Supporting Information for

Copper-Catalyzed Coupling of Anthranils and *α*-Keto Acids: Direct Synthesis of *α*-Ketoamides

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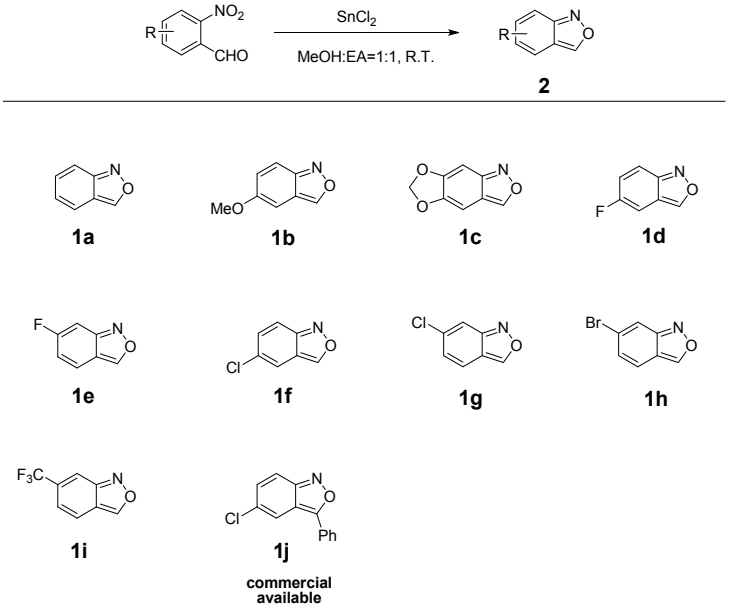
1. General Information

All solvents were dried over molecular sieves. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. $CuBr(PPh_3)_3$ was prepared according to the literature.[1] The products were isolated by column chromatography on silica gel (200-300 mesh) by using petroleum ether (30-60 °C) and ethyl acetate as eluents. Silica gel for column chromatography was purchased from AnhuiLiangchen Chemical Co, Lt. All yields described herein are the isolated yields after column chromatography. Reaction progress and product mixtures were routinely monitored by TLC using TLC SiO_2 sheets, and compounds were visualized under ultraviolet light. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer. The spectra were recorded using $CDCl_3$ as a solvent. ^{1}H NMR chemical shifts are referenced to tetramethylsilane (TMS, 0 ppm). Abbreviations are as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). High-Resolution Mass Spectra (HRMS) were recorded on Micromass Q-Tof instrument (ESI). Infrared spectra (IR) spectra were determined on a NICOLET 6700 FT-IR spectrometer. Melting points were measured with a melting point instrument and were uncorrected.

2. Synthesis of starting materials 1a-i and 2b-q.

2.1 Synthesis of compounds 1a-i



Compounds 1a-i were synthesized according to the reported literature.[2]

Benzo[c]isoxazole (1a) (Precursor to product 3a): PE/EtOAc = 30:1; Colorless oil, 343.6 mg, 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (d, J = 0.9 Hz, 1H), 7.64-7.56 (m, 2H), 7.33-7.27 (m, 1H), 7.02 (dd, J = 8.8, 6.4 Hz, 1H); The ^{1}H NMR spectra data are consistent with the reported literature.[3]

5-Methoxybenzo[c]isoxazole (1b) (Precursor to product 3b): PE/EtOAc = 20:1; Light yellow oil, 268.4 mg, 60% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, J = 1.0 Hz, 1H), 7.53 (d, J = 9.6 Hz, 1H), 7.04 (dd, J = 9.6, 2.2 Hz, 1H), 6.63 (d, J = 2.0 Hz, 1H), 3.83 (s, 3H); The ^{1}H NMR spectra data are consistent with the reported literature.[3]

[1,3]Dioxolo[4',5':4,5]benzo[1,2-c]isoxazole (1c) (Precursor to product 3c): PE/EtOAc = 10:1; Yellow solid, 244.6 mg, 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 0.9 Hz, 1H), 6.81 (d, J

= 0.7 Hz, 1H), 6.68 (d, *J* = 0.5 Hz, 1H), 5.99 (s, 2H). The ^{1}H NMR spectra data are consistent with the reported literature.[4]

5-Fluorobenzo[c]isoxazole (1d) (Precursor to product 3d): PE/EtOAc = 40:1; Light yellow solid, 242.7 mg, 59% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (s, 1H), 7.66 (dd, *J* = 9.6, 4.5 Hz, 1H), 7.18-7.11 (m, 2H); The ^{1}H NMR spectra data are consistent with the reported literature.[5]

6-Fluorobenzo[c]isoxazole (1e) (Precursor to product 3e)[6]: PE/EtOAc = 50:1; Yellow solid, 205.6 mg, 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (d, *J* = 0.9 Hz, 1H), 7.62-7.59 (m, 1H), 7.20-7.17 (m, 1H), 6.89-6.84 (m, 1H).

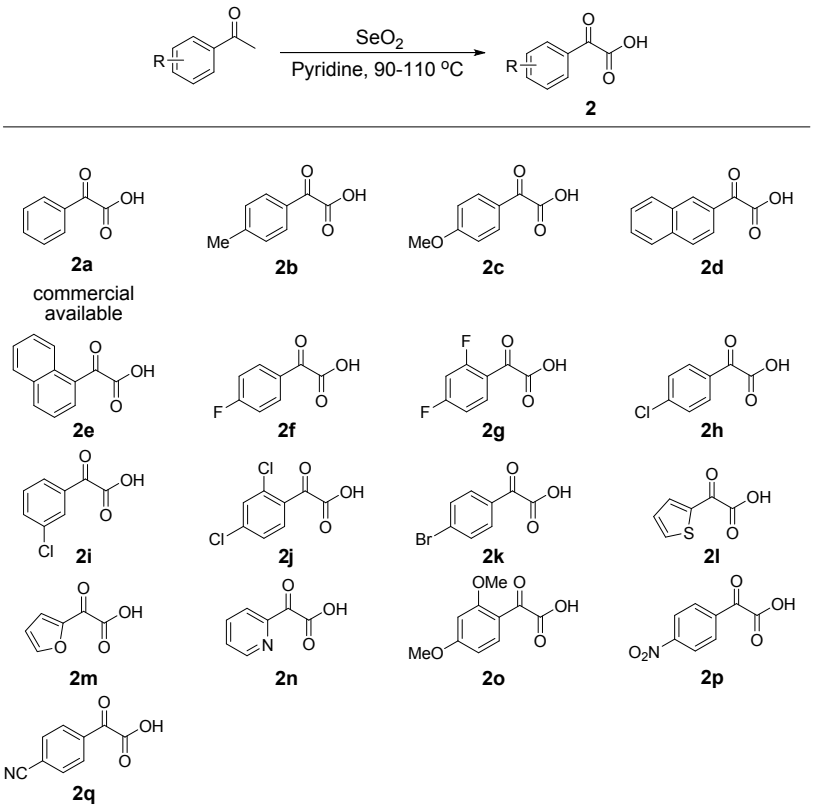
5-Chlorobenzo[c]isoxazole (1f) (Precursor to product 3f): PE/EtOAc = 40:1; White solid, 345.4 mg, 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 7.62-7.57 (m, 2H), 7.25 (t, *J* = 9.4 Hz, 1H); The ^{1}H NMR spectra data are consistent with the reported literature.[3]

6-Chlorobenzo[c]isoxazole (1g) (Precursor to product 3g): PE/EtOAc = 40:1; White solid, 340.7 mg, 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, *J* = 1.0 Hz, 1H), 7.64 (td, *J* = 1.6, 1.0 Hz, 1H), 7.54 (dd, *J* = 9.2, 0.8 Hz, 1H), 6.97 (dd, *J* = 9.2, 1.6 Hz, 1H); The ^{1}H NMR spectra data are consistent with the reported literature.[3]

6-Bromobenzo[c]isoxazole (1h) (Precursor to product 3h): PE/EtOAc = 10:1; White solid, 380.2 mg, 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, *J* = 1.0 Hz, 1H), 7.86 (d, *J* = 1.2 Hz, 1H), 7.48 (dd, *J* = 9.2, 0.8 Hz, 1H), 7.10 (dd, *J* = 9.2, 1.4 Hz, 1H); The ^{1}H NMR spectra data are consistent with the reported literature.[3]

6-(Trifluoromethyl)benzo[c]isoxazole (1i) (Precursor to product 3i): PE/EtOAc = 30:1; White solid, 364.8 mg, m.p. 40-42 ^{o}C, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (d, *J* = 0.8 Hz, 1H), 8.02-8.01 (m, 1H), 7.75 (d, *J* = 9.1 Hz, 1H), 7.18 (dd, *J* = 9.1, 1.1 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.53; The ^{1}H NMR spectra data are consistent with the reported literature.[5]

2.2 Synthesis of compounds 2b-q



Compounds 2b-m were synthesized according to the reported literature.[7]

2-Oxo-2-*p*-tolylacetic acid (2b) (Precursor to product 3k): White solid, 434.6 mg, 53% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.2 Hz, 1H), 8.00 (brs, 1H), 7.33 (d, J = 8.1 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.1, 162.7, 147.3, 131.4, 129.8, 129.2, 22.0; These NMR spectra data are consistent with the reported literature.[8]

2-(4-Methoxyphenyl)-2-oxoacetic acid (2c) (Precursor to product 3l): white solid, 558.0 mg, 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, J = 8.5 Hz, 1H), 7.00 (d, J = 9.0 Hz, 1H), 3.92 (s, 3H). The ^{1}H NMR spectra data are consistent with the reported literature.[8]

2-(Naphthalen-2-yl)-2-oxoacetic acid (2d) (Precursor to product 3m): Yellow solid, 830.8 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.20 (d, J = 8.7, 1H), 8.04 (d, J = 8.1 Hz, 1H), 7.92 (dd, J = 16.3, 8.4 Hz, 2H), 7.69 (t, J = 7.6 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.9, 160.8, 136.6, 135.7, 132.3, 130.5, 130.2, 129.0, 129.0, 127.9, 127.3, 124.7, 77.3, 77.0, 76.7; These NMR spectra data are consistent with the reported literature.[8]

2-(Naphthalen-1-yl)-2-oxoacetic acid (2e) (Precursor to product 3n): Yellow solid, 800.8 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, J = 8.6 Hz, 1H), 8.38 (d, J = 7.3 Hz, 1H), 8.16 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.71 (t, J = 7.7 Hz, 1H), 7.63-7.57 (m, 2H); The ^{1}H NMR spectra data are consistent with the reported literature.[9]

2-(4-Fluorophenyl)-2-oxoacetic acid (2f) (Precursor to product 3o): Light yellow solid, 487.5 mg, 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (dd, J = 8.6, 5.5 Hz, 2H), 7.22 (t, J = 8.5 Hz, 2H); The ^{1}H NMR spectra data are consistent with the reported literature.[10]

2-(2,4-Difluorophenyl)-2-oxoacetic acid (2g) (Precursor to product 3p)[11]: Light yellow solid, 186.1 mg, 49% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.08 (m, 1H), 7.09-7.05 (m, 1H), 6.99-6.93 (m, 1H).

2-(4-Chlorophenyl)-2-oxoacetic acid (2h) (Precursor to product 3q): White solid, 184.6 mg, 77% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 8.6 Hz, 1H), 7.56 (d, J = 8.6 Hz, 1H). The ^{1}H NMR spectra data are consistent with the reported literature data.[8]

2-(3-Chlorophenyl)-2-oxoacetic acid (2i) (Precursor to product 3r)[12]: White solid, 636.9 mg, 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 8.17 (d, J = 7.8 Hz, 1H), 7.66 (d, J = 7.9 Hz, 1H), 7.48 (t, J = 7.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.8, 162.0, 135.4, 135.3, 133.3, 130.7, 130.3, 129.2, 77.4, 77.0, 76.7.

2-(2,4-Dichlorophenyl)-2-oxoacetic acid (2j) (Precursor to product 3s)[13]: Light yellow solid, 635.1 mg, 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 8.3 Hz, 1H), 7.51 (d, J = 1.5 Hz, 1H), 7.42 (dd, J = 8.3, 1.5 Hz, 1H).

2-(4-Bromophenyl)-2-oxoacetic acid (2k) (Precursor to product 3t): White solid, 572.5 mg, 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.6 Hz, 1H), 7.69 (d, J = 8.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.7, 161.3, 132.6, 132.4, 131.6, 130.5; These NMR spectra data are consistent with the reported literature.[8]

2-Oxo-2-(thiophen-2-yl)acetic acid (2l) (Precursor to product 3u): Yellow solid, 265.5 mg, 34% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, J = 3.8 Hz, 1H), 7.96 (dd, J = 4.9, 1.0 Hz, 1H), 7.28-7.26 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.2, 159.4, 140.3, 140.0, 136.1, 129.3. These NMR spectra data are consistent with the reported literature.[8]

2-(Furan-2-yl)-2-oxoacetic acid (2m) (Precursor to product 3v): Yellow solid, 156.0 mg, 22% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 3.7 Hz, 1H), 7.87 (d, J = 1.0 Hz, 1H), 7.67 (d, J = 0.9 Hz, 1H), 6.71 (dd, J = 3.7, 1.6 Hz, 1H).

2-Oxo-2-(pyridin-2-yl)acetic acid (2n) (Precursor to product 3w): Red solid, 137.6 mg, 18% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.79 (s, 1H), 8.28 (d, J = 7.5 Hz, 1H), 8.02-7.97 (m, 1H), 7.63 (dd, J = 7.3, 4.2 Hz, 1H).

2-(2,4-Dimethoxyphenyl)-2-oxoacetic acid (2o) (Precursor to product 3x): Yellow solid, 525.5 mg, 50% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 8.8 Hz, 1H), 6.62 (dd, J = 8.8, 2.2 Hz, 2H), 6.46 (d, J = 2.2 Hz, 1H), 3.90 (s, 6H). The ^{1}H NMR spectra data are consistent with the reported literature.[14]

2-(4-Nitrophenyl)-2-oxoacetic acid (2p) (Precursor to product 3y): Yellow solid, 120.0 mg, 12% yield. ^{1}H NMR (400 MHz, DMSO) δ 8.33 (d, J = 8.9 Hz, 1H), 8.18 (d, J = 8.9 Hz, 1H). **2-(4-Cyanophenyl)-2-oxoacetic acid (2q) (Precursor to product 3z): Yellow** solid, 260.6 mg, 30% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, J = 8.5 Hz, 1H), 7.84 (d, J = 8.5 Hz, 1H).

3. Typical procedure for the synthesis of 3a starting from anthranil 1a and *α*-keto acid 2a

A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with a mixture of anthranil **1a** (0.3 mmol, 35.7 mg), α-keto acid **2a** (0.6 mmol, 90.1 mg), $CuBr_2$ (0.05 equiv, 3.3 mg) and PPh_3 (0.2 equiv, 15.7 mg). Under reduced pressure, the tube was filled with argon for three times. After the addition of DCE (3 mL), the reaction was stirred at 110 ^{o}C for 12 h. The reaction mixture was filtered through celite and concentrated in vacuo. Purification by column chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 25:1) afforded product **3a** (0.24 mmol, 60.7 mg) as a yellow solid in 80% yield.

Procedure for the synthesis of compound 9.[15] To a suspension of compound **3a** (0.2 mmol) and $CoCl_2$ (0.02 mmol) in MeCN (2 mL) was added TBHP (1.5 mmol) dropwise at room temperature over a period of 30 min. The reaction mixture was then heated at reflux and kept at that temperature until TLC analysis indicated the total consumption of compound **3a**. The solvent was evaporated under reduced pressure. Product **9** was obtained in 60% yield (0.12 mmol, 30.1 mg) as a white solid by flash column chromatography on silica gel (PE/EA = 20:1).

***N*-(2-Formylphenyl)-2-oxo-2-phenylacetamide (3a).[16]** Compound **3a** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 25:1) afforded **3a** (60.8 mg, 80%) as a yellow solid; m.p. 107-110 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.47 (s, 1H), 10.02 (s, 1H), 8.86 (d, J = 8.4 Hz, 1H), 8.39 (dd, J = 8.4, 1.2 Hz, 2H), 7.77 (dd, J = 7.6, 1.6 Hz, 1H), 7.64-7.71(m, 2H), 7.54-7.50 (m, 2H), 7.35 (td, J = 7.5, 1.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.0, 186.8, 160.7, 139.1, 136.1, 135.93, 134.5, 133.0, 131.3, 128.6, 124.2, 122.9, 120.1; ATR-FTIR(cm^{-1}): 3222, 2863, 2161, 1663, 1574, 1511, 1445, 1189, 1159, 987, 885, 760, 684.

***N*-(2-Formyl-4-methoxyphenyl)-2-oxo-2-phenylacetamide (3b).** Compound **3b** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 6:1) afforded **3b** (61.2 mg, 72%) as a yellow solid; m.p. 112-114 ^{o}C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.23 (s, 1H), 9.98 (s, 1H), 8.81 (d, J = 8.9 Hz, 1H), 8.42-8.38 (m, 2H), 7.66 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.27-7.22 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.6, 187.0, 160.2, 156.0, 134.4, 133.1, 132.6, 131.2, 128.5, 123.8, 121.8, 121.5, 120.1, 55.7; ATR-FTIR (cm^{-1}): 3236, 2049, 1666, 1592, 1520, 1464, 1331, 1278, 1166, 1129, 1033, 923, 883, 763, 679; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{16}H_{13}NO_4$ 284.0917; Found 284.0913.

***N*-(6-Formylbenzo[d][1,3]dioxol-5-yl)-2-oxo-2-phenylacetamide (3c).** Compound **3c** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica

gel (PE:EA = 8:1) afforded **3c** (55.3 mg, 62%) as a yellow solid; m.p. 145-146 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.73 (s, 1H), 9.77 (s, 1H), 8.46 (s, 1H), 8.39-8.36 (m, 2H), 7.67-7.63 (m, 1H), 7.53-7.49 (m, 2H), 7.11 (s, 1H), 6.11 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.5, 186.7, 160.6, 153.7, 144.1, 137.1, 134.5, 133.0, 131.2, 128.5, 117.1, 113.4, 102.6, 101.4; ATR-FTIR(cm^{-1}): 2924, 2161, 1979, 1678, 1596, 1516, 1497, 1367, 1283, 1190, 1032, 932, 738, 681; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{16}H_{11}NO_5$ 298.0710; Found 298.0708.

***N*-(4-Fluoro-2-formylphenyl)-2-oxo-2-phenylacetamide (3d).** Compound **3d** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3d** (57.0 mg, 70%) as a yellow solid; m.p. 133-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.33 (s, 1H), 9.97 (s, 1H), 8.89 (dd, *J* = 9.2, 4.7 Hz, 1H), 8.44-8.35 (m, 2H), 7.70-7.63 (m, 1H), 7.56-7.45 (m, 3H), 7.41 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6 (d, *J* = 1.8 Hz), 186.6, 160.1 (d, *J* = 59.8 Hz), 157.3, 135.5 (d, *J* = 2.9 Hz), 134.6, 133.0, 131.3, 128.6, 123.9 (d, *J* = 5.3 Hz), 122.9 (d, *J* = 22.0 Hz), 122.2 (d, *J* = 6.9 Hz), 121.5 (d, *J* = 22.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.62; ATR-FTIR (cm^{-1}): 3224, 2866, 1664, 1513, 1445, 1389, 1275, 1144, 1110, 948, 880, 784, 683; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}FNO_3$ 272.0717; Found 272.0715.

***N*-(5-Fluoro-2-formylphenyl)-2-oxo-2-phenylacetamide (3e).** Compound **3e** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3e** (57.8 mg, 71%) as a yellow solid; m.p. 156-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.65 (s, 1H), 9.96 (s, 1H), 8.64 (dd, *J* = 11.5, 2.3 Hz, 1H), 8.39 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.77 (dd, *J* = 8.5, 6.2 Hz, 1H), 7.70-7.64 (m, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.02 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 186.2, 167.0 (d, *J* = 257.2 Hz), 160.7, 141.5 (d, *J* = 13.6 Hz), 138.5 (d, *J* = 11.7 Hz), 134.7, 132.8, 131.3, 128.6, 119.7, 111.5 (d, *J* = 22.9 Hz), 107.8 (d, *J* = 28.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.48; ATR-FTIR (cm^{-1}): 3220, 2161, 1677, 1590, 1514, 1446, 1280, 1199, 1170, 1107, 1004, 869, 782, 678; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}FNO_3$ 272.0718; Found 272.0716.

***N*-(4-Chloro-2-formylphenyl)-2-oxo-2-phenylacetamide (3f).** Compound **3f** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3f** (60.4 mg, 70%) as a yellow solid; m.p. 135-136 °C; 1H NMR (400 MHz, $CDCl_3$) δ 12.39 (s, 1H), 9.96 (s, 1H), 8.84 (d, *J* = 8.9 Hz, 1H), 8.39-8.37 (m, 2H), 7.73 (d, J = 2.5 Hz, 1H), 7.69-7.62 (m, 2H), 7.54-7.50 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 186.4, 160.5, 137.6, 135.7, 135.3, 134.6, 132.9, 131.3, 129.4, 128.6, 123.9, 121.7; ATR-FTIR (cm^{-1}): 3222, 2857, 2752, 2162, 1686, 1662, 1572, 1499, 1444, 1383, 1274, 1187, 1152, 892, 728, 676; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}ClNO_3$ 288.0422; Found 288.0431.

***N*-(5-Chloro-2-formylphenyl)-2-oxo-2-phenylacetamide (3g).** Compound **3g** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3g** (56.1 mg, 65%) as a yellow solid; m.p. 172-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.54 (s, 1H), 9.97 (s, 1H), 8.93 (d, *J* = 1.7 Hz, 1H), 8.43-8.35 (m, 2H), 7.72-7.64 (m, 2H), 7.52 (t, *J* = 7.8 Hz, 2H), 7.31 (dd, *J* = 8.2, 1.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.8, 186.2, 160.6, 142.6, 140.0, 137.0, 134.7, 132.8, 131.3, 128.6, 124.5, 121.2, 120.3; ATR-FTIR (cm^{-1}): 3218, 2865, 2161, 1677, 1572, 1512, 1447, 1393, 1286, 1163, 1084, 987, 878, 785, 674; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}ClNO_3$ 288.0422; Found 288.0424.

***N*-(5-Bromo-2-formylphenyl)-2-oxo-2-phenylacetamide (3h).** Compound **3h** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 25:1) afforded **3h** (79.7 mg, 80%) as a yellow solid; m.p. 153-155 °C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ

12.52 (s, 1H), 9.97 (s, 1H), 9.11 (d, J = 1.3 Hz, 1H), 8.40-8.38 (m, 2H), 7.69-7.60 (m, 2H), 7.55-7.48 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.0, 186.2, 160.5, 139.8, 136.9, 134.7, 132.8, 131.5, 131.3, 128.6, 127.5, 123.2, 121.5; ATR-FTIR(cm^{-1}): 3220, 2867, 2162, 1979, 1665, 1590, 1573, 1446, 1278, 1146, 949, 880, 785, 678; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}BrNO_3$ 331.9917; Found 331.9913.

***N*-(5-Trifluoromethyl-2-formylphenyl)-2-oxo-2-phenylacetamide (3i).** Compound **3i** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3i** (58.8 mg, 61%) as a light yellow solid; m.p. 134-136 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.55 (s, 1H), 10.10 (s, 1H), 9.21 (s, 1H), 8.42-8.40 (m, 2H), 7.92 (d, J = 8.0 Hz, 1H), 7.70-7.66 (m, 1H), 7.60 (dd, J = 8.0, 1.0 Hz, 1H), 7.55-7.51 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 186.1, 160.6, 139.5, 136.9 (d, J = 33.0 Hz), 136.3, 134.7, 132.8, 131.4, 128.7, 124.5, 123.0 (q, J = 273.6 Hz), 120.7 (q, J = 3.8 Hz), 117.3 (q, J = 3.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.51; ATR-FTIR (cm^{-1}): 3221, 2866, 1679, 1665, 1580, 1525, 1446, 1328, 1280, 1158, 1113, 896, 743, 676; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{16}H_{10}F_3NO_3$ 322.0686; Found 322.0681.

***N*-(2-Benzoyl-4-chlorophenyl)-2-oxo-2-phenylacetamide (3j).** Compound **3j** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3j** (96.0 mg, 88%) as a yellow solid; m.p. 122-124 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.95 (s, 1H), 8.78-8.73 (m, 1H), 8.42-8.36 (m, 2H), 7.79-7.75 (m, 2H), 7.67-7.60 (m, 4H), 7.54-7.49 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.5, 186.6, 160.0, 137.5, 137.3, 134.5, 133.7, 133.1, 133.0, 132.8, 131.3, 130.1, 128.6, 128.6, 128.5, 126.0, 122.8; ATR-FTIR (cm^{-1}): 3220, 2162, 1691, 1674, 1574, 1509, 1446, 1306, 1277, 1159, 1100, 948, 834, 737, 677; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{21}H_{14}ClNO_3$ 364.0735; Found 364.0731.

***N*-(2-Formylphenyl)-2-oxo-2-*p*-tolylacetamide (3k).** Compound **3k** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3k** (66.6 mg, 83%) as a yellow solid; m.p. 121-123 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.45 (s, 1H), 10.01 (s, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.31 (d, J = 8.3 Hz, 2H), 7.76 (dd, J = 7.6, 1.5 Hz, 1H), 7.71-7.66 (m, 1H), 7.36-7.30 (m, 3H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 186.2, 160.9, 145.8, 139.2, 136.1, 135.9, 131.4, 130.5, 129.3, 124.1, 122.9, 120.1, 21.9; ATR-FTIR (cm^{-1}): 3218, 3105, 2833, 2749, 1670, 1583, 1521, 1452, 1414, 1287, 1261, 1195, 1158, 1118, 998, 869, 789, 672; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{16}H_{13}NO_3$ 268.0968; Found 268.0968.

***N*-(2-Formylphenyl)-2-(4-methoxyphenyl)-2-oxoacetamide (3l).** Compound **3l** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 15:1) afforded **3l** (68.0 mg, 80%) as a pink solid; m.p. 170-172 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.46 (s, 1H), 10.01 (s, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.46 (d, J = 8.9 Hz, 2H), 7.76 (dd, J = 7.6, 1.1 Hz, 1H), 7.68 (t, J = 7.9 Hz, 1H), 7.33 (t, J = 7.5 Hz, 1H), 6.98 (d, J = 8.9 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 184.7, 164.8, 161.3, 139.3, 136.1, 135.9, 134.0, 126.1, 124.1, 122.9, 120.1, 113.9, 55.6; ATR-FTIR (cm^{-1}): 3217, 2845, 2161, 2050, 1675, 1582, 1518, 1453, 1287, 1257, 1158, 1029, 868, 761, 654; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{16}H_{13}NO_4$ 284.0917; Found 284.0916.

***N*-(2-Formylphenyl)-2-(naphthalen-2-yl)-2-oxoacetamide (3m).** Compound **3m** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 15:1) afforded **3m** (73.7 mg, 81%) as a yellow solid; m.p. 156-158 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.55 (s, 1H), 10.03 (s, 1H), 9.21 (s, 1H), 8.91 (d, J = 8.4 Hz, 1H), 8.27 (dd, J = 8.7, 1.7 Hz, 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.91 (dd, J = 17.8, 8.4 Hz, 2H), 7.78 (dd, J = 7.6, 1.5 Hz, 1H), 7.74-7.69 (m, 1H),

7.67-7.63 (m, 1H), 7.59-7.55 (m, 1H), 7.36 (td, *J* = 7.5, 0.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 186.4, 160.9, 139.2, 136.2, 136.1, 135.9, 134.8, 132.3, 130.3, 130.3, 129.4, 128.5, 127.8, 126.9, 125.4, 124.2, 122.9, 120.1; ATR-FTIR (cm^{-1}): 3215, 1673, 1582, 1519, 1450, 1288, 1198, 1151, 1113, 840, 804, 756, 735, 661; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{19}H_{13}NO_3$ 304.0968; Found 304.0975.

***N*-(2-Formylphenyl)-2-(naphthalen-1-yl)-2-oxoacetamide (3n).** Compound **3n** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 15:1) afforded **3n** (59.1 mg, 65%) as a yellow solid; m.p. 180-182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.64 (s, 1H), 10.05 (s, 1H), 8.89 (d, *J* = 8.4 Hz, 1H), 8.68 (d, *J* = 8.6 Hz, 1H), 8.33 (dd, *J* = 7.3, 1.1 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.80 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.73-7.63 (m, 2H), 7.60-7.56 (m, 2H), 7.37 (td, *J* = 7.5, 0.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.1, 189.3, 161.0, 139.3, 136.2, 136.0, 134.7, 133.9, 133.0, 131.3, 129.3, 128.7, 128.5, 126.7, 125.4, 124.3, 124.2, 122.9, 120.1; ATR-FTIR (cm^{-1}): 3222, 1670, 1585, 1526, 1508, 1450, 1282, 1254, 1198, 1161, 1089, 1069, 886, 800, 760,727; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{19}H_{13}NO_3$ 304.0968; Found 304.0971.

2-(4-Fluorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3o). Compound **3o** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3o** (68.3 mg, 84%) as a yellow solid; m.p. 161-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.50 (s, 1H), 10.01 (s, 1H), 8.83 (d, *J* = 8.4 Hz, 1H), 8.52-8.47 (m, 2H), 7.78 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.72-7.67 (m, 1H), 7.35 (td, *J* = 7.5, 0.9 Hz, 1H), 7.22-7.16 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 184.9, 167.9, 165.4, 160.5, 139.0, 136.1 (d, *J* = 23.8 Hz), 134.3 (d, *J* = 9.7 Hz), 129.5 (d, *J* = 2.9 Hz), 124.3, 122.9, 120.1, 115.9 (d, *J* = 21.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.81; ATR-FTIR (cm^{-1}): 3222, 1660, 1584, 1520, 1451, 1283, 1204, 1157, 1120, 993, 869, 803, 757, 620; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}FNO_3$ 272.0718; Found 272.0716.

2-(2,4-Difluorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3p). Compound **3p** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 15:1) afforded **3p** (62.5 mg, 72%) as a white solid; m.p. 165-166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.36 (s, 1H), 10.01 (s, 1H), 8.80 (d, *J* = 8.4 Hz, 1H), 8.05-8.00 (m, 1H), 7.78 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.71-7.66 (m, 1H), 7.36 (td, *J* = 7.5, 0.9 Hz, 1H), 7.05-7.00 (m, 1H), 6.96-6.91 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.1, 185.6 (d, *J* = 1.8 Hz), 167.7 (d, *J* = 12.3 Hz), 164.7 (dd, *J* = 76.5, 12.5 Hz), 161.7 (d, *J* = 12.9 Hz), 160.0, 138.9, 136.1 (d, *J* = 12.8 Hz), 134.0 (dd, *J* = 10.8, 3.1 Hz), 124.4, 122.8, 120.2, 119.1 (dd, *J* = 11.4, 3.5 Hz), 112.0 (dd, *J* = 21.7, 3.7 Hz), 105.1 (t, *J* = 25.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -99.25 (d, *J* = 13.0 Hz), -104.26 (d, *J* = 13.0 Hz); ATR-FTIR (cm^{-1}): 3062, 1682, 1586, 1531, 1453, 1425, 1286, 1202, 1152, 1107, 996, 864, 818, 752, 634; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_9F_2NO_3$ 290.0623; Found 290.0619.

2-(4-Chlorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3q). Compound **3q** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 15:1) afforded **3q** (69.9 mg, 81%) as a yellow solid; m.p. 198-200 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.51 (s, 1H), 10.02 (s, 1H), 8.83 (d, *J* = 8.3 Hz, 1H), 8.39 (d, *J* = 8.3 Hz, 2H), 7.78 (d, *J* = 7.4 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H)；^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 185.4, 160.3, 141.3, 139.0, 136.2, 136.0, 132.8, 131.4, 129.0, 124.4, 122.9, 120.1; ATR-FTIR (cm^{-1}): 3219, 2162, 1673, 1659, 1581, 1521, 1453, 1401, 1283, 1204, 1164, 1096, 991, 868, 800, 717; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}ClNO_3$ 288.0422; Found 288.0426.

2-(3-Chlorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3r). Compound **3r** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3r** (61.3 mg, 71%) as a yellow solid; m.p. 146-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.49 (s, 1H), 10.01 (s, 1H), 8.83 (d, J = 8.4 Hz, 1H), 8.40 (t, J = 1.8 Hz, 1H), 8.30-8.28 (m, 1H), 7.78 (dd, J = 7.6, 1.6 Hz, 1H), 7.72-7.68 (m, 1H), 7.64-7.61 (m, 1H), 7.46 (t, J = 7.9 Hz, 1H), 7.36 (td, J = 7.6, 0.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 185.5, 160.0, 138.9, 136.2, 136.0, 134.7, 134.5, 134.4, 131.2, 129.9, 129.4, 124.4, 122.9, 120.1; ATR-FTIR (cm^{-1}): 3218, 1674, 1583, 1519, 1450, 1411, 1284, 1204, 1159, 1118, 993, 869, 803, 757, 666; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}ClNO_3$ 288.0422; Found 288.0425.

2-(2,4-Dichlorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3s). Compound **3s** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 15:1) afforded **3s** (67.6 mg, 70%) as a yellow solid; m.p. 182-183 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.45 (s, 1H), 10.03 (s, 1H), 8.78 (d, J = 8.4 Hz, 1H), 7.79 (dd, J = 7.6, 1.6 Hz, 1H), 7.71-7.66 (m, 2H), 7.51 (d, J = 1.9 Hz, 1H), 7.37 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.1, 188.3, 159.3, 139.1, 138.9, 136.2, 136.0, 134.3, 132.3, 132.1, 130.5, 127.1, 124.5, 122.9, 120.1; ATR-FTIR (cm^{-1}): 3182, 2161, 1670, 1588, 1530, 1451, 1374, 1280, 1208, 1153, 1066, 989, 866, 812, 753, 666; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_9Cl_2NO_3$ 322.0032; Found 322.0031.

2-(4-Bromophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3t). Compound **3t** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 10:1) afforded **3t** (62.8 mg, 63%) as a yellow solid; m.p. 190-192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.50 (s, 1H), 10.02 (s, 1H), 8.83 (d, J = 8.4 Hz, 1H), 8.31-8.28 (m, 2H), 7.78 (dd, J = 7.6, 1.5 Hz, 1H), 7.72-7.65 (m, 3H), 7.36 (td, J = 7.5, 0.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 185.7, 160.2, 139.0, 136.2, 136.0, 132.8, 132.0, 131.8, 130.3, 124.4, 122.9, 120.1; ATR-FTIR (cm^{-1}): 3220, 1673, 1578, 1522, 1452, 1278, 1203, 1163, 1074, 989, 883, 800, 664; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{15}H_{10}BrNO_3$ 331.9917; Found 331.9908.

***N*-(2-Formylphenyl)-2-oxo-2-(thiophen-2-yl)acetamide (3u).** Compound **3u** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3u** (54.5 mg, 70%) as a yellow solid; m.p. 171-173 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.64 (s, 1H), 10.02 (s, 1H), 8.84 (d, J = 8.4 Hz, 1H), 8.46 (d, J = 3.8 Hz, 1H), 7.87 (d, J = 4.8 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.69 (t, J = 7.9 Hz, 1H), 7.35 (t, J = 7.5 Hz, 1H), 7.23 (t, J = 4.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 177.7, 159.9, 138.8, 138.7, 138.2, 136.3, 136.1, 135.9, 128.3, 124.4, 123.1, 120.2; ATR-FTIR (cm^{-1}): 3182, 3103, 2922, 1670, 1645, 1584, 1526, 1497, 1406, 1276, 1202, 1053, 857, 758, 730; HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{13}H_9NO_3S$ 260.0376; Found 260.0375.

***N*-(2-Formylphenyl)-2-(furan-2-yl)-2-oxoacetamide (3v).** Compound **3v** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 10:1) afforded **3V** (14.2 mg, 20%) as a white solid; m.p. 157-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.58 (s, 1H), 10.02 (s, 1H), 8.82 (d, J = 8.4 Hz, 1H), 8.19 (dd, J = 3.6, 0.6 Hz, 1H), 7.80 (ddd, J = 9.1, 4.7, 1.1 Hz, 2H), 7.71-7.67 (m, 1H), 7.36 (td, J = 7.5, 0.9 Hz, 1H), 6.67 (dd, J = 3.6, 1.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 173.0, 159.4, 149.6, 149.4, 138.9, 136.2, 135.9, 126.6, 124.4, 123.1, 120.2, 113.2; HRMS (ESI-TOF) *m/z* $(M+Na)^+$ Calcd for $C_{13}H_9NO_4$ 266.0424; Found 266.0427.

***N*-(2-Formylphenyl)-2-oxo-2-(pyridin-2-yl)acetamide (3w').** Compound **3w'** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3w** (17.4 mg, 23%) as a white solid; m.p. 119-120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.16 (s, 1H), 10.06 (s, 1H), 9.01 (d, J = 8.4 Hz, 1H), 8.81 (dd, J = 4.0, 0.7 Hz, 1H), 8.29 (d, J = 7.8

Hz, 1H), 7.91 (td, *J* = 7.7, 1.7 Hz, 1H), 7.76 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.71-7.66 (m, 1H), 7.51 (ddd, *J* = 7.6, 4.8, 1.1 Hz, 1H), 7.31-7.27 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 164.1, 150.1, 148.8, 140.2, 137.5, 136.2, 136.0, 126.6, 123.3, 122.9, 122.8, 120.3; HRMS (ESI-TOF) *m/z* $(M+Na)^+$ Calcd for $C_{13}H_{10}N_2O_2$ 249.0635; Found 249.0649.

2-Benzoyl-4*H*-benzo[d][1,3]oxazin-4-one (9).[17] Compound **9** was synthesized in accordance with the typical procedure. Purification by column chromatography on silica gel (PE:EA = 20:1) afforded **3u** (30.1 mg, 60%) as a white solid, 127-128 °C**;** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.9 Hz, 1H), 8.24 (d, *J* = 7.5 Hz, 2H), 7.92 (t, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.5, 157.9, 151.8, 144.8, 136.9, 134.5, 133.8, 130.9, 130.6, 129.0, 128.6, 128.4, 118.4; HRMS (ESI-TOF) *m/z* $(M+Na)^+$ Calcd for $C_{15}H_9NO_3$ 249.0635; Found 249.0649.

2-Chloroethyl 2-oxo-2-phenylacetate (4).[18] Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.02 (m, 2H), 7.70-7.66 (m, 1H), 7.55-7.51 (m, 2H), 4.66-4.63 (m, 2H), 3.84-3.81 (m, 2H); HRMS (ESI-TOF) *m/z* $(M+H)^+$ Calcd for $C_{10}H_{10}ClO_3$ 213.0313; Found 213.0310.

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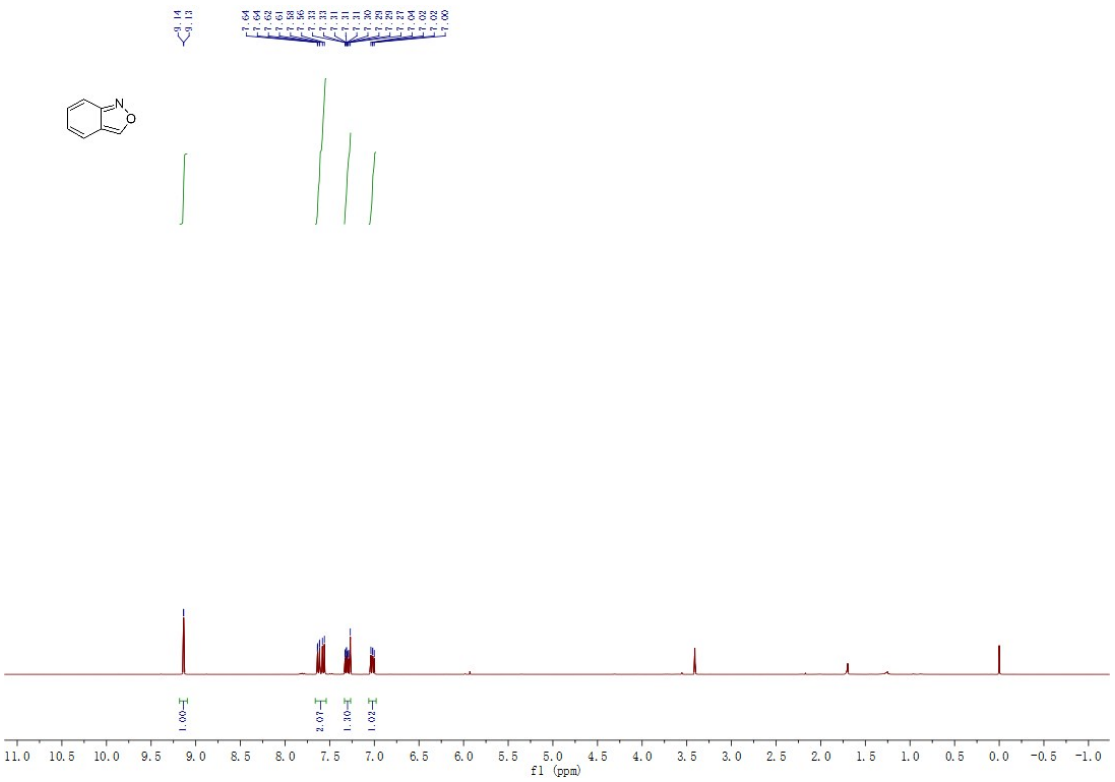
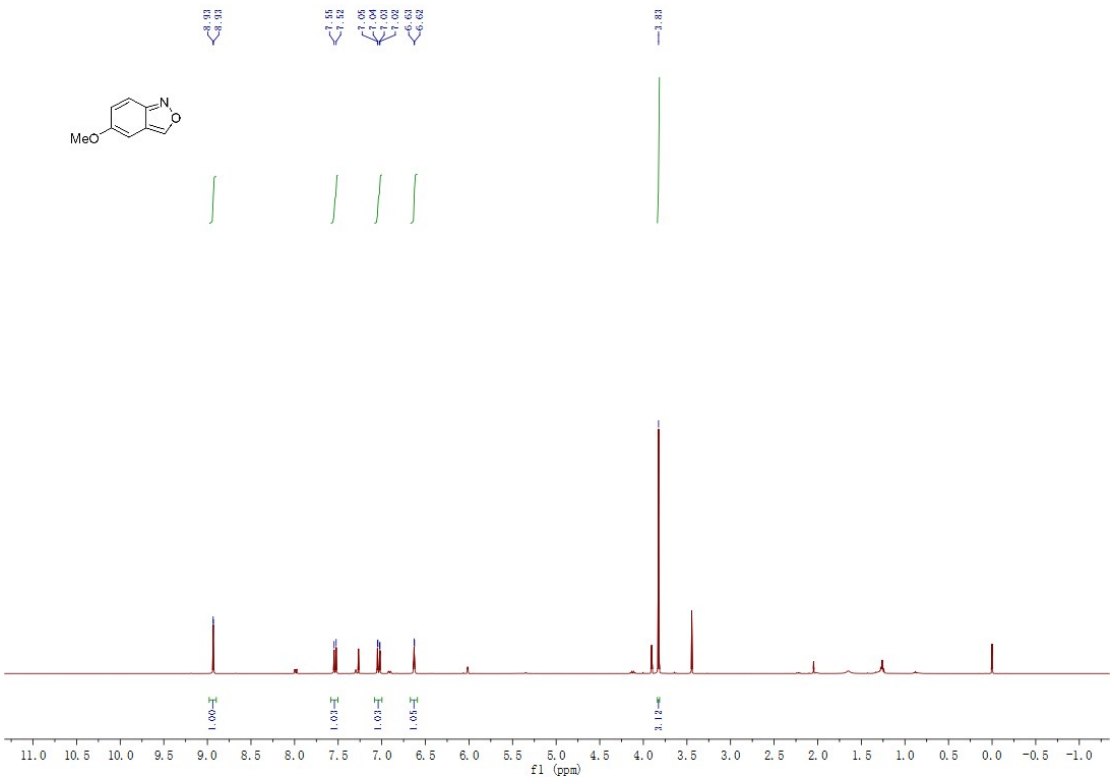
2015, *54*, 855-859.

5. NMR Spectra

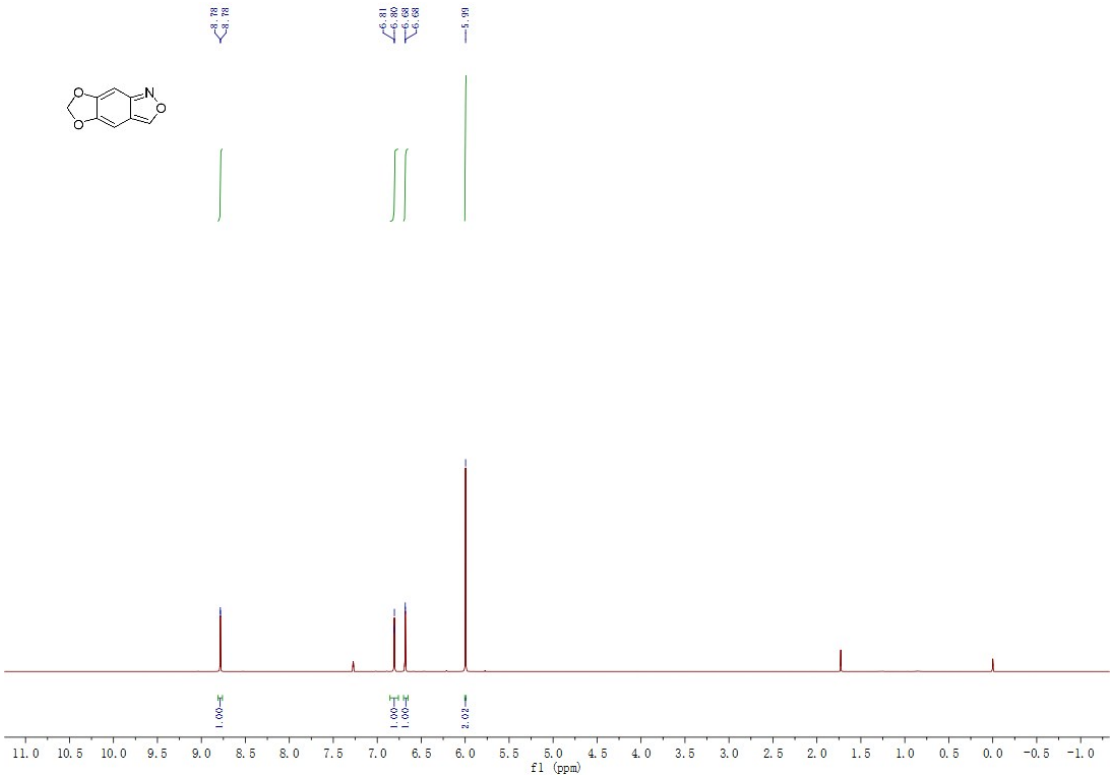
Benzo[c]isoxazole (1a)



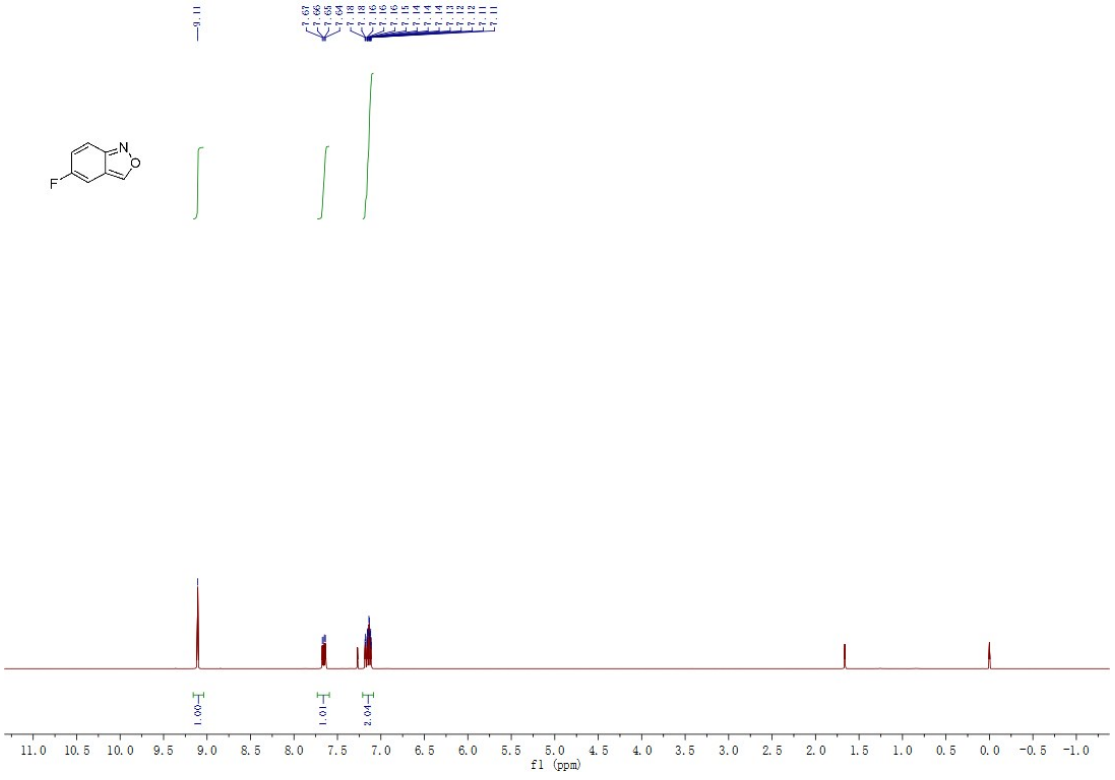
5-Methoxybenzo[c]isoxazole (1b)



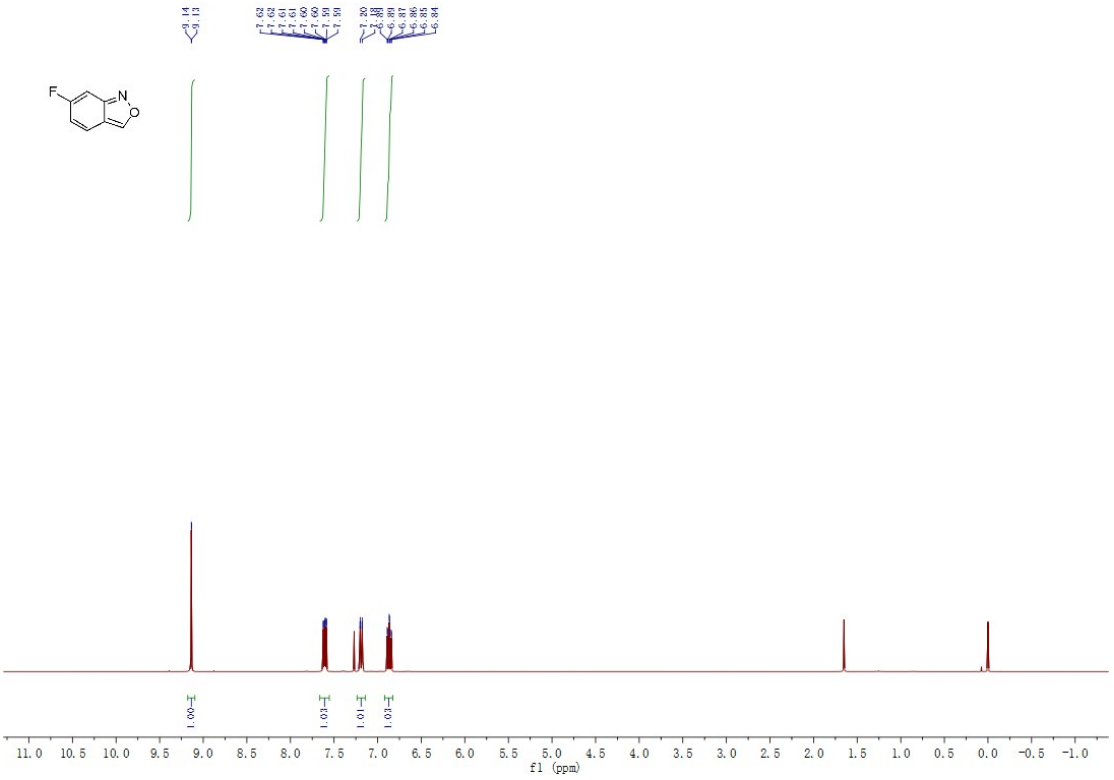
[1,3]Dioxolo[4',5':4,5]benzo[1,2-c]isoxazole (1c)



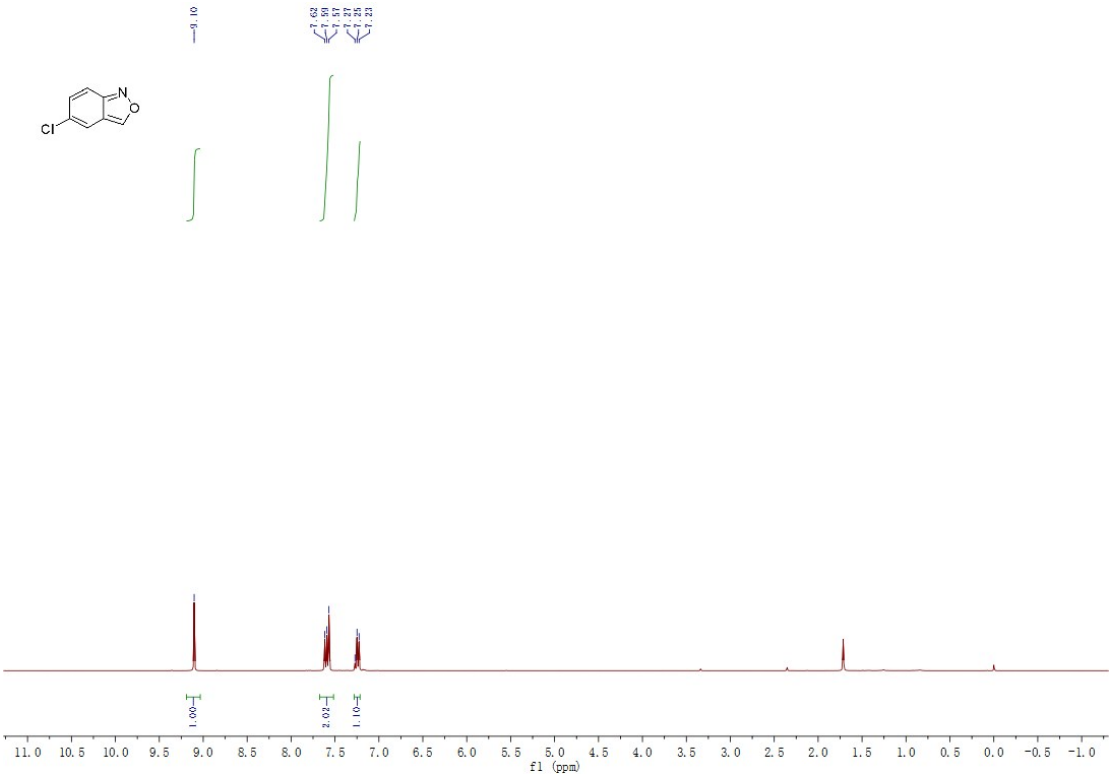
5-Fluorobenzo[c]isoxazole (1d)



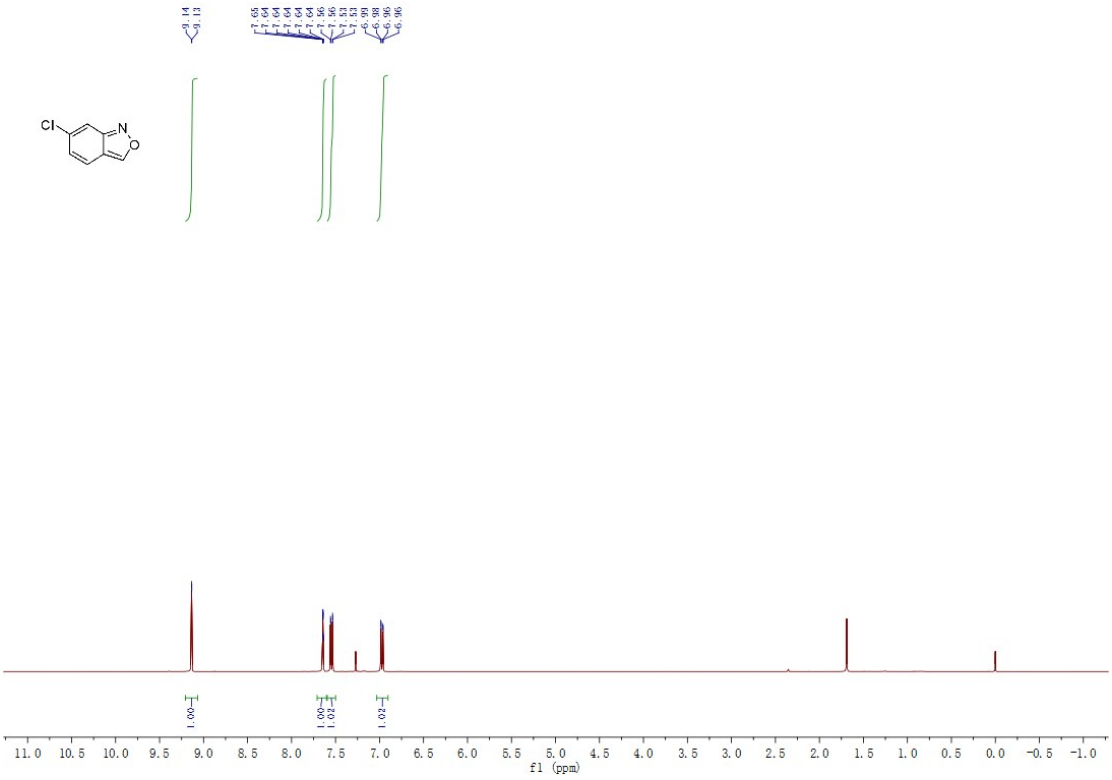
6-Fluorobenzo[c]isoxazole (1e)



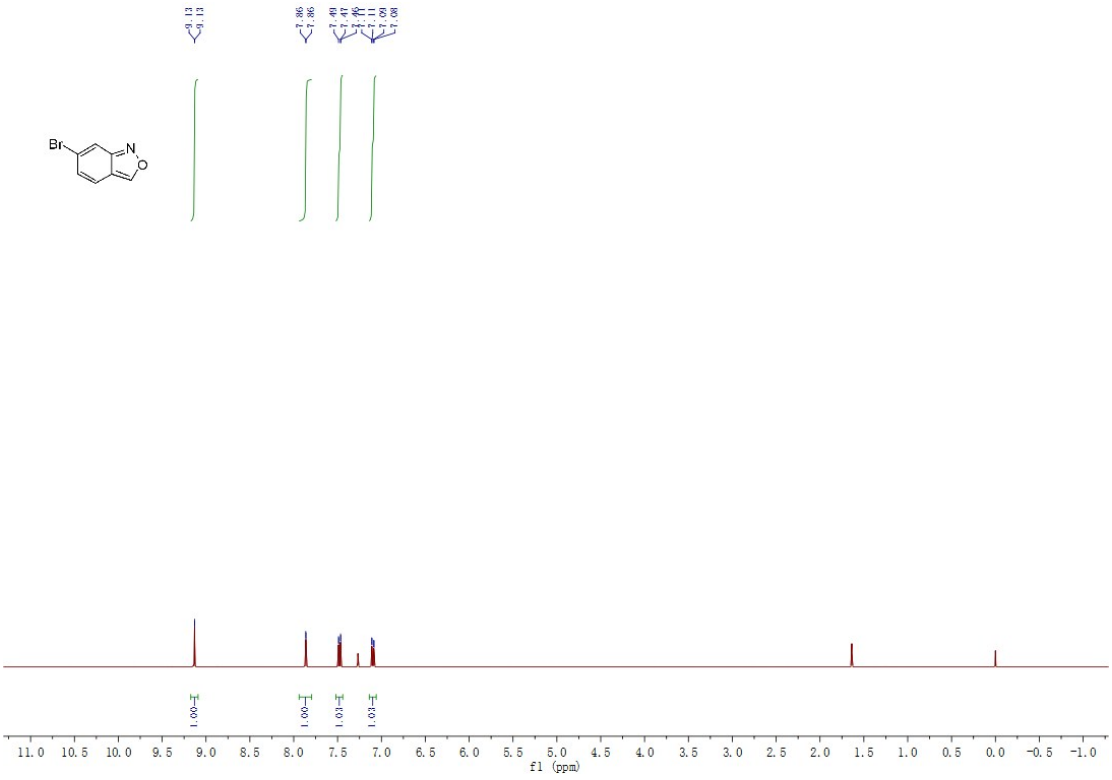
5-Chlorobenzo[c]isoxazole (1f)



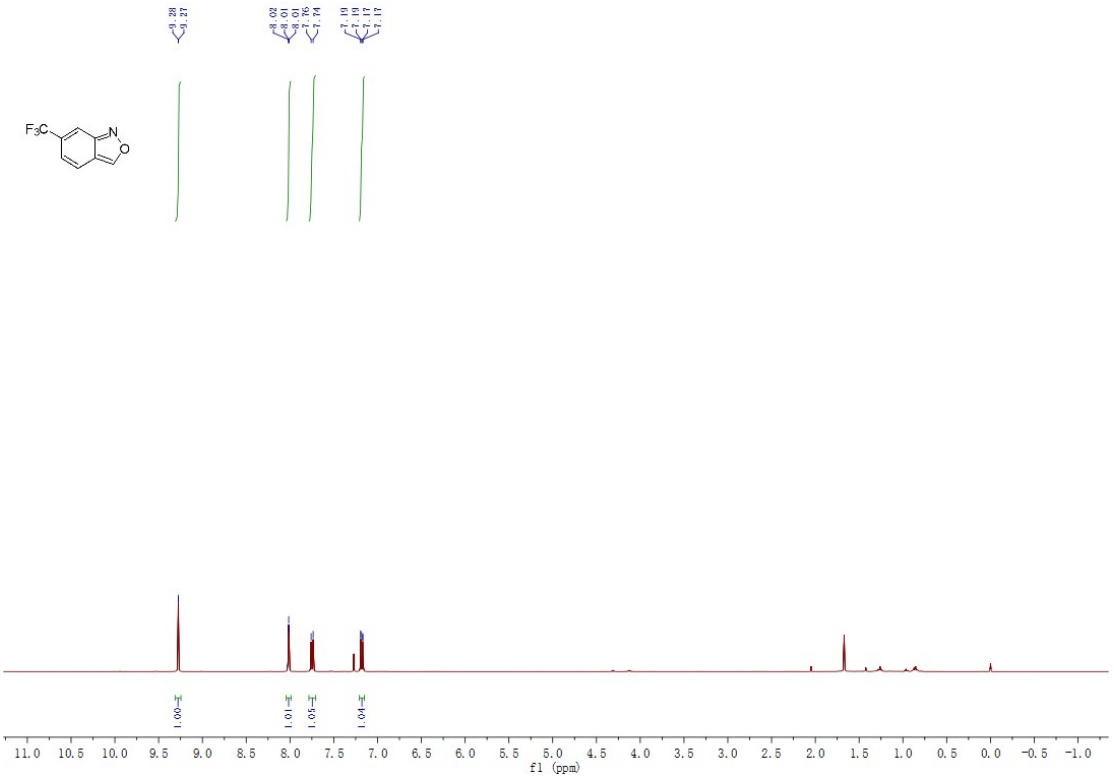
6-Chlorobenzo[c]isoxazole (1g)

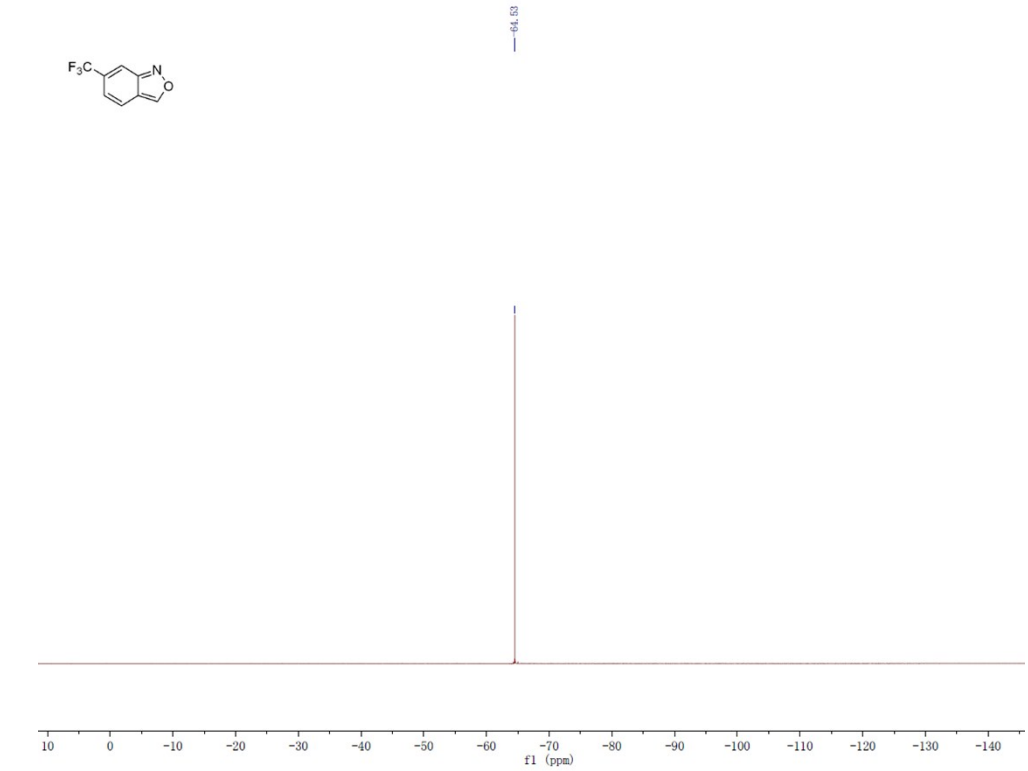


6-Bromobenzo[c]isoxazole (1h)

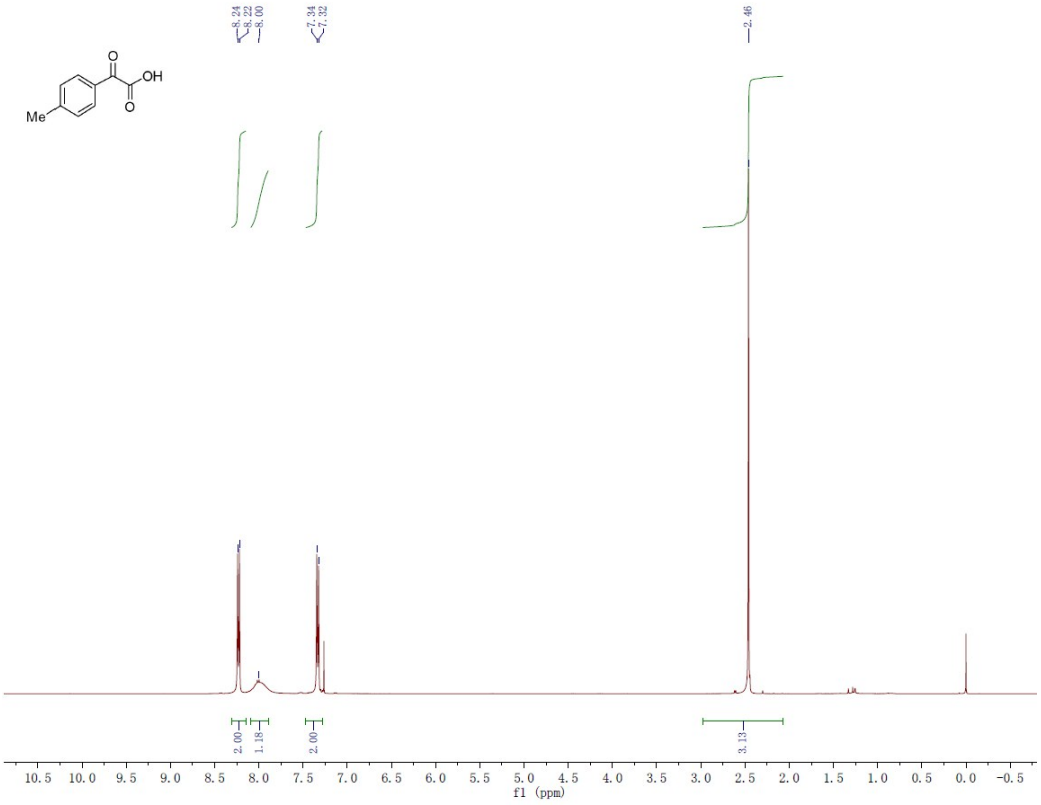


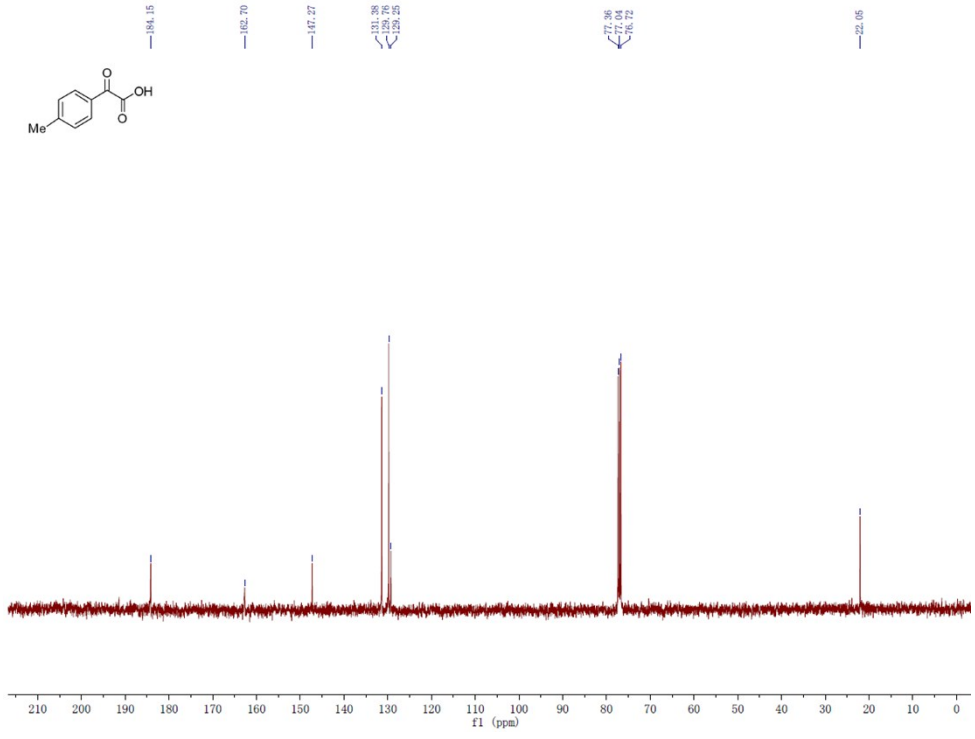
6-(Trifluoromethyl)benzo[c]isoxazole (1i)



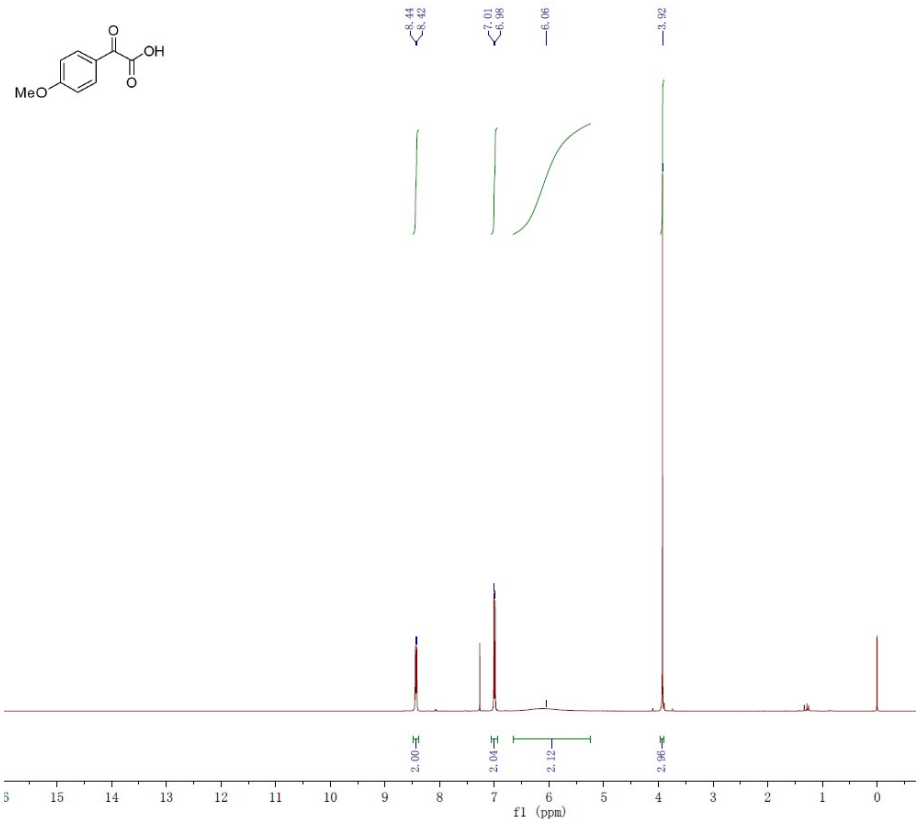


2-Oxo-2-*p*-tolylacetic acid (2b)

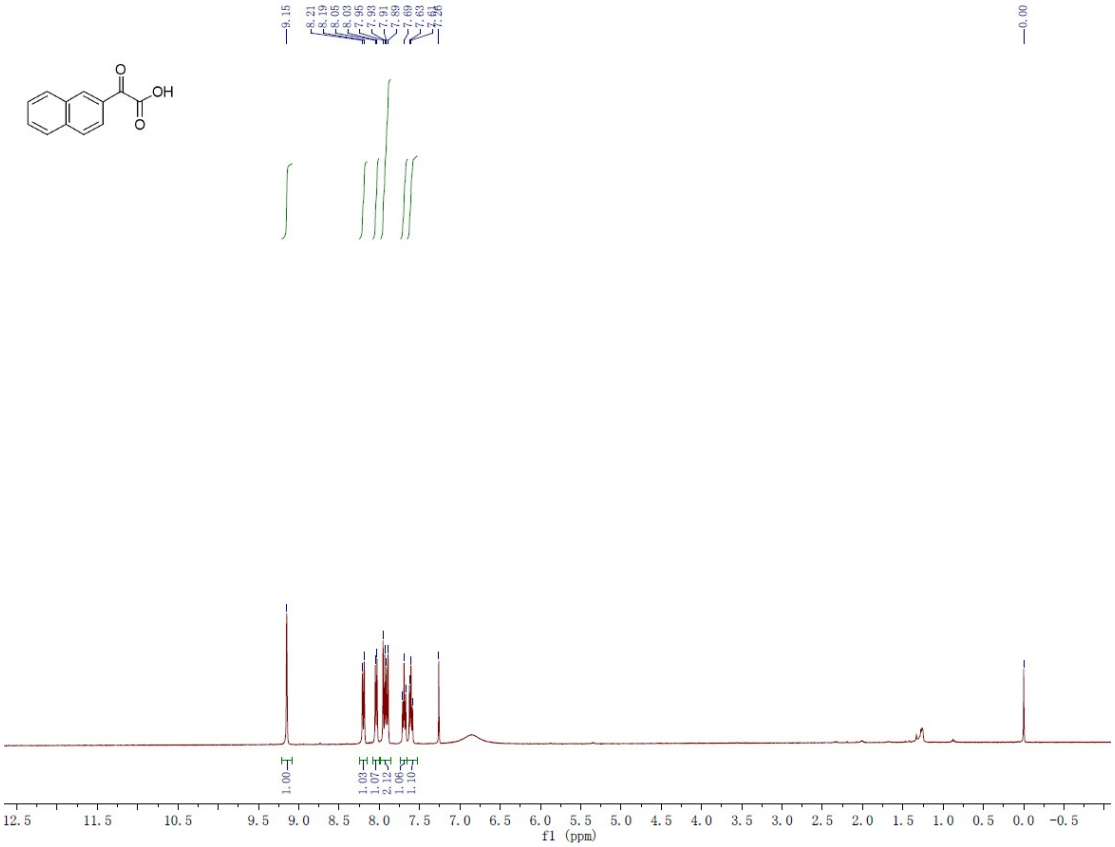


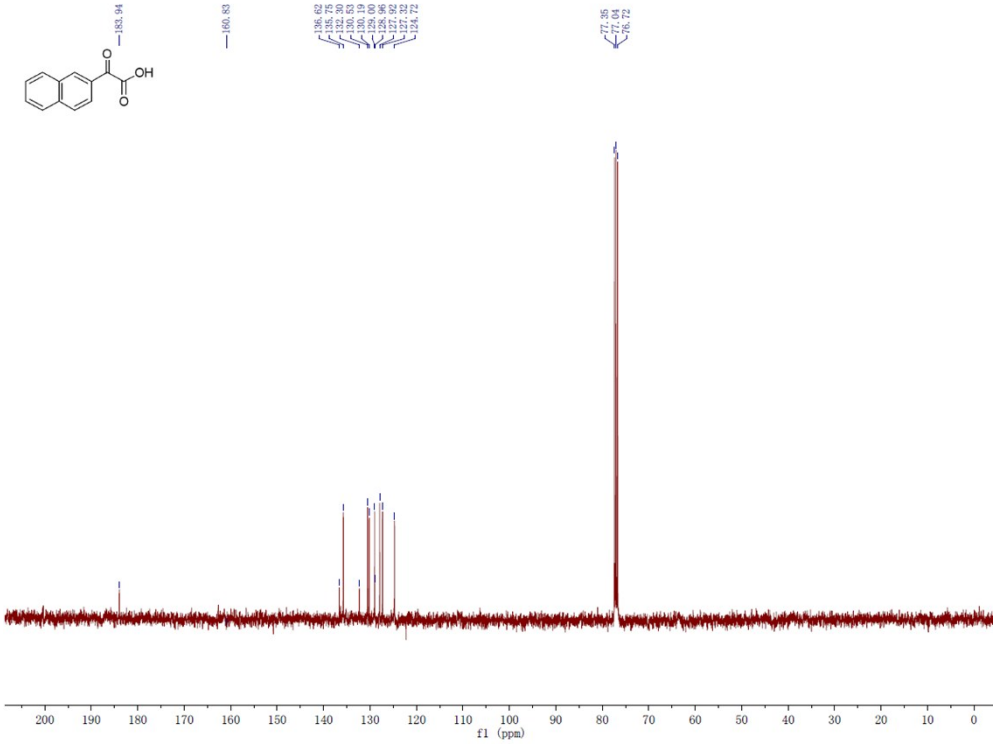


2-(4-Methoxyphenyl)-2-oxoacetic acid (2c)

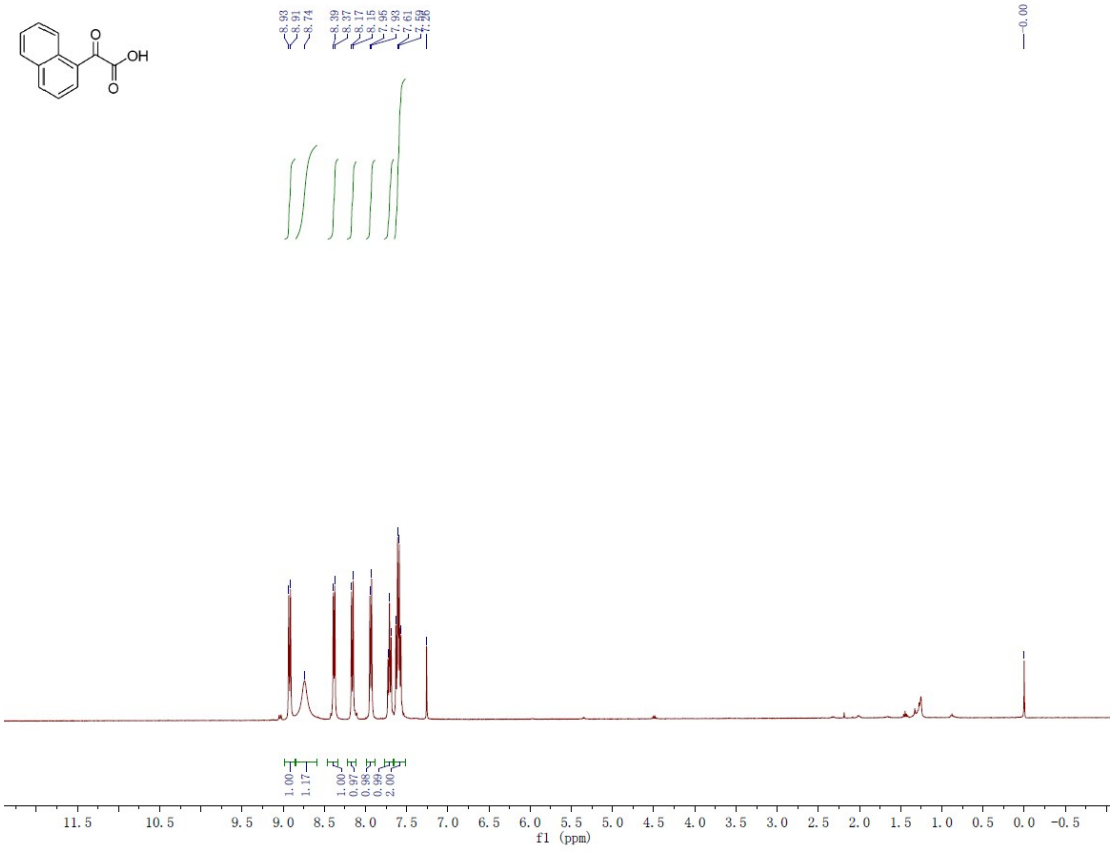


2-(Naphthalen-2-yl)-2-oxoacetic acid (2d)

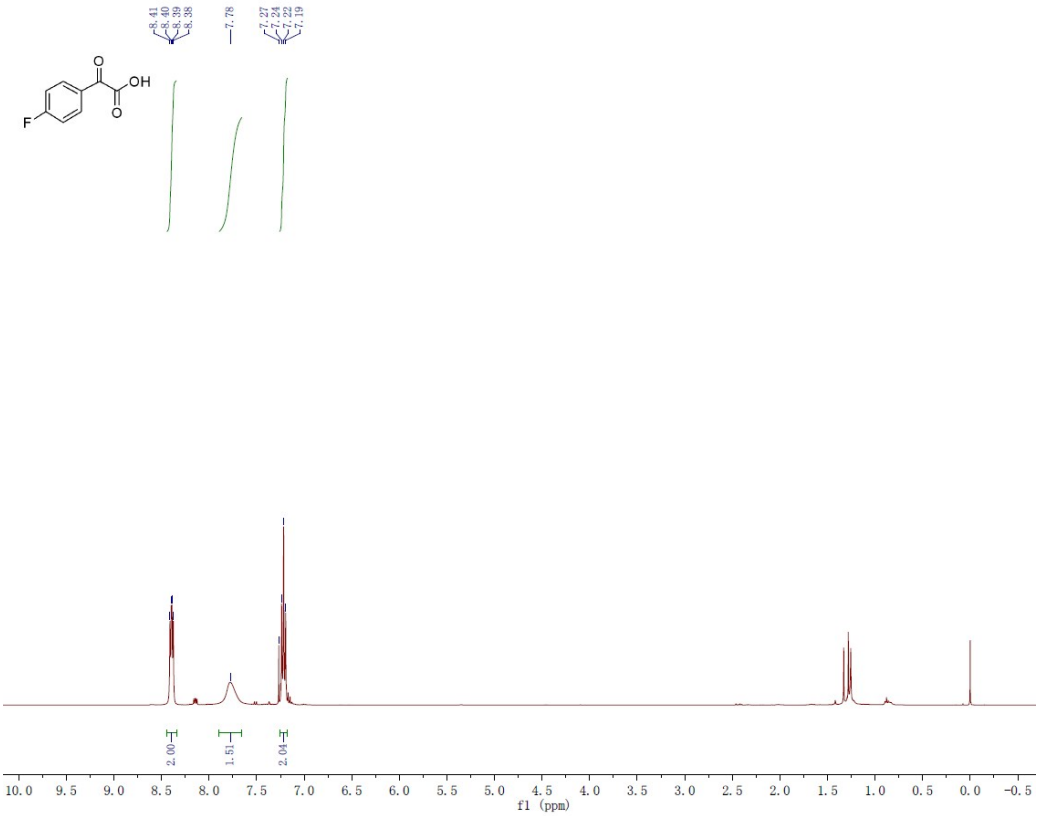




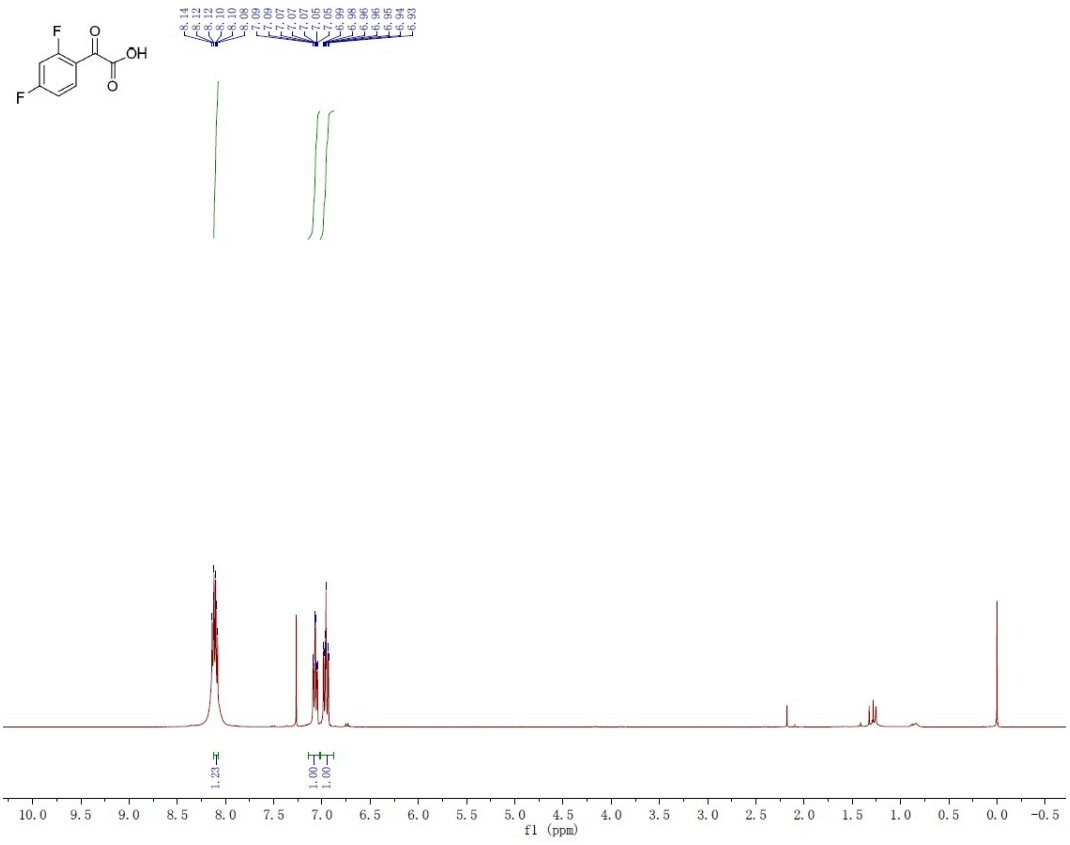
2-(Naphthalen-1-yl)-2-oxoacetic acid (2e)



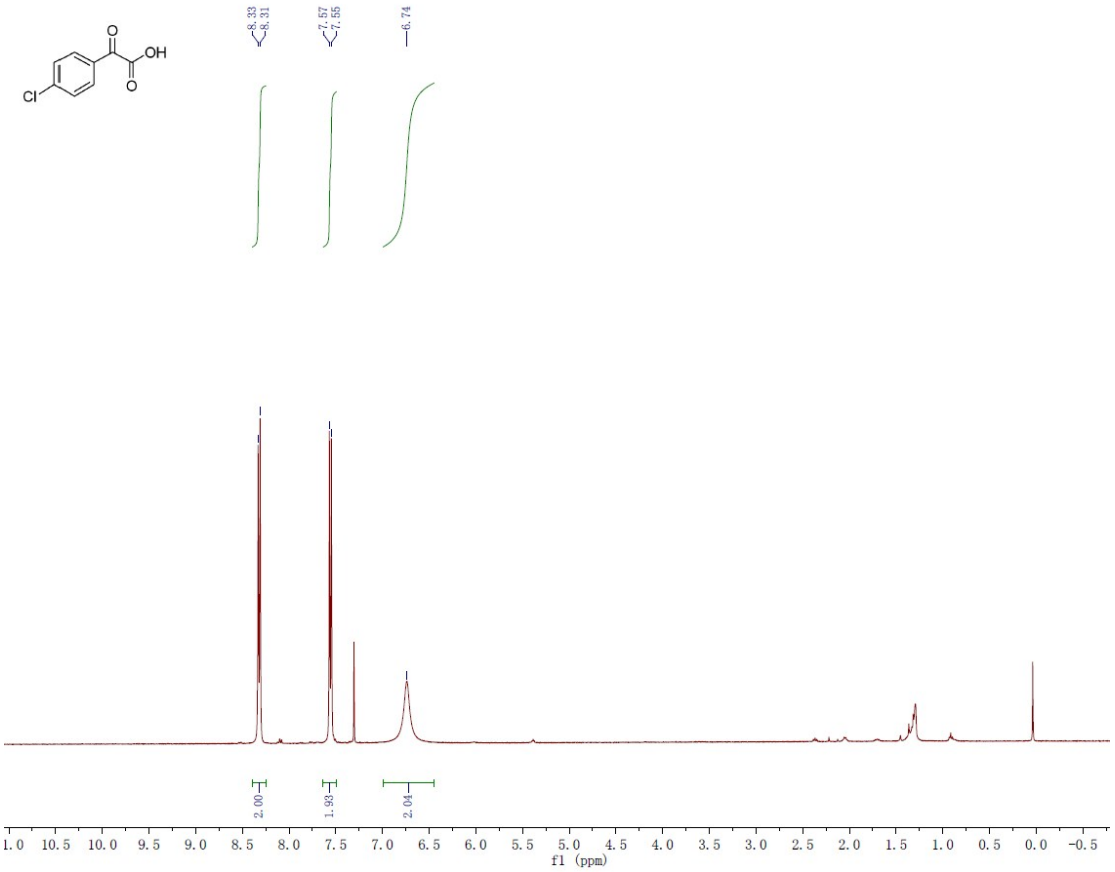
2-(4-Fluorophenyl)-2-oxoacetic acid (2f)



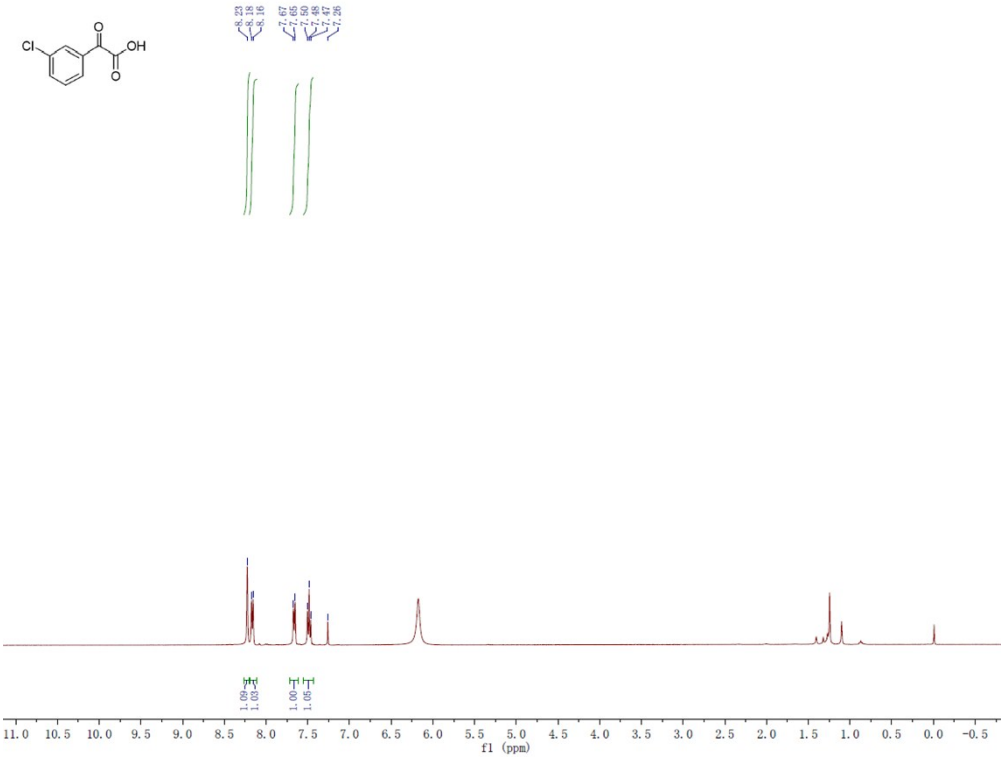
2-(2,4-Difluorophenyl)-2-oxoacetic acid (2g)

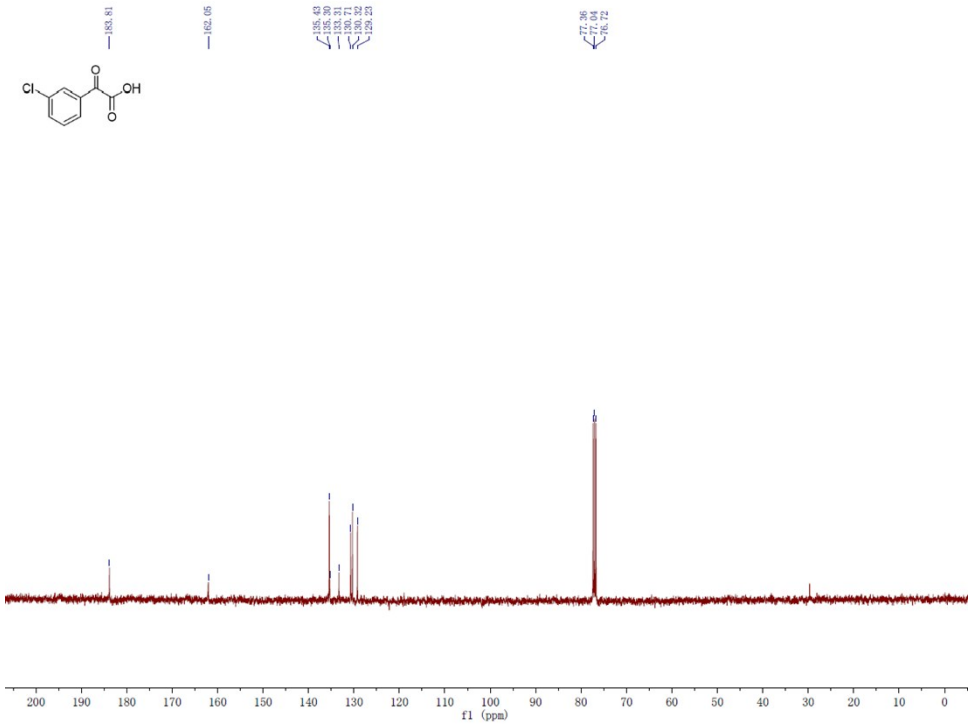


2-(4-Chlorophenyl)-2-oxoacetic acid (2h)

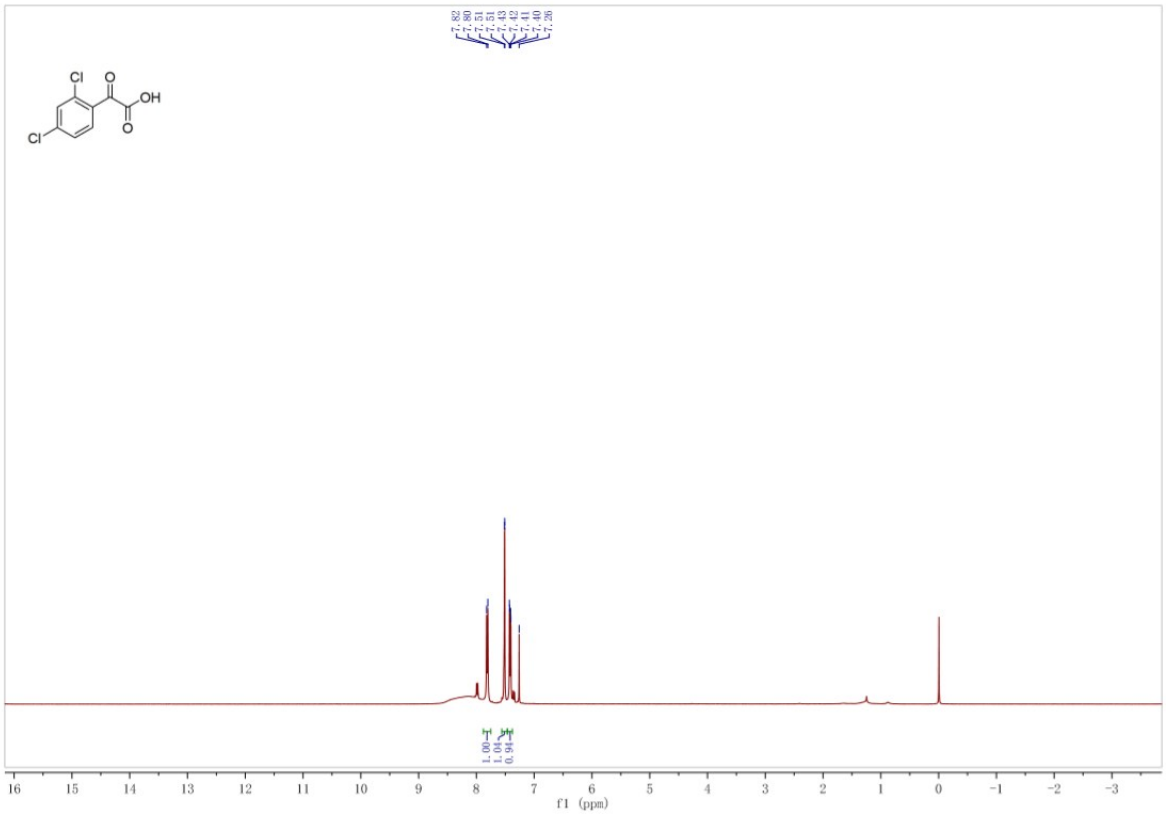


2-(3-Chlorophenyl)-2-oxoacetic acid (2i)

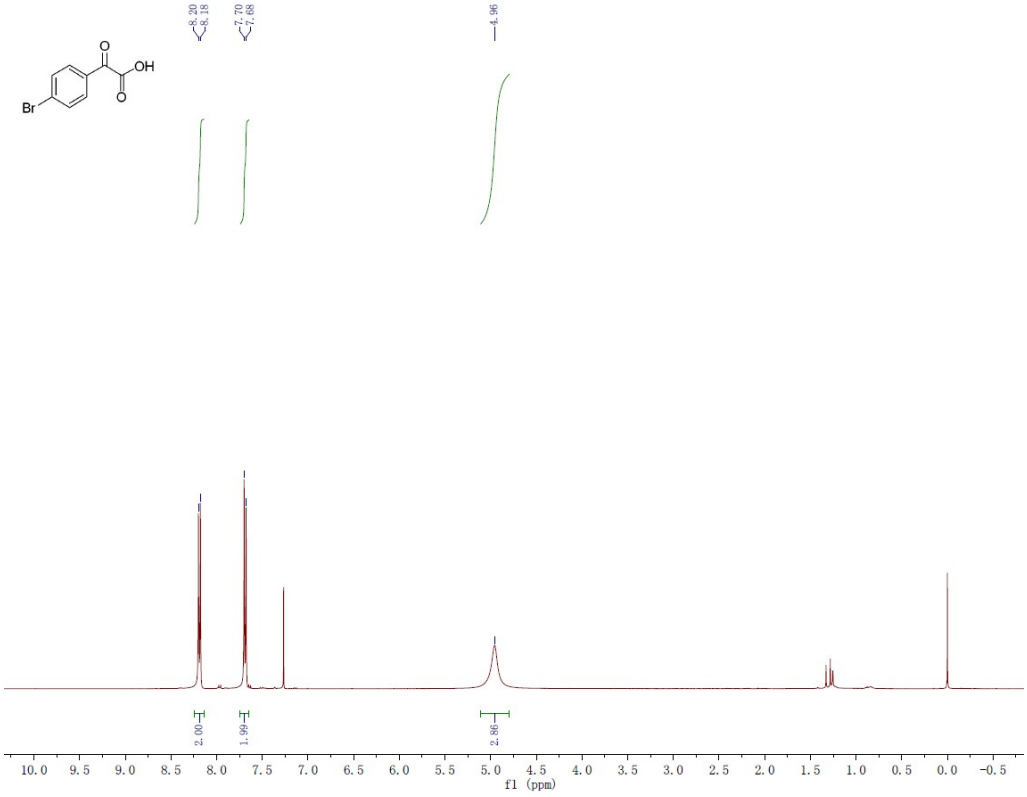


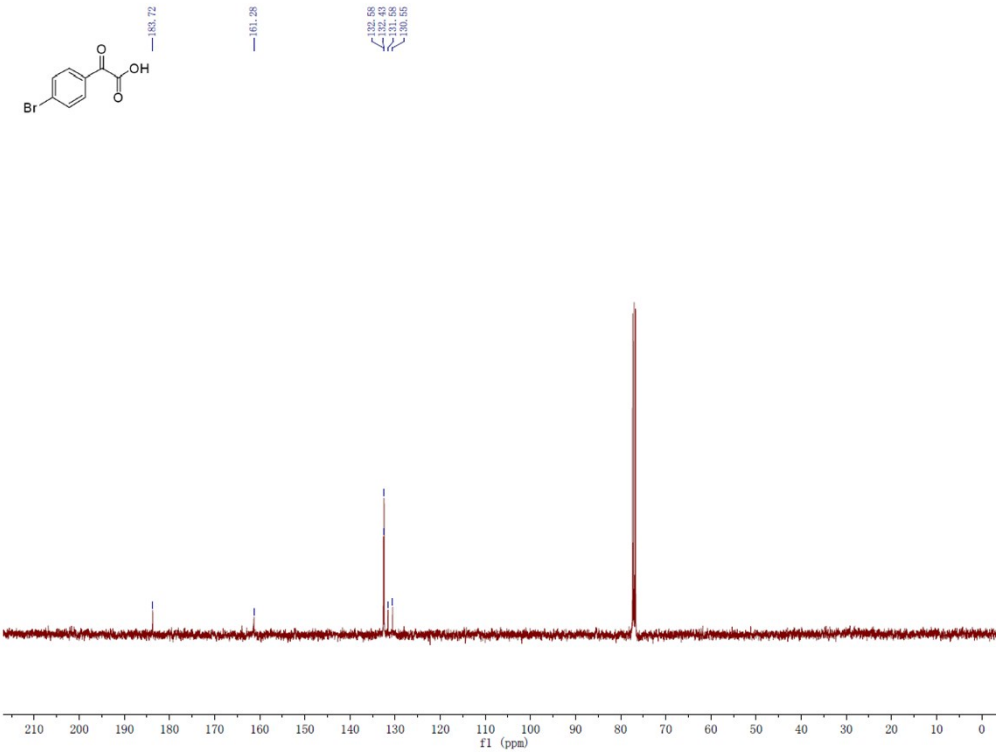


2-(2,4-Dichlorophenyl)-2-oxoacetic acid (2j)

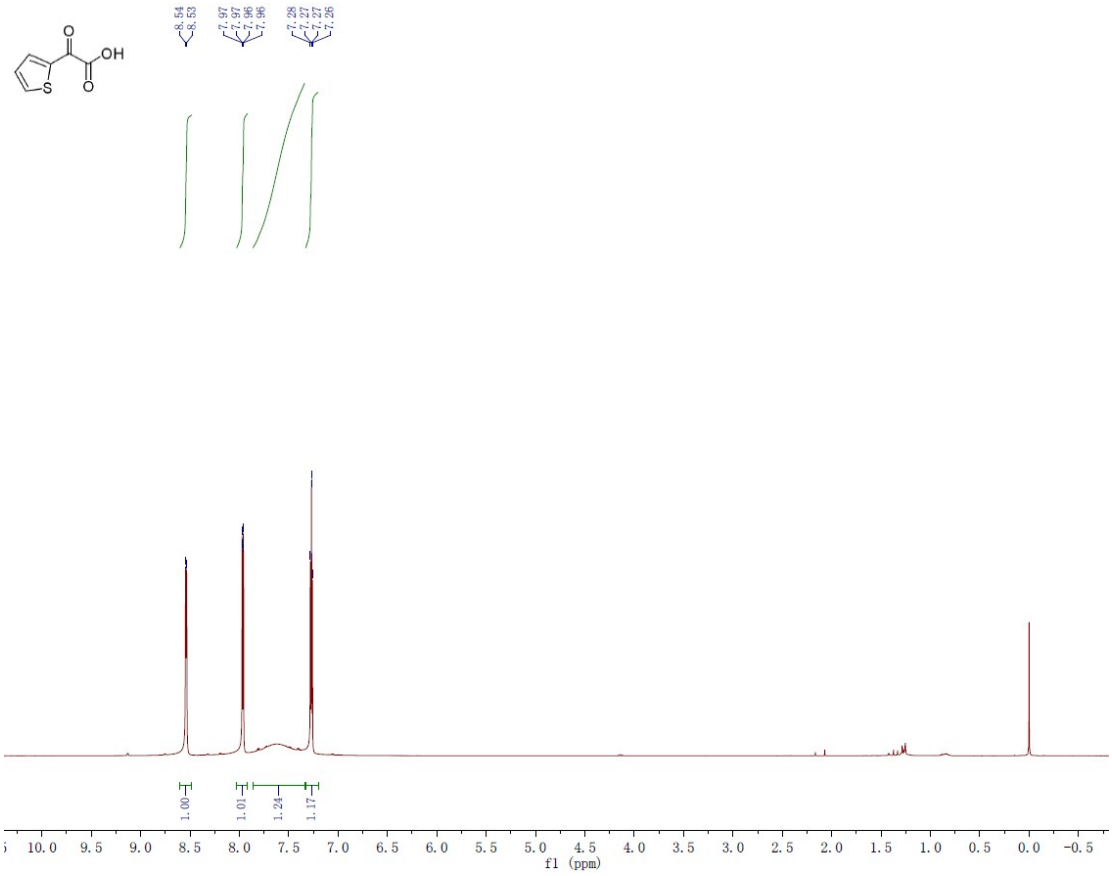


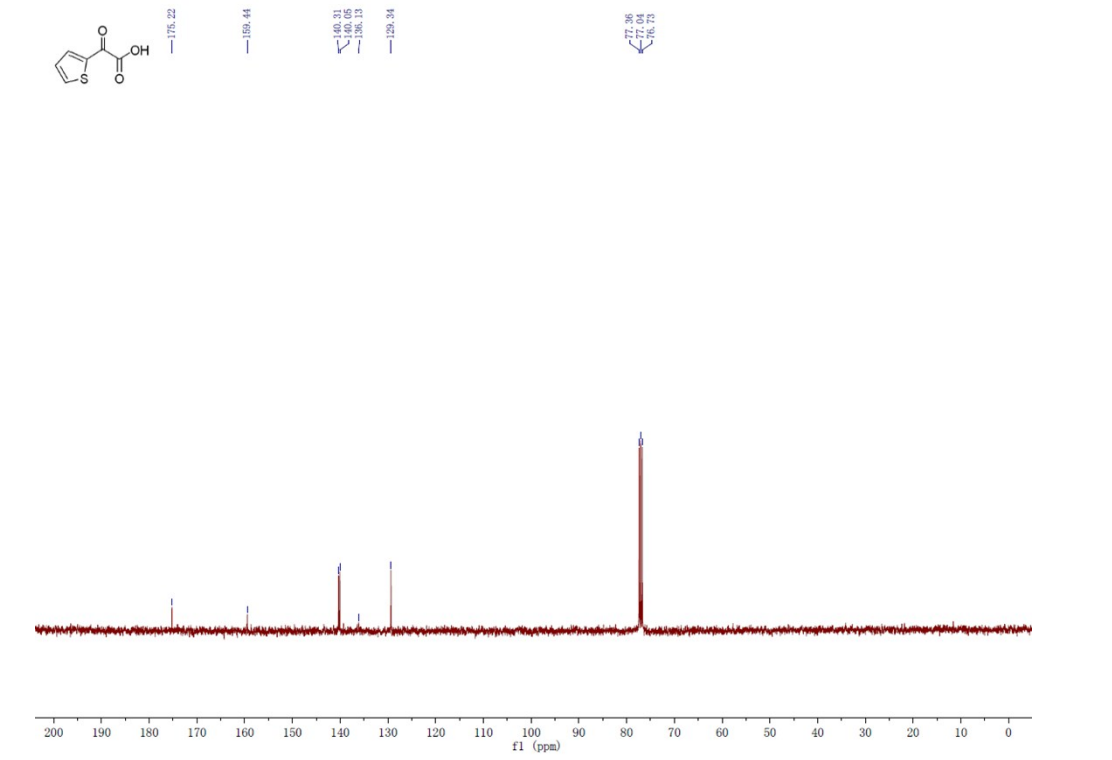
2-(4-Bromophenyl)-2-oxoacetic acid (2k)



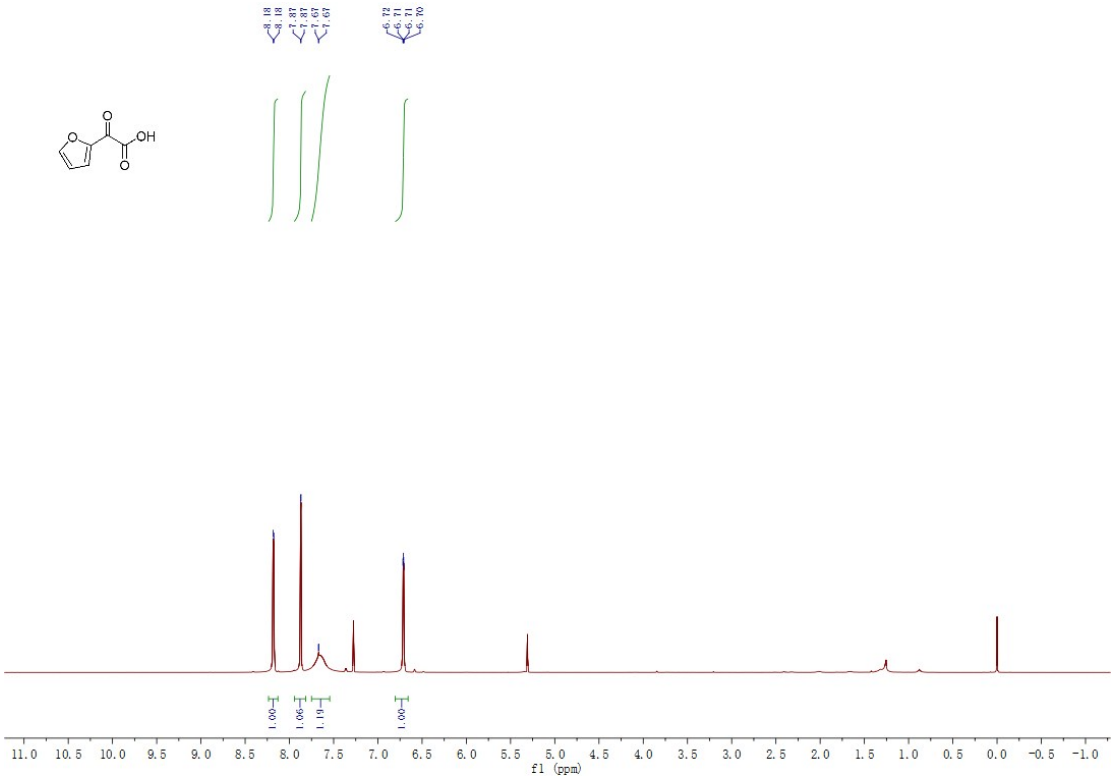


2-Oxo-2-(thiophen-2-yl)acetic acid (2l)

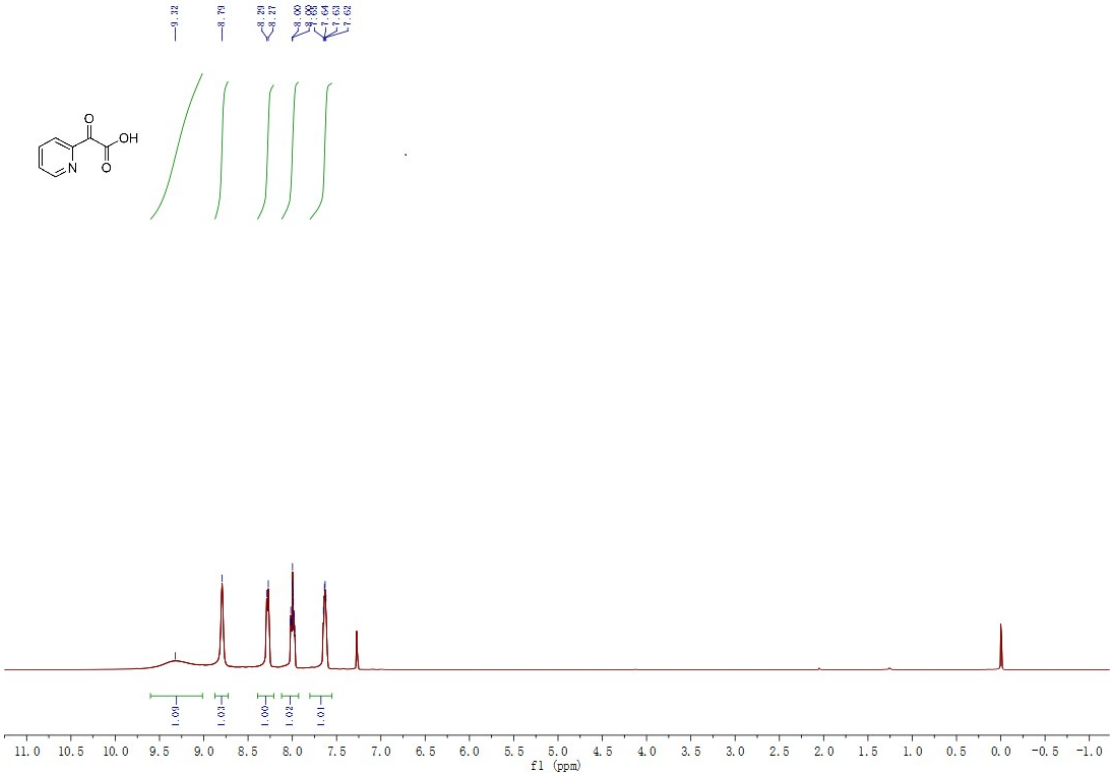




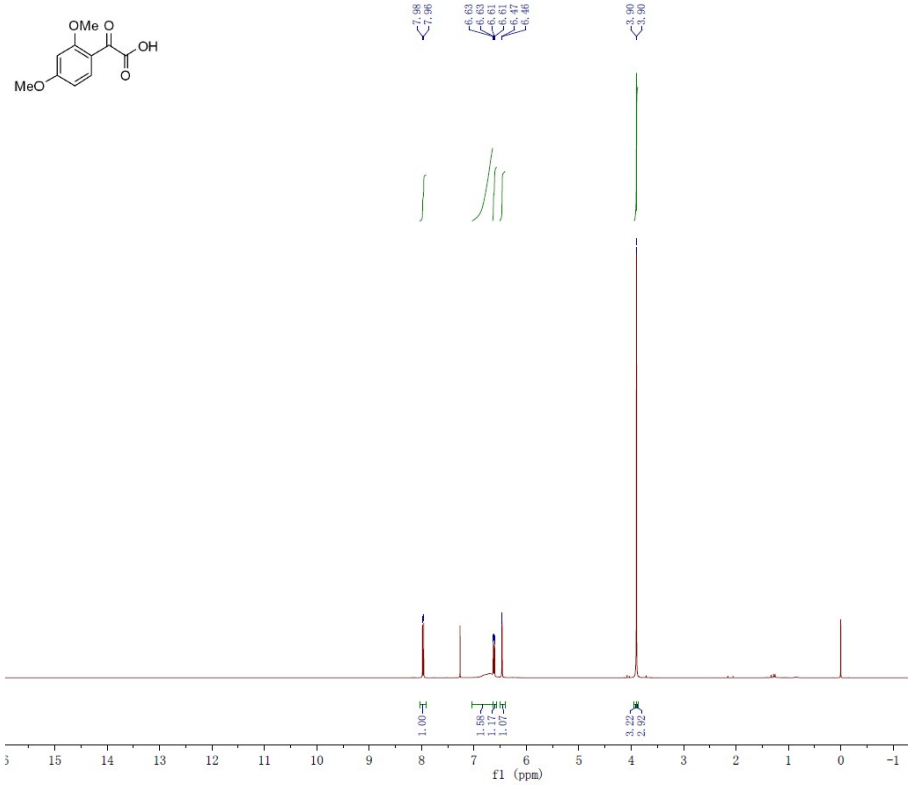
2-(Furan-2-yl)-2-oxoacetic acid (2m)



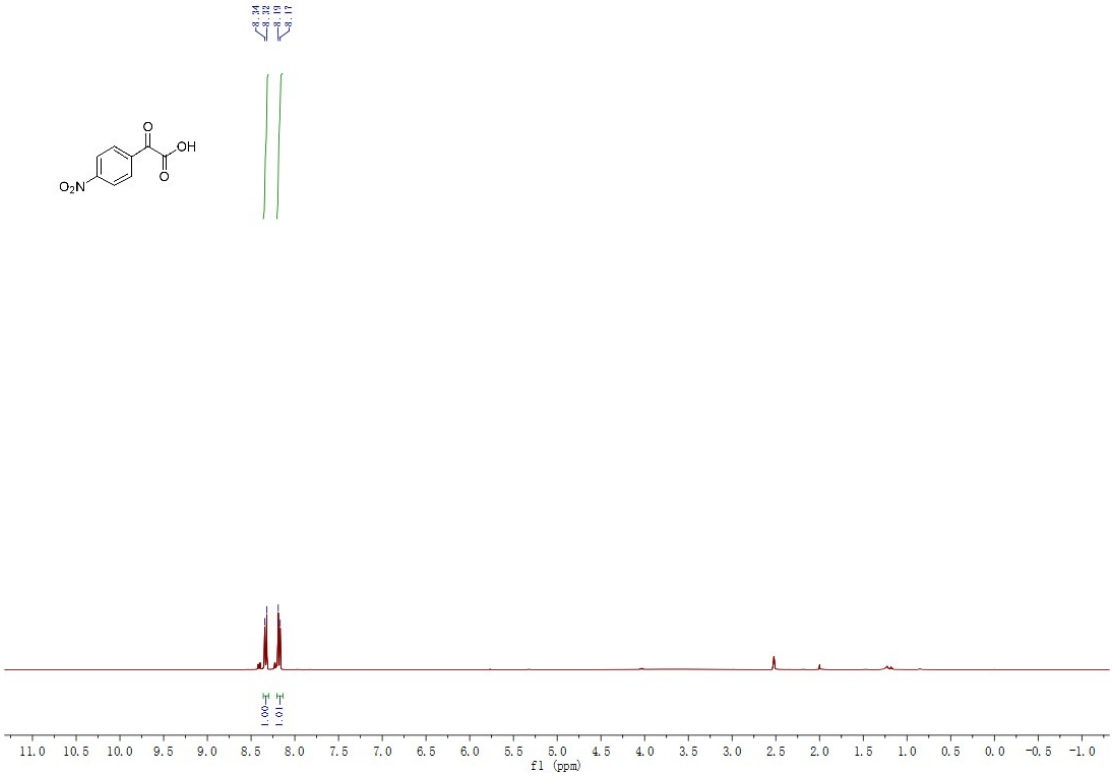
2-Oxo-2-(pyridin-2-yl)acetic acid (2n)



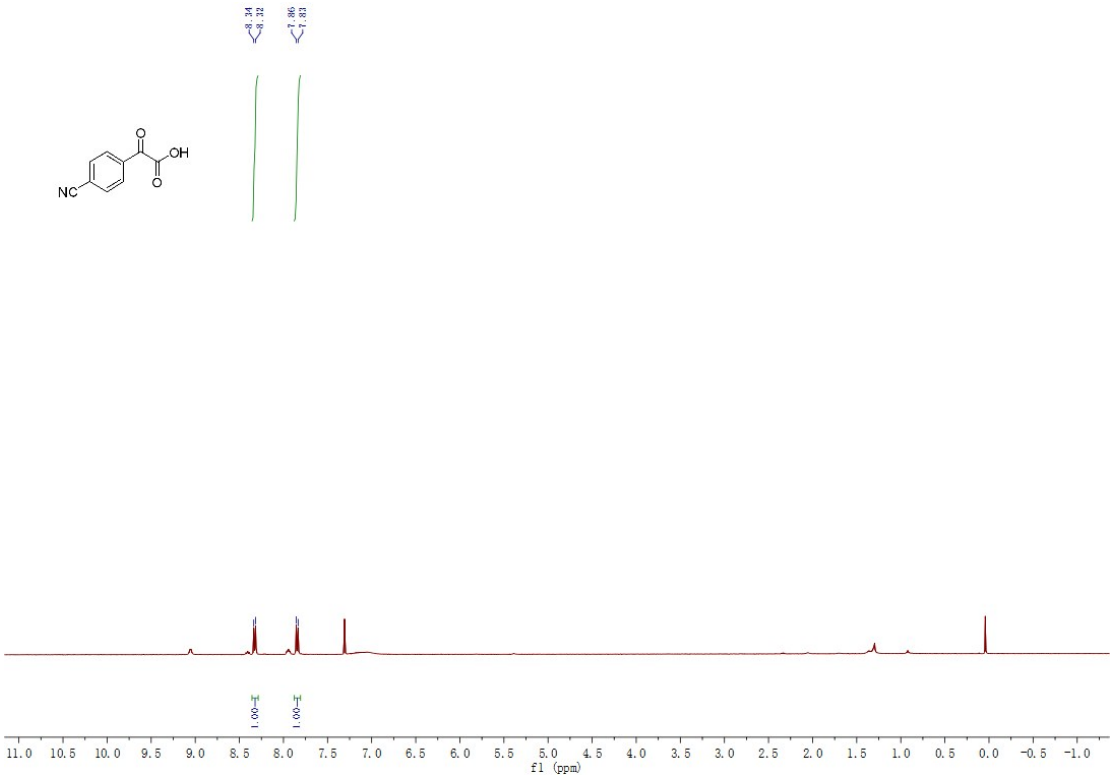
2-(2,4-Dimethoxyphenyl)-2-oxoacetic acid (2o)



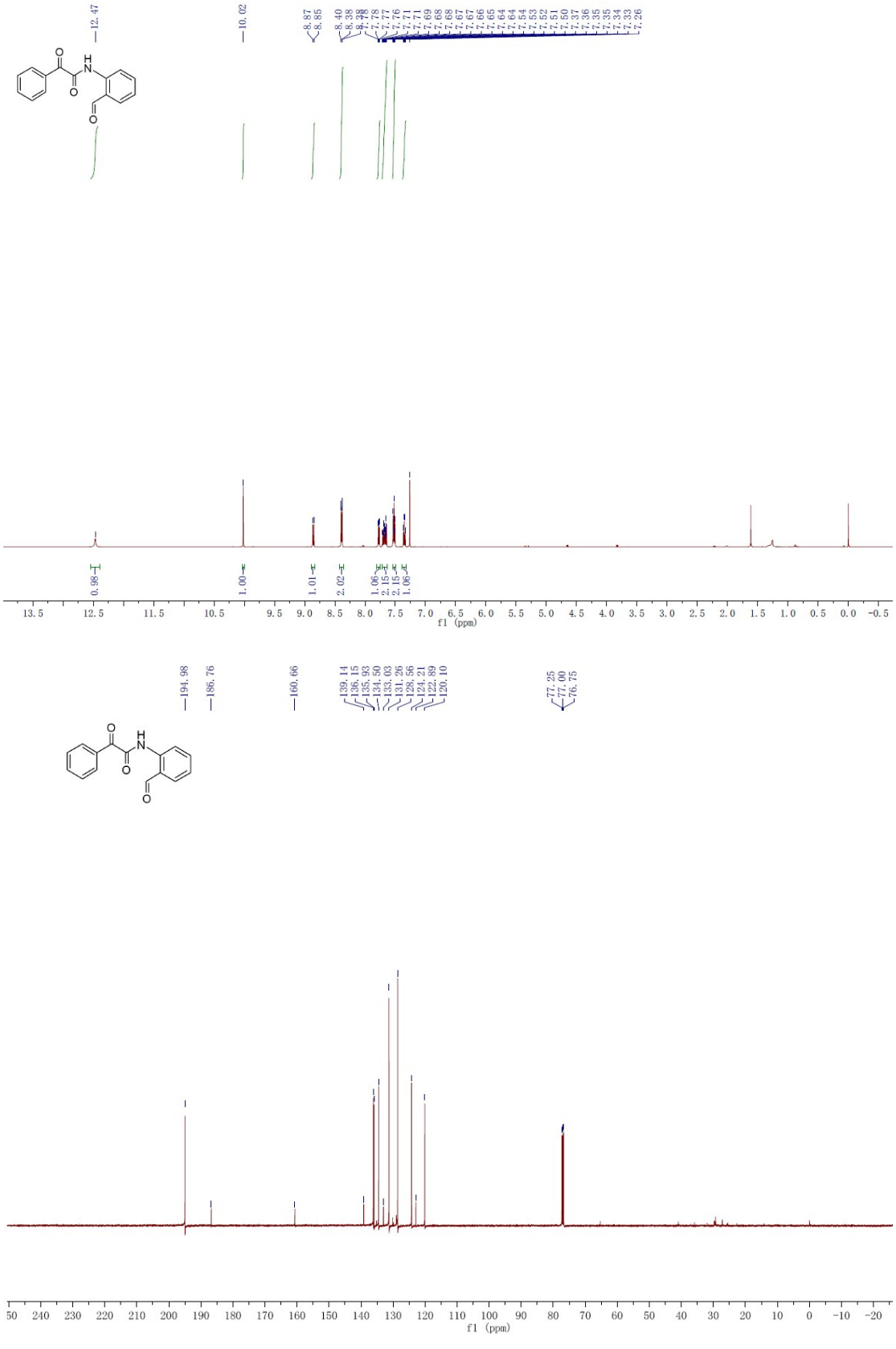
2-(4-Nitrophenyl)-2-oxoacetic acid (2p)



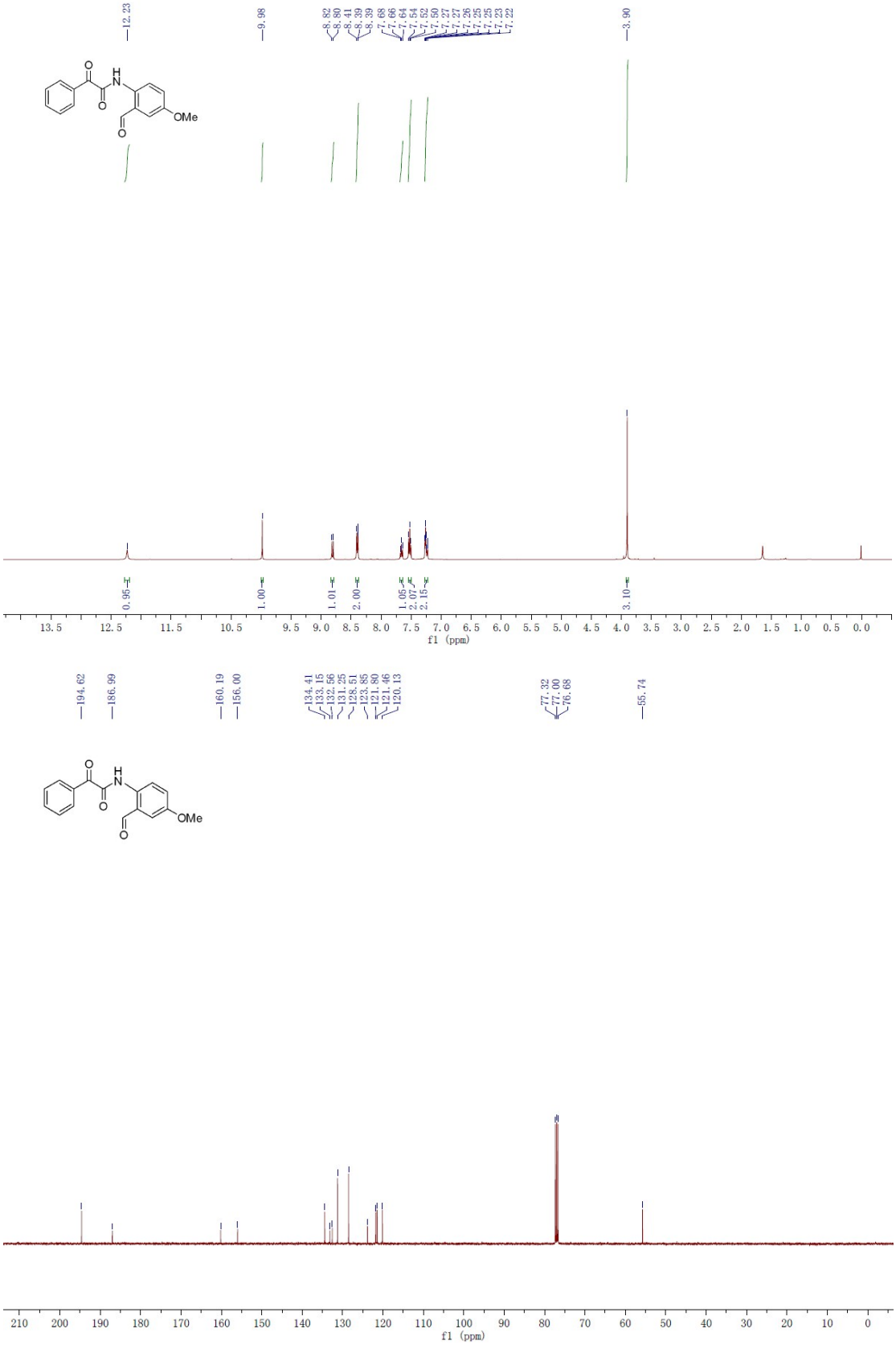
2-(4-Cyanophenyl)-2-oxoacetic acid (2q)



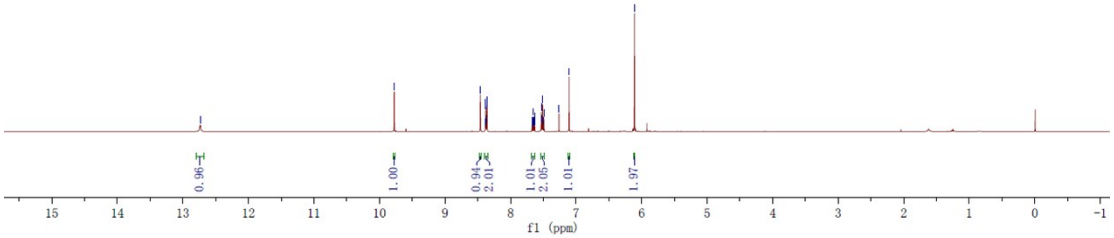
N-(2-Formylphenyl)-2-oxo-2-phenylacetamide (3a)

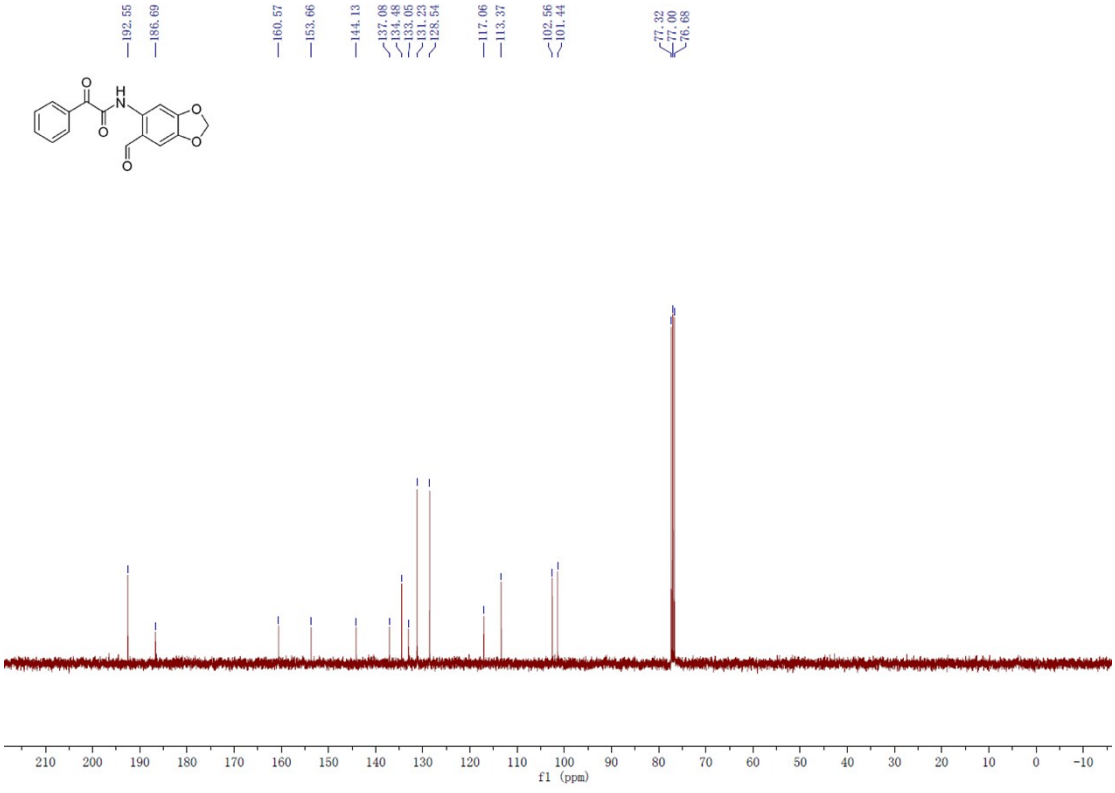


N-(2-Formyl-4-methoxyphenyl)-2-oxo-2-phenylacetamide (3b)

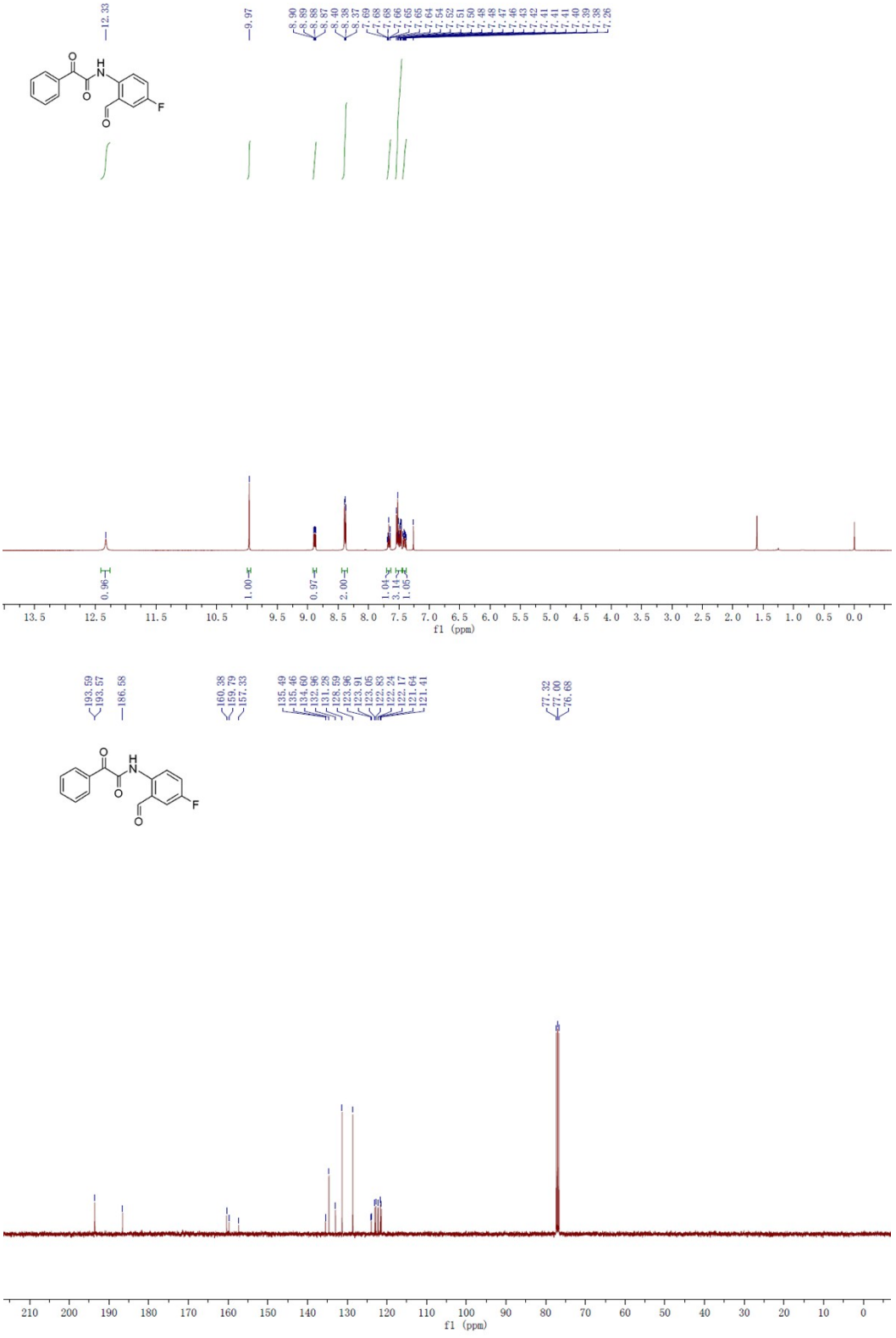


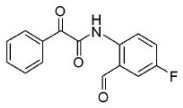
N-(6-Formylbenzo[d][1,3]dioxol-5-yl)-2-oxo-2-phenylacetamide (3c)





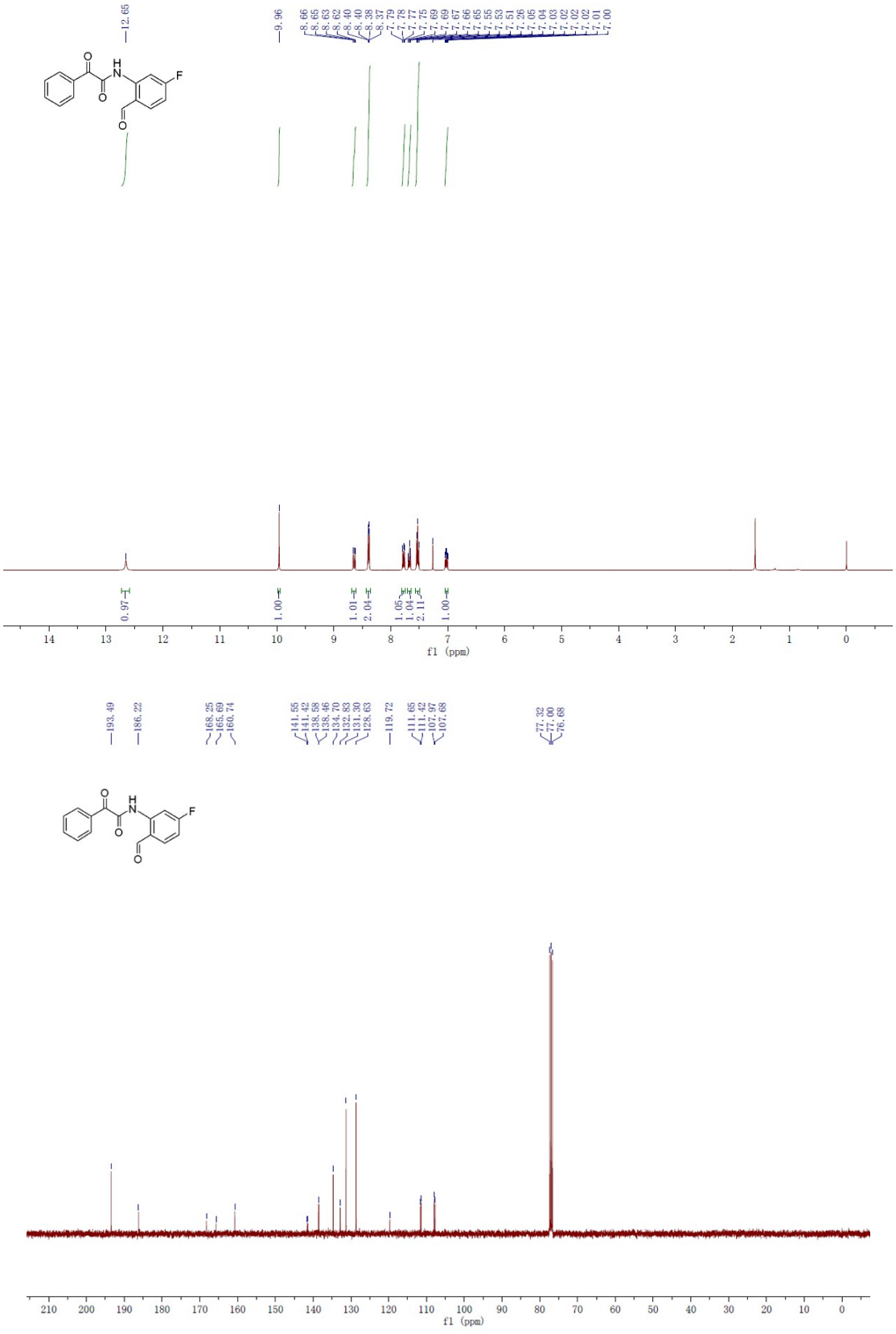
N-(4-Fluoro-2-formylphenyl)-2-oxo-2-phenylacetamide (3d)

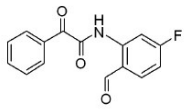



O
H
N
O
F
O

-116.62
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

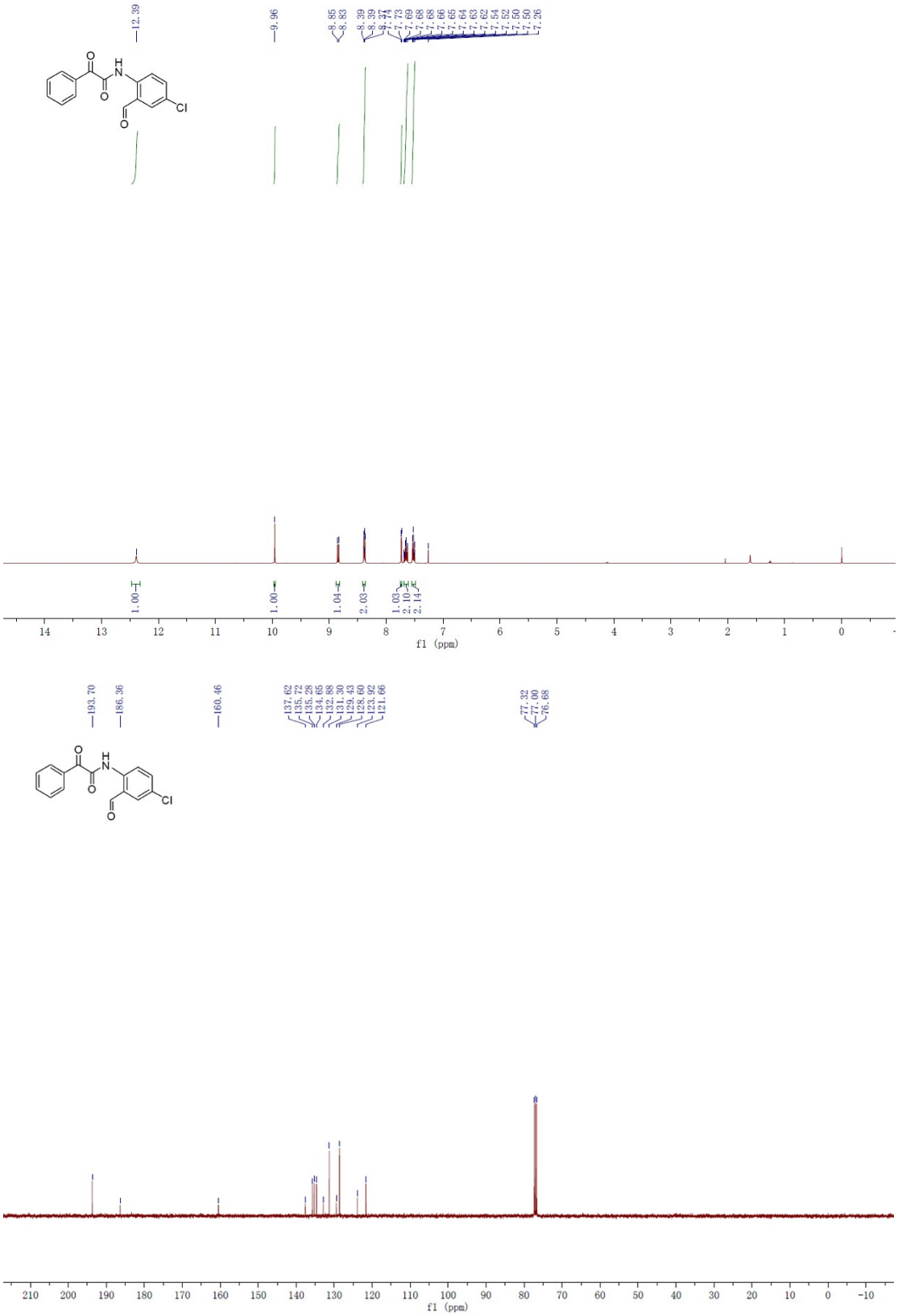
N-(5-Fluoro-2-formylphenyl)-2-oxo-2-phenylacetamide (3e)



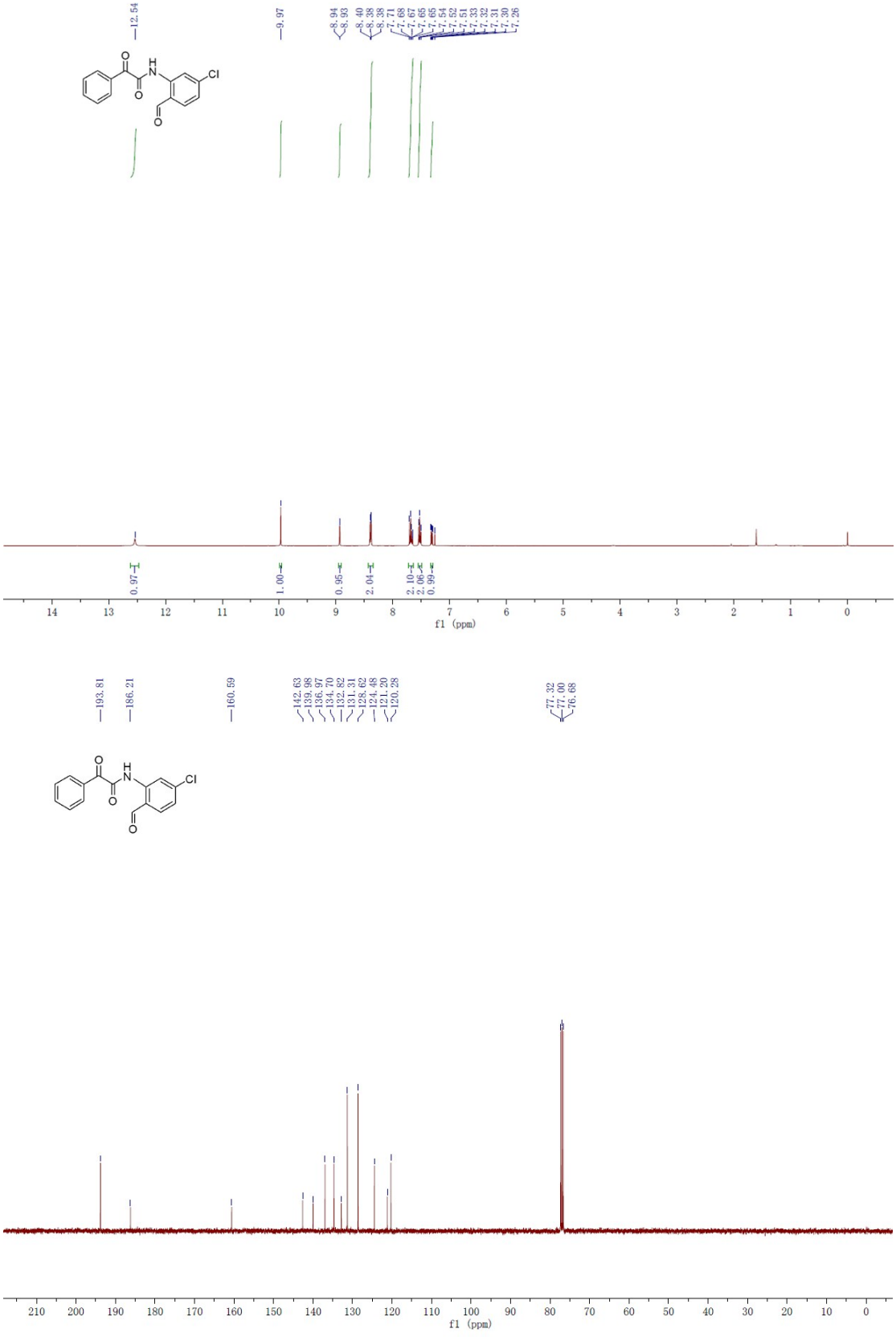

O
H
N
F
O
O

97.48
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

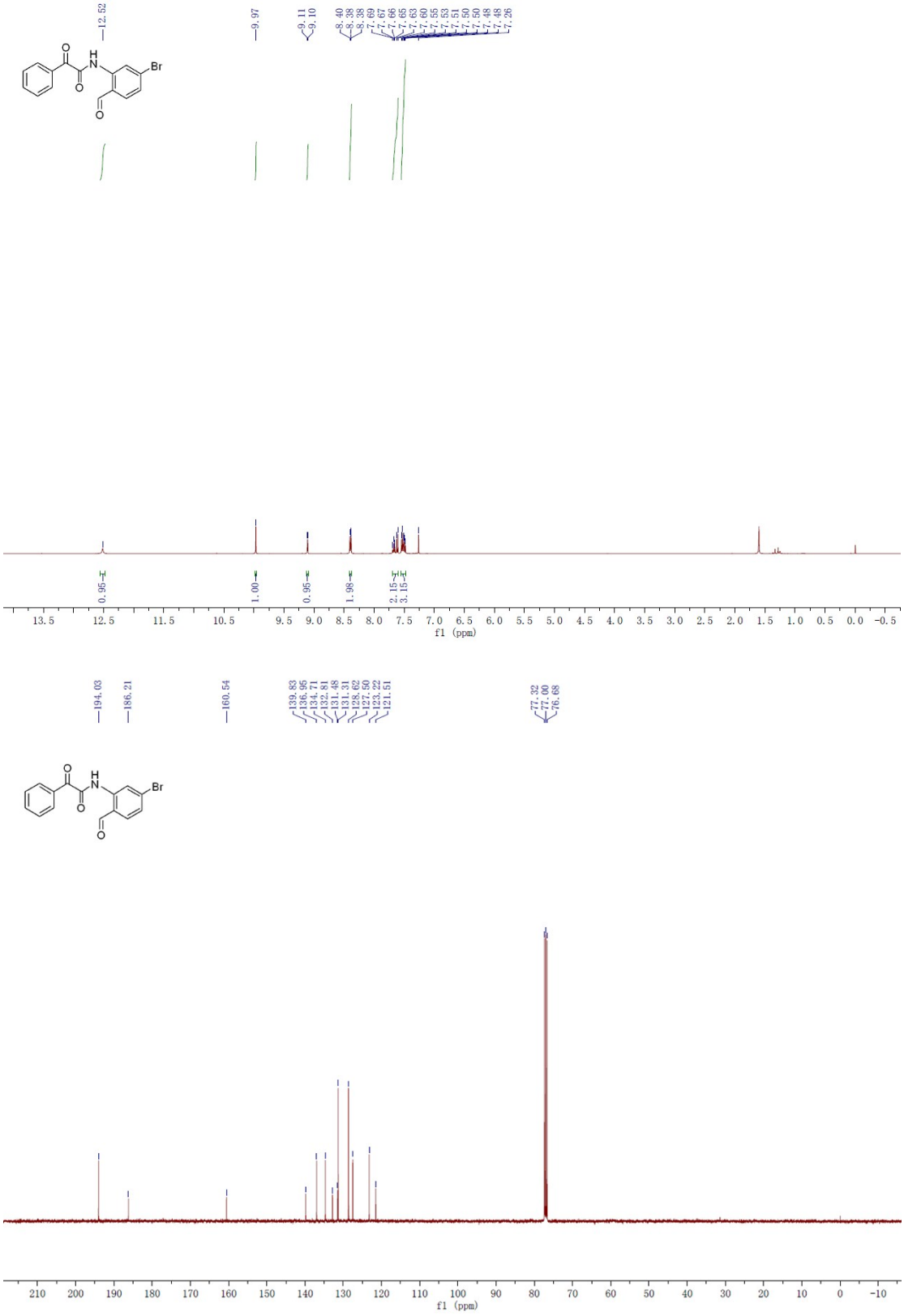
N-(4-Chloro-2-formylphenyl)-2-oxo-2-phenylacetamide (3f)



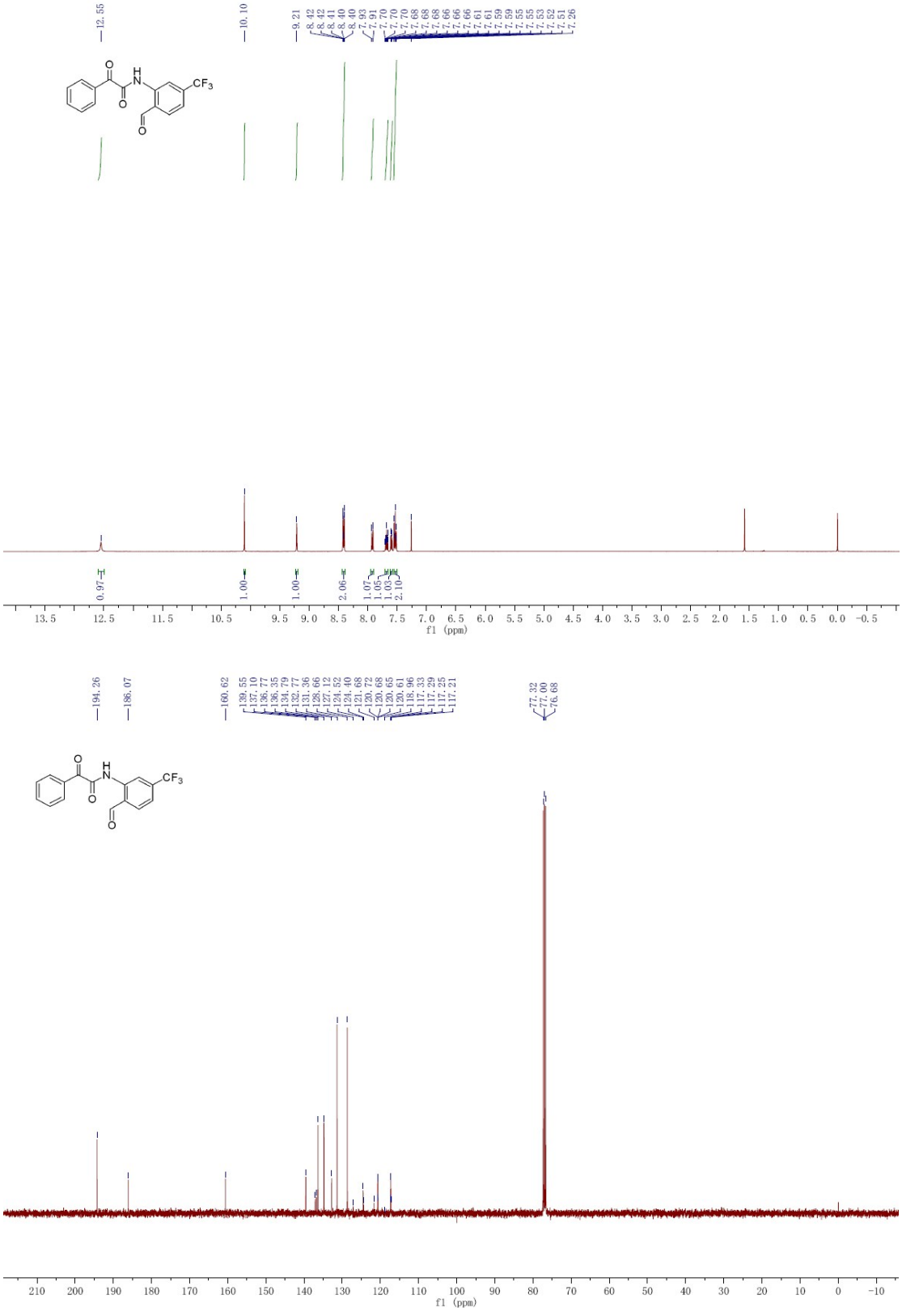
N-(5-Chloro-2-formylphenyl)-2-oxo-2-phenylacetamide (3g)

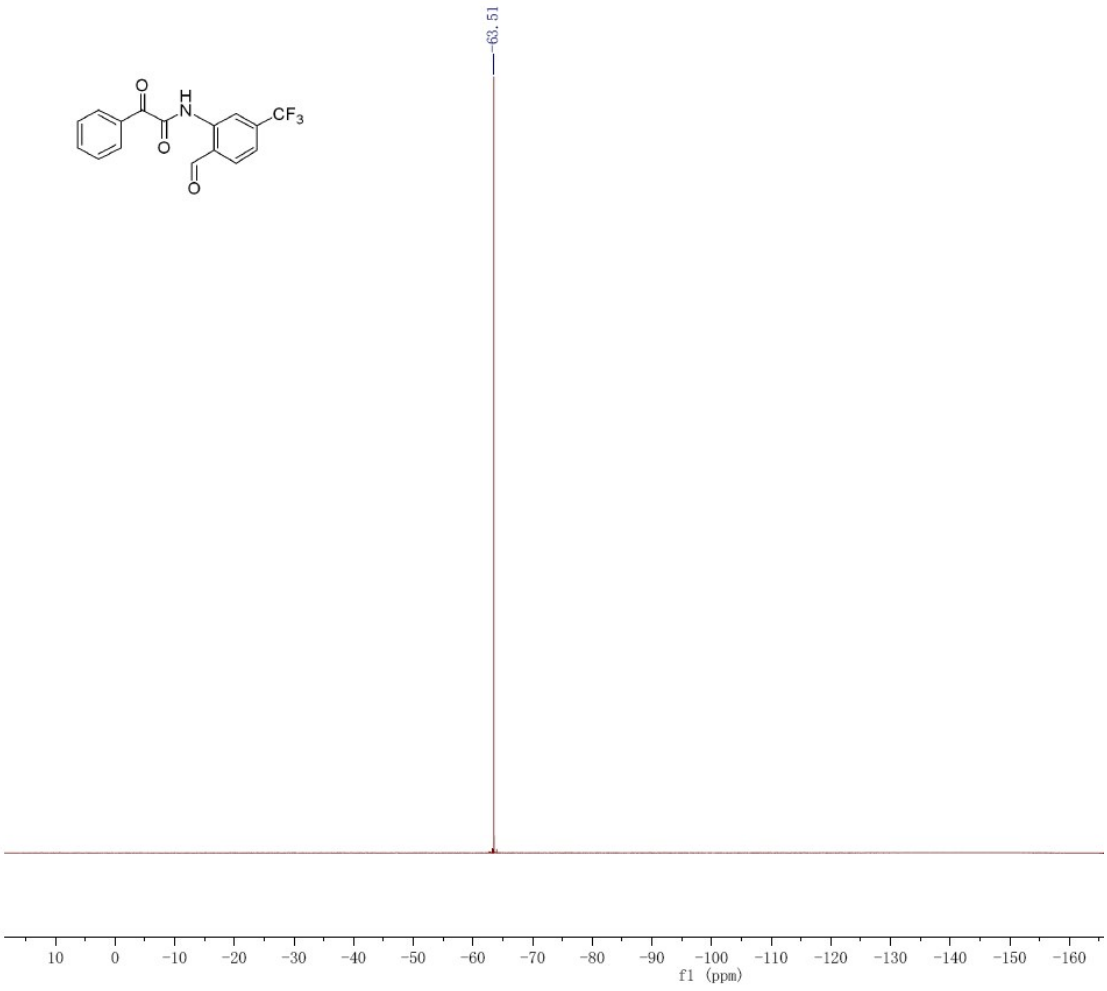


N-(5-Bromo-2-formylphenyl)-2-oxo-2-phenylacetamide (3h)

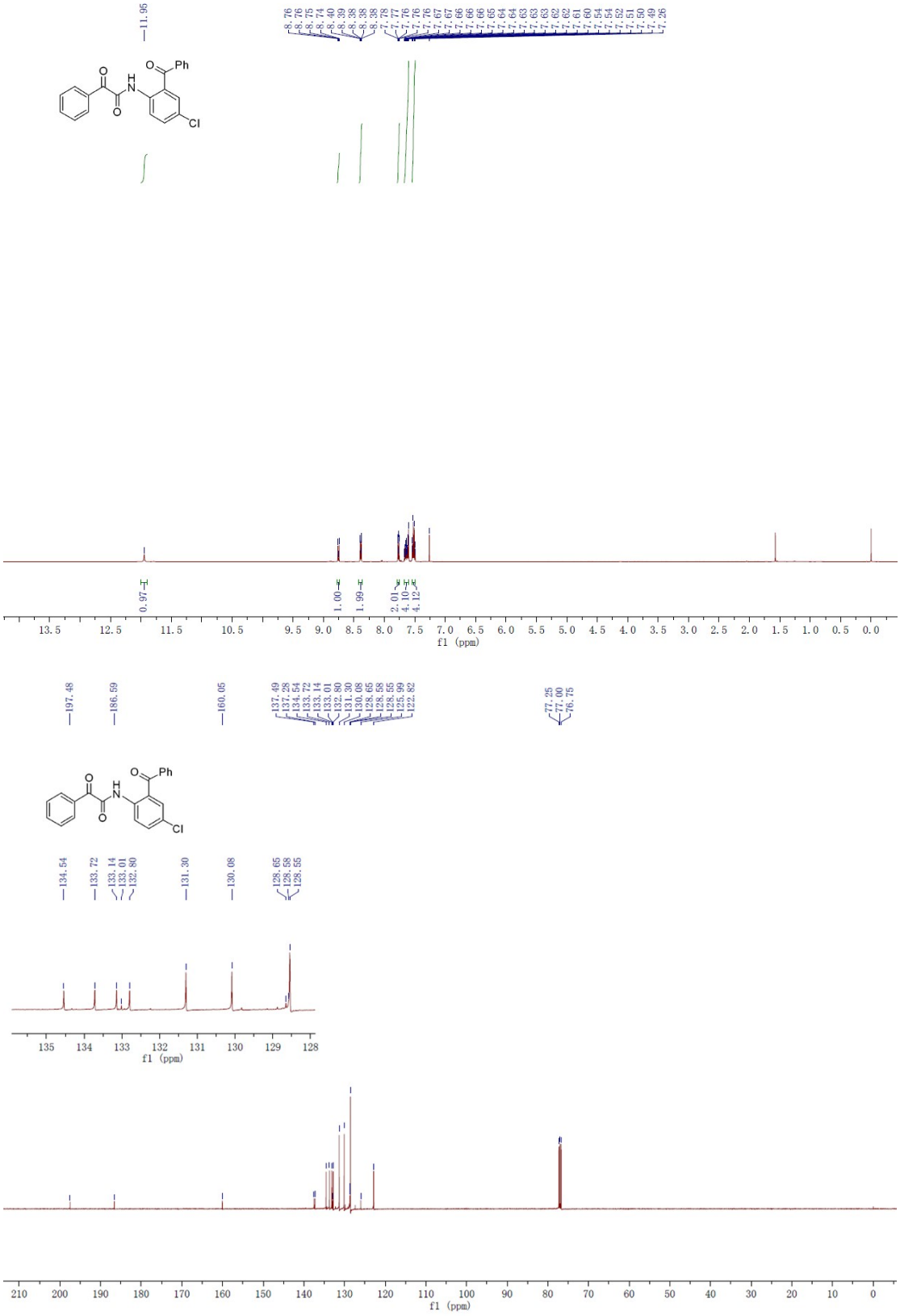


N-(5-Trifluoromethyl-2-formylphenyl)-2-oxo-2-phenylacetamide (3i)

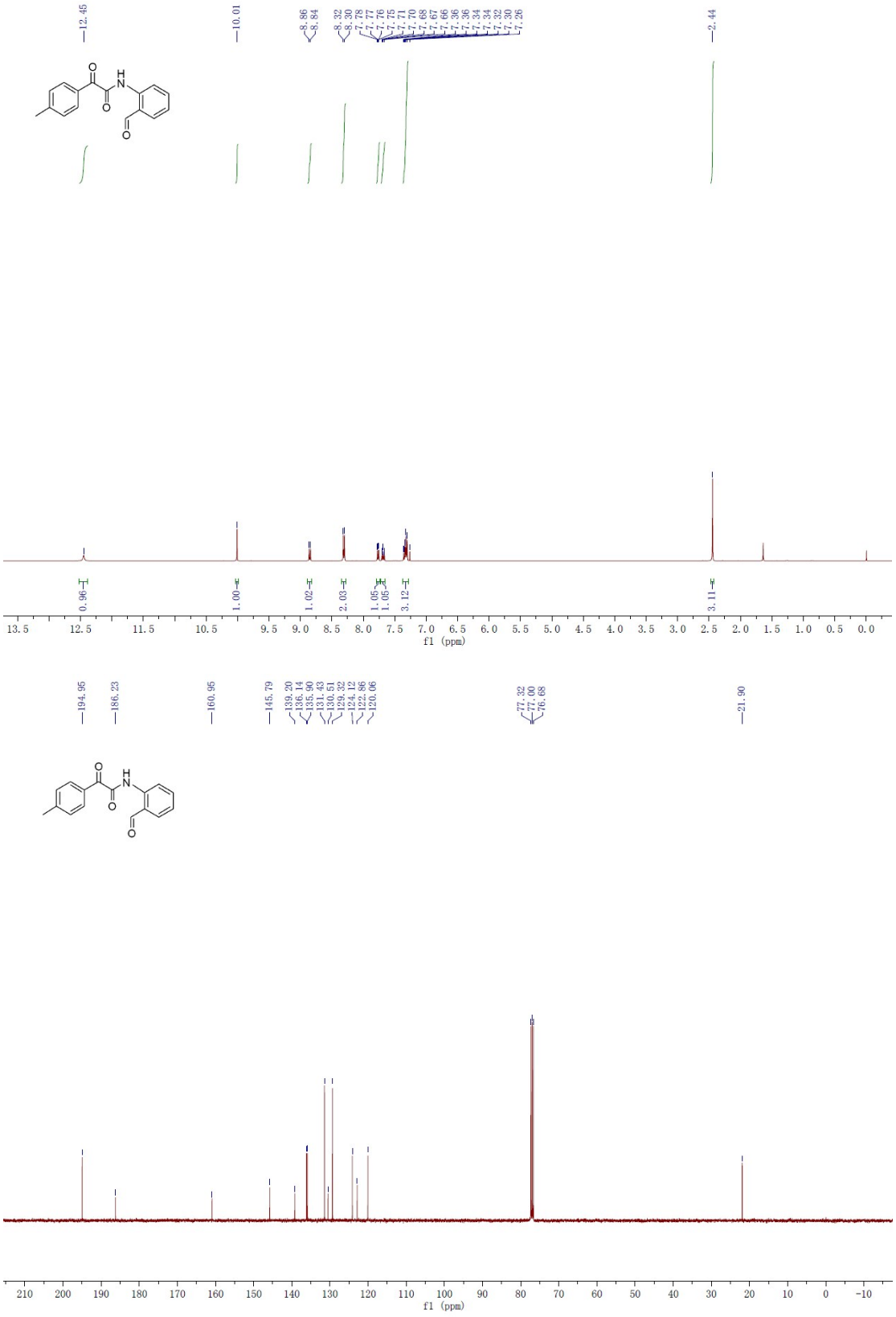



-63.51
O
H
N
O
O
CF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

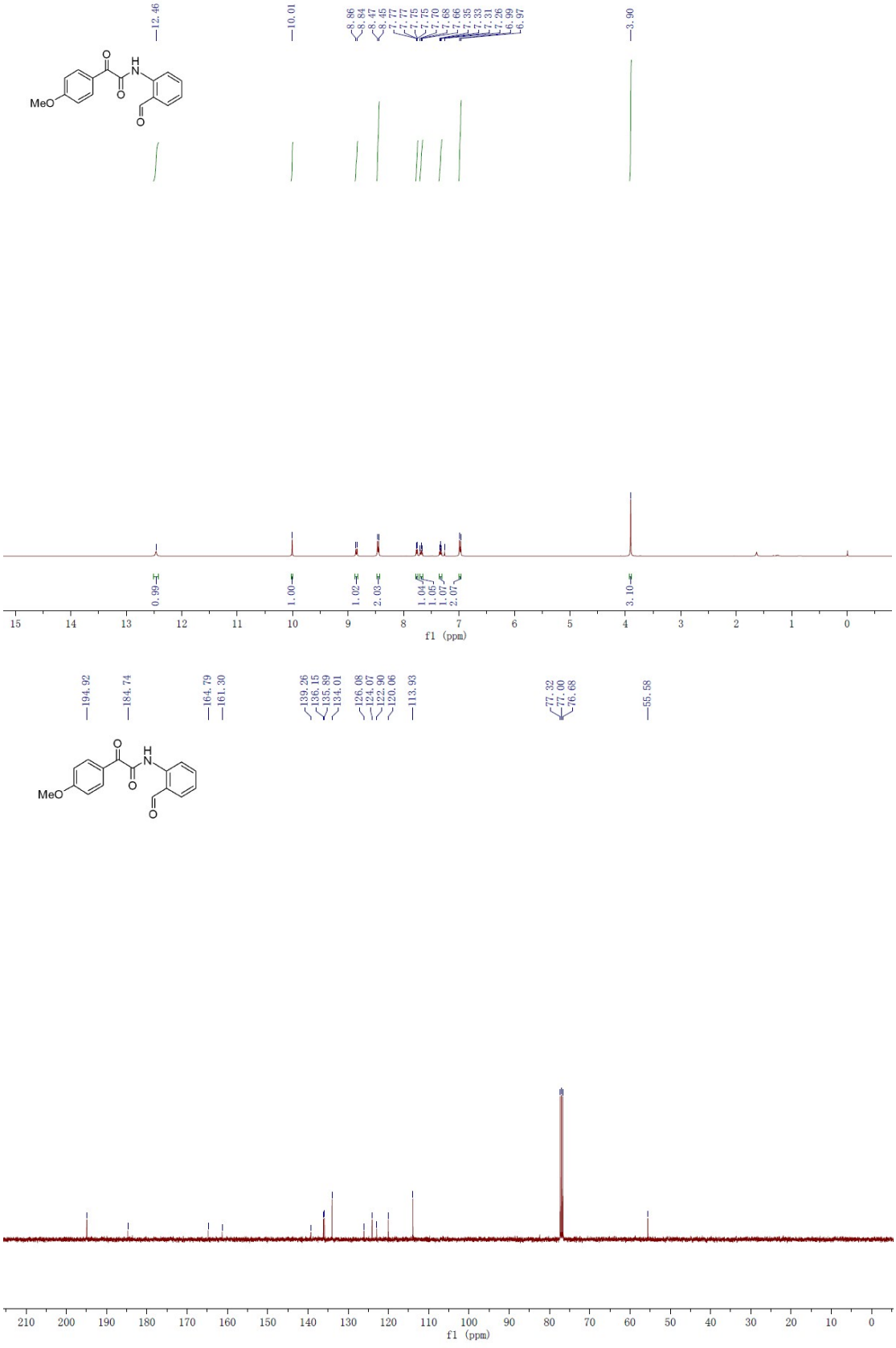
N-(2-Benzoyl-4-chlorophenyl)-2-oxo-2-phenylacetamide (3j)



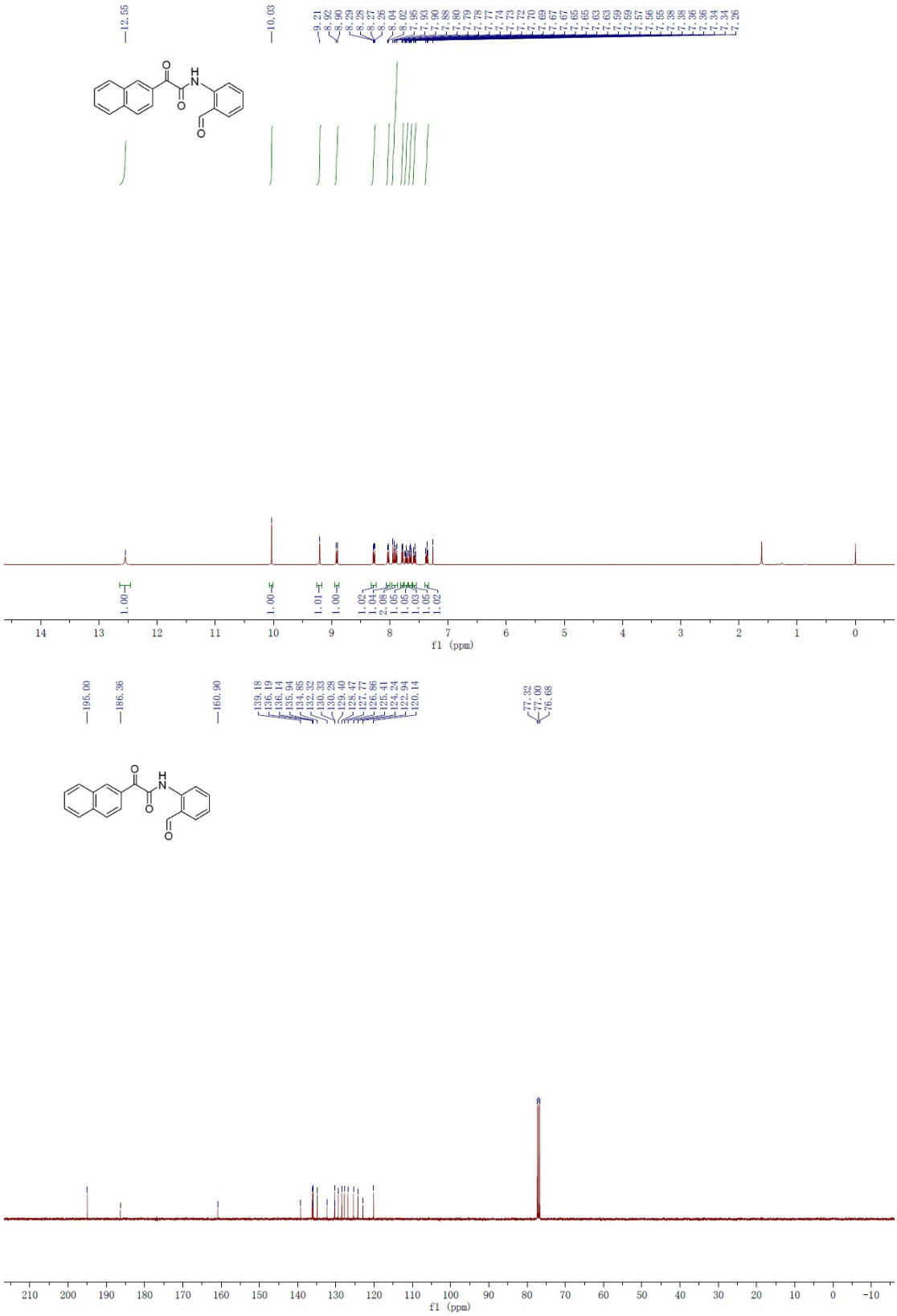
N-(2-Formylphenyl)-2-oxo-2-p-tolylacetamide (3k)



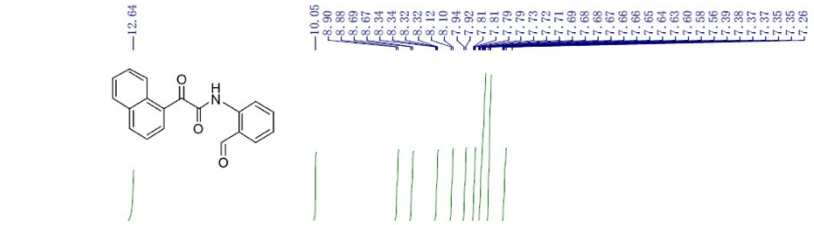
N-(2-Formylphenyl)-2-(4-methoxyphenyl)-2-oxoacetamide (3l)

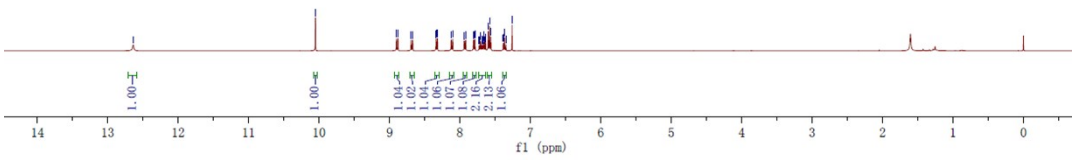


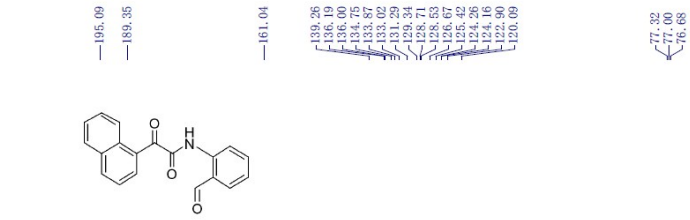
N-(2-Formylphenyl)-2-(naphthalen-2-yl)-2-oxoacetamide (3m)

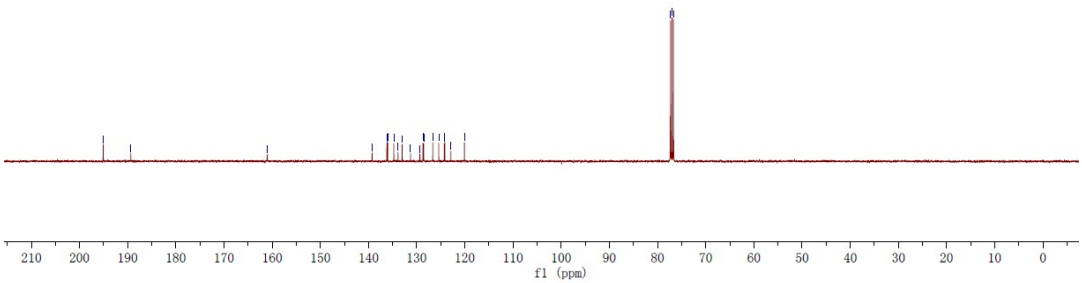


N-(2-Formylphenyl)-2-(naphthalen-1-yl)-2-oxoacetamide (3n)

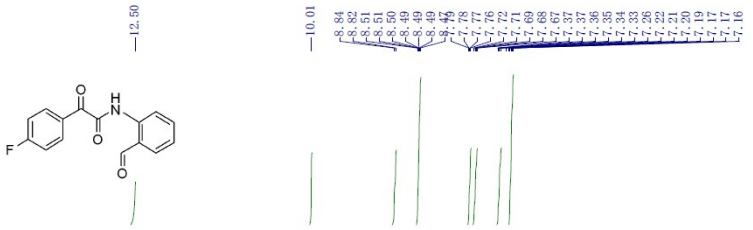


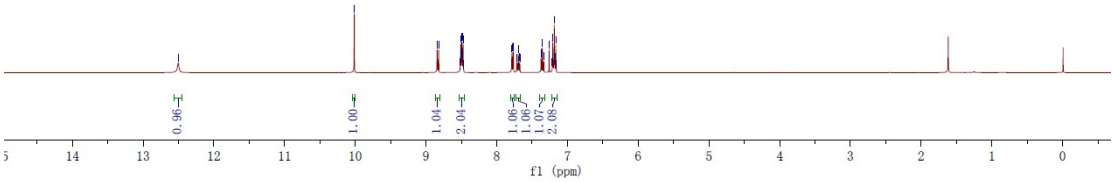


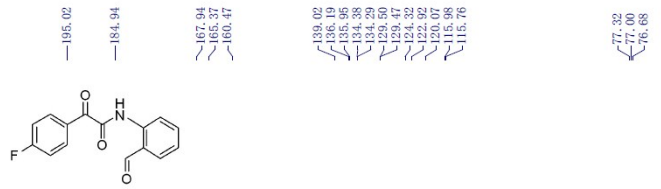


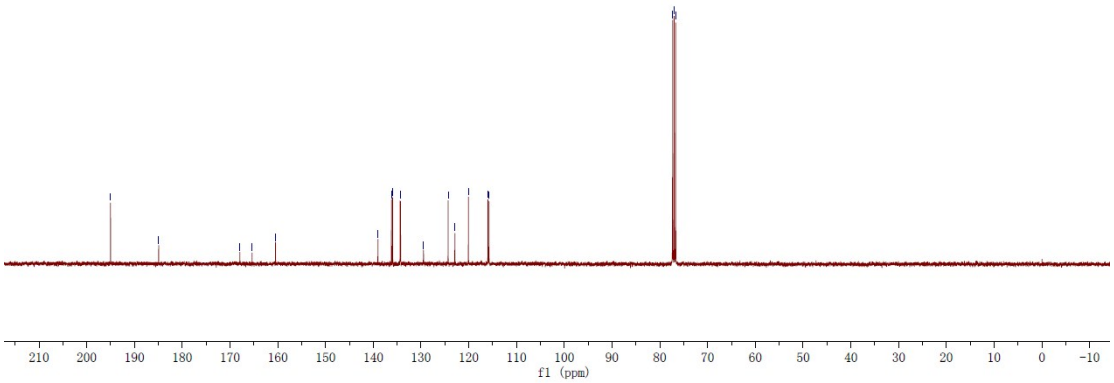


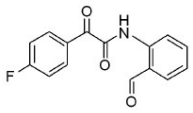
2-(4-Fluorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3o)





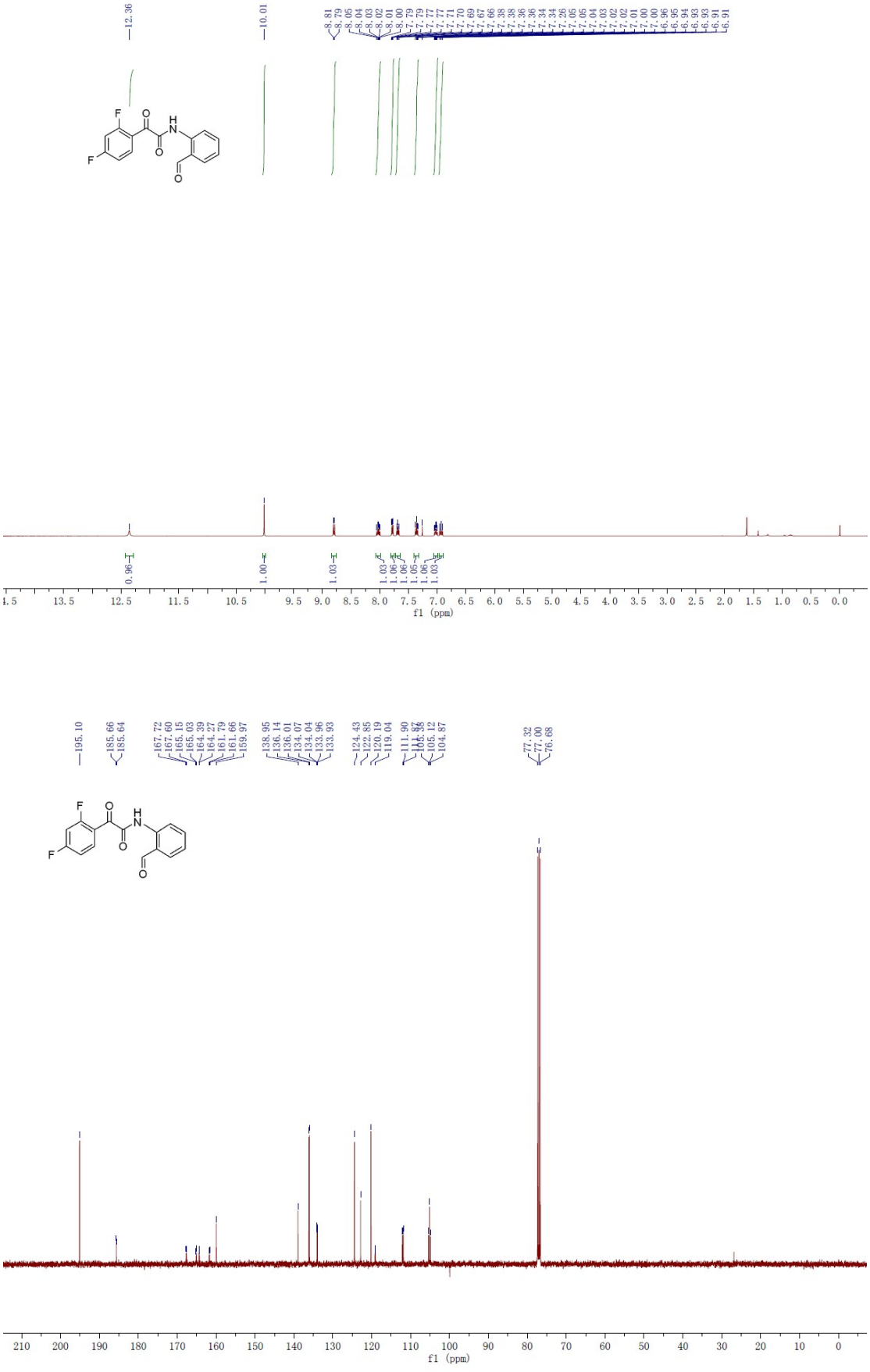


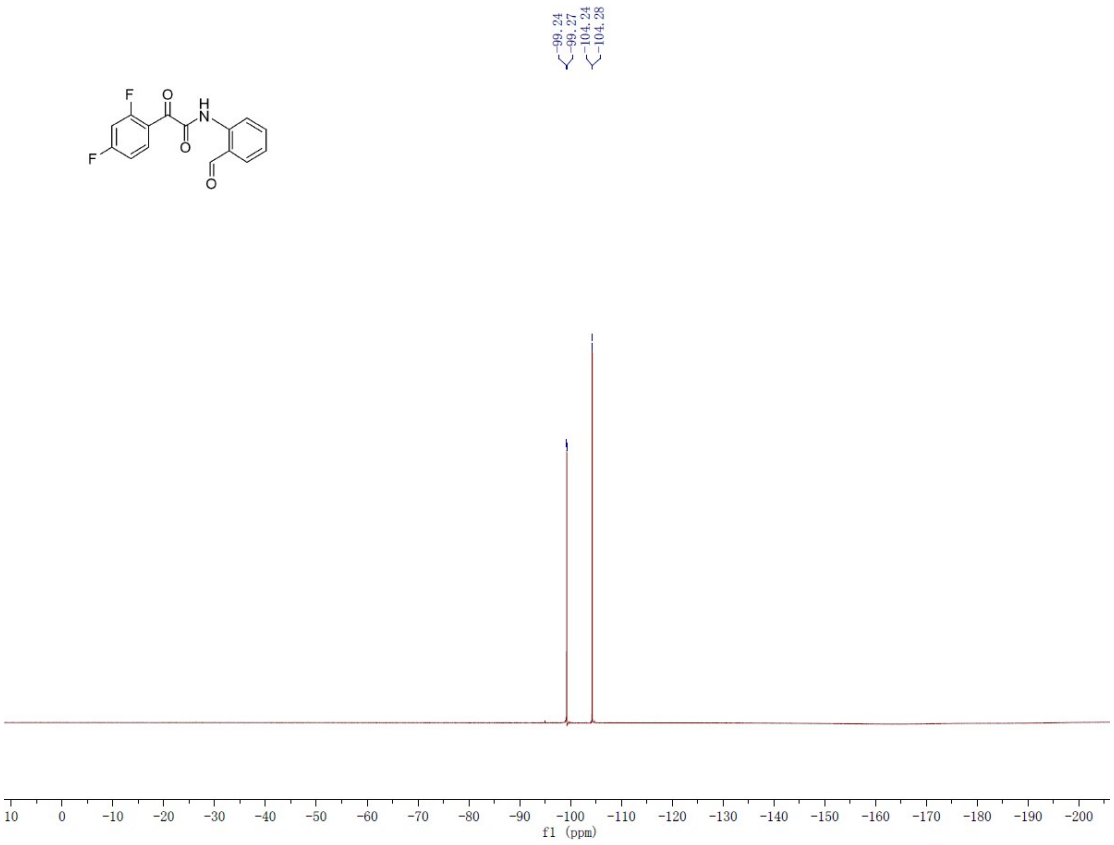



O
H
N
O
F
O

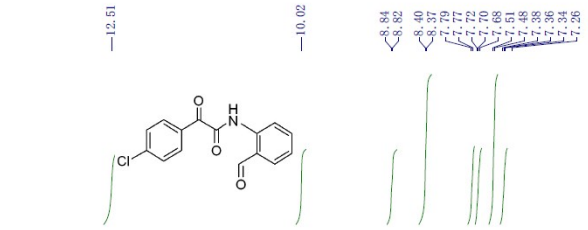
-101.81
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
f1 (ppm)

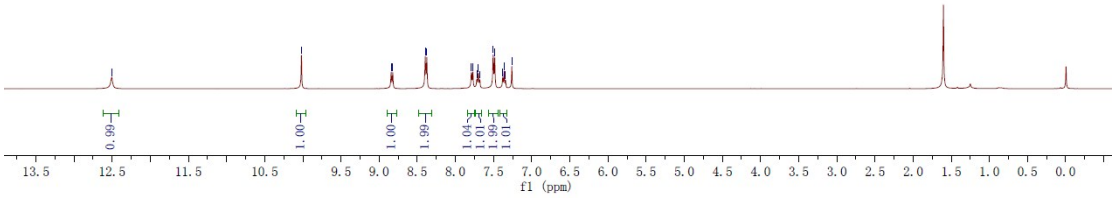
2-(2,4-Difluorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3p)

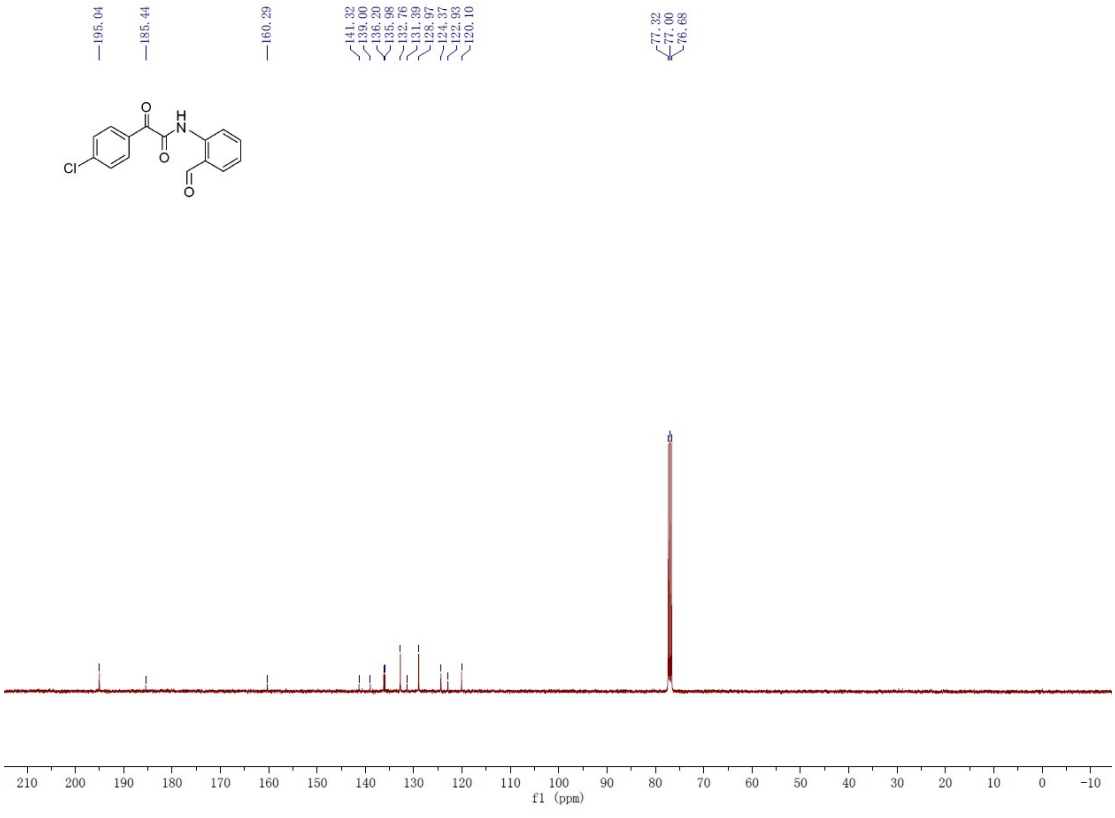



-99.24
-99.27
-104.24
-104.28
F
O
H
N
O
F
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

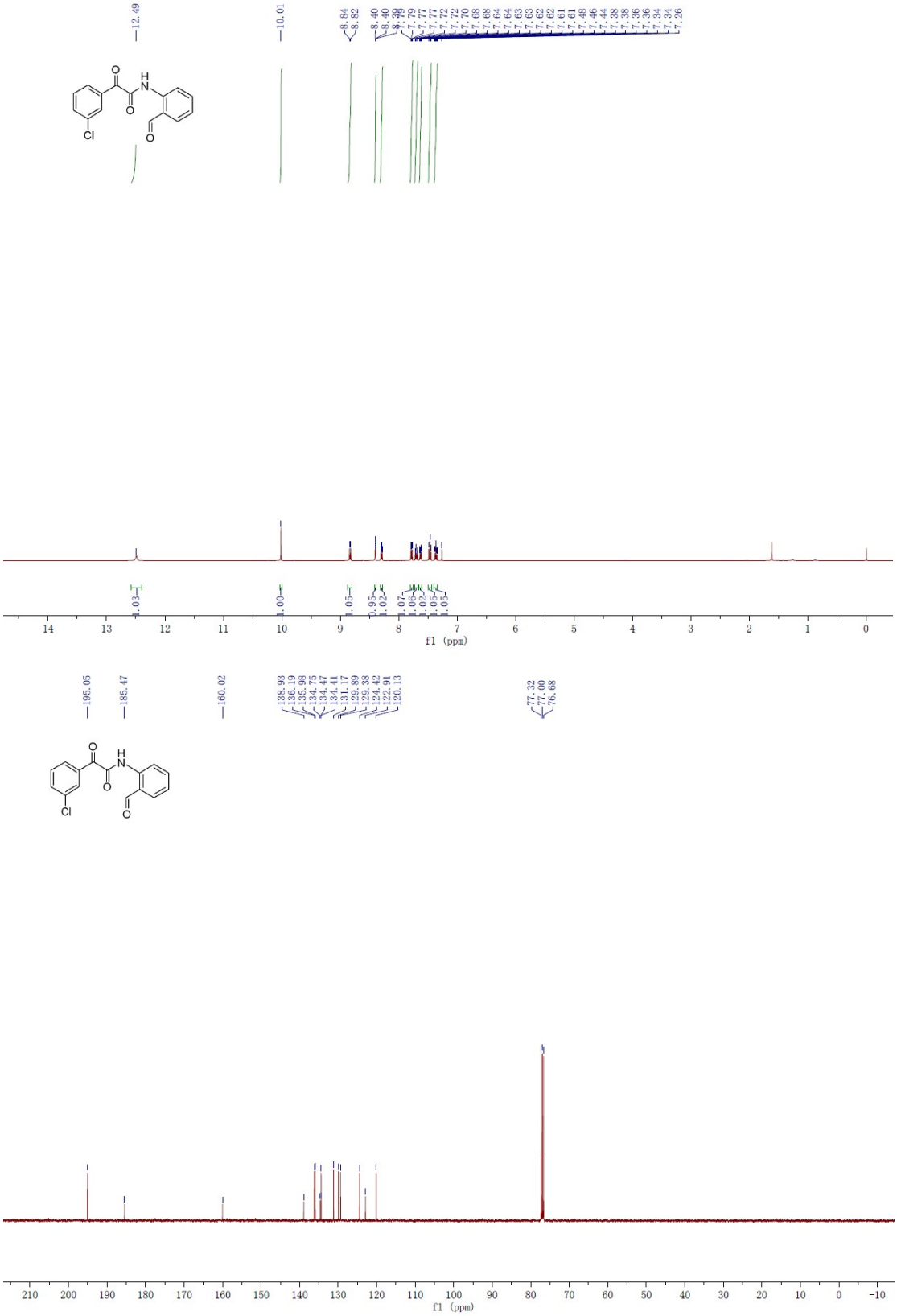
2-(4-Chlorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3q)



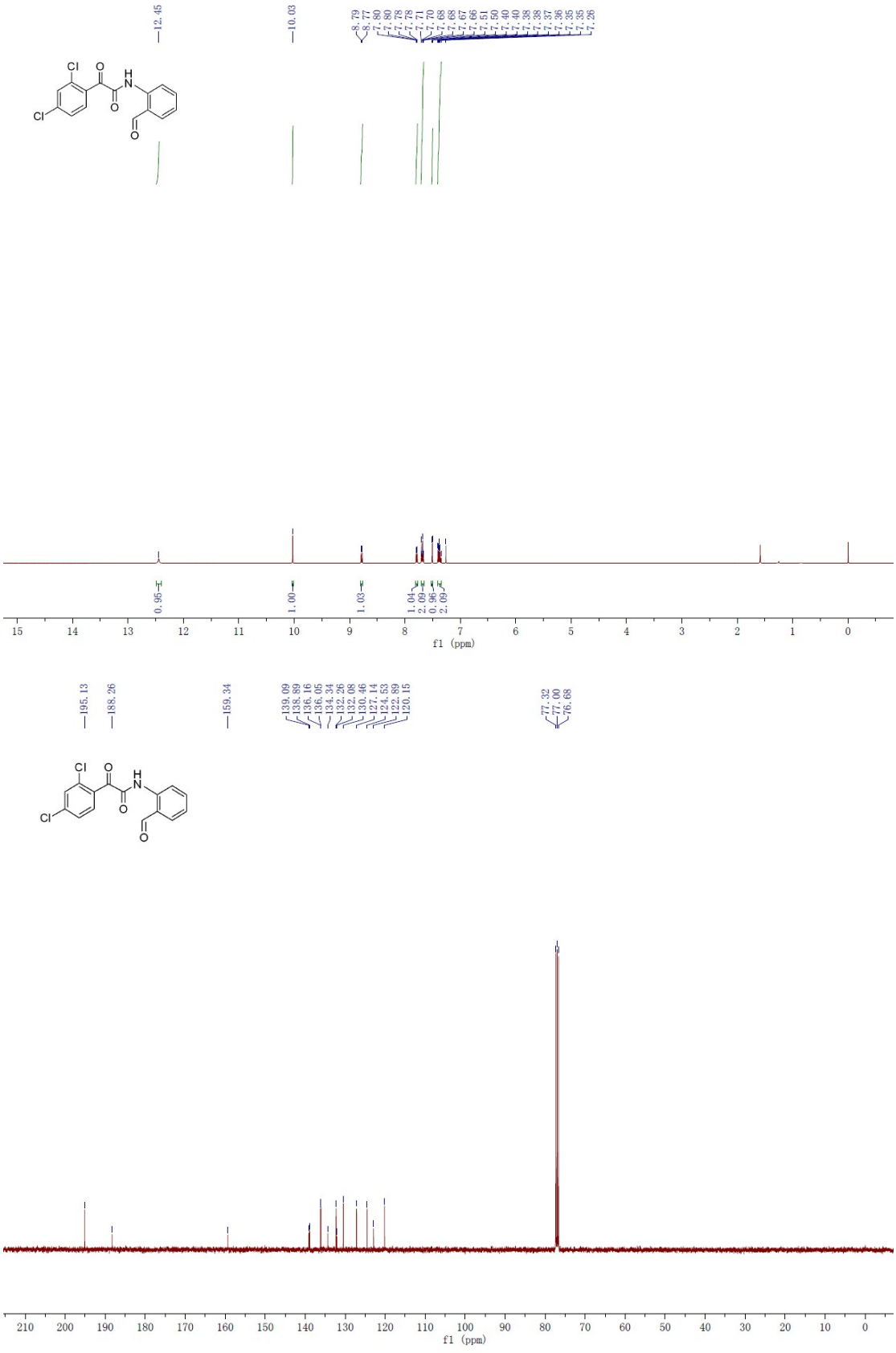




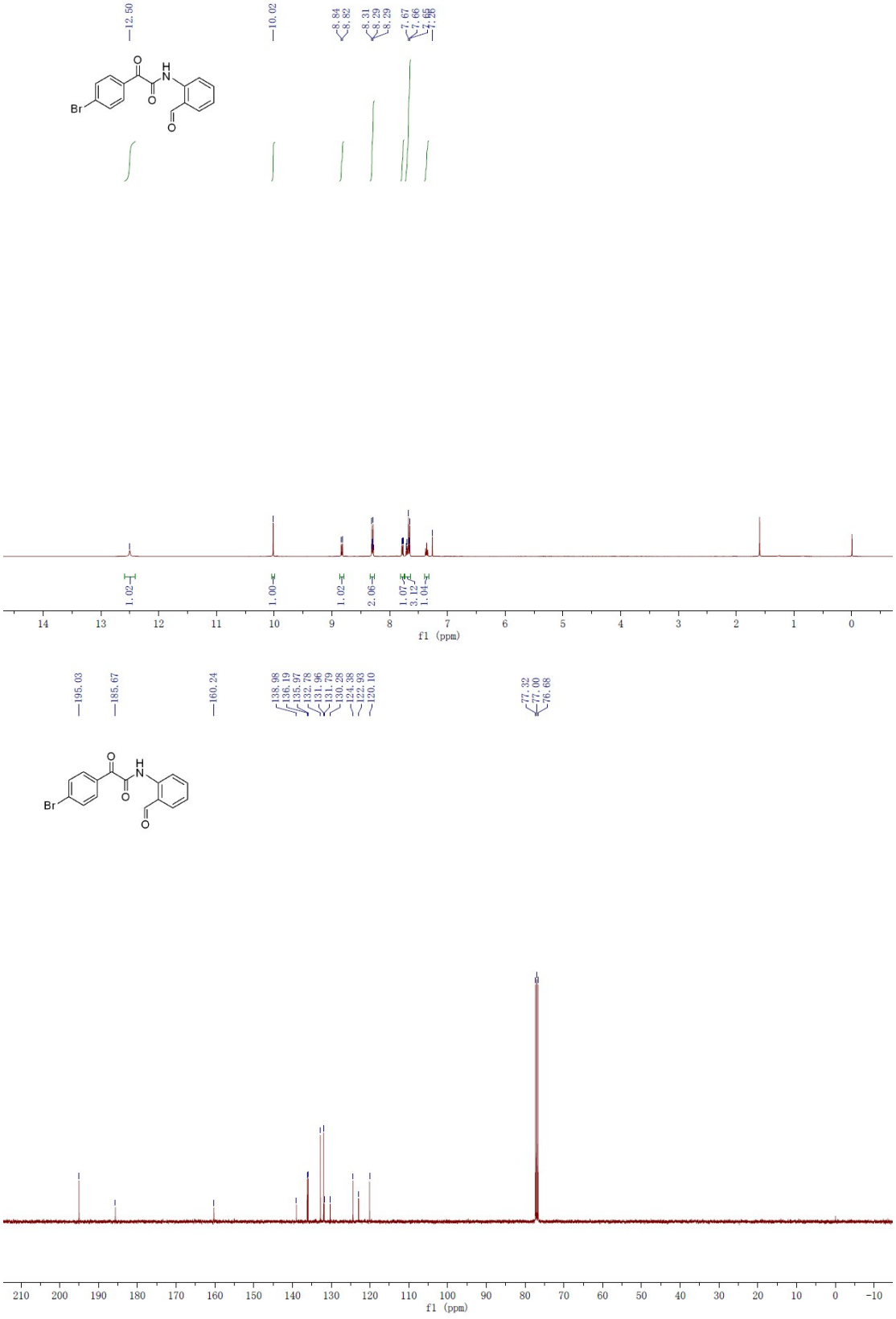
2-(3-Chlorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3r)



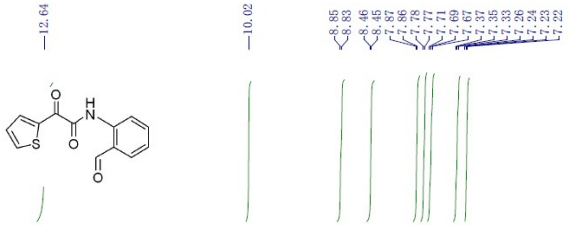
2-(2,4-Dichlorophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3s)

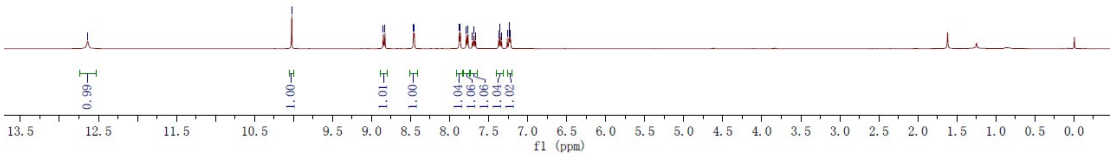


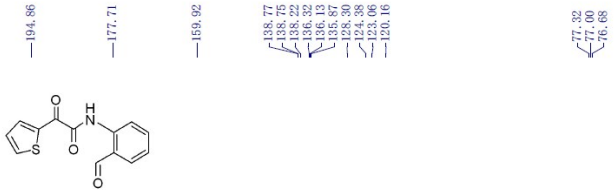
2-(4-Bromophenyl)-*N*-(2-formylphenyl)-2-oxoacetamide (3t)

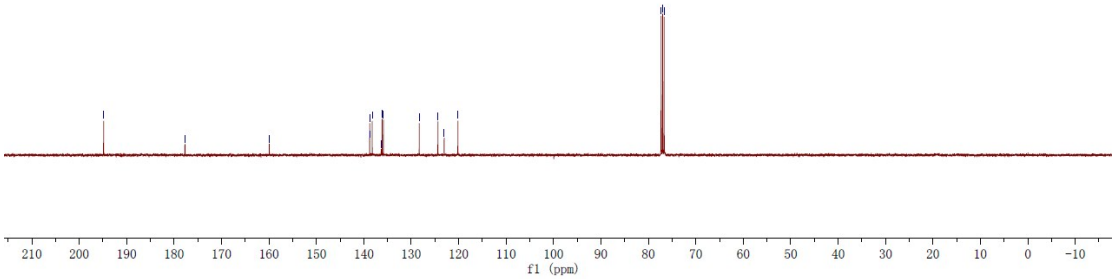


N-(2-Formylphenyl)-2-oxo-2-(thiophen-2-yl)acetamide (3u)

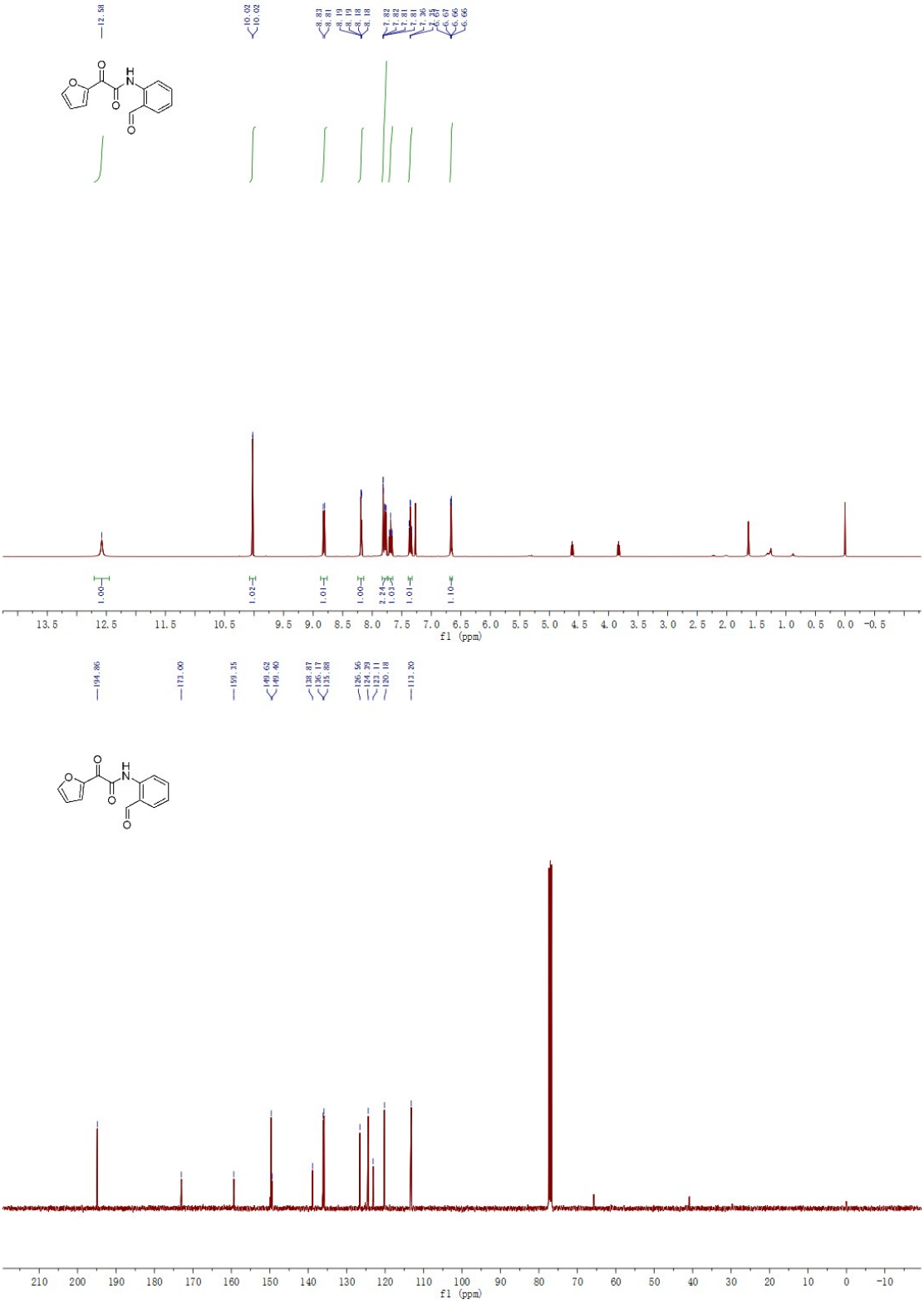




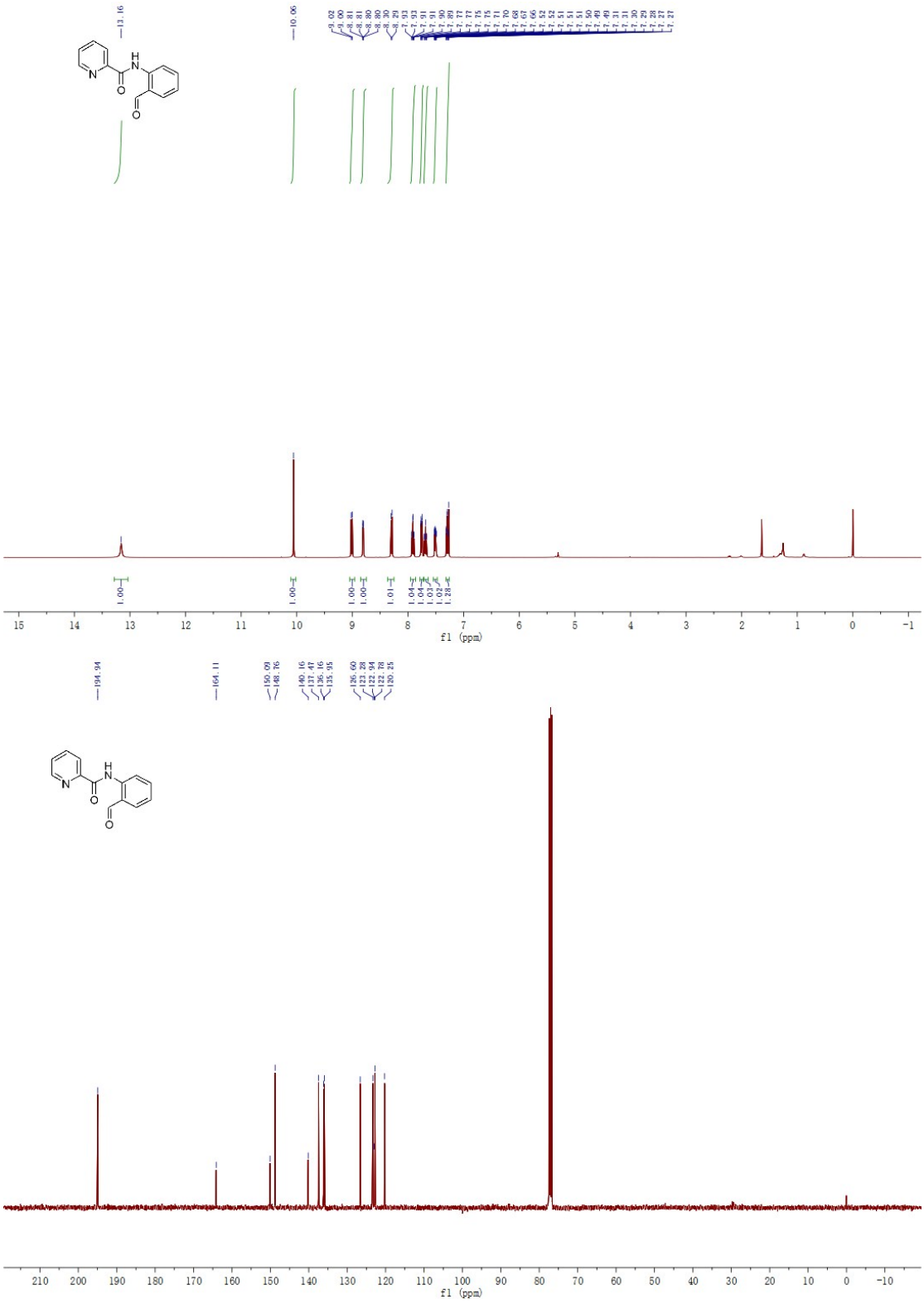




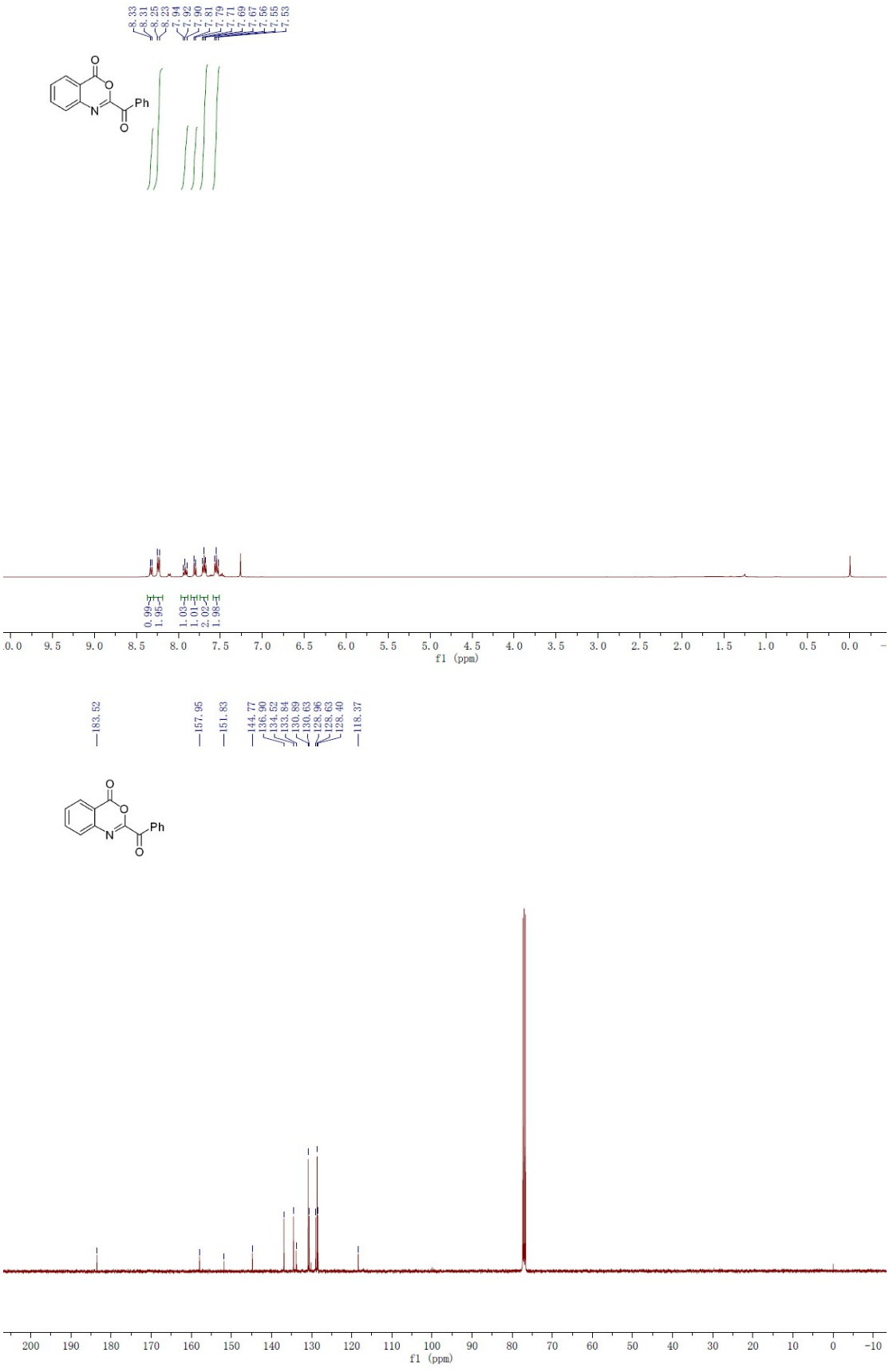
N-(2-Formylphenyl)-2-(furan-2-yl)-2-oxoacetamide (3v)



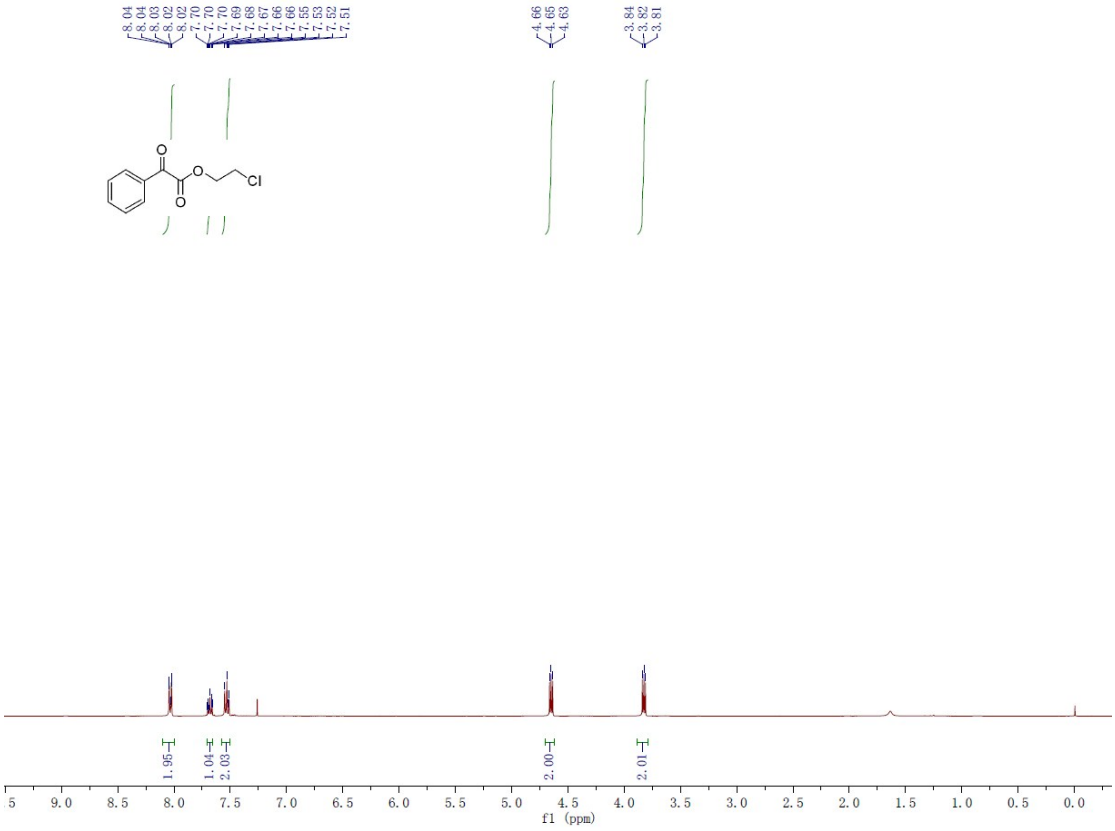
N-(2-Formylphenyl)-2-oxo-2-(pyridin-2-yl)acetamide (3w')



2-Benzoyl-4*H*-benzo[d][1,3]oxazin-4-one (11)



2-Chloroethyl 2-oxo-2-phenylacetate (4)



6. Crystallographic data for compound 3a

The method for the sample preparation: 0.1 mL solution of **3a** (1.0 mg) in 0.1 mL isopropanol was added in a 2 mL NMR tube, then 1.0 mL *n*-heptane was added. The NMR tube was kept in fridge (4 °C) for 2 weeks to form the crystal sample.

The crystallographic data collections were carried out on a Bruker Smart Apex II CCD area-detector diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) using ω-scan technique. The diffraction data were integrated by using the SAINT program,[14] which was also used for the intensity corrections for the Lorentz and polarization effects. Semi-empirical absorption correction was applied using the SADABS program.[15] The structures were solved by direct methods and all the non-hydrogen atoms were refined anisotropically on F2 by the full-matrix least-squares technique using the SHELXL-2018 crystallographic software.

Figure 1. ORTEP representation of compound **3a** displaying thermal elipsoids at 30%.

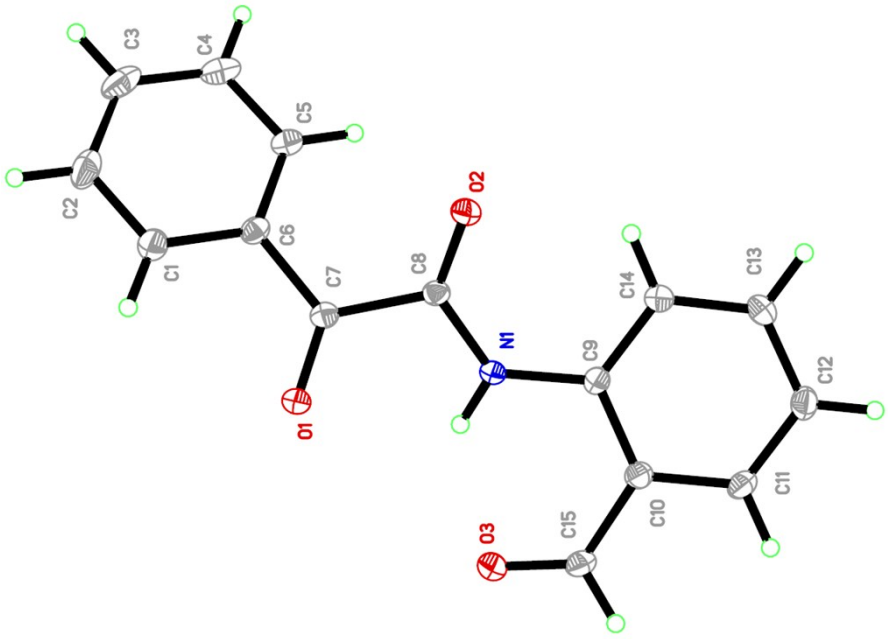


Table 1. Crystal data and structure refinement for **3a**

Identification code	**3a**
Empirical formula	$C_{15}H_{11}NO_3$
Formula weight	253.25
Temperature/K	173(2) K
Crystal system	Orthorhombic
Space group	$Pca2_1$
a/Å	a = 12.8593(8) Å
b/Å	b = 14.1412(10) Å
c/Å	c = 6.7109(5) Å
α/°	α= 90°
β/°	β= 90°
γ/°	γ = 90°
Volume /Å^3	1220.35(15) Å^3

Z	4
ρcalcg/ cm^3	1.378 $x10^{-9}$ g/ cm^3
μ/mm	0.097 mm^{-1}
F(000)	528
Crystal size/mm3	0.220 x 0.180 x 0.170 mm^3
Radiation	
2Θ range for data collection/°	3.168 to 24.999°
Index ranges	-15<=h<=14, -11<=k<=16, -7<=l<=7
Reflections collected	5786
Independent reflections	2105 [R(int) = 0.0244]
Data/restraints/parameters	2105 / 1 / 172
Goodness-of-fit on F2	1.097
Final R indexes [I>=2σ (I)]	R1 = 0.0310, wR2 = 0.0792
Final R indexes [all data]	R1 = 0.0343, wR2 = 0.0812
Largest diff. peak/hole / e $Å^{-3}$	0.149 and -0.169 e. $Å^{-3}$
CCDC	1879290

14. SAINT, Program for Data Extraction and Reduction, Bruker AXS, Inc., Madison, WI, 2001.
15. G. M. Sheldrick, SADABS, Program for Empirical Adsorption Correction of Area Detector Data. University of Gottingen, Gottingen, Germany, 2003.