Supporting Information

Ruthenium-catalyzed umpolung carboxylation of hydrazones with CO_2

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General Considerations

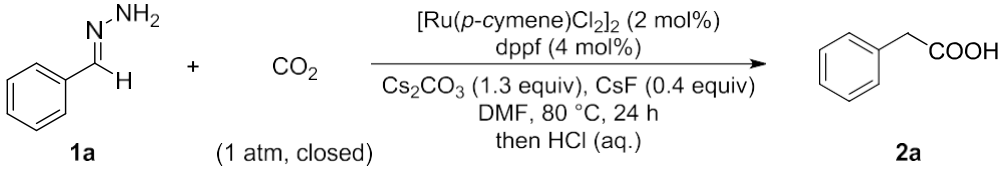
All reactions were set up using standard Schlenk techniques and carried out under a carbon dioxide atmosphere with dry solvents, unless otherwise noted. All commercially available compounds were purchased from J&K, Across, TCI or Adamas and used as received unless otherwise noted. Benzaldehyde (98% purity) was purchased from Kelong Chemicals and purified by distillation under reduced pressure prior to use. Hydrazine hydrate (98% purity) was purchased from TCI. CO_2 (99.99% purity) was commercially available. [Ru(*p*-cymene)Cl_2]$_2$ (98% purity) and 1,1'-bis(diphenylphosphino) ferrocene (98% purity) were purchased from Sinocompound. Cs_2CO_3 (99% purity) was purchased from Accela ChemBio Co., Ltd. and stored in glovebox. CsF (99% purity) was purchased from Adamas-beta® and stored in glovebox. Anhydrous DMF (99.8% purity, with molecular sieves) was purchased from J&K. The substrate of hydrazone were synthesized according to the literature procedure.[1] Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.2±0.03 mm using UV light as a visualizing agent and bromocresol green in ethanol as developing agents.

^{1}H, ^{19}F and ^{13}C NMR spectra were recorded on a Brüker Advance 400 spectrometer (^{1}H: 400 MHz, ^{13}C: 101 MHz, ^{19}F: 376 MHz). Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra are given in ppm relative to TMS, The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra and the chemical shifts converted to the TMS scale ($CDCl_3$: δH = 7.26 ppm, δC = 77.16 ppm, DMSO-d_6: δH = 2.50 ppm, δC = 39.52 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad.

GC-MS was obtained using electron ionization (Agilent Technologies 7890B/GC-System and 5977A/MSD). Exact ESI mass spectra were recorded on a SHIMADZU LCMS-IT-TOF. LRMS were obtained on a Thermo-ITQ. TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF254), and visualization was effected at 254 nm.

Reaction Conditions Optimization

Table S1. Other Reaction Conditions[a]



1a (1 atm, closed) **2a**

entry	variation from the standard conditions	yield (%)[b]
1	as shown	85
2	with H_2O (1.0 equiv) as additive	29
3	16 h instead of 24 h	68
4	THF instead of DMF	3
5	DMA instead of DMF	80
6	MeCN instead of DMF	4
7	$Ru(PPh_3)_3(CO)H_2$ instead of $[Ru(p\text{-cymene})Cl_2]_2$	12
8	$RuCl_3 \cdot 3H_2O$ instead of $[Ru(p\text{-cymene})Cl_2]_2$	12

[a]Reaction conditions: **1a** (0.4 mmol), 1 atm of CO_2, $[Ru(p\text{-cymene})Cl_2]_2$ (0.008 mol), dppf (0.016 mmol), Cs_2CO_3 (0.52 mmol), CsF (0.16 mmol), DMF (2 mL), 80 °C, 24 h. [b]Yields were determined by crude ^{1}H-NMR using dibromomethane as an internal standard.

Synthesis of the Hydrazone Substrate

General procedure for aldehyde-derived hydrazone formation (Method A)[1a]

To a solution of aldehyde (20 mmol, 1.0 equiv) in methanol (20 mL) was added hydrazine hydrate (98% purity, 1.2 mL, 24 mmol, 1.2 equiv) and the mixture stirred at room temperature for 1 h. After the aldehyde consumed completely, the mixture was then evaporated under reduced pressure at room temperature (25 ℃) to provide the desired hydrazone. Most of aldehyde-derived hydrazones were ensured by ^{1}H-NMR (> 95%) and used directly without further purification. If the purity was not good enough, the crude hydrazone was purified by a fast silica gel flash column chromatography (petroleum ether/EtOAc/NEt_3 200/20/1) to give the pure desired product. [**Note: The aldehyde-derived hydrazone is easy to deteriorate on the silica gel, so silica gel shoud be alkalified first (PE/NEt_3 =200/1). The hydrazone is also easy to deteriorate when the temperature is higher than 30 ℃, so we always keep it in the freezer under N_2 protection after purification and check the purity before use.**]

General procedure for benzophenone-derived hydrazone formation (Method B)[1b]

Hydrazine hydrate (80% purity, 6.1 mL, 100 mmol, 10 equiv) was added to benzophenone (10 mmol, 1.0 equiv) in ethanol (20 mL). Then HOAc (167 μL) was added and the mixture was heated at reflux for 12 h. After cooling to room temperature, the mixture was then evaporated under reduced pressure. The crude hydrazone was purified by a short silica gel flash column chromatography (0.1% Et_3N in

petroleum ether/EtOAc 10/1~5/1) to give the pure desired product. (**Note:** The purity of hydrazone was ensured by ^{1}H-NMR. For **3b**-**3h**, an inseparable mixture of two isomers of hydrazone was obtained, which was used in the next step without further purification.)

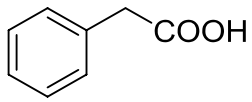
General procedure for ketone-derived hydrazone formation(3i, 3j, Method C)[1c]

To a solution of ketone (10 mmol, 1.0 equiv) in ethanol (20 mL) was added hydrazine hydrate (98% purity, 1 mL, 20 mmol, 2 equiv). The mixture was heated at reflux for 2 h. After cooling to room temperature, the mixture was then evaporated under reduced pressure. The crude hydrazone was purified by a short silica gel flash column chromatography (0.1% Et_3N in petroleum ether/EtOAc 10/1~5/1) to give the pure desired product. (The purity of hydrazone was ensured by ^{1}H-NMR.)

Experimental Procedures and Characterization Data

A flame-dried Schlenk tube (25 mL) containing a stirring bar was charged with 1,1'-bis(diphenylphosphino)ferrocene (8.9 mg, 0.016mmol, 4 mol%) and hydrazone substrate (0.40 mmol, 1.0 equiv for non-liquid substrates). The reaction tube was transferred to the glovebox and charged with $[Ru(p\text{-cymene})Cl_2]_2$ (4.9 mg, 0.008 mmol, 2 mol%), Cs_2CO_3 (169 mg, 0.52 mmol, 1.3 equiv) and CsF (24 mg, 0.16 mmol, 0.4 equiv). The reaction tube was moved out of the glovebox and the tube was then evacuated and back-filled with carbon dioxide for 3 times. Subsequently anhydrous DMF (1 mL), hydrazone substrate (0.40 mmol, 1.0 equiv for liquid substrates) and another anhydrous DMF (1 mL) were added via syringes under CO_2. Once added, the Schlenk tube was sealed at atmospheric pressure of CO_2 (1 atm). The resulting mixture was stirred for 24 h at 80 °C (380 r/min). After cooling to room temperature, the resulting mixture was diluted with 2 mL EtOAc and quenched by 2 mL 2N HCl. The reaction mixture was extracted by EtOAc (3 x 5 mL) and the combined organic phases were concentrated in vacuo. The residue was purified by a short silica gel flash column chromatography (0.1% AcOH in petroleum ether/EtOAc 10/1~5/1) to give the pure desired product with bromocresol green as chromogenic agent.

2-phenylacetic acid (2a)



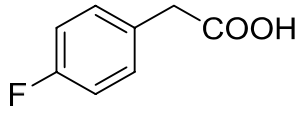
45 mg, 83% yield, white solid;

R_f (PE/EA 3:1): 0.35;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.23 (m, 5H), 3.63 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.3, 133.2, 129.4, 128.7, 127.4, 41.1. The spectroscopic data correspond to those previously reported in the literature.[2]

LRMS (ESI-): calc. for $C_8H_7O_2^-$ $[M-H]^-$ 135.04, found 134.90.

2-(4-fluorophenyl)acetic acid (2b)



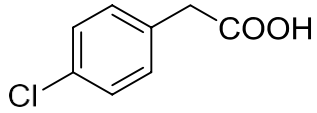
48 mg, 77% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.19 (m, 2H), 7.05 – 6.97 (m, 2H), 3.61 (s, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -115.18; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.2, 162.1 (d, J = 245.8 Hz), 131.0 (d, J = 8.2 Hz), 128.9 (d, J = 3.4 Hz), 115.5 (d, J = 21.4 Hz), 40.1. The spectroscopic data correspond to those previously reported in the literature.[2]

LRMS (ESI-): calc. for $C_8H_6FO_2^-$ $[M-H]^-$ 153.04, found 152.86.

2-(4-chlorophenyl)acetic acid (2c)



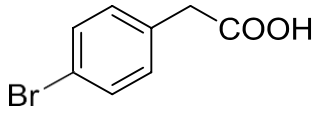
56 mg, 82% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 3.60 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.7, 133.4, 131.6, 130.8, 128.8, 40.4. The spectroscopic data correspond to those previously reported in the literature.[6]

LRMS (ESI-): calc. for $C_8H_6ClO_2^-$ $[M-H]^-$ 169.01, found 168.91.

2-(4-bromophenyl)acetic acid (2d)



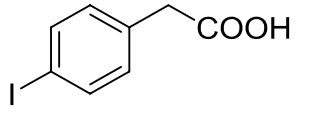
76 mg, 88% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 3.59 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.8, 132.2, 131.8, 131.2, 121.5, 40.5. The spectroscopic data correspond to those previously reported in the literature.[6]

LRMS (ESI-): calc. for $C_8H_6BrO_2^-$ $[M-H]^-$ 212.96, found 212.88.

2-(4-iodophenyl)acetic acid (2e)



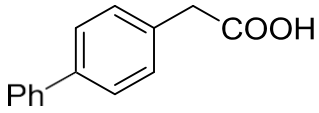
85 mg, 81% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.02 (d, *J* = 8.3 Hz, 2H), 3.59 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.5, 137.8, 132.8, 131.4, 93.0, 40.5. The spectroscopic data correspond to those previously reported in the literature.[7]

LRMS (ESI-): calc. for $C_8H_6IO_2^-$ $[M-H]^-$ 260.94, found 260.82.

4-biphenylacetic acid (2f)



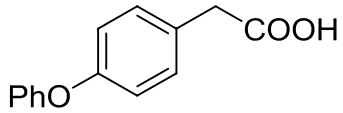
65 mg, 77% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.66 – 7.52 (m, 4H), 7.47 – 7.38 (m, 2H), 7.36 – 7.27 (m, 3H), 3.59 (s, 2H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 173.2, 140.4, 139.0, 134.8, 130.5 , 129.4, 127.8, 127.1, 127.0, 40.8. The spectroscopic data correspond to those previously reported in the literature10.[4]

LRMS (ESI-): calc. for $C_{14}H_{11}O_2^-$ $[M-H]^-$ 211.08, found 210.84.

2-(4-phenoxyphenyl)acetic acid (2g)



65 mg, 71% yield, white solid;

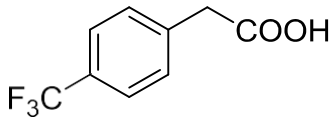
R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 2H), 7.25 – 7.20 (m, 2H), 7.13 – 7.06 (m, 1H), 7.03 – 6.92 (m, 4H), 3.61 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.3, 157.1, 156.7, 130.8, 129.8, 128.0, 123.5, 119.1, 118.9, 40.4. The spectroscopic data correspond to those previously reported in the literature.[11]

LRMS (ESI-): calc. for $C_{14}H_{11}O_3^-$ $[M-H]^-$ 227.07, found 226.97.

2-(4-(trifluoromethyl)phenyl)acetic acid (2h)

75 mg, 92% yield, white solid;

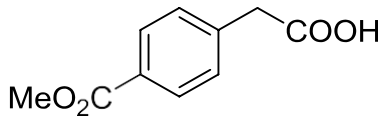


R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 8.1 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 3.71 (s, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.61; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.4, 137.1, 129.9, 129.8 (q, *J* = 32.6 Hz), 125.6 (q, *J* = 3.7 Hz), 124.1 (q, *J* = 272.1 Hz), 40.8. The spectroscopic data correspond to those previously reported in the literature.[3]

LRMS (ESI-): calc. for $C_9H_6F_3O_2^-$ [M-H]$^-$ 203.03, found 202.93.

2-(4-(methoxycarbonyl)phenyl)acetic acid (2i)



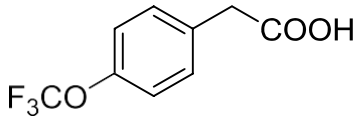
62 mg, 80% yield, white solid;

R_f (PE/EA 3:1): 0.20;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 3.90 (s, 3H), 3.70 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.8, 166.9, 138.4, 129.9, 129.5, 129.2, 52.2, 40.9. The spectroscopic data correspond to those previously reported in the literature.[8]

LRMS (ESI-): calc. for $C_{10}H_9O_4^-$ [M-H]$^-$ 193.05, found 192.72.

2-(4-(trifluoromethoxy)phenyl)acetic acid (2j)



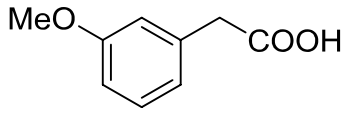
68 mg, 78% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 8.6 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 3.65 (s, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.92; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.5, 148.5, 131.8, 130.8, 121.1 (d, *J* = 0.6 Hz), 120.4 (q, *J* = 257.1 Hz), 40.3. The spectroscopic data correspond to those previously reported in the literature.[12]

LRMS (ESI-): calc. for $C_9H_6F_3O^-$ [M-H]$^-$ 219.03, found 218.90.

2-(3-methoxyphenyl)acetic acid (2k)



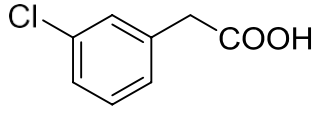
62 mg, 93% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.21 (m, 1H), 6.89 – 6.79 (m, 3H), 3.79 (s, 3H), 3.61 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.8, 159.7, 134.6, 129.6, 121.7, 115.0, 112.8, 55.2, 41.1. The spectroscopic data correspond to those previously reported in the literature.[2]

LRMS (ESI-): calc. for $C_9H_9O_3^-$ [M-H]$^-$ 165.05, found 164.94.

2-(3-chlorophenyl)acetic acid (2l)



63 mg, 92% yield, white solid;

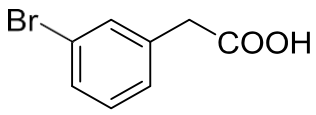
R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 3H), 7.19 – 7.13 (m, 1H), 3.63 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.4, 135.0, 134.5, 129.9, 129.6, 127.7, 127.6, 40.6. The spectroscopic data correspond to those previously reported in the literature.[9]

LRMS (ESI-): calc. for $C_8H_6ClO_2^-$ [M-H]$^-$ 169.01, found 168.84.

2-(3-bromophenyl)acetic acid (2m)

79 mg, 92% yield, white solid;

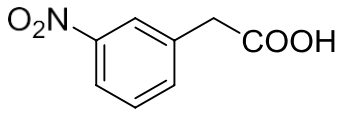


R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.39 (m, 2H), 7.24 – 7.17 (m, 2H), 3.63 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.0, 135.3, 132.5, 130.6 , 130.2, 128.1, 122.6, 40.5. The spectroscopic data correspond to those previously reported in the literature.[6]

LRMS (ESI-): calc. for $C_8H_6BrO_2^-$ [M-H]$^-$ 212.96, found 212.93.

2-(3-nitrophenyl)acetic acid (2n)



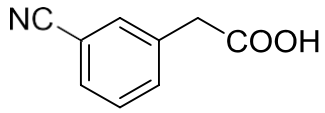
59 mg, 81% yield, light yellow solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.03 (m, 2H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.9 Hz, 1H), 3.79 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.3, 148.4, 135.7, 135.0, 129.6, 124.5, 122.6, 40.3. The spectroscopic data correspond to those previously reported in the literature.[6]

LRMS (ESI-): calc. for $C_8H_6NO_4^-$ [M-H]$^-$ 180.03, found 179.87.

2-(3-cyanophenyl)acetic acid (2o)



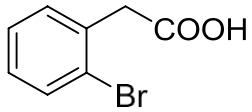
53 mg, 82% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.56 (m, 2H), 7.55 – 7.51 (m, 1H), 7.49 – 7.42 (m, 1H), 3.70 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.6, 134.7, 134.1, 133.0, 131.2, 129.5, 118.5, 112.7, 40.4. The spectroscopic data correspond to those previously reported in the literature.[8]

LRMS (ESI-): calc. for $C_9H_6NO_2^-$ [M-H]$^-$ 160.04, found 159.86.

2-(2-bromophenyl)acetic acid (2p)



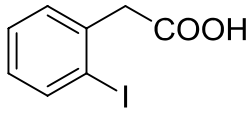
67 mg, 78% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.9 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.20 – 7.13 (m, 1H), 3.85 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.0, 133.4, 132.9, 131.6, 129.2, 127.6, 125.1, 41.4. The spectroscopic data correspond to those previously reported in the literature.[13]

LRMS (ESI-): calc. for $C_8H_6BrO_2^-$ [M-H]$^-$ 212.96, found 212.82.

2-(2-iodophenyl)acetic acid (2q)



83 mg, 79% yield, white solid;

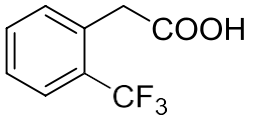
R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 7.9, 0.9 Hz, 1H), 7.36 – 7.28 (m, 2H), 7.02 – 6.95 (m, 1H), 3.86 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.7, 139.6, 137.0, 130.7, 129.2, 128.5, 101.0, 45.9. The spectroscopic data correspond to those previously reported in the literature.[10]

LRMS (ESI-): calc. for $C_8H_6IO_2^-$ [M-H]$^-$ 260.94, found 260.78.

2-(2-(trifluoromethyl)phenyl)acetic acid (2r)

67 mg, 82% yield, white solid;

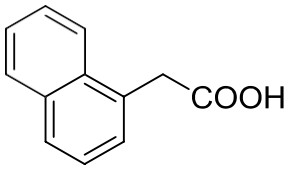


R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.42 – 7.34 (m, 2H), 3.86 (s, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -59.97; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2, 132.6, 132.0 (d, *J* = 0.9 Hz), 131.5 (q, *J* = 1.7 Hz), 129.0 (q, *J* = 30.2 Hz), 127.7, 126.1 (q, *J* = 5.5 Hz), 124.2 (q, *J* = 273.7 Hz), 38.0 (d, *J* = 1.9 Hz). The spectroscopic data correspond to those previously reported in the literature.[14]

LRMS (ESI-): calc. for $C_9H_6F_3O_2^-$ $[M-H]^-$ 203.03, found 202.84.

2-(naphthalen-1-yl)acetic acid (2s)



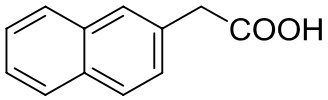
60 mg, 81% yield, light yellow solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.91 (m, 1H), 7.86 – 7.80 (m, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.41 – 7.32 (m, 2H), 4.03 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.2, 133.9, 132.1, 129.8, 128.9, 128.4, 128.3, 126.6, 126.0, 125.5, 123.8, 38.9. The spectroscopic data correspond to those previously reported in the literature.[4]

LRMS (ESI-): calc. for $C_{12}H_9O_2^-$ $[M-H]^-$ 185.06, found 184.92.

2-(naphthalen-2-yl)acetic acid (2t)



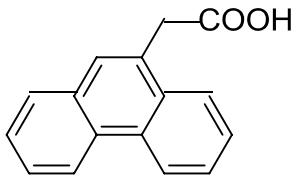
59 mg, 79% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.76 (m, 3H), 7.72 (s, 1H), 7.49 – 7.42 (m, 2H), 7.40 (dd, *J* = 8.4, 1.8 Hz, 1H), 3.80 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.8, 133.4, 132.5, 130.7, 128.3, 128.2, 127.7, 127.7, 127.3, 126.2, 126.0, 41.2. The spectroscopic data correspond to those previously reported in the literature.[2]

LRMS (ESI-): calc. for $C_{12}H_9O_2^-$ $[M-H]^-$ 185.06, found 184.89.

2-(phenanthren-9-yl)acetic acid (2u)



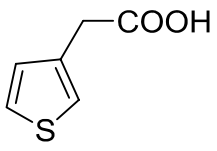
87 mg, 92% yield, brown solid;

R_f (PE/EA 3:1): 0.20;

^{1}H NMR (400 MHz, DMSO-d_6) δ 12.51 (s, 1H), 8.91 – 8.54 (m, 2H), 8.05 – 7.97 (m, 1H), 7.93 – 7.87 (m, 1H), 7.75 (s, 1H), 7.70 – 7.57 (m, 4H), 4.08 (s, 2H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 173.3, 131.6, 131.4, 130.6, 130.5, 129.9, 128.9, 128.5, 127.4, 127.4, 127.2, 127.0, 125.1, 123.8, 123.2, 39.4. The spectroscopic data correspond to those previously reported in the literature.[15]

LRMS (ESI-): calc. for $C_{16}H_{11}O_2^-$ $[M-H]^-$ 235.08, found 234.83.

2-(thiophen-3-yl)acetic acid (2v)



27 mg, 47% yield, white solid;

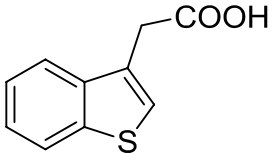
R_f (PE/EA 3:1): 0.4;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 4.9, 3.0 Hz, 1H), 7.20 – 7.14 (m, 1H), 7.05 (d, *J* = 4.9 Hz, 1H), 3.70 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.5,

132.7, 128.5, 125.9, 123.3, 35.5. The spectroscopic data correspond to those previously reported in the literature.[16]

LRMS (ESI-): calc. for $C_6H_5O_2S^-$ $[M-H]^-$ 141.00, found 140.89.

2-(benzo[*b*]thiophen-3-yl)acetic acid (2w)

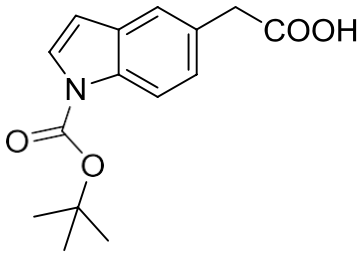


63 mg, 81% yield, yellow solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.42 – 7.31 (m, 3H), 3.87 (s, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2, 140.2, 138.4, 127.4, 125.1, 124.6, 124.3, 122.9, 121.7, 34.2; **HRMS (ESI-):** calcd for $C_{10}H_7O_2S^-$ $[M-H]^-$ 191.0172, found 191.0183.

2-(1-(*tert*-butoxycarbonyl)-1*H*-indol-5-yl)acetic acid (2x)

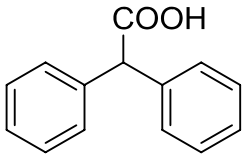


65 mg, 59% yield, yellow solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 3.5 Hz, 1H), 7.45 (d, *J* = 0.9 Hz, 1H), 7.21 (dd, *J* = 8.5, 1.6 Hz, 1H), 6.52 (d, *J* = 3.6 Hz, 1H), 3.72 (s, 2H), 1.66 (s, 9H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.3, 149.7, 134.4, 130.9, 127.6, 126.4, 125.5, 121.6, 115.3, 107.1, 83.8, 40.9, 28.2; **HRMS (ESI-):** calcd for $C_{15}H_{16}NO_4^-$ $[M-H]^-$ 274.1085, found 274.1085.

2,2-diphenylacetic acid (4a)



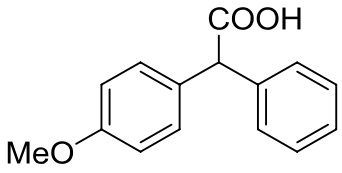
61 mg, 72% yield, white solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.23 (m, 10H), 5.04 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.9, 138.0, 128.8, 128.7, 127.6, 57.1. The spectroscopic data correspond to those previously reported in the literature.[3]

LRMS (ESI-): calc. for $C_{14}H_{11}O_2^-$ $[M-H]^-$ 211.08, found 210.72.

2-(4-methoxyphenyl)-2-phenylacetic acid (4b)



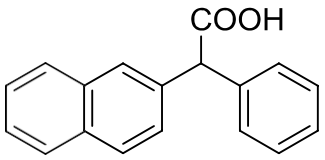
69 mg, 71% yield, light yellow solid;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.21 (m, 7H), 6.88 – 6.82 (m, 2H), 4.99 (s, 1H), 3.76 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 179.0, 158.9, 138.3, 130.0, 129.8, 128.7, 128.6, 127.4, 114.1, 56.2, 55.3. The spectroscopic data correspond to those previously reported in the literature.[5]

LRMS (ESI-): calc. for $C_{15}H_{13}O_3^-$ $[M-H]^-$ 241.09, found 240.74.

2-(naphthalen-2-yl)-2-phenylacetic acid (4c)



63 mg, 60% yield, light yellow solid;

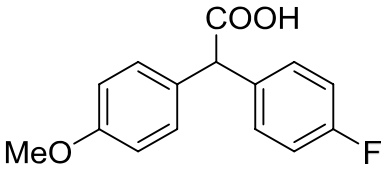
R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.73 (m, 4H), 7.45 – 7.39 (m, 3H), 7.38 – 7.23 (m, 5H), 5.20 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ

178.7, 137.8, 135.3, 133.3, 132.6, 128.8, 128.7, 128.4, 128.0, 127.6, 127.6, 127.5, 126.7, 126.3, 126.2, 57.1. The spectroscopic data correspond to those previously reported in the literature.[4]

LRMS (ESI-): calc. for $C_{17}H_{13}^-$[M-COOH]$^-$ 217.10, found 217.06.[4]

2-(4-fluorophenyl)-2-(4-methoxyphenyl)acetic acid (4d)

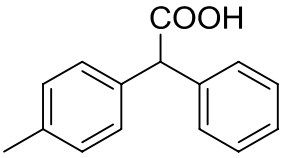


84 mg, 81% yield, light yellow solid;

R_f (PE/EA 3:1): 0.25;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 2H), 7.24 – 7.19 (m, 2H), 7.03 – 6.96 (m, 2H), 6.89 – 6.84 (m, 2H), 4.96 (s, 1H), 3.77 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -115.03; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.8, 162.1 (d, J = 246.4 Hz), 159.0, 134.0 (d, J = 3.3 Hz), 130.2 (d, J = 8.1 Hz), 129.8, 129.7, 115.5 (d, J = 21.5 Hz), 114.2, 55.4, 55.3. **HRMS (ESI-):** calcd for $C_{15}H_{12}FO_3^-$ [M-H]$^-$ 259.0776, found 259.0784.

2-phenyl-2-(*p*-tolyl)acetic acid (4e)



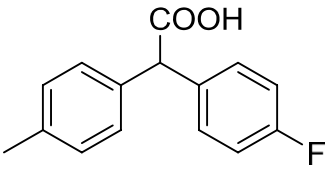
72 mg, 80% yield, light yellow solid;

R_f (PE/EA 3:1): 0.20;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.23 (m, 5H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.01 (s, 1H), 2.32 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.9, 138.1, 137.3, 135.0, 129.4, 128.7, 128.7, 128.6, 127.5, 56.7, 21.1. The spectroscopic data correspond to those previously reported in the literature.[17]

LRMS (ESI-): calc. for $C_{14}H_{13}^-$[M-COOH]$^-$ 181.10, found 181.01.[5]

2-(4-fluorophenyl)-2-(*p*-tolyl)acetic acid (4f)

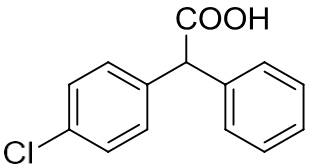


78 mg, 80% yield, light yellow solid;

R_f (PE/EA 3:1): 0.20;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (dd, *J* = 8.7, 5.3 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.90 (t, *J* = 8.7 Hz, 2H), 4.89 (s, 1H), 2.23 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -114.98; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.8, 162.2 (d, *J* = 246.4 Hz), 137.5, 134.9, 134.0 (d, *J* = 3.1 Hz), 130.3 (d, *J* = 8.1 Hz), 129.5, 128.5, 115.5 (d, *J* = 21.5 Hz), 55.9, 21.1. **HRMS (ESI-):** calcd for $C_{15}H_{12}FO_2^-$ [M-H]$^-$ 243.0827, found 243.0837.

2-(4-chlorophenyl)-2-phenylacetic acid (4g)



62 mg, 63% yield, light yellow solid;

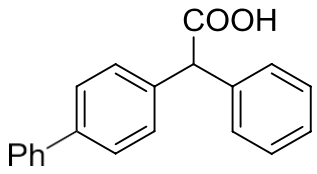
R_f (PE/EA 3:1): 0.25;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 6.47 (m, 9H), 5.00 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.6, 137.4, 136.4, 133.6, 130.1, 128.9, 128.6, 127.8, 56.4. The spectroscopic data correspond to those previously reported in the literature.[5]

LRMS (ESI-): calc. for $C_{13}H_{10}Cl^-$ [M-COOH]$^-$ 201.05, found 201.02.[4]

2-([1,1'-biphenyl]-4-yl)-2-phenylacetic acid (4h)

90 mg, 78% yield, light yellow solid;

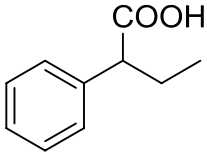


R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.50 (m, 4H), 7.45 – 7.24 (m, 10H), 5.09 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.8, 140.6, 140.5, 137.9, 137.0, 129.2, 128.8, 128.8, 128.8, 127.7 , 127.5, 127.4, 127.2, 56.8. The spectroscopic data correspond to those previously reported in the literature.[18]

HRMS (ESI-): calc. for $C_{19}H_{15}^-$ [M-COOH]$^-$ 243.1179, found 243.1183.[4]

2-phenylbutanoic acid (4i)



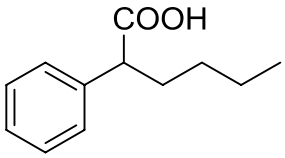
33 mg, 50% yield, light yellow oil;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.22 (m, 5H), 3.45 (t, *J* = 7.7 Hz, 1H), 2.15 – 2.04 (m, 1H), 1.86 – 1.75 (m, 1H), 0.90 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.6, 138.4, 128.7, 128.1, 127.5, 53.4, 26.3, 12.1. The spectroscopic data correspond to those previously reported in the literature.[19]

LRMS (ESI-): calc. for $C_{10}H_{11}O_2^-$ [M-H]$^-$ 163.08, found 162.99.

2-phenylhexanoic acid (4j)

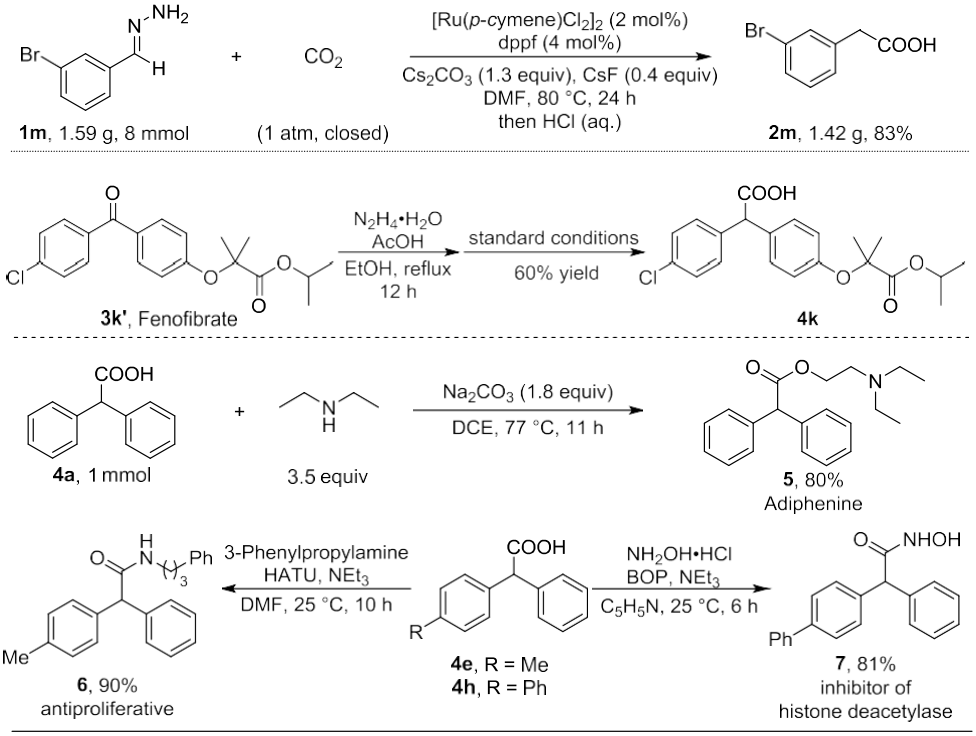


46 mg, 60% yield, light yellow oil;

R_f (PE/EA 3:1): 0.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.21 (m, 5H), 3.53 (t, *J* = 7.7 Hz, 1H), 2.14 – 2.00 (m, 1H), 1.84 – 1.71 (m, 1H), 1.37 – 1.17 (m, 4H), 0.86 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.5, 138.6, 128.7, 128.1, 127.4, 51.6, 32.8, 29.7, 22.5, 13.9; **HRMS (ESI-):** calcd for $C_{12}H_{15}O_2^-$ [M-H]$^-$ 191.1078, found 191.1075.

The Application of the Reaction



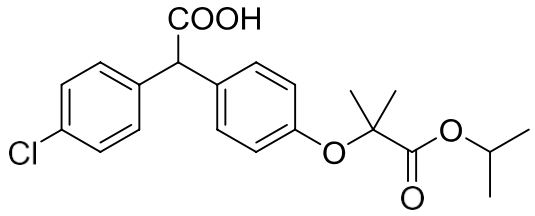
Synthesis of 2m in gram scale

A flame-dried Schlenk flask (500 mL) containing a stirring bar was charged with 1,1'-bis(diphenylphosphino)ferrocene (177 mg, 0.32 mmol, 4 mol%) and hydrazone substrate **1m** (1.59 g, 8 mmol, 1.0 equiv). The reaction tube was transferred to the glovebox and charged with [Ru(*p*-cymene)Cl_2]$_2$ (98 mg, 0.16 mmol, 2 mol%), Cs_2CO_3 (3.39 g, 10.4 mmol, 1.3 equiv) and CsF (486 mg, 3.2 mmol, 0.4 equiv) before being sealed. The reaction tube was moved out of the glovebox and the tube was then evacuated and back-filled with carbon dioxide for 3 times. Subsequently anhydrous DMF (40 mL) was added via syringe under CO_2. Once added, the Schlenk tube was sealed at atmospheric pressure of CO_2 (1 atm). The resulting mixture was stirred for 24 h at 80 ℃. Then the resulting mixture was diluted with 40 mL EtOAc and quenched by 40 mL 2N HCl. The reaction mixture was extracted by EtOAc with three times and the combined organic phases were concentrated in vacuo. The residue was purified by silica gel flash column chromatography (petroleum ether/EtOAc/AcOH 10/1/1%) to give the pure desired product **2m** as a white solid (1.42 g, 83% yield).

Synthesis of 4k

Following the general procedure, using hydrazone (150 mg, 0.4 mmol) which was prepared from Fenofibrate (**3k'**) according to method B provided the corresponding acid **4k** as a light yellow solid (94 mg, 60% yield).

2-(4-chlorophenyl)-2-(4-((1-isopropoxy-2-methyl-1-oxopropan-2-yl)oxy)phenyl)acetic acid (4k)



94 mg, 60% yield, light yellow solid;

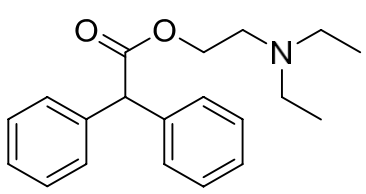
R_f (PE/EA 3:1): 0.15;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (dd, *J* = 22.9, 8.5 Hz, 4H), 7.15 (d, *J* = 8.7 Hz, 2H), 6.79 (d, *J* = 8.7 Hz, 2H), 5.06 (m, 1H), 4.93 (s, 1H), 1.57 (s, 6H), 1.19 (d, *J* = 6.3 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.2, 173.6, 155.0, 136.6, 133.4, 130.6, 123.0, 129.3, 128.7, 118.9, 79.1, 69.0, 55.5, 25.4, 25.3, 21.5; **HRMS (ESI-):** calcd for $C_{20}H_{22}ClO_3^-$ [M-COOH]$^-$ 345.1263, found 345.1266.[4]

Synthesis of 5

To a solution of **4a** (212 mg, 1 mmol), anhydrous Na_2CO_3 (1.8 mmol, 1.8 equiv) in dry 1,2-dichloroethane (DCE, 1.69 mL, 21.5 mmol) was added diethylamine (3.5 mmol, 3.5 equiv) and the reaction mixture was stirred at 77 ℃ for 11 h. The solvents were removed under vacuum and the residue was purified by silica chromatography (PE/EtOAc 2/1) to give the 2-(diethylamino)ethyl 2,2-diphenylacetate **5** as a light yellow oil (248 mg, 80% yield).

2-(diethylamino)ethyl 2,2-diphenylacetate (5)



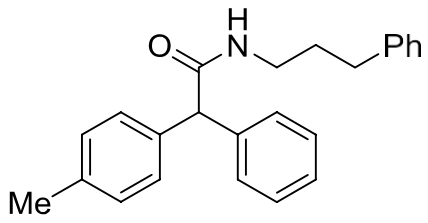
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 10H), 5.03 (s, 1H), 4.22 (t, *J* = 6.2 Hz, 2H), 2.67 (t, *J* = 6.2 Hz, 2H), 2.50 (q, *J* = 7.1 Hz, 4H), 0.96 (t, *J* = 7.1 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.5, 138.7, 128.7, 128.6, 127.3, 63.5, 57.2, 51.0, 47.6, 11.9. The spectroscopic data correspond to those previously reported in the literature.[20]

LRMS (ESI+): calc. for $C_{20}H_{26}NO_2^+$ [M+H]$^+$ 312.19, found 312.28.

Synthesis of 6

In a flame-dried Schlenk tube (25 mL), to a solution of acid **4e** (45 mg, 0.2 mmol), 3-phenylpropanamine (0.3 mmol, 1.5 equiv), Et_3N (0.6 mmol, 3 equiv) in DMF (2 mL) was added *o*-(7-Azabenzotriazol-1-yl)-N,N,N',N'-tramethyluronium hexafluorophosphate (HATU, 0.4 mmol, 2 equiv) at room temperature and the resulting mixture was stirred for 10 h at 25 ℃. The reaction was quenched with $NaHCO_3$ solution and extracted with ethyl acetate for three times. The combined organic layer was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica chromatography (PE/EtOAc 2/1) to give the 2-phenyl-*N*-(3-phenylpropyl)-2-(p-tolyl)acetamide **6** as a white solid (62 mg, 90% yield).

2-phenyl-*N*-(3-phenylpropyl)-2-(p-tolyl)acetamide (6)



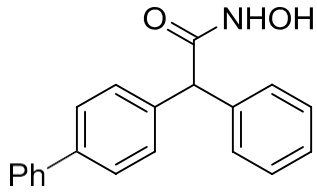
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.20 (m, 7H), 7.19 – 7.04 (m, 7H), 5.72 (t, *J* = 5.8 Hz, 1H), 4.85 (s, 1H), 3.26 (dd, *J* = 13.3, 6.9 Hz, 2H), 2.55 (t, *J* = 8 Hz, 2H), 2.31 (s, 3H), 1.81 – 1.73 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.0, 141.3, 139.7, 136.9, 136.5, 129.5, 128.9, 128.8, 128.7, 128.5, 128.3, 127.1, 126.0, 58.8, 39.4, 33.2, 31.2, 21.1. The spectroscopic data correspond to those previously reported in the literature.[17]

LRMS (ESI+): calc. for $C_{24}H_{26}NO^+$ $[M+H]^+$ 344.20, found 344.19.

Synthesis of 7

To a solution of **4h** (58 mg, 0.2 mmol), benzotriazol-1-yloxytris(dimethylamino)-phosphonium hexafluorophosphate (BOP, 0.4 mmol, 2 equiv), and hydroxylamine hydrochloride (0.3 mmol, 1.5 equiv) in pyridine (5 mL) was added Et_3N (0.6 mmol, 3 equiv) and the reaction mixture was stirred at 25 ℃ for 6 h. The solvents were removed under vacuum and the residue was purified by silica chromatography (PE/EtOAc 2/1) to give the 2-([1,1'-biphenyl]-4-yl)-*N*-hydroxy-2-phenylacetamide **7** as a white solid (49 mg, 81% yield).

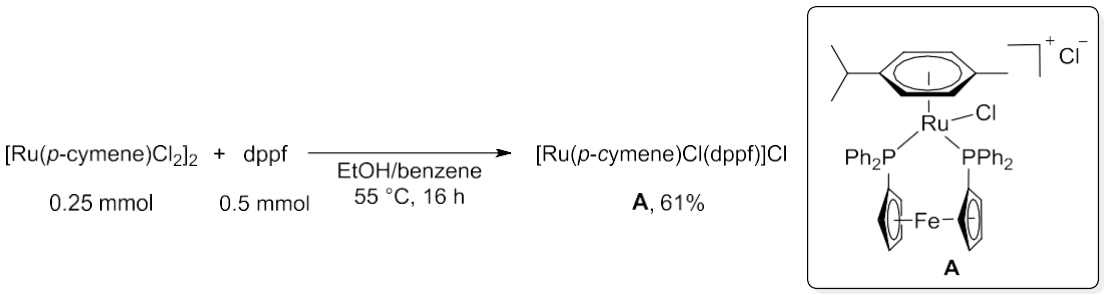
2-([1,1'-biphenyl]-4-yl)-*N*-hydroxy-2-phenylacetamide (7)

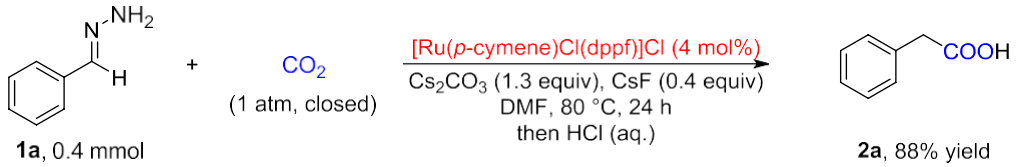


^{1}H NMR (400 MHz, DMSO-d_6) δ 11.02 (s, 1H), 9.05 (s, 1H), 7.76 – 7.55 (m, 4H), 7.51 – 7.19 (m, 10H), 4.80 (s, 1H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 168.4, 140.3, 139.6, 139.1, 129.4, 129.3, 128.9, 128.7, 127.8 , 127.2, 127.0, 127.0, 53.4. The spectroscopic data correspond to those previously reported in the literature.[17]

LRMS (ESI+): calc. for $C_{20}H_{18}NO_2^+$ $[M+H]^+$ 304.13, found 304.13.

Mechanistic Studies





First of all, the Ru-DPPF complex **A** was confirmed to be active catalyst in this transformation.

Synthesis of A

A mixture of [Ru(*p*-cymene)Cl_2]$_2$ (153 mg, 0.25 mmol) and 1,1-bis(diphenylphosphino)ferrocene (277 mg, 0.5 mmol) in ethanol (8 mL) and benzene (1 mL) was heated to 55 ℃ for 50 min and then stirred at 55 ℃ for 16 h. After evaporating the solvent, dichloromethane was used to dissolve the residue and diethyl ether was added to precipitate a dark yellow solid. This solid was then recrystallized from methanol/diethyl ether to give the [RuCl(*p*-cymene)(dppf)]Cl complex **A** (262 mg, 61% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 6H), 7.65 – 7.55 (m, 8H), 7.46 (s, 6H), 5.83 (s, 2H), 5.18 (d, *J* = 4.7 Hz, 2H), 5.06 (s, 2H), 4.37 (s, 2H), 4.27 (s, 2H), 4.09 (s, 2H), 2.73 – 2.62 (m, 1H), 1.06 (s, 3H), 0.89 (d, *J* = 6.9 Hz, 6H); **^{31}P NMR** (162 MHz, $CDCl_3$) δ 36.33; **^{13}C NMR** (101 MHz, $CDCl_3$) *δ* = 138.5–128.4 [$(C_6H_5)_4P_2Fe(C_5H_4)_2$], 99.0, 96.2, 90.5 (t, *J* = 5.1 Hz), 84.5 – 82.3 (m), 78.5(t, *J* = 4.8 Hz), 74.8, 73.8 (t, *J* = 2.9 Hz), 69.2, 30.9, 20.7, 14.9. The spectroscopic data correspond to those previously reported in the literature.[21]

Experimental procedures of using [RuCl(*p*-cymene)(dppf)]Cl as catalyst

A flame-dried Schlenk tube (25 mL) containing a stirring bar was charged with [RuCl(*p*-cymene)(dppf)][Cl] (13.8 mg, 0.016mmol, 4 mol%). The reaction tube was transferred to the glovebox and charged with Cs_2CO_3 (169 mg, 0.52 mmol, 1.3 equiv) and CsF (24 mg, 0.16 mmol, 0.4 equiv) before being sealed. The reaction tube was moved out of the glovebox and the tube was then evacuated and back-filled with carbon dioxide for 3 times. Subsequently anhydrous DMF (1 mL), benzaldehyde hydrazone (48 mg, 0.40 mmol, 1.0 equiv) and another anhydrous DMF (1 mL) were added via syringes under CO_2. Once added, the Schlenk tube was sealed at atmospheric pressure of CO_2 (1 atm). The resulting mixture was stirred for 24 h at 80 ℃ (380 r/min). After cooling to room temperature, the resulting mixture was diluted with 2 mL EtOAc and quenched by 2 mL 2N HCl. The reaction mixture was extracted by EtOAc (3 x 5 mL) and the combined organic phases were concentrated in vacuo. The residue was purified by a short silica gel flash column chromatography (0.1% AcOH in petroleum ether/EtOAc 10/1~5/1) to give the pure desired product (48 mg, 88% yield) with bromocresol green as chromogenic agent.

General Computational Calculation Details

1. Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

2. Computational Methods

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. DFT method B3-LYP[22] with a standard 6–31G(d) basis set (lanl2dz[23] basis set for Ru and Fe atoms) was used for geometry optimizations. Harmonic vibrational frequency calculations were performed for all of the stationary points to confirm them as a local minima or transition structures, and to derive the thermochemical corrections for the enthalpies and free energies. The M06-L[24] functional in combination with the 6–311+G(d,p) basis set (lanl2dz basis set for Ru and Fe atoms) was used to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with an SMD[25] solvation model in the N,N-dimethylformamide solvent.

3. Ligand Exchange of Ru Catalyst

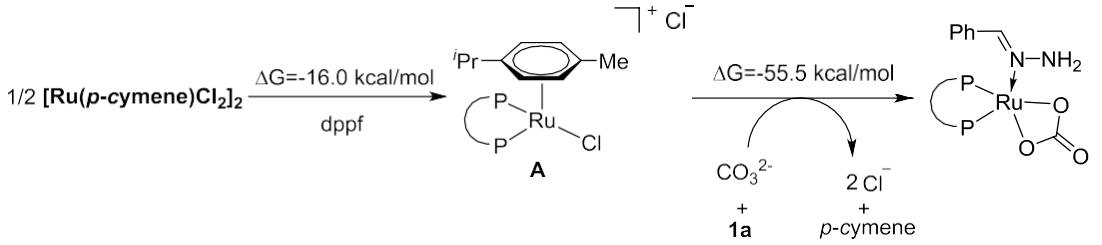


Figure S1. Ligand exchange of Ru catalyst.

4. Free Energy Profile for the Generation of Ruthenium-nitrenoid

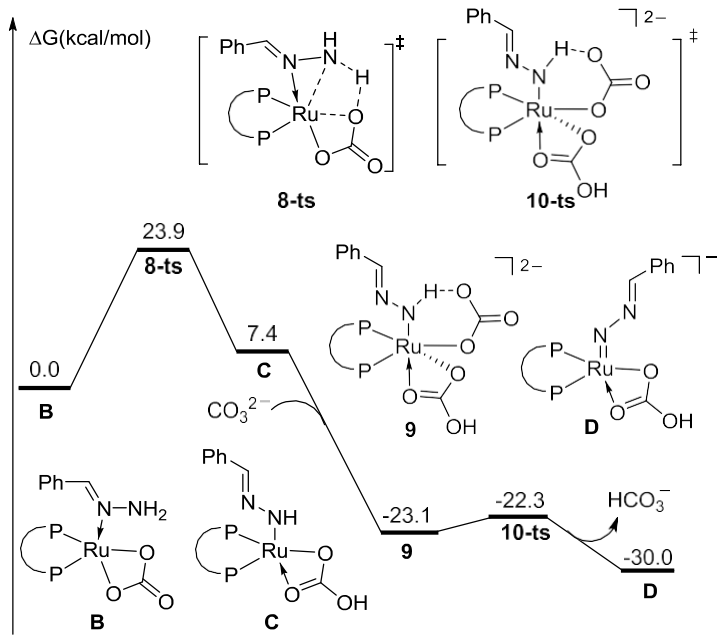


Figure S2. Free energy profile for the two steps N-H cleavage to generate ruthenium-nitrenoid.

5. Cycloaddition Between Amino-ruthenium Complex and CO_2

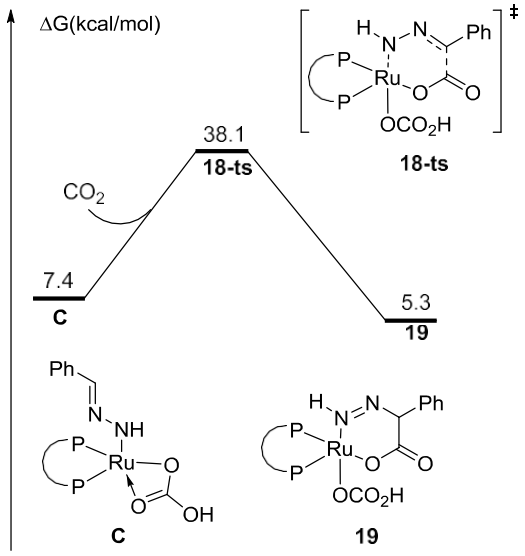


Figure S3. Free energy profile for the cycloaddition between amino-ruthenium complex and CO_2.

6. Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{(\text{elec-B3-LYP})}$ [1]	$G_{(\text{corr-B3-LYP})}$ [2]	$H_{(\text{corr-B3-LYP})}$ [3]	$E_{(\text{solv, M06-L})}$ [4]	IF[5]
[Ru(*p*-cymene)Cl_2]$_2$	-2807.735283	0.371511	0.470051	-2808.033473	-
DPPF	-2118.591843	0.447709	0.549544	-2118.88024	-
Cl^-	-460.248732	-0.01502	0.00236	-460.378806	-

A	-3062.079715	0.661294	0.785546	-3062.556433	-
CO_3^{2-}	-263.58037	-0.01158	0.018135	-264.058828	-
1a	-381.015769	0.107156	0.148181	-381.085441	-
***p*-cymene**	-389.503565	0.176222	0.224665	-389.555812	-
CO_2	-188.577571	-0.0091	0.015204	-188.632974	-
HCO_3^-	-264.42022	0.000479	0.03072	-264.600221	-
N_2	-109.520718	-0.01285	0.008905	-109.538605	-
B	-2857.360738	0.599097	0.725903	-2857.857881	-
C	-2857.37189	0.595864	0.725434	-2857.84281	-
D	-2856.808117	0.578253	0.709732	-2857.355469	-
E	-3045.426155	0.595206	0.728436	-3046.013669	-
F	-2935.938236	0.588743	0.717046	-2936.510161	-
G	-2856.779827	0.581001	0.70951	-2857.337517	-
H	-2747.300208	0.573983	0.697867	-2857.333174	-
8-ts	-2857.32579	0.594438	0.719708	-2857.815154	-737.00
9	-3121.195269	0.603443	0.741418	-3121.969405	-
10-ts	-3121.190695	0.59973	0.736525	-3121.964526	-1052.00
11-ts	-3045.369361	0.586831	0.725389	-3045.970529	-26.72
12-ts	-3045.413794	0.590293	0.725423	-3046.011998	-82.13
13	-2935.945709	0.587197	0.717384	-2936.501326	-
14	-459.552604	0.095695	0.139554	-459.733168	-
15-ts	-2856.76065	0.580268	0.707947	-2857.315117	-393.27
16-ts	-2856.7754	0.579471	0.707569	-2857.333174	-236.54
17-ts	-2935.866998	0.583039	0.713439	-2936.444327	-132.84
18-ts	-3045.902122	0.604042	0.740409	-3046.444243	-383.72
19	-3045.968872	0.60971	0.743345	-3046.502184	-

[1]The electronic energy calculated by B3-LYP in gas phase. [2]The thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. [3]The thermal correction to enthalpy calculated by B3-LYP in gas phase. [4]The electronic energy calculated by M06-L in N,N-dimethylformamide solvent. [5]The B3-LYP calculated imaginary frequencies for the transition states.

7. B3LYP Geometries for All the Optimized Compounds and Transition State

[Ru(*p*-cymene)Cl_2]$_2$

Ru	1.86012400	-0.15613100	0.19090400
Cl	-0.05745300	-0.00913600	-1.40625500
Cl	1.68327000	2.25641400	0.50193600
C	3.27384100	-0.88869400	-1.35384300
C	2.59622700	-2.02547100	-0.79593800
C	2.59453500	-2.27205300	0.59314300
C	3.27518600	-1.31512000	1.42892200
C	3.95909400	-0.20676200	0.88129300
C	3.98435400	0.02692600	-0.53990200
H	3.16554800	-0.69338100	-2.41382400
H	1.98676600	-2.64517400	-1.44471000
H	3.19146300	-1.40555100	2.50716600
H	4.38924000	0.53482600	1.54571000
C	1.83574100	-3.42329700	1.19189500
H	2.50787500	-4.27907700	1.34009300
H	1.40909700	-3.14659500	2.15955700
H	1.01036300	-3.72984000	0.54411300
C	4.71540400	1.24153700	-1.08192500
C	4.18100300	1.74743100	-2.42787400
C	6.22672600	0.93395200	-1.15634300
H	4.56060600	2.04155500	-0.34781400
H	3.10924100	1.95872900	-2.36983200
H	4.69561900	2.67584600	-2.69752700
H	4.36132400	1.03095700	-3.23914900
H	6.62740700	0.61875200	-0.18606600
H	6.43148100	0.13680200	-1.88144400
H	6.77583500	1.82746800	-1.47341800
Ru	-1.89171200	-0.02184600	0.30367600
Cl	0.02327000	-0.42112400	1.87213600
Cl	-2.03191300	-2.42665900	0.00549800
C	-3.04961800	1.41826100	-0.89780000
C	-2.32479100	2.17961400	0.07710200
C	-2.42923500	1.87729400	1.45169700
C	-3.28471600	0.78132400	1.83158800
C	-4.02111500	0.05757700	0.86725400
C	-3.93138000	0.36611900	-0.53518300
H	-2.84754800	1.60637100	-1.94570800
H	-1.59293400	2.90834000	-0.25333600
H	-3.30393700	0.45978600	2.86759500
H	-4.58105200	-0.81819900	1.17771600
C	-1.61562500	2.61511900	2.47761000
H	-2.15972800	3.51089200	2.80606600
H	-1.42624100	1.98821200	3.35280700
H	-0.64983700	2.91632200	2.06256000
C	-4.71751900	-0.45937400	-1.53752100
C	-4.06007000	-0.54899400	-2.92116900
C	-6.16036000	0.08059600	-1.63193200
H	-4.75482200	-1.47663000	-1.12866000
H	-3.03276600	-0.91772900	-2.84347200
H	-4.62563600	-1.24493900	-3.55001900
H	-4.05212600	0.41924500	-3.43717000
H	-6.65162200	0.10223300	-0.65226500
H	-6.17333800	1.09927700	-2.03862000
H	-6.75847600	-0.55480200	-2.29468200

DPPF

C	1.97572300	0.54819800	0.26669100
C	1.66617100	-0.07222300	1.52531700
C	0.57941300	0.63101300	2.12235500
C	0.20616600	1.69392000	1.24521300
C	1.05278400	1.63867700	0.10156100
H	2.15232600	-0.95197400	1.92442300
H	0.09169700	0.37565700	3.05412400
H	-0.61233300	2.38506900	1.39274800
H	0.99862100	2.28990100	-0.76149200
C	-2.01800900	-0.62631800	0.06691300
C	-1.45051900	-0.27707800	-1.20621600
C	-0.38280100	-1.17852400	-1.48773400
C	-0.27496200	-2.09478400	-0.39733000
C	-1.27073300	-1.75145100	0.56149300
H	-1.75886100	0.55597500	-1.82280500
H	0.26729000	-1.13677600	-2.35198800
H	0.46983200	-2.87223100	-0.29118700
H	-1.42739100	-2.23490400	1.51727500
Fe	0.00496400	-0.14407900	0.27651500
P	3.24984100	0.12873500	-0.98324300
P	-3.40985700	0.11093500	1.00550400
C	3.77952900	-1.56590000	-0.43748000
C	3.35273300	-2.65984400	-1.20680300
C	4.59219500	-1.81070200	0.68114300
C	3.70331400	-3.96546500	-0.85505700
H	2.74773900	-2.48562700	-2.09343300
C	4.94723400	-3.11443500	1.03231100
H	4.95743200	-0.97712500	1.27438300

C	4.50011300	-4.19519900	0.26808100
H	3.36427200	-4.79976400	-1.46389900
H	5.57739000	-3.28607700	1.90142400
H	4.78046000	-5.20929300	0.54058300
C	4.68799300	1.16231200	-0.42718200
C	5.78454900	1.25137600	-1.30203600
C	4.72904600	1.88862500	0.77261600
C	6.89919400	2.02402800	-0.97771200
H	5.76193800	0.71319700	-2.24729600
C	5.84077000	2.67255000	1.09275000
H	3.88937200	1.84487300	1.45994200
C	6.92933700	2.73962000	0.22192700
H	7.73936500	2.07618000	-1.66550000
H	5.85457900	3.23031300	2.02589900
H	7.79287500	3.35027600	0.47223600
C	-3.73215800	1.68312100	0.07147000
C	-3.43713100	2.89488200	0.71524300
C	-4.27676800	1.72753600	-1.22232300
C	-3.65140700	4.11856500	0.07597200
H	-3.04854800	2.87829900	1.73090900
C	-4.49457300	2.94870300	-1.86189900
H	-4.54322000	0.80309800	-1.72699200
C	-4.17804400	4.14696900	-1.21608900
H	-3.41679000	5.04678500	0.59063700
H	-4.91648300	2.96539100	-2.86369000
H	-4.35130500	5.09720300	-1.71435400
C	-4.83508500	-0.94261400	0.45006700
C	-6.04781300	-0.79341100	1.14464400
C	-4.76498900	-1.89708800	-0.57601200
C	-7.16444200	-1.55847900	0.80920100
H	-6.11586800	-0.07376300	1.95777400
C	-5.88019100	-2.67236700	-0.90473700
H	-3.83559400	-2.03850800	-1.11954600
C	-7.08270300	-2.50324800	-0.21695400
H	-8.09492200	-1.42494500	1.35514000
H	-5.80736300	-3.40859600	-1.70145200
H	-7.94895900	-3.10741700	-0.47355500
Cl-			
Cl	0.00000000	0.00000000	0.00000000
A			
Ru	0.06452300	1.03307200	-0.85542300
Cl	-0.00118600	-0.35957600	-2.85428400
C	1.60030100	2.80913300	-0.95155300
C	0.99275500	2.68641300	-2.20833200
C	-0.42323700	2.86429500	-2.36652400
C	-1.18051600	3.03312300	-1.19871600
C	-0.55619600	3.12622600	0.08616400
C	0.84295100	3.10573900	0.23123500
H	2.67528700	2.69166600	-0.88304600
H	1.59880200	2.44829200	-3.07587400
H	-2.26003900	3.10844100	-1.26616200
H	-1.18927200	3.27089800	0.95219400
C	-1.04321000	2.83426100	-3.73322100
H	-0.73481300	1.93306000	-4.27355400
H	-2.13461500	2.86006200	-3.68013100
H	-0.70807000	3.70530500	-4.30988800
C	1.56567400	3.48656300	1.51554400
C	0.64443500	3.66404100	2.72902400
C	2.36874000	4.78691700	1.27238800
H	2.28505100	2.68977100	1.74136100
H	0.02229800	2.78485200	2.92031200
H	1.24893000	3.84719300	3.62282700
H	-0.01963500	4.52744400	2.60282600
H	3.09087300	4.68444600	0.45582500
H	1.69991900	5.62094600	1.03047400
H	2.92462200	5.05259800	2.17756800
Fe	-0.21487100	-3.25352600	0.51788600
P	1.75928500	-0.52966500	-0.14331700
P	-1.83347800	-0.15145700	0.11347100
C	2.38628700	-0.32917100	1.58424700
C	3.27214300	-0.30129400	-1.18432200
C	1.55040300	0.20526000	2.57324300
H	0.56748400	0.57097100	2.29733200
C	-1.70075800	-1.84565000	0.81996100
C	-3.29764400	0.05965600	-2.33860500
H	-2.38581000	0.43293600	-2.78392700
C	-5.62200800	-0.58175600	-2.57242300
H	-6.51667500	-0.67574700	-3.18126900
C	1.45560400	-2.33421900	-0.20945600
C	4.53443000	-0.81625300	-3.19640600
H	4.63660600	-1.39002100	-4.11295000
C	3.66390200	-0.78549100	1.95769500
H	4.33099200	-1.20942100	1.21439500
C	-2.60980800	0.86968300	1.47026900
C	5.50887300	0.11732700	-2.84137500
H	6.37383400	0.27464600	-3.47912400
C	3.23921900	-0.17453200	4.26270600
H	3.56948400	-0.11466800	5.29567300

C	-3.30386700	-0.34608400	-0.99932600
C	-4.49269900	-0.86905800	-0.45256500
H	-4.52617500	-1.18057000	0.58695300
C	-1.12809100	-2.28513000	2.07133900
H	-0.57411100	-1.68844600	2.77943300
C	-4.45193300	-0.06009300	-3.12016700
H	-4.42648200	0.24802500	-4.16166800
C	4.26086000	0.63607400	-0.83436800
H	4.18790300	1.18916000	0.09766700
C	5.37078900	0.84147400	-1.65522500
H	6.13129900	1.55959900	-1.36128700
C	4.08532800	-0.70518000	3.28550900
H	5.07519000	-1.06125700	3.55605300
C	-2.24762500	-3.01686500	0.18408000
H	-2.71996100	-3.03991200	-0.78690800
C	1.41874100	-4.56561300	0.43699600
H	1.51575400	-5.46297300	1.03373300
C	3.42360000	-1.02586100	-2.37687000
H	2.67805600	-1.75350600	-2.67240700
C	-2.03918200	-4.13620200	1.03663300
H	-2.31572500	-5.15816300	0.81353900
C	-5.63929000	-0.98706000	-1.23389700
H	-6.54705200	-1.39361100	-0.79731100
C	-3.75866100	2.54891200	3.43157000
H	-4.20542700	3.18851200	4.18698700
C	-2.80804900	1.59331400	3.78985600
H	-2.51425500	1.47869500	4.82951800
C	-2.23557200	0.76706600	2.81886000
H	-1.51475100	0.02619400	3.13590300
C	1.96990000	0.28081500	3.90396900
H	1.30776500	0.70019400	4.65641900
C	-4.14209700	2.66342200	2.09395500
H	-4.89495300	3.39031500	1.80208300
C	0.82965100	-3.10914700	-1.25453100
H	0.40838600	-2.71291800	-2.16395600
C	-3.57833100	1.83101900	1.12566900
H	-3.92120600	1.91517200	0.09974100
C	1.82329400	-3.26198600	0.83399800
H	2.28292500	-3.00887000	1.77714500
C	-1.35655600	-3.68546700	2.20229000
H	-1.01871100	-4.30346800	3.02369300
C	0.81262500	-4.47099100	-0.84814700
H	0.36594400	-5.28549800	-1.40313900

CO_3^{2-}

C	0.00022200	-0.00004800	-0.00006000
O	1.19258200	-0.54979400	0.00003200
O	-1.07274000	-0.75746200	0.00003300
O	-0.12000800	1.30729300	-0.00002100

1a

C	2.78230200	-0.26576200	0.01104500
C	2.30204500	1.04445300	0.01008600
C	0.92791800	1.28494600	-0.00035500
C	0.01221200	0.22048200	-0.00967000
C	0.50693400	-1.09692800	-0.01059500
H	3.85219300	-0.45595400	0.01857000
H	2.99627000	1.88070000	0.01689900
H	0.55712000	2.30790500	-0.00185400
H	-0.20034600	-1.91991500	-0.02162400
C	-1.42509000	0.50877800	-0.01541800
H	-1.71485500	1.57013900	-0.04392500
N	-2.31133000	-0.41943800	0.00897300
N	-3.62957500	-0.05647200	-0.08178600
H	-4.21158800	-0.75185800	0.37075300
H	-3.84114500	0.88460700	0.25898000
C	1.87745200	-1.33391800	0.00040500
H	2.24605000	-2.35656600	-0.00110100

***p*-cymene**

C	1.36439100	1.18545800	0.01517200
C	-0.02173500	1.04676700	0.00873300
C	-0.62558400	-0.22031900	-0.00225100
C	0.21712200	-1.33715400	-0.00533200
C	1.60694200	-1.19879000	0.00108900
C	2.20740100	0.06441700	0.00862900
H	1.80119900	2.18225500	0.02692200
H	-0.64104000	1.94079600	0.01587500
H	-0.21891300	-2.33417800	-0.00940500
H	2.23284500	-2.08882900	0.00127400
C	-2.13994000	-0.38270300	-0.00633200
H	-2.34840700	-1.46154700	-0.01725800
C	3.71054100	0.22210100	-0.00968100
H	4.21376700	-0.70733400	0.27666600
H	4.07269000	0.49604100	-1.00979100
H	4.04085600	1.00946100	0.67789800
C	-2.78404100	0.19694500	1.26775400
H	-3.86605500	0.01754500	1.27093000
H	-2.35923400	-0.25876200	2.16889000
H	-2.62650200	1.28009300	1.33570700
C	-2.77950400	0.22188900	-1.27104200

H	-2.35211100	-0.21664800	-2.17944900
H	-3.86161900	0.04339700	-1.28111500
H	-2.62103400	1.30604000	-1.31758000

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16958400
O	0.00000000	0.00000000	-1.16958400

HCO_3^-

C	-0.15878700	-0.07259800	-0.00001500
O	0.13801900	-1.29193500	0.00002500
O	-1.24086400	0.53306600	-0.00002200
O	1.00726900	0.79655900	0.00006400
H	1.71732400	0.13406300	-0.00045400

N_2

N	0.00000000	0.00000000	0.55265200
N	0.00000000	0.00000000	-0.55265200

B

Fe	-1.67507200	-2.90491500	0.38315400
P	1.15994900	-1.03603000	-0.05581500
P	-2.13125100	0.47703900	0.04142100
C	1.74319400	-1.20157900	1.69219200
C	2.68546000	-1.41883000	-1.05838800
C	1.36693500	-0.22062600	2.62338100
H	0.78816400	0.63965100	2.29925800
C	-2.59073300	-1.12034200	0.81749700
C	-2.56685700	0.35203900	-2.74225500
H	-1.48176900	0.30115200	-2.81552700
C	-4.71774700	0.42617800	-3.84362100
H	-5.31214100	0.41270100	-4.75331500
C	0.21391900	-2.59034900	-0.33939900
C	3.63678500	-2.11701400	-3.18987200
H	3.49097700	-2.46507500	-4.20930100
C	2.54076800	-2.27718400	2.12187300
H	2.87296600	-3.02559400	1.40870400
C	-3.02506000	1.69408000	1.11914200
C	4.92763900	-1.93692100	-2.68650100
H	5.79256500	-2.14358400	-3.31142000
C	2.53593200	-1.41227000	4.38148000
H	2.84122800	-1.49486300	5.42139300
C	-3.18145500	0.46856200	-1.48734400
C	-4.58000700	0.57965100	-1.43130700
H	-5.07264300	0.69786000	-0.47071000
C	-1.97592100	-1.66935000	1.99856000
H	-1.16779200	-1.21861000	2.55795700
C	-3.32738600	0.32816800	-3.91364000
H	-2.83232600	0.24241500	-4.87730300
C	3.98541900	-1.22492100	-0.57077600
H	4.14094400	-0.86163900	0.43894400
C	5.09635400	-1.48802800	-1.37717400
H	6.09412400	-1.33241600	-0.97585000
C	2.93139100	-2.38304000	3.45705500
H	3.54827300	-3.22008400	3.77382100
C	-3.57389900	-2.07337600	0.37783000
H	-4.18762400	-1.97995100	-0.50650900
C	-0.75364900	-4.69859400	-0.17894000
H	-1.03214000	-5.67374100	0.19952300
C	2.52836500	-1.85945400	-2.38392100
H	1.53395000	-2.01407900	-2.79185500
C	-3.55234500	-3.18696900	1.26612400
H	-4.14837000	-4.08515600	1.16861600
C	-5.34193700	0.55463200	-2.60011500
H	-6.42345100	0.64374400	-2.54004400
C	-4.37088300	3.58749700	2.70363200
H	-4.88699600	4.32091900	3.31773300
C	-4.17480500	2.29012400	3.17675100
H	-4.54155100	2.00407100	4.15929700
C	-3.50662400	1.34848500	2.39110300
H	-3.37110800	0.34378900	2.77557200
C	1.76012900	-0.33134600	3.96114800
H	1.46131900	0.43610900	4.67026000
C	-3.89489100	3.93975300	1.43956500
H	-4.02856900	4.95114600	1.06649600
C	-0.71389000	-2.76235100	-1.42772400
H	-0.96873100	-2.01352600	-2.16520700
C	-3.22794100	3.00383300	0.65020100
H	-2.83603000	3.29636000	-0.31671100
C	0.18179000	-3.80870200	0.42443400
H	0.72099400	-3.99281700	1.34184400
C	-2.57163300	-2.93480200	2.26995200
H	-2.28908100	-3.60734300	3.06946900
C	-1.30499300	-4.05414000	-1.32469700
H	-2.07318800	-4.45286400	-1.97425200
Ru	0.07083900	1.00709300	-0.62817800
C	-0.14968000	3.36754100	0.27172500
O	-0.14294100	4.50355000	0.70458200
O	-0.62158500	2.97108200	-0.91529200
O	0.32784100	2.29421700	0.93784200

C	4.41815200	2.13446500	1.75164100	H	-3.78538600	0.42455000	0.88864300
C	5.78797700	2.14683300	1.47161300	C	1.79072400	1.46998500	-3.28553600
C	6.22673500	2.17680300	0.14510600	H	2.67722100	0.88517500	-3.51454500
C	5.29653200	2.18184100	-0.89103500	C	2.47239700	-1.95480300	-1.04245500
C	3.91712800	2.14301900	-0.61656400	H	2.70262500	-1.06204600	-0.46614700
C	3.48039000	2.13781600	0.72033700	C	3.44917100	-2.51850400	-1.87165700
H	4.07321800	2.13127400	2.78169800	H	4.41917500	-2.03552900	-1.95544900
H	6.51055500	2.14916400	2.28351100	C	0.69372800	-4.98004700	2.76058900
H	7.28946500	2.20187800	-0.08027900	H	1.42094900	-5.78419600	2.83757400
H	5.63683300	2.20342400	-1.92390600	C	-3.07602200	0.91410100	-2.35840400
H	2.41664700	2.17196000	0.93903500	H	-2.45378800	1.15842800	-3.20729600
C	3.00251000	2.16674500	-1.75634800	C	-3.68126700	-2.95823500	-1.52415700
H	3.44542400	2.49752500	-2.70353600	H	-4.70460900	-3.30920800	-1.49525500
N	1.75218900	1.85905700	-1.76291400	C	0.95456600	-3.73601000	-1.64615600
N	1.04831000	1.97629800	-2.97593400	H	-0.01024600	-4.22556100	-1.56185900
H	0.28157900	2.62588100	-2.76995100	C	-4.40492900	0.40412200	-2.41203800
H	1.64175200	2.36535900	-3.71516900	H	-4.96154800	0.18571600	-3.31445000
C				C	0.25980700	3.26428500	-3.81088000
Fe	-3.13615400	-0.95306100	-1.46505100	H	-0.04822600	4.08255200	-4.45653200
P	-0.09552500	-1.80976200	0.16916200	C	-1.80934900	5.82467900	1.35640100
P	-1.07094900	1.53058600	-0.30004200	H	-1.96181400	6.82796900	1.74547700
C	-0.17015800	-3.05122500	1.55658000	C	-2.89190300	5.08537600	0.88126100
C	1.20833600	-2.54749700	-0.93513600	H	-3.89254200	5.50947300	0.89775700
C	-1.14524600	-2.89221600	2.55965000	C	-2.69791600	3.79512300	0.37796900
H	-1.83944600	-2.05910400	2.51857600	H	-3.54912800	3.23338400	0.00792700
C	-2.68288800	0.99869000	-0.97724800	C	-1.20907500	-3.78244000	3.63270700
C	1.05479000	1.18048000	-2.13325800	H	-1.97292200	-3.64693300	4.39399500
H	1.37652200	0.39068000	-1.46777100	C	-0.52646000	5.26908400	1.33131800
C	1.39326100	2.50849900	-4.12704600	H	0.32216400	5.83798500	1.70192800
H	1.96727000	2.73727200	-5.02115300	C	-1.66244400	-2.13805700	-2.28204000
C	-1.58949400	-2.21443600	-0.84584500	H	-0.87546200	-1.78531000	-2.93405700
C	1.93410900	-4.30058500	-2.46158000	C	-0.33250400	3.98169000	0.83656600
H	1.71966400	-5.21847000	-3.00284500	H	0.66490700	3.55049000	0.83173100
C	0.75517400	-4.09952500	1.67825700	C	-2.85308400	-2.71370300	-0.38879000
H	1.52918800	-4.23279600	0.93138200	H	-3.13560800	-2.86433300	0.64311000
C	-1.41546000	3.23171900	0.34885300	C	-4.84797600	0.17547500	-1.07461800
C	3.18383300	-3.68657200	-2.58444000	H	-5.80106000	-0.24758100	-0.78468100
H	3.94415300	-4.12114200	-3.22836500	C	-2.94343400	-2.60938100	-2.69442200
C	-0.29140600	-4.82961600	3.73680400	H	-3.30646100	-2.64798200	-3.71334300
H	-0.33835800	-5.51736300	4.57706300	Ru	-0.15243700	0.23232600	1.30880600
C	-0.08771000	1.92161700	-1.81591800	C	-1.77552800	1.04779100	3.14313600
C	-0.47423400	2.97706800	-2.66096800	O	-2.57889300	1.46605500	4.14060500
H	-1.34448300	3.57884800	-2.41536100	O	-0.63766400	1.59285700	2.98783400
C	-3.79397200	0.53190200	-0.18670600	O	-2.19291800	0.12150500	2.39143300

C	7.02567400	-0.14055500	-0.38366200
C	7.92673900	0.92481900	-0.27826200
C	7.51112400	2.11553600	0.32203500
C	6.20893000	2.24245000	0.80130100
C	5.28542500	1.18543800	0.68507300
C	5.72472900	-0.01723100	0.09473900
H	7.34714200	-1.07934600	-0.82876800
H	8.94328200	0.82238600	-0.64836200
H	8.20385500	2.94779000	0.41902200
H	5.89222900	3.17376000	1.26601100
H	5.04016800	-0.85693600	0.04483300
C	3.93082200	1.36379200	1.19260500
H	3.76013100	2.21892500	1.86438100
N	2.94491700	0.56654000	0.90737800
N	1.76790900	0.74762000	1.51570200
H	1.77389400	1.59228300	2.11052300
H	-2.09837300	2.18008400	4.59508700

D

Fe	-0.31120700	0.09022700	2.95047700
P	0.65098000	1.49326300	0.00150500
P	-1.90771100	-0.87462700	-0.00536700
C	-0.30043700	3.07642600	0.26165700
C	2.25675400	2.19432500	-0.61746800
C	-1.61637900	3.16929400	-0.21391900
H	-2.04405800	2.33420100	-0.76093700
C	-1.93562000	-0.57094500	1.82110500
C	-0.73598600	-3.41496900	-0.52747900
H	0.08493600	-2.83346600	-0.93753600
C	-1.74156800	-5.55947600	-0.00960600
H	-1.69819900	-6.64660900	-0.01045700
C	1.07548700	0.99257500	1.72122200
C	4.68174100	2.37540200	-0.59934400
H	5.63509500	2.09566200	-0.15808400
C	0.27236500	4.19658900	0.88807300
H	1.30730100	4.15920500	1.21703200
C	-3.72488200	-0.65196800	-0.42174500
C	4.64030400	3.22013700	-1.70691000
H	5.56163400	3.61525500	-2.12907800
C	-1.78653300	5.43888900	0.62081800
H	-2.36157000	6.35168400	0.76048100
C	-1.85520100	-2.74750100	-0.01394800
C	-2.92075200	-3.50864900	0.49726400
H	-3.80154700	-3.00824300	0.88970700
C	-2.22225500	0.68318400	2.46686100
H	-2.44256300	1.61448700	1.96298100
C	-0.68136300	-4.81263600	-0.52337600
H	0.19474400	-5.31269400	-0.92916700
C	2.22750800	3.03473600	-1.74439700
H	1.27496500	3.28079600	-2.20639500
C	3.40659500	3.54801500	-2.27993100
H	3.36386900	4.19932400	-3.15001000
C	-0.46628900	5.36594700	1.07427800
H	-0.00838500	6.22299300	1.56346400
C	-1.63818000	-1.51211500	2.86333500
H	-1.34293600	-2.53986100	2.70716500
C	1.31321900	0.82892300	4.02653700
H	1.27822300	1.06569400	5.08297900
C	3.49771600	1.86366500	-0.05782700
H	3.54861300	1.19954800	0.79834500
C	-1.74896900	-0.85302300	4.12395200
H	-1.54467200	-1.29540400	5.09101600
C	-2.86462700	-4.90245800	0.50195600
H	-3.69941900	-5.47538700	0.90034000
C	-6.38835500	-0.29252500	-1.28892400
H	-7.41335300	-0.15043400	-1.62410300
C	-6.02350500	0.02865800	0.01810400
H	-6.76575600	0.41667900	0.71300200
C	-4.70476900	-0.15046200	0.44841900
H	-4.44885600	0.09466000	1.47369900
C	-2.35444700	4.34327000	-0.03084900
H	-3.37103700	4.40000200	-0.41214200
C	-5.42246300	-0.79696500	-2.16446400
H	-5.69143200	-1.04747600	-3.18802300
C	1.50504400	-0.34133000	2.04479700
H	1.66195600	-1.12624800	1.31658900
C	-4.10735100	-0.97202800	-1.73809000
H	-3.36119000	-1.35588100	-2.42764800
C	0.96569400	1.71202700	2.96149700
H	0.61284400	2.72722300	3.07331000
C	-2.11920300	0.50330700	3.87943100
H	-2.24517000	1.27648700	4.62705500
C	1.64921800	-0.43692400	3.45780800
H	1.92109400	-1.32937600	4.00708800
Ru	-0.25527700	-0.01698600	-1.38603900
C	-1.72600500	0.25910600	-3.59101700
O	-2.36701700	0.43601500	-4.79274300
O	-1.23131900	-0.88488500	-3.35861900
O	-1.68516700	1.23958000	-2.81022900

C	5.85124200	-3.08102900	0.94414200
C	7.12027600	-2.85565400	0.39306300
C	7.21301200	-2.10849000	-0.78620700
C	6.07145400	-1.59799900	-1.39688000
C	4.77952600	-1.81134800	-0.85349900
C	4.70639200	-2.57623600	0.33972200
H	5.75573700	-3.66476700	1.85869100
H	8.01221300	-3.25489700	0.87010300
H	8.18748400	-1.92128600	-1.23515100
H	6.16239200	-1.01700100	-2.31282600
H	3.72854800	-2.76729900	0.77132900
C	3.62394200	-1.26072100	-1.51312600
H	3.75856600	-0.73776400	-2.46378700
N	2.40412600	-1.36529000	-1.00280100
N	1.34699800	-0.98767000	-1.58556600
H	-2.25947200	-0.41698900	-5.24668500

E

Fe	2.91305000	-0.25453800	-2.03755900
P	0.66895500	-1.83572700	0.06926100
P	0.92483300	1.77527600	-0.08980800
C	-0.15053300	-3.12946700	-0.99267800
C	1.10060600	-2.81863900	1.59515300
C	-0.89815000	-2.71819200	-2.10716900
H	-1.04573800	-1.65941100	-2.28929000
C	1.84741800	1.45704100	-1.64928800
C	2.63952200	1.64831900	2.15084200
H	2.08153700	0.74654900	2.38401200
C	4.34641300	3.26650400	2.73651400
H	5.14354900	3.59910200	3.39767400
C	2.31430900	-1.76841100	-0.76551000
C	2.60973000	-4.20273100	2.91504700
H	3.57521800	-4.69226500	3.02447100
C	-0.01312500	-4.50397500	-0.74364000
H	0.55050400	-4.84506900	0.11833800
C	0.08994700	3.38633100	-0.54542100
C	1.64710000	-4.31249600	3.91933000
H	1.85820600	-4.88674300	4.81906100
C	-1.33581300	-5.02526100	-2.70342100
H	-1.79892900	-5.75796700	-3.36052100
C	2.28222300	2.40668900	1.02564500
C	2.95510800	3.61669000	0.78759700
H	2.66506000	4.23654300	-0.05608000
C	1.25712300	0.76492600	-2.76213000
H	0.24503900	0.37867900	-2.75682400
C	3.66831600	2.07499400	2.99661600
H	3.92835200	1.47690500	3.86677400
C	0.13508300	-2.93734600	2.61082700
H	-0.82877800	-2.45252200	2.48848100
C	0.41184300	-3.68187100	3.75897600
H	-0.34721100	-3.76327100	4.53330100
C	-0.60191200	-5.44346900	-1.59188800
H	-0.49062800	-6.50418100	-1.37813300
C	3.19705800	1.78584800	-2.02164000
H	3.92379100	2.27342600	-1.38693100
C	4.04064500	-1.98959200	-2.30649400
H	4.58603700	-2.23055600	-3.21038700
C	2.33748000	-3.46396300	1.76079400
H	3.09565800	-3.39743600	0.98778700
C	3.43364700	1.28559500	-3.33750300
H	4.37364800	1.33134100	-3.87357100
C	3.98243300	4.04110400	1.63159700
H	4.49268900	4.98074300	1.43145000
C	-1.16838600	5.83735000	-1.14617100
H	-1.65745400	6.78064100	-1.37902800
C	-0.24440400	5.28655100	-2.03402200
H	-0.00853600	5.79656200	-2.96555400
C	0.37889500	4.07181900	-1.73638000
H	1.09027800	3.65750800	-2.44272500
C	-1.48232400	-3.66064600	-2.95687200
H	-2.06651000	-3.32168400	-3.80892800
C	-1.46802800	5.16071400	0.03783100
H	-2.19682000	5.57242600	0.73207500
C	3.47863900	-1.09701200	-0.25305200
H	3.52696900	-0.54500000	0.67514100
C	-0.84931300	3.94598700	0.33756800
H	-1.11895100	3.41119700	1.24207700
C	2.67990700	-2.32253400	-2.03809400
H	2.01354300	-2.86153500	-2.69648600
C	2.23387400	0.65726200	-3.79268900
H	2.10358200	0.14524400	-4.73780000
C	4.53744400	-1.23917700	-1.19827900
H	5.52602300	-0.80632400	-1.11077000
Ru	-0.52465000	0.09105200	0.67967800
C	-0.97425100	1.10124300	3.09702200
O	-1.41495100	1.61408900	4.28535300
O	-0.04599700	0.25802400	3.10494000
O	-1.55000600	1.54162200	2.05613800
H	-0.88588700	1.15217600	4.95753700

C	-3.26241800	-1.15411100	0.90861700
C	-3.55491200	0.14750000	0.10925500
H	-3.22369300	0.98227500	0.73447200
N	-2.70582800	0.17806100	-1.16637500
N	-1.47823000	0.19063500	-1.09743600
C	-4.99803400	0.33066800	-0.27697300
C	-5.66493800	-0.62095500	-1.06345100
C	-5.69653000	1.47872700	0.11206700
C	-6.98996400	-0.42479100	-1.44783900
H	-5.13608500	-1.52099400	-1.35737500
C	-7.02751200	1.67802900	-0.26615200
H	-5.18924900	2.22542800	0.71960800
C	-7.67900500	0.72583500	-1.05024400
H	-7.49176100	-1.17484000	-2.05609100
H	-7.55117100	2.57800600	0.05017600
H	-8.71461400	0.87575700	-1.34923000
O	-2.02829600	-1.28644600	1.28974900
O	-4.15725300	-1.96349400	1.14545800

F

Fe	-0.18291100	-0.36579900	3.00947400
P	1.73891500	-0.58343600	0.14929300
P	-1.84552600	-0.15412800	0.03003100
C	3.12850000	0.63690100	0.40440400
C	2.73011800	-2.08518800	-0.37801100
C	3.00513000	1.70549600	1.30682400
H	2.08488900	1.84167200	1.86289000
C	-1.65896500	0.37135800	1.78886400
C	-2.33745000	-2.94623300	-0.11518100
H	-1.35909100	-2.97815800	-0.58527600
C	-4.35218100	-4.08674100	0.60315500
H	-4.92051600	-5.00452400	0.73733200
C	1.37350000	-1.10187600	1.88699700
C	4.15159800	-3.99099300	0.15477500
H	4.66549800	-4.59646500	0.89854400
C	4.30657000	0.54499300	-0.35389600
H	4.41798800	-0.24879700	-1.08358600
C	-3.20840900	1.00899900	-0.51072300
C	4.23438000	-4.32053600	-1.19989900
H	4.81198600	-5.18602400	-1.51812300
C	5.22511800	2.49396800	0.75280100
H	6.03534800	3.20627100	0.89031400
C	-2.87959900	-1.70692500	0.25635100
C	-4.18483500	-1.67818900	0.77699100
H	-4.64120900	-0.72696400	1.03529000
C	-0.78592700	1.43956000	2.18916800
H	-0.20243800	2.04242800	1.50657900
C	-3.06759100	-4.12640400	0.06081000
H	-2.62996500	-5.07607400	-0.23839100
C	2.82309800	-2.42097200	-1.73830500
H	2.32307500	-1.80221100	-2.47364100
C	3.57372300	-3.52970700	-2.14050800
H	3.63632300	-3.77291000	-3.19866200
C	5.34102100	1.46672100	-0.18482100
H	6.23969500	1.37781500	-0.79023400
C	-2.23282200	-0.17161500	2.99194600
H	-2.90079300	-1.01972300	3.04081800
C	1.22800500	-1.35788300	4.19537800
H	1.36362900	-1.19289300	5.25708900
C	3.40903900	-2.88110200	0.56017500
H	3.36063400	-2.63481200	1.61647100
C	-1.70327900	0.54246400	4.10863600
H	-1.90817800	0.33241400	5.15118800
C	-4.91246700	-2.85576200	0.95544500
H	-5.92078000	-2.81099400	1.36161800
C	-5.26416800	2.71582000	-1.41078200
H	-6.05351200	3.37786500	-1.75983700
C	-4.89448300	2.71085900	-0.06541400
H	-5.39337100	3.37009700	0.64178800
C	-3.87575800	1.86421200	0.38070400
H	-3.59581800	1.88108500	1.42907700
C	4.05002900	2.61183800	1.49575500
H	3.93046500	3.42545800	2.20707700
C	-4.60513400	1.87046200	-2.30623500
H	-4.87678300	1.87272100	-3.35926100
C	0.42824500	-2.14432900	2.18176700
H	-0.15099800	-2.68557100	1.44748800
C	-3.58504300	1.02551800	-1.86489300
H	-3.05752500	0.39417000	-2.57324500
C	1.87722200	-0.63612000	3.15055200
H	2.59806900	0.15567100	3.28900300
C	-0.81174900	1.54005600	3.61001900
H	-0.22374100	2.22591800	4.20677900
C	0.33671300	-2.29620900	3.59508600
H	-0.33031400	-2.97024600	4.11745500
Ru	0.03825400	-0.20680700	-1.36252100
C	-0.98156900	-1.73062600	-3.26645100
O	-1.46214300	-2.39621200	-4.35971600
O	-0.30199700	-2.37416700	-2.42138200

O	-1.26707200	-0.50376800	-3.18013000	C	0.17989100	-2.94506800	-1.57680800
H	-1.12918500	-3.30362600	-4.25537800	H	0.75169600	-3.30418800	-0.73190600
C	1.50690800	1.47858000	-2.74154300	C	-4.27858800	1.25264700	-1.74245500
C	0.30122600	1.86996500	-1.88504500	H	-4.26783400	2.15556700	-2.34668300
H	-0.58311800	1.91337900	-2.53438100	C	3.50817600	2.02559600	1.55714900
C	0.37203500	3.12288000	-1.08431600	H	2.91286300	1.66597100	2.39113800
C	1.58650800	3.75479900	-0.74826300	C	4.49553500	2.98502300	1.77544000
C	-0.81535600	3.76113300	-0.66454700	H	4.67331800	3.34995800	2.78385900
C	1.60781100	4.93785700	-0.00729100	C	4.85459300	-2.58262700	0.96776200
H	2.51367500	3.32954500	-1.11111900	H	5.89975600	-2.75794500	0.72170400
C	-0.79519900	4.94162100	0.07664900	C	-1.29001300	-1.72759200	-2.86694200
H	-1.76996700	3.32023700	-0.93483000	H	-2.03266600	-1.00366200	-3.17220600
C	0.42155900	5.53954000	0.41892200	C	2.42685300	-0.83746500	-3.89100900
H	2.56596400	5.39758400	0.22891700	H	2.81463600	-1.43813300	-4.70463200
H	-1.73515400	5.39902100	0.38055700	C	3.99400000	2.06591000	-0.80817300
H	0.44298500	6.46377500	0.99303700	H	3.80562000	1.71781700	-1.81925100
O	1.56199700	0.16270500	-2.79181600	C	-0.58260000	-2.61958100	-3.72951700
O	2.30264800	2.23987100	-3.28256800	H	-0.68909200	-2.67892200	-4.80573100
G				C	-5.47622300	-0.46101100	-0.54213100
Fe	0.75728700	-1.36105300	-2.76103900	H	-6.41241000	-0.91685600	-0.22600200
P	1.91871200	0.25225300	0.07541800	C	-2.53433800	-4.99448800	2.36005100
P	-1.36919400	-1.07075300	0.03788900	H	-2.79094500	-5.90044800	2.90510200
C	2.84721800	-1.22165000	0.74833000	C	-2.79021500	-4.90342100	0.98833900
C	3.25110600	1.54447800	0.26116700	H	-3.24805100	-5.73795600	0.46101800
C	2.18615900	-2.09610600	1.62163700	C	-2.45716200	-3.74260400	0.29053900
H	1.16281900	-1.88083600	1.91071600	H	-2.66195100	-3.68650800	-0.77490900
C	-0.82750100	-1.92000300	-1.52429400	C	2.84421300	-3.21215200	2.14695100
C	-3.07042900	0.70872000	-1.30582300	H	2.31252000	-3.87677600	2.82336500
H	-2.13939000	1.20401800	-1.55732300	C	-1.94410200	-3.91773200	3.02030400
C	-5.48849900	0.66640000	-1.36418300	H	-1.73549500	-3.97684700	4.08603600
H	-6.43253300	1.09588100	-1.69236300	C	1.15639500	0.66341100	-2.68382300
C	1.98698100	-0.04513200	-1.74709200	H	0.41204500	1.39709900	-2.41010500
C	4.97901000	3.03371400	-0.58831400	C	-1.60886600	-2.75320900	2.31949500
H	5.54295400	3.42856400	-1.43086100	H	-1.12812100	-1.93155600	2.84232500
C	4.19714500	-1.46754100	0.44588800	C	2.77381200	-0.97322400	-2.51347900
H	4.74261900	-0.77319500	-0.18722500	H	3.46765200	-1.69456300	-2.10540100
C	-1.86355500	-2.64642200	0.94427600	C	0.32146600	-3.38013700	-2.92831100
C	5.23572500	3.49204900	0.70388200	H	1.02952000	-4.11687700	-3.28688100
H	5.99985400	4.24699500	0.87531400	C	1.42913600	0.17853600	-3.99586100
C	4.17617300	-3.46344300	1.81483500	H	0.92735900	0.48786400	-4.90406800
H	4.68933200	-4.33044800	2.22501100	Ru	-0.07093000	0.71831800	1.05643300
C	-3.04195200	-0.44311900	-0.50154700	C	-1.15268800	0.53706700	3.47089200
C	-4.26510700	-1.01161300	-0.11446700	O	-1.70693100	0.62277300	4.71852700
H	-4.28007000	-1.88622600	0.52620900	O	-1.76225100	1.12171200	2.52189800

O	-0.09993200	-0.13163400	3.34162300	H	-0.68549000	-0.77233000	-2.38346700
C	-3.40613500	4.49166000	0.27972900	C	-0.85003300	4.26405600	2.40178600
C	-3.47927000	5.09534600	-0.98063500	H	-0.08869100	4.61819100	3.09355400
C	-2.43836700	4.88151600	-1.88961000	C	3.96418600	-1.17805600	1.64250600
C	-1.35112600	4.08250500	-1.53896400	H	3.24669600	-1.95537000	1.88603100
C	-1.26663300	3.45462600	-0.27499400	C	5.19085800	-1.14211700	2.30482500
C	-2.32683500	3.68505500	0.63144400	H	5.42690300	-1.91321100	3.03436400
H	-4.20708400	4.64855500	1.00020700	C	3.71687900	-2.98153600	-2.75762800
H	-4.32668800	5.72350600	-1.24659200	H	4.67554400	-3.08315300	-3.26214500
H	-2.46697100	5.34838300	-2.87316000	C	-1.48331600	2.47299700	-2.20784100
H	-0.53777600	3.94284300	-2.24991300	H	-1.72655800	3.40602000	-1.72025700
H	-2.29939900	3.20371400	1.60255600	C	2.26906600	2.44198600	-3.18371000
C	-0.09046300	2.64431400	0.05700100	H	2.40926800	2.75328900	-4.21176600
H	0.75096600	2.83386100	-0.61063500	C	4.54618400	0.84182400	0.45854200
N	0.39386300	2.65127600	1.46688100	H	4.30954300	1.62213200	-0.25814100
N	0.62102800	3.44239900	2.32555700	C	-1.17291100	2.31300400	-3.59193800
H	-2.47922500	1.20227600	4.60215200	H	-1.14551800	3.10333900	-4.33235700
H				C	-2.91453300	4.60000400	1.20513400
Fe	0.45498000	1.77424700	-2.40984600	H	-3.77408900	5.21864300	0.95432800
P	1.93558400	-0.30121800	-0.09945300	C	-6.07767400	-0.34799800	0.50418100
P	-1.52130800	0.75312200	0.25191100	H	-7.13111200	-0.60646900	0.58741600
C	2.26738800	-1.75079900	-1.23551000	C	-5.56212100	0.12146000	-0.70353800
C	3.62392300	-0.18852300	0.70160700	H	-6.21203300	0.23189100	-1.56943100
C	1.27619500	-2.72074000	-1.43125600	C	-4.20627000	0.44684100	-0.81024100
H	0.34424000	-2.62568900	-0.88055700	H	-3.82165300	0.81043200	-1.75861100
C	-1.34072600	1.20244500	-1.54856300	C	1.49611500	-3.80310200	-2.28848900
C	-0.74015700	2.97841000	1.86150100	H	0.71332400	-4.54598200	-2.42173000
H	0.08012600	2.33559100	2.16345100	C	-5.22666500	-0.49548500	1.60274300
C	-1.93200000	5.08202500	2.07308000	H	-5.61514400	-0.87234500	2.54623300
H	-2.01810800	6.07959200	2.49905200	C	1.73381000	2.45945100	-0.93884800
C	2.05905600	1.10320400	-1.29141900	H	1.39164100	2.78667400	0.03360400
C	5.77450500	0.87747500	1.12468900	C	-3.87334600	-0.17935300	1.49183000
H	6.47483700	1.68427400	0.91674300	H	-3.20358600	-0.33289300	2.33369100
C	3.49598800	-1.90176100	-1.90088900	C	2.39426500	1.10910300	-2.68937100
H	4.28854000	-1.17683200	-1.73784900	H	2.64236300	0.23666300	-3.27700300
C	-3.34295300	0.30261800	0.28524300	C	-0.84010300	0.94233100	-3.81083800
C	6.10400300	-0.11606500	2.04769000	H	-0.51351100	0.50523700	-4.74615300
H	7.05894700	-0.08730200	2.56806400	C	1.86470400	3.27768800	-2.09894000
C	2.71400900	-3.93456400	-2.95723700	H	1.64330100	4.33606400	-2.15597700
H	2.88737800	-4.77912900	-3.62084400	Ru	0.00739100	-0.55467500	1.26636200
C	-1.70780000	2.49146200	0.97023500	C	1.50778500	-0.25161000	3.50220100
C	-2.80386700	3.31723400	0.66411400	O	2.22466900	-0.17506000	4.67407700
H	-3.58785900	2.95203100	0.00751300	O	1.23718400	0.83172300	2.91284200
C	-0.93915000	0.26305100	-2.56108900	O	1.18483100	-1.39911700	3.10906000

H	2.39014100	0.77581100	4.78806900
C	-0.95997100	-2.19049500	1.21443300
C	-2.00690600	-2.98975800	0.58929300
C	-2.50088500	-4.13881600	1.26441300
C	-2.56477200	-2.73299100	-0.68638300
C	-3.49038000	-4.94982000	0.72016000
H	-2.08539600	-4.37801200	2.24169000
C	-3.54921700	-3.55019600	-1.23723000
H	-2.20865000	-1.87765900	-1.24781400
C	-4.02715100	-4.66441200	-0.54139100
H	-3.84245000	-5.81675100	1.27758700
H	-3.94911000	-3.31304500	-2.22171400
H	-4.79693800	-5.30006000	-0.97351100
H	-0.43527900	-2.78612900	1.98217300

8-ts

Fe	1.68951900	2.91175100	0.33646800
P	-1.14852900	1.02266200	-0.06542600
P	2.15386600	-0.44545300	0.04409000
C	-1.74481200	1.23470400	1.67114100
C	-2.65156700	1.37983900	-1.10374600
C	-1.39001500	0.26876800	2.62572500
H	-0.81698600	-0.60325800	2.32525200
C	2.61447500	1.15013600	0.81987400
C	2.69571800	-0.49909400	-2.72550900
H	1.61447500	-0.51831100	-2.84262000
C	4.89779100	-0.54224500	-3.72682800
H	5.53171300	-0.56353500	-4.60934000
C	-0.18639400	2.55641300	-0.39178800
C	-3.55529500	2.00569800	-3.27615200
H	-3.38788300	2.29637000	-4.31004400
C	-2.53278300	2.32831400	2.07153400
H	-2.85093100	3.06555200	1.34073700
C	2.97065900	-1.67945600	1.16433400
C	-4.85610500	1.89653600	-2.77812700
H	-5.70720800	2.10129700	-3.42227300
C	-2.56075000	1.50795700	4.34778100
H	-2.87586600	1.61440500	5.38247600
C	3.26014500	-0.49268300	-1.44259600
C	4.65937900	-0.53133800	-1.31838400
H	5.11335200	-0.55622900	-0.33190200
C	1.97717900	1.71669500	1.98137900
H	1.16288000	1.27281500	2.53728200
C	3.50957100	-0.52077300	-3.86151400
H	3.05534900	-0.53197100	-4.84868600
C	-3.96100500	1.25530700	-0.62031700
H	-4.14004800	0.94040900	0.40133700
C	-5.05366800	1.51817400	-1.45096500
H	-6.05987100	1.41335500	-1.05486600
C	-2.93433100	2.46517600	3.40061600
H	-3.54414300	3.31548000	3.69462200
C	3.59535900	2.10463300	0.37607400
H	4.22099700	2.00297000	-0.49863700
C	0.76458900	4.67621400	-0.30800300
H	1.03196100	5.66833600	0.03232400
C	-2.46441200	1.74982500	-2.44671400
H	-1.46152700	1.84726500	-2.85126900
C	3.55051500	3.23419700	1.24288300
H	4.14025400	4.13548300	1.13683300
C	5.47158300	-0.55150000	-2.45206700
H	6.55226100	-0.58255800	-2.34075700
C	4.14906500	-3.61734900	2.82877100
H	4.60104200	-4.36713800	3.47262500
C	3.86881400	-2.34395400	3.32358800
H	4.10655300	-2.09298100	4.35414800
C	3.28384200	-1.38086700	2.49850400
H	3.08388500	-0.39430600	2.90154400
C	-1.79465000	0.40916900	3.95687200
H	-1.51380600	-0.34844200	4.68353300
C	3.84287300	-3.92351600	1.50143400
H	4.05005400	-4.91427500	1.10677200
C	0.75138100	2.68970700	-1.47723600
H	1.01757500	1.91267000	-2.18106600
C	3.25966900	-2.96458300	0.67391200
H	3.01323200	-3.22126700	-0.34971700
C	-0.17131300	3.80565600	0.32187200
H	-0.72183100	4.02432500	1.22473600
C	2.55706400	2.99272600	2.23631600
H	2.25667000	3.67738200	3.01878200
C	1.33249800	3.98885100	-1.42022900
H	2.10544900	4.36566400	-2.07716900
Ru	-0.07001000	-1.00031100	-0.59117300
C	0.03194700	-3.41913500	0.30936300
O	-0.08323900	-4.58288100	0.59691300
O	0.64540900	-2.99492100	-0.91139100
O	-0.30587000	-2.35204300	0.99004200
C	-4.56956600	-1.95490600	1.68546500
C	-5.92618900	-1.97944900	1.34644100
C	-6.29768500	-2.07920900	0.00313300

C	-5.32073900	-2.13820600	-0.98822400
C	-3.95271600	-2.08991200	-0.65967800
C	-3.58780600	-2.01576400	0.69843900
H	-4.27031700	-1.89794600	2.72870600
H	-6.68584400	-1.93730400	2.12255500
H	-7.34875100	-2.11438700	-0.27219400
H	-5.61449100	-2.21234400	-2.03292000
H	-2.53845900	-2.03774400	0.97225400
C	-2.97963600	-2.17533400	-1.74392800
H	-3.34746300	-2.55258200	-2.70427200
N	-1.71663200	-1.89165500	-1.67230700
N	-0.82712100	-2.10804900	-2.68306500
H	0.05358600	-2.97880300	-1.84666100
H	-1.31320800	-2.35420700	-3.55621900

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Fe	-2.08340000	2.58069300	-1.34994300
P	-1.86738900	-0.83431300	-0.39953900
P	0.76059100	1.47086700	0.16787000
C	-3.51872900	-1.25953500	0.36974500
C	-1.67651100	-2.24833100	-1.60693800
C	-3.78600600	-0.89159500	1.69740700
H	-3.00409600	-0.44553600	2.29943600
C	-0.38620600	2.87389100	-0.20376300
C	1.59437300	0.23037900	-2.23798700
H	1.01385600	-0.60972700	-1.87224400
C	3.05339300	1.19846300	-3.91330100
H	3.57796400	1.12412700	-4.86389200
C	-2.47106100	0.52313500	-1.53223000
C	-1.86291100	-3.30040900	-3.79783800
H	-2.14053900	-3.23181600	-4.84877000
C	-4.52689700	-1.88853800	-0.37756100
H	-4.32939400	-2.19501300	-1.40082900
C	2.04959700	2.31731900	1.21461900
C	-1.34645600	-4.48934300	-3.28042200
H	-1.21271100	-5.35530200	-3.92738400
C	-6.04731900	-1.75618400	1.49770500
H	-7.02324400	-1.95395300	1.93880800
C	1.70493000	1.38214500	-1.44576300
C	2.53257900	2.42422800	-1.89279500
H	2.66956700	3.30532000	-1.27133700
C	-1.56076300	3.13124900	0.58628500
H	-1.83198000	2.56311500	1.46736800
C	2.25723800	0.14262500	-3.46501600
H	2.16654000	-0.76467800	-4.05707400
C	-1.16339300	-3.45167300	-1.08809100
H	-0.88129700	-3.54258300	-0.02861600
C	-1.00477000	-4.55722400	-1.92814400
H	-0.60286700	-5.47686400	-1.50894400
C	-5.78287100	-2.13587600	0.17966100
H	-6.54956900	-2.63133800	-0.41394700
C	-0.41440800	3.79434300	-1.30864800
H	0.30183000	3.82626500	-2.11740600
C	-3.79983300	2.20219300	-2.45386800
H	-4.59769200	2.92278700	-2.58807200
C	-2.02830500	-2.18909700	-2.96571300
H	-2.44112500	-1.27735600	-3.38463700
C	-1.59257100	4.59382800	-1.20333900
H	-1.91854800	5.34142900	-1.91739500
C	3.19629500	2.33872100	-3.11946500
H	3.83402100	3.15770300	-3.44765600
C	4.05713200	3.45353600	2.82740300
H	4.83469100	3.89212800	3.45061500
C	2.95739400	4.21693400	2.43553200
H	2.86990300	5.25496500	2.75262200
C	1.96106600	3.65223800	1.63170100
H	1.10937200	4.25621100	1.33213100
C	-5.04766100	-1.13655600	2.24889500
H	-5.23477100	-0.85786400	3.28337300
C	4.15000000	2.11852500	2.42051900
H	4.99885900	1.51095000	2.72556000
C	-1.81576700	1.04760700	-2.70052400
H	-0.84475000	0.74481800	-3.06562100
C	3.15270900	1.55004900	1.62980400
H	3.21557200	0.50643900	1.33233400
C	-3.69520100	1.25779200	-1.38877700
H	-4.40217800	1.12721800	-0.58178300
C	-2.29707000	4.18344900	-0.02907900
H	-3.25329500	4.56674700	0.30590200
C	-2.63788900	2.06594900	-3.27312200
H	-2.39129100	2.66567700	-4.14102700
Ru	-0.24583700	-0.39436400	1.15830300
C	-0.35683500	0.69497500	3.51232700
O	-0.47186300	1.06468200	4.82548600
O	0.71301500	0.13484000	3.14802500
O	-1.32388900	0.96387300	2.74733500
C	6.45234400	-1.01611800	-1.11483600
C	7.34336300	-2.09707300	-1.01837800

C	6.85435600	-3.30800000	-0.51092300	H	-2.67026800	-3.25572400	-1.29840500
C	5.52849000	-3.43438700	-0.11142800	C	1.54223700	-3.10503200	0.59075400
C	4.60786000	-2.35139500	-0.19629400	H	1.80964500	-2.53445600	1.47181100
C	5.12564600	-1.13165900	-0.72221900	C	-2.23197300	-0.08158700	-3.47032400
H	6.80213400	-0.06289300	-1.51243300	H	-2.13612800	0.82955900	-4.05559700
H	8.38108100	-1.99834400	-1.33181000	C	1.17010900	3.43933700	-1.09337600
H	7.51954900	-4.16826300	-0.42464500	H	0.84781000	3.51244900	-0.05482900
H	5.17272000	-4.38554000	0.28223400	C	1.02681300	4.55310900	-1.92430100
H	4.45264300	-0.28613200	-0.81979500	H	0.59523300	5.46195000	-1.51190400
C	3.24887000	-2.52773600	0.22261100	C	5.79109100	2.07769300	0.28409300
H	2.93491300	-3.52110300	0.56164900	H	6.56453800	2.61188900	-0.26547800
N	2.36085200	-1.53427000	0.19905400	C	0.39276700	-3.78326000	-1.29665400
N	1.12560700	-1.75199200	0.51478200	H	-0.32359100	-3.82008200	-2.10513700
H	0.84763800	-2.69151700	0.91260300	C	3.77766100	-2.22590100	-2.47969000
H	0.32917700	0.69823000	5.23784300	H	4.56727100	-2.95474800	-2.61807900
C	-0.87154800	-3.14816500	2.58237000	C	2.11794600	2.20749800	-2.94642300
O	-1.15252400	-1.83140500	2.34896600	H	2.55237600	1.30256600	-3.35884900
O	-1.36678300	-3.63899800	3.61530500	C	1.56668100	-4.58803500	-1.18219400
O	-0.14927900	-3.78635200	1.71906400	H	1.88878900	-5.34551200	-1.88758800
10-ts				C	-3.17788000	-2.27802700	-3.14628000
Fe	2.06790300	-2.58014200	-1.35489900	H	-3.81525100	-3.09328100	-3.48424400
P	1.87474700	0.81505900	-0.40856900	C	-4.09848700	-3.40169700	2.79425400
P	-0.76727000	-1.43655200	0.16557200	H	-4.88535600	-3.83758000	3.40769500
C	3.52292600	1.19866000	0.39027500	C	-3.01427900	-4.17916000	2.38685700
C	1.71947800	2.24695800	-1.59994800	H	-2.94757900	-5.22493900	2.68283200
C	3.77836500	0.73525700	1.69042100	C	-2.00671300	-3.61806600	1.59469700
H	2.99362800	0.24220600	2.25259900	H	-1.16703900	-4.23274400	1.28335900
C	0.36985300	-2.85024400	-0.20231100	C	5.03570500	0.93232000	2.26861100
C	-1.58003000	-0.17768000	-2.23823600	H	5.21390900	0.57719800	3.28106100
H	-1.00186200	0.65866400	-1.86084300	C	-4.16452700	-2.05723300	2.41487500
C	-3.02581900	-1.13360700	-3.93193100	H	-5.00194900	-1.43939900	2.73052000
H	-3.54280700	-1.05213000	-4.88606800	C	1.80259300	-1.05289600	-2.71468100
C	2.47209100	-0.53223300	-1.55315800	H	0.83094700	-0.74215300	-3.07142300
C	1.96894600	3.32520000	-3.77277200	C	-3.15617600	-1.49256000	1.63507400
H	2.28422100	3.27083000	-4.81374900	H	-3.19829500	-0.44291700	1.35602400
C	4.53901800	1.87581100	-0.30077800	C	3.69236200	-1.27564100	-1.41831600
H	4.35201800	2.25384400	-1.30182200	H	4.40746800	-1.14905800	-0.61799900
C	-2.06897400	-2.27357200	1.20438900	C	2.27371300	-4.16738200	-0.01295200
C	1.42001500	4.50298600	-3.26312100	H	3.22760100	-4.55244800	0.32666100
H	1.29825300	5.37360900	-3.90565500	C	2.60934100	-2.08236700	-3.28863400
C	6.04378200	1.60131800	1.57229700	H	2.34902300	-2.68404100	-4.15115800
H	7.01686000	1.76170100	2.03418400	Ru	0.24873400	0.39952300	1.15296000
C	-1.69890600	-1.33440000	-1.45457200	C	0.27577800	-0.68407600	3.56038700
C	-2.52483600	-2.37200800	-1.91421400	O	0.25280400	-1.02363700	4.89049900

O	-0.73527700	-0.07153200	3.10810700
O	1.28329100	-1.02212400	2.89154200
C	-6.36389800	0.94537700	-1.14254000
C	-7.27313100	2.01468600	-1.08290000
C	-6.80465300	3.24301400	-0.59487500
C	-5.48748100	3.39696200	-0.18035100
C	-4.54544600	2.32504300	-0.22673100
C	-5.04480400	1.08646700	-0.73480800
H	-6.69396400	-0.02167900	-1.52433900
H	-8.30507900	1.89489200	-1.40806700
H	-7.48204900	4.09667000	-0.53606200
H	-5.15160200	4.36210400	0.19720100
H	-4.36202400	0.24647600	-0.80729600
C	-3.20181500	2.53315600	0.20655100
H	-2.90917700	3.53759800	0.52878100
N	-2.28344400	1.55280400	0.22218500
N	-1.07241900	1.80377500	0.55601000
H	-0.67141000	2.82461300	1.14807000
H	-0.57007700	-0.62008000	5.21592200
C	0.84361300	3.13969200	2.58652700
O	1.19800400	1.88101600	2.31464200
O	1.38924900	3.75023400	3.51508200
O	-0.07473200	3.70003000	1.80820900

11-ts

Fe	2.69230500	0.42339800	-2.40156600
P	1.25524800	-1.60256400	-0.00800600
P	0.48825500	1.79100900	-0.04279600
C	0.66609700	-3.23405900	-0.71107400
C	2.24399700	-2.15654400	1.47678400
C	-0.29979200	-3.18591900	-1.73116400
H	-0.71294900	-2.22184800	-2.01885700
C	1.34296100	1.79885200	-1.67438000
C	2.34457100	1.84064800	2.07777200
H	2.02626400	0.81164500	2.21590500
C	3.68769200	3.72899000	2.77706000
H	4.43039800	4.16470700	3.44162100
C	2.64061900	-1.25339100	-1.18570900
C	4.19512200	-3.18227400	2.51681600
H	5.16959700	-3.65543500	2.41630300
C	1.12821700	-4.48716200	-0.28031200
H	1.85803800	-4.55466400	0.51931700
C	-0.69123200	3.21567900	-0.32550300
C	3.63854600	-2.98144000	3.78274300
H	4.17896900	-3.29618500	4.67289300
C	-0.29187300	-5.60440700	-1.89355800
H	-0.66337400	-6.52026000	-2.34801100
C	1.75970300	2.60512700	1.05804600
C	2.13928300	3.95144900	0.92850600
H	1.67199400	4.57329500	0.17048500
C	0.79926300	1.15378900	-2.83732200
H	-0.10007300	0.54867700	-2.82028200
C	3.30513500	2.39531100	2.92780900
H	3.74281300	1.78406400	3.71319700
C	1.69458400	-1.95920400	2.75397400
H	0.73436600	-1.46020400	2.87348100
C	2.38997300	-2.36889600	3.89602600
H	1.94764100	-2.19665500	4.87392700
C	0.65198100	-5.66233900	-0.86682100
H	1.01904000	-6.62443200	-0.51564400
C	2.55677400	2.45569000	-2.07889500
H	3.22471900	3.00148900	-1.42700800
C	3.91908600	-1.09700300	-3.11987500
H	4.23739500	-1.18938800	-4.15071200
C	3.50400700	-2.77268800	1.37507300
H	3.95023400	-2.93121500	0.39783600
C	2.75927200	2.20552800	-3.46960900
H	3.61397500	2.52480300	-4.05331600
C	3.09782200	4.50745300	1.77762400
H	3.37711200	5.55272800	1.66442400
C	-2.45665400	5.38789900	-0.66380800
H	-3.14167100	6.22242800	-0.79656900
C	-1.41238300	5.18527900	-1.56693700
H	-1.27784600	5.86011900	-2.40964500
C	-0.53869300	4.10830700	-1.40078300
H	0.26077000	3.96408500	-2.11939500
C	-0.76662200	-4.36284200	-2.32118500
H	-1.51768200	-4.30561800	-3.10552000
C	-2.62224900	4.50197900	0.40139600
H	-3.44285800	4.63655400	1.10180700
C	3.80119900	-0.45042200	-0.90636900
H	4.02092900	0.02821400	0.03846000
C	-1.75147700	3.42358100	0.57139300
H	-1.91502600	2.71774200	1.37843400
C	2.72657700	-1.64710300	-2.56170800
H	1.98681900	-2.23348400	-3.08874800
C	1.67206500	1.40339800	-3.93522300
H	1.55787400	1.00993100	-4.93759800
C	4.58759700	-0.36229900	-2.09439400

H	5.50354800	0.20400200	-2.20789300
Ru	-0.42709000	-0.14395200	0.67592100
C	-1.61110500	0.60865300	3.26692500
O	-2.47808300	1.29512100	4.09605000
O	-0.72834700	-0.09063700	3.78784300
O	-1.86270500	0.80388800	2.02980000
H	-2.18161500	1.05380100	4.98942500
C	-2.87220900	-2.16798100	1.67131300
C	-3.70185400	-0.17162200	-0.25679300
H	-3.46864700	0.27925600	0.70687700
N	-2.72008300	-0.38290300	-1.14303200
N	-1.48619400	-0.35899900	-1.16043200
C	-5.08030100	-0.35657400	-0.64161300
C	-6.11818700	-0.07886100	0.28370700
C	-5.47863700	-0.82565700	-1.92038300
C	-7.45801800	-0.25880400	-0.04628600
H	-5.85006100	0.28024700	1.27542600
C	-6.81927900	-1.00080800	-2.24266600
H	-4.70465700	-1.04303000	-2.65126400
C	-7.83038700	-0.72220800	-1.31316300
H	-8.22331400	-0.03411500	0.69584000
H	-7.08377500	-1.36074000	-3.23673200
H	-8.87798700	-0.86300900	-1.56995300
O	-1.73994200	-2.08653000	1.35666600
O	-3.93775700	-2.39658400	2.09381000

12-ts

Fe	2.82869200	-1.05562000	-1.95928100
P	0.05812100	-1.84598000	0.02753200
P	1.56884500	1.52759400	-0.09688500
C	-1.09035700	-2.82461600	-1.05734800
C	0.08279100	-2.92229900	1.54878600
C	-2.19151800	-2.22799900	-1.67946800
H	-2.41466900	-1.18569600	-1.51718200
C	2.37959200	0.91430400	-1.62583400
C	3.16052100	0.87627000	2.14189000
H	2.38203200	0.14794800	2.34417000
C	5.22548400	1.97069400	2.78128800
H	6.07605800	2.06110700	3.45283700
C	1.68240700	-2.27874600	-0.74236300
C	1.03054300	-4.67517300	2.94519800
H	1.82549400	-5.39355600	3.13450700
C	-0.88058800	-4.20528700	-1.23177500
H	-0.05598300	-4.69619900	-0.72315100
C	1.22780100	3.29268900	-0.59602400
C	-0.04928300	-4.57222500	3.82228900
H	-0.10145800	-5.20987900	4.70243200
C	-2.81208100	-4.34552300	-2.67848900
H	-3.48090800	-4.93354000	-3.30291700
C	3.02269600	1.74049500	1.04501300
C	3.99174000	2.73785000	0.84522900
H	3.88456200	3.43718400	0.02119400
C	1.64915400	0.43092700	-2.76698400
H	0.57165700	0.37238100	-2.83691100
C	4.25776400	0.98969600	3.00068100
H	4.34606400	0.31554800	3.84920100
C	-1.00350200	-2.82236800	2.43595900
H	-1.78058700	-2.08642000	2.23216500
C	-1.06294700	-3.64775100	3.55959100
H	-1.91156400	-3.56232900	4.23423800
C	-1.72885100	-4.95864100	-2.03986500
H	-1.55267100	-6.02519200	-2.16068200
C	3.77726000	0.77794000	-1.93301100
H	4.59246800	1.01690400	-1.26436000
C	3.33327700	-3.06225100	-2.18417800
H	3.82257500	-3.47247500	-3.05859100
C	1.09540600	-3.85782400	1.81327400
H	1.93878400	-3.96376000	1.13967600
C	3.89869600	0.20258700	-3.23284200
H	4.82578800	-0.07125300	-3.72082200
C	5.08659500	2.84919600	1.70353700
H	5.82717700	3.62751300	1.53458200
C	0.68345800	5.96797200	-1.28855400
H	0.46679400	6.99887600	-1.55866200
C	1.50093700	5.18529600	-2.10439600
H	1.92648300	5.60190400	-3.01458300
C	1.77074600	3.85825400	-1.76157500
H	2.40328900	3.26303000	-2.41197900
C	-3.04299500	-2.98536500	-2.49069300
H	-3.90161000	-2.50318800	-2.94890400
C	0.13705300	5.41392300	-0.12944200
H	-0.51145400	6.01000200	0.50761800
C	2.97083100	-2.02827700	-0.15395500
H	3.14253600	-1.52358300	0.78606000
C	0.40190900	4.08769600	0.21677500
H	-0.04672300	3.66108100	1.10753300
C	1.92544000	-2.91895700	-2.00594300
H	1.16358300	-3.20999000	-2.71440900
C	2.58386500	-0.00533600	-3.74885700

H	2.33647700	-0.46332600	-4.69801000
C	3.98020800	-2.51691300	-1.03505600
H	5.04859500	-2.43654400	-0.87957800
Ru	-0.38961500	0.38527000	0.63807600
C	-0.33898100	1.25650500	3.05993900
O	-0.42902000	1.54802600	4.38024400
O	0.20201900	0.14820800	2.72932900
O	-0.76811800	2.08414000	2.22432000
H	-0.10445200	0.75519600	4.84089100
C	-3.43622300	-0.25117100	0.79667200
C	-3.93851100	1.07108800	0.51658100
H	-3.35590900	1.89253800	0.92371400
N	-2.33709100	1.34111500	-1.44429600
N	-1.34305800	0.98730700	-1.02768100
C	-5.24364500	1.39924700	0.01326200
C	-6.20273000	0.43966100	-0.42139500
C	-5.63325100	2.76464800	-0.08905900
C	-7.44072000	0.83157400	-0.91976300
H	-5.93580100	-0.60720100	-0.33661500
C	-6.87264700	3.14475500	-0.59003200
H	-4.92797100	3.52861000	0.23553200
C	-7.79813500	2.18299000	-1.01508000
H	-8.14737000	0.06513200	-1.23922800
H	-7.12342200	4.20389100	-0.64902400
H	-8.76980100	2.47844100	-1.40614500
O	-2.21594100	-0.31346000	1.38773600
O	-4.04390200	-1.31682200	0.56106600

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Fe	2.56162900	1.94756800	-1.52404100
P	-0.53262400	1.61910900	-0.10504100
P	2.00866000	-0.93929000	0.22676800
C	-0.43507500	2.82812900	1.30106700
C	-2.20349600	1.99613600	-0.81697400
C	0.53979500	3.82492300	1.46263500
H	1.30965700	3.96310200	0.71422500
C	3.14564800	0.44191400	-0.23100000
C	2.05981700	-2.61314800	-2.06561300
H	1.10014900	-2.16435700	-2.29630200
C	3.81906100	-4.19033200	-2.60636100
H	4.24253500	-4.93821800	-3.27306000
C	0.52891200	2.21169500	-1.48087200
C	-3.95093100	3.56516900	-1.43490000
H	-4.33887600	4.58153100	-1.44710500
C	-1.38889100	2.64947600	2.32470200
H	-2.11819000	1.84600400	2.25224900
C	2.65374500	-1.45446500	1.89419100
C	-4.69327400	2.52199000	-1.99433500
H	-5.66451400	2.72373100	-2.44087200
C	-0.41115900	4.47150500	3.59397300
H	-0.40370500	5.10669800	4.47685200
C	2.71385500	-2.26981900	-0.87278000
C	3.92540000	-2.90831300	-0.55716300
H	4.44083800	-2.66547500	0.36728300
C	3.20465300	1.71908800	0.42474200
H	2.62228900	2.00437800	1.29009800
C	2.61210800	-3.56834200	-2.92417100
H	2.08031200	-3.83632900	-3.83336500
C	-2.94925300	0.95478500	-1.38700000
H	-2.56155800	-0.05858300	-1.36888600
C	-4.19097700	1.22017300	-1.96984600
H	-4.77040200	0.39871800	-2.38178600
C	-1.37400700	3.46851200	3.45342700
H	-2.11792500	3.30980700	4.22990500
C	4.04577400	0.50710600	-1.34960600
H	4.20172700	-0.28340400	-2.06966000
C	1.91671000	3.27481500	-3.01235200
H	2.54445300	4.02086700	-3.48375300
C	-2.71293700	3.30301800	-0.84735200
H	-2.14901100	4.11681300	-0.39904000
C	4.63970300	1.80365800	-1.38179100
H	5.33048300	2.16640000	-2.13248400
C	4.47463600	-3.85899600	-1.41743700
H	5.41133100	-4.34598500	-1.15523500
C	3.47046100	-2.30620200	4.44790600
H	3.78231600	-2.63101800	5.43796100
C	4.18755600	-1.31483000	3.77731900
H	5.06328900	-0.86518000	4.24021300
C	3.78390600	-0.89321600	2.50715600
H	4.35348800	-0.12404600	1.99528100
C	0.54968100	4.64149600	2.59816600
H	1.31371500	5.40959400	2.69875800
C	2.34858600	-2.87698100	3.84121100
H	1.78368500	-3.65019100	4.35600400
C	0.87985100	1.27603700	-2.51748300
H	0.56297100	0.24103600	-2.53856500
C	1.93650500	-2.45633100	2.57607800
H	1.06090900	-2.89803900	2.10631800
C	1.16056800	3.45869500	-1.81704100

H	1.10756400	4.37893300	-1.25458000
C	4.12376200	2.55178600	-0.28099000
H	4.35730400	3.58209600	-0.04364300
C	1.73601900	1.92826900	-3.44741100
H	2.20441000	1.46701200	-4.30731400
Ru	-0.27360500	-0.6334170(	0.48753600
C	-0.81816000	-2.81257500	-0.70636300
O	-1.16916200	-3.80498100	-1.33600300
O	-0.72178300	-1.58512000	-1.26682200
O	-0.49383600	-2.75723600	0.57301400
C	-3.12939200	-0.87106400	2.03871100
C	-3.56397700	-2.26347700	1.54157800
H	-2.70051600	-2.81259000	1.16353300
C	-4.64875800	-2.17250500	0.48194800
C	-5.85520000	-1.50841400	0.75876800
C	-4.47710800	-2.75481200	-0.78241300
C	-6.86751300	-1.43626300	-0.19760700
H	-5.97580900	-1.03563800	1.72994200
C	-5.49358100	-2.68137700	-1.74069700
H	-3.54505100	-3.26365500	-1.01914300
C	-6.69305800	-2.02631400	-1.45361600
H	-7.79470700	-0.91624400	0.03617000
H	-5.34186700	-3.14084000	-2.71526700
H	-7.48399900	-1.97442700	-2.19944600
O	-2.14230300	-0.28918100	1.42256400
O	-3.75413800	-0.33403900	2.95909600
H	-3.96154600	-2.79537200	2.41508200

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C	2.31670400	0.08190100	-0.13075400
C	1.18900000	-0.64927100	0.74098900
H	1.35138900	-1.73179700	0.70064200
C	-0.23078200	-0.32084700	0.37115400
C	-0.67892500	1.01475400	0.32597600
C	-1.15666300	-1.32745100	0.04995200
C	-1.99654500	1.31762700	-0.01266900
H	0.05864300	1.78931100	0.51007100
C	-2.47841800	-1.02581900	-0.28990500
H	-0.83049900	-2.36630200	0.06925600
C	-2.91001400	0.30149500	-0.31807900
H	-2.31640400	2.35861400	-0.04420500
H	-3.17137500	-1.83082400	-0.53215100
H	-3.93933500	0.54239100	-0.57877600
O	3.17876400	-0.68222300	-0.61280700
O	2.21473900	1.33323200	-0.17731600
H	1.37342200	-0.32380100	1.77616800

15-ts

Fe	0.30303800	-0.21736200	3.02202000
P	-1.42400200	-0.89597200	0.18092100
P	1.88242300	0.23133700	-0.03063100
C	-1.42972700	-2.75262800	0.43363700
C	-3.20572600	-0.67041300	-0.30524500
C	-0.33849000	-3.51529800	-0.00890200
H	0.46754100	-3.02446000	-0.54681700
C	1.93840100	-0.27147600	1.74766100
C	1.68776600	3.02187400	0.35805000
H	0.61934100	2.84998500	0.31013900
C	3.54393700	4.55170700	0.62882700
H	3.92016600	5.55630100	0.80861900
C	-1.44578500	-0.31806600	1.93477300
C	-5.51185800	-0.03417900	0.13273300
H	-6.26332000	0.34777100	0.82049800
C	-2.50881700	-3.41680000	1.04125900
H	-3.38354500	-2.85134600	1.35010900
C	3.34398900	-0.66199000	-0.74587100
C	-5.86092400	-0.36088600	-1.17806400
H	-6.88729000	-0.23820500	-1.51724500
C	-1.37787000	-5.54441300	0.81698300
H	-1.35801400	-6.62203600	0.96389100
C	2.57023200	1.95308700	0.15673700
C	3.95040600	2.20606500	0.18596600
H	4.65298700	1.39439600	0.02818600
C	1.65000800	-1.58148600	2.26596000
H	1.35094100	-2.43788900	1.67855300
C	2.16977800	4.31027200	0.59984200
H	1.46415100	5.12317700	0.75051600
C	-3.56178200	-0.99269100	-1.62752200
H	-2.79894800	-1.35261700	-2.31603500
C	-4.88216500	-0.84042300	-2.05386500
H	-5.14354900	-1.09281200	-3.07884500
C	-2.48100100	-4.79813100	1.23981100
H	-3.32559200	-5.29264700	1.71500600
C	2.22432600	0.56819900	2.87931700
H	2.44752900	1.62424400	2.83235800
C	-1.37604600	-0.15296800	4.25401700
H	-1.36315800	-0.42113600	5.30342800
C	-4.19137900	-0.18731100	0.56666900
H	-3.93221200	0.07862300	1.58692300
C	2.11012900	-0.21206400	4.06681100

H	2.22707600	0.15393600	5.07930200
C	4.43309600	3.49573600	0.41663600
H	5.50609800	3.67376200	0.42876000
C	5.52293000	-1.92860600	-1.98875700
H	6.36436100	-2.42142400	-2.47133200
C	5.28007000	-2.12787900	-0.62936000
H	5.93259400	-2.77312700	-0.04495000
C	4.19820300	-1.49393900	-0.00977300
H	4.02718900	-1.64958900	1.05083500
C	-0.31373400	-4.90036100	0.18500600
H	0.53610200	-5.47600100	-0.17429500
C	4.67816500	-1.09396800	-2.72721100
H	4.86077700	-0.93445700	-3.78746700
C	-1.17343000	1.04665100	2.29404300
H	-1.00128400	1.84695200	1.58746800
C	3.58904700	-0.47079100	-2.11804400
H	2.91900200	0.16670500	-2.69262800
C	-1.57994800	-1.05167400	3.16407200
H	-1.73918700	-2.11774400	3.24342200
C	1.76158300	-1.54298100	3.68733800
H	1.56117200	-2.36788400	4.35956700
C	-1.12832400	1.14527200	3.71390800
H	-0.90021600	2.03960900	4.27990200
Ru	0.04827300	0.11228800	-1.35710300
C	0.11375900	-2.17374000	-3.16930900
O	0.75483400	-3.11819200	-3.95004400
O	0.87261400	-1.69602800	-2.24267800
O	-1.06155500	-1.91233000	-3.41888700
C	-1.05690800	1.99735400	-1.99729400
N	0.26269200	2.28857900	-2.50195100
H	1.66908800	-3.12324700	-3.61913100
H	-1.62629100	1.34018200	-2.66381900
C	-1.82319100	3.06137000	-1.36032500
C	-1.23875600	4.29615400	-0.98433900
C	-3.21522000	2.92042300	-1.14428300
C	-2.00255700	5.31670200	-0.42024000
H	-0.18395600	4.44861400	-1.18463500
C	-3.96810600	3.93862800	-0.56739800
H	-3.70125900	1.99485200	-1.43831600
C	-3.37183600	5.14876000	-0.19225000
H	-1.52126700	6.25841800	-0.15844700
H	-5.03445900	3.78528900	-0.41048300
H	-3.96165300	5.94161900	0.26229800
N	0.86004500	1.24946600	-2.89931300

16-ts

Fe	-0.81207300	-1.39366100	2.73643100
P	-1.92491400	0.30800600	-0.05783200
P	1.35780100	-1.06896900	-0.01629800
C	-2.92686800	-1.11383400	-0.73669500
C	-3.19623300	1.65981800	-0.21824600
C	-2.31672900	-2.02215700	-1.61238900
H	-1.28512400	-1.86124400	-1.90671300
C	0.76094200	-1.95610500	1.50150100
C	3.00615200	0.56792700	1.56094900
H	2.06429100	0.95983900	1.92763700
C	5.42202700	0.67642400	1.49759200
H	6.35574200	1.11042300	1.84765900
C	-1.98929400	-0.01065800	1.75843900
C	-4.71980400	3.33107800	0.67819800
H	-5.16325800	3.82693900	1.53894900
C	-4.28708900	-1.28709900	-0.42901800
H	-4.79104400	-0.56570000	0.20812000
C	1.87777300	-2.62580100	-0.93185900
C	-5.08026300	3.71332500	-0.61365000
H	-5.80524900	4.50944800	-0.76702900
C	-4.37898000	-3.27923200	-1.80008200
H	-4.93977700	-4.11631700	-2.20987900
C	3.00108200	-0.44080800	0.58152100
C	4.23060500	-0.85337400	0.04525100
H	4.25801800	-1.60804000	-0.73311400
C	-0.28826500	-2.93959600	1.48116700
H	-0.86261000	-3.22346800	0.60985200
C	4.20374100	1.11320400	2.02164500
H	4.17854500	1.90858200	2.76139100
C	-3.55692100	2.06326100	-1.51544900
H	-3.08463000	1.59325000	-2.37325900
C	-4.49437900	3.07526800	-1.71066600
H	-4.75475000	3.37751100	-2.72192100
C	-5.00579400	-2.36415900	-0.94948000
H	-6.05784300	-2.48304500	-0.69942600
C	1.21122100	-1.86178500	2.85975700
H	1.97750500	-1.18993400	3.21897500
C	-2.45085600	-0.82162300	3.88977800
H	-2.85965400	-1.41919200	4.69533700
C	-3.78477200	2.31006100	0.87510300
H	-3.51520600	2.02217200	1.88647000
C	0.44957100	-2.76652000	3.65928200
H	0.53439200	-2.88968400	4.73194900

C	5.42957400	-0.30080700	0.50155900
H	6.37116200	-0.63516100	0.07094900
C	2.57967500	-4.98709400	-2.30578800
H	2.85003200	-5.89807600	-2.83546200
C	2.94059800	-4.82076600	-0.96471100
H	3.49208200	-5.60209100	-0.44591700
C	2.59062200	-3.65411700	-0.28702300
H	2.87388800	-3.53858400	0.75549800
C	-3.03655000	-3.10028600	-2.13624400
H	-2.54503500	-3.79173800	-2.81614500
C	1.86861900	-3.97946200	-2.95477300
H	1.57920400	-4.09741700	-3.99639100
C	-1.12676300	0.64918700	2.70178500
H	-0.36391000	1.36532400	2.42936500
C	1.51801500	-2.80675500	-2.27421500
H	0.95147400	-2.03719500	-2.78912300
C	-2.81053400	-0.91953900	2.51267700
H	-3.53458100	-1.60592500	2.09736300
C	-0.47314500	-3.43992700	2.80367300
H	-1.21883900	-4.16296200	3.10966500
C	-1.41230100	0.15122600	4.00592900
H	-0.89341500	0.42447500	4.91602900
Ru	0.06971200	0.69972400	-1.07947800
C	1.06923200	0.36991900	-3.51623700
O	1.56992900	0.36763600	-4.78861100
O	1.75365800	0.94804200	-2.61880400
O	-0.02331600	-0.21623800	-3.31702800
C	3.72637400	4.09847600	-0.31366900
C	3.71911900	5.04079800	0.72415600
C	2.58489100	5.11606200	1.54205600
C	1.49951200	4.27222900	1.33101100
C	1.49028400	3.29162500	0.29619600
C	2.64988400	3.24559700	-0.52807700
H	4.59409100	4.02598200	-0.96869200
H	4.56779000	5.70229300	0.88455900
H	2.54456600	5.84562400	2.35098200
H	0.62484000	4.35453000	1.97552400
H	2.68241700	2.52559900	-1.33746000
C	0.32654700	2.46237200	0.10313300
H	-0.52172400	2.77132900	0.71595800
N	-0.39628300	2.60167300	-1.56227600
N	-0.66963000	3.46074200	-2.28743200
H	2.38597600	0.89370500	-4.73094500

17-ts

Fe	-0.50196100	-1.15132900	2.87687300
P	1.54383500	-0.79302800	0.07676600
P	-1.96280800	0.20626300	0.09819400
C	3.03769400	0.10197000	0.75430400
C	2.37806300	-2.25872500	-0.74832500
C	2.91706900	0.94889300	1.86759700
H	1.95042600	1.08835400	2.33674400
C	-1.79458800	0.13811700	1.93253400
C	-3.16212300	-2.22145100	-0.73156900
H	-2.17736200	-2.42651300	-1.14077300
C	-5.47693600	-2.86661200	-0.41933200
H	-6.27889600	-3.59190600	-0.53844900
C	1.00116100	-1.72163100	1.59132900
C	3.84185900	-4.20286700	-0.63238300
H	4.51473400	-4.83635500	-0.05806700
C	4.29549000	-0.00877200	0.14283100
H	4.40788900	-0.61007800	-0.75045500
C	-2.88087500	1.82772000	-0.08658200
C	3.57094100	-4.49609400	-1.97218300
H	4.03289900	-5.35936500	-2.44684600
C	5.27707600	1.47262200	1.79076900
H	6.14156500	1.99644000	2.19262300
C	-3.40179600	-0.98572500	-0.11285400
C	-4.70406200	-0.69811500	0.32966800
H	-4.91708800	0.26261200	0.78994300
C	-0.81020800	0.88274700	2.66679600
H	-0.10733100	1.57457700	2.22257500
C	-4.19193600	-3.15620900	-0.87899200
H	-3.98750200	-4.10715600	-1.36578800
C	2.10914500	-2.56490000	-2.08742100
H	1.41713400	-1.94726600	-2.64744100
C	2.70229500	-3.67751800	-2.69294900
H	2.48070500	-3.89831700	-3.73441300
C	5.40330900	0.66670400	0.65895800
H	6.36777800	0.56338100	0.16675700
C	-2.50837900	-0.66435500	2.88923100
H	-3.29327200	-1.36913200	2.65419100
C	0.71521400	-2.62644300	3.71586800
H	0.81846200	-2.80263300	4.77957600
C	3.24723900	-3.09609800	-0.02749600
H	3.46453400	-2.87919100	1.01474800
C	-1.95530000	-0.42670300	4.18336500
H	-2.24962200	-0.92293700	5.09982100
C	-5.73191200	-1.63054100	0.18171200

H	-6.73379100	-1.39022800	0.53145000
C	-4.28927200	4.24555900	-0.44405800
H	-4.82818300	5.18015100	-0.58338100
C	-4.00841200	3.78044200	0.84022100
H	-4.32738900	4.34925800	1.71112800
C	-3.31238700	2.58063600	1.01768400
H	-3.10564300	2.23615800	2.02553000
C	4.02465500	1.61839700	2.38903000
H	3.90197900	2.26708400	3.25299900
C	-3.86573400	3.50313400	-1.54908500
H	-4.07095800	3.85849000	-2.55617300
C	-0.07773800	-2.66859600	1.55204900
H	-0.68040800	-2.88523700	0.68064400
C	-3.16605800	2.30820400	-1.37720500
H	-2.81849000	1.75321300	-2.24280800
C	1.49614700	-1.71834400	2.94002500
H	2.29487900	-1.09495800	3.31491900
C	-0.90833300	0.53432700	4.04579900
H	-0.26928300	0.90009300	4.83961900
C	-0.25515900	-3.21957400	2.85407800
H	-1.02388200	-3.92414100	3.14548600
Ru	-0.06933600	0.15541800	-1.27228400
C	-1.42279000	-0.72798700	-3.43445900
O	-2.09619900	-1.01205200	-4.59219500
O	-0.87562800	-1.68014500	-2.81313800
O	-1.41556600	0.47901100	-3.07236600
H	-1.97776300	-1.96945600	-4.70981500
C	1.95486600	0.91238700	-3.13418500
C	0.71622200	1.90084100	-1.51136500
H	0.04764000	2.41989700	-2.21695900
C	1.48685200	2.89903000	-0.72185700
C	2.86259600	3.14923300	-0.88021400
C	0.78496000	3.70703100	0.20159400
C	3.49924900	4.16082100	-0.15724600
H	3.42845200	2.53740200	-1.57243600
C	1.42423200	4.70968300	0.92928000
H	-0.28201000	3.54357500	0.33107600
C	2.79074100	4.94692200	0.75216900
H	4.56457200	4.32758000	-0.30426700
H	0.85001500	5.31561000	1.62852800
H	3.29239900	5.73228300	1.31407500
O	1.35471200	1.14638600	-4.14983400
O	3.01527200	0.54897100	-2.66868500

18-ts

Fe	3.37515100	-0.14192000	-1.62097900
P	0.80451100	-1.84021800	0.08154900
P	1.11749600	1.71989700	0.17619600
C	-0.03319100	-3.19505900	-0.86390900
C	1.21546900	-2.61256800	1.71896900
C	-0.55340900	-2.90926100	-2.14003200
H	-0.48953200	-1.90347800	-2.54164800
C	2.36009100	1.58574000	-1.16206400
C	2.28952800	1.04425400	2.65111500
H	1.76604400	0.10106300	2.53345000
C	3.75466100	2.46352500	3.95043900
H	4.36793500	2.63075600	4.83179600
C	2.46201300	-1.76358900	-0.70331300
C	2.50936300	-4.16047600	3.08218800
H	3.29095500	-4.91157400	3.15753100
C	-0.18223300	-4.48862200	-0.34078400
H	0.19664900	-4.73268000	0.64545900
C	0.36766300	3.38895000	-0.11520900
C	1.79769900	-3.77252300	4.22049400
H	2.02439700	-4.21947000	5.18451600
C	-1.32720800	-5.19699400	-2.35204700
H	-1.83041000	-5.96998300	-2.92668700
C	2.16260900	2.03738700	1.67046900
C	2.83960200	3.25567900	1.85331400
H	2.74029700	4.04515200	1.11459500
C	2.10732000	1.21078600	-2.53280300
H	1.15146200	0.93626000	-2.95416500
C	3.08122700	1.25324600	3.78359400
H	3.16372800	0.47105300	4.53345300
C	0.50611600	-2.23648900	2.87103300
H	-0.28309400	-1.49128200	2.80871200
C	0.79490700	-2.80919300	4.11270200
H	0.23381700	-2.50050100	4.99035800
C	-0.82710300	-5.48168100	-1.08195800
H	-0.93906500	-6.47676100	-0.65946500
C	3.77710200	1.80326600	-1.03786800
H	4.29843300	2.05919200	-0.12687600
C	4.18851400	-1.96058600	-2.23862800
H	4.72425400	-2.10498700	-3.16768100
C	2.22302400	-3.58567200	1.84388500
H	2.78630100	-3.89469300	0.96935000
C	4.38137800	1.55788900	-2.30330900
H	5.44254500	1.59289600	-2.51384300
C	3.63104400	3.46467000	2.98271400

H	4.14756700	4.41232900	3.10989700
C	-0.90063500	5.86687000	-0.51047600
H	-1.39212900	6.82371800	-0.66390500
C	-0.23923900	5.24097000	-1.56643200
H	-0.21330900	5.70550000	-2.54819100
C	0.39208800	4.00985300	-1.37205500
H	0.90207000	3.53869300	-2.20524900
C	-1.18787900	-3.90997100	-2.87653700
H	-1.58613700	-3.67354400	-3.85934200
C	-0.93303600	5.25524200	0.74569800
H	-1.44815900	5.73467700	1.57378700
C	3.70031800	-1.42709300	-0.04598600
H	3.80659200	-1.12077400	0.98543800
C	-0.30885000	4.02436500	0.94122300
H	-0.34454300	3.55884800	1.92190100
C	2.78027000	-2.08591800	-2.06538700
H	2.06717300	-2.35887800	-2.82986200
C	3.35171300	1.20225300	-3.22310800
H	3.49194100	0.91912300	-4.25828800
C	4.75732100	-1.56091600	-0.99259500
H	5.80203100	-1.34774200	-0.80725900
Ru	-0.57152600	-0.00139600	0.35282900
C	-1.37091100	0.82306400	-2.52287700
O	-2.23183800	1.72980200	-1.97496900
O	-0.61888200	0.11811600	-1.70991700
O	-1.30959700	0.70306900	-3.73412300
H	-2.08716400	1.79142600	-1.01437300
C	-3.34180800	1.53435000	1.32144400
C	-4.02687000	-0.30543800	0.18410200
H	-3.51199200	0.10196200	-0.68767000
N	-3.40176300	-1.19700600	0.94964200
N	-2.10198400	-1.32608600	0.88298500
H	-1.85336100	-2.16396200	1.40575900
C	-5.49474900	-0.25186600	0.17005600
C	-6.13943300	0.45208900	-0.86196600
C	-6.28281800	-0.86171500	1.16214300
C	-7.53012800	0.53774200	-0.90673200
H	-5.54024400	0.93171000	-1.63323800
C	-7.67167000	-0.77663500	1.11266600
H	-5.79194300	-1.40432000	1.96381900
C	-8.30401400	-0.07649600	0.08009200
H	-8.00934500	1.08413200	-1.71518700
H	-8.26653400	-1.25648000	1.88622800
H	-9.38834300	-0.00983900	0.04722100
O	-2.18749700	1.60475300	0.95360100
O	-4.27652000	1.94672400	1.90571300

19

Fe	3.29610900	-0.83029600	-1.47514800
P	0.36030900	-1.93745000	0.01425800
P	1.30482500	1.63650900	-0.09215200
C	-0.66273300	-2.63387100	-1.35735400
C	0.24640600	-3.24687000	1.31881700
C	-0.38104700	-2.39038700	-2.71270000
H	0.52495600	-1.86682000	-2.99747700
C	2.51077900	1.06815100	-1.35747400
C	2.83521800	1.63063800	2.27925300
H	2.39129100	0.65636700	2.44551100
C	4.27456600	3.42912100	3.02496900
H	4.97932300	3.83407900	3.74638600
C	2.11004600	-2.17348800	-0.47555100
C	0.60809300	-5.56173500	1.96511000
H	0.91475500	-6.57148000	1.70509100
C	-1.85789000	-3.29412000	-1.02528800
H	-2.11951100	-3.45554000	0.01480800
C	0.57857000	3.12574500	-0.93340600
C	0.17821300	-5.26802600	3.26254000
H	0.14871200	-6.05081500	4.01609300
C	-2.43202800	-3.49457900	-3.37090700
H	-3.11417200	-3.82951600	-4.14748300
C	2.44699900	2.38533200	1.16177700
C	2.97711200	3.67525600	0.99627100
H	2.68024300	4.27931300	0.14481000
C	2.16949400	0.46385100	-2.61759200
H	1.16763200	0.27503700	-2.97812200
C	3.74706400	2.14909700	3.20177400
H	4.03626100	1.55372600	4.06394000
C	-0.18527400	-2.95845300	2.61935400
H	-0.50535300	-1.95715000	2.87241300
C	-0.21508700	-3.96998600	3.58436400
H	-0.55696200	-3.73733400	4.58930700
C	-2.73185200	-3.72051000	-2.02613700
H	-3.65276400	-4.22489400	-1.74769200
C	3.94526600	1.13142000	-1.30401800
H	4.52343900	1.50302500	-0.46997400
C	4.11651300	-2.76087700	-1.48474200
H	4.83317400	-3.12024800	-2.21191300
C	0.64484900	-4.55732800	1.00045700
H	0.98208300	-4.79551600	-0.00459800

C	4.46944300	0.56494300	-2.50214500
H	5.51834600	0.42932900	-2.73165800
C	3.88398400	4.19233500	1.92230800
H	4.28248400	5.19375200	1.78276700
C	-0.58026800	5.38846700	-2.13857200
H	-1.03193500	6.25894500	-2.60687700
C	0.53452600	4.78059200	-2.71674200
H	0.95866700	5.17673300	-3.63578500
C	1.11206700	3.65798200	-2.11848700
H	1.98160800	3.20101100	-2.57871100
C	-1.25544900	-2.82605700	-3.71143400
H	-1.01512400	-2.63912000	-4.75495200
C	-1.11197800	4.87193600	-0.95515200
H	-1.97861700	5.34023300	-0.49640500
C	3.19467100	-1.74387000	0.36627300
H	3.09115500	-1.20803200	1.29922400
C	-0.54103100	3.74894400	-0.35502700
H	-0.95863000	3.35705300	0.56595300
C	2.69921100	-2.82052700	-1.61583500
H	2.16376200	-3.25206600	-2.44866900
C	3.37291800	0.15877200	-3.31769700
H	3.44023800	-0.33302300	-4.27948300
C	4.42191900	-2.10194400	-0.25841500
H	5.41190700	-1.86954000	0.11154000
Ru	-0.42461300	0.17482600	0.69524800
C	-0.58709200	1.25276400	3.00724200
O	-0.78321500	1.74919200	4.24031300
O	0.17531200	0.24776400	2.84413100
O	-1.17218600	1.81574000	2.03801800
H	-0.27522900	1.18588300	4.84970900
C	-3.30085000	-0.73466600	0.96700200
C	-3.47595600	0.60795100	0.13597400
H	-3.00444500	1.38507500	0.75063400
N	-2.72639800	0.49189800	-1.11966600
N	-1.48606900	0.35802000	-0.99864200
C	-4.91188900	0.96295700	-0.15357000
C	-5.48503600	2.08950900	0.44387300
C	-5.69317500	0.17748600	-1.01067500
C	-6.81629700	2.43088100	0.19298700
H	-4.88682300	2.70292600	1.11460600
C	-7.01888300	0.51978700	-1.26908500
H	-5.25754800	-0.70540800	-1.46780100
C	-7.58548000	1.64748100	-0.66725200
H	-7.24786200	3.30877600	0.66702800
H	-7.61548500	-0.09789700	-1.93571100
H	-8.62101400	1.91085100	-0.86753900
O	-2.09069500	-0.96225500	1.36914100
O	-4.26965800	-1.44729500	1.17569600
H	-1.06240000	0.27255000	-1.92841000

Reference:

[1] (a) J.-S. Poh, D. N. Tran, C. Battilocchio, J. M. Hawkins and S. V. Ley, *Angew. Chem. Int. Ed.* 2015*,* **54***,* 7920; (b) M. Hu, C. Ni, L. Li, Y. Han and J. Hu, *J. Am. Chem. Soc.* 2015, **137**, 14496; (c) L.-M. Zhao, H.-S. Jin, J. Liu, T. C. Skaar, J. Ipe, W. Lv, D. A. Flockhart and M. Cushman, *Bioorg. Med. Chem.* 2016, **24***,* 5400*.*

[2] T. Moragas, M. Gaydou and R. Martin, *Angew. Chem. Int. Ed.* 2016, **55**, 5053.

[3] T. León, A. Correa and R. Martin, *J. Am. Chem. Soc.* 2013, **135**, 1221.

[4] The observed exact mass on mass spectroscopy matches with calculated mass of [M-COOH], such cases were also observed in A. Correa, T. León and R. Martin, *J. Am. Chem. Soc.* 2014, **136**, 1062. (Compound 8k, 8m, 8n, 8o, 10j). However, both NMR (^{1}H and ^{13}C) indicate the existence of carboxylic acid group.

[5] S.-C. Sha, J. Zhang and P. J. Walsh, *Org. Lett.* 2015, **17**, 410.

[6] S. Kodumuri, S. Peraka, N. Mameda, D. Chevella, R. Banothu and N. Nama, *RSC Adv.* 2016, **6**, 6719.

[7] S. M. Waybright, C. P. Singleton, K. Wachter, C. J. Murphy and U. H. F. Bunz, *J. Am. Chem. Soc.* 2001, **123**, 1828.

[8] M. Ohkoshi, J. Y. Michinishi, S. Hara and H. Senboku, *Tetrahedron* 2010, **66**, 7732.

[9] M.-Y. She, D.-W. Xiao, B. Yin, Z. Yang, P. Liu, J.-L. Li and Z. Shi, *Tetrahedron* 2013, **69**, 7264.

[10] T.-S. Mei, D.-H. Wang and J.-Q. Yu, *Org. Lett.* 2010, **12**, 3140.

[11] D. D. Tanner and S. A. A. Osman, *J. Org. Chem.* 1987, **52**, 4689.

[12] Patent: R. B. William, S. Cai and L. K. Eric, US6087358, 2000.

[13] J. McNulty and P. Das, *Tetrahedron* 2009, **65**, 7794.

[14] C. Dalvit and A. Vulpetti, *Magn. Reson. Chem.* 2012, **50**, 592.

[15] F. Fernandez, G. Gomez, C. Lopez and A. Santos, *Synthesis* 1988, **10**, 802.

[16] G. Arena, R. Cali, E. Maccarone and A. Passerini, *J. Chem. Soc., Perkin Trans. 2* 1993, **0**,1941.

[17] B. Ma, Z. Chu, B. Huang, Z. Liu, L. Liu and J. Zhang, *Angew. Chem. Int. Ed.* 2017, **56**,2749.

[18] Patent: T. Pierre and L. Silvana, WO2008122115, 2008.

[19] J. A. Mukhlall, B. C. Noll and W. H. Hersh, *J. Sulfur Chem.* 2011, **32**, 199.

[20] M. C. Lu, W. E. Wung, L. B. Shih, S. Callejas, J. E. Gearien and E. B. Thompson, *J. Med. Chem.* 1987, **30**, 273.

[21] A. Rodríguez-Bárzano, J. D. A. Fonseca, A. J. Blacker and P. C. McGowan, *Eur. J. Inorg. Chem.*2014, **11**, 1974.

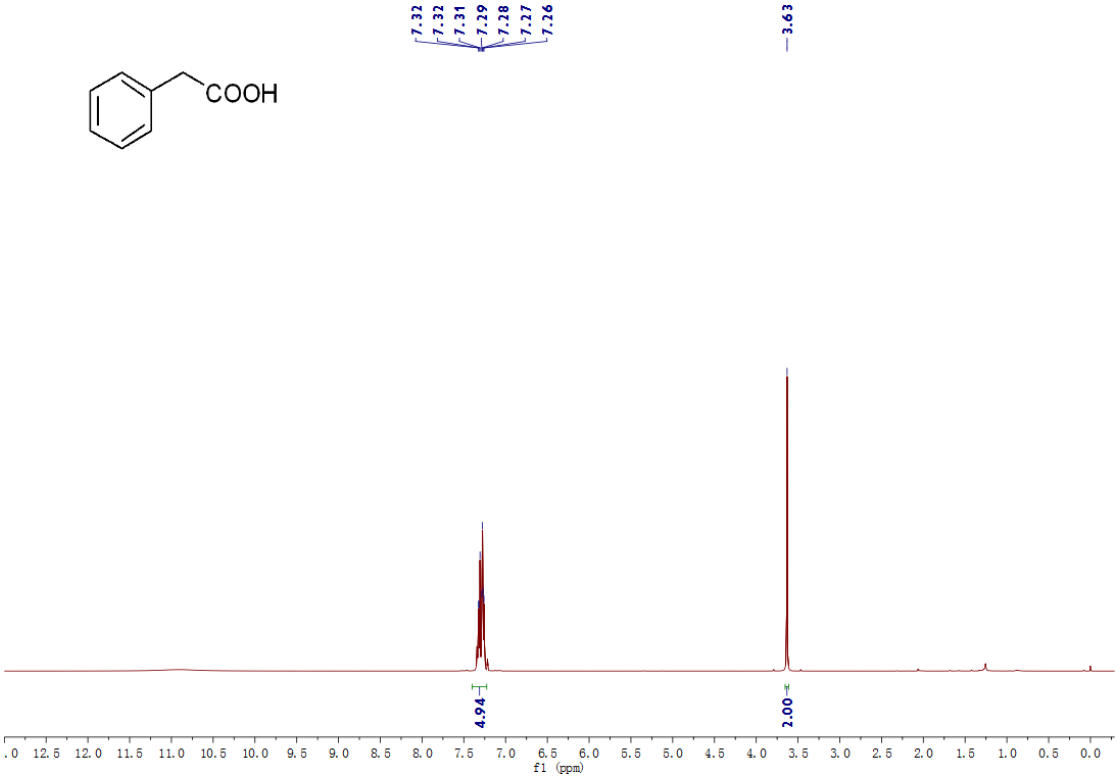
[22] a) A. D. Becke, *J. Chem. Phys*. 1993, **98**, 5648; b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785.

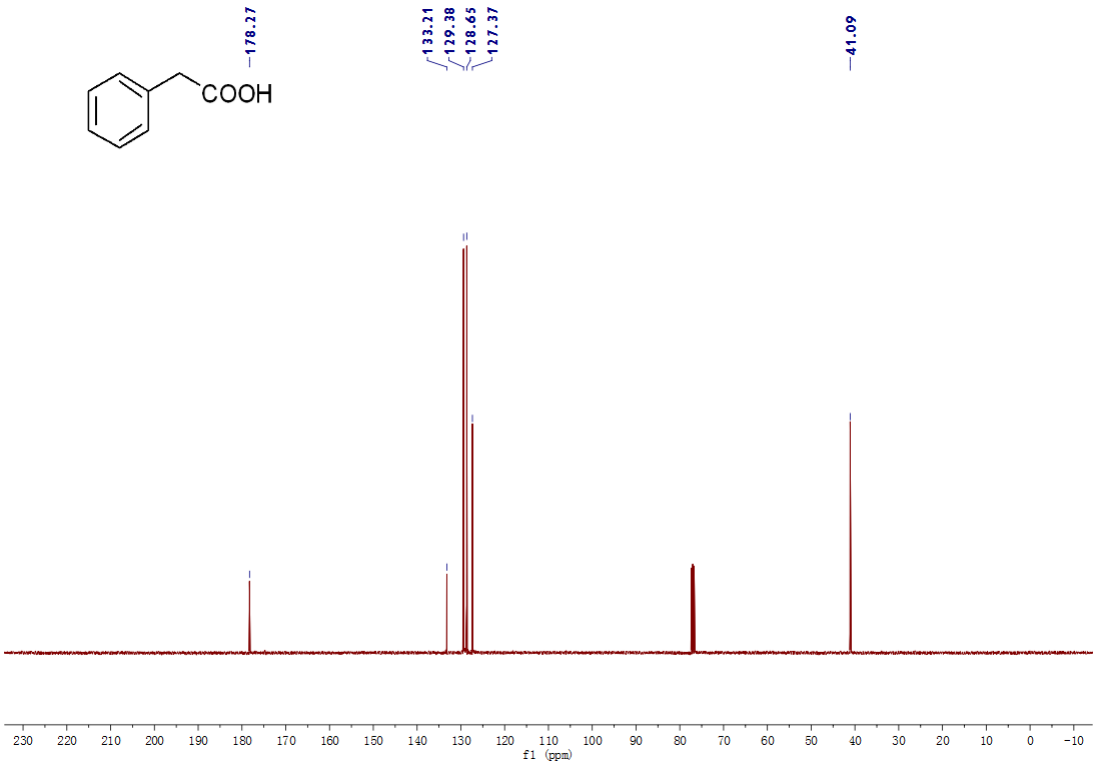
[23] a) P. J. Hay and W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 270-283; b) W. R. Wadt and P. J. Hay, *J. Chem. Phys.* 1985, **82**, 284-298; c) P. J. Hay and W. R. Wadt, *J. Chem. Phys.* 1985, **82**,299-310.

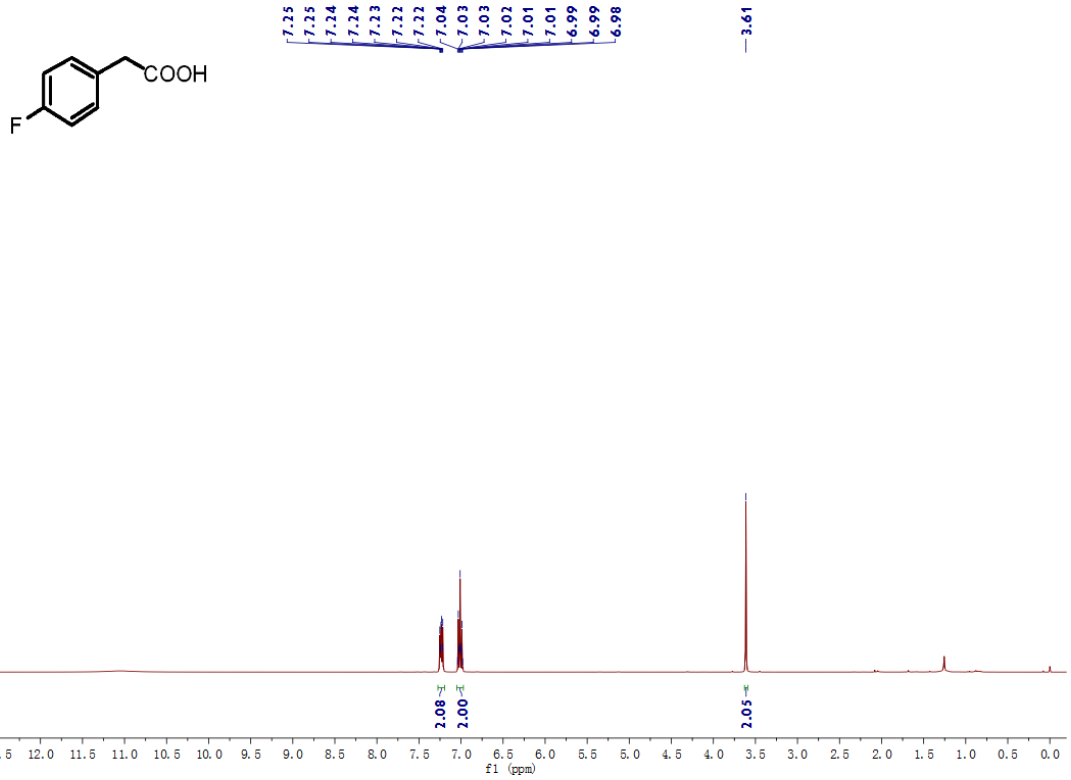
[24] Y. Zhao and D. G. Truhlar, *J. Chem. Phys.* 2006, **125**, 194101.

[25] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B* 2009, **113**, 6378.

^{1}H NMR, ^{19}F NMR and ^{13}C NMR Spectra



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7.24
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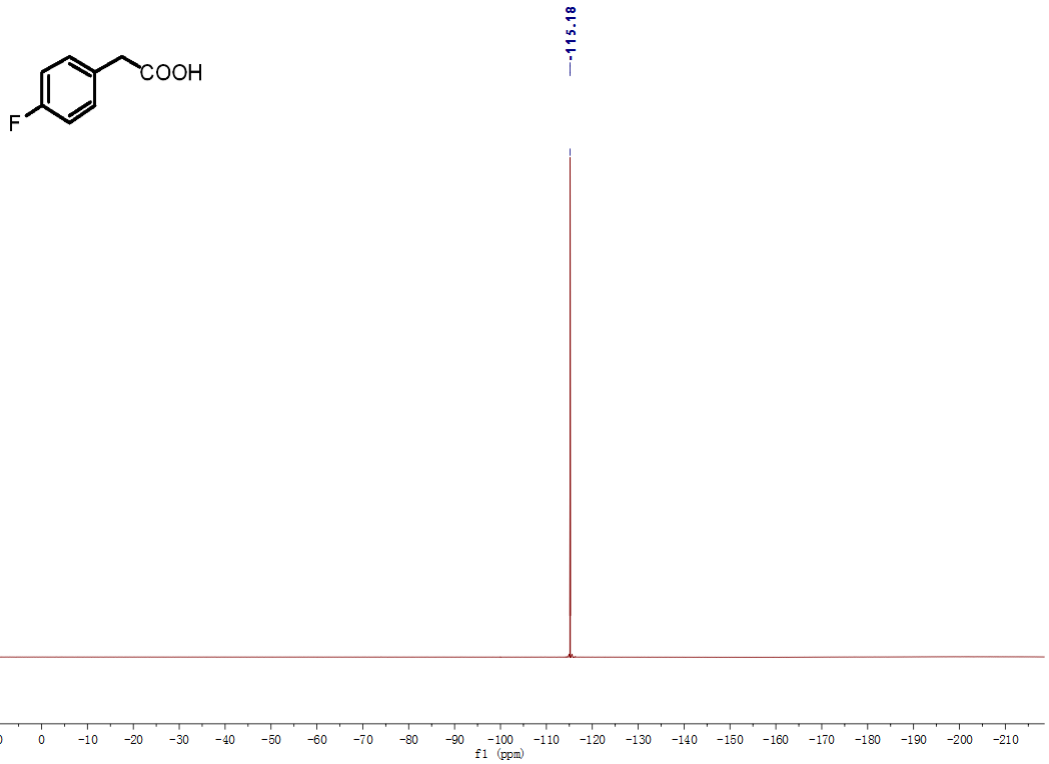
7.22
7.22
7.04
7.03
7.03
7.02
7.01
7.01
6.99
6.99
6.98
3.61
2.08
2.00
2.05
f1 (ppm)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F
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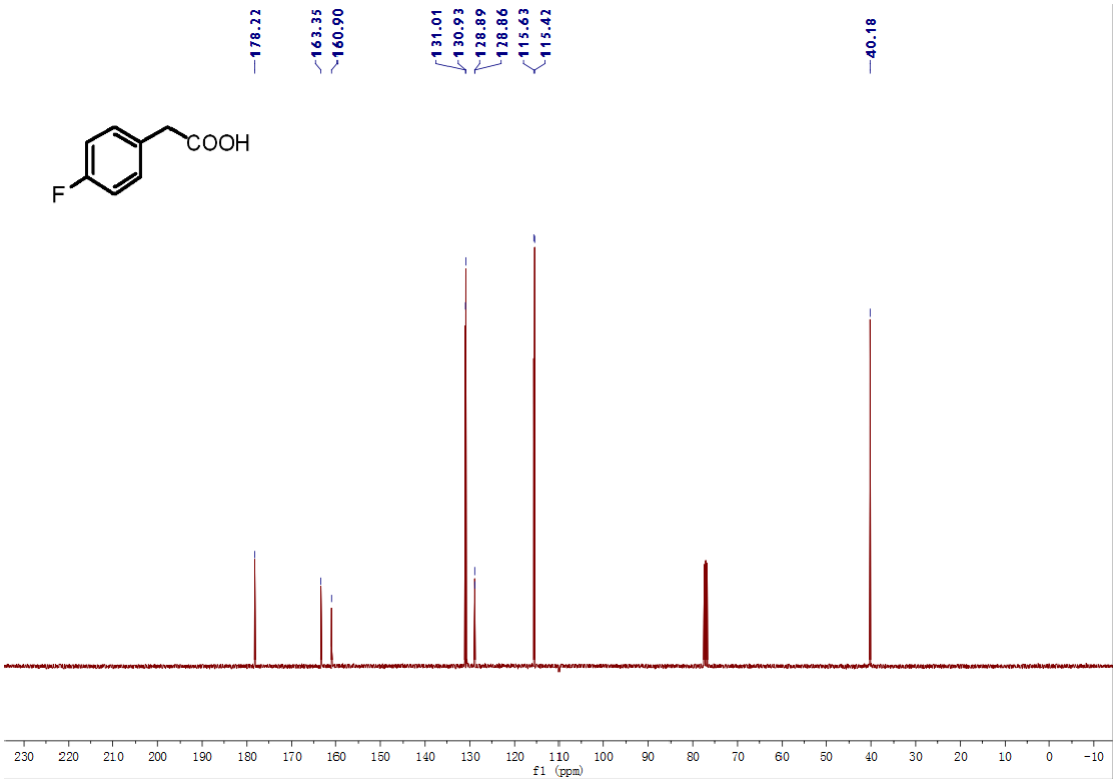
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115.42
40.18
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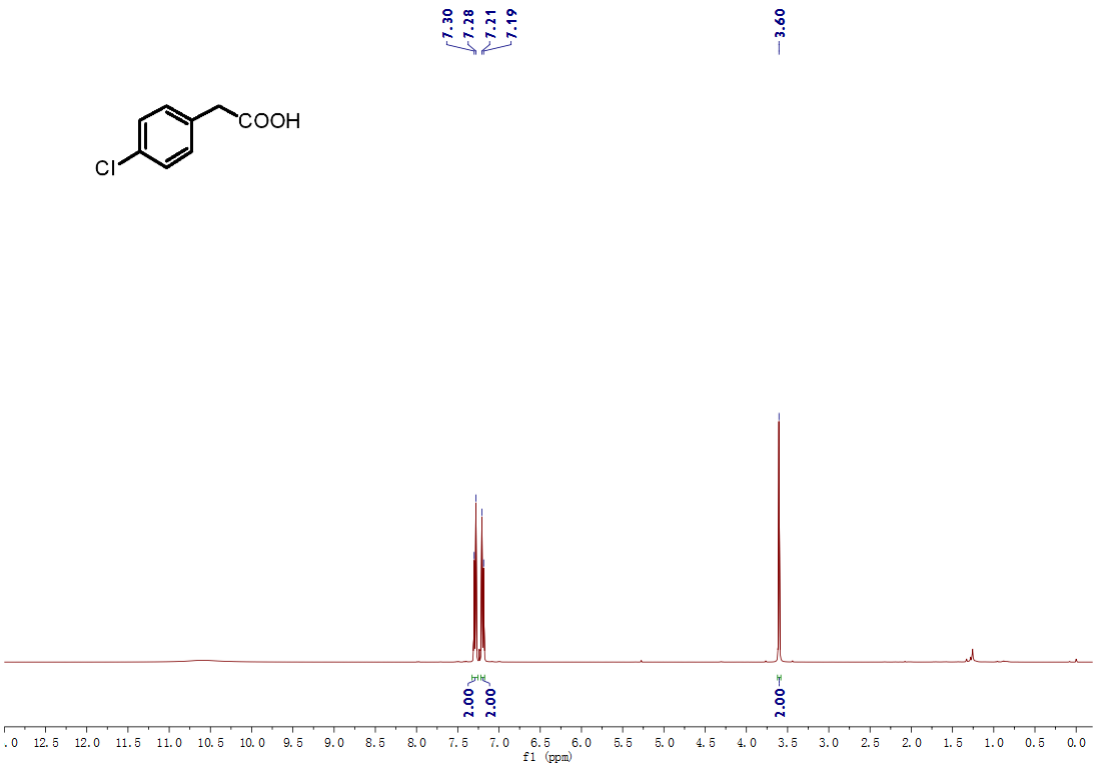
F
f1 (ppm)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Cl
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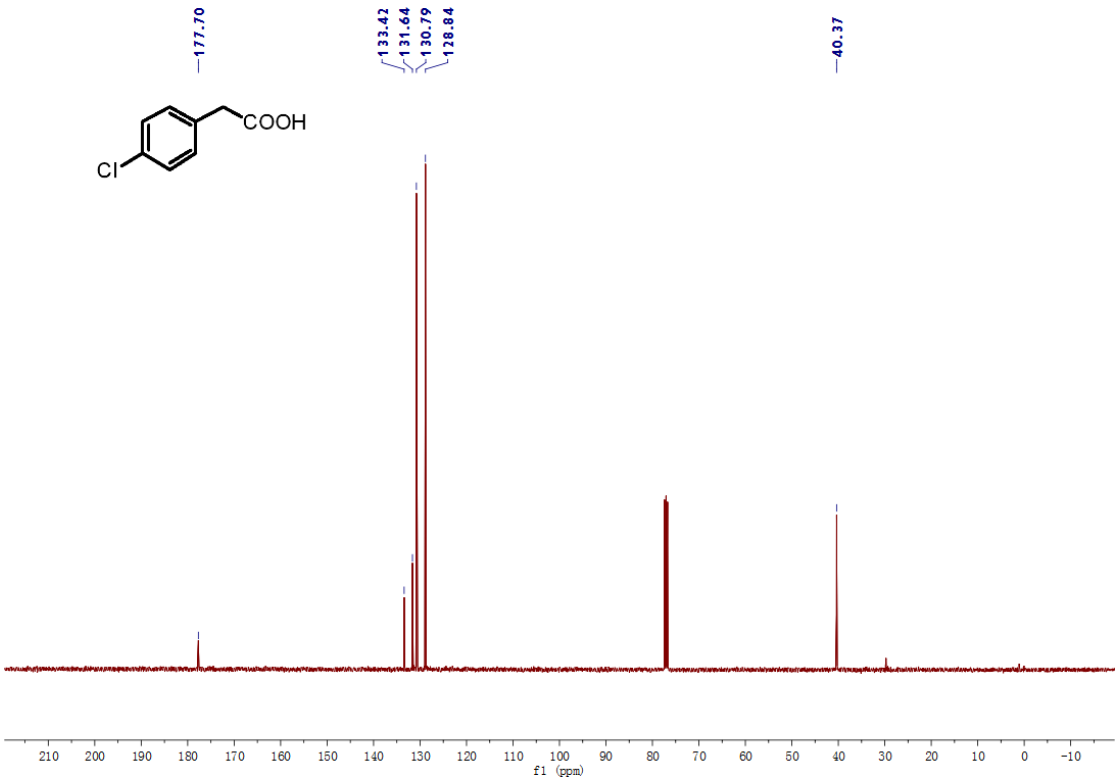
2.00
2.00
f1 (ppm)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Cl
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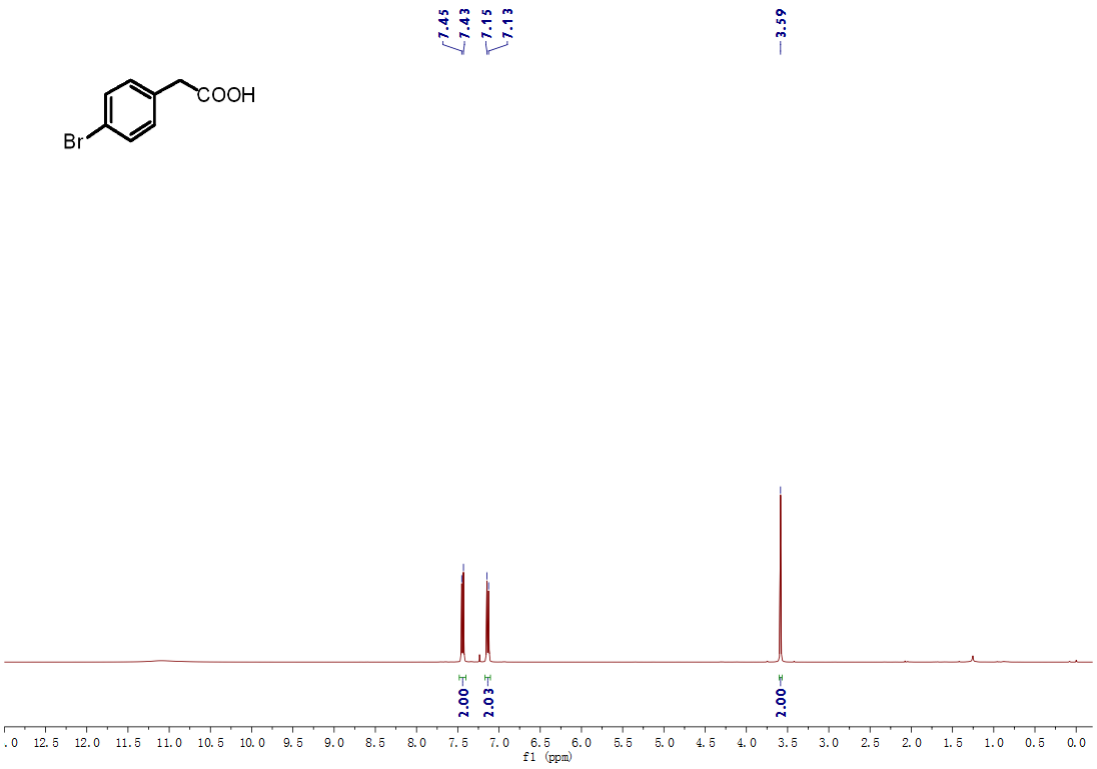
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Br
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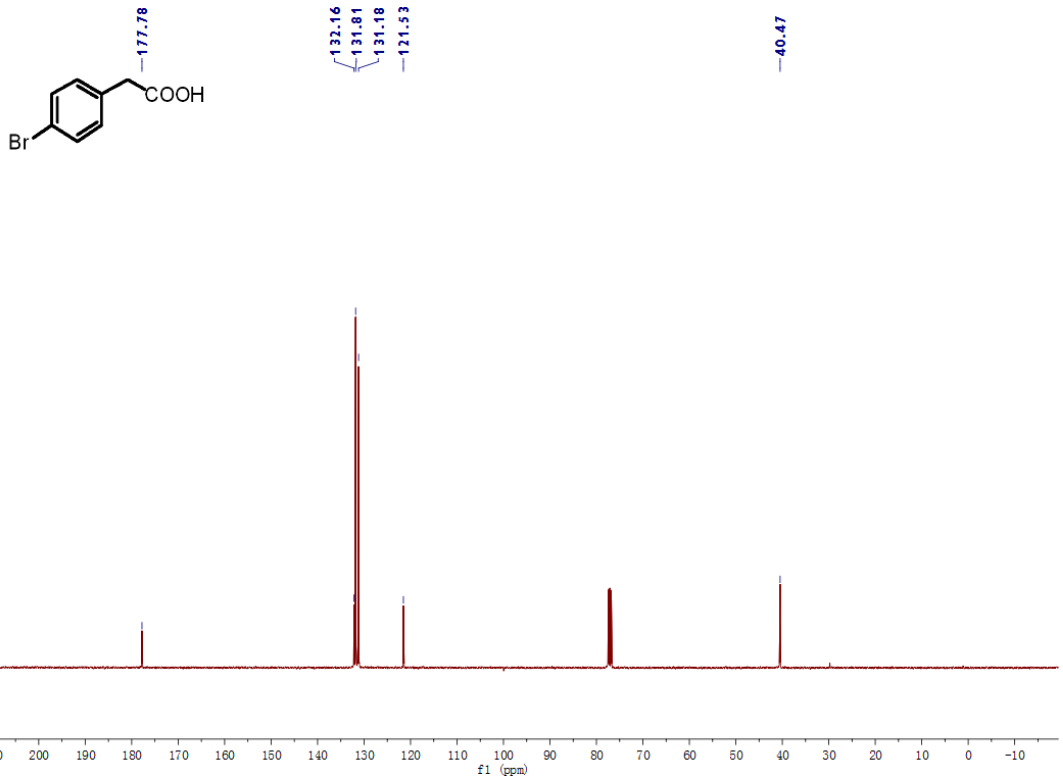
2.03
2.00
f1 (ppm)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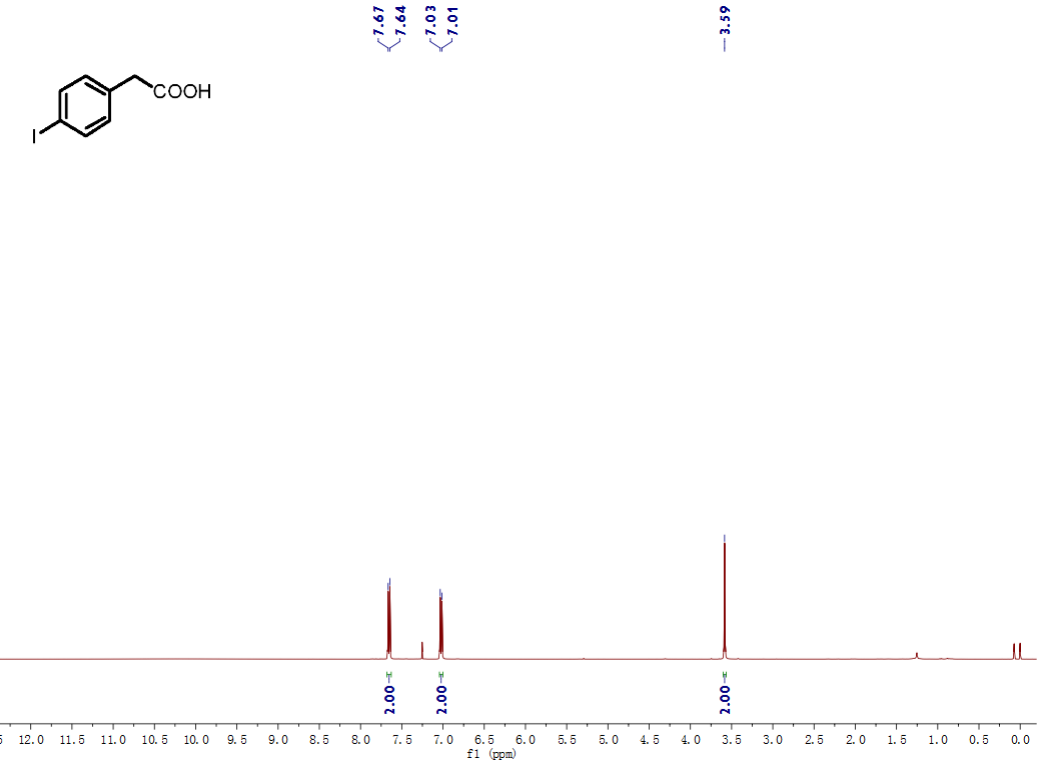
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I
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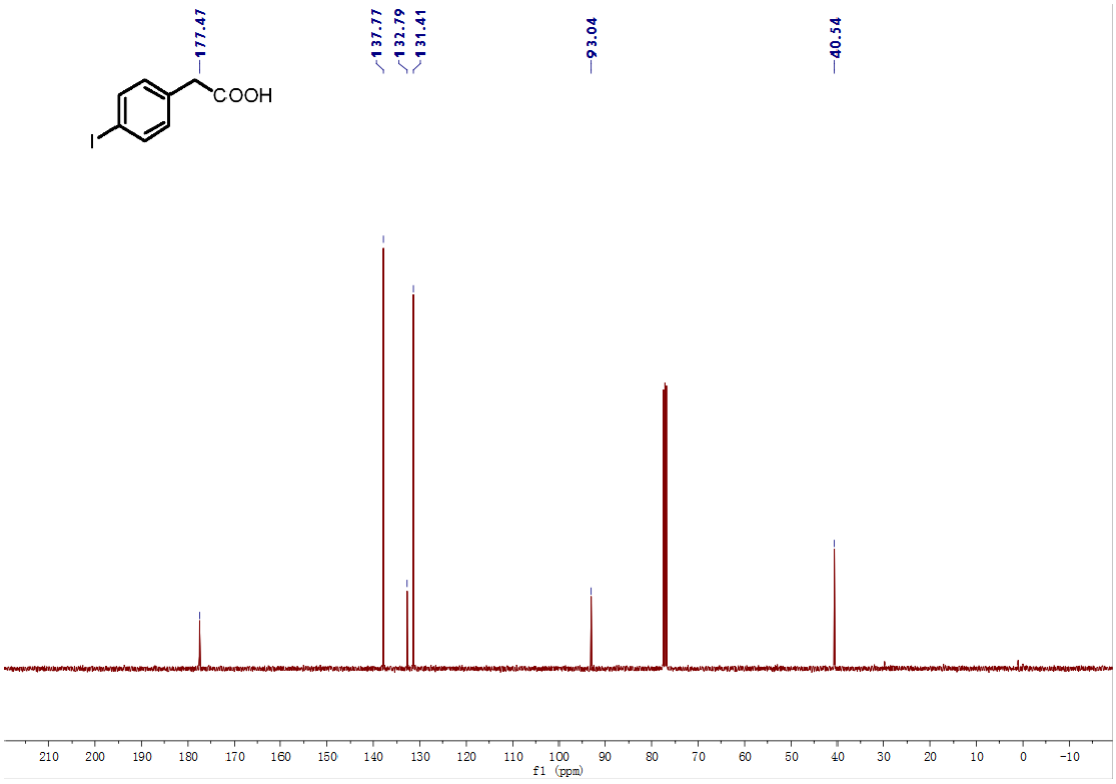
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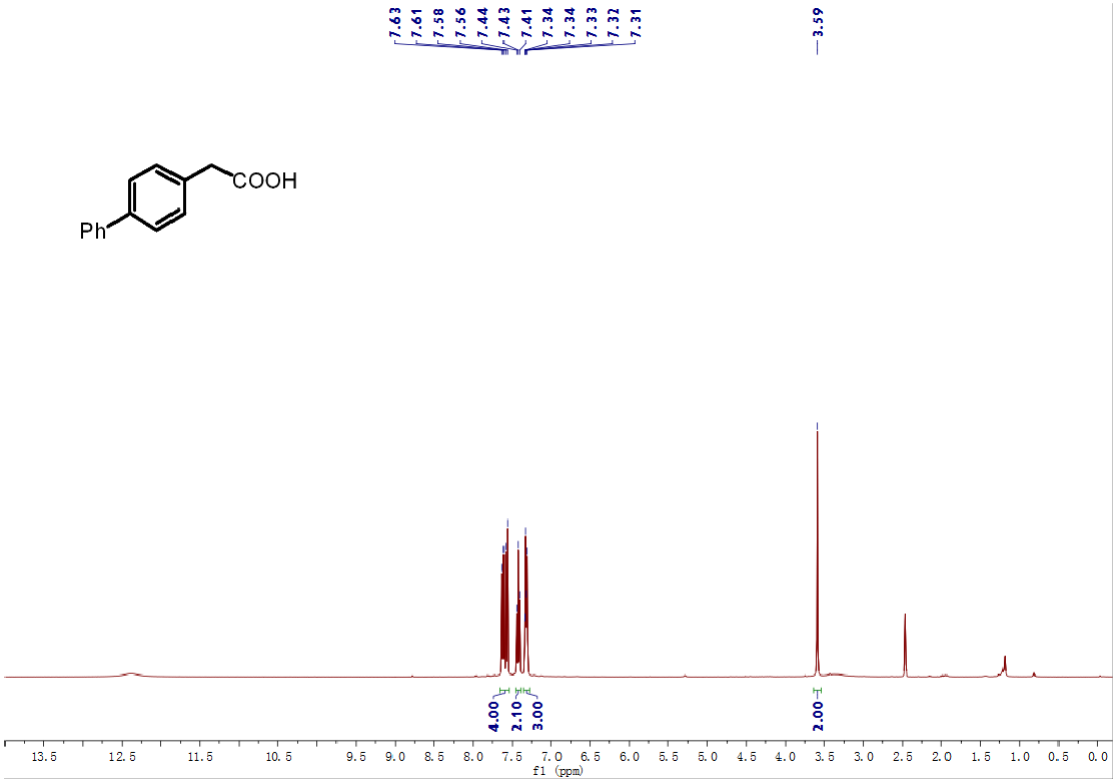
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Ph
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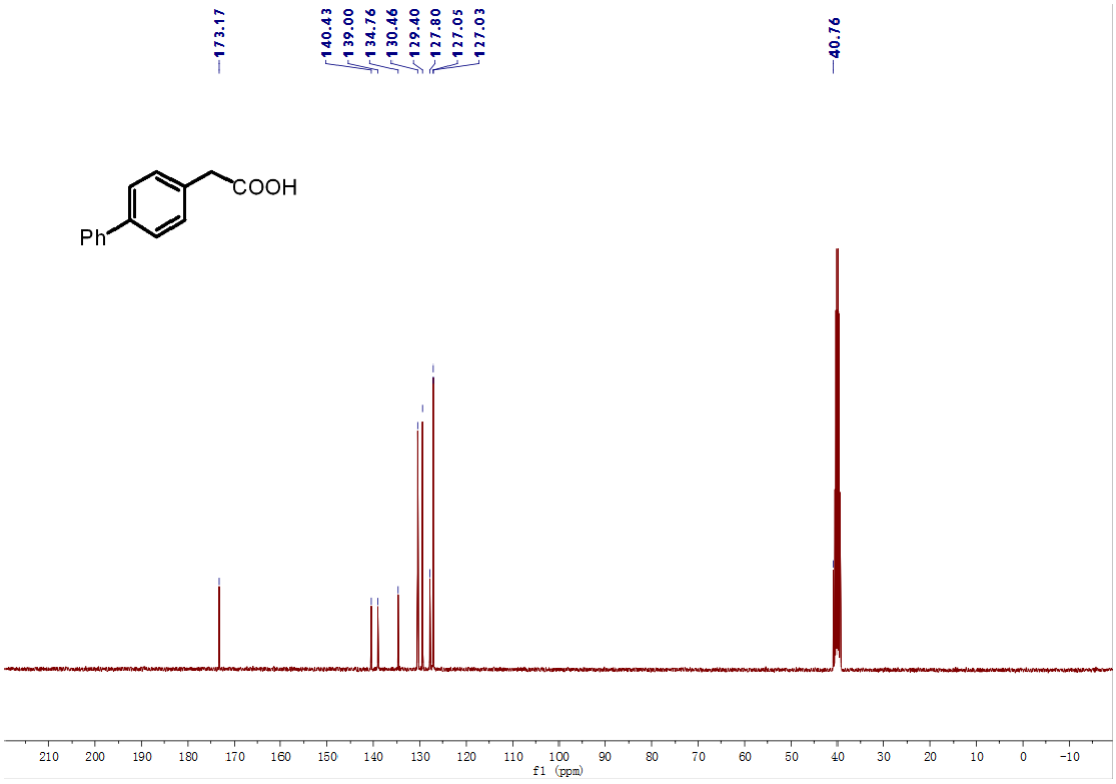
3.00
2.00
f1 (ppm)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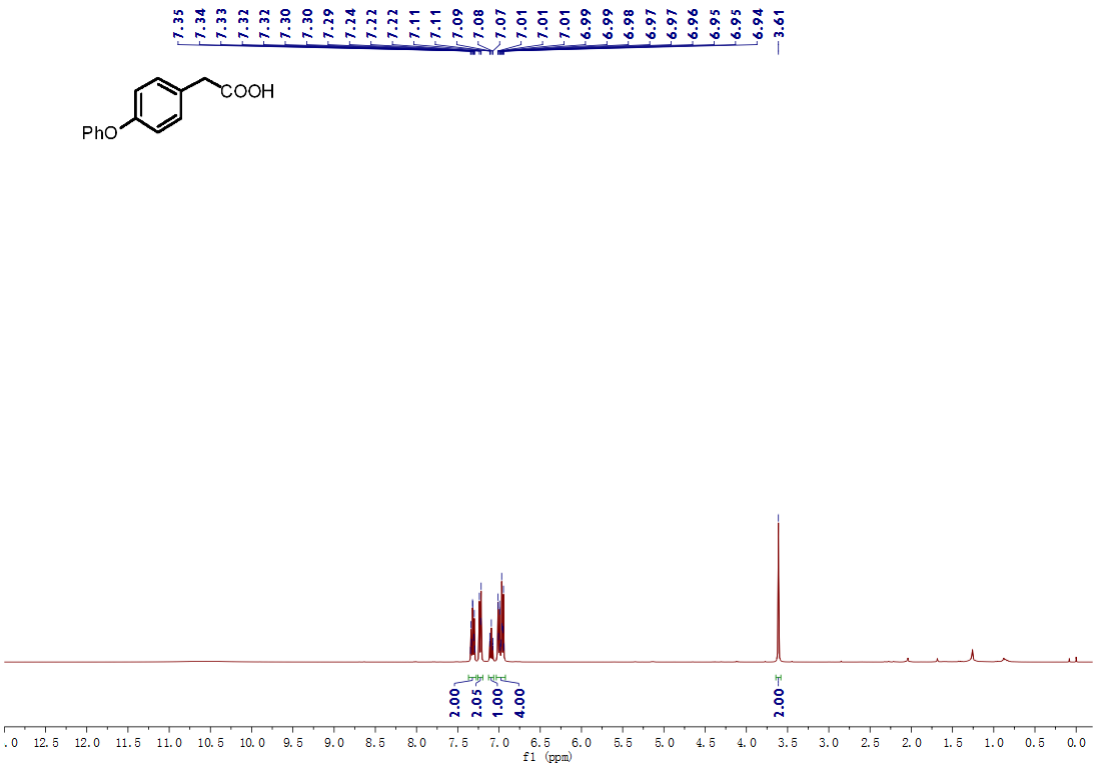
Ph
f1 (ppm)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7.01
6.99
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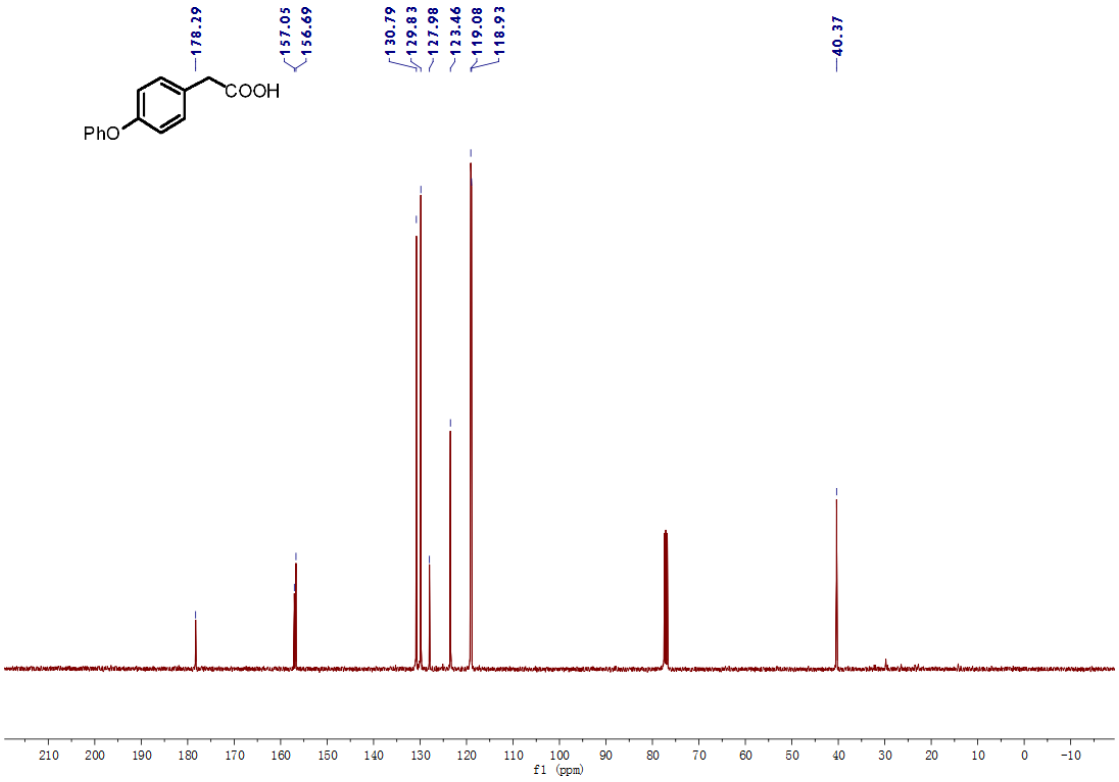
f1 (ppm)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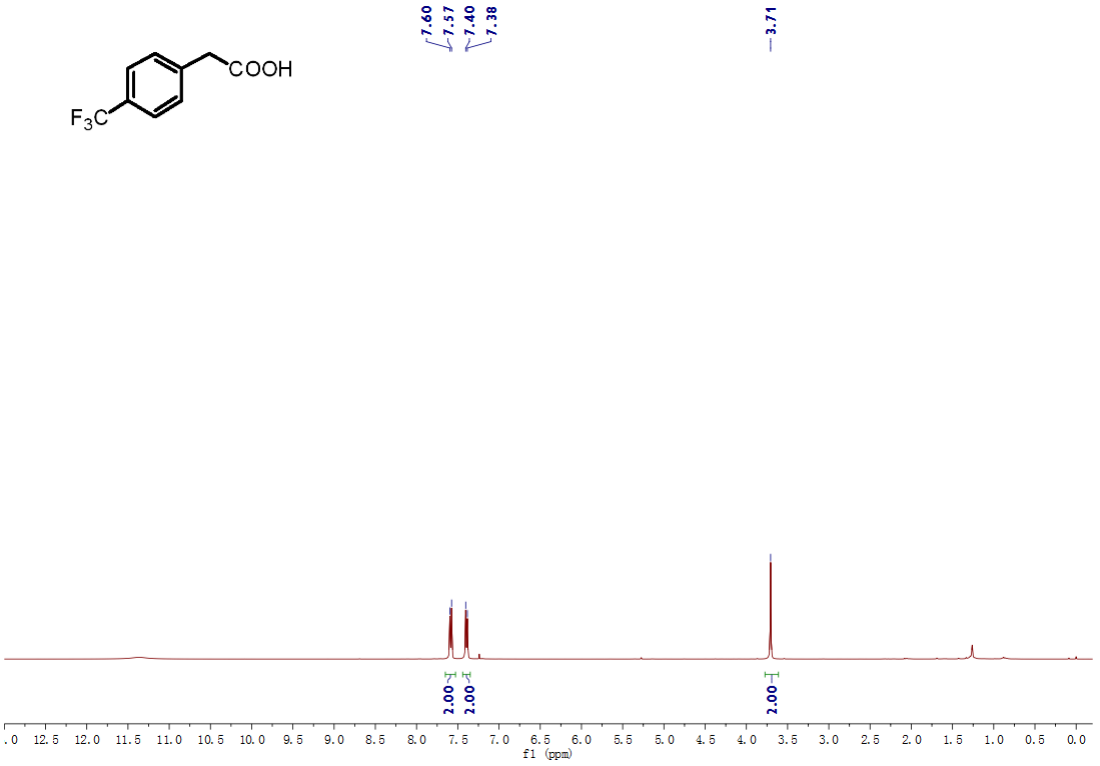
f1 (ppm)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2.00
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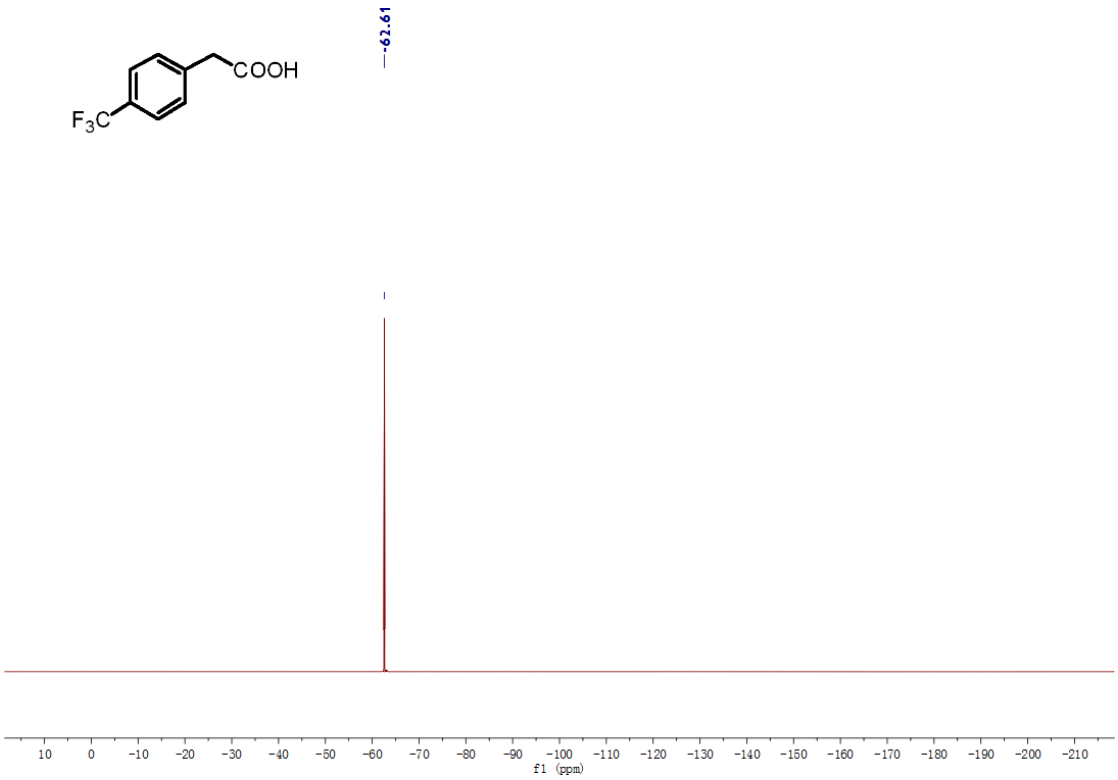
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F3C
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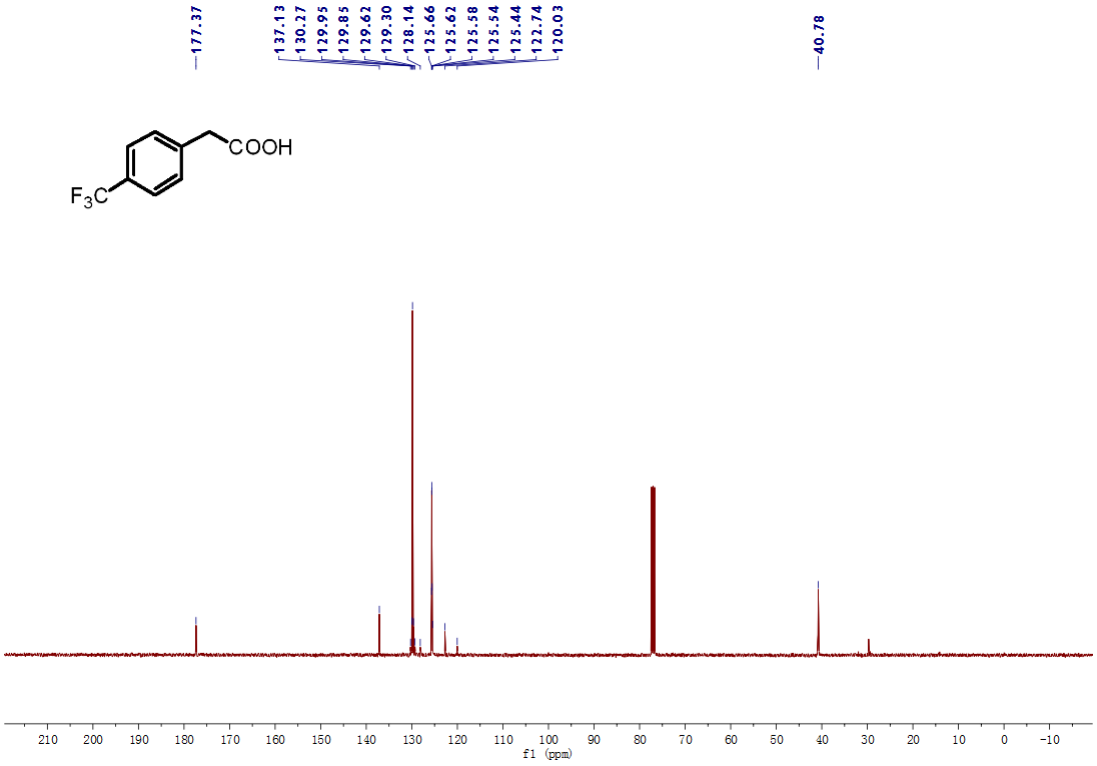
f1 (ppm)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125.62
125.58
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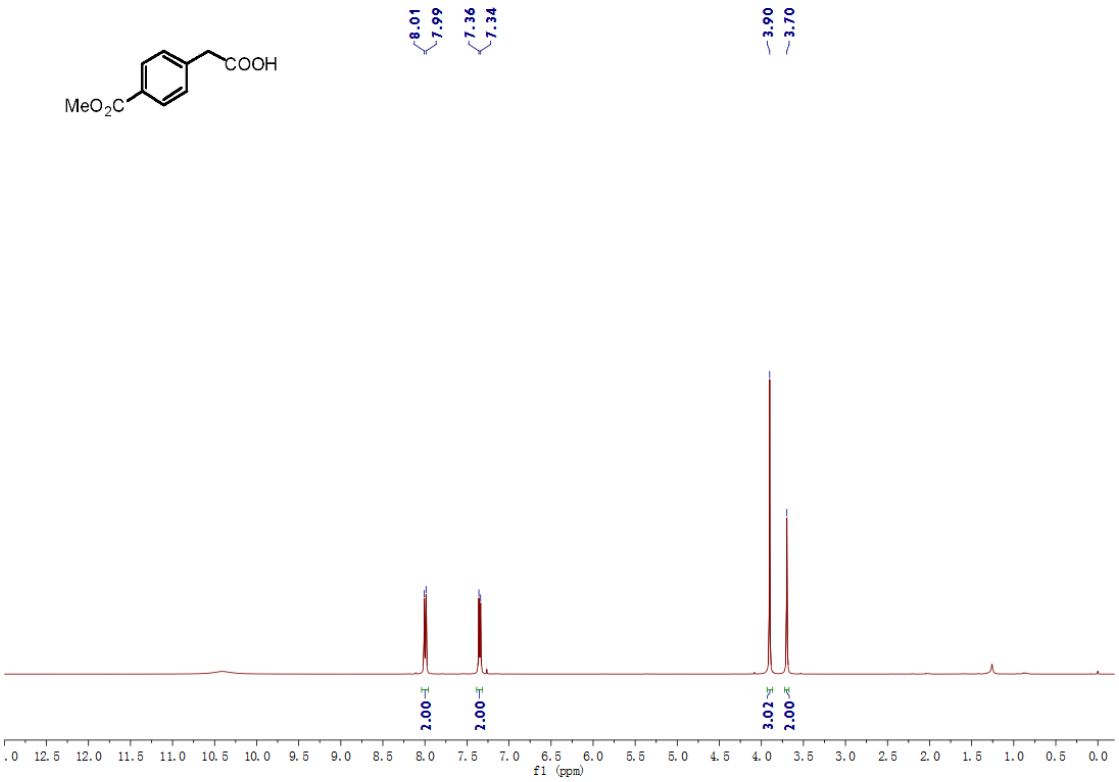
f1 (ppm)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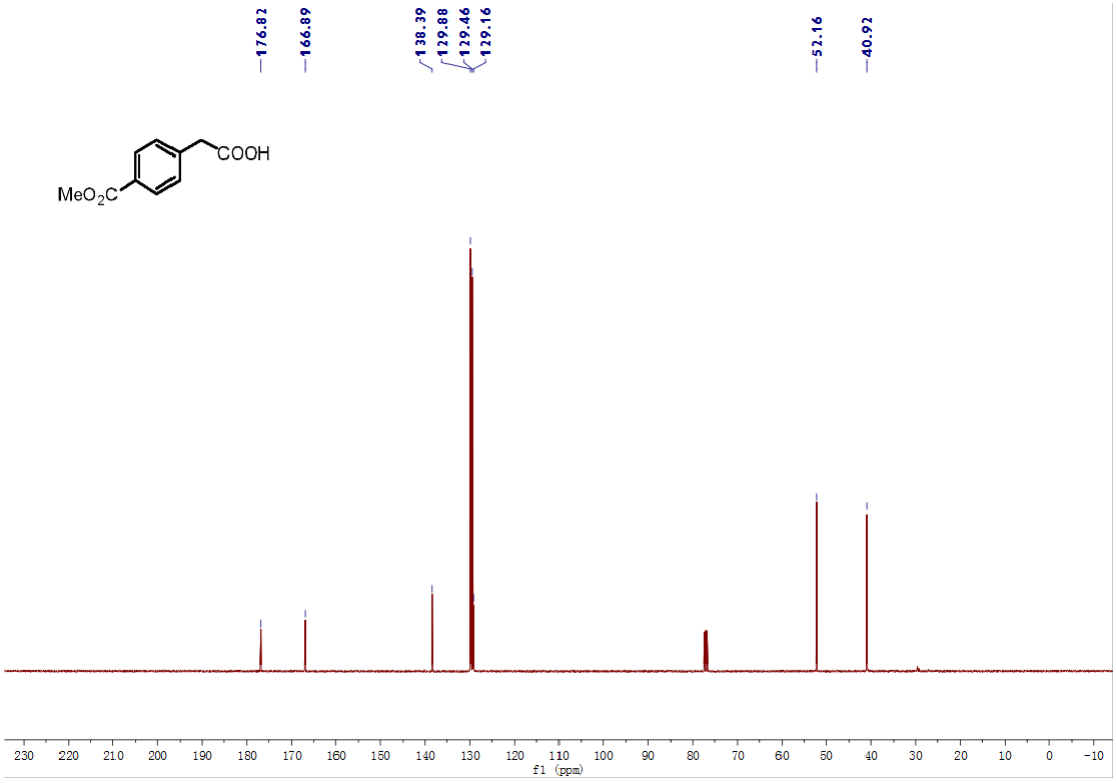
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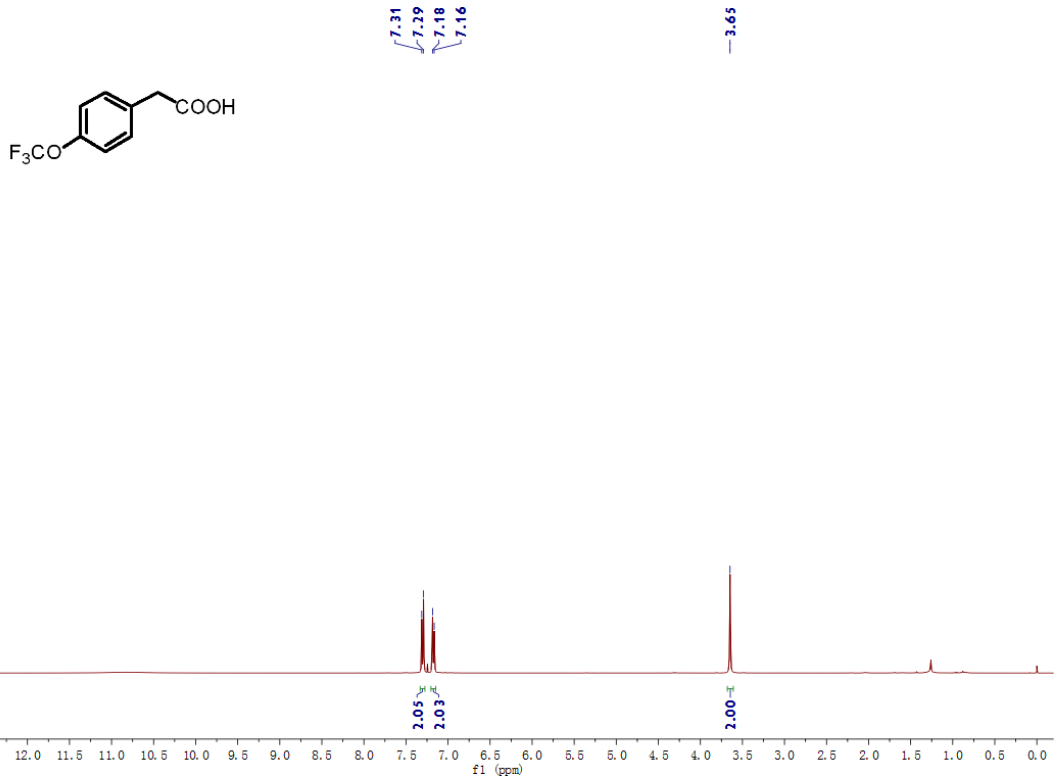
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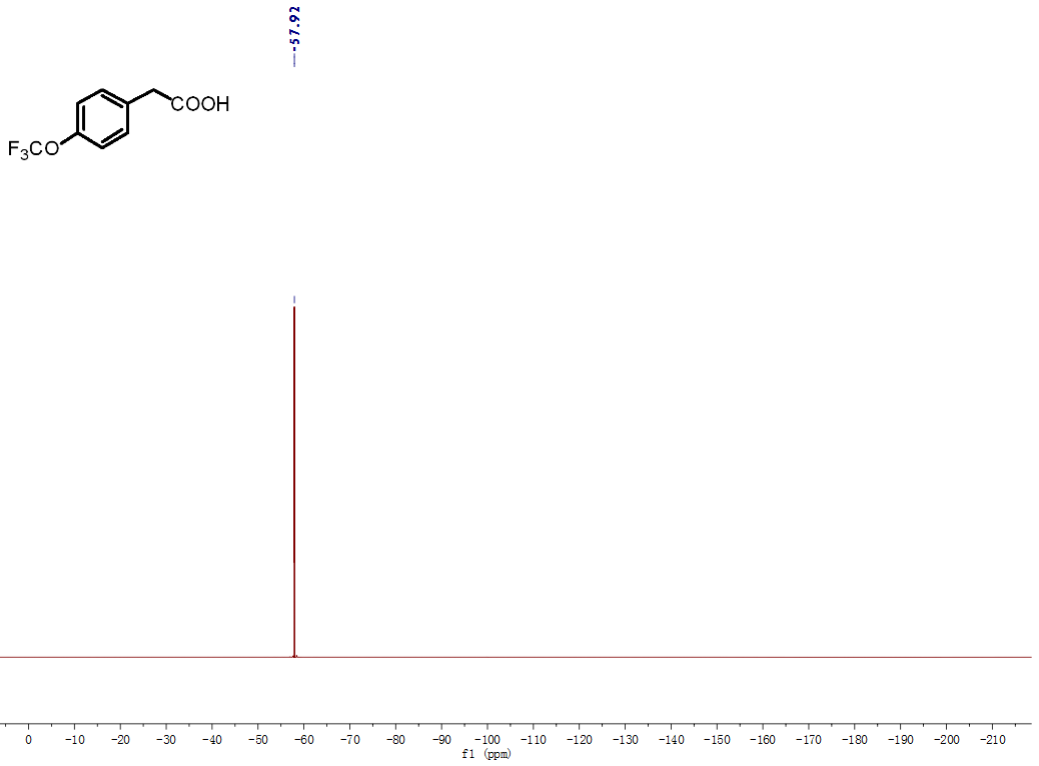
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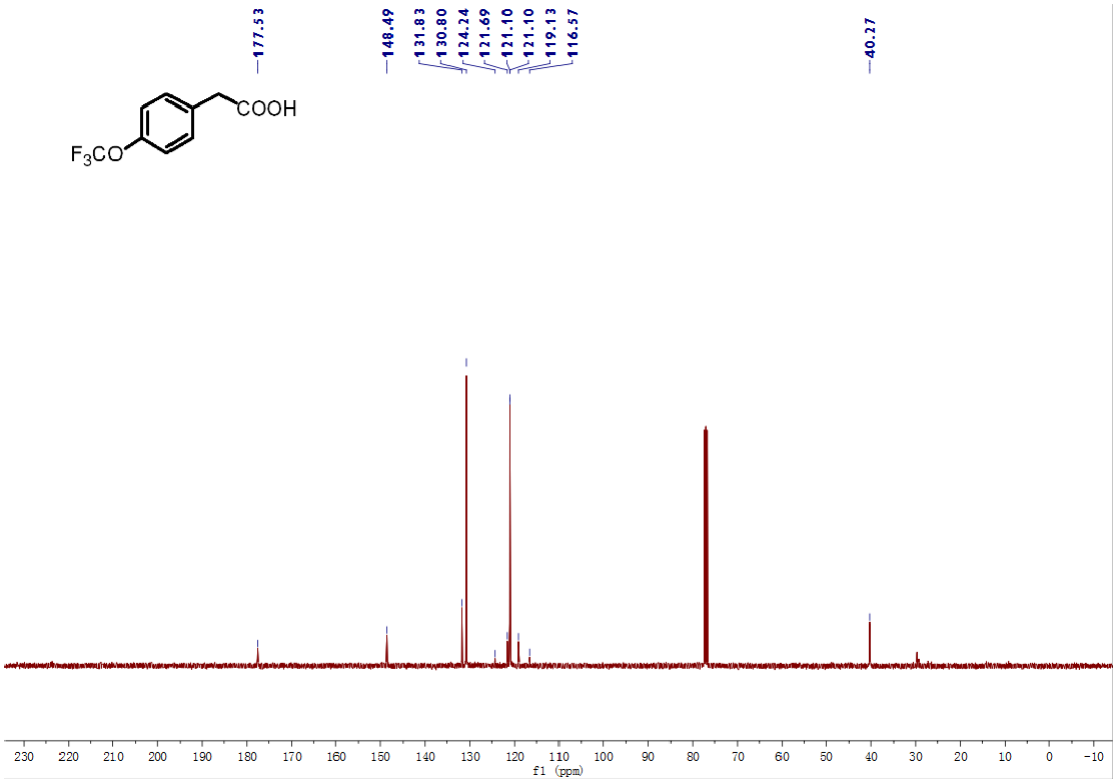
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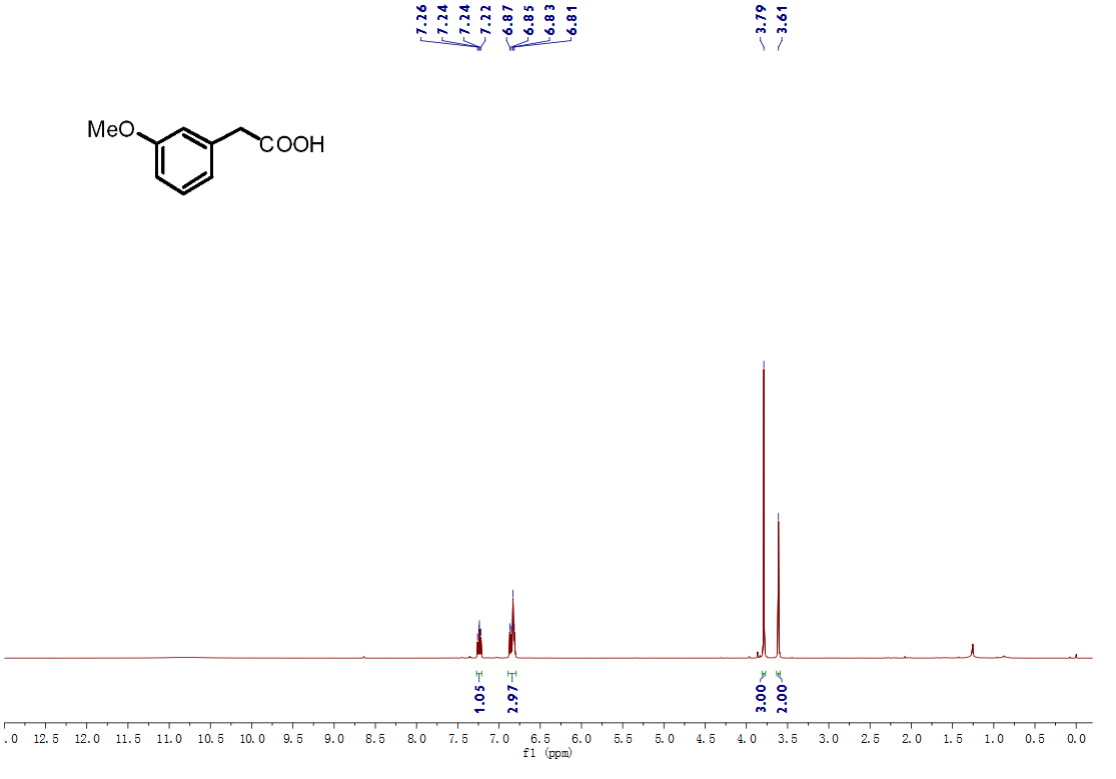
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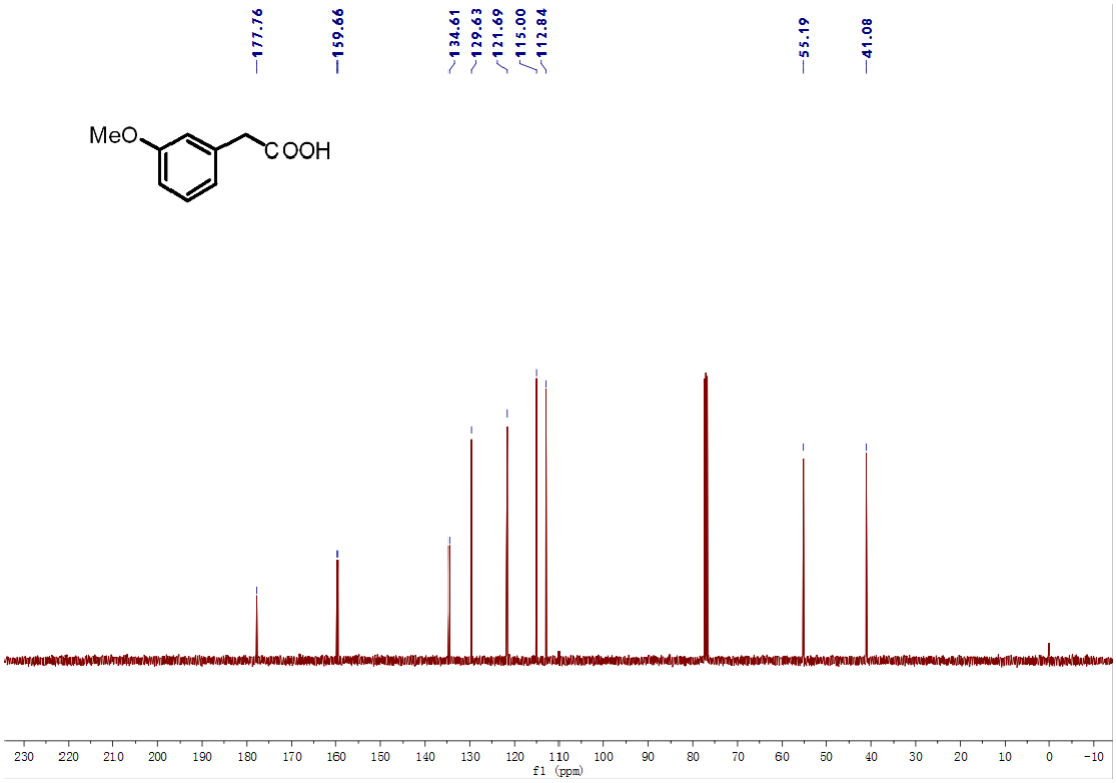
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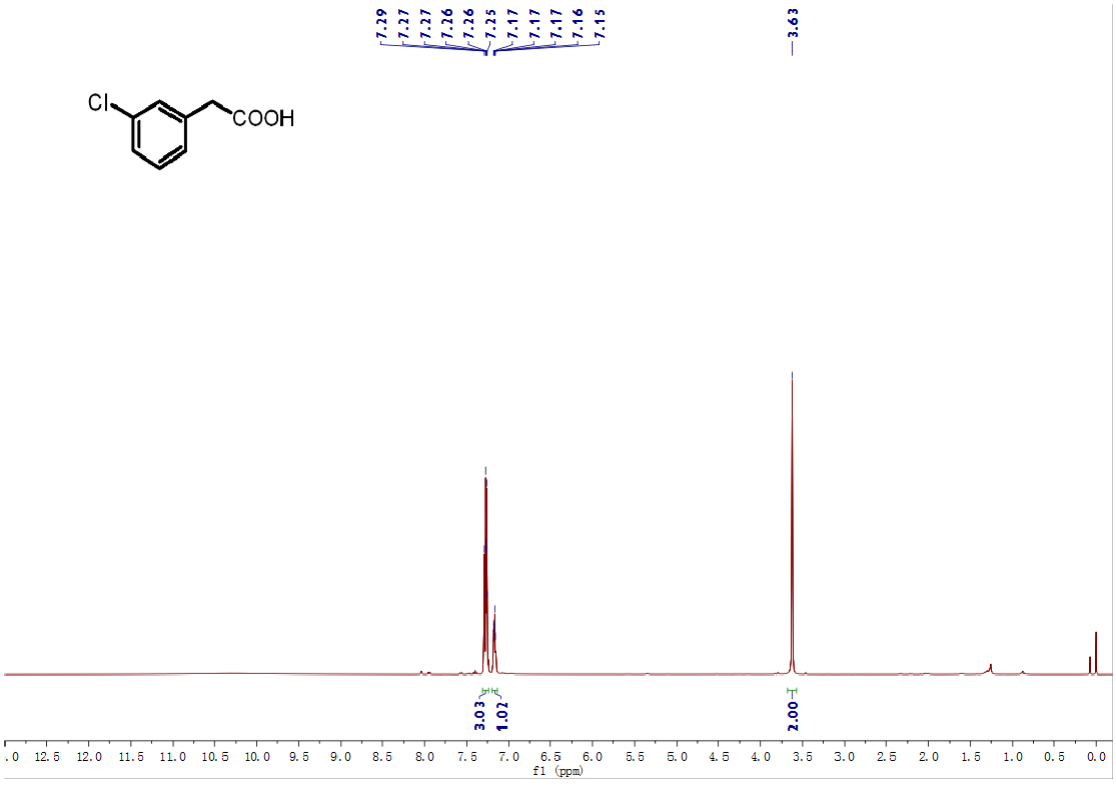
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2.00
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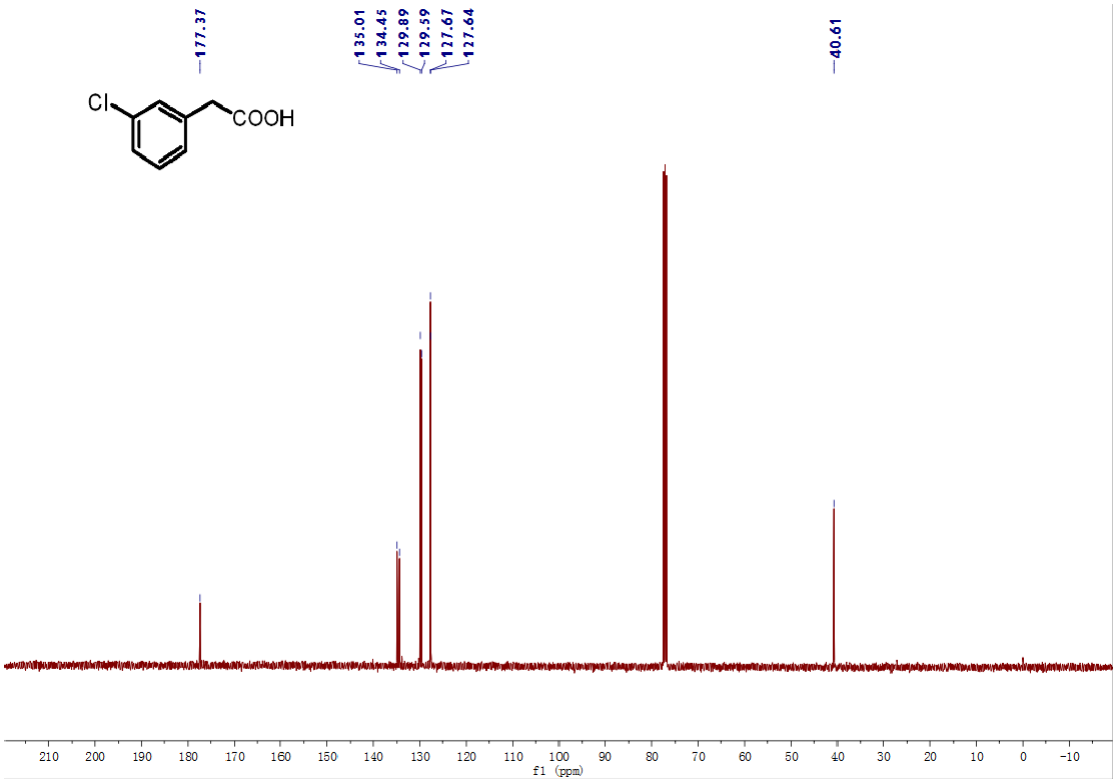
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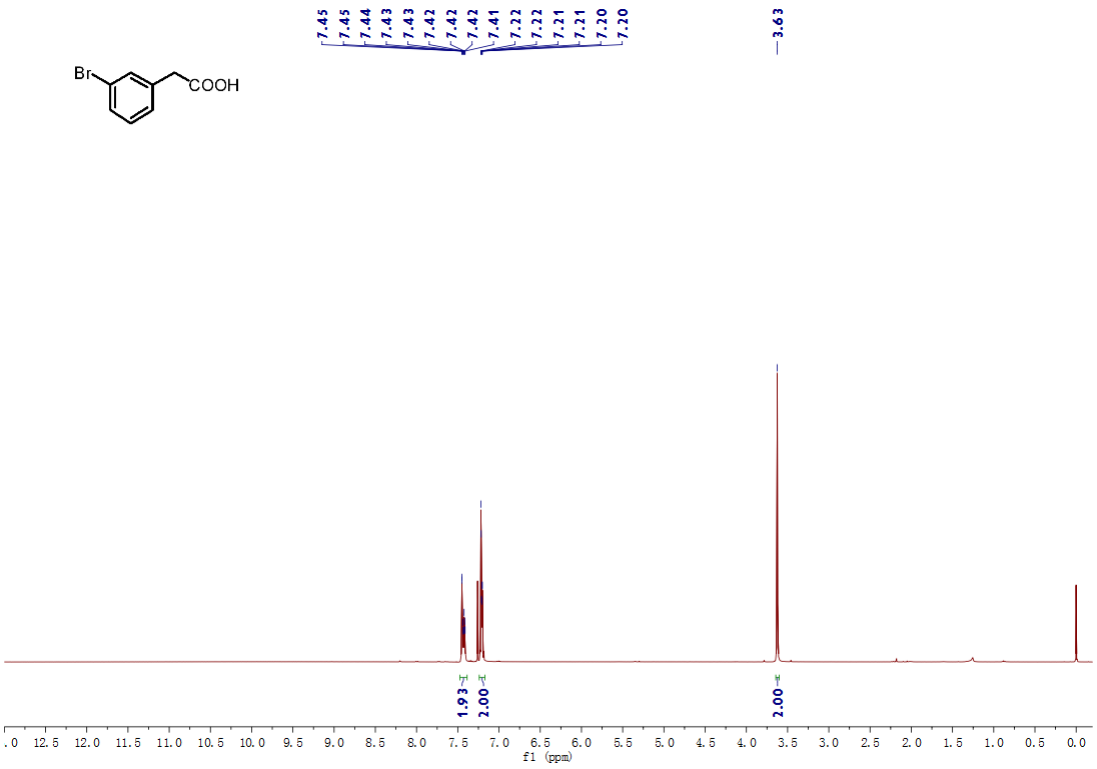
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2.00
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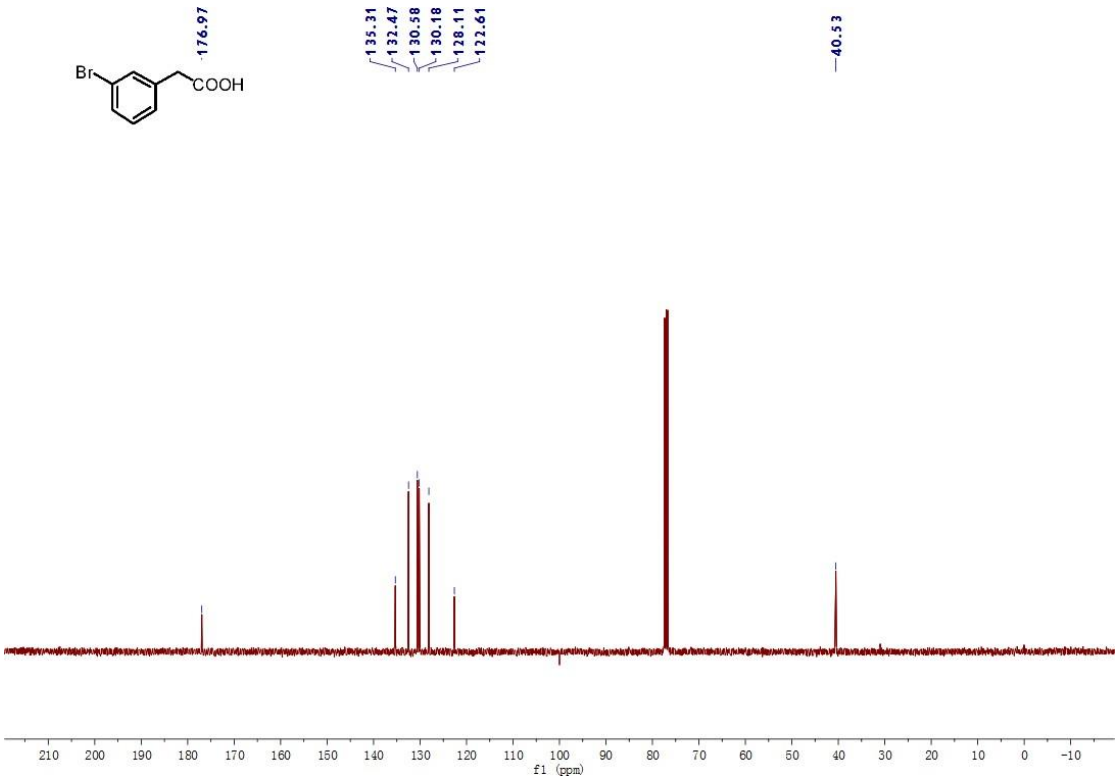
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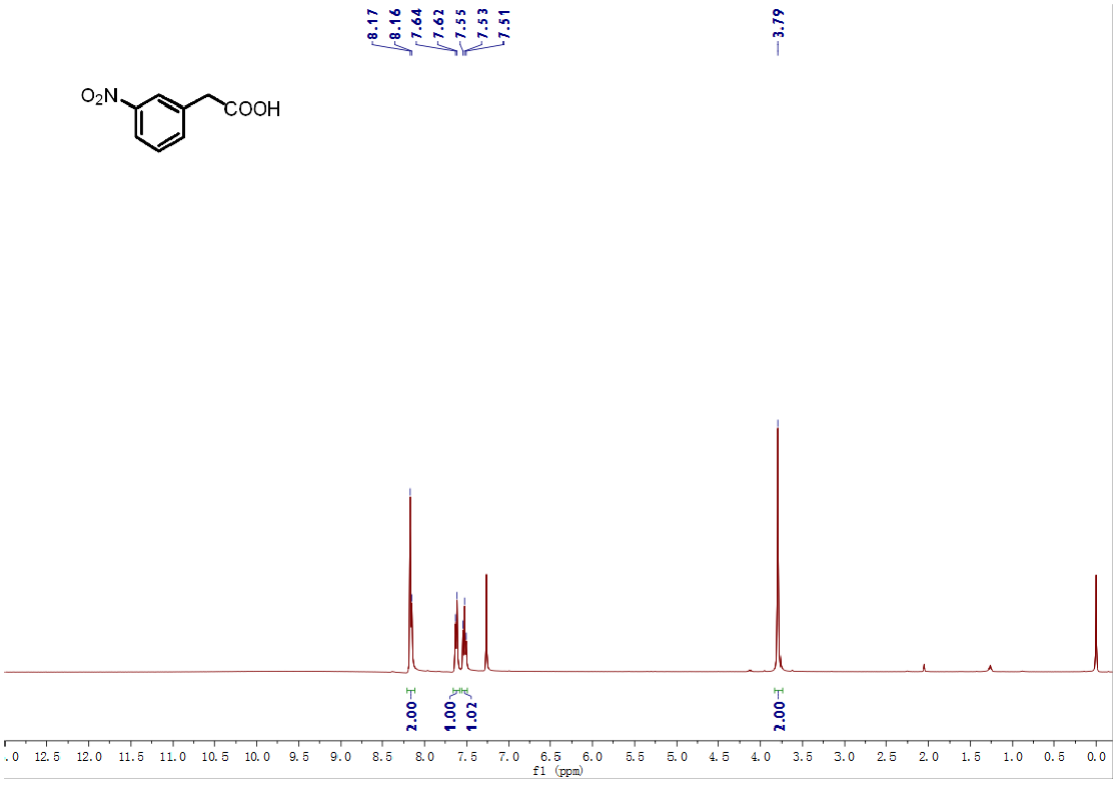
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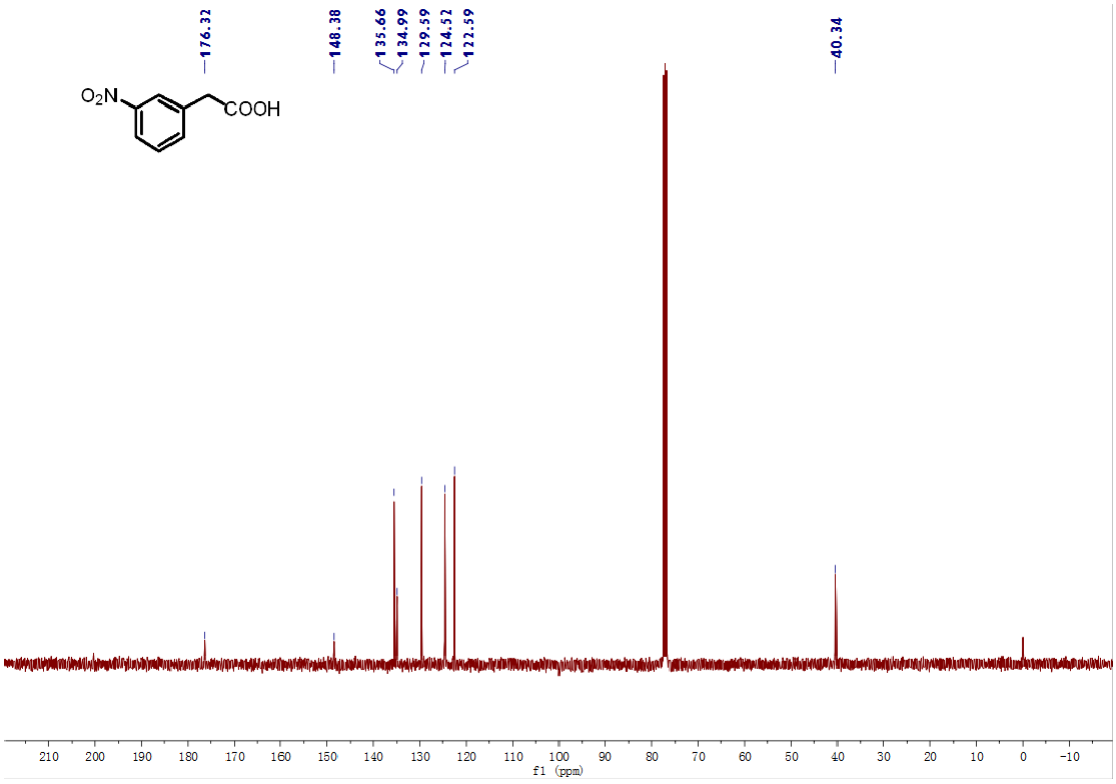
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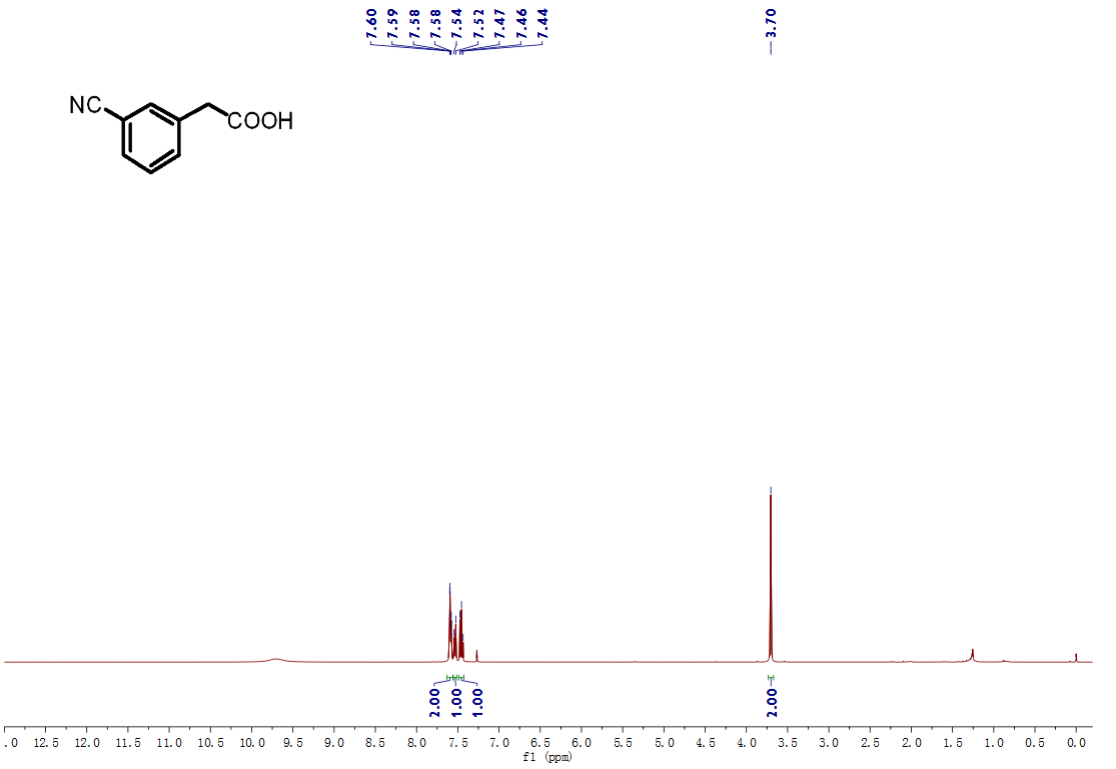
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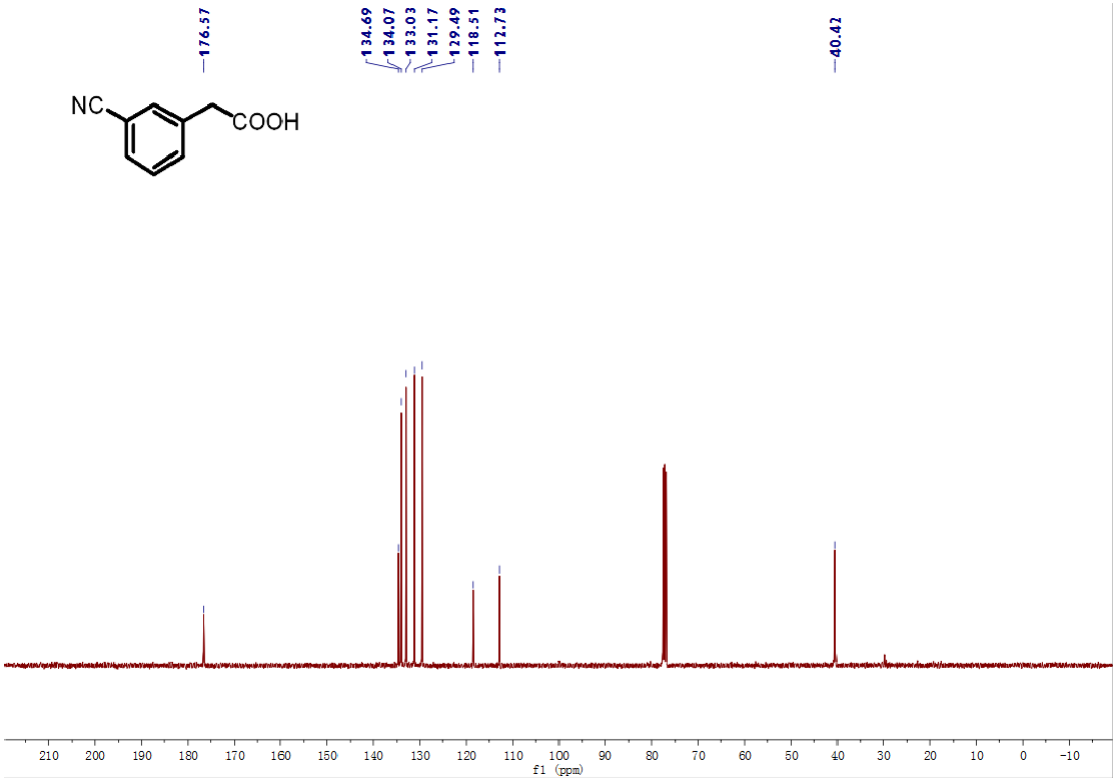
1.00
2.00
.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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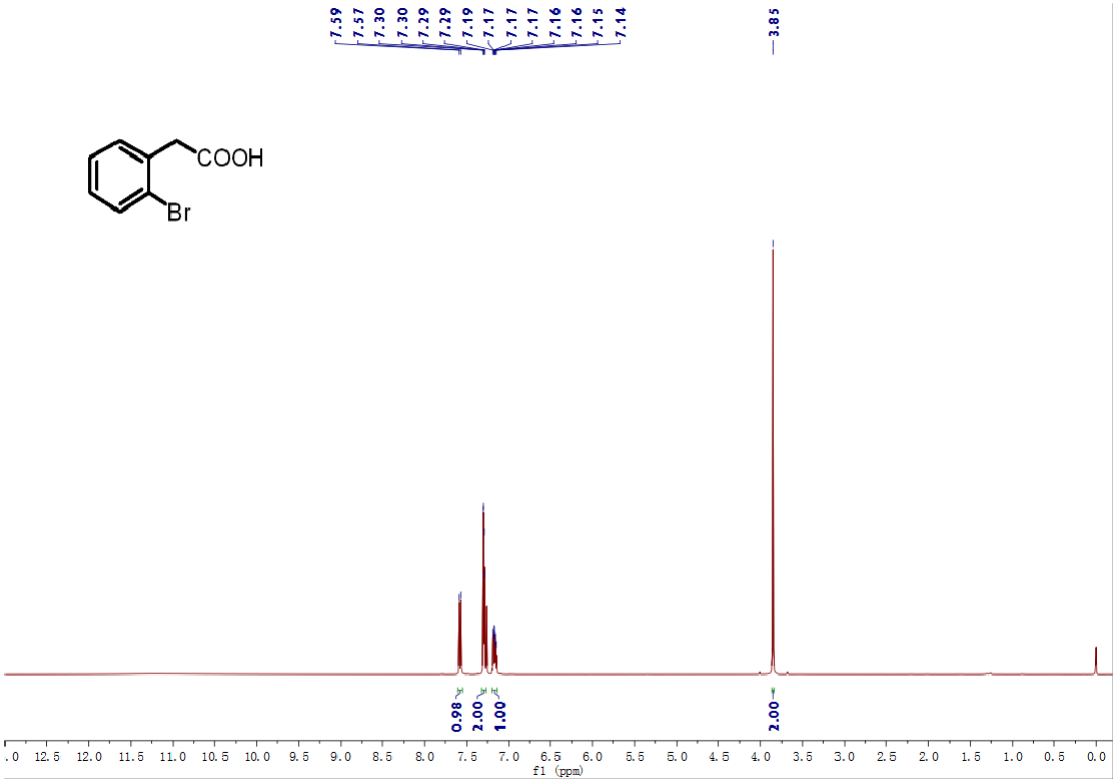
134.69
134.07
133.03
131.17
129.49
118.51
112.73
40.42
NC
COOH
f1 (ppm)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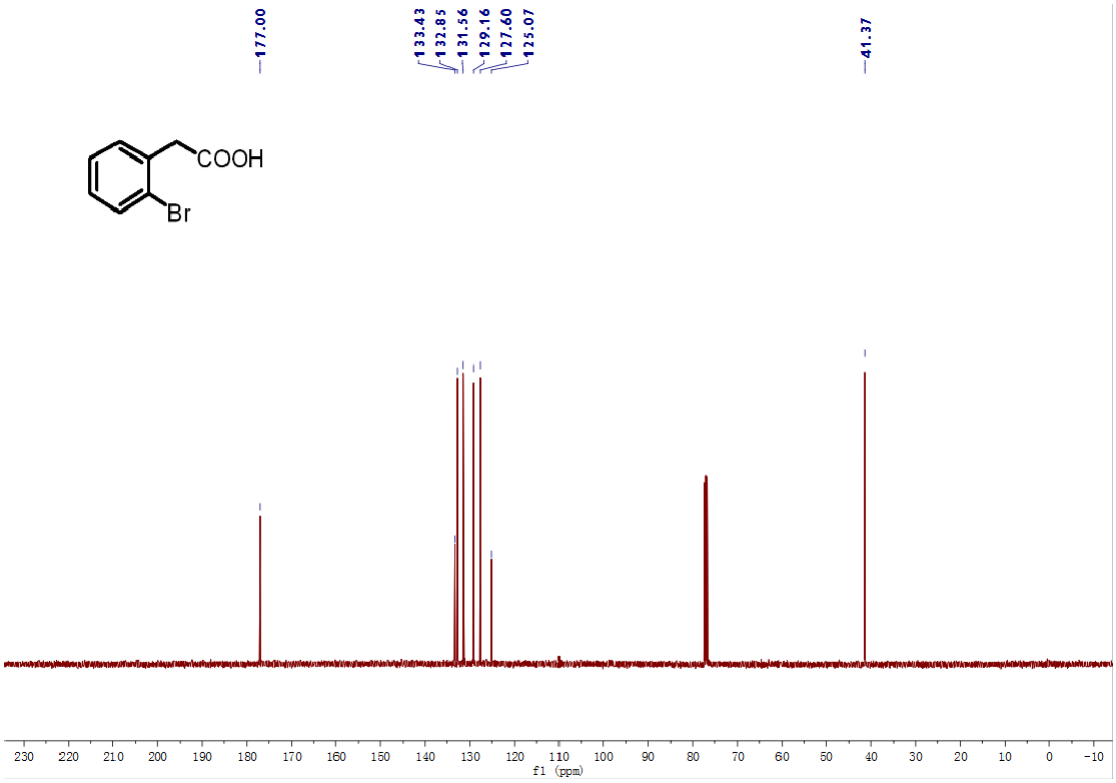
7.57
7.30
7.30
7.29
7.29
7.19
7.17
7.17
7.17
7.16
7.16
7.15
7.14
3.85
COOH
Br
0.98
2.00
1.00
2.00
f1 (ppm)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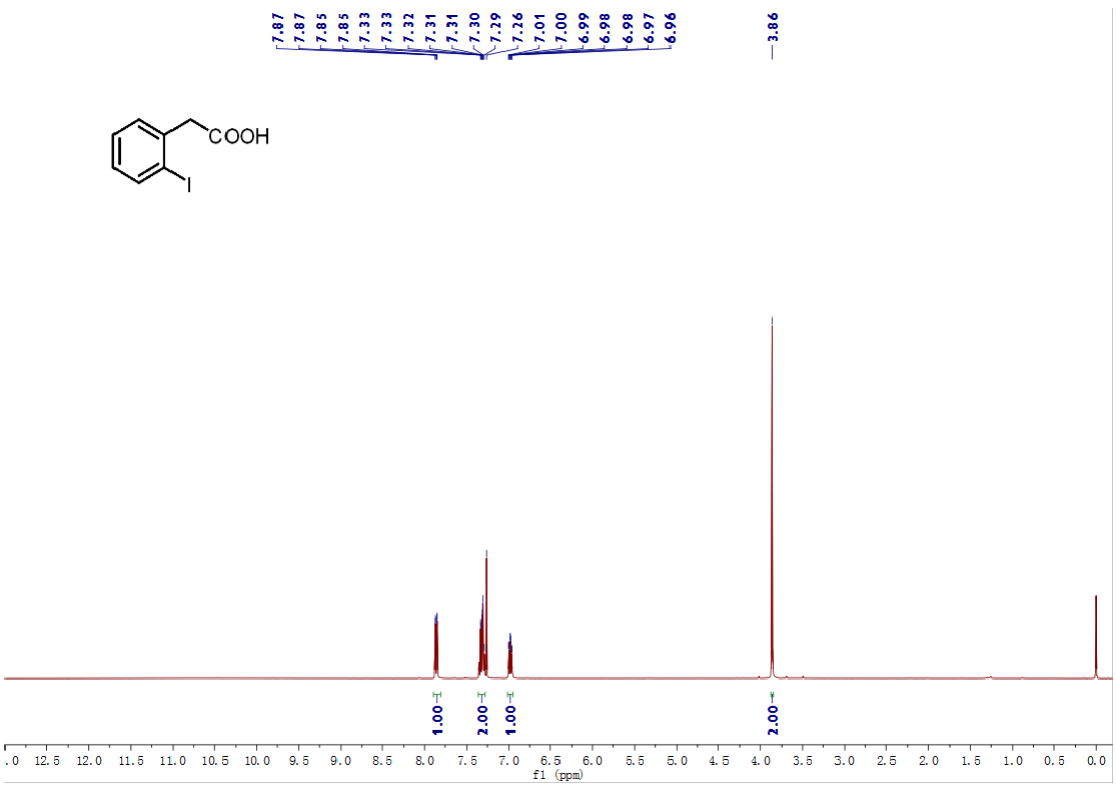
127.60
125.07
41.37
COOH
Br
f1 (ppm)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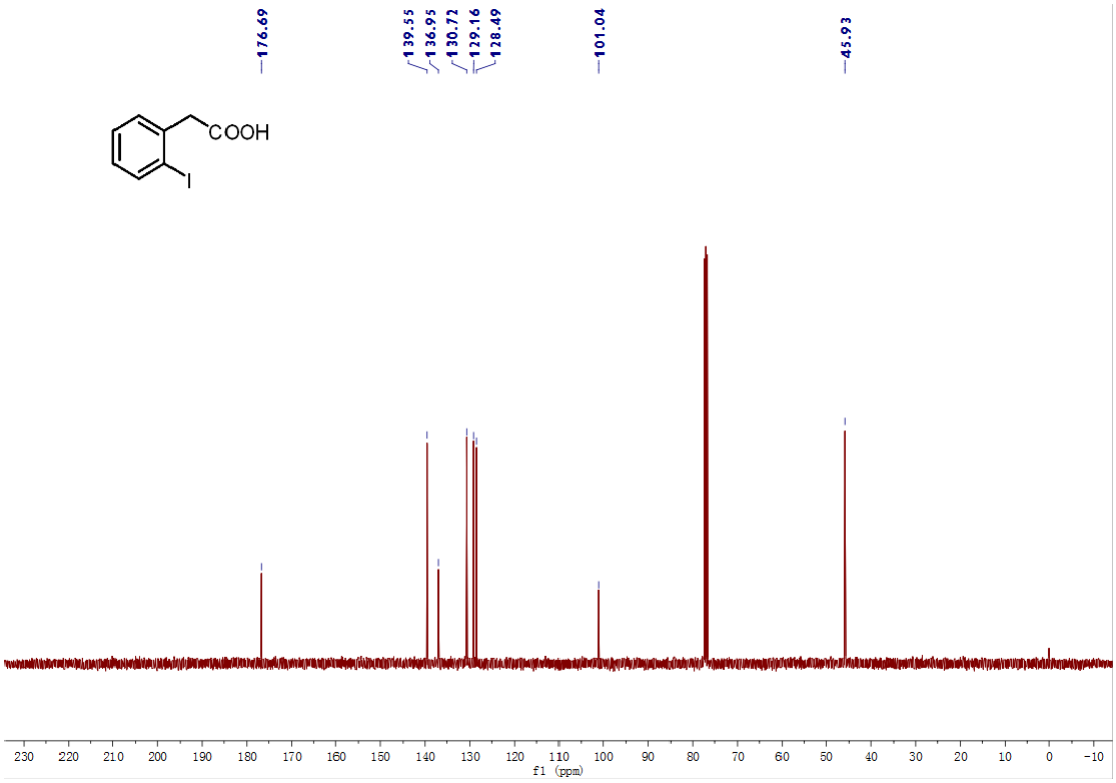
7.87
7.85
7.85
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.26
7.01
7.00
6.99
6.98
6.98
6.97
6.96
3.86
COOH
I
1.00
2.00
1.00
2.00
f1 (ppm)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136.95
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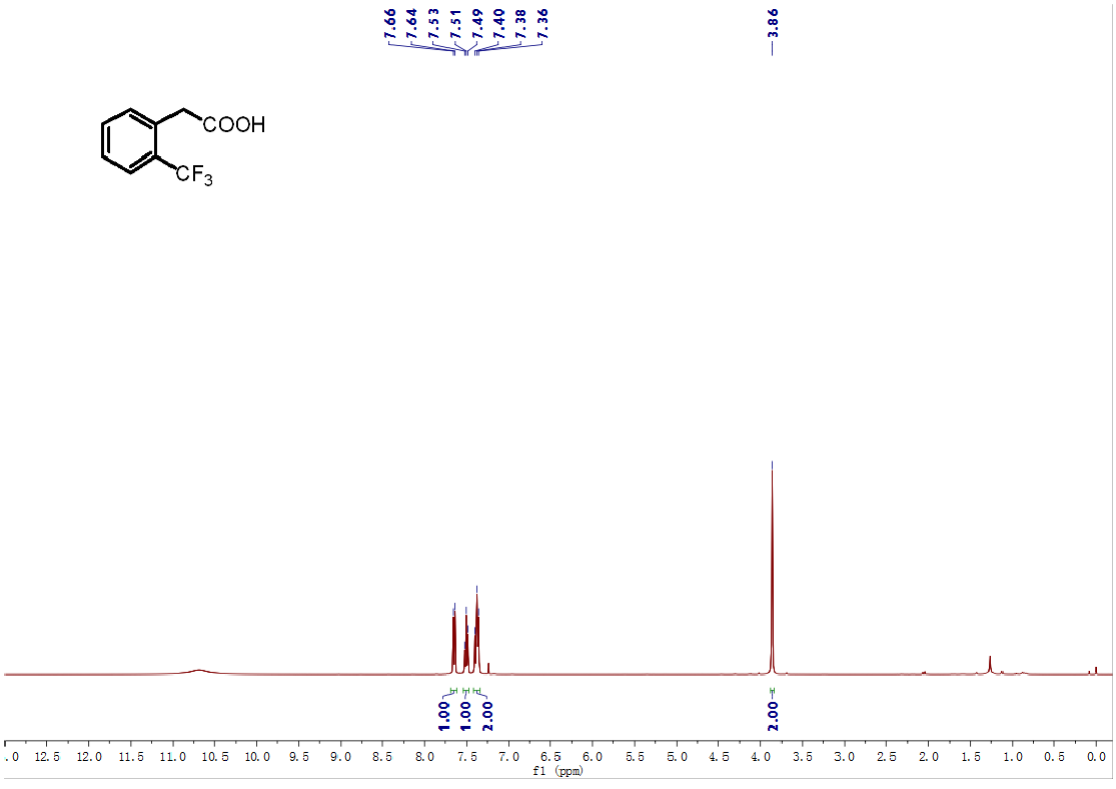
129.16
128.49
101.04
45.93
COOH
I
f1 (ppm)


7.66
7.64
7.53
7.51
7.49
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7.38
7.36
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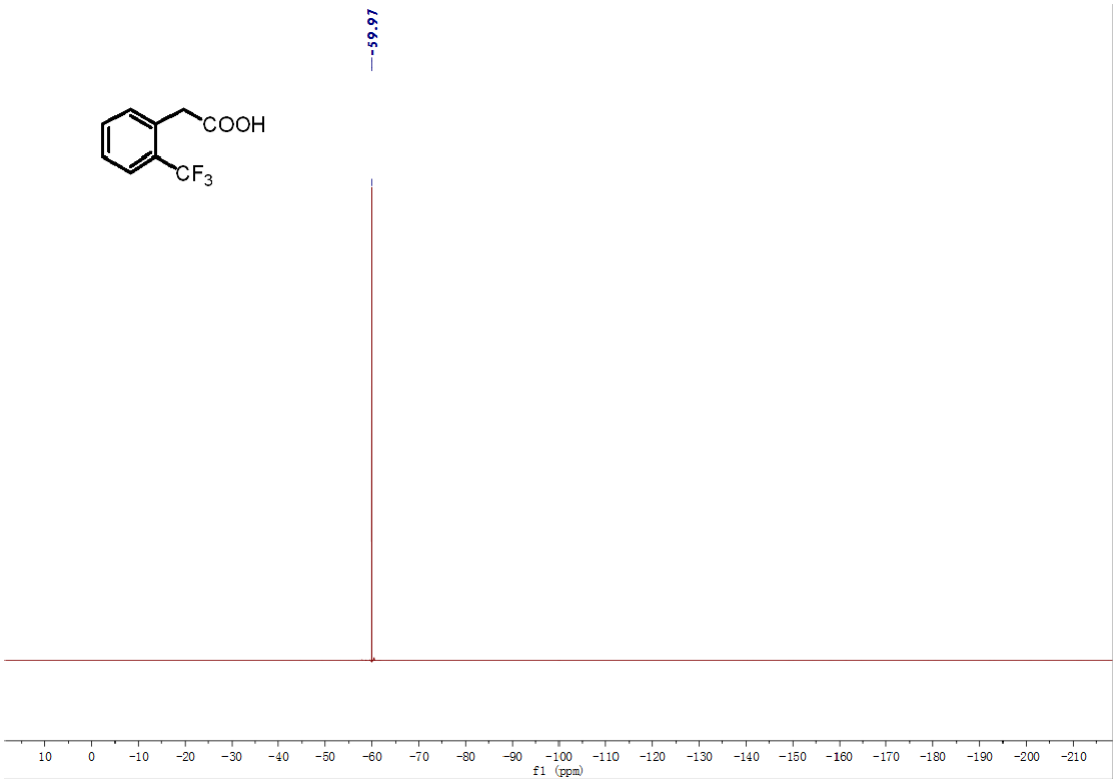
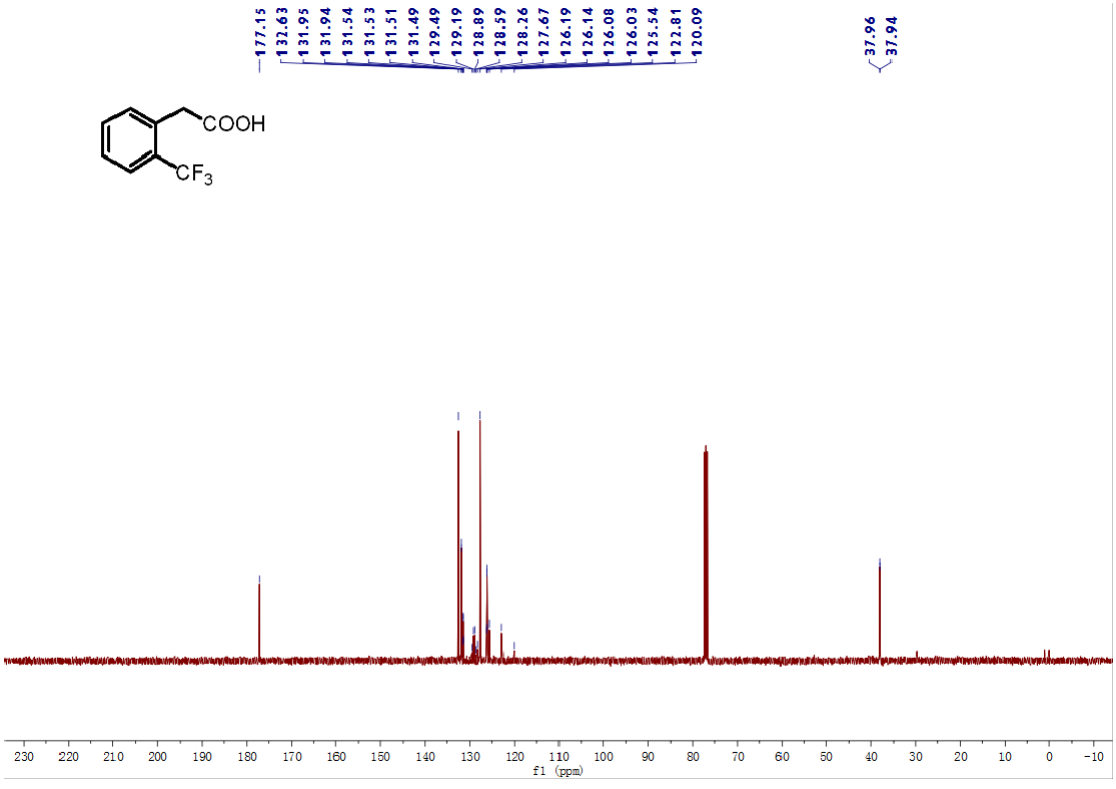
COOH
CF3
1.00
1.00
2.00
2.00
f1 (ppm)


-59.97
COOH
CF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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131.49
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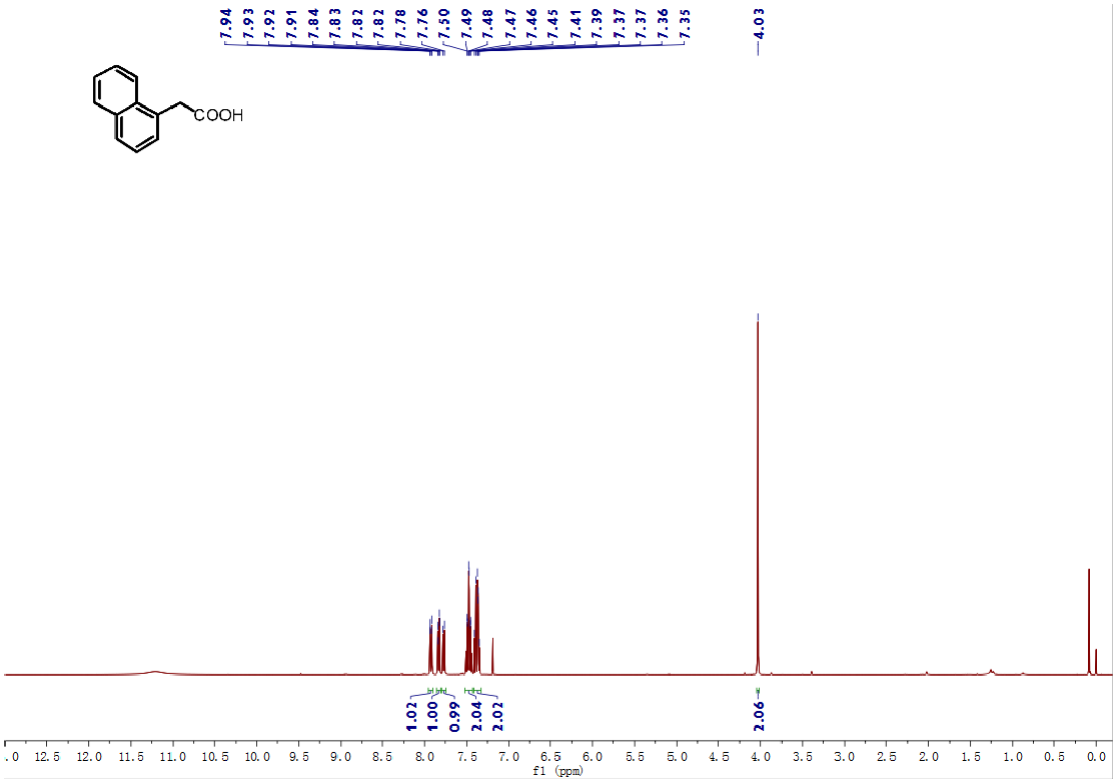
129.19
128.89
128.59
128.26
127.67
126.19
126.14
126.08
126.03
125.54
122.81
120.09
37.96
37.94
COOH
CF3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.93
7.92
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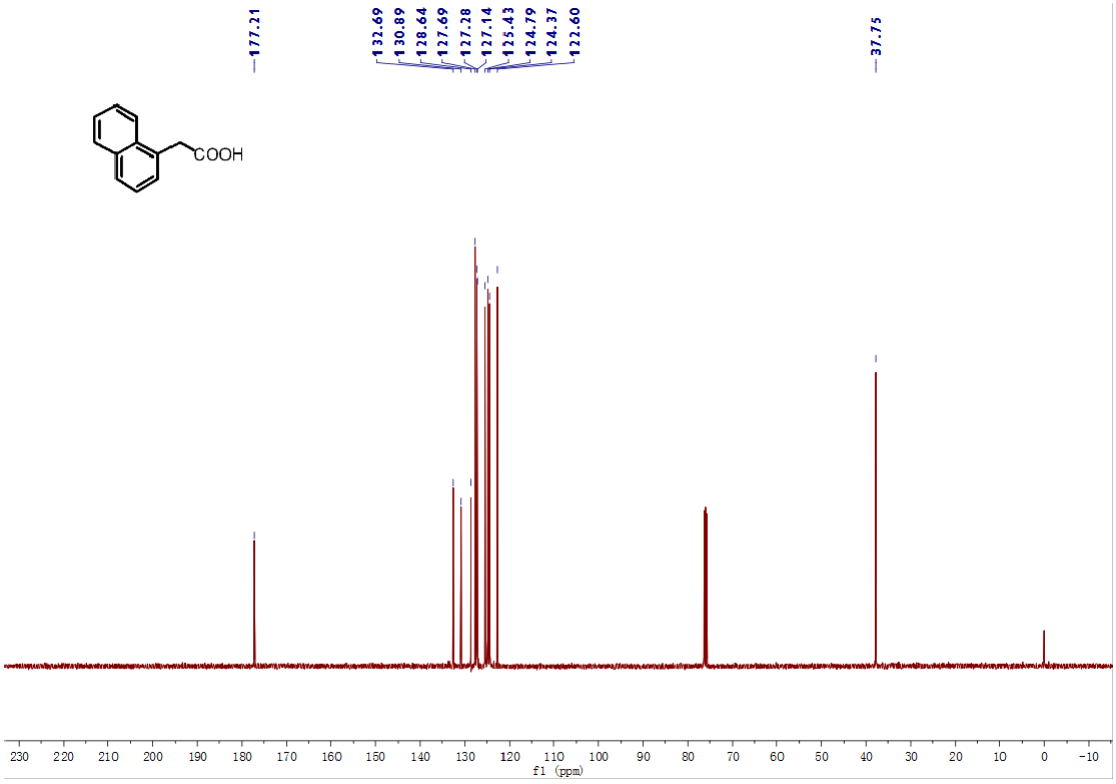
7.83
7.82
7.82
7.78
7.76
7.50
7.49
7.48
7.47
7.46
7.45
7.41
7.39
7.37
7.37
7.36
7.35
4.03
COOH
1.02
1.00
0.99
2.04
2.02
2.06
f1 (ppm)


177.21
132.69
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128.64
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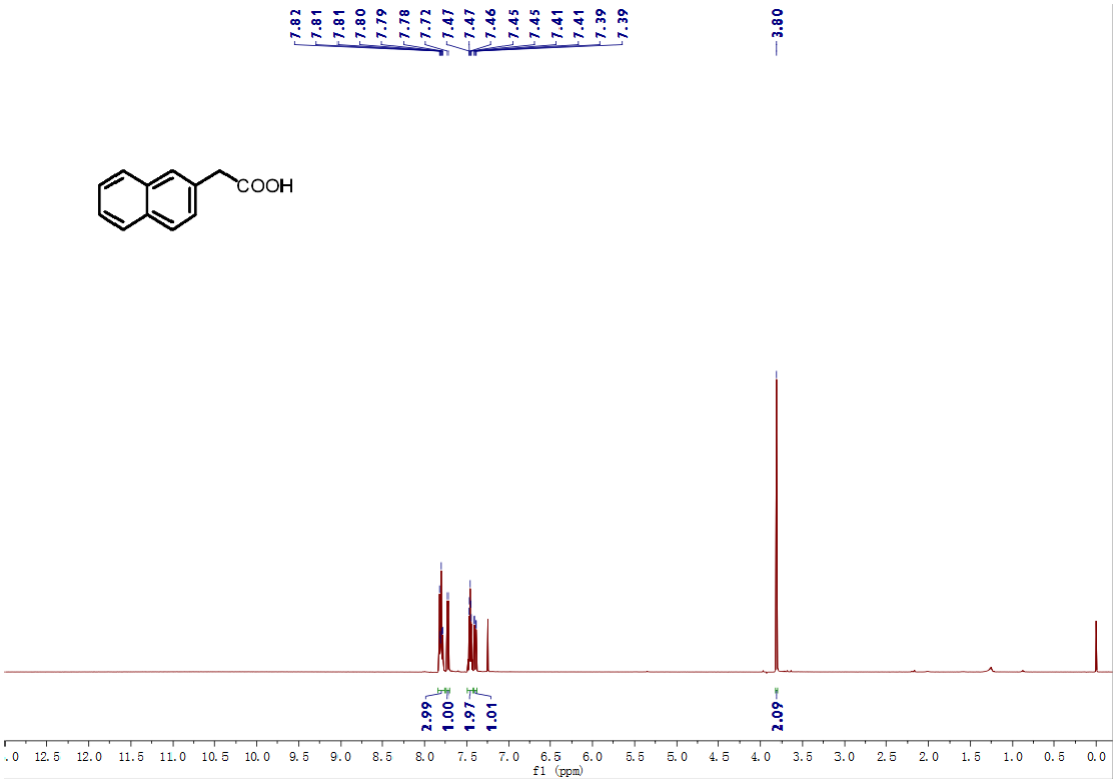
127.28
127.14
125.43
124.79
124.37
122.60
37.75
COOH
f1 (ppm)


7.82
7.81
7.81
7.80
7.79
7.78
7.72
7.47
7.47
7.46
7.45
7.45
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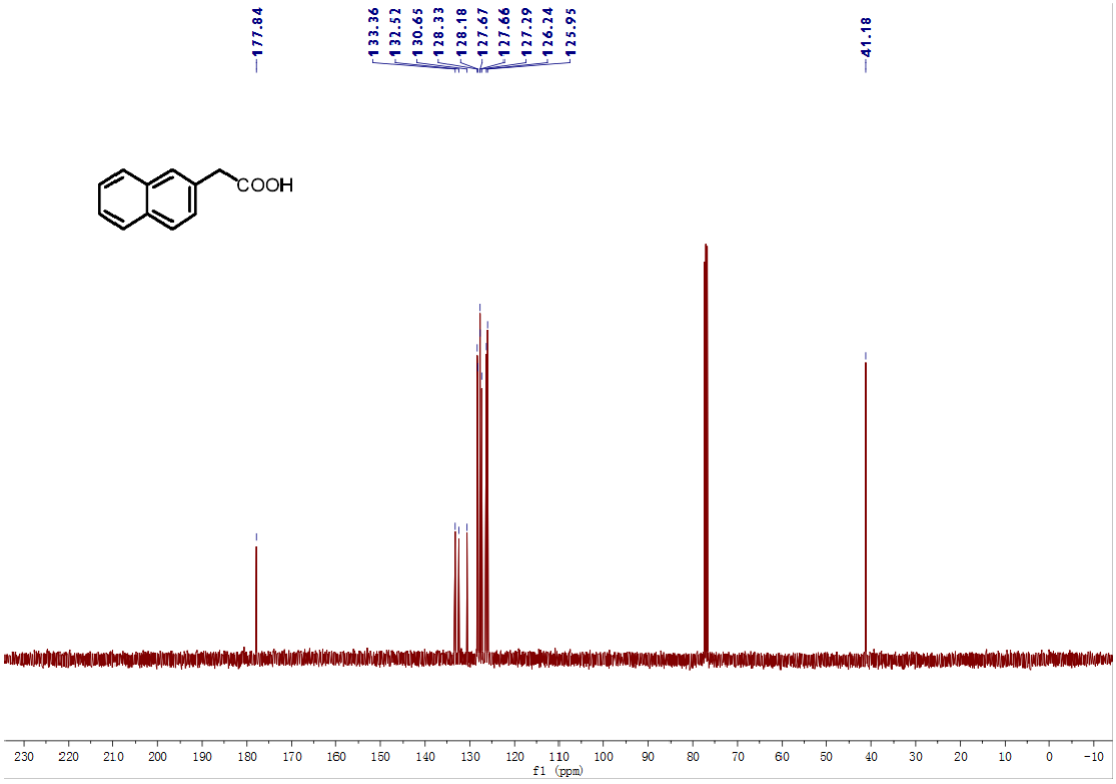
1.00
1.97
1.01
2.09
f1 (ppm)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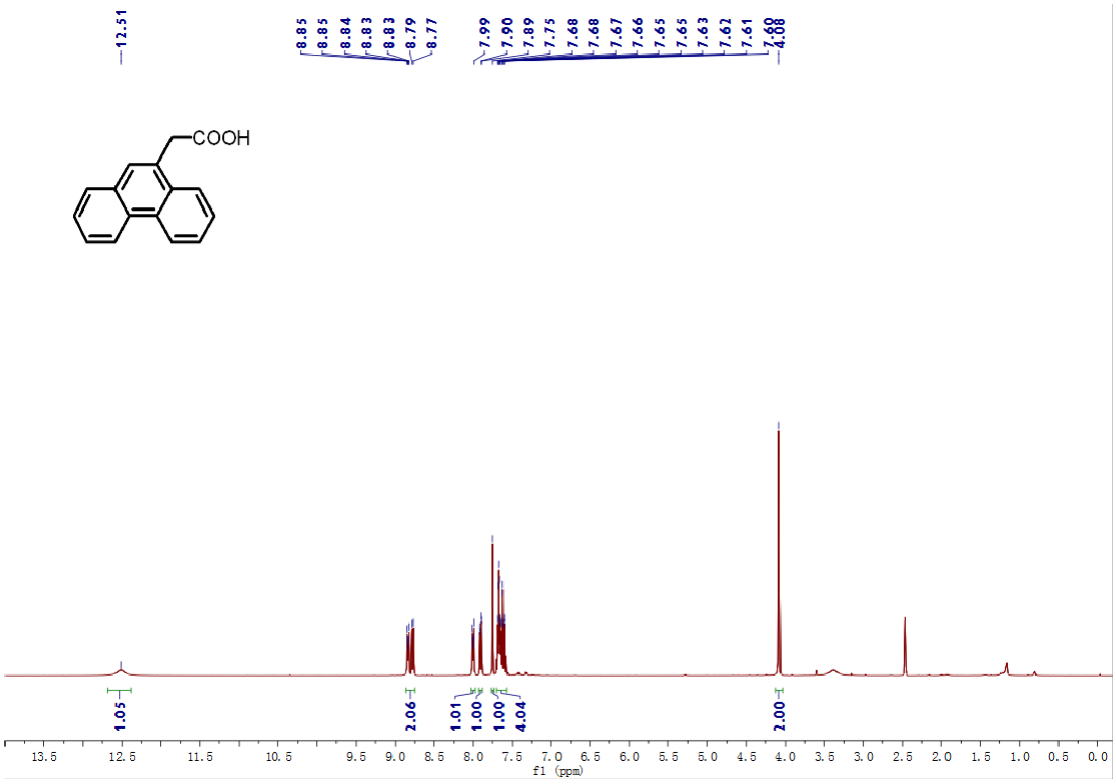
133.36
132.52
130.65
128.33
128.18
127.67
127.66
127.29
126.24
125.95
41.18
COOH
f1 (ppm)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8.85
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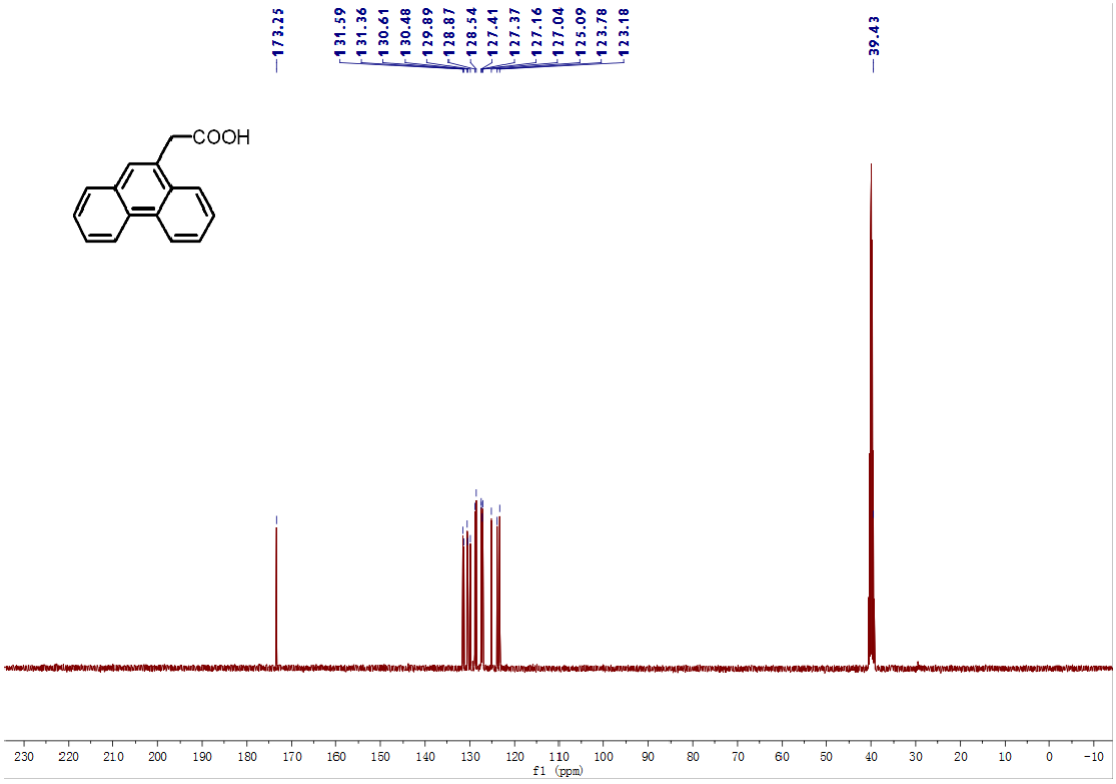
8.83
8.83
8.79
8.77
7.99
7.90
7.89
7.75
7.68
7.68
7.67
7.66
7.65
7.65
7.63
7.62
7.61
7.60
4.08
COOH
1.05
2.06
1.01
1.00
1.00
4.04
2.00
f1 (ppm)


173.25
131.59
131.36
130.61
130.48
129.89
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128.54
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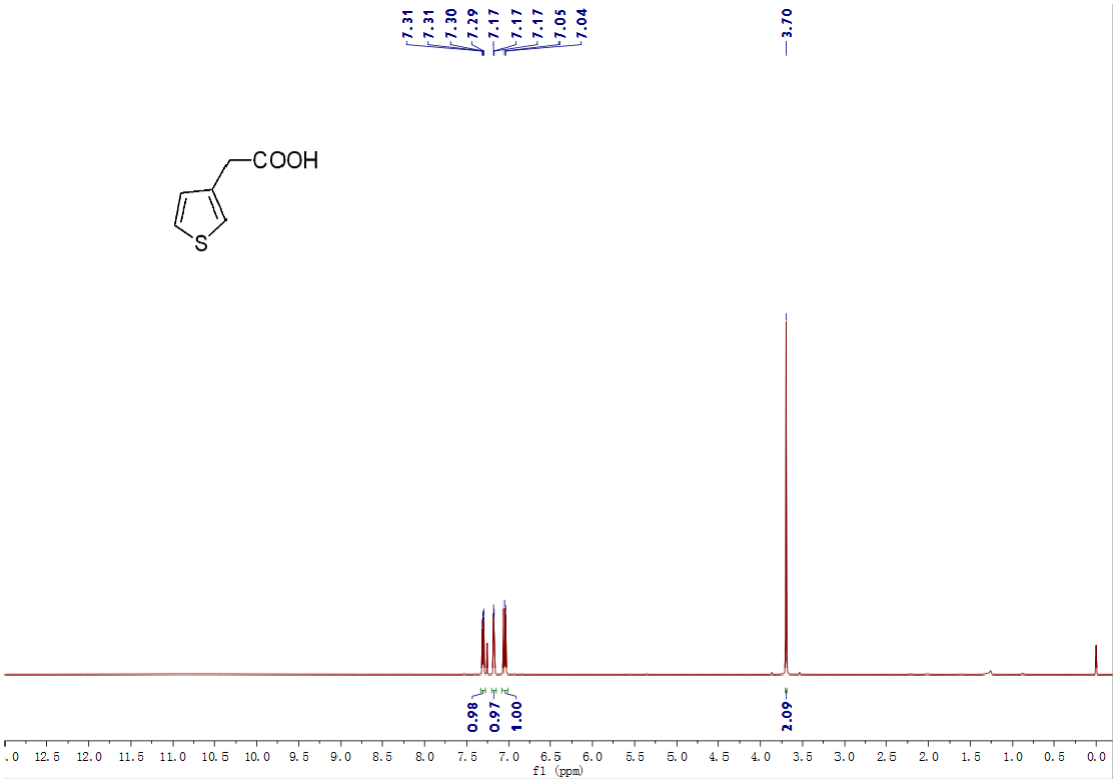
127.37
127.16
127.04
125.09
123.78
123.18
39.43
COOH
f1 (ppm)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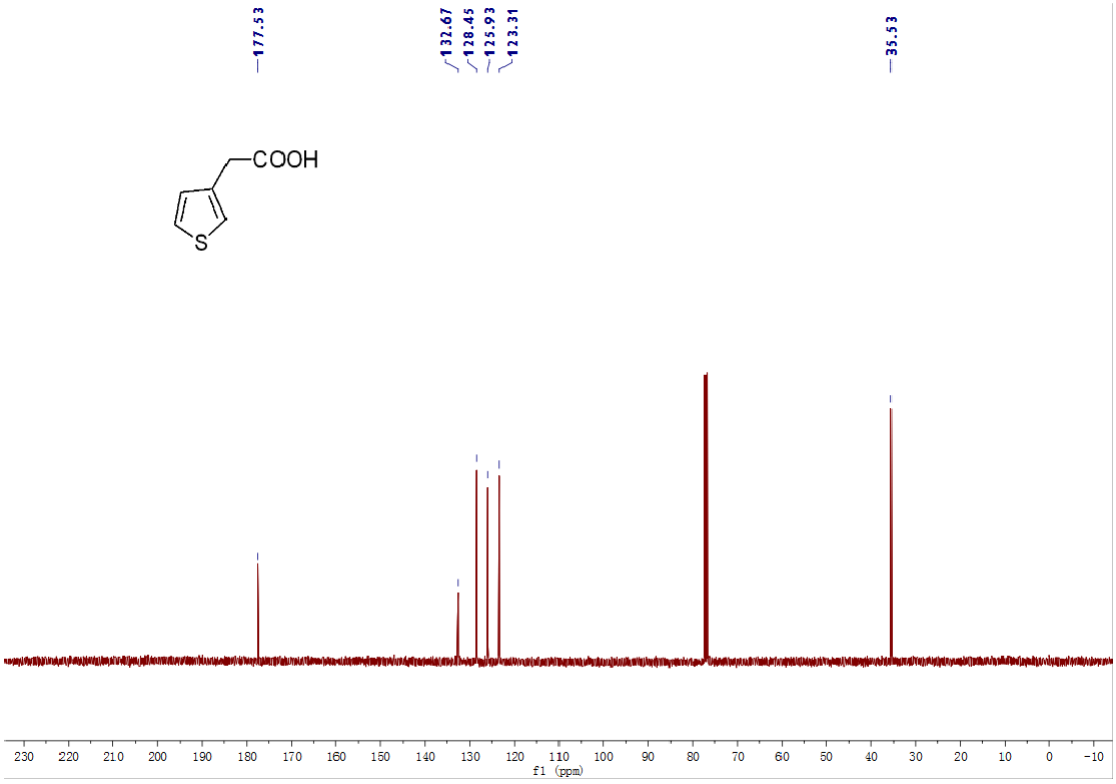
7.31
7.30
7.29
7.17
7.17
7.17
7.05
7.04
3.70
COOH
S
0.98
0.97
1.00
2.09
f1 (ppm)


177.53
132.67
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123.31
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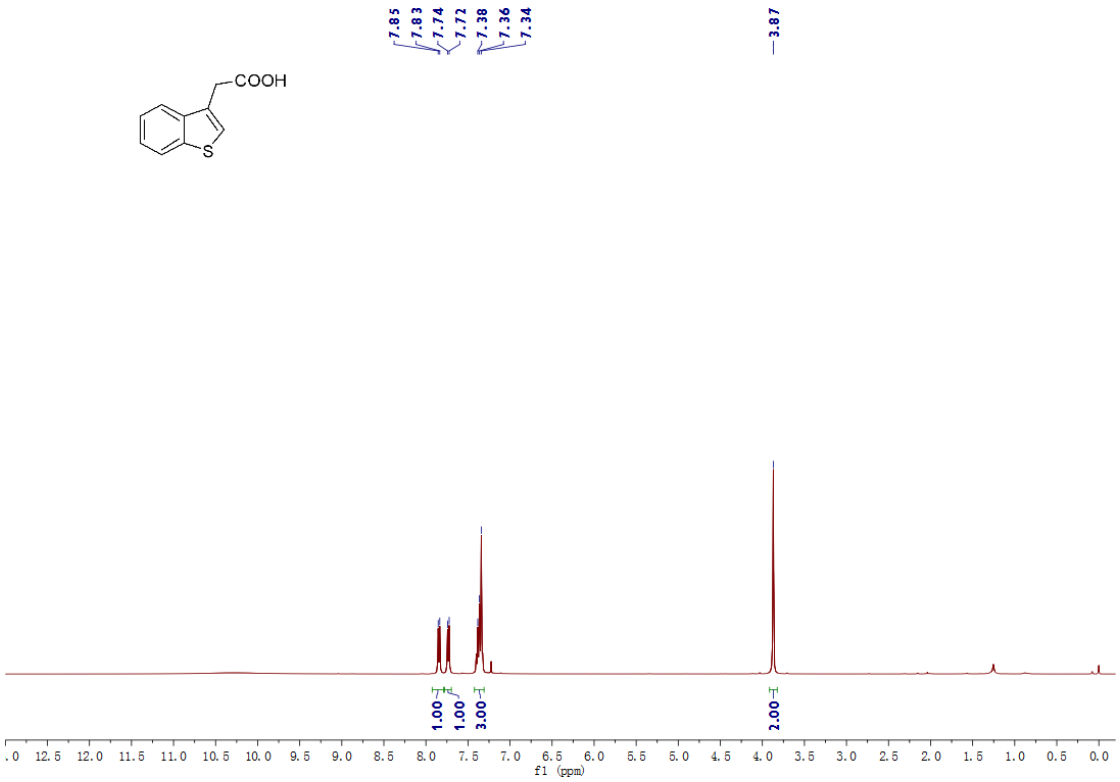
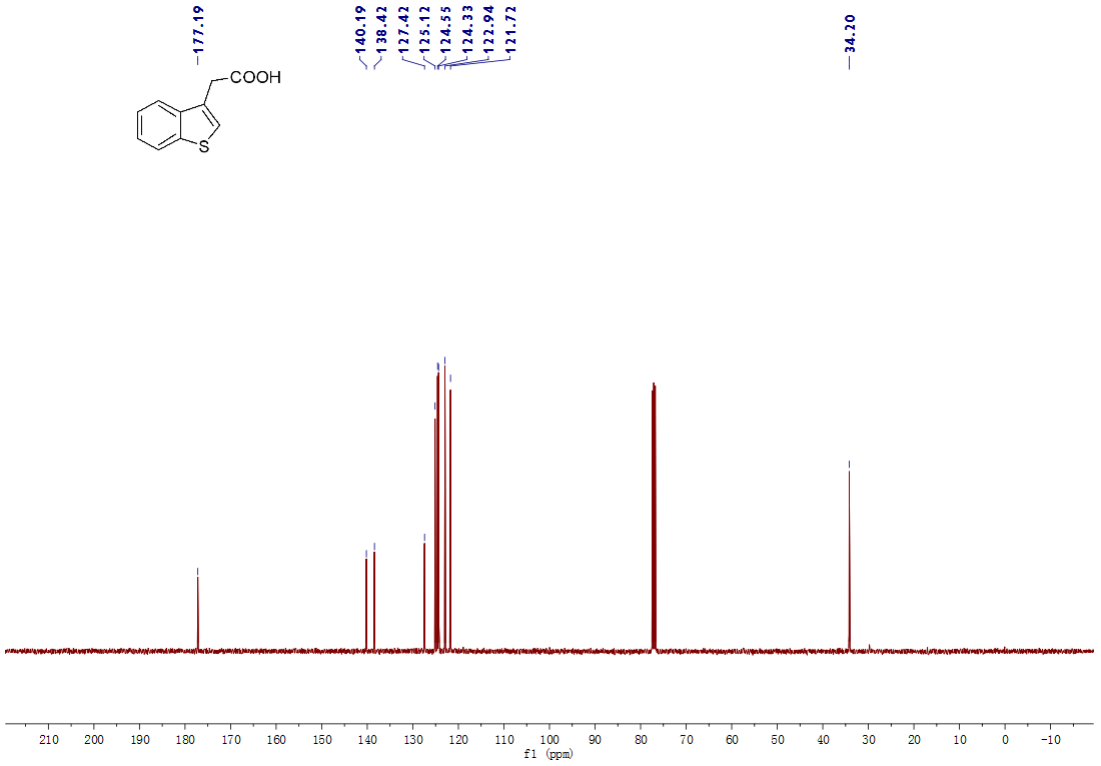
COOH
S
f1 (ppm)


7.85
7.83
7.74
7.72
7.38
7.36
7.34
3.87
COOH
S
1.00
1.00
3.00
2.00
f1 (ppm)


177.19
140.19
138.42
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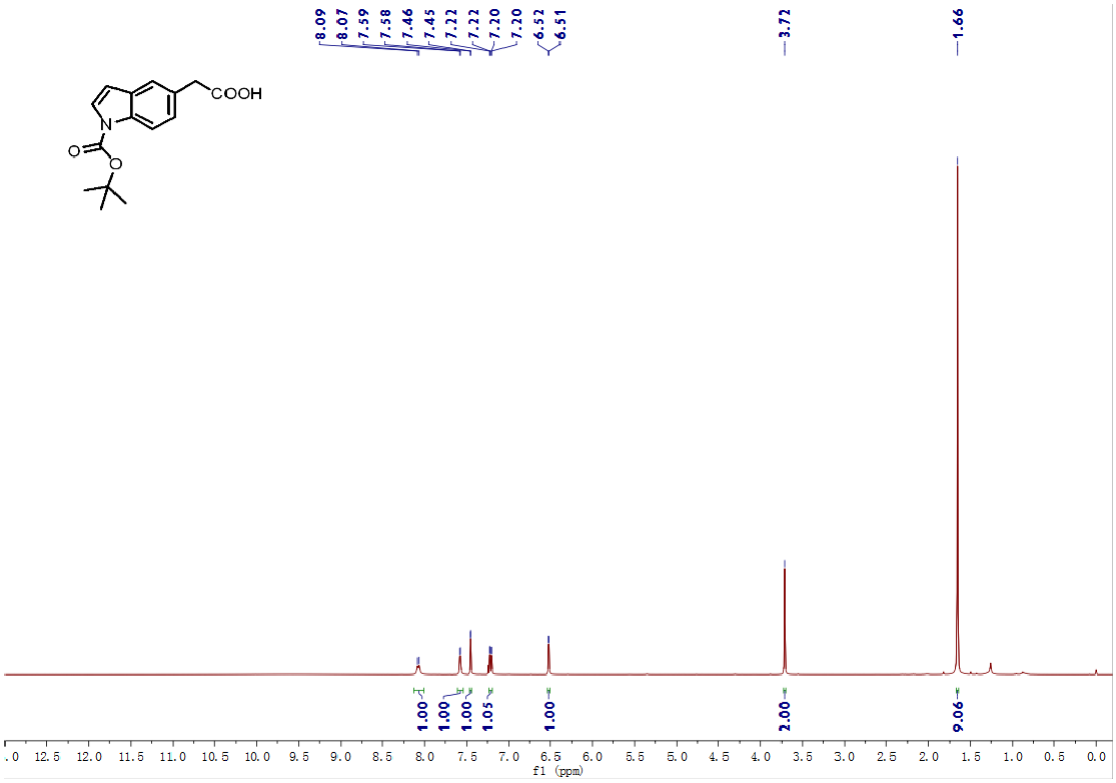
125.12
124.55
124.33
122.94
121.72
34.20
COOH
S
f1 (ppm)


8.09
8.07
7.59
7.58
7.46
7.45
7.22
7.22
7.20
7.20
6.52
6.51
3.72
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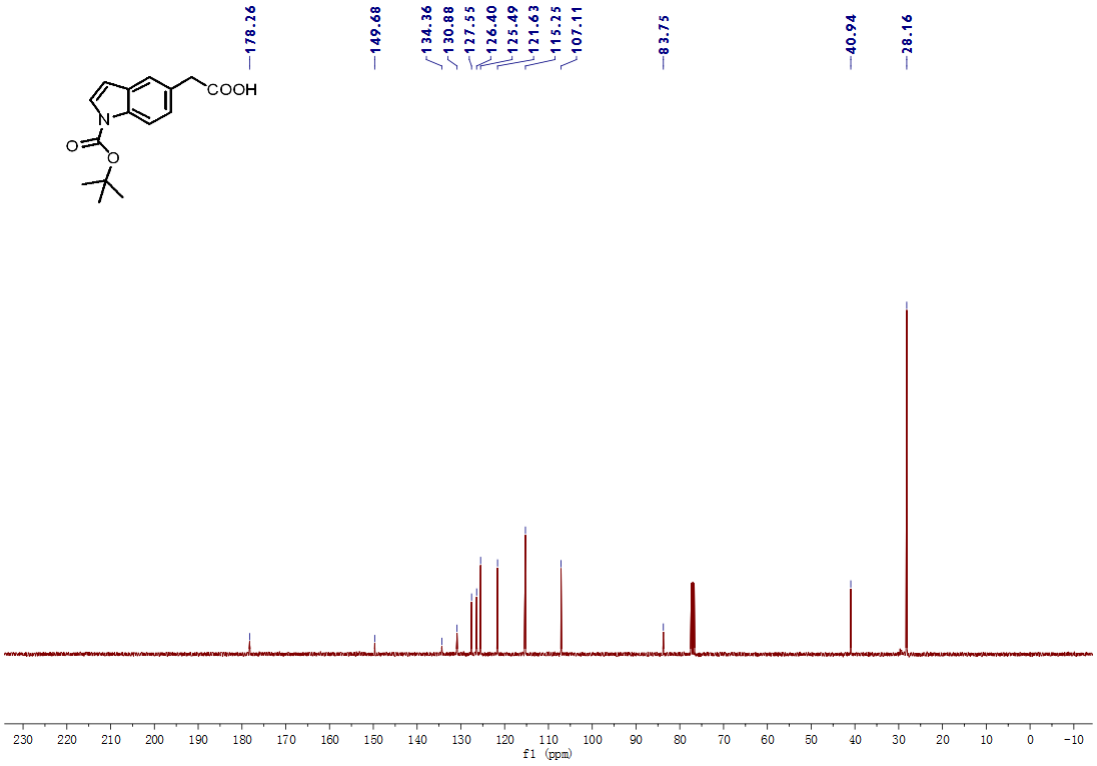
COOH
1.00
1.00
1.00
1.05
1.00
2.00
9.06
f1 (ppm)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149.68
134.36
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127.55
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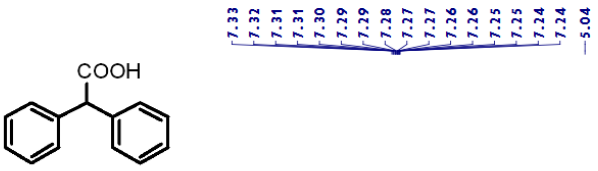
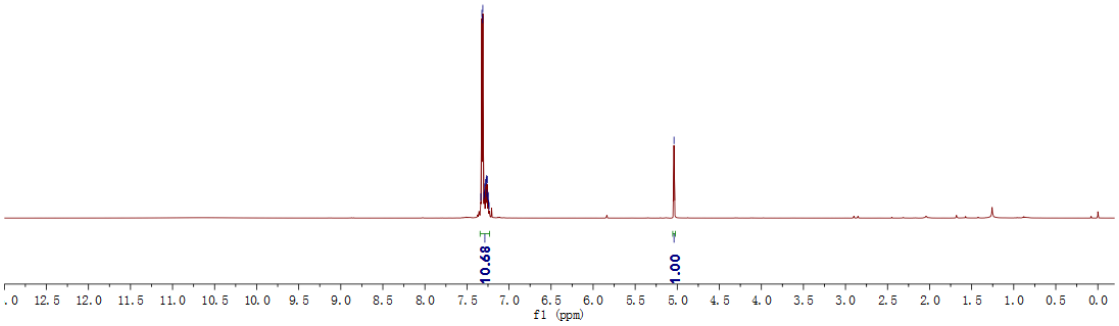
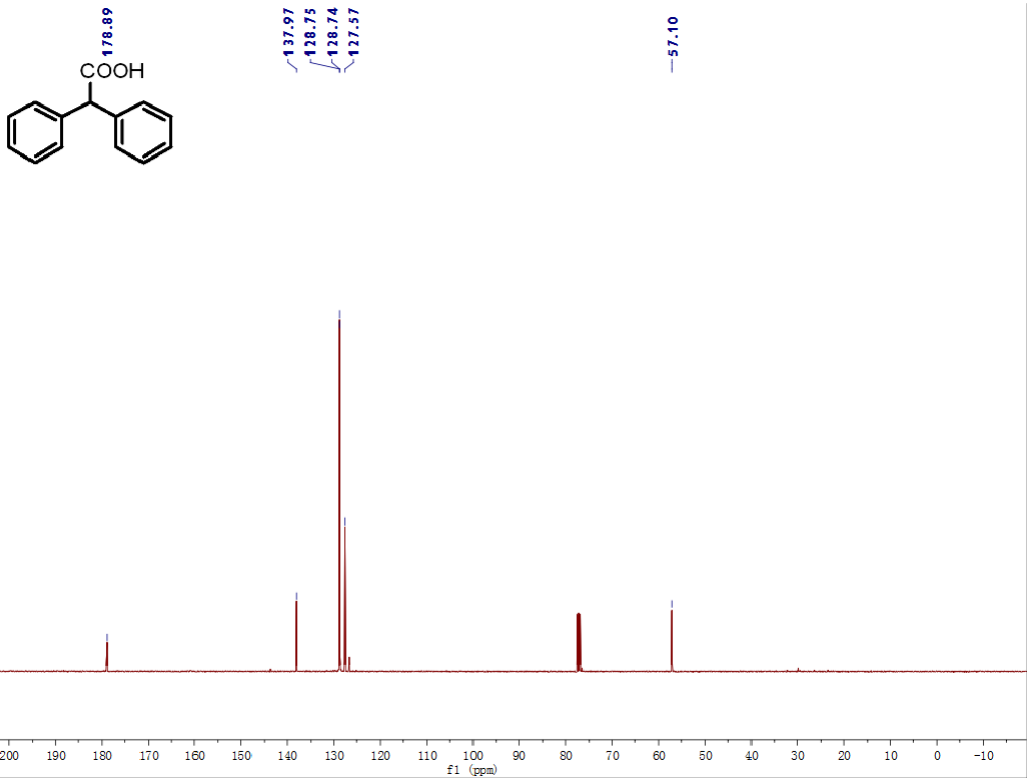
125.49
121.63
115.25
107.11
83.75
40.94
28.16
COOH
f1 (ppm)


COOH
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.24
5.04


10.68
1.00
f1 (ppm)


COOH
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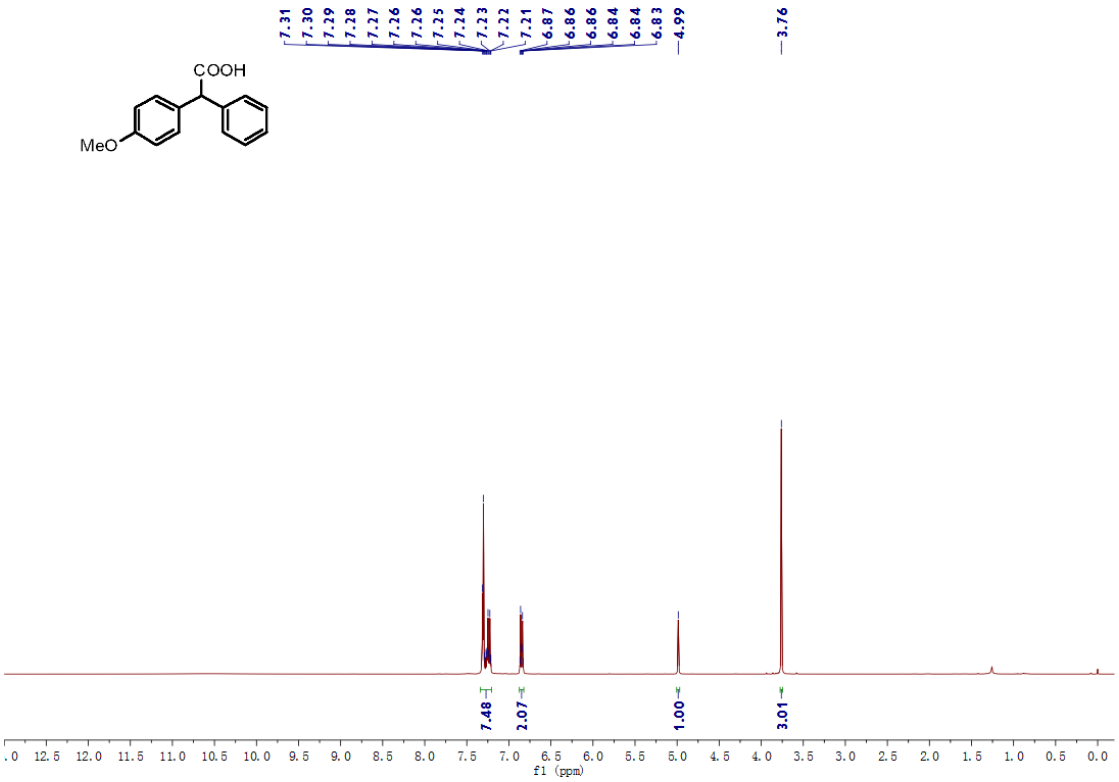
57.10
f1 (ppm)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7.25
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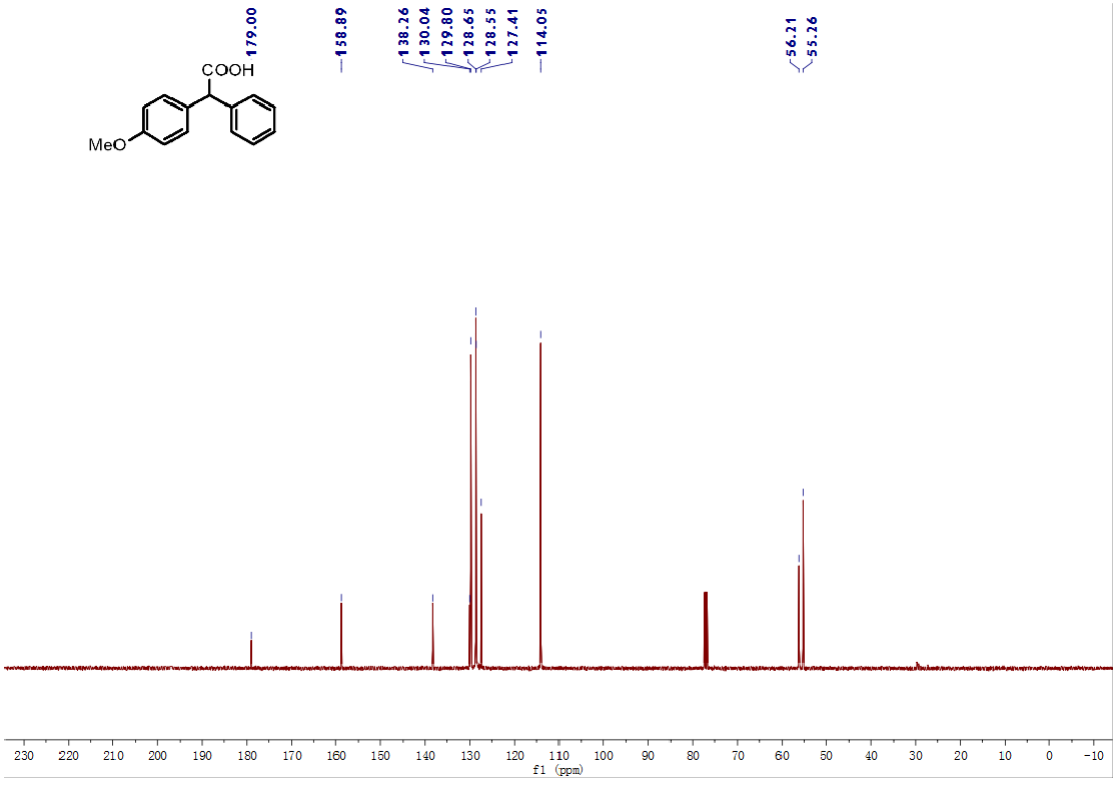
7.23
7.22
7.21
6.87
6.86
6.86
6.84
6.84
6.83
4.99
3.76
COOH
MeO
7.48
2.07
1.00
3.01
f1 (ppm)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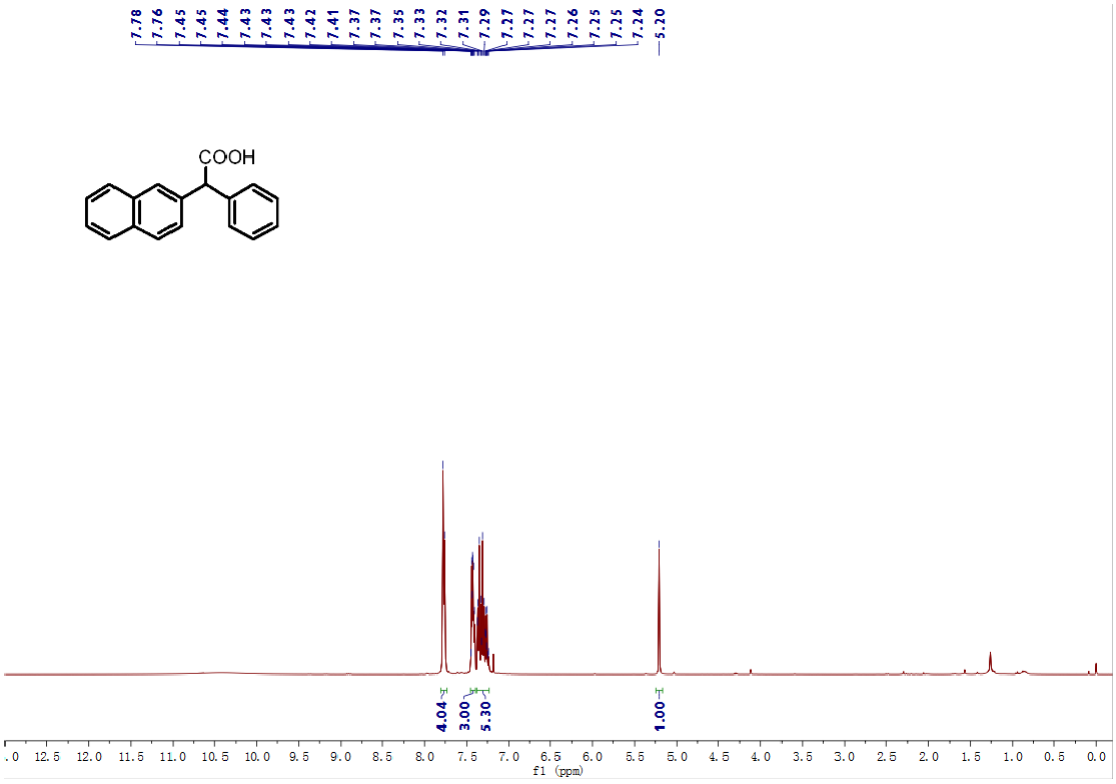
129.80
128.65
128.55
127.41
114.05
56.21
55.26
COOH
MeO
f1 (ppm)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7.76
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7.43
7.43
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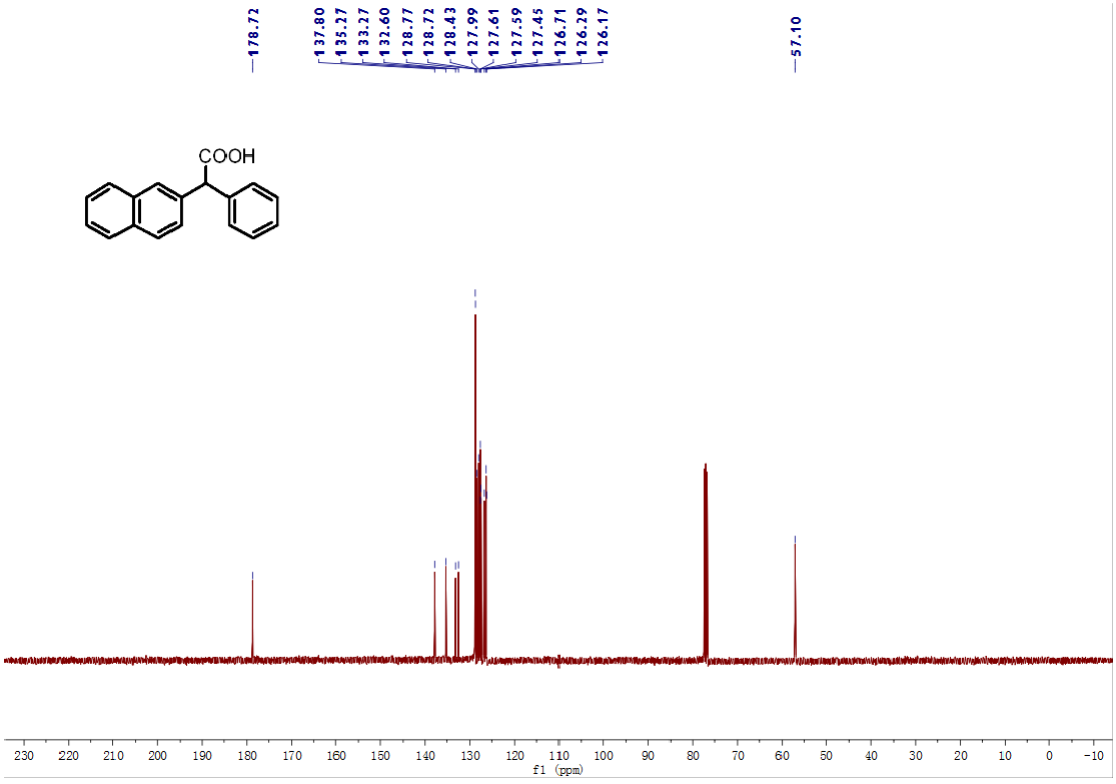
7.41
7.37
7.37
7.35
7.33
7.32
7.31
7.29
7.27
7.27
7.27
7.26
7.25
7.25
7.24
5.20
COOH
4.04
3.00
5.30
1.00
f1 (ppm)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133.27
132.60
128.77
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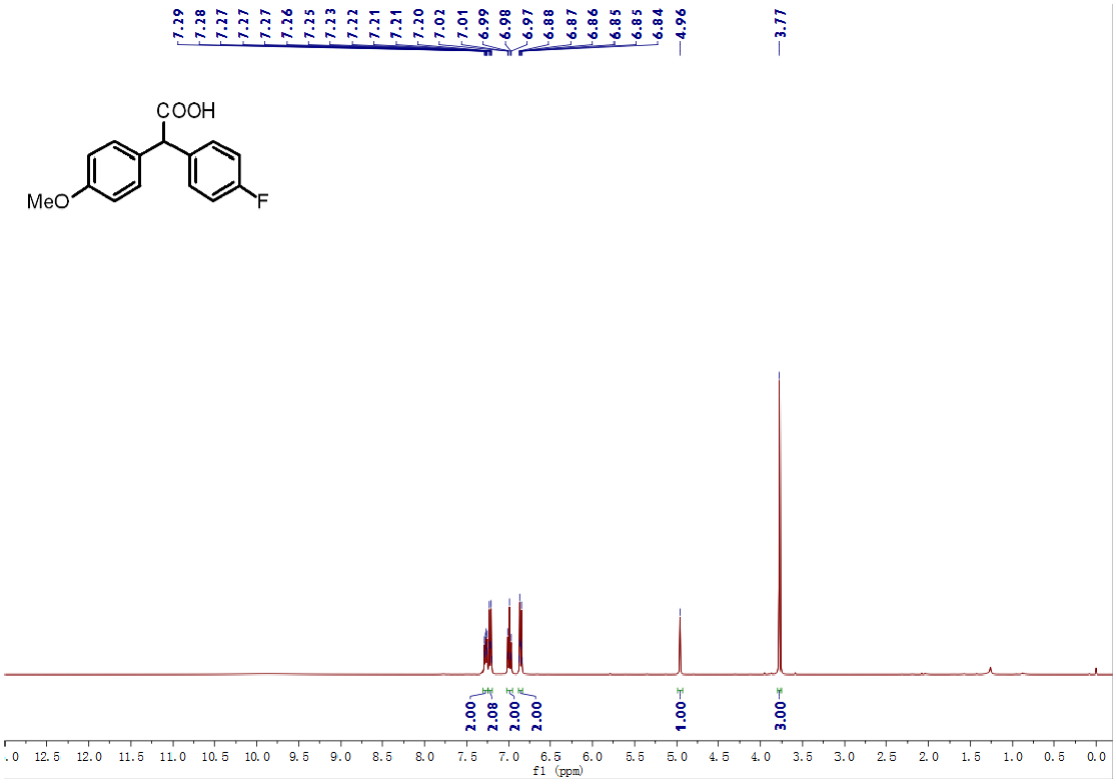
127.61
127.59
127.45
126.71
126.29
126.17
57.10
COOH
f1 (ppm)


7.29
7.28
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7.27
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7.26
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7.22
7.21
7.21
7.20
7.02
7.01
6.99
6.98
6.97
6.88
6.87
6.86
6.85
6.84
4.96
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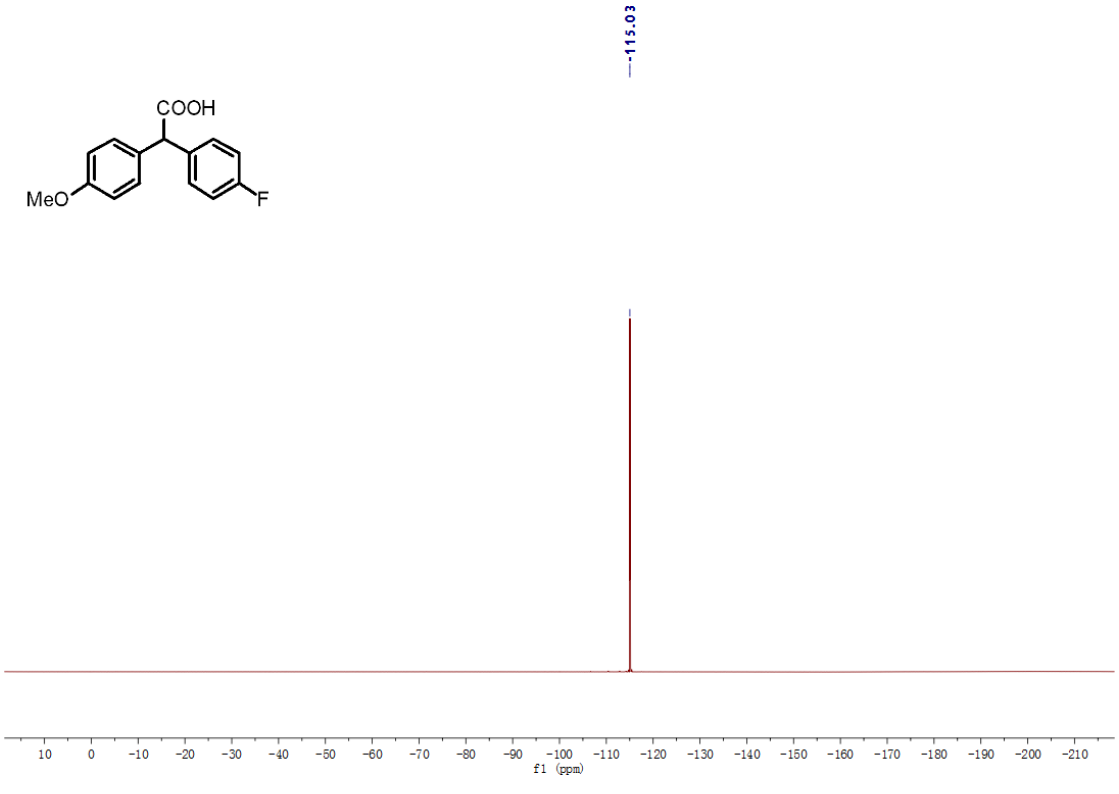
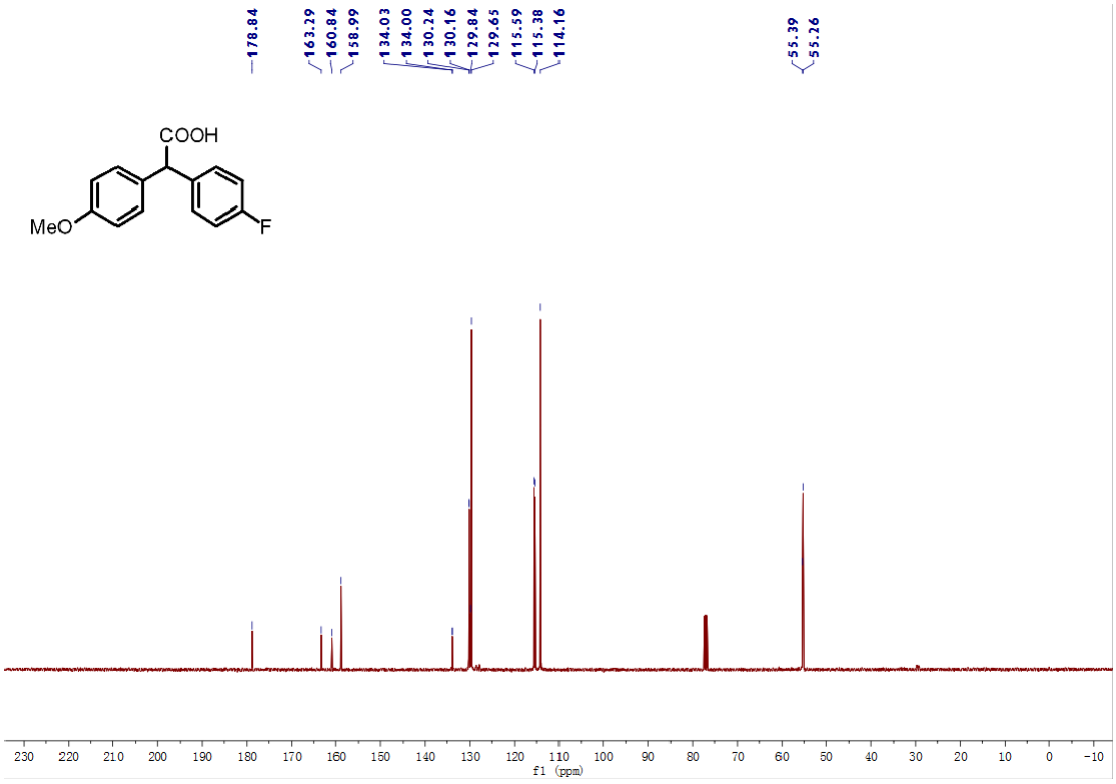
COOH
MeO
F
2.00
2.08
2.00
2.00
1.00
3.00
f1 (ppm)


-115.03
COOH
MeO
F
f1 (ppm)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163.29
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158.99
134.03
134.00
130.24
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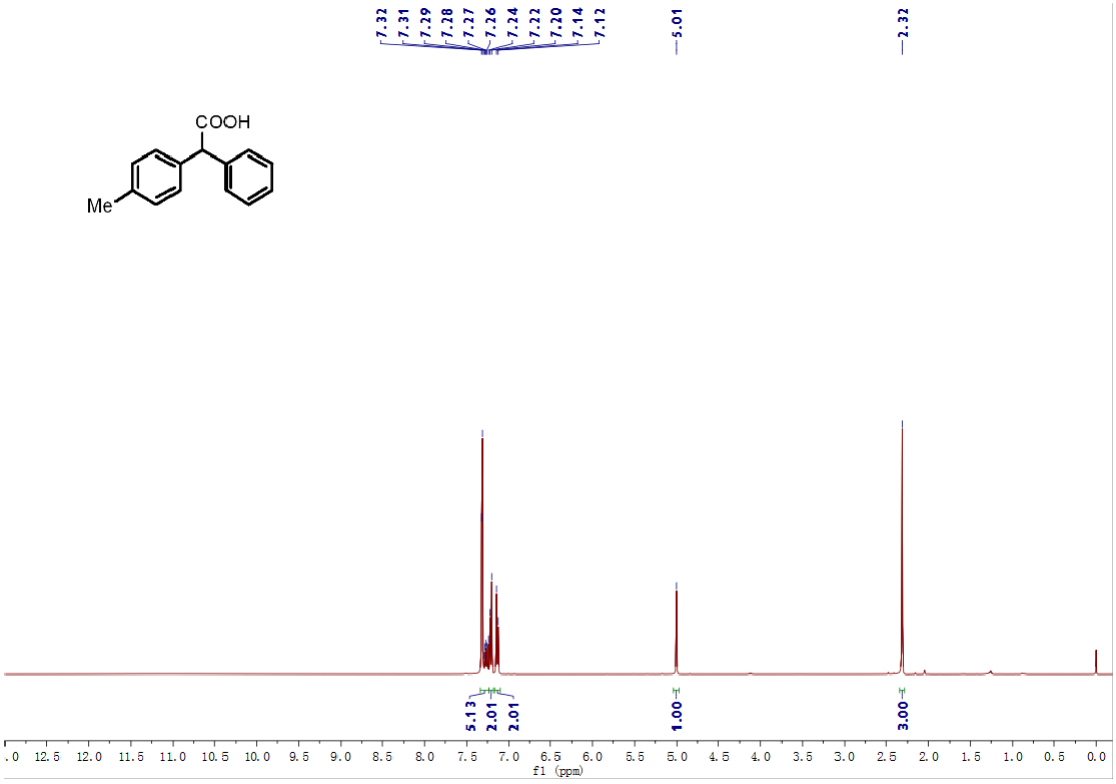
129.84
129.65
115.59
115.38
114.16
55.39
55.26
COOH
MeO
F
f1 (ppm)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7.31
7.29
7.28
7.27
7.26
7.24
7.22
7.20
7.14
7.12
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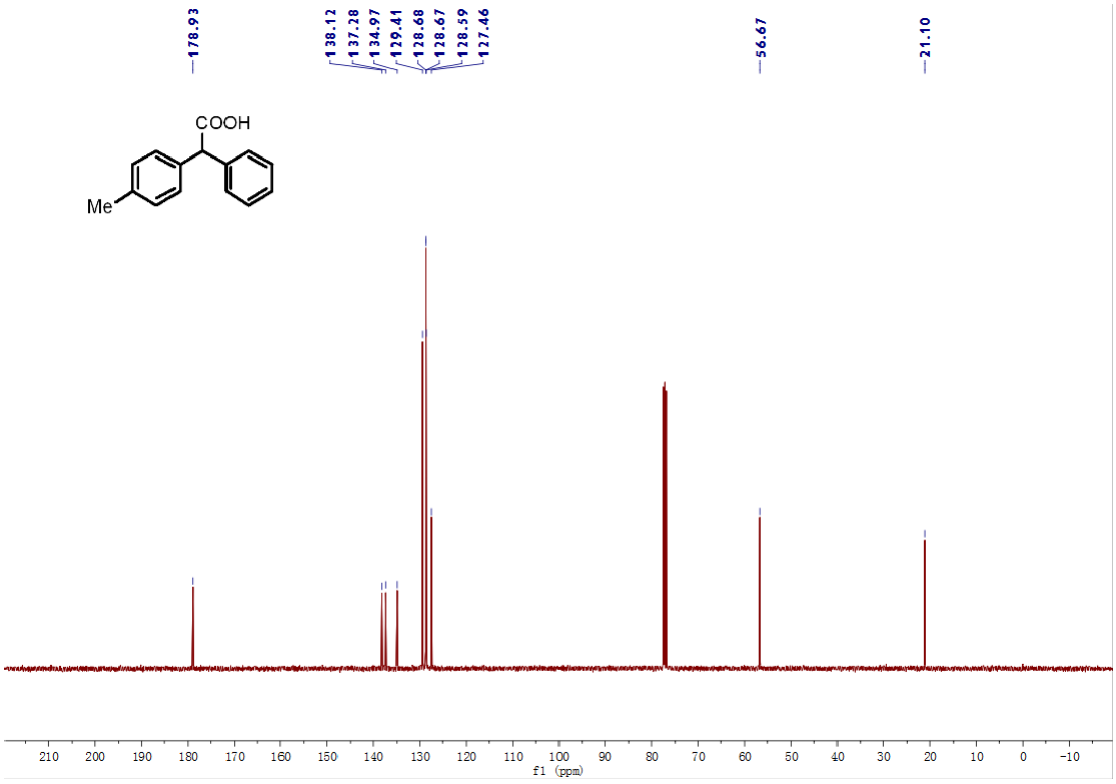
2.32
COOH
Me
5.13
2.01
2.01
1.00
3.00
f1 (ppm)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138.12
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127.46
56.67
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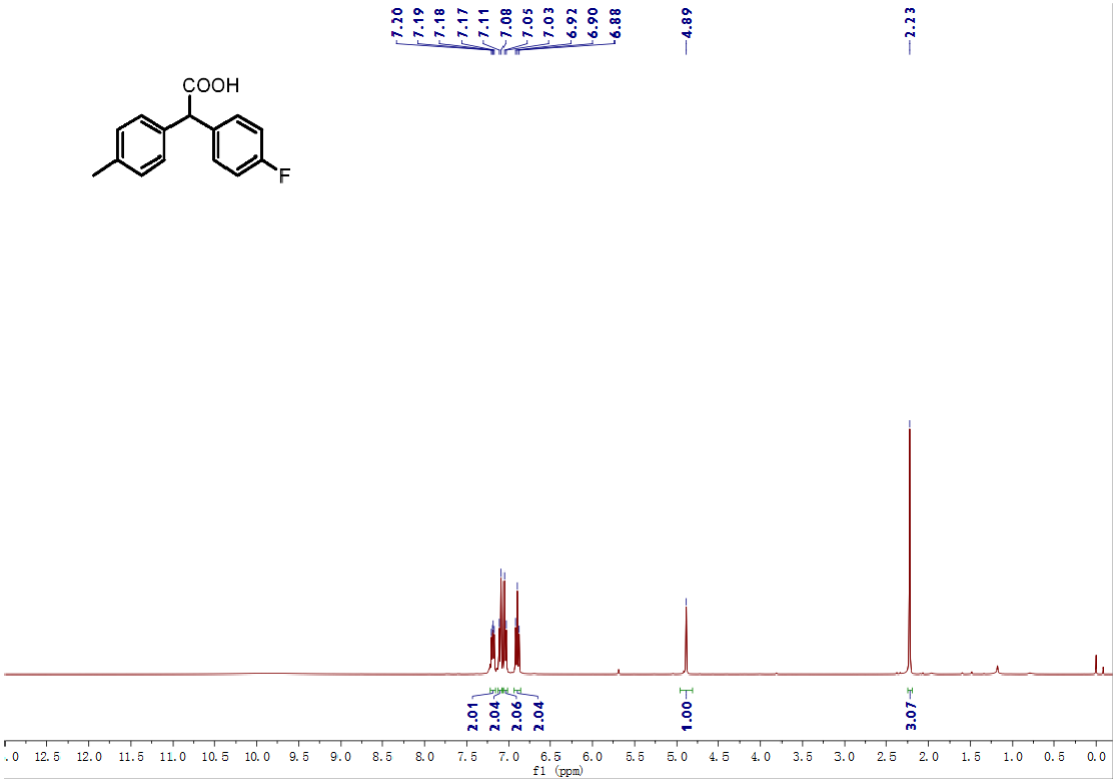
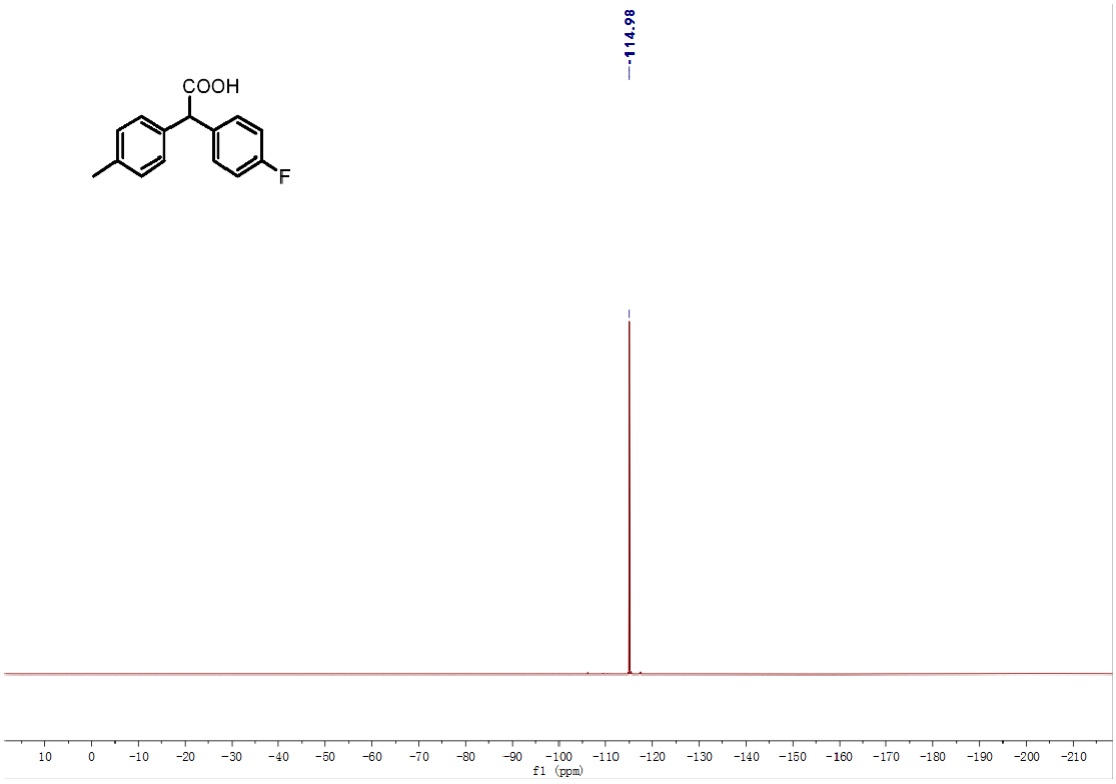
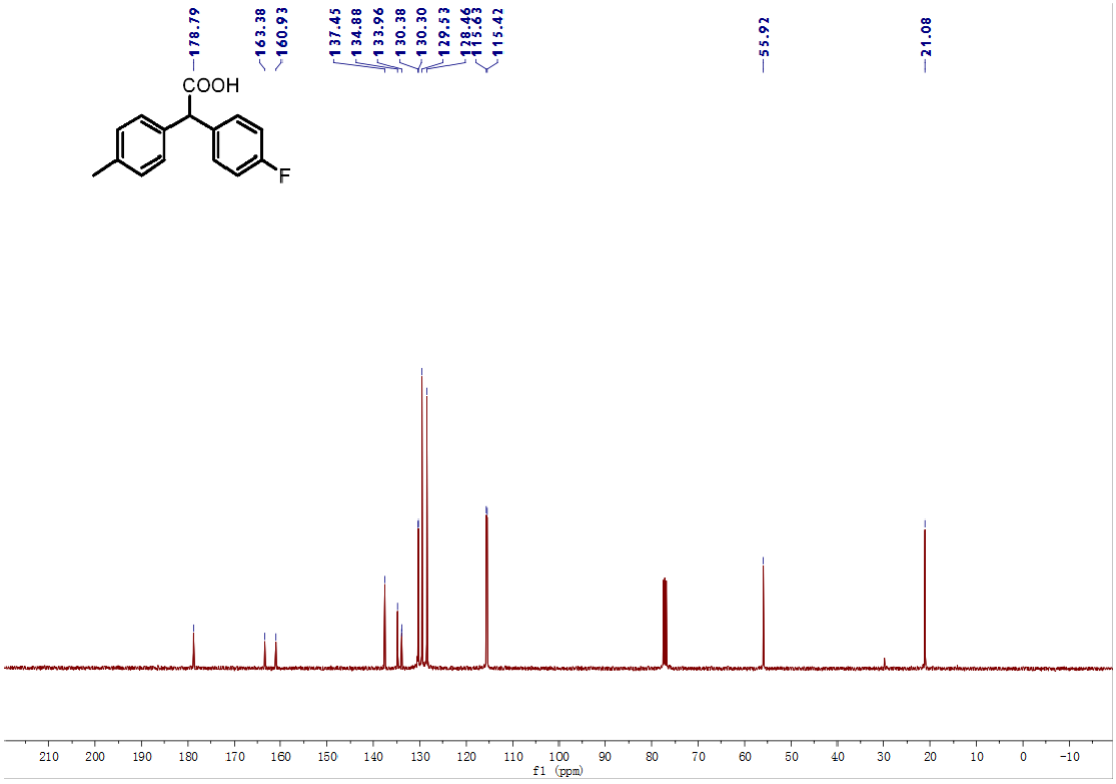
COOH
Me
f1 (ppm)


7.20
7.19
7.18
7.17
7.11
7.08
7.05
7.03
6.92
6.90
6.88
4.89
2.23
COOH
F
2.01
2.04
2.06
2.04
1.00
3.07
f1 (ppm)


COOH
F
-114.98
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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137.45
134.88
133.96
130.38
130.30
129.53
128.46
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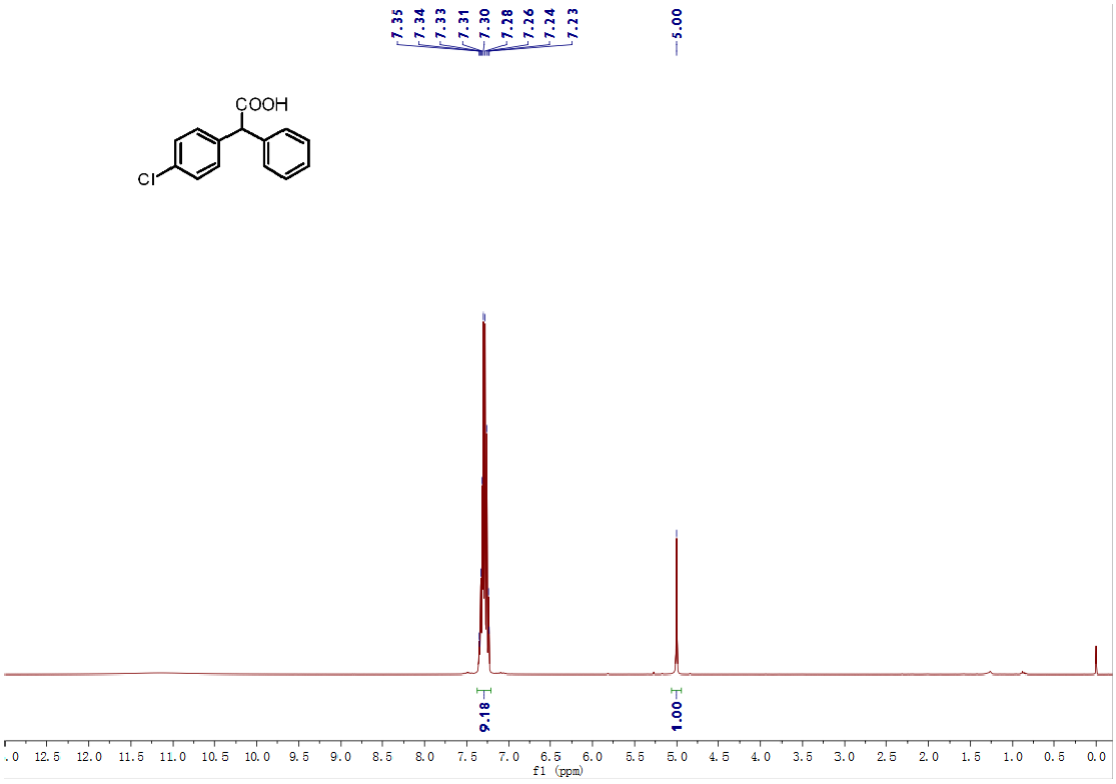
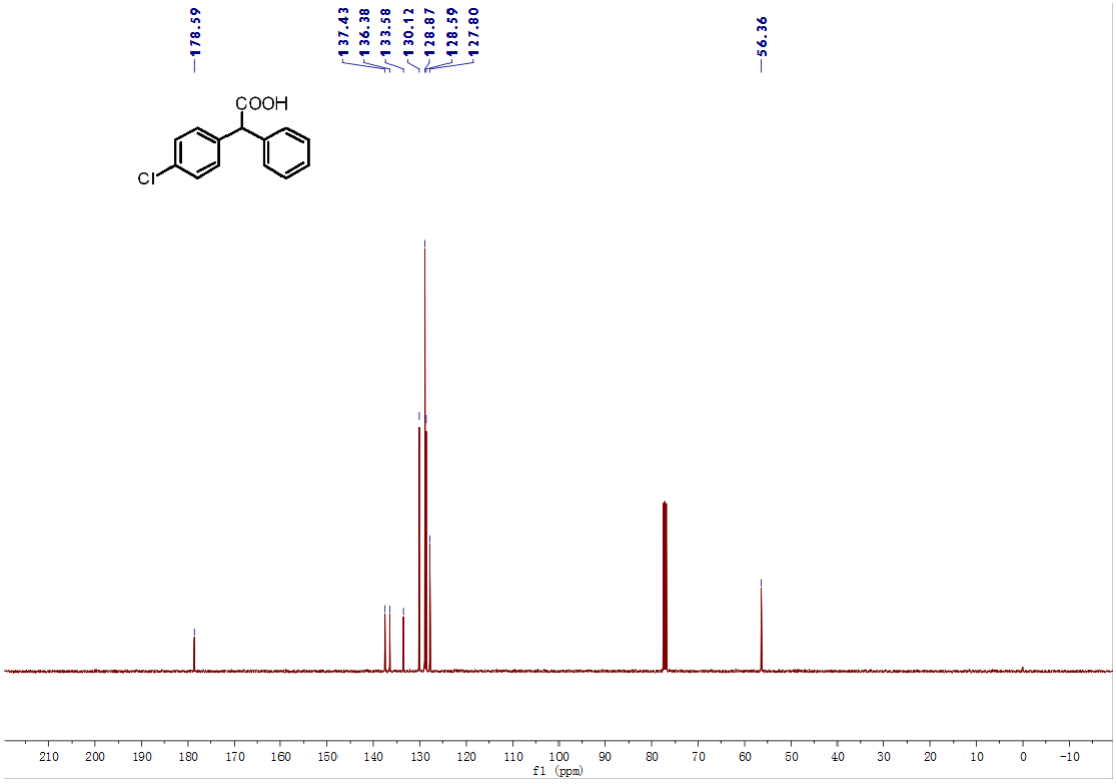
115.42
55.92
21.08
COOH
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.35
7.34
7.33
7.31
7.30
7.28
7.26
7.24
7.23
5.00
COOH
Cl
9.18
1.00
f1 (ppm)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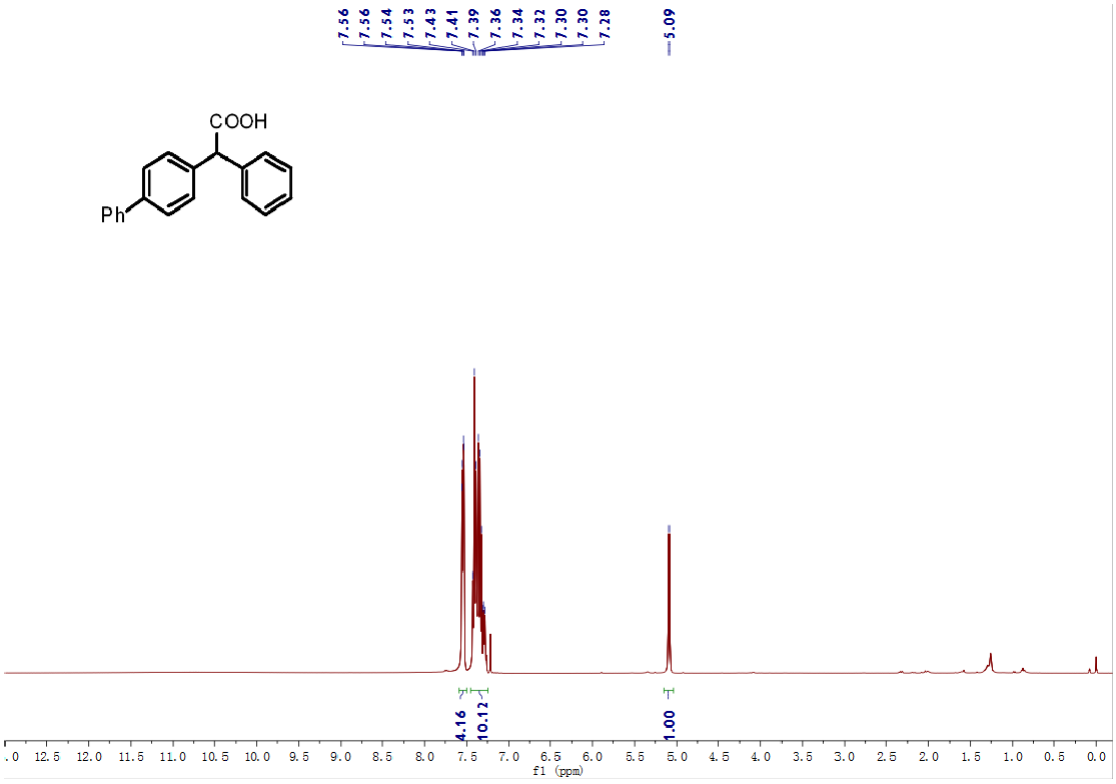
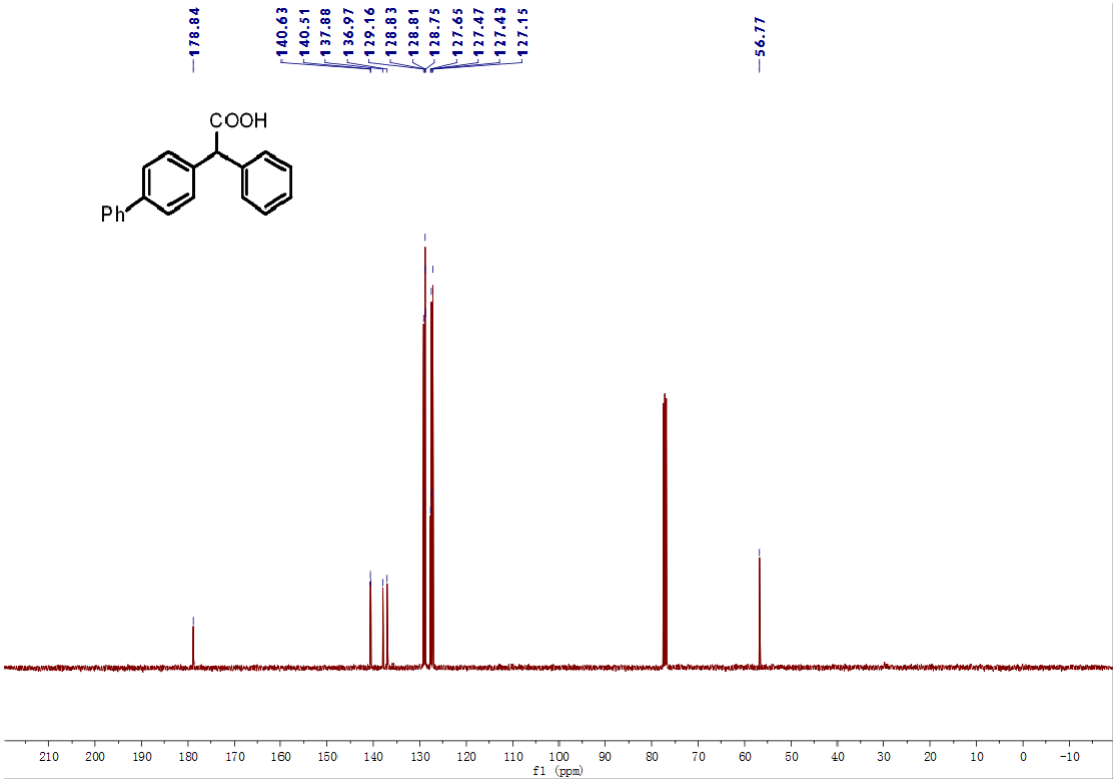
136.38
133.58
130.12
128.87
128.59
127.80
56.36
COOH
Cl
f1 (ppm)


7.56
7.56
7.54
7.53
7.43
7.41
7.39
7.36
7.34
7.32
7.30
7.30
7.28
5.09
COOH
Ph
4.16
10.12
1.00
f1 (ppm)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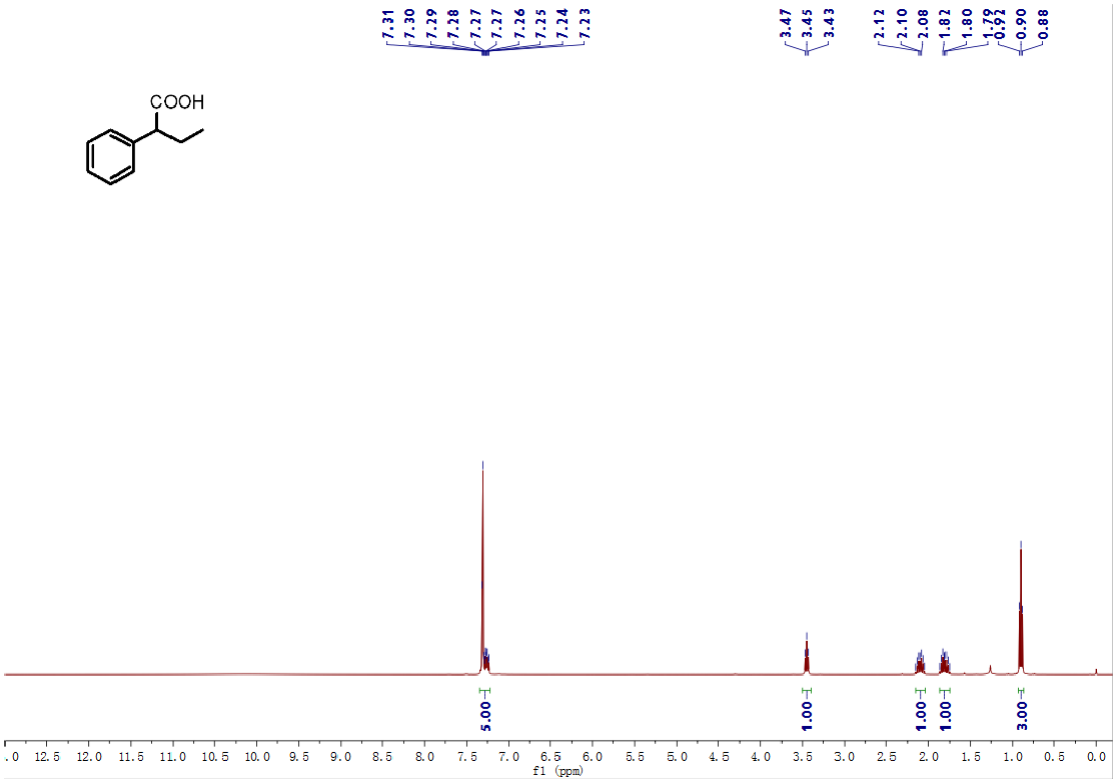
140.63
140.51
137.88
136.97
129.16
128.83
128.81
128.75
127.65
127.47
127.43
127.15
56.77
COOH
Ph
f1 (ppm)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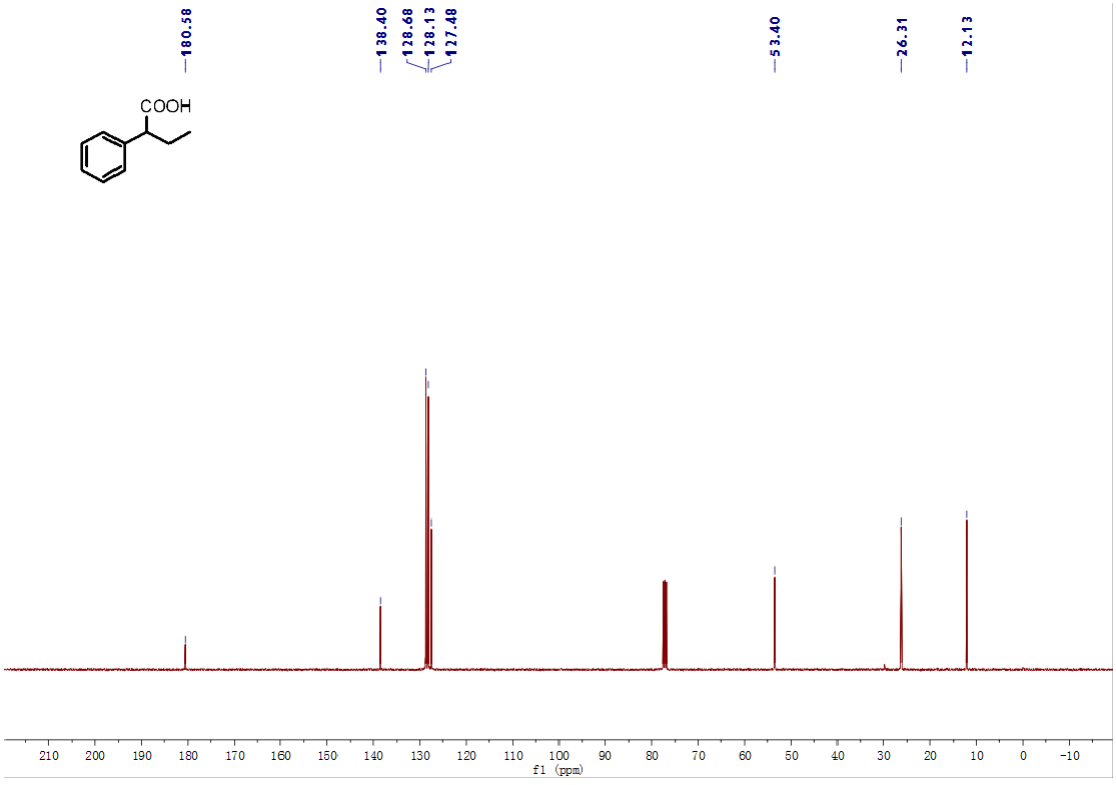
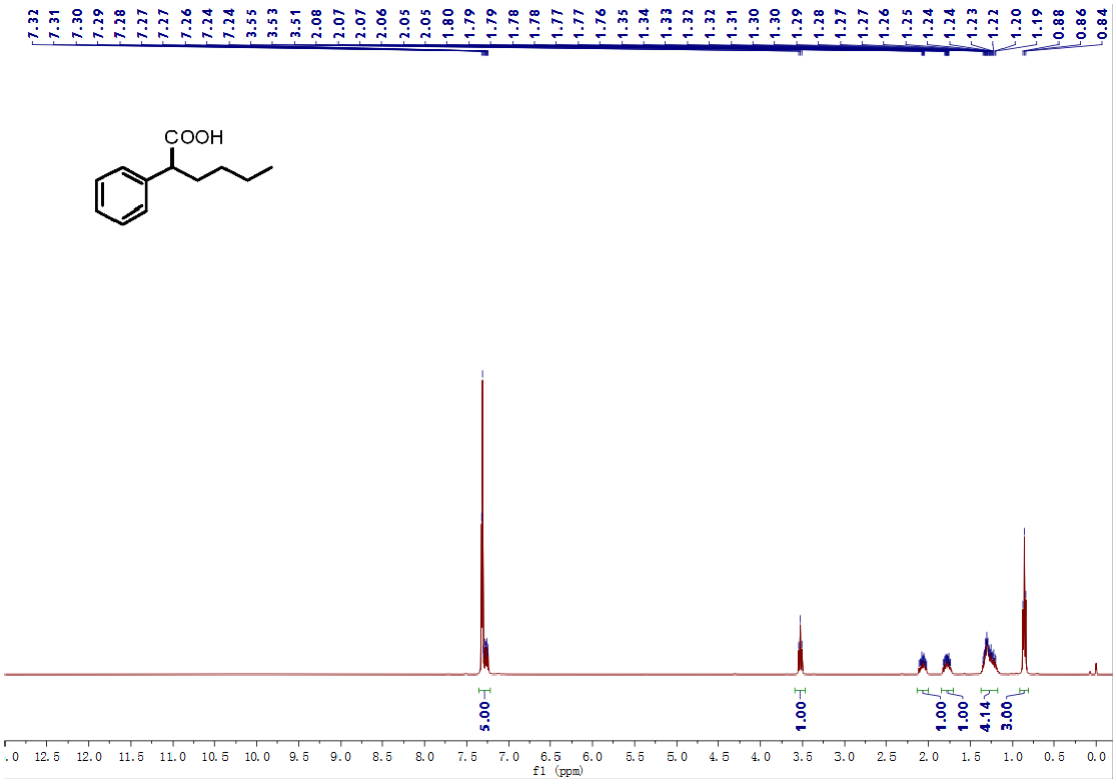
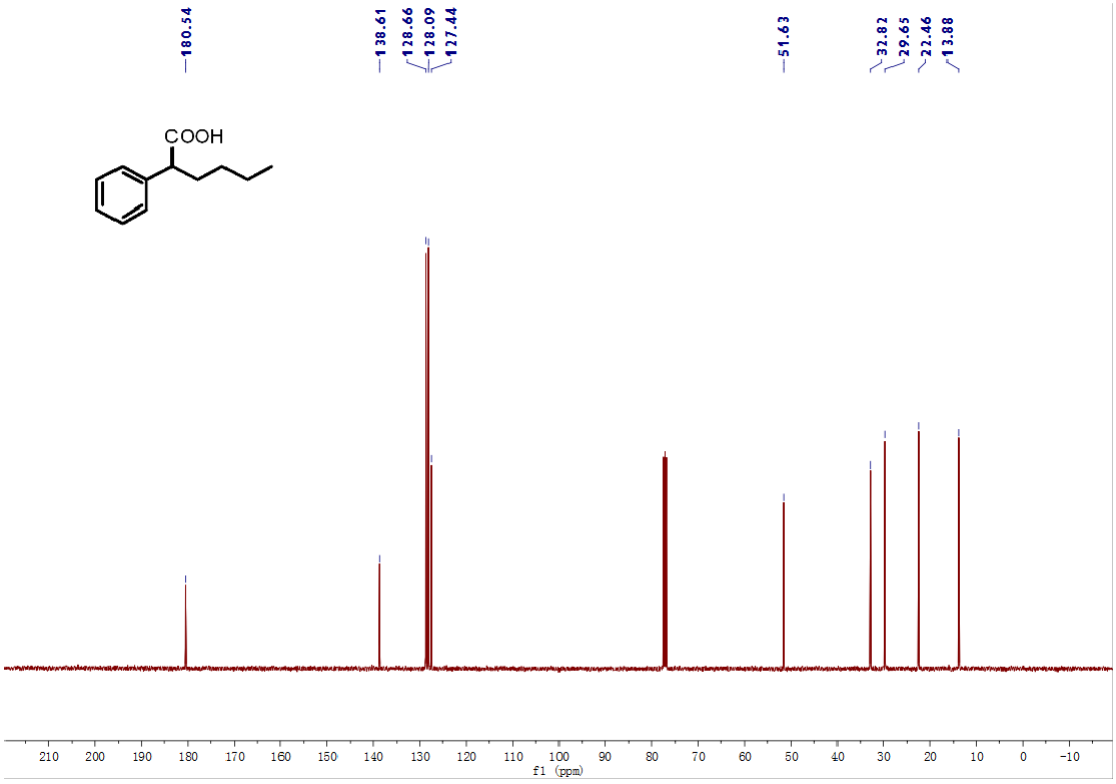
7.30
7.29
7.28
7.27
7.27
7.26
7.25
7.24
7.23
3.47
3.45
3.43
2.12
2.10
2.08
1.82
1.80
1.79
0.92
0.90
0.88
COOH
5.00
1.00
1.00
1.00
3.00
f1 (ppm)


180.58
138.40
128.68
128.13
127.48
53.40
26.31
12.13
COOH
f1 (ppm)


7.32 7.31 7.30 7.29 7.28 7.27 7.27 7.26 7.24 7.24 3.55 3.53 3.51 2.08 2.07 2.07 2.06 2.05 2.05 1.80 1.79 1.79 1.78 1.78 1.77 1.77 1.76 1.35 1.34 1.33 1.32 1.32 1.31 1.30 1.30 1.29 1.28 1.27 1.27 1.26 1.25 1.24 1.24 1.23 1.22 1.20 1.19 0.88 0.86 0.84
COOH
5.00
1.00
1.00
1.00
4.14
3.00
f1 (ppm)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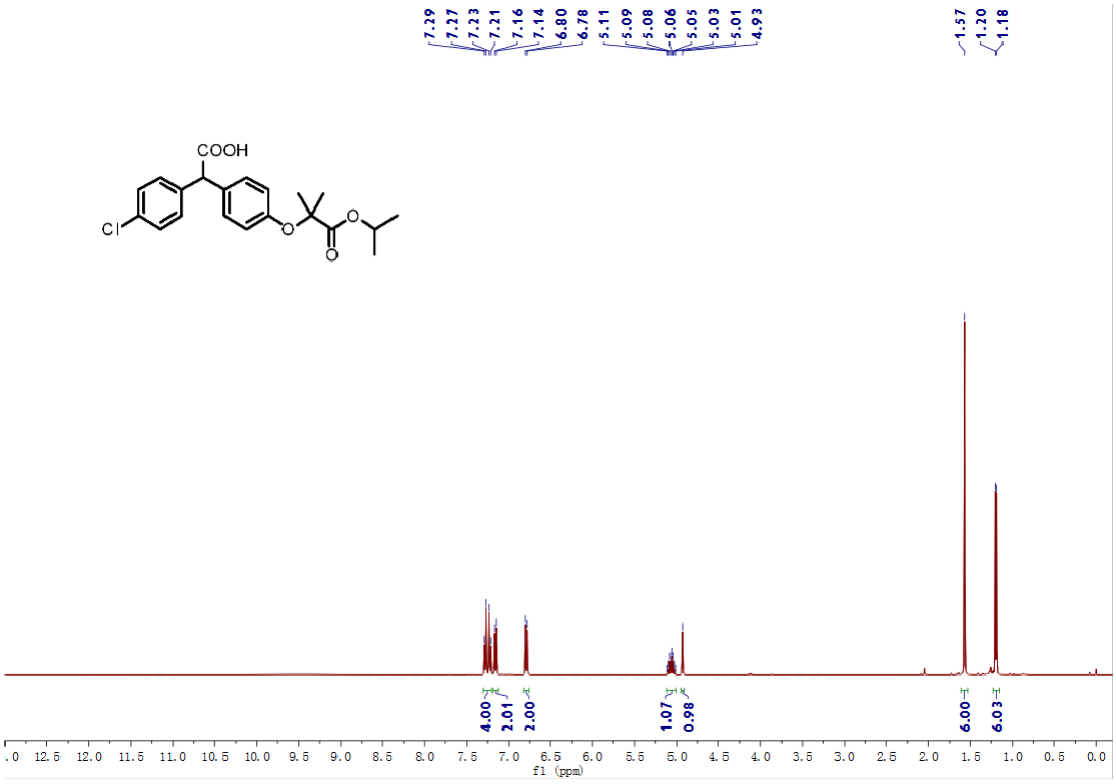
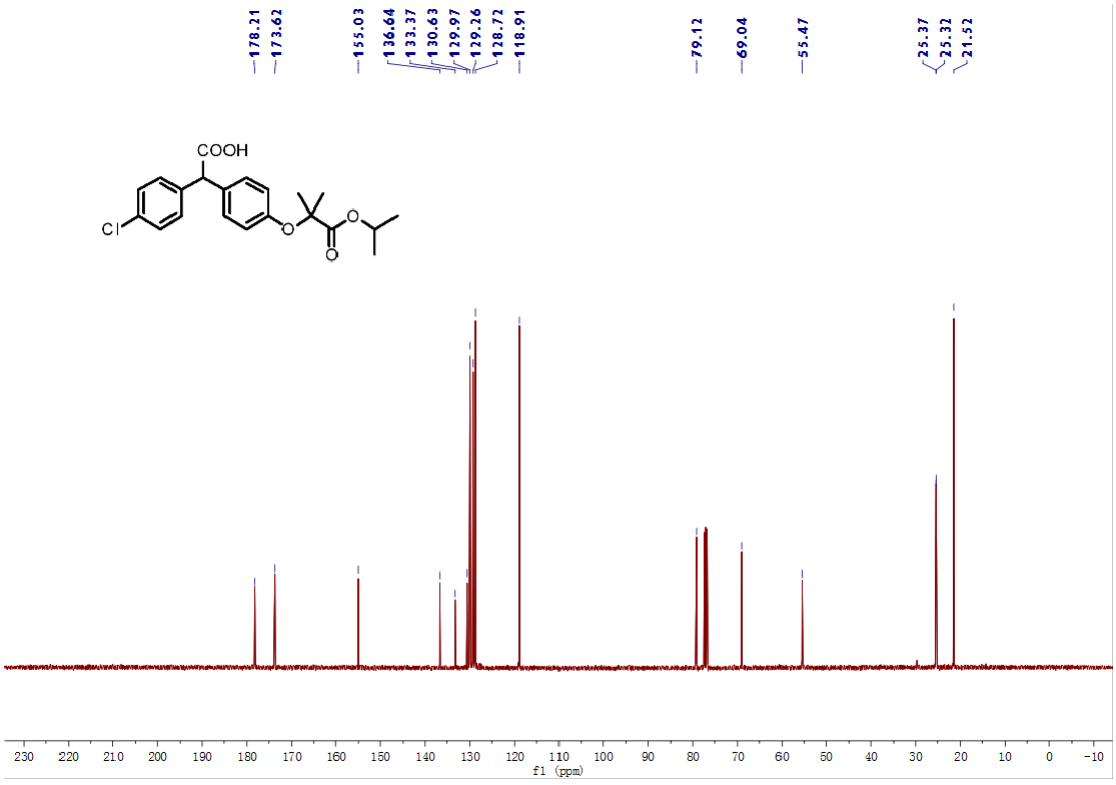
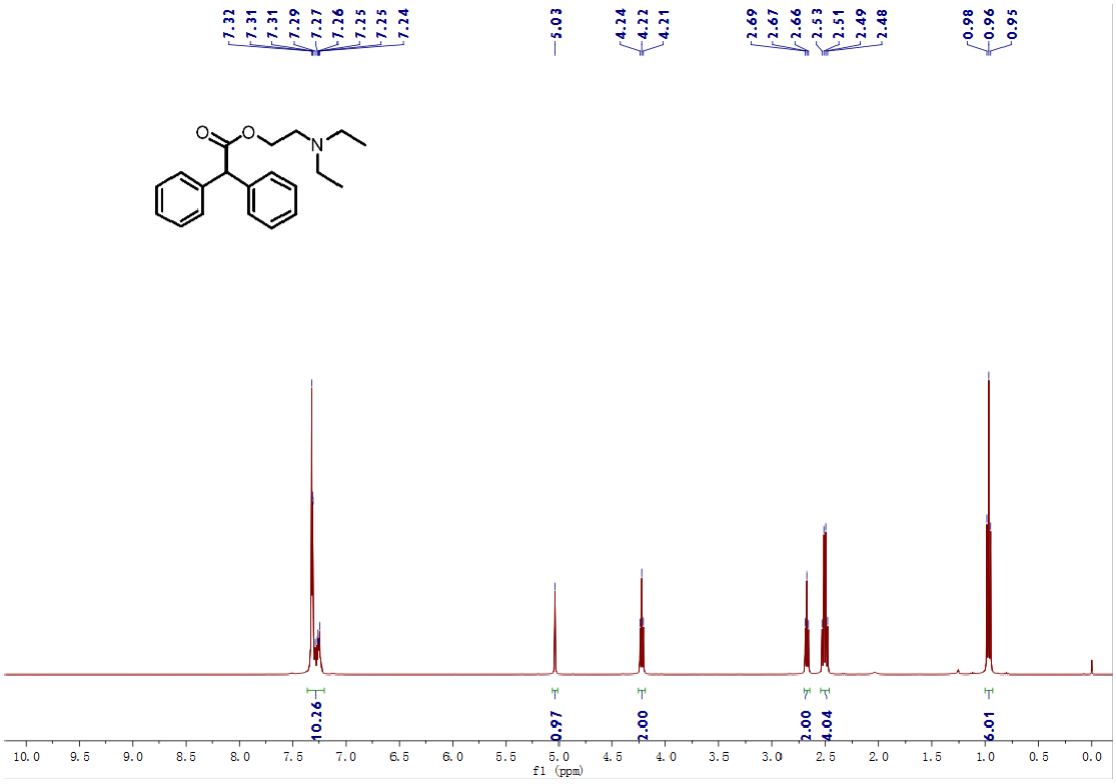
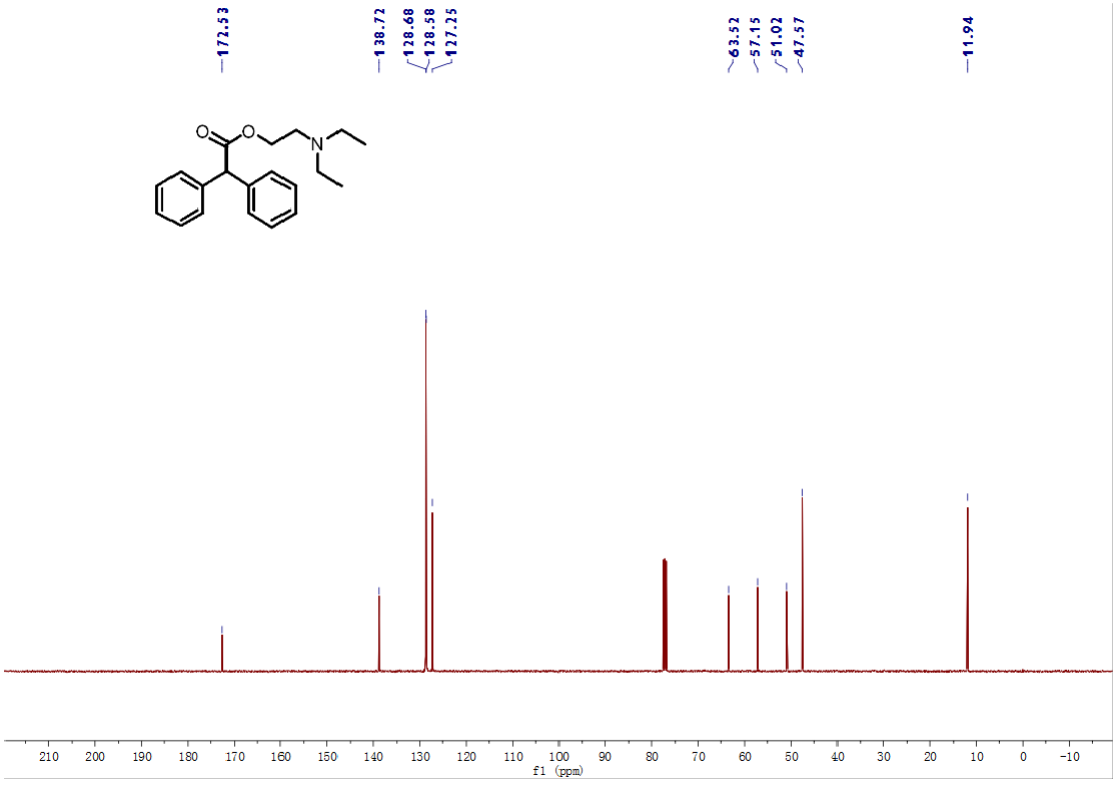
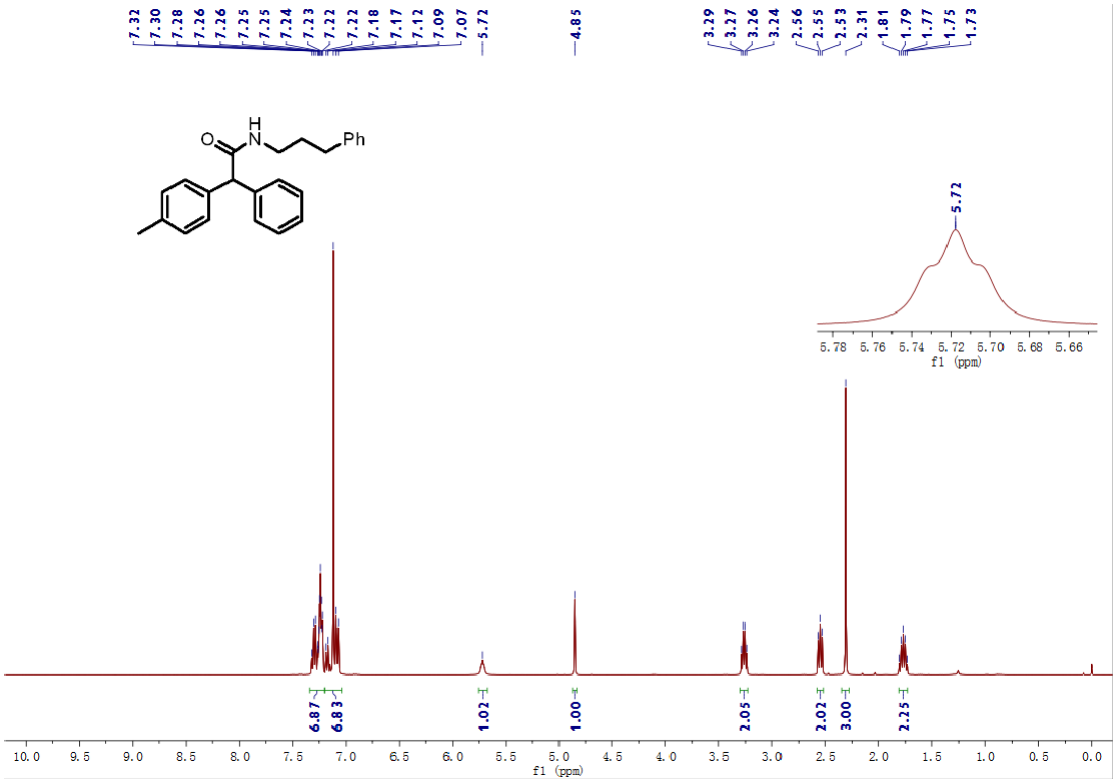
128.66
128.09
127.44
51.63
32.82
29.65
22.46
13.88
COOH
f1 (ppm)

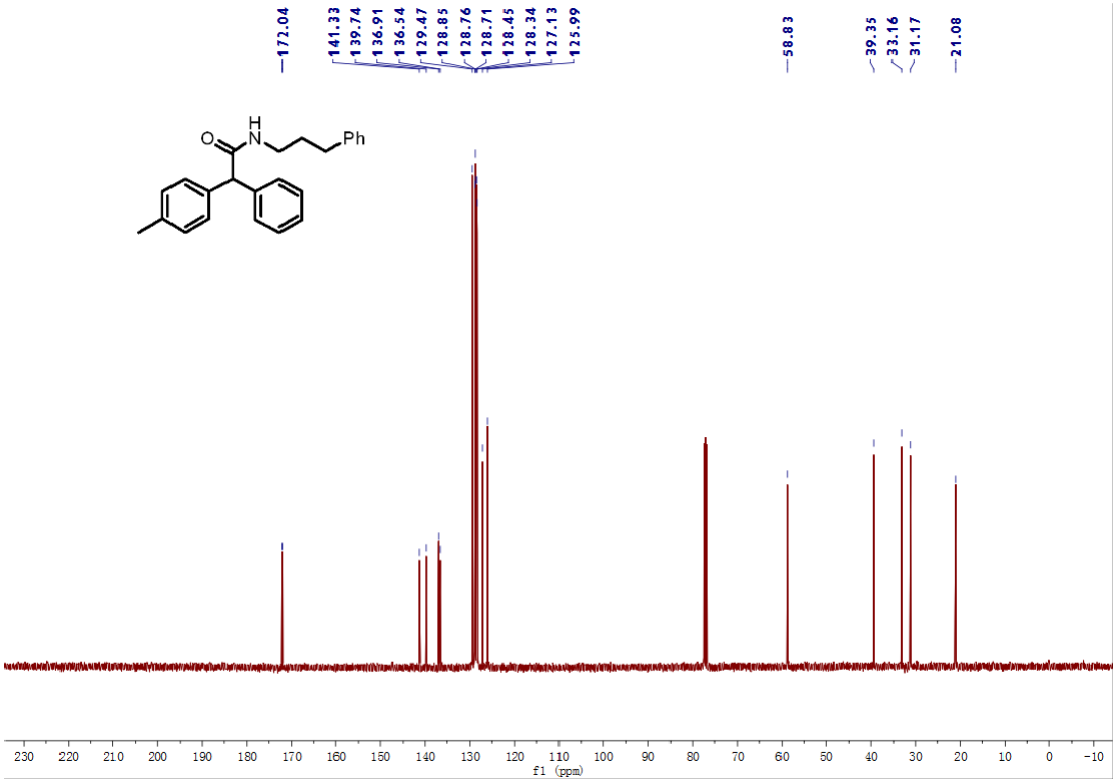

7.29
7.27
7.23
7.21
7.16
7.14
6.80
6.78
5.11
5.09
5.08
5.06
5.05
5.03
5.01
4.93
1.57
1.20
1.18
COOH
Cl
O
O
O
4.00
2.01
2.00
1.07
0.98
6.00
6.03
f1 (ppm)

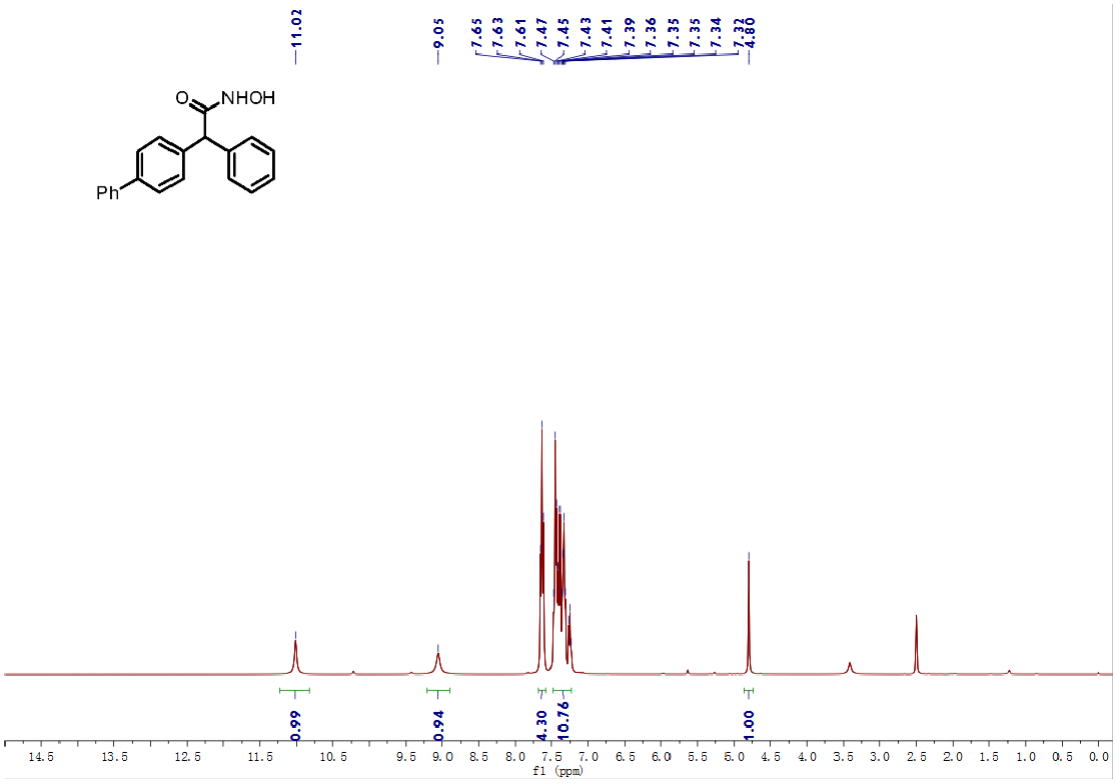

178.21
173.62
155.03
136.64
133.37
130.63
129.97
129.26
128.72
118.91
79.12
69.04
55.47
25.37
25.32
21.52
COOH
Cl
O
O
O
f1 (ppm)

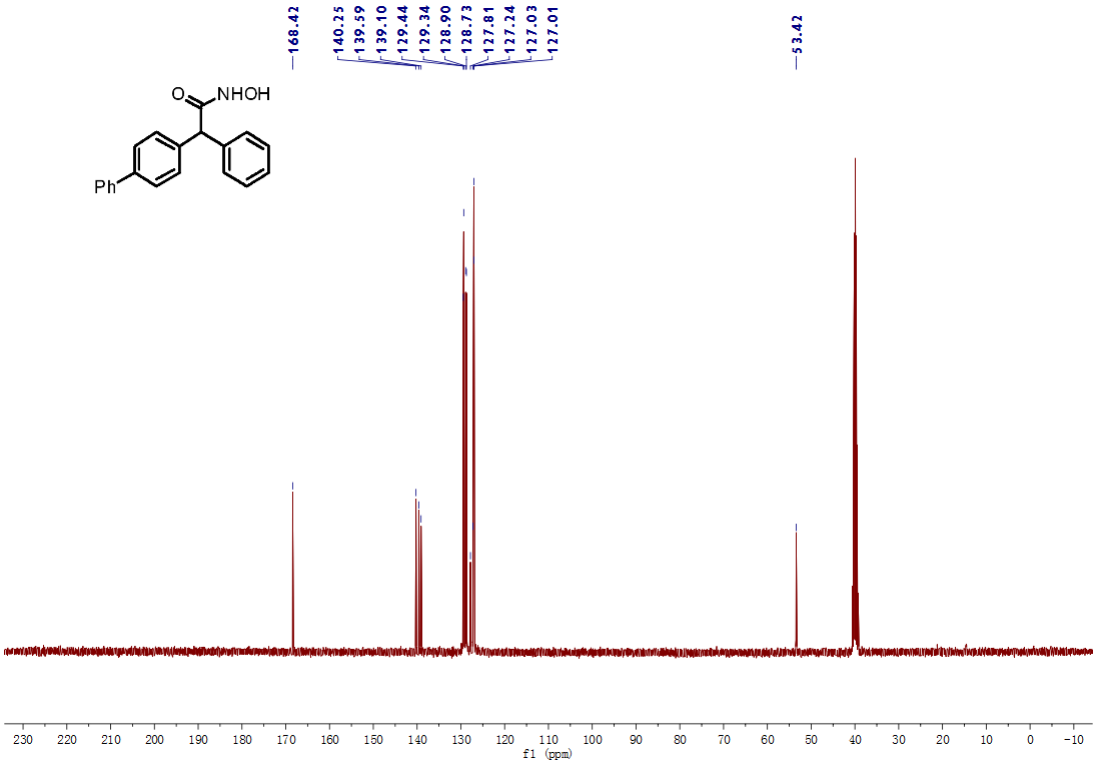

7.32
7.31
7.31
7.29
7.27
7.26
7.25
7.25
7.24
5.03
4.24
4.22
4.21
2.69
2.67
2.66
2.53
2.51
2.49
2.48
0.98
0.96
0.95
O
O
N
10.26
0.97
2.00
2.00
4.04
6.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

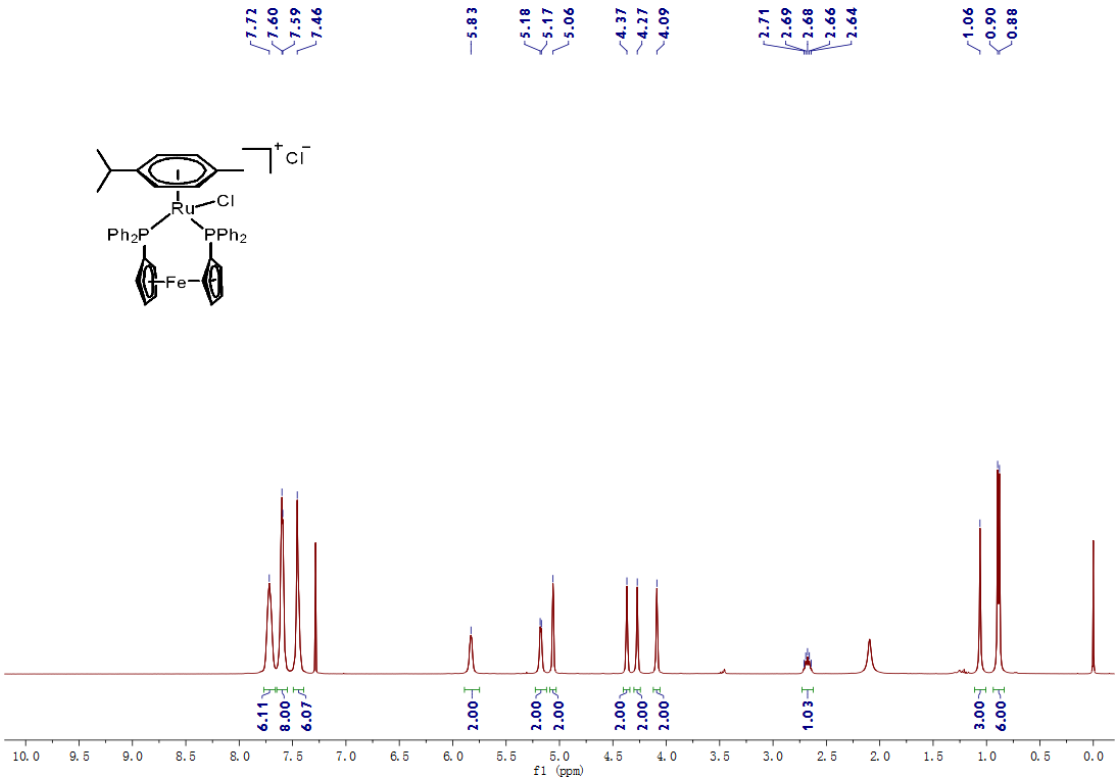

172.53
138.72
128.68
128.58
127.25
63.52
57.15
51.02
47.57
11.94
O
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

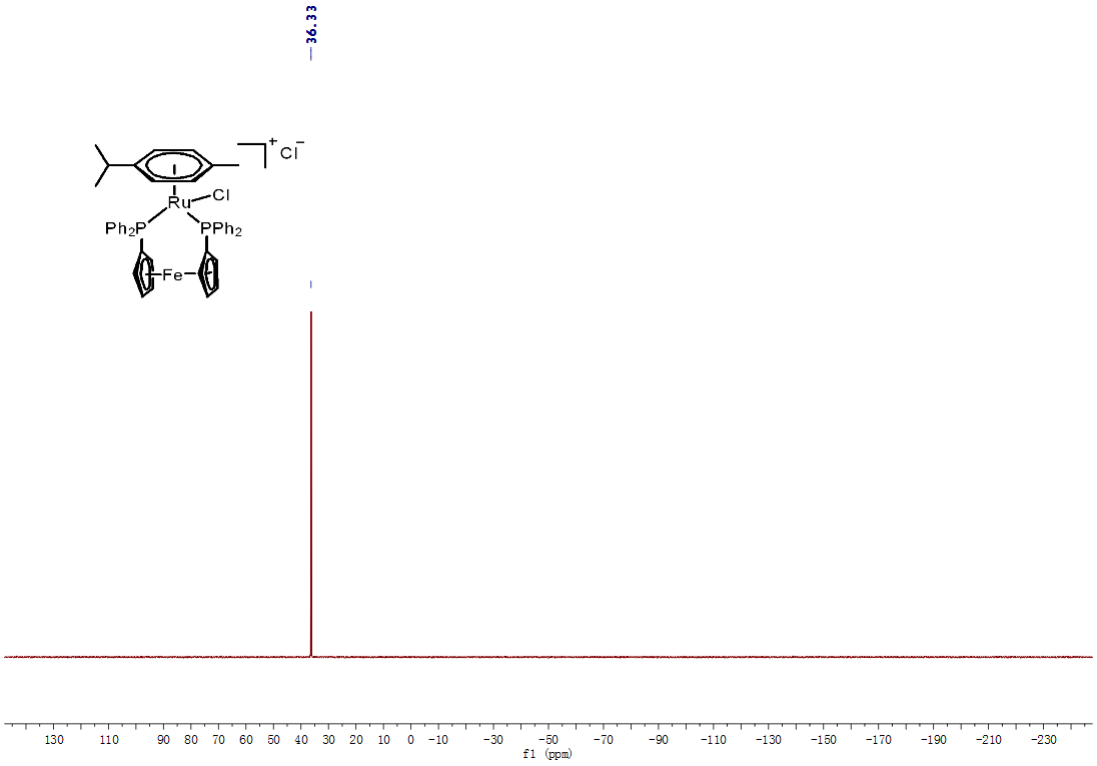

7.32
7.30
7.28
7.26
7.26
7.25
7.25
7.24
7.23
7.22
7.22
7.18
7.17
7.12
7.09
7.07
5.72
4.85
3.29
3.27
3.26
3.24
2.56
2.55
2.53
2.31
1.81
1.79
1.77
1.75
1.73
O
N
H
Ph
5.72
5.78 5.76 5.74 5.72 5.70 5.68 5.66
f1 (ppm)
6.87
6.83
1.02
1.00
2.05
2.02
3.00
2.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

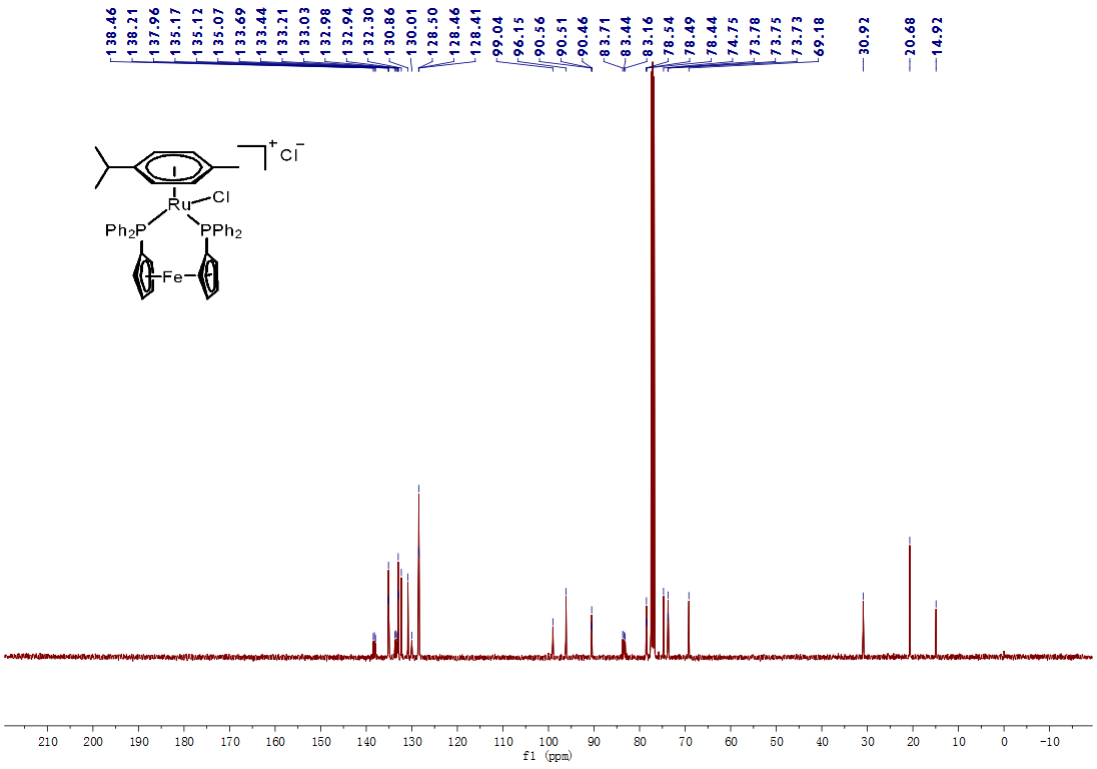

172.04
141.33
139.74
136.91
136.54
129.47
128.85
128.76
128.71
128.45
128.34
127.13
125.99
58.83
39.35
33.16
31.17
21.08
O
N
H
Ph
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.02
9.05
7.65
7.63
7.61
7.47
7.45
7.43
7.41
7.39
7.36
7.35
7.35
7.34
7.32
4.80
O
NHOH
Ph
0.99
0.94
4.30
10.76
1.00
f1 (ppm)


168.42
140.25
139.59
139.10
129.44
129.34
128.90
128.73
127.81
127.24
127.03
127.01
53.42
O
NHOH
Ph
f1 (ppm)


7.72
7.60
7.59
7.46
5.83
5.18
5.17
5.06
4.37
4.27
4.09
2.71
2.69
2.68
2.66
2.64
1.06
0.90
0.88
Cl
Ru
Cl
Ph2P
PPh2
Fe
6.11
8.00
6.07
2.00
2.00
2.00
2.00
2.00
2.00
1.03
3.00
6.00
f1 (ppm)


36.33
Cl
Ru
Cl
Ph2P
PPh2
Fe
f1 (ppm)


138.46
138.21
137.96
135.17
135.12
135.07
133.69
133.44
133.21
133.03
132.98
132.94
132.30
130.86
130.01
128.50
128.46
128.41
99.04
96.15
90.56
90.51
90.46
83.71
83.44
83.16
78.54
78.49
78.44
74.75
73.78
73.75
73.73
69.18
30.92
20.68
14.92
Cl
Ru
Cl
Ph2P
PPh2
Fe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)