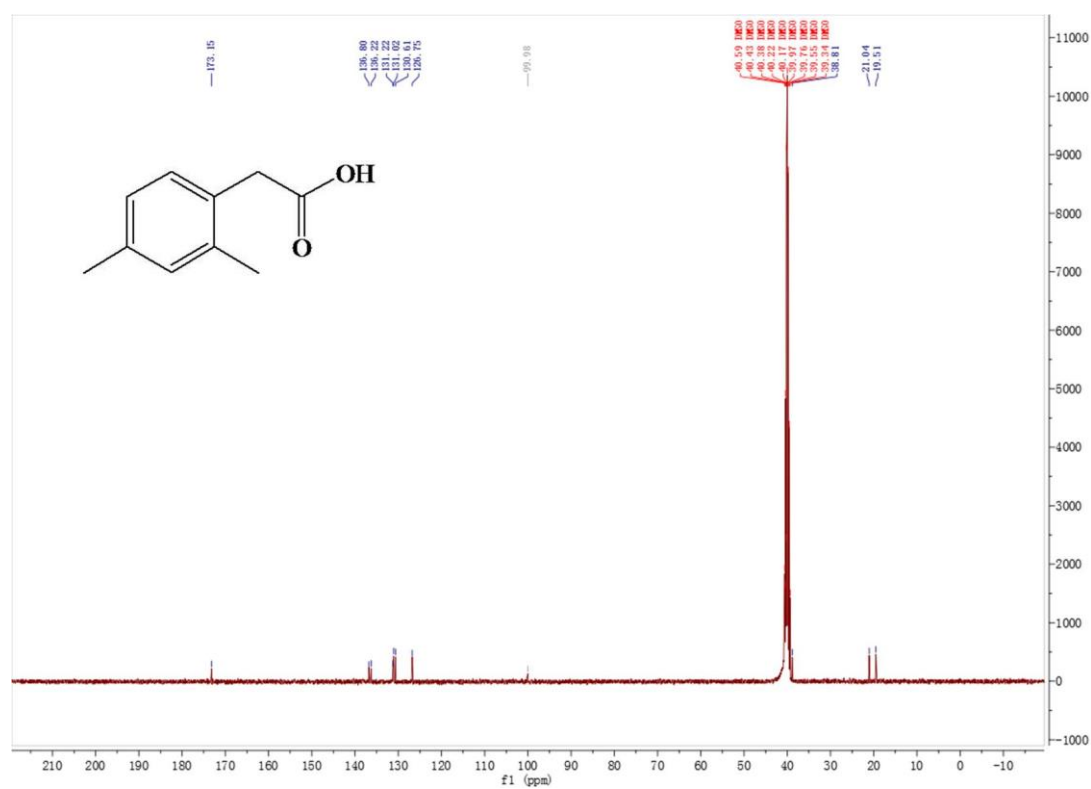
¹³C NMR peaks (ppm):

- 173.36
- 135.97
- 132.57
- 129.66
- 125.23
- 40.93
- 40.53
- 40.13
- 40.42
- 40.36
- 40.16
- 39.95
- 39.75
- 39.53
- 39.32
- 39.60
- 21.12

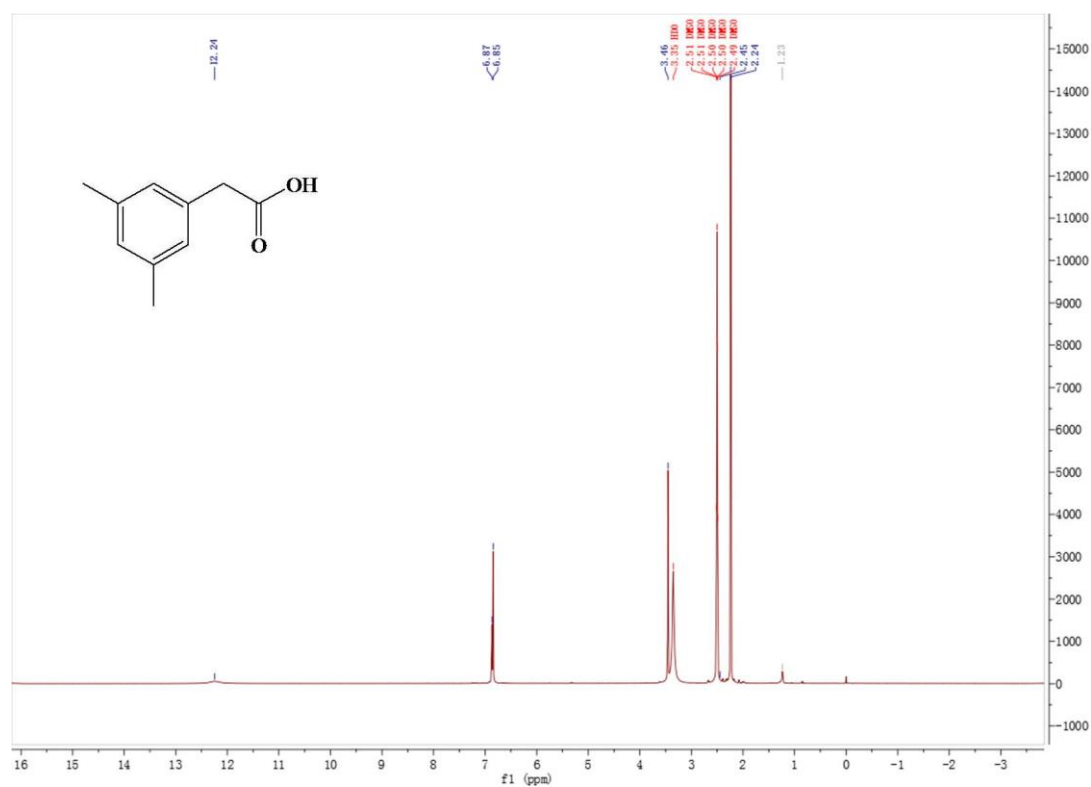
¹H NMR of 10b



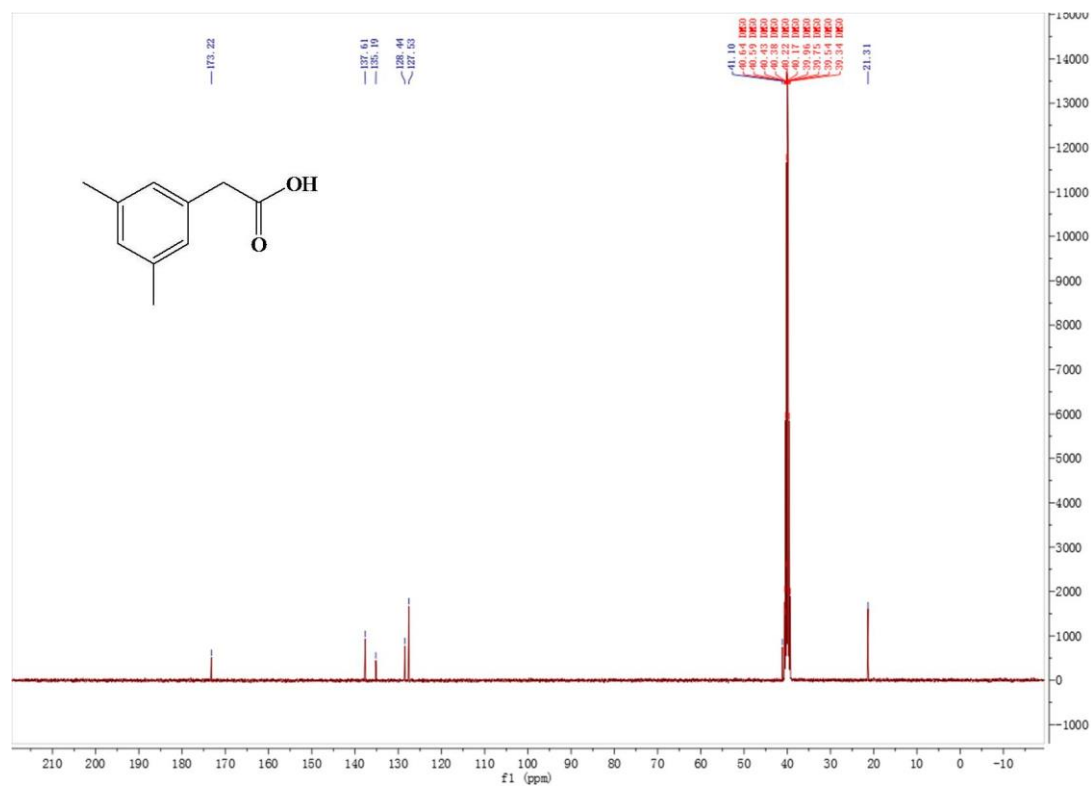
¹³C NMR of 10b



¹H NMR of 11b



¹³C NMR of 11b



Chemical structure: O=C(O)Cc1ccccc1F

¹H NMR spectrum (ppm):

- 12.47 (s, 1H, integration 1.00)
- 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.20, 7.19, 7.17, 7.15, 7.14, 7.13 (m, 7H, integration 7.36)
- 3.74 (s, 2H, integration 2.36)
- 0.00 (s, 3H, integration 3.00)

[illegible]

Chemical structure: OC(=O)Cc1ccc(F)cc1

¹H NMR spectrum (ppm):

- 12.46 (broad, integration 12.46)
- 7.39, 7.38, 7.36, 7.35, 7.34, 7.33, 7.32, 7.16, 7.15, 7.12, 7.11, 7.10, 7.09, 7.08, 7.06, 7.05 (aromatic region, integration 7.16, 7.15, 7.12, 7.11, 7.10, 7.09, 7.08, 7.06, 7.05)
- 3.69 (singlet, integration 3.69)
- 2.50 (doublet, integration 2.50, 2.51, 2.52, 2.53, 2.54, 2.55, 2.56, 2.57, 2.58, 2.59, 2.60, 2.61, 2.62, 2.63, 2.64, 2.65, 2.66, 2.67, 2.68, 2.69, 2.70, 2.71, 2.72, 2.73, 2.74, 2.75, 2.76, 2.77, 2.78, 2.79, 2.80, 2.81, 2.82, 2.83, 2.84, 2.85, 2.86, 2.87, 2.88, 2.89, 2.90, 2.91, 2.92, 2.93, 2.94, 2.95, 2.96, 2.97, 2.98, 2.99, 3.00, 3.01, 3.02, 3.03, 3.04, 3.05, 3.06, 3.07, 3.08, 3.09, 3.10, 3.11, 3.12, 3.13, 3.14, 3.15, 3.16, 3.17, 3.18, 3.19, 3.20, 3.21, 3.22, 3.23, 3.24, 3.25, 3.26, 3.27, 3.28, 3.29, 3.30, 3.31, 3.32, 3.33, 3.34, 3.35, 3.36, 3.37, 3.38, 3.39, 3.40, 3.41, 3.42, 3.43, 3.44, 3.45, 3.46, 3.47, 3.48, 3.49, 3.50, 3.51, 3.52, 3.53, 3.54, 3.55, 3.56, 3.57, 3.58, 3.59, 3.60, 3.61, 3.62, 3.63, 3.64, 3.65, 3.66, 3.67, 3.68, 3.69, 3.70, 3.71, 3.72, 3.73, 3.74, 3.75, 3.76, 3.77, 3.78, 3.79, 3.80, 3.81, 3.82, 3.83, 3.84, 3.85, 3.86, 3.87, 3.88, 3.89, 3.90, 3.91, 3.92, 3.93, 3.94, 3.95, 3.96, 3.97, 3.98, 3.99, 4.00, 4.01, 4.02, 4.03, 4.04, 4.05, 4.06, 4.07, 4.08, 4.09, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17, 4.18, 4.19, 4.20, 4.21, 4.22, 4.23, 4.24, 4.25, 4.26, 4.27, 4.28, 4.29, 4.30, 4.31, 4.32, 4.33, 4.34, 4.35, 4.36, 4.37, 4.38, 4.39, 4.40, 4.41, 4.42, 4.43, 4.44, 4.45, 4.46, 4.47, 4.48, 4.49, 4.50, 4.51, 4.52, 4.53, 4.54, 4.55, 4.56, 4.57, 4.58, 4.59, 4.60, 4.61, 4.62, 4.63, 4.64, 4.65, 4.66, 4.67, 4.68, 4.69, 4.70, 4.71, 4.72, 4.73, 4.74, 4.75, 4.76, 4.77, 4.78, 4.79, 4.80, 4.81, 4.82, 4.83, 4.84, 4.85, 4.86, 4.87, 4.88, 4.89, 4.90, 4.91, 4.92, 4.93, 4.94, 4.95, 4.96, 4.97, 4.98, 4.99, 5.00, 5.01, 5.02, 5.03, 5.04, 5.05, 5.06, 5.07, 5.08, 5.09, 5.10, 5.11, 5.12, 5.13, 5.14, 5.15, 5.16, 5.17, 5.18, 5.19, 5.20, 5.21, 5.22, 5.23, 5.24, 5.25, 5.26, 5.27, 5.28, 5.29, 5.30, 5.31, 5.32, 5.33, 5.34, 5.35, 5.36, 5.37, 5.38, 5.39, 5.40, 5.41, 5.42, 5.43, 5.44, 5.45, 5.46, 5.47, 5.48, 5.49, 5.50, 5.51, 5.52, 5.53, 5.54, 5.55, 5.56, 5.57, 5.58, 5.59, 5.60, 5.61, 5.62, 5.63, 5.64, 5.65, 5.66, 5.67, 5.68, 5.69, 5.70, 5.71, 5.72, 5.73, 5.74, 5.75, 5.76, 5.77, 5.78, 5.79, 5.80, 5.81, 5.82, 5.83, 5.84, 5.85, 5.86, 5.87, 5.88, 5.89, 5.90, 5.91, 5.92, 5.93, 5.94, 5.95, 5.96, 5.97, 5.98, 5.99, 6.00, 6.01, 6.02, 6.03, 6.04, 6.05, 6.06, 6.07, 6.08, 6.09, 6.10, 6.11, 6.12, 6.13, 6.14, 6.15, 6.16, 6.17, 6.18, 6.19, 6.20, 6.21, 6.22, 6.23, 6.24, 6.25, 6.26, 6.27, 6.28, 6.29, 6.30, 6.31, 6.32, 6.33, 6.34, 6.35, 6.36, 6.37, 6.38, 6.39, 6.40, 6.41, 6.42, 6.43, 6.44, 6.45, 6.46, 6.47, 6.48, 6.49, 6.50, 6.51, 6.52, 6.53, 6.54, 6.55, 6.56, 6.57, 6.58, 6.59, 6.60, 6.61, 6.62, 6.63, 6.64, 6.65, 6.66, 6.67, 6.68, 6.69, 6.70, 6.71, 6.72, 6.73, 6.74, 6.75, 6.76, 6.77, 6.78, 6.79, 6.80, 6.81, 6.82, 6.83, 6.84, 6.85, 6.86, 6.87, 6.88, 6.89, 6.90, 6.91, 6.92, 6.93, 6.94, 6.95, 6.96, 6.97, 6.98, 6.99, 7.00, 7.01, 7.02, 7.03, 7.04, 7.05, 7.06, 7.07, 7.08, 7.09, 7.10, 7.11, 7.12, 7.13, 7.14, 7.15, 7.16, 7.17, 7.18, 7.19, 7.20, 7.21, 7.22, 7.23, 7.24, 7.25, 7.26, 7.27, 7.28, 7.29, 7.30, 7.31, 7.32, 7.33, 7.34, 7.35, 7.36, 7.37, 7.38, 7.39, 7.40, 7.41, 7.42, 7.43, 7.44, 7.45, 7.46, 7.47, 7.48, 7.49, 7.50, 7.51, 7.52, 7.53, 7.54, 7.55, 7.56, 7.57, 7.58, 7.59, 7.60, 7.61, 7.62, 7.63, 7.64, 7.65, 7.66, 7.67, 7.68, 7.69, 7.70, 7.71, 7.72, 7.73, 7.74, 7.75, 7.76, 7.77, 7.78, 7.79, 7.80, 7.81, 7.82, 7.83, 7.84, 7.85, 7.86, 7.87, 7.88, 7.89, 7.90, 7.91, 7.92, 7.93, 7.94, 7.95, 7.96, 7.97, 7.98, 7.99, 8.00, 8.01, 8.02, 8.03, 8.04, 8.05, 8.06, 8.07, 8.08, 8.09, 8.10, 8.11, 8.12, 8.13, 8.14, 8.15, 8.16, 8.17, 8.18, 8.19, 8.20, 8.21, 8.22, 8.23, 8.24, 8.25, 8.26, 8.27, 8.28, 8.29, 8.30, 8.31, 8.32, 8.33, 8.34, 8.35, 8.36, 8.37, 8.38, 8.39, 8.40, 8.41, 8.42, 8.43, 8.44, 8.45, 8.46, 8.47, 8.48, 8.49, 8.50, 8.51, 8.52, 8.53, 8.54, 8.55, 8.56, 8.57, 8.58, 8.59, 8.60, 8.61, 8.62, 8.63, 8.64, 8.65, 8.66, 8.67, 8.68, 8.69,

Chemical structure: O=C(O)Cc1ccc(F)cc1

¹³C NMR peaks (ppm):

- 172.73
- 163.66
- 161.25
- 138.75
- 138.77
- 130.73
- 130.42
- 126.09
- 126.06
- 116.82
- 116.61
- 115.74
- 113.74
- 40.57, 40.55, 40.53, 40.38, 40.36, 40.34, 40.15, 40.13, 40.11, 39.97, 39.95, 39.79, 39.78, 39.49, 39.28 (CDCl₃ solvent)

Chemical structure: OC(=O)Cc1ccc(F)cc1

¹H NMR spectrum (DMSO-d₆) showing peaks for 4-fluorophenylacetic acid. The x-axis represents the chemical shift in ppm (f1), ranging from -3 to 16. The y-axis represents intensity, ranging from -2000 to 25000.

Key peaks and integration values:

- Carboxylic acid proton: ~12.37 ppm (Integration: 12.37)
- Aromatic protons: 7.11-7.31 ppm (Integration: 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91, 0.90, 0.89, 0.88, 0.87, 0.86, 0.85, 0.84, 0.83, 0.82, 0.81, 0.80, 0.79, 0.78, 0.77, 0.76, 0.75, 0.74, 0.73, 0.72, 0.71, 0.70, 0.69, 0.68, 0.67, 0.66, 0.65, 0.64, 0.63, 0.62, 0.61, 0.60, 0.59, 0.58, 0.57, 0.56, 0.55, 0.54, 0.53, 0.52, 0.51, 0.50, 0.49, 0.48, 0.47, 0.46, 0.45, 0.44, 0.43, 0.42, 0.41, 0.40, 0.39, 0.38, 0.37, 0.36, 0.35, 0.34, 0.33, 0.32, 0.31, 0.30, 0.29, 0.28, 0.27, 0.26, 0.25, 0.24, 0.23, 0.22, 0.21, 0.20, 0.19, 0.18, 0.17, 0.16, 0.15, 0.14, 0.13, 0.12, 0.11, 0.10, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, 0.01, 0.00)
- Methylene protons: ~3.4 ppm (Integration: 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91, 0.90, 0.89, 0.88, 0.87, 0.86, 0.85, 0.84, 0.83, 0.82, 0.81, 0.80, 0.79, 0.78, 0.77, 0.76, 0.75, 0.74, 0.73, 0.72, 0.71, 0.70, 0.69, 0.68, 0.67, 0.66, 0.65, 0.64, 0.63, 0.62, 0.61, 0.60, 0.59, 0.58, 0.57, 0.56, 0.55, 0.54, 0.53, 0.52, 0.51, 0.50, 0.49, 0.48, 0.47, 0.46, 0.45, 0.44, 0.43, 0.42, 0.41, 0.40, 0.39, 0.38, 0.37, 0.36, 0.35, 0.34, 0.33, 0.32, 0.31, 0.30, 0.29, 0.28, 0.27, 0.26, 0.