Enantioconvergent deoxygenative reductive cross-coupling of lactic acid derivatives

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Supporting Information

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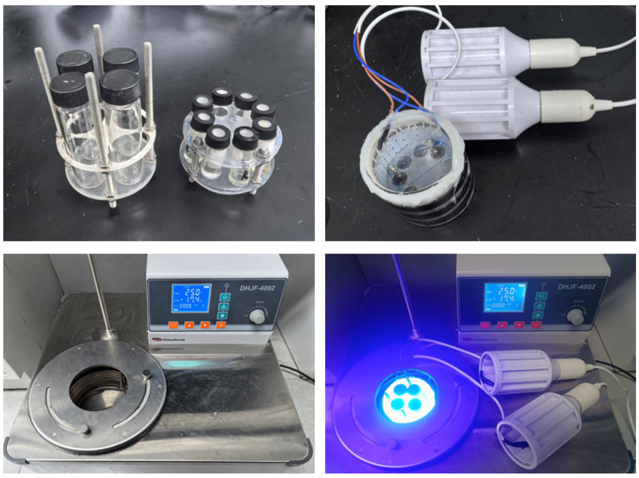
I. General Information

Unless otherwise noted, all other reagents and starting materials were purchased from commercial sources and used without further purification. Anhydrous MTBE (methyl *tert*-butyl ether) and CF_3Ph ((trifluoromethyl)benzene) were purchased from *J&K* and stored under nitrogen. Ligand (*S*)-**L1** and NHC were prepared according to the literature procedure, and all analytical data matched the reports.[1,2] Unless otherwise noted, all reactions were performed under an atmosphere of dry nitrogen.

NMR spectra were collected on a Bruker 400 MHz, or a Bruker 600 MHz spectrometer at ambient temperature; chemical shifts (δ) are reported in ppm downfield from tertramethylsilane, using the solvent resonance as the internal standard. HPLC analysis was performed on an Agilent 1260 Infinity II system with Daicel CHIRALPAK® or Daicel CHIRALCEL® columns (4.6 × 250 mm, particle size 3 μm). FT-IR measurements were carried out on a Thermo Scientific Nicolet iS10 spectrometer. HRMS were obtained from a Bruker micro TOF-II instrument. GC data were acquired by a Shimadzu GC-2030AF spectrometer. Optical rotation data were measured on a Rudolph AUTOPOL VI polarimeter. X-ray crystallographic analyses were carried out on a Bruker APEX-III CMOS diffractometer. Flash column chromatography was performed using silica gel (particle size 200-400 mesh ASTM, purchased from Yantai, China).

The blue LEDs (455 mm, 30 W) were purchased from www.taobao.com. As shown in **Figure S1**, the reaction vials were positioned 2-3 cm from the LEDs, and the temperature was controlled using a cooler (Greatwall DHJF-4002).

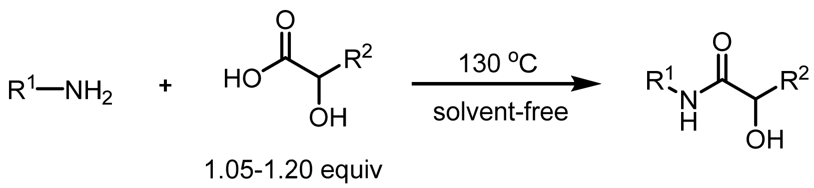
Figure S1. Photoreaction setup



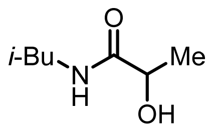
II. Preparation of α-Hydroxy Amides

The yields have not been optimized.

General Procedure 1 (GP-1).



Preparation of α-hydroxy amide from primary amine and α-hydroxy carboxylic acid. A mixture of primary amine (1.0 equiv) and α-hydroxy carboxylic acid (1.05-1.20 equiv) in the absence of solvent was stirred at 130 °C for 2-12 hours, until TLC indicated the disappearance of primary amine. The mixture was cooled to room temperature and dissolved in ethyl acetate. The organic layer was washed with water, brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel to give the target product.



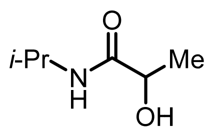
2-Hydroxy-*N*-isobutylpropanamide. The title compound was synthesized according to **GP-1** from isobutylamine (1.46 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 2.12 g (14.6 mmol, 73% yield). Yellow oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.98 (s, 1H), 4.48 (d, *J* = 4.4 Hz, 1H), 4.20 (dt, *J* = 11.1, 5.5 Hz, 1H), 3.18 – 2.99 (m, 2H), 1.84 – 1.72 (m, 1H), 1.41 (d, *J* = 6.8 Hz, 3H), 0.92 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.4, 68.0, 46.2, 28.3, 21.0, 19.9, 19.8.

FT-IR (film): 3670, 3307, 2970, 1642, 1398, 1055 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_7H_{15}NNaO_2$: 168.0995, found: 168.1003.



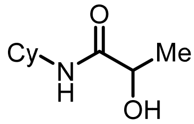
2-Hydroxy-*N*-isopropylpropanamide. The title compound was synthesized according to **GP-1** from isopropylaminei (1.18 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 1.47 g (11.2 mmol, 56% yield). Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.71 (s, 1H), 4.45 (s, 1H), 4.11 (q, *J* = 6.9 Hz, 1H), 4.02 – 3.93 (m, 1H), 1.35 (d, *J* = 6.8 Hz, 3H), 1.12 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.3, 68.0, 40.9, 22.52, 22.51, 21.0.

FT-IR (film): 3664, 3324, 2973, 1632, 1390, 1058 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_6H_{14}NO_2$: 132.1019, found: 132.1021.



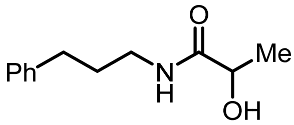
***N*-Cyclohexyl-2-hydroxypropanamide.** The title compound was synthesized according to **GP-1** from cyclohexylamine (1.98 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 2.57 g (15.0 mmol, 75% yield). Yellow oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.82 (d, *J* = 8.5 Hz, 1H), 4.72 (s, 1H), 4.10 (q, *J* = 6.8 Hz, 1H), 3.69 – 3.59 (m, 1H), 1.89 – 1.76 (m, 2H), 1.68 – 1.63 (m, 2H), 1.58 – 1.48 (m, 1H), 1.34 – 1.31 (m, 3H), 1.31 – 1.24 (m, 2H), 1.17 – 1.07 (m, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 67.9, 47.6, 32.71, 32.70, 25.3, 24.6, 21.0.

FT-IR (film): 3672, 2976, 1636, 1530, 1252, 1070, 894 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_9H_{17}NNaO_2$: 194.1151, found: 194.1151.



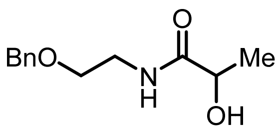
2-Hydroxy-*N*-(3-phenylpropyl)propanamide. The title compound was synthesized according to **GP-1** from 3-phenyl-1-aminopropane (2.70 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.14 g (15.2 mmol, 76% yield). Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (t, *J* = 8.2 Hz, 2H), 7.24 – 7.20 (m, 3H), 7.10 (t, *J* = 6.1 Hz, 1H), 4.67 (s, 1H), 4.24 (q, *J* = 6.8 Hz, 1H), 3.31 (q, *J* = 6.8 Hz, 2H), 2.69 (t, *J* = 7.7 Hz, 2H), 1.88 (p, *J* = 7.4 Hz, 2H), 1.45 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.3, 141.0, 128.3, 128.1, 125.8, 68.0, 38.4, 32.9, 30.8, 20.9.

FT-IR (film): 3670, 2976, 1642, 1249, 1070 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{12}H_{18}NO_2$: 208.1332, found: 208.1331.



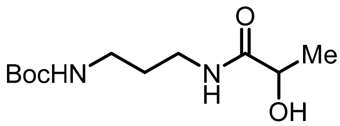
***N*-(2-(Benzyloxy)ethyl)-2-hydroxypropanamide.** The title compound was synthesized according to **GP-1** from 2-(benzyloxy)ethylamine (3.02 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.66 g (16.4 mmol, 82% yield). Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.23 (m, 5H), 7.02 (s, 1H), 4.51 (s, 2H), 4.14 (q, *J* = 6.8 Hz, 1H), 3.62 – 3.51 (m, 3H), 3.49 – 3.34 (m, 2H), 1.36 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 137.6, 128.4, 127.8, 127.7, 73.0, 68.7, 68.2, 38.8, 21.1.

FT-IR (film): 3667, 3257, 2970, 1630, 1055, 727 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{12}H_{17}NNaO_3$: 246.1101, found: 246.1102.



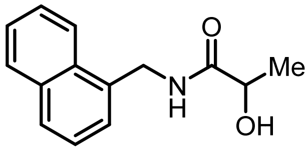
***tert*-Butyl (3-(2-hydroxypropanamido)propyl)carbamate.** The title compound was synthesized according to **GP-1** from *tert*-butyl (3-aminopropyl)carbamate (3.48 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (3:1 EtOAc/hexanes). 3.54 g (14.4 mmol, 72% yield). Yellow solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.15 (s, 1H), 5.17 (s, 1H), 4.34 – 4.07 (m, 2H), 3.28 (m, 2H), 3.10 (q, *J* = 6.4 Hz, 2H), 1.62 (p, *J* = 6.4 Hz, 2H), 1.43 – 1.36 (m, 12H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 175.8, 156.4, 79.2, 68.0, 37.1, 35.7, 29.7, 28.2, 20.9.

FT-IR (film): 3673, 3316, 2979, 1694, 1252, 1061 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{11}H_{23}N_2O_4$: 247.1652, found: 247.1657.



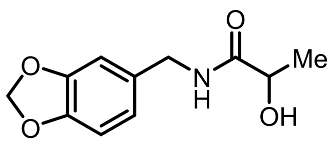
2-Hydroxy-*N*-(naphthalen-1-ylmethyl)propanamide. The title compound was synthesized according to **GP-1** from naphthalen-1-ylmethanamine (3.14 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). 3.21 g (14.0 mmol, 70% yield). Brown solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.90 (m, 1H), 7.87 – 7.83 (m, 1H), 7.80 – 7.76 (m, 1H), 7.53 – 7.45 (m, 2H), 7.41 – 7.35 (m, 2H), 6.97 (s, 1H), 4.83 (d, *J* = 3.7 Hz, 2H), 4.20 (q, *J* = 6.7 Hz, 1H), 3.31 (s, 1H), 1.38 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.7, 133.7, 133.0, 131.1, 128.6, 128.4, 126.4, 126.1, 125.8, 125.2, 123.1, 68.2, 40.9, 20.9.

FT-IR (film): 3664, 3321, 2970, 1639, 1067, 780 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{14}H_{16}NO_2$: 230.1176, found: 230.1177.



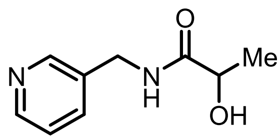
***N*-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-2-hydroxypropanamide.** The title compound was synthesized according to **GP-1** from benzo[*d*][1,3]dioxol-5-ylmethanamine (3.02 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.03 g (13.6 mmol, 68% yield). Brown oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.14 (s, 1H), 6.75 – 6.71 (m, 2H), 6.69 (d, *J* = 8.0 Hz, 1H), 5.91 (s, 2H), 4.29 (d, *J* = 5.9 Hz, 2H), 4.21 (q, *J* = 6.8 Hz, 1H), 4.12 (s, 1H), 1.40 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 147.7, 146.8, 131.6, 120.8, 108.1, 108.0, 100.9, 68.1, 42.7, 21.0.

FT-IR (film): 3673, 3339, 2976, 1648, 1486, 1038 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+ Na]$^+$ calcd for $C_{11}H_{13}NNaO_4$: 246.0737, found: 246.0744.



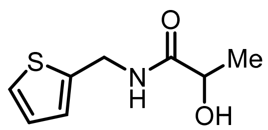
2-Hydroxy-*N*-(pyridin-3-ylmethyl)propanamide. The title compound was synthesized according to **GP-1** from pyridin-3-ylmethanamine (2.16 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:12 MeOH/DCM). 2.63 g (14.6 mmol, 73% yield). Yellow solidl.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.43 (dd, *J* = 4.5, 1.9 Hz, 2H), 7.64 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.49 – 7.41 (m, 1H), 7.28 – 7.25 (m, 1H), 4.54 (s, 1H), 4.50 (dd, *J* = 15.1, 6.3 Hz, 1H), 4.40 (dd, *J* = 15.2, 5.9 Hz, 1H), 4.28 (q, *J* = 6.8 Hz, 1H), 1.43 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.3, 148.4, 148.3, 136.0, 134.3, 123.8, 68.3, 40.4, 21.1.

FT-IR (film): 3671, 3197, 2966, 1653, 1024, 836 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_9H_{13}N_2O_2$: 181.0972, found: 181.0970.



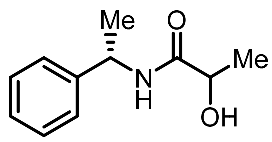
2-Hydroxy-*N*-(thiophen-2-ylmethyl)propanamide. The title compound was synthesized according to **GP-1** from thiophen-2-ylmethanamine (2.26 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 2.96 g (16.0 mmol, 80% yield). Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.20 (dd, *J* = 4.8, 1.5 Hz, 1H), 7.16 (s, 1H), 6.98 – 6.88 (m, 2H), 4.57 (d, *J* = 5.8 Hz, 2H), 4.21 (q, *J* = 6.8 Hz, 1H), 3.78 (s, 1H), 1.40 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 140.4, 126.8, 125.8, 125.1, 68.1, 37.7, 20.9.

FT-IR (film): 3670, 3324, 2973, 1642, 1064, 692 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_8H_{12}NO_2S$: 186.0583, found: 186.0589.



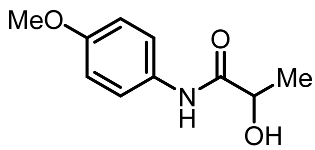
2-Hydroxy-*N*-((*S*)-1-phenylethyl)propanamide. The title compound was synthesized according to **GP-1** from (*S*)-1-phenylethan-1-amine (2.42 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). 2.66 g (13.8 mmol, 69% yield). Yellow oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.31 – 7.25 (m, 4H), 7.23 (t, *J* = 6.9 Hz, 1H), 7.11 (d, *J* = 8.3 Hz, 1H), 5.03 (p, *J* = 7.3 Hz, 1H), 4.15 – 4.06 (m, 2H), 1.45 (d, *J* = 6.9 Hz, 3H), 1.35 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 142.8, 128.4, 127.1, 125.8, 67.9, 48.3, 21.9, 20.8.

FT-IR (film): 3670, 2973, 1648, 1404, 1070, 698 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{11}H_{16}NO_2$: 194.1176, found: 194.1173.



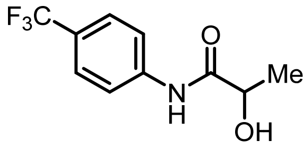
2-Hydroxy-*N*-(4-methoxyphenyl)propanamide. The title compound was synthesized according to **GP-1** from 4-methoxyaniline (2.46 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). 2.54 g (13.0 mmol, 65% yield). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.58 (s, 1H), 7.39 (d, *J* = 9.0 Hz, 2H), 6.81 (d, *J* = 9.0 Hz, 2H), 4.26 (q, *J* = 6.8 Hz, 1H), 3.75 (s, 3H), 1.45 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.0, 156.5, 130.1, 121.7, 114.1, 68.5, 55.4, 21.0.

FT-IR (film): 3667, 3254, 2987, 2970, 1648, 1406, 1068 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{10}H_{14}NO_3$: 196.0968, found: 196.0968.



2-Hydroxy-*N*-(4-(trifluoromethyl)phenyl)propanamide. The title compound was synthesized according to **GP-1** from 4-(trifluoromethyl)aniline (3.22 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). 2.90 g (12.4 mmol, 62% yield). White solid.

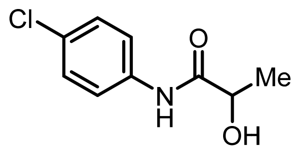
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.81 (s, 1H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 4.37 (q, *J* = 6.9 Hz, 1H), 3.73 (s, 1H), 1.51 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.3, 140.0, 126.4 (q, *J* = 32.9 Hz), 126.2 (q, *J* = 3.9 Hz), 123.9 (q, *J* = 271.6 Hz), 119.4, 68.8, 20.9.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.2.

FT-IR (film): 3673, 3260, 2984, 1668, 1316, 1117, 836 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{10}H_{11}F_3NO_2$: 234.0736, found: 234.0731.



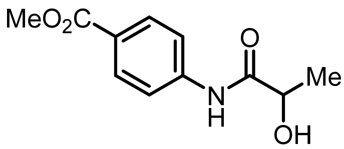
***N*-(4-Chlorophenyl)-2-hydroxypropanamide.** The title compound was synthesized according to **GP-1** from 4-chloroaniline (2.54 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). 2.83 g (14.2 mmol, 71% yield). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.62 (s, 1H), 7.47 (d, *J* = 7.0 Hz, 2H), 7.26 (d, *J* = 8.7 Hz, 2H), 4.33 (d, *J* = 6.1 Hz, 1H), 3.50 (s, 1H), 1.49 (d, *J* = 8.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.0, 135.6, 129.6, 129.0, 121.1, 68.7, 21.0.

FT-IR (film): 3667, 3298, 2973, 1653, 1395, 1076, 824 cm^{-1}.

HRMS (ESI-MS) m/z [M+H]$^+$ calcd for $C_9H_{11}ClNO_2$: 200.0473, found: 200.0471.



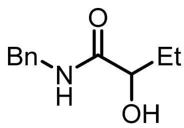
Methyl 4-(2-hydroxypropanamido)benzoate. The title compound was synthesized according to **GP-1** from methyl 4-aminobenzoate (2.27 g, 15.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). 1.81 g (8.1 mmol, 54% yield). White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 (s, 1H), 7.98 (d, *J* = 8.2Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 2H), 4.38 (q, *J* = 6.8 Hz, 1H), 3.89 (s, 3H), 3.33 (s, 1H), 1.52 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.9, 166.7, 141.4, 130.8, 125.7, 118.9, 68.9, 52.1, 21.0.

FT-IR (film): 3676, 3266, 2972, 1631, 1176, 699 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{11}H_{14}NO_4$: 224.1907, found: 224.1910.



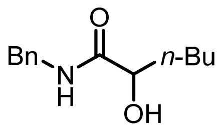
***N*-Benzyl-2-hydroxybutanamide.** The title compound was synthesized according to **GP-1** from phenylmethanamine (2.14 g, 20.0 mmol) and 2-hydroxybutanoic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.40 g (17.6 mmol, 88% yield). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29 (t, *J* = 7.2 Hz, 2H), 7.25 (d, *J* = 7.1 Hz, 1H), 7.23 – 7.18 (m, 3H), 4.41 (dd, *J* = 14.8, 6.1 Hz, 1H), 4.35 (dd, *J* = 14.8, 5.8 Hz, 1H), 4.06 – 4.04 (m, 1H), 1.92 – 1.78 (m, 1H), 1.70 – 1.62 (m, 1H), 0.93 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.2, 137.8, 128.6, 127.52, 127.50, 127.4, 72.9, 42.9, 27.7, 9.0.

FT-IR (film): 3673, 3254, 2970, 1615, 1252, 1082, 695 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{11}H_{15}NNaO_2$: 216.0995, found: 216.0991.



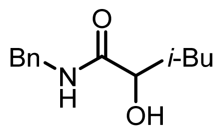
N-Benzyl-2-hydroxyhexanamide. The title compound was synthesized according to **GP-1** from phenylmethanamine (2.14 g, 20.0 mmol) and 2-hydroxyhexanoic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.54 g (16.0 mmol, 80% yield). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.33 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.25 (m, 3H), 6.87 (s, 1H), 4.48 – 4.43 (m, 2H), 4.16 – 4.14 (m, 1H), 2.84 (s, 1H), 1.94 – 1.82 (m, 1H), 1.72 – 1.61 (m, 1H), 1.49 – 1.29 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.1, 137.9, 128.6, 127.6, 127.5, 72.1, 43.0, 34.5, 27.1, 22.4, 13.9.

FT-IR (film): 3670, 3251, 2970, 1624, 1536, 1061, 724 cm^{-1}.

HRMS (ESI-MS) *m/z* $[2M+H]^+$ calcd for $C_{26}H_{39}N_2O_4$: 443.2904, found: 443.2892.



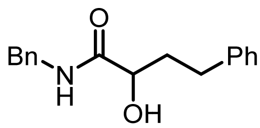
N-Benzyl-2-hydroxy-4-methylpentanamide. The title compound was synthesized according to **GP-1** from phenylmethanamine (2.14 g, 20.0 mmol) and 2-hydroxy-4-methylpentanoic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.71 g (16.8 mmol, 84% yield). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 7.2 Hz, 2H), 7.29 – 7.24 (m, 3H), 6.90 (s, 1H), 4.44 (d, *J* = 3.8 Hz, 2H), 4.19 – 4.16 (m, 1H), 2.65 (s, 1H), 1.96 – 1.78 (m, 1H), 1.72 – 1.63 (m, 1H), 1.60 – 1.50 (m, 1H), 0.96 (d, *J* = 6.0 Hz, 3H), 0.94 (d, *J* = 5.4 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 137.8, 128.6, 127.5, 127.4, 70.6, 43.7, 42.9, 24.3, 23.4, 21.3.

FT-IR (film): 3667, 3348, 2964, 1642, 1076, 698 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{13}H_{19}NNaO_2$: 244.1308, found: 244.1285.



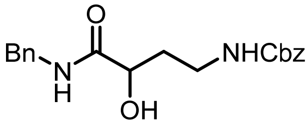
N-Benzyl-2-hydroxy-4-phenylbutanamide. The title compound was synthesized according to **GP-1** from phenylmethanamine (2.14 g, 20.0 mmol) and 2-hydroxy-4-phenylbutanoic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 4.47 g (16.6 mmol, 83% yield). White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.27 (m, 3H), 7.27 – 7.22 (m, 4H), 7.20 – 7.14 (m, 3H), 7.04 (s, 1H), 4.53 – 4.31 (m, 2H), 4.19 – 4.06 (m, 1H), 3.70 (s, 1H), 2.89 – 2.64 (m, 2H), 2.22 – 2.12 (m, 1H), 2.01 – 1.91 (m, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 141.2, 137.8, 128.7, 128.4, 127.6, 127.5, 126.0, 71.5, 43.1, 36.4, 31.2.

FT-IR (film): 3673, 2975, 1615, 1407, 1055, 698 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_2$: 292.1308, found: 292.1309.



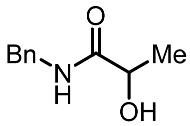
Benzyl (4-(benzylamino)-3-hydroxy-4-oxobutyl)carbamate. The title compound was synthesized according to **GP-1** from phenylmethanamine (2.14 g, 20.0 mmol) and 4-(((benzyloxy)carbonyl)amino)-2-hydroxybutanoic acid. The product was purified by column chromatography on silica gel (3:1 EtOAc/hexanes). 2.80 g (8.2 mmol, 41% yield). White solid.

^1H NMR (600 MHz, Chloroform-*d*) δ 7.38 – 7.29 (m, 7H), 7.27 – 7.22 (m, 3H), 5.40 (s, 1H), 5.08 – 5.04 (m, 2H), 4.48 – 4.37 (m, 2H), 4.13 (d, *J* = 6.5 Hz, 1H), 3.59 – 3.43 (m, 1H), 3.28 – 3.15 (m, 1H), 2.08 (td, *J* = 10.6, 4.9 Hz, 1H), 1.70 (td, *J* = 10.0, 5.0 Hz, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.5, 158.1, 137.9, 136.1, 128.6, 128.5, 128.2, 128.0, 127.6, 127.4, 68.9, 67.1, 43.0, 37.0, 35.1.

FT-IR (film): 3670, 3333, 2970, 1692, 1064 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{19}H_{23}N_2O_4$: 343.1652, found: 343.1640.



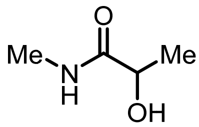
***N*-Benzyl-2-hydroxypropanamide.** The title compound was synthesized according to **GP-1** from benzylamine (2.14 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). 3.20 g (17.9 mmol, 89% yield). Yellow oil.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.26 (m, 2H), 7.25 – 7.19 (m, 3H), 4.37 (d, *J* = 5.9 Hz, 2H), 4.20 (q, *J* = 6.8 Hz, 1H), 1.38 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.1, 137.7, 128.6, 127.5, 127.4, 68.2, 42.9, 21.0.

FT-IR (film): 3672, 3253, 2970, 1616, 1252, 1080, 695 cm^{-1}.

HRMS (ESI-MS) m/z $[M+H]^+$ calcd for $C_{10}H_{14}NO_2$: 180.1019, found: 180.1025.



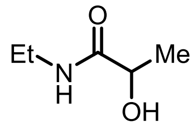
2-Hydroxy-*N*-methylpropanamide. The title compound was synthesized according to **GP-1** from methanamine solution in alcohol (2.06 g, 27%-32%, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:15 MeOH/DCM). 1.28 g (12.4 mmol, 62% yield). Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.07 (s, 1H), 4.95 (d, *J* = 4.3 Hz, 1H), 4.13 – 4.06 (m, 1H), 2.71 (d, *J* = 5.0 Hz, 3H), 1.29 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 176.1, 68.0, 25.6, 20.8.

FT-IR (film): 3672, 3317, 2978, 1643, 1532, 1072 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_4H_9NNaO_2$: 126.0525, found: 126.0529.



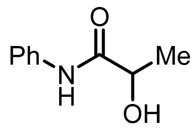
***N*-Ethyl-2-hydroxypropanamide.** The title compound was synthesized according to **GP-1** from ethanamine (0.90 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:15 MeOH/DCM). 1.76 g (15.0 mmol, 75% yield). Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.85 (s, 1H), 4.17 (s, 2H), 3.29 (qd, *J* = 7.3, 5.7 Hz, 2H), 1.40 (d, *J* = 6.3 Hz, 3H), 1.15 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 175.1, 68.1, 33.9, 21.0, 14.6.

FT-IR (film): 3670, 3316, 2976, 1642, 1533, 1073 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_5H_{12}NO_2$: 118.0863, found: 118.0870.



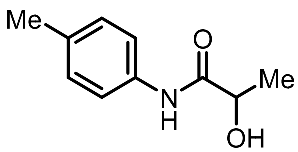
2-Hydroxy-*N*-phenylpropanamide. The title compound was synthesized according to **GP-1** from aniline (1.86 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). 2.57 g (15.6 mmol, 78% yield). Yellow oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.61 (s, 1H), 7.52 (d, *J* = 7.9 Hz, 2H), 7.32 – 7.29 (m, 2H), 7.12 (t, *J* = 7.3 Hz, 1H), 4.31 (q, *J* = 7.0 Hz, 1H), 3.88 – 3.69 (s, 1H), 1.49 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.0, 137.0, 129.0, 124.6, 119.9, 68.7, 21.0.

FT-IR (film): 3670, 3253, 2972, 1620, 1252, 1081, 696 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_9H_{12}NO_2$: 166.0863, found: 166.0869.



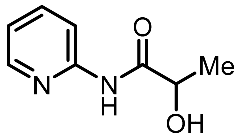
2-Hydroxy-*N*-(*p*-tolyl)propanamide. The title compound was synthesized according to **GP-1** from *p*-toluidine (1.61 g, 15.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). 2.04 g (11.4 mmol, 76% yield). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.64 (s, 1H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 4.29 (s, 1H), 4.27 (q, *J* = 6.9 Hz, 1H), 2.29 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.3, 134.33, 134.30, 129.4, 120.0, 68.5, 20.9, 20.8.

FT-IR (film): 3675, 3258, 2970, 1650, 1179, 903, 705 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{10}H_{14}NO_2$: 180.1019, found: 180.1021.



2-Hydroxy-*N*-(pyridin-2-yl)propanamide. The title compound was synthesized according to **GP-1** from pyridin-2-amine (1.88 g, 20.0 mmol) and (±)-lactic acid. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). 1.23 g (7.4 mmol, 37% yield). White solid.

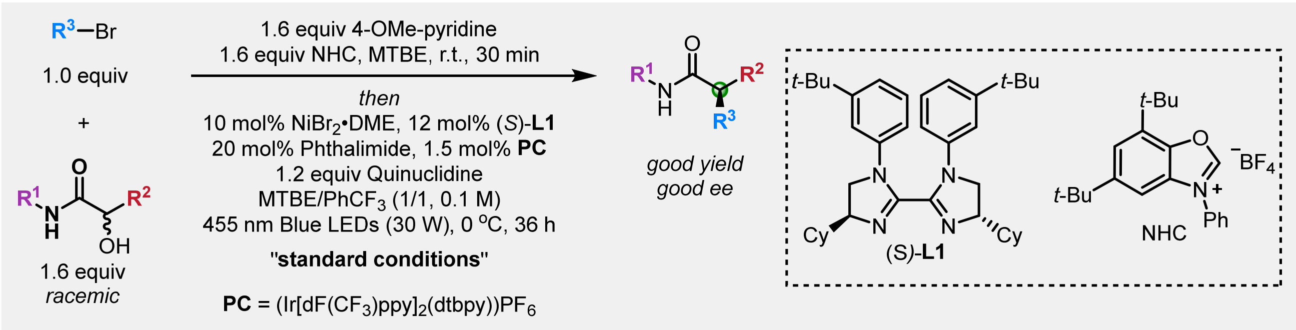
^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.66 (s, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 8.20 (d, *J* = 3.3 Hz, 1H), 7.71 (dd, *J* = 8.8, 7.6 Hz, 1H), 7.04 (dd, *J* = 7.4, 5.0 Hz, 1H), 6.38 (s, 1H), 4.42 (q, *J* = 6.8 Hz, 1H), 1.54 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.8, 150.8, 146.9, 139.0, 119.9, 114.2, 68.4, 21.0.

FT-IR (film): 3670, 3297, 2972, 1653, 1076, 823 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_8H_{11}N_2O_2$: 167.0815, found: 167.0825.

III. Catalytic Enantioconvergent Cross-Couplings



General Procedure 2 (GP-2): Enantioconvergent deoxygenative reductive cross-coupling of α-hydroxy amide and aryl bromide.

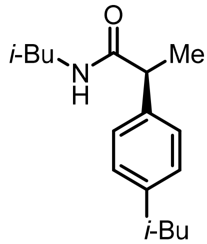
Preparation of the catalyst solution: In a nitrogen-filled glovebox, an oven-dried 4 mL vial that contained a stir bar was charged with $NiBr_2$·DME (15.5 mg, 0.051 mmol, 10.0 mol%), (*S*)-**L1** (34.0 mg, 0.060 mmol, 12.0 mol%), and Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (9.0 mg, 0.0075 mmol, 1.5 mol%). Anhydrous (trifluoromethyl)benzene (2.5 mL) was added, and the vial was capped with a PTFE septum cap. The mixture was stirred at room temperature for 30 min, leading to a crimson solution.

Preparation of the NHC-alcohol adduct solution: In a nitrogen-filled glovebox, a separate oven-dried 4 mL vial was charged with the α-hydroxy amide (0.80 mmol, 1.6 equiv), NHC (316.5 mg, 0.80 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (2.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (81.2 μL, 0.80 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution.

Cross-coupling: In a nitrogen-filled glovebox, an oven-dried 20 mL vial was charged with the aryl bromide (0.50 mmol, 1.0 equiv), quinuclidine (67 mg, 0.60 mmol, 1.2 equiv), phthalimide (14.7 mg, 0.10 mmol, 20.0 mol%), and a stir bar. The catalyst solution and NHC-alcohol adduct solution were transferred via syringe to the 20 mL reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours.

Work-up: The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel.

The racemic example was obtained by using 4,4'-di-*tert*-butyl-2,2'-bipyridine as ligand without further optimization.



(*S*)-*N*-Isobutyl-2-(4-isobutylphenyl)propanamide (1). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-isobutylpropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 110.9 mg, 85% yield, 96% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 9.2 min (major), 9.7 min (minor).

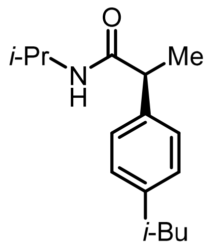
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 5.37 (s, 1H), 3.53 (q, *J* = 7.2 Hz, 1H), 3.06 – 2.94 (m, 2H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.89 – 1.80 (m, 1H), 1.69 – 1.61 (m, 1H), 1.51 (d, *J* = 7.2 Hz, 3H), 0.89 (d, *J* = 6.6 Hz, 6H), 0.77 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 140.7, 138.7, 129.6, 127.3, 46.82, 46.77, 45.0, 30.1, 28.4, 22.3, 19.8, 18.3.

FT-IR (film): 3270, 2919, 1642, 1541, 1230, 1068, 703 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{17}H_{27}NNaO$: 284.1985, found: 284.1987.

$[\alpha]^{15}_{D}$ = +6.2 (c 1.0, $CHCl_3$); 96% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-isopropylpropanamide (2). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-isopropylpropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 102.5 mg, 83% yield, 95% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.1 min (major), 11.0 min (minor).

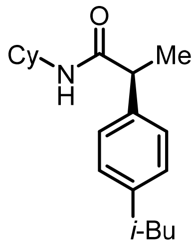
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.17 (d, *J* = 7.7 Hz, 2H), 7.10 (d, *J* = 7.8 Hz, 2H), 5.14 (s, 1H), 4.07 – 3.96 (m, 1H), 3.47 (q, *J* = 7.2 Hz, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.89 – 1.80 (m, 1H), 1.48 (d, 3H), 1.06 (d, *J* = 6.5 Hz, 3H), 1.01 (d, *J* = 6.5 Hz, 3H), 0.89 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.5, 140.5, 138.8, 129.5, 127.2, 46.8, 45.0, 41.3, 30.1, 22.6, 22.5, 22.3, 18.5.

FT-IR (film): 3314, 2973, 2916, 1637, 1534, 1228, 1058 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{16}H_{25}NNaO$: 270.1828, found: 270.1819.

$[\alpha]^{15}_D$ = +2.1 (c 1.0, $CHCl_3$); 95% ee, from (*S*)-**L1**.



(*S*)-*N*-Cyclohexyl-2-(4-isobutylphenyl)propanamide (3). The title compound was synthesized according to **GP-2** from *N*-cyclohexyl-2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 114.8 mg, 80% yield, 96% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.0 min (major), 10.6 min (minor).

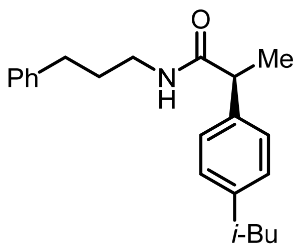
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.17 (d, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.18 (s, 1H), 3.77 – 3.67 (m, 1H), 3.48 (q, *J* = 7.2 Hz, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.88 – 1.73 (m, 3H), 1.61 – 1.51 (m, 3H), 1.49 (d, *J* = 7.2 Hz, 3H), 1.36 – 1.28 (m, 2H), 1.12 – 0.95 (m, 3H), 0.89 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.4, 140.5, 138.8, 129.5, 127.3, 48.0, 46.8, 45.0, 32.9, 32.8, 30.1, 25.5, 24.62, 24.56, 22.3, 18.5.

FT-IR (film): 3304, 2981, 2906, 1644, 1531, 1066, 772 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{19}H_{29}NNaO$: 310.2141, found: 310.2141.

$[\alpha]^{15}_D$ = +1.7 (c 1.0, $CHCl_3$); 96% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(3-phenylpropyl)propanamide (4). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(3-phenylpropyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 145.4 mg, 90% yield, 94% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 9.2 min (major), 10.8 min (minor).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.23 (m, 2H), 7.21 – 7.16 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 6.8 Hz, 2H), 5.36 (s, 1H), 3.51 (q, *J* = 7.2 Hz, 1H), 3.27 – 3.18 (m, 2H), 2.53 (t, *J*

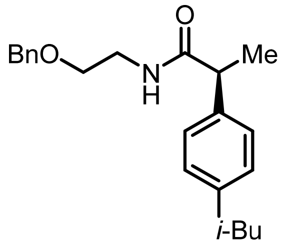
= 6.9 Hz, 2H), 2.47 (d, *J* = 7.2 Hz, 2H), 1.91 – 1.82 (m, 1H), 1.78 – 1.71 (m, 2H), 1.52 (d, *J* = 7.2 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 141.4, 140.7, 138.6, 129.6, 128.4, 128.3, 127.3, 125.9, 46.8, 45.0, 39.1, 33.1, 31.1, 30.1, 22.3, 18.3.

FT-IR (film): 3316, 2979, 2902, 1645, 1558, 1238, 1052, 699 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{22}H_{29}NNaO$: 346.2141, found: 346.2122.

$[\alpha]^{15}_{D}$ = +3.5 (c 1.0, $CHCl_3$); 94% ee, from (*S*)-**L1**.



(*S*)-*N*-(2-(Benzyloxy)ethyl)-2-(4-isobutylphenyl)propanamide (5). The title compound was synthesized according to **GP-2** from *N*-(2-(benzyloxy)ethyl)-2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 147.5 mg, 87% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 13.5 min (major), 15.0 min (minor).

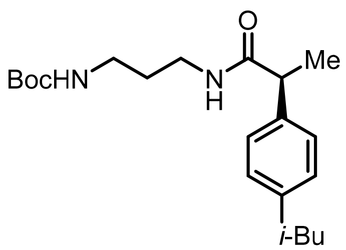
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.35 – 7.29 (m, 3H), 7.22 – 7.17 (m, 4H), 7.13 – 7.09 (m, 2H), 5.78 (s, 1H), 4.41 (s, 2H), 3.54 – 3.51 (m, 1H), 3.49 – 3.45 (m, 2H), 3.45 – 3.38 (m, 2H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.87 – 1.82 (m, 1H), 1.51 (d, *J* = 7.2 Hz, 3H), 0.89 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.4, 140.6, 138.5, 137.8, 129.5, 128.4, 127.7, 127.6, 127.3, 73.0, 68.8, 46.7, 45.0, 39.3, 30.1, 22.3, 18.4.

FT-IR (film): 3301, 2974, 2893, 1649, 1386, 1059, 700 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{22}H_{29}NNaO_2$: 362.2091, found: 362.2094.

$[\alpha]^{15}_{D}$ = –3.5 (c 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



***tert*-Butyl (*S*)-(3-(2-(4-isobutylphenyl)propanamido)propyl)carbamate (6).** The title compound was synthesized according to **GP-2** from *tert*-butyl (3-(2-hydroxypropanamido)propyl)carbamate and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). White solid, 143.0 mg, 79% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 9.1 min (major), 10.5 min (minor).

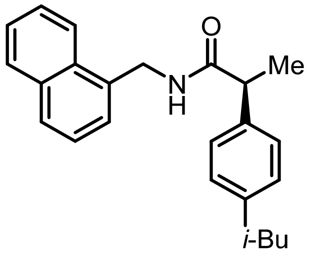
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.20 (d, *J* = 7.7 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.05 (s, 1H), 5.02 (s, 1H), 3.52 (q, *J* = 7.1 Hz, 1H), 3.21 (q, *J* = 6.3 Hz, 2H), 3.03 (q, *J* = 6.3 Hz, 2H), 2.43 (d, *J* = 7.2 Hz, 2H), 1.88 – 1.77 (m, 1H), 1.56 – 1.47 (m, 5H), 1.41 (s, 9H), 0.88 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 156.4, 140.5, 138.6, 129.5, 127.2, 79.1, 46.7, 45.0, 36.9, 36.0, 30.1, 28.3, 22.3, 18.4.

FT-IR (film): 3292, 2973, 2894, 1639, 1527, 1221, 1051, 686 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{21}H_{35}N_2O_3$: 363.2642, found: 363.2643.

$[\alpha]^{15}_D$ = +5.7 (c 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(naphthalen-1-ylmethyl)propanamide (7). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(naphthalen-1-ylmethyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 134.6 mg, 78% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 11.3 min (major), 15.9 min (minor).

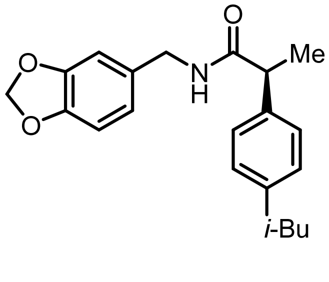
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.79 – 7.73 (m, 2H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.26 (t, *J* = 8.3 Hz, 1H), 7.18 – 7.16 (m, 1H), 7.11 – 7.07 (m, 2H), 7.00 – 6.94 (m, 2H), 5.62 (s, 1H), 4.76 (dd, *J* = 14.7, 5.5 Hz, 1H), 4.71 (dd, *J* = 14.8, 5.4 Hz, 1H), 3.46 (q, *J* = 7.1 Hz, 1H), 2.34 (d, *J* = 7.2 Hz, 2H), 1.75 – 1.71 (m, 1H), 1.45 (d, *J* = 7.1 Hz, 3H), 0.79 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.0, 140.6, 138.4, 133.7, 133.5, 131.2, 129.5, 128.6, 128.4, 127.2, 126.4, 126.1, 125.9, 125.2, 123.4, 46.7, 44.9, 41.8, 30.1, 22.3, 18.4.

FT-IR (film): 3267, 2977, 2896, 1635, 1384, 1056, 786 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+K]$^+$ calcd for $C_{24}H_{27}KNO$: 384.1724, found: 384.1722.

$[\alpha]^{15}_D$ = –4.2 (c 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-*N*-(Benzo[d][1,3]dioxol-5-ylmethyl)-2-(4-isobutylphenyl)propanamide (8). The title compound was synthesized according to **GP-2** from *N*-(benzo[d][1,3]dioxol-5-ylmethyl)-2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 149.2 mg, 88% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 17.3 min (major), 23.4 min (minor).

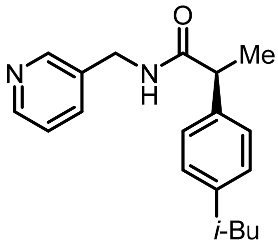
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H), 6.68 (d, *J* = 7.9 Hz, 1H), 6.63 (s, 1H), 6.60 – 6.56 (m, 1H), 5.91 (s, 2H), 5.62 (s, 1H), 4.33 – 4.22 (m, 2H), 3.55 (q, *J* = 7.2 Hz, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.89 – 1.79 (m, 1H), 1.53 (d, *J* = 7.2 Hz, 3H), 0.89 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 147.8, 146.8, 140.8, 138.4, 132.3, 129.6, 127.3, 120.6, 108.2, 108.0, 101.0, 46.8, 45.0, 43.3, 30.1, 22.3, 18.4.

FT-IR (film): 3298, 2960, 2897, 1634, 1246, 1038, 826 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{21}H_{25}NNaO_3$: 362.1727, found: 362.1719.

$[\alpha]^{15}_{D}$ = +1.1 (c 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(pyridin-3-ylmethyl)propanamide (9). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(pyridin-3-ylmethyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). Yellow oil, 102.1 mg, 69% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (40% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 14.1 min (major), 32.4 min (minor).

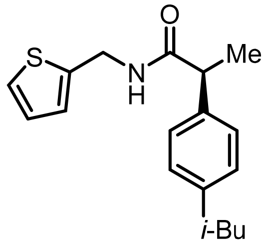
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 4.8 Hz, 1H), 8.39 (s, 1H), 7.49 – 7.44 (m, 1H), 7.20 – 7.16 (m, 3H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.87 (s, 1H), 4.38 (d, *J* = 6.0 Hz, 2H), 3.58 (q, *J* = 7.2 Hz, 1H), 2.44 (d, *J* = 7.2 Hz, 2H), 1.86 – 1.80 (m, 1H), 1.53 (d, *J* = 7.2 Hz, 3H), 0.88 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.6, 148.7, 148.6, 140.9, 138.2, 135.3, 134.1, 129.7, 127.3, 123.5, 46.6, 44.9, 40.9, 30.1, 22.3, 18.3.

FT-IR (film): 3304, 2977, 2907, 1634, 1534, 1229, 1045, 706 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{19}H_{24}N_2NaO$: 319.1781, found: 319.1775.

$[\alpha]^{15}_{D}$ = +3.6 (c 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(thiophen-2-ylmethyl)propanamide (10). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(thiophen-2-ylmethyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 106.9 mg, 71% yield, 94% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.4 min (major), 12.7 min (minor).

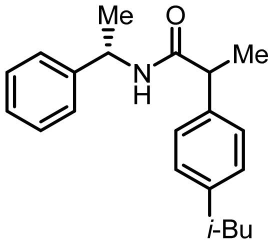
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 5.1 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.90 – 6.87 (m, 1H), 6.84 – 6.81 (m, 1H), 5.76 (s, 1H), 4.58 – 4.51 (m, 2H), 3.56 (q, *J* = 7.2 Hz, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.87 – 1.82 (m, 1H), 1.53 (d, *J* = 7.2 Hz, 3H), 0.90 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.1, 141.2, 140.8, 138.2, 129.6, 127.4, 126.7, 125.4, 124.9, 46.6, 45.0, 38.4, 30.1, 22.3, 18.3.

FT-IR (film): 3299, 2975, 2899, 1636, 1525, 1225, 1070, 686 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{18}H_{23}NNaOS$: 324.1393, found: 324.1391.

$[\alpha]^{15}_{D}$ = +37.6 (c 1.0, $CHCl_3$); 94% ee, from (*S*)-**L1**.



2-(4-Isobutylphenyl)-*N*-((*S*)-1-phenylethyl)propanamide (11, 12). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-((*S*)-1-phenylethyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil.

(*S*)-**L1**: 136.0 mg, 88% yield, 95:5 dr; (*R*)-**L1**: 132.9 mg, 86% yield, 5:95 dr.

HPLC analysis: The dr was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.8 min (major), 12.0 min (minor).

NMR data for the product from (*S*)-**L1**:

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.26 – 7.18 (m, 3H), 7.18 – 7.15 (m, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 7.09 – 7.04 (m, 2H), 5.58 (s, 1H), 5.10 – 5.04 (m, 1H), 3.56 (q, *J* = 7.2 Hz, 1H), 2.46 (d, *J* =

7.2 Hz, 2H), 1.89 – 1.82 (m, 1H), 1.51 (d, J = 7.2 Hz, 3H), 1.39 (d, J = 6.9 Hz, 3H), 0.90 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-d) δ 173.4, 143.3, 140.7, 138.6, 129.6, 128.4, 127.3, 127.0, 125.7, 48.5, 46.7, 45.0, 30.2, 22.31, 22.28, 21.9, 18.2.

NMR data for the product from (*R*)-**L1**:

^{1}H NMR (400 MHz, Chloroform-d) δ 7.35 – 7.31 (m, 1H), 7.31 – 7.28 (m, 1H), 7.28 – 7.19 (m, 5H), 7.15 (d, J = 7.9 Hz, 2H), 5.62 (s, 1H), 5.11 (p, J = 7.1 Hz, 1H), 3.55 (q, J = 7.2 Hz, 1H), 2.49 (d, J = 7.2 Hz, 2H), 1.94 – 1.84 (m, 1H), 1.53 (d, J = 7.2 Hz, 3H), 1.37 (d, J = 6.9 Hz, 3H), 0.93 (d, J = 6.6 Hz, 6H).

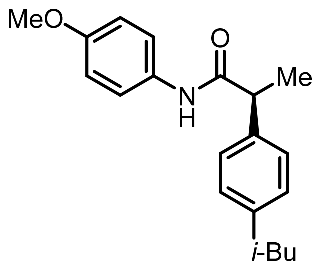
^{13}C NMR (101 MHz, Chloroform-d) δ 173.5, 143.3, 140.6, 138.6, 129.6, 128.5, 127.3, 127.2, 125.9, 48.6, 46.7, 45.0, 30.1, 22.3, 21.6, 18.4.

FT-IR (film): 3287, 2974, 2899, 1635, 1541, 1066, 696 cm^{-1}.

HRMS (ESI-MS) m/z [M+K]$^+$ calcd for $C_{21}H_{27}KNO$: 348.1724, found: 348.1723.

$[\alpha]^{15}_{D}$ = +13.1 (c 1.0, $CHCl_3$); 95:5 dr, from (*S*)-**L1**.

$[\alpha]^{15}_{D}$ = +8.2 (c 1.0, $CHCl_3$); 5:95 dr, from (*R*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(4-methoxyphenyl)propanamide (13). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(4-methoxyphenyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 144.8 mg, 93% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 11.0 min (major), 12.3 min (minor).

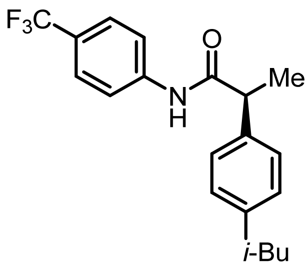
^{1}H NMR (600 MHz, Chloroform-d) δ 7.34 – 7.29 (m, 2H), 7.25 (d, J = 7.9 Hz, 2H), 7.19 – 7.16 (m, 1H), 7.13 (d, J = 7.8 Hz, 2H), 6.81 – 6.76 (m, 2H), 3.74 (s, 3H), 3.67 (q, J = 7.1 Hz, 1H), 2.46 (d, J = 7.2 Hz, 2H), 1.89 – 1.82 (m, 1H), 1.57 (d, J = 7.0 Hz, 3H), 0.90 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-d) δ 172.5, 156.2, 140.9, 138.2, 131.1, 129.7, 127.3, 121.6, 113.9, 55.4, 47.4, 45.0, 30.1, 22.3, 18.5.

FT-IR (film): 3326, 2969, 2903, 1666, 1507, 1243, 1064, 813 cm^{-1}.

HRMS (ESI-MS) m/z [M+Na]$^+$ calcd for $C_{20}H_{25}NNaO_2$: 334.1778, found: 334.1785.

$[\alpha]^{15}_{D}$ = +39.2 (c 1.0, $CHCl_3$); 92% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(4-(trifluoromethyl)phenyl)propanamide (14). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(4-(trifluoromethyl)phenyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 148.5 mg, 85% yield, 89% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IG-3 column (5% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 12.0 min (major), 17.1 min (minor).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 8.9 Hz, 2H), 7.27 – 7.24 (m, 3H), 7.17 (d, *J* = 8.1 Hz, 2H), 3.71 (q, *J* = 7.1 Hz, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 1.90 – 1.83 (m, 1H), 1.61 – 1.58 (m, 3H), 0.91 (d, *J* = 6.6 Hz, 6H).

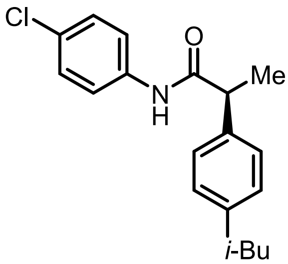
^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.9, 141.4, 140.9, 137.6, 130.0, 127.4, 126.1 (q, *J* = 3.9 Hz), 125.9 (q, *J* = 32.9 Hz), 124.0 (q, *J* = 271.6 Hz), 119.2, 47.8, 45.0, 30.1, 22.3, 18.4.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -62.1.

FT-IR (film): 3309, 2969, 2889, 1670, 1549, 1323, 1059, 833 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{20}H_{22}F_3NNaO$: 372.1546, found: 372.1538.

$[\alpha]^{15}_D$ = +26.6 (c 1.0, $CHCl_3$); 89% ee, from (*S*)-**L1**.



(*S*)-*N*-(4-Chlorophenyl)-2-(4-isobutylphenyl)propanamide (15). The title compound was synthesized according to **GP-2** from *N*-(4-chlorophenyl)-2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 142.1 mg, 90% yield, 90% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (2% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 23.7 min (major), 25.3 min (minor).

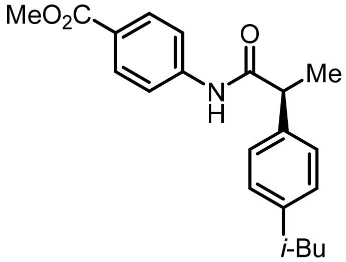
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.38 – 7.35 (m, 2H), 7.29 (s, 1H), 7.24 (d, *J* = 7.9 Hz, 2H), 7.22 – 7.19 (m, 2H), 7.15 (d, *J* = 7.8 Hz, 2H), 3.68 (q, *J* = 7.1 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 1.90 – 1.83 (m, 1H), 1.57 (d, *J* = 7.1 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.7, 141.1, 137.8, 136.5, 129.8, 129.1, 128.8, 127.3, 121.0, 47.6, 45.0, 30.1, 22.3, 18.4.

FT-IR (film): 3292, 2978, 2906, 1653, 1404, 1246, 1066, 818 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{19}H_{22}ClNNaO$: 338.1282, found: 338.1285.

$[\alpha]^{15}_{D}$ = +40.3 (c 1.0, $CHCl_3$); 90% ee, from (*S*)-**L1**.



Methyl (*S*)-4-(2-(4-isobutylphenyl)propanamido)benzoate (16). The title compound was synthesized according to **GP-2** from methyl 4-(2-hydroxypropanamido)benzoate and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 151.1mg, 89% yield, 90% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALCEL OD-3 column (10% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 7.3 min (major), 8.9 min (minor).

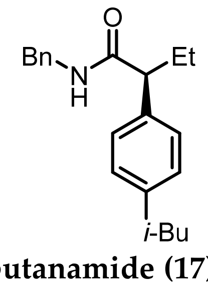
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.93 (d, 2H), 7.63 (s, 1H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.13 (d, 2H), 3.86 (s, 3H), 3.72 (q, *J* = 7.1 Hz, 1H), 2.46 (d, *J* = 7.2 Hz, 2H), 1.88 – 1.81 (m, 1H), 1.57 (d, *J* = 7.0, 1.9 Hz, 3H), 0.90 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.9, 166.6, 142.2, 141.2, 137.6, 130.6, 129.8, 127.3, 125.3, 118.7, 51.9, 47.7, 44.9, 30.1, 22.3, 18.4.

FT-IR (film): 3300, 2936, 2906, 1653, 1526, 1233, 1053, 816 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{21}H_{26}NO_3$: 340.1907, found: 340.1905.

$[\alpha]^{15}_{D}$ = +32.3 (c 1.0, $CHCl_3$); 90% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-isobutylphenyl)butanamide (17). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxybutanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 136.0 mg, 88% yield, 95% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.8 min (major), 14.5 min (minor).

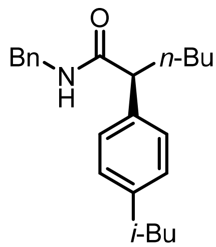
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.20 (m, 5H), 7.16 – 7.10 (m, 4H), 5.80 (s, 1H), 4.44 (dd, *J* = 15.0, 5.7 Hz, 1H), 4.37 (dd, *J* = 15.0, 5.7 Hz, 1H), 3.27 (t, *J* = 7.6 Hz, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 2.27 – 2.20 (m, 1H), 1.91 – 1.80 (m, 2H), 0.94 – 0.90 (m, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.6, 140.6, 138.4, 137.2, 129.5, 128.5, 127.7, 127.4, 127.2, 54.9, 45.0, 43.4, 30.1, 26.2, 22.3, 12.4.

FT-IR (film): 3300, 2965, 2899, 1636, 1525, 1211, 1052, 686 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{21}H_{27}NNaO$: 332.1985, found: 332.1980.

$[\alpha]^{15}_D$ = +9.6 (c 1.0, $CHCl_3$); 95% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-isobutylphenyl)hexanamide (18). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxyhexanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 118.0 mg, 70% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 8.5 min (major), 11.0 min (minor).

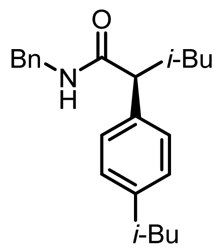
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.20 (m, 5H), 7.17 – 7.08 (m, 4H), 5.80 (s, 1H), 4.43 (dd, *J* = 15.0, 5.7 Hz, 1H), 4.37 (dd, *J* = 15.0, 5.6 Hz, 1H), 3.35 (t, *J* = 7.6 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 2.27 – 2.14 (m, 1H), 1.93 – 1.77 (m, 2H), 1.39 – 1.27 (m, 3H), 1.25 – 1.18 (m, 1H), 0.92 (d, *J* = 6.6 Hz, 6H), 0.88 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.8, 140.6, 138.4, 137.3, 129.5, 128.5, 127.6, 127.4, 127.2, 53.1, 45.0, 43.4, 32.8, 30.1, 29.9, 22.5, 22.3, 13.9.

FT-IR (film): 3285, 2967, 2916, 1645, 1558, 1240, 699 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{23}H_{32}NO$: 338.2478, found: 338.2476.

$[\alpha]^{15}_D$ = +7.7 (c 1.0, $CHCl_3$); 92% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-isobutylphenyl)-4-methylpentanamide (19). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxy-4-methylpentanamide and 1-bromo-

4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 107.9 mg, 64% yield, 87% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 7.3 min (major), 9.7 min (minor).

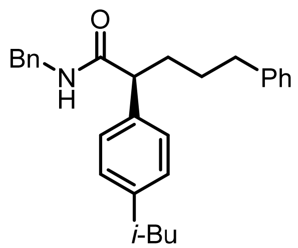
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.22 (m, 5H), 7.16 – 7.10 (m, 4H), 5.83 (s, 1H), 4.42 (dd, *J* = 15.0, 5.7 Hz, 1H), 4.36 (dd, *J* = 15.0, 5.7 Hz, 1H), 3.49 (t, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 2.10 – 2.02 (m, 1H), 1.92 – 1.83 (m, 1H), 1.81 – 1.73 (m, 1H), 1.54 – 1.46 (m, 1H), 0.92 (d, *J* = 6.7 Hz, 12H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.8, 140.6, 138.4, 137.3, 129.5, 128.5, 127.6, 127.3, 127.2, 50.8, 45.0, 43.4, 41.9, 30.1, 25.6, 22.9, 22.3, 22.0.

FT-IR (film): 3266, 2960, 2917, 1646, 1559, 1061, 680 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{23}H_{32}NO$: 338.2478, found: 338.2476.

$[\alpha]^{15}_{D}$ = +6.9 (c 1.0, $CHCl_3$); 87% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-isobutylphenyl)-5-phenylpentanamide (20). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxy-5-phenylpentanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). Yellow oil, 127.9 mg, 64% yield, 87% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (15% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 14.9 min (major), 15.6 min (minor).

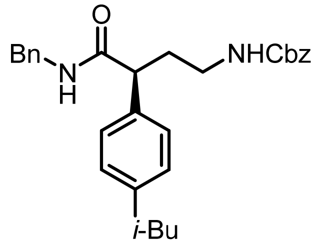
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.22 (m, 5H), 7.22 – 7.17 (m, 3H), 7.16 – 7.08 (m, 6H), 5.66 (s, 1H), 4.42 (dd, *J* = 15.0, 5.8 Hz, 1H), 4.35 (dd, *J* = 15.0, 5.7 Hz, 1H), 3.46 – 3.16 (m, 1H), 2.65 – 2.50 (m, 3H), 2.46 (d, *J* = 7.2 Hz, 2H), 2.18 – 2.08 (m, 1H), 1.90 – 1.81 (m, 1H), 0.90 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.3, 141.5, 140.8, 138.3, 136.9, 129.6, 128.6, 128.5, 128.3, 127.7, 127.4, 127.3, 125.9, 52.0, 45.0, 43.5, 34.4, 33.6, 30.2, 22.3.

FT-IR (film): 3240, 2922, 1616, 1534, 1450, 1073, 690 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{28}H_{33}NNaO$: 422.2454, found: 422.2452.

$[\alpha]^{15}_{D}$ = +6.6 (c 1.0, $CHCl_3$); 87% ee, from (*S*)-**L1**.



Benzyl (*S*)-(4-(benzylamino)-3-(4-isobutylphenyl)-4-oxobutyl)carbamate (21). The title compound was synthesized according to **GP-2** from benzyl (4-(benzylamino)-3-hydroxy-4-oxobutyl)carbamate and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). White solid, 144.3 mg, 63% yield, 88% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 17.8 min (major), 25.4 min (minor).

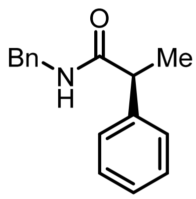
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.28 (m, 5H), 7.28 – 7.20 (m, 3H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.12 – 7.09 (m, 4H), 5.86 (s, 1H), 5.07 (s, 2H), 4.97 (s, 1H), 4.37 (d, *J* = 5.6 Hz, 2H), 3.42 (t, *J* = 7.4 Hz, 1H), 3.27 – 3.13 (m, 2H), 2.44 (d, *J* = 7.2 Hz, 2H), 2.43 – 2.35 (m, 1H), 2.03 – 1.94 (m, 1H), 1.87 – 1.79 (m, 1H), 0.89 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.2, 156.5, 141.1, 138.2, 136.6, 129.7, 128.6, 128.5, 128.1, 127.6, 127.4, 127.3, 66.6, 50.4, 45.0, 43.6, 39.6, 33.3, 30.1, 22.3.

FT-IR (film): 3670, 3333, 2922, 1695, 1616, 1534, 1450, 1068, 690 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{29}H_{35}N_2O_3$: 459.2642, found: 459.2645.

$[\alpha]^{15}_{D}$ = +2.1 (c 1.0, $CHCl_3$); 88% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-phenylpropanamide (22). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and bromobenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 101.6 mg, 85% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 11.9 min (major), 13.5 min (minor).

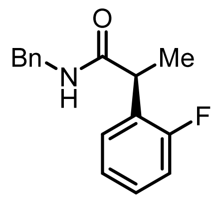
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.34 – 7.29 (m, 4H), 7.28 – 7.24 (m, 3H), 7.23 – 7.20 (m, 1H), 7.13 (d, *J* = 7.2 Hz, 2H), 5.81 (s, 1H), 4.39 (dd, *J* = 15.0, 5.8 Hz, 1H), 4.34 (dd, *J* = 15.0, 5.8 Hz, 1H), 3.59 (q, *J* = 7.2 Hz, 1H), 1.54 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.0, 141.2, 138.3, 128.8, 128.5, 127.6, 127.4, 127.3, 127.2, 47.0, 43.4, 18.5.

FT-IR (film): 3280, 2971, 1643, 1519, 1226, 1064, 701 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{16}H_{18}NO$: 240.1383, found: 240.1384.

$[\alpha]^{15}_{D}$ = +2.8 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(2-fluorophenyl)propanamide (23). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-2-fluorobenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 65.5 mg, 51% yield, 83% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.5 min (major), 12.7 min (minor).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.42 – 7.38 (m, 1H), 7.30 – 7.27 (m, 2H), 7.26 – 7.22 (m, 2H), 7.19 – 7.12 (m, 3H), 7.07 – 7.02 (m, 1H), 5.81 (s, 1H), 4.43 (dd, *J* = 14.9, 5.8 Hz, 1H), 4.38 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.92 (q, *J* = 7.1 Hz, 1H), 1.54 (d, *J* = 7.1 Hz, 3H).

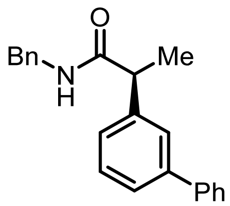
^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.0, 160.3 (d, *J* = 245.1 Hz), 138.2, 128.8, 128.7 (d, *J* = 3.5 Hz), 128.6, 128.1 (d, *J* = 14.6 Hz), 127.5, 127.4, 124.7 (d, *J* = 3.5 Hz), 115.4 (d, *J* = 22.4 Hz), 43.6, 39.2 (d, *J* = 2.6 Hz), 17.1.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -118.2.

FT-IR (film): 3285, 2916, 1649, 1544, 1455, 1222, 1005, 683 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{16}H_{17}FNO$: 258.1289, found: 258.1287.

$[\alpha]^{15}_{D}$ = +2.1 (*c* 1.0, $CHCl_3$); 83% ee, from (*S*)-**L1**.



(*S*)-2-([1,1'-Biphenyl]-3-yl)-*N*-benzylpropanamide (24). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 3-bromo-1,1'-biphenyl. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). Yellow oil, 144.9 mg, 92% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 11.6 min (major), 13.6 min (minor).

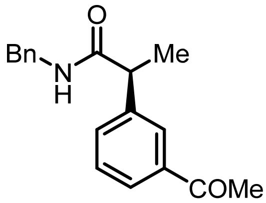
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.54 – 7.52 (m, 2H), 7.49 (s, 1H), 7.48 – 7.46 (m, 1H), 7.42 – 7.36 (m, 3H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.24 – 7.18 (m, 3H), 7.13 (d, *J* = 6.6 Hz, 2H), 5.88 (s, 1H), 4.39 – 4.33 (m, 2H), 3.64 (q, *J* = 7.1 Hz, 1H), 1.56 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.9, 141.83, 141.80, 140.7, 138.3, 129.3, 128.7, 128.5, 127.4, 127.3, 127.1, 126.5, 126.0, 47.1, 43.5, 18.6.

FT-IR (film): 3305, 2926, 1646, 1539, 1223, 1064, 689 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{22}H_{22}NO$: 316.1696, found: 316.1697.

$[\alpha]^{15}_{D}$ = +6.2 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-2-(3-Acetylphenyl)-*N*-benzylpropanamide (25). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-(3-bromophenyl)ethan-1-one. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 125.1 mg, 89% yield, 91% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 14.4 min (major), 18.9 min (minor).

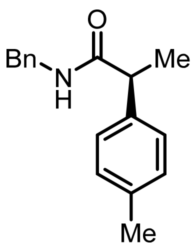
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.30 – 7.23 (m, 3H), 7.15 (d, *J* = 7.2 Hz, 2H), 5.85 (s, 1H), 4.42 (dd, *J* = 14.9, 5.8 Hz, 1H), 4.36 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.64 (q, *J* = 7.1 Hz, 1H), 2.57 (s, 3H), 1.56 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 198.0, 173.4, 142.0, 138.1, 137.5, 132.2, 129.1, 128.6, 127.5, 127.4, 127.3, 47.0, 43.6, 26.6, 18.7.

FT-IR (film): 3312, 2919, 1641, 1525, 1262, 1076, 690 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{18}H_{20}NO_2$: 282.1489, found: 282.1489.

$[\alpha]^{15}_{D}$ = +6.7 (*c* 1.0, $CHCl_3$); 91% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(*p*-tolyl)propanamide (26). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-methylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 94.9 mg, 75% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 12.6 min (major), 15.4 min (minor).

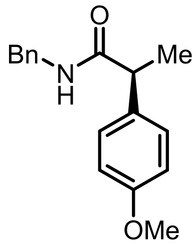
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29 – 7.26 (m, 2H), 7.24 – 7.21 (m, 1H), 7.19 (d, *J* = 7.8 Hz, 2H), 7.14 – 7.13 (m, 4H), 5.70 (s, 1H), 4.40 (dd, *J* = 15.0, 5.8 Hz, 1H), 4.34 (dd, *J* = 15.0, 5.7 Hz, 1H), 3.56 (q, *J* = 7.2 Hz, 1H), 2.32 (s, 3H), 1.53 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.3, 138.3, 138.2, 136.9, 129.6, 128.5, 127.5, 127.4, 127.3, 46.7, 43.5, 21.0, 18.5.

FT-IR (film): 3307, 2980, 2921, 1641, 1542, 1226, 1069, 691 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{17}H_{20}NO$: 254.1539, found: 254.1529.

$[\alpha]^{15}_{D}$ = +1.5 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-methoxyphenyl)propanamide (27). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-methoxybenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 86.1 mg, 64% yield, 94% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 19.1 min (major), 22.2 min (minor).

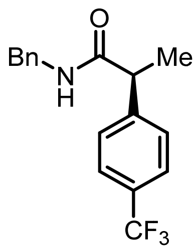
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 2H), 7.24 – 7.19 (m, 3H), 7.14 (d, *J* = 7.2 Hz, 2H), 6.86 (d, *J* =8.4 Hz, 2H), 5.72 (s, 1H), 4.39 (dd, *J* = 14.9, 5.8 Hz, 1H), 4.35 (dd, *J* = 15.0, 5.8 Hz, 1H), 3.78 (s, 3H), 3.55 (q, *J* = 7.2 Hz, 1H), 1.52 (d, *J* = 7.8 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.4, 158.7, 138.3, 133.2, 128.7, 128.6, 127.4, 127.3, 114.3, 55.2, 46.2, 43.5, 18.6.

FT-IR (film): 3332, 2985, 2891, 1634, 1381, 1233, 1063 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_2$: 292.1308, found: 292.1307.

$[\alpha]^{15}_{D}$ = –0.8 (*c* 1.0, $CHCl_3$); 94% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-(trifluoromethyl)phenyl)propanamide (28). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-(trifluoromethyl)benzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 142.8 mg, 93% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 6.3 min (major), 7.0 min (minor).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.24 (m, 3H), 7.18 – 7.11 (m, 2H), 5.86 (s, 1H), 4.41 (dd, *J* = 14.9, 5.8 Hz, 1H), 4.35 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.62 (q, *J* = 7.1 Hz, 1H), 1.54 (d, *J* = 7.1 Hz, 3H).

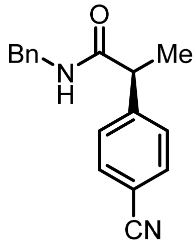
^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.0, 145.3, 138.0, 129.5 (q, *J* = 32.8 Hz), 128.7, 127.9, 127.52, 127.50, 125.7 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 272.1 Hz), 47.0, 43.7, 18.7.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -62.5.

FT-IR (film): 3297, 2916, 1635, 1513, 1324, 1176, 1101, 682 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^{+}$ calcd for $C_{17}H_{17}F_3NO$: 308.1257, found: 308.1254.

$[\alpha]^{15}_{D}$ = –1.4 (*c* 1.0, $CHCl_3$); 92% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-cyanophenyl)propanamide (29). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 4-bromobenzonitrile. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 112.2 mg, 85% yield, 90% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 22.5 min (major), 24.0 min (minor).

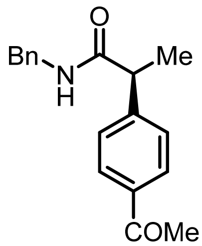
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.51 – 7.47 (m, 2H), 7.36 – 7.33 (m, 2H), 7.23 – 7.16 (m, 3H), 7.10 – 7.04 (m, 2H), 6.04 (s, 1H), 4.32 (dd, *J* = 14.8, 5.7 Hz, 1H), 4.26 (dd, *J* = 14.8, 5.6 Hz, 1H), 3.53 (q, *J* = 7.1 Hz, 1H), 1.44 (d, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.6, 146.7, 137.9, 132.4, 128.6, 128.3, 127.49, 127.47, 118.6, 110.9, 47.0, 43.6, 18.6.

FT-IR (film): 3278, 2924, 2877, 2220, 1647, 1233, 1103, 698 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^{+}$ calcd for $C_{17}H_{17}N_2O$: 265.1335, found: 265.1332.

$[\alpha]^{15}_{D}$ = –4.1 (*c* 1.0, $CHCl_3$); 90% ee, from (*S*)-**L1**.



(*S*)-2-(4-Acetylphenyl)-*N*-benzylpropanamide (30). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-(4-bromophenyl)ethan-1-one. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 130.7 mg, 93% yield, 94% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALCEL OD-3 column (15% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 16.1 min (major), 18.7 min (minor).

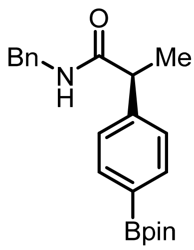
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.31 – 7.23 (m, 3H), 7.18 – 7.13 (m, 2H), 5.90 (s, 1H), 4.42 (dd, *J* = 14.8, 5.5 Hz, 1H), 4.36 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.65 (q, *J* = 7.1 Hz, 1H), 2.57 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.6, 173.0, 146.7, 138.0, 136.1, 128.9, 128.6, 127. 8, 127.5, 127.4, 47.1, 43.7, 26.5, 18.6.

FT-IR (film): 3291, 2926, 1638, 1537, 1263, 1069, 701 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^{+}$ calcd for $C_{18}H_{19}NNaO_2$: 304.1308, found: 304.1308.

$[\alpha]^{15}_{D}$ = –7.1 (*c* 1.0, $CHCl_3$); 94% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)propanamide (31). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 2-(4-bromophenyl)-4,4,5-trimethyl-1,3,2-dioxaborolane. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). Yellow oil, 157.0 mg, 86% yield, 94% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 9.2 min (major), 10.5 min (minor).

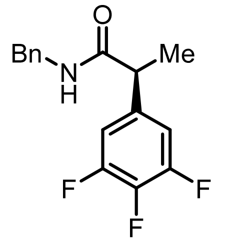
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.25 – 7.21 (m, 1H), 7.14 (d, *J* = 7.2 Hz, 2H), 5.60 (s, 1H), 4.40 (dd, *J* = 15.0, 5.8 Hz, 1H), 4.35 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.61 (q, *J* = 7.1 Hz, 1H), 1.55 (d, *J* = 7.2 Hz, 3H), 1.34 (s, 12H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.7, 144.4, 138.2, 135.4, 128.6, 127.5, 127.4, 127.1, 83.8, 47.4, 43.6, 24.84, 24.82, 18.4.

FT-IR (film): 3315, 2988, 2899, 1653, 1364, 1097, 860, 637 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^{+}$ calcd for $C_{22}H_{29}BNO_3$: 366.2235, found: 366.2229.

$[\alpha]^{15}_{D}$ = –1.3 (*c* 1.0, $CHCl_3$); 94% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(3,4,5-trifluorophenyl)propanamide (32). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 5-bromo-1,2,3-trifluorobenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 123.1 mg, 84% yield, 91% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 5.8 min (major), 6.5 min (minor).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.33 – 7.28 (m, 2H), 7.28 – 7.24 (m, 1H), 7.20 – 7.14 (m, 2H), 7.00 – 6.88 (m, 2H), 5.99 (s, 1H), 4.40 (dd, *J* = 14.8, 5.8 Hz, 1H), 4.34 (dd, *J* = 14.8, 5.6 Hz, 1H), 3.46 (q, *J* = 7.1 Hz, 1H), 1.47 (d, *J* = 7.1 Hz, 3H).

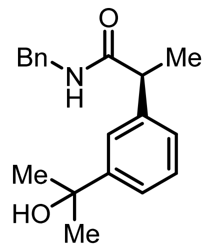
^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.6, 151.2 (d, *J* = 246.1 Hz), 138.8 (d, *J* = 251.3 Hz), 137.8, 137.4, 128.7, 127.62, 127.57, 111.6 (dd, *J* = 16.9, 4.7 Hz), 46.3, 43.7, 18.7.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -133.7, -133.8, -162.3.

FT-IR (film): 3309, 2994, 2908, 1646, 1533, 1238, 1044, 702 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{16}H_{15}F_3NO$: 294.1100, found: 294.1090.

$[\alpha]^{15}_{D}$ = –2.6 (*c* 1.0, $CHCl_3$); 91% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(3-(2-hydroxypropan-2-yl)phenyl)propanamide (33). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 2-(3-bromophenyl)propan-2-ol. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). Yellow oil, 98.0 mg, 66% yield, 91% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.7 min (minor), 18.2 min (major).

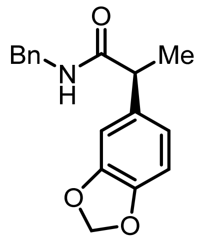
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.30 – 7.20 (m, 5H), 7.13 (d, *J* = 6.0 Hz, 2H), 5.86 (s, 1H), 4.39 (dd, *J* = 14.9, 5.8 Hz, 1H), 4.32 (dd, *J* = 15.0, 5.8 Hz, 1H), 3.58 (q, *J* = 7.2 Hz, 1H), 1.55 (s, 6H), 1.52 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 148.2, 139.5, 138.3, 128.5, 127.4, 127.2, 124.9, 72.2, 46.6, 43.4, 31.7, 31.4, 18.5.

FT-IR (film): 3296, 2971, 2923, 1643, 1532, 1235, 704 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{19}H_{24}NO_2$: 298.1802, found: 298.1801.

$[\alpha]^{15}_D$ = –5.1 (*c* 1.0, $CHCl_3$); 91% ee, from (*S*)-**L1**.



(*S*)-2-(Benzo[*d*][1,3]dioxol-5-yl)-*N*-benzylpropanamide (34). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 5-bromobenzo[*d*][1,3]dioxole. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). White solid, 100.5 mg, 71% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 20.6 min (major), 26.2 min (minor).

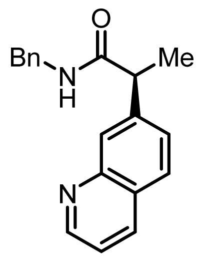
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 2H), 7.24 – 7.21 (m, 1H), 7.15 (d, *J* = 7.2 Hz, 2H), 6.80 (s, 1H), 6.75 – 6.70 (m, 2H), 5.92 (s, 2H), 5.80 (s, 1H), 4.39 (dd, *J* = 14.9, 5.9 Hz, 1H), 4.33 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.50 (q, *J* = 7.2 Hz, 1H), 1.49 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.1, 148.0, 146.7, 138.3, 135.0, 128.6, 127.4, 127.3, 120.8, 108.4, 107.9, 101.0, 46.7, 43.5, 18.6.

FT-IR (film): 3287, 2971, 1646, 1489, 1220, 1046, 944, 687 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{17}H_{18}NO_3$: 284.1281, found: 284.1279.

$[\alpha]^{15}_D$ = –4.7 (*c* 1.0, $CHCl_3$); 92% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(quinolin-7-yl)propanamide (35). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 7-bromoquinoline. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). White solid, 123.3 mg, 85% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 17.1 min (major), 21.5 min (minor).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.84 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.98 (s, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.57 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.37 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.25 –

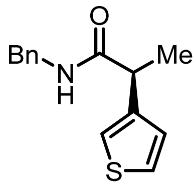
7.21 (m, 2H), 7.21 – 7.16 (m, 1H), 7.13 (d, J = 7.0 Hz, 2H), 6.10 (t, J = 5.9 Hz, 1H), 4.41 (dd, J = 14.9, 5.9 Hz, 1H), 4.34 (dd, J = 14.9, 5.8 Hz, 1H), 3.82 (q, J = 7.1 Hz, 1H), 1.63 (d, J = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.4, 150.5, 148.0, 143.0, 138.1, 136.0, 128.5, 128.4, 127.6, 127.5, 127.33, 127.29, 126.4, 121.0, 47.2, 43.6, 18.4.

FT-IR (film): 3270, 2919, 1642, 1541, 1230, 1068, 703 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{19}H_{19}N_2O$: 291.1492, found: 291.1473.

$[\alpha]^{15}_{D}$ = –0.9 (*c* 1.0, $CHCl_3$); 92% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(thiophen-3-yl)propanamide (36). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 3-bromothiophene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 95.6 mg, 78% yield, 87% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 12.0 min (major), 13.4 min (minor).

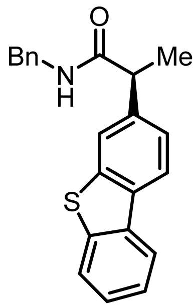
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.25 (m, 4H), 7.20 – 7.13 (m, 3H), 7.06 (d, J = 5.0 Hz, 1H), 5.83 (s, 1H), 4.41 (d, J = 5.8 Hz, 2H), 3.75 (q, J = 7.2 Hz, 1H), 1.58 (d, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.8, 141.6, 138.3, 128.6, 127.4, 127.3, 127.0, 126.5, 121.5, 43.5, 42.6, 18.4.

FT-IR (film): 3322, 2979, 2920, 1652, 1524, 1237, 1074, 683 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{14}H_{16}NOS$: 246.0947, found: 246.0947.

$[\alpha]^{15}_{D}$ = –4.0 (*c* 1.0, $CHCl_3$); 87% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(dibenzo[*b,d*]thiophen-3-yl)propanamide (37). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 3-bromodibenzo[*b,d*]thiophene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 151.8 mg, 88% yield, 91% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 14.0 min (major), 16.1 min (minor).

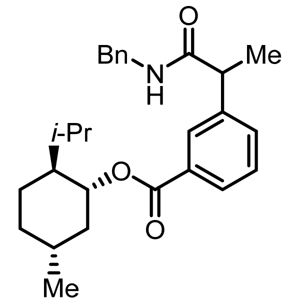
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 – 8.10 (m, 2H), 7.91 – 7.80 (m, 2H), 7.53 – 7.46 (m, 2H), 7.45 – 7.41 (m, 1H), 7.32 – 7.23 (m, 3H), 7.22 – 7.14 (m, 2H), 5.94 (s, 1H), 4.46 (dd, *J* = 14.8, 5.7 Hz, 1H), 4.40 (dd, *J* = 14.9, 5.8 Hz, 1H), 3.80 (q, *J* = 7.2 Hz, 1H), 1.68 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 139.8, 138.3, 138.2, 137.8, 136.0, 135.1, 128.5, 127.4, 127.3, 126.9, 126.4, 124.4, 123.1, 122.8, 121.6, 120.5, 47.0, 43.6, 19.0.

FT-IR (film): 3283, 2969, 1630, 1539, 1230, 1077, 686 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{22}H_{20}NOS$: 346.1260, found: 346.1258.

$[\alpha]^{15}_{D}$ = –11.8 (*c* 1.0, $CHCl_3$); 91% ee, from (*S*)-**L1**.



(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 3-(1-(benzylamino)-1-oxopropan-2-yl) benzoate (38, 39). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and (1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 3-bromobenzoate. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). White solid.

(*S*)-**L1**: 168.4 mg, 80% yield, 95:5 dr; (*R*)-**L1**: 162.1 mg, 77% yield, 5:95 dr.

HPLC analysis: The dr was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 9.3 min (major), 11.3 min (minor).

NMR data for the product from (*S*)-**L1**:

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.02 – 7.89 (m, 2H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.43 – 7.37 (m, 1H), 7.29 – 7.21 (m, 3H), 7.15 (d, *J* = 7.0 Hz, 2H), 5.87 (s, 1H), 4.97 – 4.90 (m, 1H), 4.41 (dd, *J* = 14.9, 5.8 Hz, 1H), 4.36 (dd, *J* = 14.9, 5.8 Hz, 1H), 3.64 (q, *J* = 7.1 Hz, 1H), 2.12 – 2.07 (m, 1H), 1.97 – 1.90 (m, 1H), 1.76 – 1.70 (m, 2H), 1.59 – 1.53 (m, 5H), 1.17 – 1.07 (m, 2H), 0.96 – 0.90 (m, 7H), 0.79 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.5, 165.8, 141.6, 138.1, 131.8, 131.3, 128.9, 128.8, 128.6, 128.4, 127.5, 127.3, 75.0, 47.1, 46.9, 43.6, 40.9, 34.2, 31.4, 26.5, 23.6, 22.0, 20.7, 18.6, 16.5.

NMR data for the product from (*R*)-**L1**:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.91 (m, 2H), 7.60 – 7.54 (m, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.32 – 7.22 (m, 3H), 7.20 – 7.12 (m, 2H), 5.80 (s, 1H), 5.00 – 4.91 (m, 1H), 4.45 (dd, *J* = 14.9, 5.7 Hz, 1H), 4.37 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.66 (q, *J* = 7.1 Hz, 1H), 2.15 – 2.08 (m, 1H), 1.99 – 1.90 (m, 1H), 1.79 – 1.70 (m, 2H), 1.61 – 1.54 (m, 5H), 1.19 – 1.06 (m, 2H), 0.99 – 0.89 (m, 7H), 0.81 (d, *J* = 6.9 Hz, 3H).

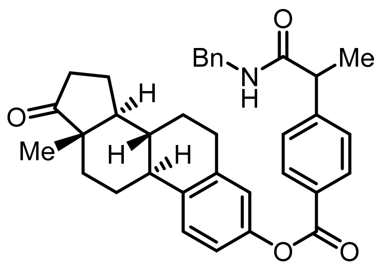
^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.4, 165.8, 141.7, 138.1, 131.8, 131.3, 128.93, 128.87, 128.6, 128.4, 127.5, 127.4, 75.0, 47.2, 47.0, 43.6, 40.9, 34.3, 31.4, 26.5, 23.6, 22.0, 20.7, 18.6, 16.5.

FT-IR (film): 3300, 2956, 1705, 1657, 1541, 1451, 1275, 687 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{27}H_{36}NO_3$: 422.2690, found: 422.2680.

$[\alpha]^{15}_D$ = +36.5 (*c* 1.0, $CHCl_3$); 95:5 dr, from (*S*)-**L1**.

$[\alpha]^{15}_D$ = +46.0 (*c* 1.0, $CHCl_3$); 5:95 dr, from (*R*)-**L1**.



(8*R*,9*S*,13*S*,14*S*)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a] phenanthren-3-yl 4-(1-(benzylamino)-1-oxopropan-2-yl)benzoate (40, 41). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and (8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a] phenanthren-3-yl 4-bromobenzoate. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). White solid.

(*S*)-**L1**: 205.9 mg, 77% yield, 93:7 dr; (*R*)-**L1**: 192.6 mg, 72% yield, 8:92 dr.

HPLC analysis: The dr was determined via HPLC on a CHIRALPAK AD-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 19.6 min (major), 21.8 min (minor).

NMR data for the product from (*S*)-**L1**:

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 1H), 7.32 – 7.26 (m, 3H), 7.21 – 7.13 (m, 2H), 7.01 – 6.94 (m, 2H), 5.96 (s, 1H), 4.43 (dd, 1H), 4.38 (dd, *J* = 14.8, 5.6 Hz, 1H), 3.68 (q, *J* = 7.1 Hz, 1H), 2.98 – 2.91 (m, 2H), 2.51 (dd, *J* = 18.6, 8.7 Hz, 1H), 2.43 (dd, *J* = 13.0, 4.3 Hz, 1H), 2.36 – 2.29 (m, 1H), 2.16 (q, *J* = 9.2 Hz, 1H), 2.09 – 2.00 (m, 2H), 2.00 – 1.94 (m, 1H), 1.69 – 1.62 (m, 2H), 1.59 (d, *J* = 7.3 Hz, 3H), 1.57 – 1.54 (m, 1H), 1.54 – 1.44 (m, 3H), 0.93 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.0, 165.2, 148.8, 147.3, 138.2, 138.1, 137.5, 130.7, 128.7, 128.6, 127.9, 127.8, 127.6, 127.5, 126.5, 121.7, 118.9, 50.5, 48.0, 47.2, 44.2, 43.7, 38.0, 35.9, 31.6, 29.4, 26.4, 25.8, 21.6, 18.7, 13.9.

NMR data for the product from (*R*)-**L1**:

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.11 (d, *J* = 7.9 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.29 – 7.22 (m, 3H), 7.15 (d, *J* = 7.6 Hz, 2H), 6.98 – 6.90 (m, 2H), 6.11 (s, 1H), 4.39 (dd, *J* = 14.9, 5.7 Hz, 1H), 4.35 (dd, *J* = 14.9, 5.7 Hz, 1H), 3.66 (q, *J* = 7.1 Hz, 1H), 2.96 – 2.88 (m, 2H), 2.48 (dd, *J* = 19.0, 8.7 Hz, 1H), 2.41 (dd, *J* = 13.5, 3.6 Hz, 1H), 2.32 – 2.25 (m, 1H), 2.16 – 2.08

(m, 1H), 2.07 – 1.99 (m, 2H), 1.96 – 1.92 (m, 1H), 1.65 – 1.58 (m, 2H), 1.55 (d, *J* = 7.2 Hz, 3H), 1.53 – 1.51 (m, 1H), 1.51 – 1.40 (m, 3H), 0.90 (s, 3H).

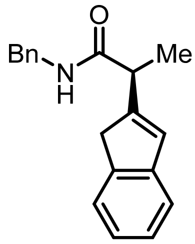
^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.0, 165.0, 148.7, 147.3, 138.1, 138.0, 137.4, 130.5, 128.6, 128.5, 127.7, 127.4, 127.3, 126.3, 121.5, 118.7, 50.3, 47.8, 47.0, 44.0, 43.6, 37.9, 35.7, 31.5, 29.3, 26.2, 25.7, 21.5, 18.6, 13.7.

FT-IR (film): 3296, 2975, 2914, 1739, 1254, 1066, 691 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{35}H_{38}NO_4$: 536.2795, found: 536.2786.

$[\alpha]^{15}_{D}$ = +52.0 (*c* 1.0, $CHCl_3$); 93:7 dr, from (*S*)-**L1**.

$[\alpha]^{15}_{D}$ = +36.7 (*c* 1.0, $CHCl_3$); 8:92 dr, from (*R*)-**L1**.



(*S*)-*N*-Benzyl-2-(1*H*-inden-2-yl)propanamide (42). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 2-bromo-1*H*-indene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 90.1 mg, 65% yield, 90% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 13.6 min (major), 19.1 min (minor).

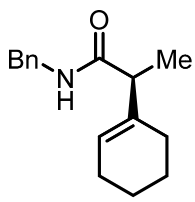
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.24 (t, *J* = 7.2 Hz, 2H), 7.20 (d, *J* = 6.6 Hz, 2H), 7.18 – 7.13 (m, 1H), 6.71 (s, 1H), 5.93 (s, 1H), 4.40 (d, *J* = 5.8 Hz, 2H), 3.55 (q, *J* = 7.1 Hz, 1H), 3.43 (dd, *J* = 22.8, 1.6 Hz, 1H), 3.35 (dd, *J* = 22.6, 1.6 Hz, 1H), 1.51 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.3, 148.6, 144.3, 143.1, 138.2, 128.7, 128.6, 127.6, 127.4, 126.4, 124.6, 123.7, 120.6, 43.61, 43.58, 39.5, 17.3.

FT-IR (film): 3295, 2919, 1644, 1528, 1215, 754, 701 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{19}H_{20}NO$: 278.1539, found: 278.1538.

$[\alpha]^{15}_{D}$ = –5.9 (*c* 1.0, $CHCl_3$); 90% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(cyclohex-1-en-1-yl)propanamide (43). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-bromocyclohex-1-

ene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 87.5 mg, 72% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 31.2 min (major), 33.4 min (minor).

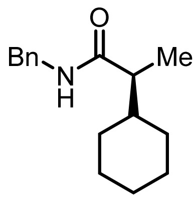
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.29 (m, 2H), 7.28 – 7.21 (m, 3H), 5.99 (s, 1H), 5.64 (s, 1H), 4.46 (dd, *J* = 14.9, 5.9 Hz, 1H), 4.39 (dd, *J* = 14.9, 5.7 Hz, 1H), 2.95 (q, *J* = 7.1 Hz, 1H), 2.06 – 1.96 (m, 3H), 1.93 – 1.84 (m, 1H), 1.64 – 1.50 (m, 4H), 1.27 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 138.7, 138.1, 128.7, 127.5, 127.4, 124.5, 49.0, 43.5, 26.2, 25.3, 22.8, 22.3, 15.2.

FT-IR (film): 3292, 2927, 1646, 1549, 1448, 1222, 691 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{16}H_{22}NO$: 244.1696, found: 244.1699.

$[\alpha]^{15}_{D}$ = +12.1 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-cyclohexylpropanamide (44). An oven-dried 10 mL Schlenk tube was charged with a magnetic stir bar, (*S*)-*N*-benzyl-2-(cyclohex-1-en-1-yl)propanamide (**43**, 93% ee, 24.3 mg, 0.10 mmol, 1.0 equiv), Pd/C (2.43 mg, 10% w/w), and then it was sealed with a rubber septum cap. The flask was placed under a H_2 atmosphere by evacuating and backfilling the tube (three cycles), followed by the addition of MeOH (1.0 mL). The reaction mixture was stirred at 80 °C for 24 h and then cooled down to room temperature. The reaction mixture was filtered through Celite and the filtrate was concentrated in vacuo. The residue was then purified by column chromatography on silica gel (1:8 EtOAc/hexanes) to afford the desired product. White solid, 22.1 mg, 90% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK AD-3 column (5% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 8.3 min (major), 9.2 min (minor).

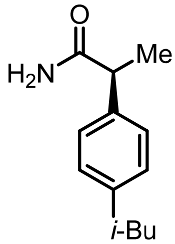
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.31 (m, 2H), 7.30 – 7.25 (m, 3H), 5.73 – 5.60 (m, 1H), 4.45 (d, *J* = 5.5 Hz, 2H), 1.98 – 1.89 (m, 1H), 1.84 – 1.77 (m, 1H), 1.74 – 1.61 (m, 4H), 1.60 – 1.51 (m, 1H), 1.31 – 1.19 (m, 3H), 1.13 (d, *J* = 6.9 Hz, 3H), 1.03 – 0.94 (m, 1H), 0.91 – 0.84 (m, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.1, 138.5, 128.7, 127.8, 127.4, 47.8, 43.4, 40.9, 31.5, 30.0, 26.4, 26.2, 15.0.

FT-IR (film): 3300, 2925, 1711, 1610, 1433, 1107, 701 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{16}H_{24}NO$: 246.1852, found: 246.1861.

$[\alpha]^{15}_{D}$ = +95.5 (*c* 0.1, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(S)-2-(4-Isobutylphenyl)propanamide (45). The title compound was synthesized according to **GP-2** from 2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (2:1 EtOAc/hexanes). White solid, 77.9 mg, 76% yield, 80% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (S)-**L1**: 8.4 min (major), 10.2 min (minor).

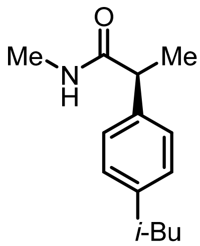
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.21 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 7.8 Hz, 2H), 5.55 (s, 1H), 5.32 (s, 1H), 3.57 (q, J = 7.2 Hz, 1H), 2.45 (d, J = 7.2 Hz, 2H), 1.90 – 1.80 (m, 1H), 1.51 (d, J = 7.2 Hz, 3H), 0.90 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 177.2, 140.8, 138.4, 129.6, 127.3, 46.2, 44.9, 30.1, 22.3, 18.2.

FT-IR (film): 3343, 3200, 2979, 2892, 1638, 1401, 1063, 688 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{13}H_{20}NO$: 206.1539, found: 206.1538.

$[\alpha]^{15}_{D}$ = +4.6 (c 1.0, $CHCl_3$); 80% ee, from (S)-**L1**.



(S)-2-(4-Isobutylphenyl)-*N*-methylpropanamide (46). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-methylpropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). Yellow oil, 90.9 mg, 83% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (S)-**L1**: 6.8 min (major), 7.9 min (minor).

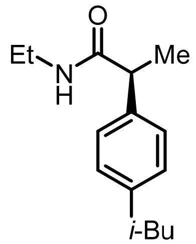
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.18 (d, J = 8.2 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 5.55 (s, 1H), 3.52 (q, J = 7.2 Hz, 1H), 2.72 (d, J = 4.8 Hz, 3H), 2.44 (d, J = 7.2 Hz, 2H), 1.89 – 1.80 (m, 1H), 1.50 (d, J = 7.2 Hz, 3H), 0.89 (d, J = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.1, 140.7, 138.6, 129.6, 127.4, 46.7, 45.0, 30.2, 26.5, 22.4, 18.5.

FT-IR (film): 3285, 2970, 1630, 1530, 1219, 1053, 693 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{14}H_{21}NNaO$: 242.1515, found: 242.1517.

$[\alpha]^{15}_{D}$ = +14.1 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-*N*-Ethyl-2-(4-isobutylphenyl)propanamide (47). The title compound was synthesized according to **GP-2** from *N*-ethyl-2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). Yellow oil, 99.0 mg, 85% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 12.0 min (major), 13.6 min (minor).

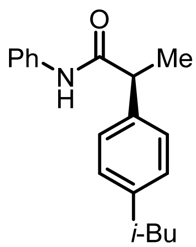
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.18 (d, *J* = 7.9 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 5.36 (s, 1H), 3.50 (q, *J* = 7.2 Hz, 1H), 3.27 – 3.15 (m, 2H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.89 – 1.81 (m, 1H), 1.50 (d, *J* = 7.2 Hz, 3H), 1.03 (t, *J* = 7.2 Hz, 3H), 0.90 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 140.6, 138.7, 129.5, 127.3, 46.7, 45.0, 34.4, 30.1, 22.3, 18.5, 14.7.

FT-IR (film): 3317, 2977, 2905, 1641, 1538, 1237, 1065, 683 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+K]^+$ calcd for $C_{15}H_{23}KNO$: 272.1411, found: 272.1420.

$[\alpha]^{15}_{D}$ = +5.4 (c 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-phenylpropanamide (48). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-phenylpropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 120.8 mg, 86% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 5.9 min (major), 6.5 min (minor).

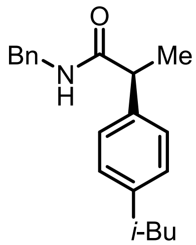
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.22 (m, 4H), 7.14 (d, *J* = 7.7 Hz, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 7.02 (s, 1H), 3.67 (q, *J* = 7.2 Hz, 1H), 2.46 (d, *J* = 7.2 Hz, 2H), 1.88 – 1.81 (m, 1H), 1.57 (d, *J* = 7.2 Hz, 3H), 0.89 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.5, 141.1, 138.0, 137.9, 129.9, 128.9, 127.4, 124.1, 119.6, 47.8, 45.0, 30.2, 22.4, 18.5.

FT-IR (film): 3296, 2970, 2904, 1659, 1435, 1249, 1065, 750 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^{+}$ calcd for $C_{19}H_{23}NNaO$: 304.1672, found: 304.1666.

$[\alpha]^{15}_{D}$ = +7.5 (c 1.0, $CHCl_3$); 92% ee, from (*S*)-**L1**.



(*S*)-*N*-Benzyl-2-(4-isobutylphenyl)propanamide (49). The title compound was synthesized according to **GP-2** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 122.4 mg, 83% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 9.6 min (major), 12.3 min (minor).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.24 (m, 3H), 7.24 – 7.21 (m, 2H), 7.17 – 7.10 (m, 4H), 5.67 (s, 1H), 4.41 (d, *J* = 5.8 Hz, 2H), 3.60 (q, *J* = 7.2 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 1.92 – 1.82 (m, 1H), 1.57 (d, *J* = 7.2 Hz, 3H), 0.92 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 140.8, 138.5, 138.4, 129.6, 128.6, 127.34, 127.28, 46.8, 45.0, 43.5, 30.1, 22.3, 18.4.

FT-IR (film): 3310, 2969, 2903, 1645, 1538, 1231, 1069, 690 cm^{-1}.

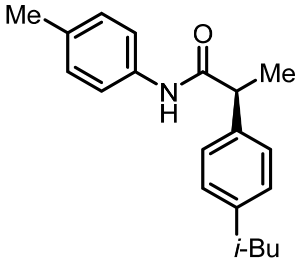
HRMS (ESI-MS) *m/z* [M+Na]$^{+}$ calcd for $C_{20}H_{25}NNaO$: 318.1828, found: 318.1828.

$[\alpha]^{15}_{D}$ = +4.2 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.

Gram-scale reaction: In the air, $NiBr_2$·glyme (217.0 mg, 0.71 mmol, 10.0 mol%), Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (126.0 mg, 0.105 mmol, 1.5 mol%), and (*S*)-**L1** (476.0 mg, 0.84 mmol, 12.0 mol%) were added to an oven-dried 50 mL round-bottom flask equipped with a stir bar. The flask was closed with a rubber septum cap and the flask was placed under a nitrogen atmosphere by evacuating and back-filling the flask (three cycles). A balloon filled with nitrogen was attached to the reaction flask. Anhydrous (trifluoromethyl)benzene (35 mL) was added to the flask, and the mixture was stirred at room temperature for 30 min, at which time it was a crimson solution. In the air, an oven-dried 100 mL flask was charged with benzyl *N*-benzyl-2-hydroxypropanamide (2.0 g, 11.2 mmol, 1.6 equiv), NHC (4.43 g, 11.2 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (35 mL) was added, and the reaction was stirred at room temperature for 10 min. Next, 4-methoxypyridine (1.14 mL, 11.2 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution. In the air, a separate oven-dried 100 mL flask was charged with 1-bromo-4-isobutylbenzene (1.48

g, 7.0 mmol, 1.0 equiv), quinuclidine (0.94 g, 8.4 mmol, 1.2 equiv), phthalimide (203.0 mg, 1.4 mmol, 20.0 mol%), and a stir bar. The catalyst solution and NHC-alcohol adduct solution were transferred via syringe to this 100 mL reaction flask. The reaction mixture was stirred at 0 °C in an EtOH cooling bath for 10 min before being irradiated with blue LEDs (455 nm, 30 W). The reaction was stirred under irradiation at 0 °C for 48 hours. Next, the reaction mixture was passed through a column of silica gel (5 cm), and the flask, the septum, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid.

(*S*)-**L1**: 1.75 g, 85% yield, 92% ee.



(*S*)-2-(4-Isobutylphenyl)-*N*-(*p*-tolyl)propanamide (50). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(*p*-tolyl)propanamide and 1-bromo-4-isobutylbenzene. The product was purified by column chromatography on silica gel (1:5 EtOAc/hexanes). White solid, 134.2 mg, 91% yield, 93% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 7.7 min (major), 9.1 min (minor).

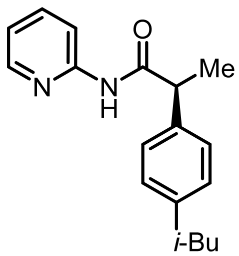
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.20 (s, 1H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.05 (d, *J* = 8.3 Hz, 2H), 3.67 (q, *J* = 7.2 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 2.27 (s, 3H), 1.89 – 1.83 (m, 1H), 1.57 (d, *J* = 7.2 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.5, 140.9, 138.2, 135.4, 133.7, 129.7, 129.3, 127.4, 119.7, 47.6, 45.0, 30.1, 22.3, 20.8, 18.5.

FT-IR (film): 3300, 2961, 2926, 1657, 1513, 1251, 813 cm^{-1}.

HRMS (ESI-MS) *m*/*z* $[M+H]^+$ calcd for $C_{20}H_{26}NO$: 296.2009, found: 296.2003.

$[\alpha]^{15}_D$ = +45.0 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-2-(4-Isobutylphenyl)-*N*-(pyridin-2-yl)propanamide (51). The title compound was synthesized according to **GP-2** from 2-hydroxy-*N*-(pyridin-2-yl)propanamide and 1-bromo-4-

isobutylbenzene. The product was purified by column chromatography on silica gel (1:1 EtOAc/hexanes). White solid, 38.1 mg, 27% yield, 90% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 5.9 min (minor), 6.5 min (major).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.02 (s, 1H), 7.73 – 7.67 (m, 1H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.03 – 6.98 (m, 1H), 3.72 (q, *J* = 7.1 Hz, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.93 – 1.84 (m, 1H), 1.59 (d, *J* = 7.1 Hz, 3H), 0.90 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.0, 151.3, 147.2, 141.2, 138.7, 137.5, 129.9, 127.4, 119.6, 113.9, 48.0, 45.0, 30.1, 22.4, 18.4.

FT-IR (film): 3300, 2981, 2911, 1655, 1214, 835, 690 cm^{-1}.

HRMS (ESI-MS) *m*/*z* [M+H]$^+$ calcd for $C_{18}H_{23}N_2O$: 283.1805, found: 283.1802.

$[\alpha]^{15}_D$ = +16.4 (*c* 1.0, $CHCl_3$); 90% ee, from (*S*)-**L1**.

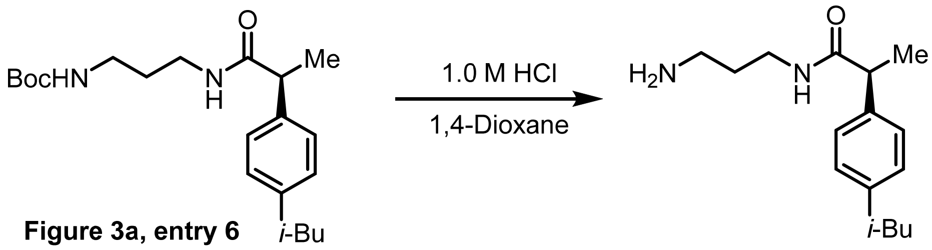


Figure 3a, entry 6

(*S*)-*N*-(3-Aminopropyl)-2-(4-isobutylphenyl)propanamide (52). In a nitrogen-filled glovebox, an oven-dried 4 mL vial that contained a stir bar was charged with *tert*-butyl (*S*)-(3-(2-(4-isobutylphenyl)propanamido)propyl)carbamate (**6**, 93% ee, 72.4 mg, 0.20 mmol, 1.0 equiv), 1.0 M aqueous HCl (1.0 mL, 1.0 mmol, 5.0 equiv), and 1,4-Dioxane (2.0 mL). The vial was transferred out of the glovebox and stirred at 40 °C for 24 h. It was then cooled down to room temperature. The reaction mixture was filtered through Celite and the filtrate was concentrated in vacuo. The residue was then purified by column chromatography on silica gel (1:5 MeOH/DCM) to afford the desired product. White solid, 45.6 mg, 87% yield, 93% ee (the ee value was determined under the assumption that this process would not cause racemization).

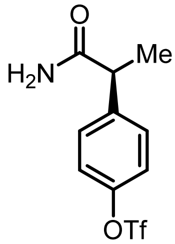
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.17 (d, *J* = 8.2 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.20 (s, 1H), 3.50 (q, *J* = 7.2 Hz, 1H), 3.30 – 3.24 (m, 2H), 2.64 (t, *J* = 6.4 Hz, 2H), 2.43 (d, *J* = 7.3 Hz, 2H), 1.86 – 1.79 (m, 1H), 1.53 – 1.49 (m, 2H), 1.48 (d, *J* = 7.2 Hz, 3H), 1.37 (s, 2H), 0.87 (d, *J* = 6.5 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.5, 140.5, 138.7, 129.4, 127.3, 46.7, 44.9, 39.8, 37.8, 32.2, 30.1, 22.3, 18.4.

FT-IR (film): 2922, 2851, 1676, 1489, 1451, 1214, 983, 835, 749, 690 cm^{-1}.

HRMS (ESI-MS) *m*/*z* [M+H]$^+$ calcd for $C_{16}H_{27}N_2O$: 263.2118, found: 263.2115.

$[\alpha]^{15}_D$ = +6.6 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.



(*S*)-4-(1-Amino-1-oxopropan-2-yl)phenyl trifluoromethanesulfonate (53). The title compound was synthesized according to **GP-2** from 2-hydroxypropanamide and 4-bromophenyl trifluoromethanesulfonate. The product was purified by column chromatography on silica gel (3:1 EtOAc/hexanes). White solid, 104.0 mg, 70% yield, 84% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 7.9 min (major), 8.5 min (minor).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, 8.8 Hz, 2H), 7.21 (d, *J* = 8.7 Hz, 2H), 6.24 (s, 1H), 5.63 (s, 1H), 3.61 (q, *J* = 7.1 Hz, 1H), 1.48 (d, *J* = 7.1 Hz, 3H).

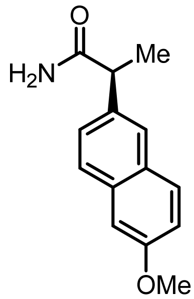
^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.0, 148.5, 141.7, 129.3, 121.6, 118.6 (q, *J* = 322.0 Hz), 45.8, 18.6.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -72.9.

FT-IR (film): 3419, 3183, 1655, 1426, 1215, 1144, 891, 616 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{10}H_{11}F_3NO_4S$: 298.0355, found: 298.0351.

$[\alpha]^{15}_{D}$ = +32.9 (c 1.0, $CHCl_3$); 84% ee, from (*S*)-**L1**.



(*S*)-2-(6-Methoxynaphthalen-2-yl)propanamide (54). The title compound was synthesized according to **GP-2** from 2-hydroxypropanamide and 2-bromo-6-methoxynaphthalene. The product was purified by column chromatography on silica gel (5:1 EtOAc/hexanes). White solid, 84.7 mg, 74% yield, 80% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (40% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 14.8 min (major), 16.4 min (minor).

^{1}H NMR (400 MHz, Methanol-*d*$_4$) δ 7.72 – 7.58 (m, 3H), 7.36 (d, *J* = 8.6 Hz, 1H), 7.12 (d, *J* = 2.5 Hz, 1H), 7.06 – 6.97 (m, 1H), 3.81 (s, 3H), 3.72 (q, *J* = 7.1 Hz, 1H), 1.44 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Methanol-*d*$_4$) δ 179.9, 158.9, 137.9, 135.0, 130.2, 130.0, 127.9, 127.0, 126.6, 119.7, 106.4, 55.5, 46.8, 18.6.

FT-IR (film): 3343, 3163, 2990, 1628, 1382, 1250, 1017, 819 cm^{-1}.

HRMS (ESI-MS) *m/z* $[M+H]^+$ calcd for $C_{14}H_{16}NO_2$: 230.1176, found: 230.1173.
$[\alpha]^{15}_{D}$ = +19.0 (c 1.0, $CHCl_3$); 80% ee, from (*S*)-**L1**.

IV. Effect of Reaction Parameters

General Procedure 3 (GP-3).

Preparation of the catalyst solution: In a nitrogen-filled glovebox, an oven-dried 4 mL vial that contained a stir bar was charged with $NiBr_2$·DME (3.1 mg, 0.010 mmol, 10.0 mol%), (*S*)-**L1** (6.8 mg, 0.012 mmol, 12.0 mol%), and Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (1.8 mg, 0.0015 mmol, 1.5 mol%). Anhydrous (trifluoromethyl)benzene (0.5 mL) was added, and the vial was capped with a PTFE septum cap. The mixture was stirred at room temperature for 30 min, leading to a crimson solution.

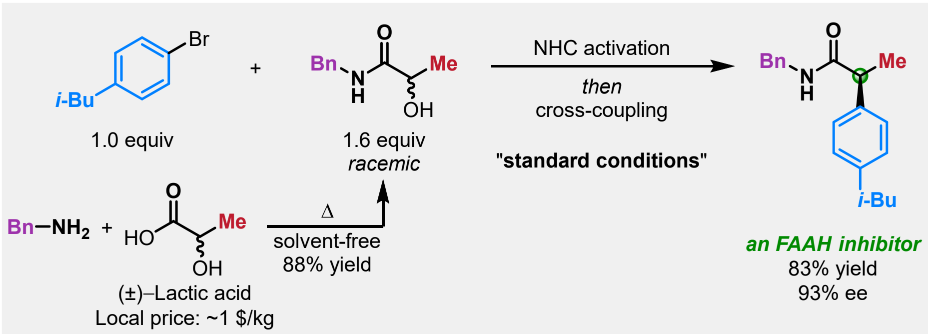
Preparation of the NHC-alcohol adduct solution: In a nitrogen-filled glovebox, a separate oven-dried 4 mL vial was charged with α-hydroxy amide (0.16 mmol, 1.6 equiv), NHC (63.3 mg, 0.16 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (0.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (16.3 μL, 0.16 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution.

Cross-coupling: In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with the aryl bromide (0.10 mmol, 1.0 equiv), quinuclidine (13.4 mg, 0.12 mmol, 1.2 equiv), phthalimide (2.9 mg, 0.020 mmol, 20.0 mol%), and a stir bar. The catalyst solution and NHC-alcohol adduct solution were transferred via syringe to the 4 mL reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours.

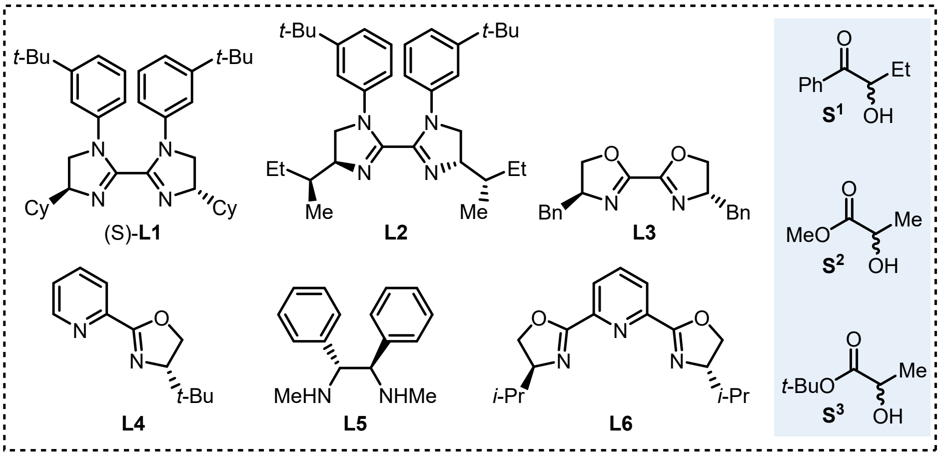
Work-up: The reaction was stopped by ending the irradiation. The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel.

Figure S2: *N*-Benzyl-2-hydroxypropanamide was reacted with 1-bromo-4-isobutylbenzene according to **GP-3**.

Figure S2. Effect of reaction parameters

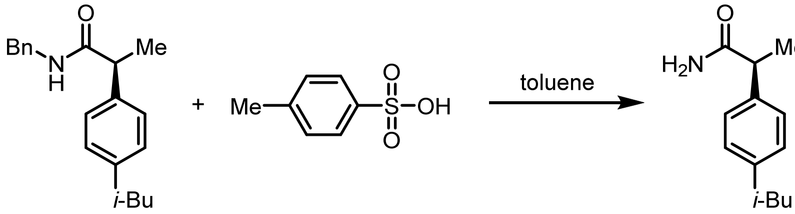


entry	variation from the "**standard conditions**"	yield (%)[a]	ee (%)[b]
1	None	83	93
2	No Ni, photocatalyst, quinuclidine, or light	0	–
3	No (*S*)-**L1**	11	0
4	No phthalimide	67	73
5	**L2**, instead of (*S*)-**L1**	81	89
6	**L3**, instead of (*S*)-**L1**	13	46
7	**L4**, instead of (*S*)-**L1**	37	-33
8	**L5**, instead of (*S*)-**L1**	0	–
9	**L6**, instead of (*S*)-**L1**	0	–
10	THF, instead of MTBE	18	85
11	*m*-Xylene, instead of $PhCF_3$	80	92
12	Pure MTBE	60	89
13	Pure $PhCF_3$	67	92
14	NaOAc, instead of quinuclidine	8	72
15	Pyridine, instead of 4-OMe-pyridine	78	92
16	5 mol% $NiBr_2$•DME, 6 mol% (*S*)-**L1**	70	93
17	18 h, instead of 36 h	67	93
18	r.t., instead of 0 °C	80	87
19	0.05 M, instead of 0.1 M	79	92
20	1.4 equiv of NHC, alkyl alcohol, and 4-OMe-pyridine	78	93
21	1.2 equiv of NHC, alkyl alcohol, and 4-OMe-pyridine	67	93
22	1.0 equiv of NHC, alkyl alcohol, and 4-OMe-pyridine	52	93
23	1.0 mL air added (4 mL vial)	75	93
24	3.0 mL air added	10	92
25	0.1 equiv H_2O added	33	93
26	$\mathbf{S^1}$ or $\mathbf{S^3}$, instead of α-hydroxy amide	0	–
27	$\mathbf{S^2}$, instead of α-hydroxy amide	31	22



[a]Isolated yield. [b]Determined through HPLC analysis.

V. Applications

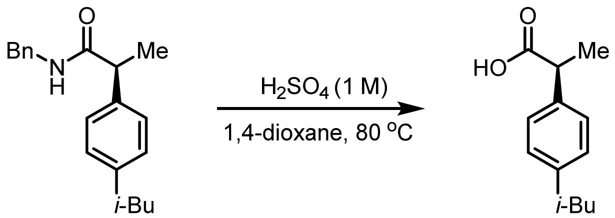


49, 92% ee **45**, 76% yield, 92% ee

(*S*)-2-(4-Isobutylphenyl)propanamide (45). In a nitrogen-filled glovebox, a 10 mL Schlenk tube was equipped with a magnetic stir bar, (*S*)-*N*-benzyl-2-(4-isobutylphenyl)propanamide (**49**, 92% ee, 29.5 mg, 0.10 mmol, 1.0 equiv), 4-methylbenzenesulfonic acid (68.9 mg, 0.40 mmol, 4.0 equiv), and toluene (1 mL), and the vial was capped with a PTFE septum cap. The Schlenk tube was transferred out of the glovebox, and the reaction mixture was stirred at 50 °C for 8 h. Then, the mixture was allowed to warm to 100 °C and stirred for another 16 h. Upon completion, saturated $NaHCO_3$ aqueous solution (5 mL) was added, and the aqueous phase was extracted with EtOAc (3 x 5 mL). The combined organic layers were concentrated, and the residue was purified by flash chromatography (2:1 EtOAc/hexanes) to afford the desired product. White solid, 15.6 mg, 76% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IG-3 column (10% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 25.3 min (major), 28.7 min (minor).

$[\alpha]^{15}_{D}$ = +6.5 (c 0.2, $CHCl_3$); 92% ee, from (*S*)-**L1**.



49, 92% ee **55**, 84% yield, 92% ee

(*S*)-2-(4-Isobutylphenyl)propanoic acid (55). A solution of (*S*)-*N*-benzyl-2-(4-isobutylphenyl)propanamide (**49**, 92% ee, 29.5 mg, 0.10 mmol, 1.0 equiv), 1 M aqueous H_2SO_4 (1.0 mL), and 1,4-dioxane (2.0 mL) was stirred at 80 °C for 12 h. After the reaction was completed, the reaction mixture was cooled down to room temperature. The mixture was extracted with CH_2Cl_2 (3 x 10 mL). The organic layer was dried over sodium sulfate, filtered, and concentrated. The residue was then purified by column chromatography on silica gel (1:1 EtOAc/hexanes) to give the desired product. White solid, 17.3 mg, 84% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (10% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 10.2 min (major), 11.3 min (minor).

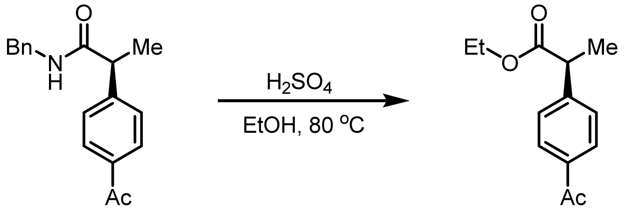
^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.71 (s, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 3.75 (q, *J* = 7.1 Hz, 1H), 2.50 (d, *J* = 7.1 Hz, 2H), 1.95 – 1.84 (m, 1H), 1.54 (d, *J* = 7.2 Hz, 3H), 0.95 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.2, 140.8, 136.9, 129.4, 127.3, 45.03, 44.98, 30.1, 22.4, 18.1.

FT-IR (film): 2989, 2905, 1717, 1418, 1233, 1069, 782 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{13}H_{19}O_2$: 207.1380, found: 207.1368.

$[\alpha]^{15}_D$ = +53.6 (c 0.2, $CHCl_3$); 92% ee, from (*S*)-**L1**.



30, 94% ee

56, 63% yield, 94% ee

Ethyl (*S*)-2-(4-acetylphenyl)propanoate (56). A solution of (*S*)-2-(4-acetylphenyl)-*N*-benzylpropanamide (**30**, 94% ee, 28.1 mg, 0.10 mmol, 1.0 equiv), 1 M aqueous H_2SO_4 (1.0 mL), and EtOH (2.0 mL) was stirred at 80 °C for 12 h. After the reaction was completed, the reaction mixture was cooled down to room temperature. The mixture was extracted with CH_2Cl_2 (3 x 5 mL). The organic layer was dried over sodium sulfate, filtered, and concentrated. The residue was then purified by column chromatography on silica gel (1:10 EtOAc/hexanes) to afford the desired product. Yellow oil, 13.9 mg, 63% yield, 94% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALCEL OD-3 column (5% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 15.7 min (minor), 18.3 min (major).

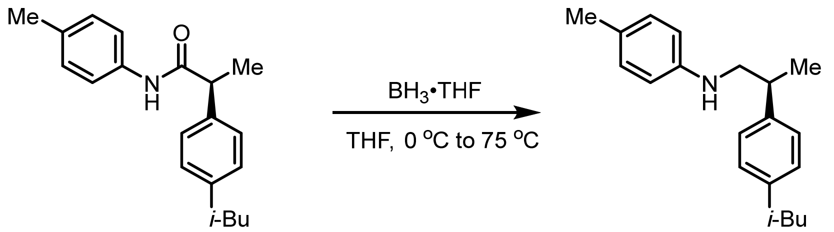
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 4.17 – 4.08 (m, 2H), 3.76 (q, *J* = 7.2 Hz, 1H), 2.58 (s, 3H), 1.51 (d, *J* = 7.1 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.6, 173.7, 146.0, 136.0, 128.7, 127.7, 60.9, 45.6, 26.5, 18.4, 14.0.

FT-IR (film): 2925, 2851, 1758, 1711, 1610, 1433, 1276, 1193, 1107, 731 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{13}H_{17}O_3$: 221.1172, found: 221.1172.

$[\alpha]^{15}_D$ = +11.4 (*c* 0.1, $CHCl_3$); 94% ee, from (*S*)-**L1**.



50, 93% ee　　　　**57**, 85% yield, 92% ee

(*S*)-*N*-(2-(4-Isobutylphenyl)propyl)-4-methylaniline (57). A solution of methyl (*S*)-2-(4-isobutylphenyl)-*N*-(*p*-tolyl)propanamide (**50**, 29.5 mg, 0.10 mmol, 1.0 equiv) in anhydrous THF (2 mL) was placed into a 10 mL round bottom flask under N_2 atmosphere. The mixture was cooled to 0 °C and a solution of BH_3•THF (1.0 M, 1.0 mL, 1.0 mmol, 10 equiv) was then slowly added over 5 min. The reaction mixture was allowed to gradually warm up to room temperature and then stirred at 75 °C for 12 hours. The reaction was quenched upon the addition of MeOH (1.0 mL) and the solvent was removed on the rotary evaporator. The residue was added an aqueous solution of HCl (2 M, 4 mL) and stirred at 75 °C for 1 hour. The reaction was quenched by adding a saturated solution of K_2CO_3 and extracted with EtOAc (3 x 5 mL). The organic layers were combined, dried over $MgSO_4$, and filtered. The solvent was removed on the rotary evaporator and the residue was further purified by flash column chromatography (1:5 EtOAc/hexanes) to afford the desired product. White solid, 23.9 mg, 85% yield, 92% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALCEL OD-3 column (100% hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 5.3 min (major), 5.9 min (minor).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.13 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.1 Hz, 2H), 6.51 (d, *J* = 8.4 Hz, 2H), 3.47 (s, 1H), 3.30 (dd, *J* = 12.2, 6.2 Hz, 1H), 3.20 (dd, *J* = 12.2, 8.2 Hz, 1H), 3.06 – 2.99 (m, 1H), 2.46 (d, *J* = 7.2 Hz, 2H), 2.24 (s, 3H), 1.89 – 1.83 (m, 1H), 1.32 (d, *J* = 6.9 Hz, 3H), 0.92 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.9, 141.7, 139.9, 129.7, 129.3, 126.9, 126.5, 113.2, 51.4, 45.0, 38.8, 30.2, 22.4, 20.3, 19.8.

FT-IR (film): 2922, 2854, 1513, 1451, 1030, 817, 698 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{20}H_{27}NNa$: 304.2036, found: 304.2040.

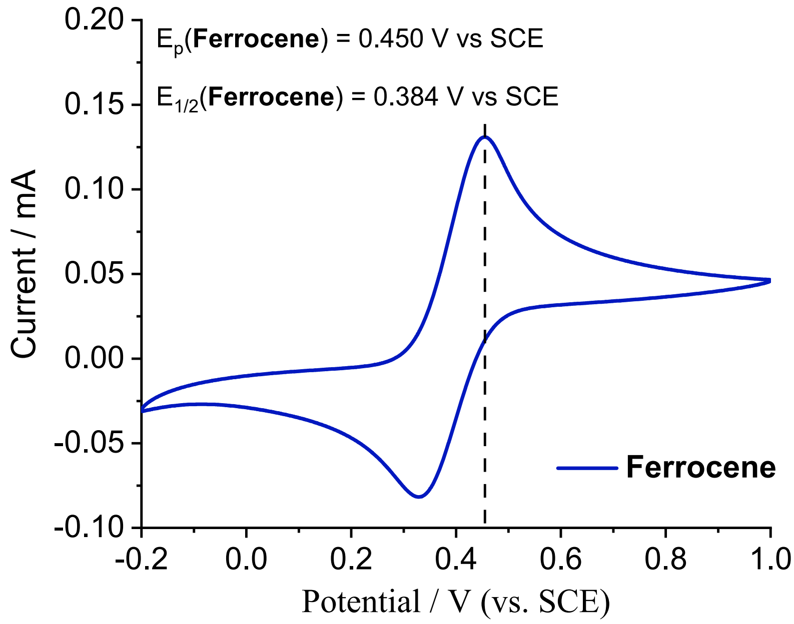
$[\alpha]^{26}_D$ = +36.2 (*c* 0.1, $CHCl_3$); 92% ee, from (*S*)-**L1**.

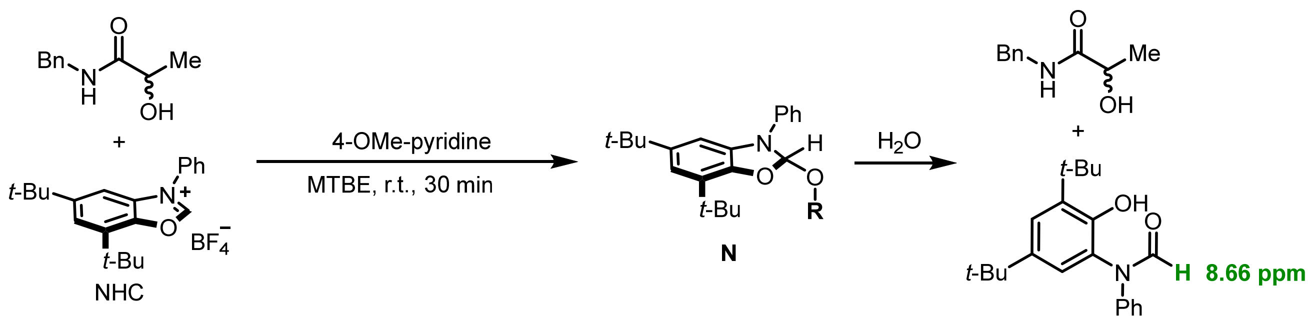
VI. Mechanistic Experiments

1. Cyclic voltammograms profiles.

Cyclic voltammogram of ferrocene. Cyclic voltammograms were collected with a CorrTest CS2350M electrochemical workstation. Samples were prepared by mixing 0.050 mmol of ferrocene (9.3 mg) in 10 mL of 0.1 M *n*-Bu_4NPF_6 (387.4 mg, 1.0 mmol) in anhydrous MeCN. Measurements employed a glassy carbon working electrode, platinum wire counter electrode, saturated calomel electrode (SCE) reference electrode, and a scan rate of 100 mV/s. The glassy carbon electrode was polished between each scan. The samples were sparged with N_2 for at least 15 minutes prior to data collection.

Figure S3. Cyclic voltammogram of ferrocene



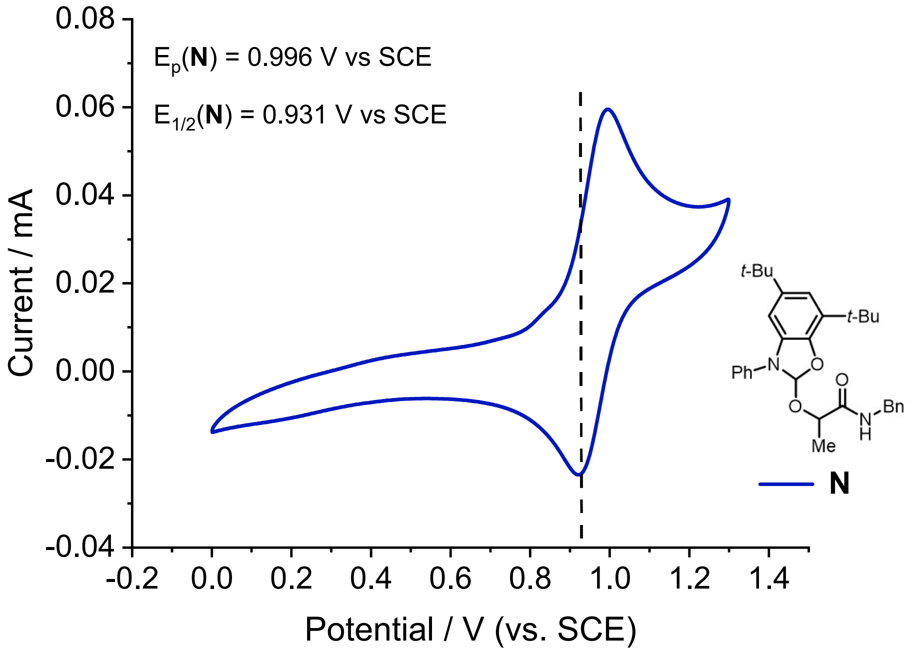


Preparation of the NHC-alcohol adduct (N) solution. In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with *N*-benzyl-2-hydroxypropanamide (17.9 mg, 0.10 mmol, 1.0 equiv), NHC (39.6 mg, 0.10 mmol, 1.0 equiv), and a stir bar. MTBE (1.0 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (10.2 μL, 0.10 mmol, 1.0 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution.

Note: *The solution of* **N** *was treated with water for 30 minutes, leading to the production of alkyl alcohol and amide. The concentration of* **N** *was determined by* ^{1}*H NMR analysis of the amide using 1,2-dibromoethane as the internal standard. The concentration of* **N** *is 0.067 M.*

Cyclic voltammogram of NHC-alcohol adduct (N). Cyclic voltammograms were collected with a CorrTest CS2350M electrochemical workstation. Samples were prepared by mixing 0.030 mmol of **N** in 10 mL of 0.1 M n-Bu_4NPF_6 (387.4 mg, 1.0 mmol) in anhydrous MeCN. Measurements employed a glassy carbon working electrode, platinum wire counter electrode, saturated calomel electrode (SCE) reference electrode, and a scan rate of 100 mV/s. The glassy carbon electrode was polished between each scan. The samples were sparged with N_2 for at least 15 minutes prior to data collection.

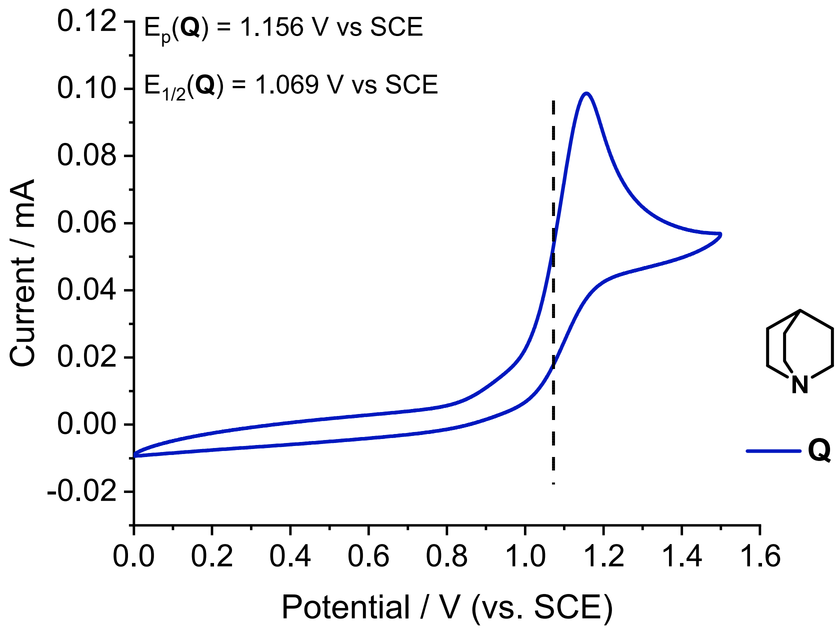
Figure S4. Cyclic voltammogram of **N**



Cyclic voltammogram of quinuclidine (Q). Cyclic voltammograms were collected with a CorrTest CS2350M electrochemical workstation. Samples were prepared by mixing 0.030 mmol of quinuclidine (3.3 mg) in 10 mL of 0.1 M n-Bu_4NPF_6 (387.4 mg, 1.0 mmol) in anhydrous MeCN. Measurements employed a glassy carbon working electrode, platinum wire counter electrode, saturated calomel electrode (SCE) reference electrode, and a scan rate of 100 mV/s.

The glassy carbon electrode was polished between each scan. The samples were sparged with N_2 for at least 15 minutes prior to data collection.

Figure S5. Cyclic voltammogram of **Q**

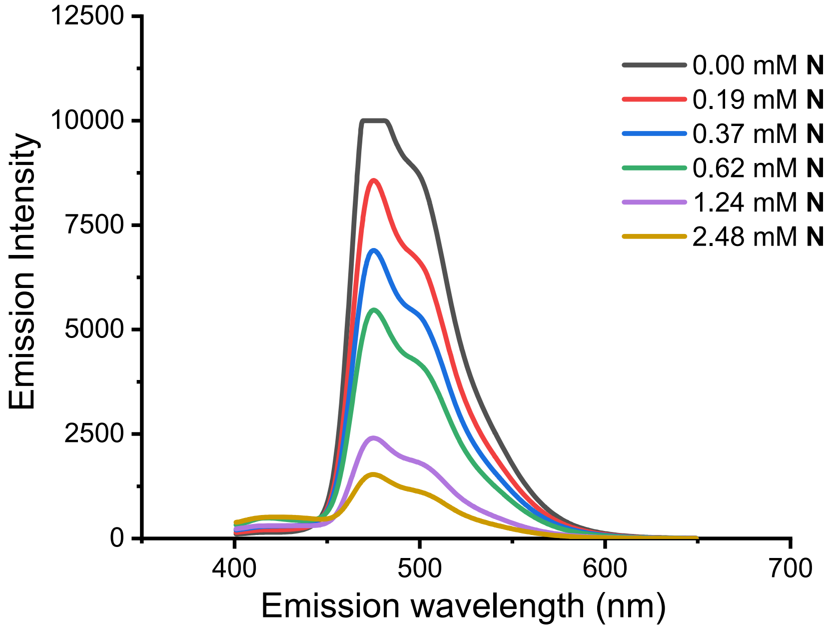


2. Stern–Volmer luminescence quenching studies.

The fluorescence quenching experiments were carried out in degassed MTBE: $PhCF_3$(1:1) at room temperature upon excitation by 455 nm light.

Emission quenching of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 as a function of concentration of NHC-alcohol adduct. A 1.0×10^{-3} M solution of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 (11.2 mg, 0.010 mmol) in anhydrous degassed MTBE:$PhCF_3$ (1:1, 10 mL) and a 1.24×10^{-2} M solution of **N** in anhydrous degassed MTBE:$PhCF_3$ (1:1) were prepared in a nitrogen filled glovebox. To six sample vials were added 20 uL of 1.0×10^{-3} M solution of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 and 0 uL, 30 uL, 60 uL, 100 uL, 200 uL, and 400 uL of 1.24×10^{-2} M solution of **N**. Anhydrous degassed MTBE:$PhCF_3$ (1:1) was then added to each sample vial to a quantity of 2.0 mL. These were then transferred to a 3.5 mL quartz cuvette (path length: l = 10 mm) and sealed with Teflon caps under an atmosphere of nitrogen in the glove box. The cuvette caps were wrapped with parafilm and the quartz cuvettes were removed out of the glove box. The emission quenching of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 (1.0×10^{-5} M) as a function of the concentration of **N** in deaerated MTBE:$PhCF_3$ with excitation at 455 nm is shown in **Figure S6.**

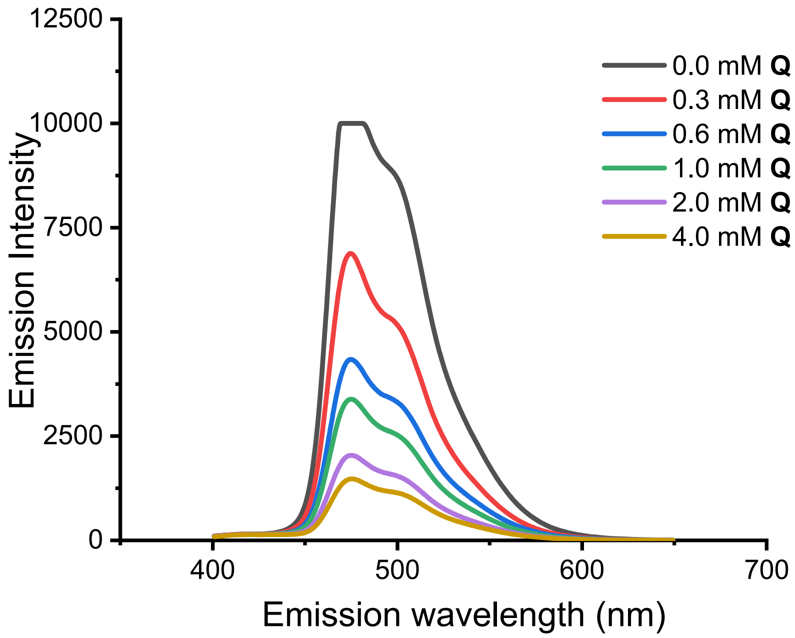
Figure S6. The emission quenching of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 (0.01 mM) as a function of concentration of **N** in deaerated TBME:$PhCF_3$ (1:1) with excitation at 455 nm



Conditions: (black curve) **N** (0.0 mM); (red curve) **N** (0.19 mM); (blue curve) **N** (0.37 mM); (green curve) **N** (0.62 mM); (purple curve) **N** (1.24 mM); (yellow curve) **N** (2.48 mM).

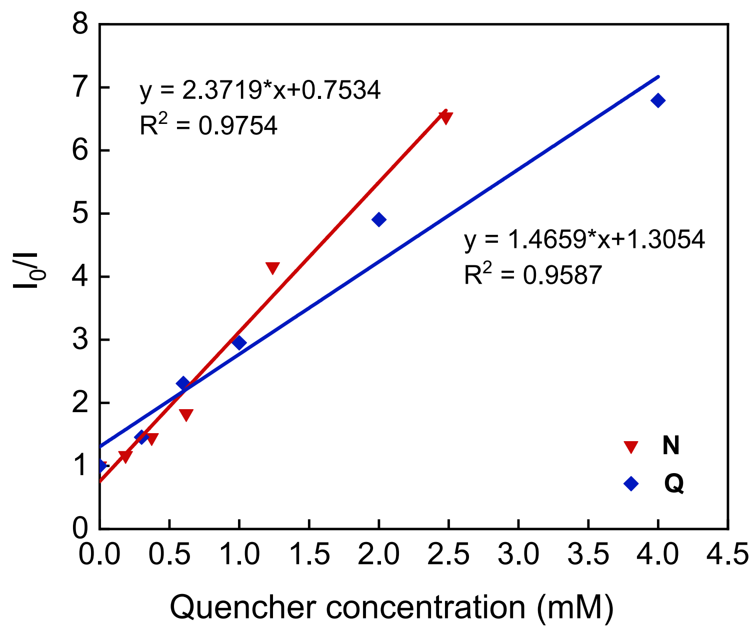
Emission quenching of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 as a function of concentration of quinuclidine (Q). A 1.0×10^{-3} M solution of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 (11.2 mg, 0.010 mmol) in anhydrous degassed MTBE:$PhCF_3$ (1:1, 10 mL) and a 2.0×10^{-2} M solution of **Q** (2.2 mg, 0.020 mmol) in anhydrous degassed MTBE:$PhCF_3$ (1:1, 1 mL) were prepared in a nitrogen filled glovebox. To six sample vials were added 20 uL of 1.0×10^{-3} M solution of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 and 0 uL, 30 uL, 60 uL, 100 uL, 200 uL, and 400 uL of 1.0×10^{-2} M solution of quinuclidine. Anhydrous degassed MTBE:$PhCF_3$ (1:1) was then added to each sample vial to a quantity of 2.0 mL. These were then transferred to a 3.5 mL quartz cuvette (path length: l = 10 mm) and sealed with Teflon caps under an atmosphere of nitrogen in the glove box. The cuvette caps were wrapped with parafilm and the quartz cuvettes were removed out of the glove box. The emission quenching of [Ir(dF(CF_3)ppy)$_2$(dtbbpy)]PF_6 (1.0×10^{-5} M) as a function of the concentration of **Q** in deaerated TBME:$PhCF_3$ with excitation at 455 nm is shown in **Figure S7.**

Figure S7. The emission quenching of $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (0.01 mM) as a function of concentration of **Q** in deaerated TBME:$PhCF_3$ (1:1) with excitation at 455 nm

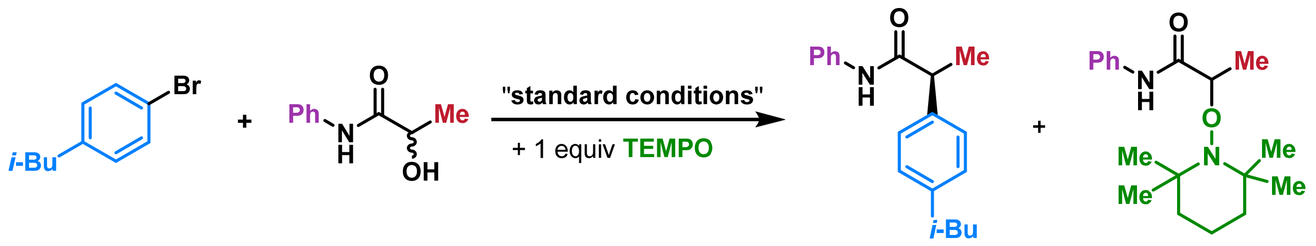


Conditions: (black curve) **Q** (0.0 mM); (red curve) **Q** (0.3 mM); (blue curve) **Q** (0.6 mM); (green curve) **Q** (1.0 mM); (purple curve) **Q** (2.0 mM); (yellow curve) **Q** (4.0 mM).

Figure S8. Comparison of Stern-Volmer quenching for **N** and **Q**

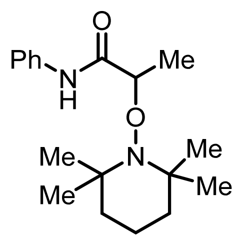


3. Radical trapping experiment using TEMPO as the trapping agent.



1.0 equiv | 1.6 equiv | **48**, not observed | **T**, 40% yield

Procedure. In a nitrogen-filled glovebox, an oven-dried 4 mL vial that contained a stir bar was charged with $NiBr_2$·DME (3.1 mg, 0.010 mmol, 10.0 mol%), (*S*)-**L1** (6.8 mg, 0.012 mmol, 12.0 mol%), and Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (1.8 mg, 0.0015 mmol, 1.5 mol%). Anhydrous (trifluoromethyl)benzene (0.5 mL) was added, and the vial was capped with a PTFE septum cap. The mixture was stirred at room temperature for 30 min, leading to a crimson solution. Then, a separate oven-dried 4 mL vial was charged with 2-hydroxy-*N*-phenylpropanamide (26.4 mg, 0.16 mmol, 1.6 equiv), NHC (63.3 mg, 0.16 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (0.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (16.3 μL, 0.16 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution. In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with 1-bromo-4-isobutylbenzene (21.3 mg, 0.10 mmol, 1.0 equiv), quinuclidine (13.4 mg, 0.12 mmol, 1.2 equiv), phthalimide (2.9 mg, 0.02 mmol, 20.0 mol%), TEMPO (15.6 mg, 0.10 mmol, 1.0 equiv), and a stir bar. The catalyst solution and NHC-alcohol adduct solution were transferred via syringe to the 4 mL reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours. The reaction was stopped by ending the irradiation. The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel.



***N*-Phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)propanamide (T).** White solid, 12.7 mg, 42% yield.

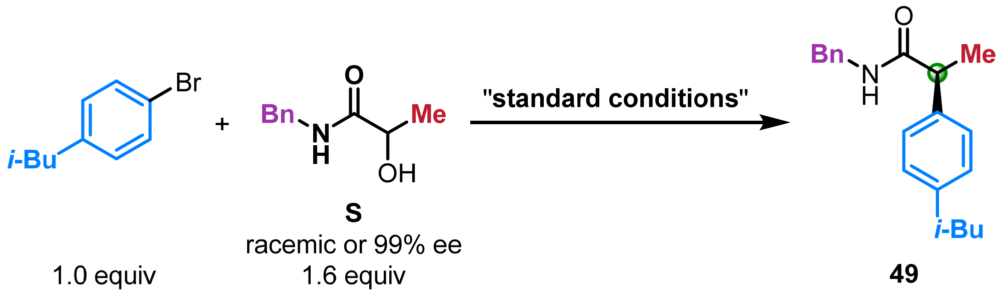
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (s, 1H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.15 (t, *J* = 7.4 Hz, 1H), 4.45 (q, *J* = 7.0 Hz, 1H), 1.58 (d, *J* = 7.0 Hz, 3H), 1.56 – 1.53 (m, 5H), 1.28 – 1.24 (m, 7H), 1.19 (s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.9, 137.5, 129.1, 124.2, 119.5, 82.7, 40.3, 31.7, 29.7, 19.2, 17.0.

FT-IR (film): 3261, 2933, 1628, 1382, 1060. 651 cm^{-1}.

HRMS (ESI-MS) m/z $[M+Na]^+$ calcd for $C_{18}H_{28}N_2NaO_2$: 327.2043, found: 327.2043.

4. Cross-coupling reactions starting from racemic or enantioenriched alkyl alcohols.



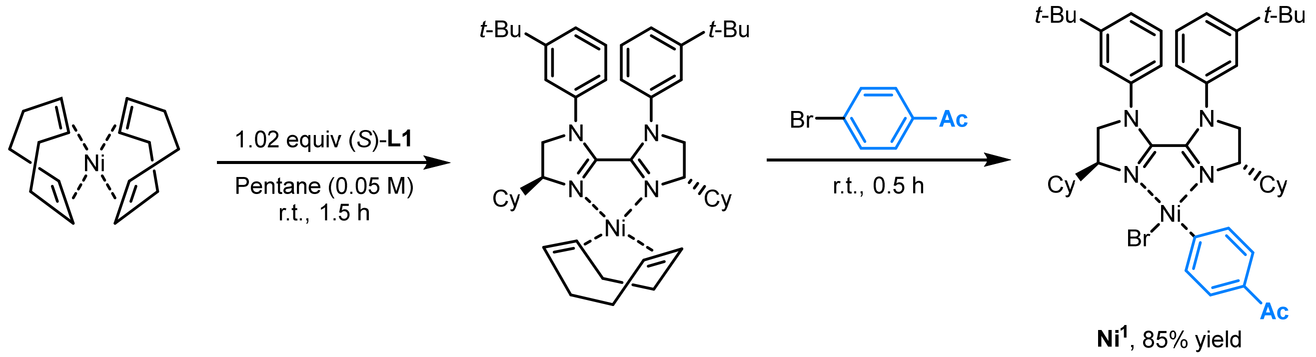
entry	S	remaining **S** recovery (%)^a	remaining **S** ee (%)^b	product **49** yield (%)^a	product **49** ee (%)^b
1	racemic	42	racemic	83	93
2	*R*, 99% ee	47	*R*, 99% ee	82	93
3	*S*, 99% ee	45	*S*, 99% ee	83	93

^{a}Isolated yield. ^{b}Determined through HPLC analysis.

Procedure. In a nitrogen-filled glovebox, an oven-dried 4 mL vial that contained a stir bar was charged with $NiBr_2$·DME (3.1 mg, 0.010 mmol, 10.0 mol%), (*S*)-**L1** (6.8 mg, 0.012 mmol, 12.0 mol%), and $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (1.8 mg, 0.0015 mmol, 1.5 mol%). Anhydrous (trifluoromethyl)benzene (0.5 mL) was added, and the vial was capped with a PTFE septum cap. The mixture was stirred at room temperature for 30 min, leading to a crimson solution. Then, a separate oven-dried 4 mL vial was charged with the racemic or enantioenriched alkyl alcohol (28.6 mg, 0.16 mmol, 1.6 equiv), NHC (63.3 mg, 0.16 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (0.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (16.3 μL, 0.16 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution. In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with 1-bromo-4-isobutylbenzene (21.3 mg, 0.10 mmol, 1.0 equiv), quinuclidine (13.4 mg, 0.12 mmol, 1.2 equiv), phthalimide (2.9 mg, 0.02 mmol, 20.0 mol%), and a stir bar. The catalyst solution and NHC-alcohol adduct solution were transferred via syringe to the 4 mL reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours. The reaction was stopped by ending the irradiation and H_2O (0.5 mL) was introduced to the reaction mixture, which was then stirred for 1 hour. The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel to afford the alcohol **S** and cross-coupling product **49**. The results are displayed in the table.

***N*-Benzyl-2-hydroxypropanamide (S)**. The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for this compound: 19.5 min, 23.5 min.

5. Independently prepared nickel complexes.

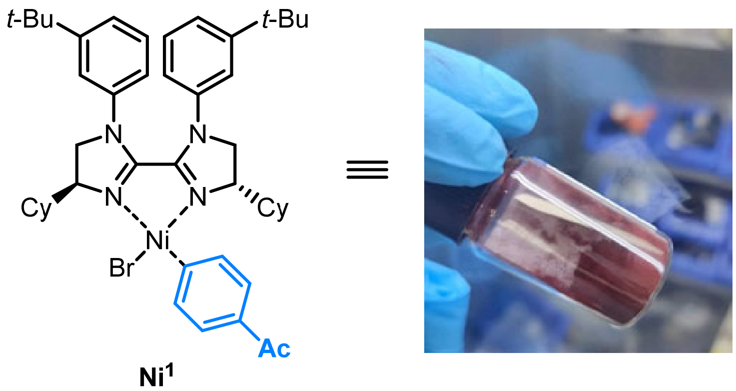


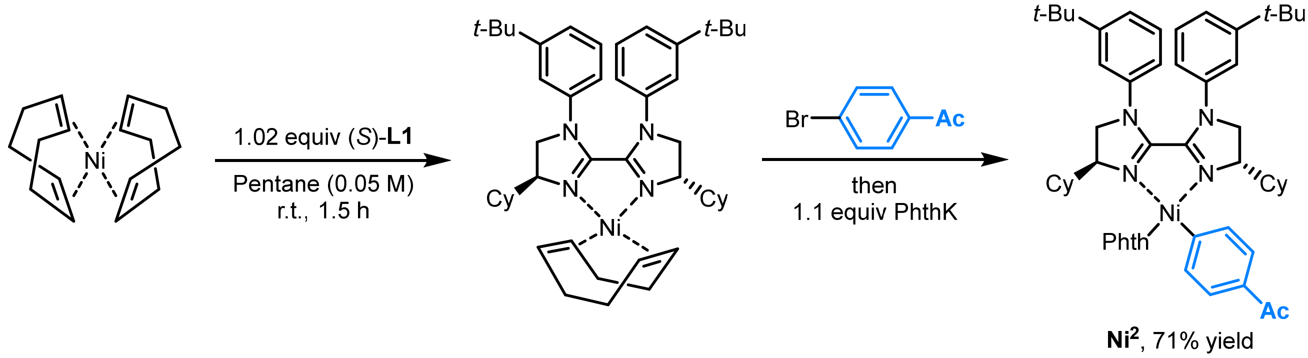
Preparation of Ni¹: In a nitrogen-filled glovebox, an oven-dried 20 mL vial that contained a stir bar was charged with (*S*)-**L1** (288.9 mg, 0.51 mmol, 1.02 equiv), $Ni(COD)_2$ (137.5 mg , 0.50 mmol, 1.0 equiv), and dry pentane (10 mL). The reaction was stirred at 20 °C for 1.5 hours, then 4-bromoacetophenone (108.9 mg, 0.55 mmol, 1.1 equiv) was added. The reaction was stirred at room temperature. After 0.5 hours, a dark red solid formed, which was filtered and washed with pentane (5 × 10 mL). The solid was dried in vacuo, affording **Ni¹** as a dark red powder (350.2 mg, 85%), which was stored in the glovebox at −30 °C. This complex is not sensitive to dry air, but it degrades slowly in the presence of moisture.

Note: *The sample is paramagnetic. The ^1H and ^{13}C NMR spectra show signal broadening, preventing a comprehensive analytical characterization.*

HRMS (ESI-MS) *m/z* $[M]^+$ calcd for $C_{46}H_{61}BrN_4NiO$: 822.3382, found: 822.3392.

Figure S9. Picture of Ni–aryl bromide complex **Ni¹**



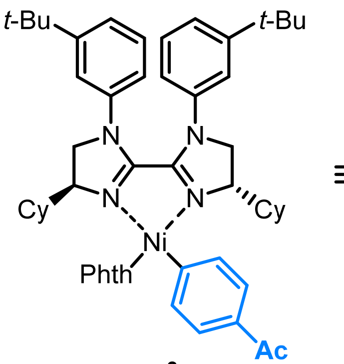


Preparation of Ni²: In a nitrogen-filled glovebox, an oven-dried 20 mL vial that contained a stir bar was charged with (*S*)-**L1** (288.9 mg, 0.51 mmol, 1.02 equiv), $Ni(COD)_2$ (137.5 mg , 0.50 mmol, 1.0 equiv), and dry pentane (10 mL). The reaction was stirred at 20 °C for 1.5 hours, then 4-bromoacetophenone (108.9 mg, 0.55 mmol, 1.1 equiv) were added. The reaction was stirred at room temperature. After 0.5 hours, potassium phthalimide (101.9 mg, 0.55 mmol, 1.1 equiv) was added and the mixture was stirred for another 12 hours. The resulting deep red solution was filtered and removed under reduced pressure to obtain a dark red solid, which is washed with pentane (3 × 5 mL). The solid was redissolved in Et_2O (5 mL), and pentane (10 mL) was slowly added. An orange powder precipitated, which was then washed with pentane (5 × 10 mL). The solid was dried in vacuo, affording **Ni²** an orange powder (315.8 mg, 71%). This complex remains stable in the solid state outside the glovebox for short periods of time, but it rapidly decomposes when in solution under aerobic conditions.

Note: *The sample is paramagnetic. The ^{1}H and ^{13}C NMR spectra show signal broadening, preventing a comprehensive analytical characterization.*

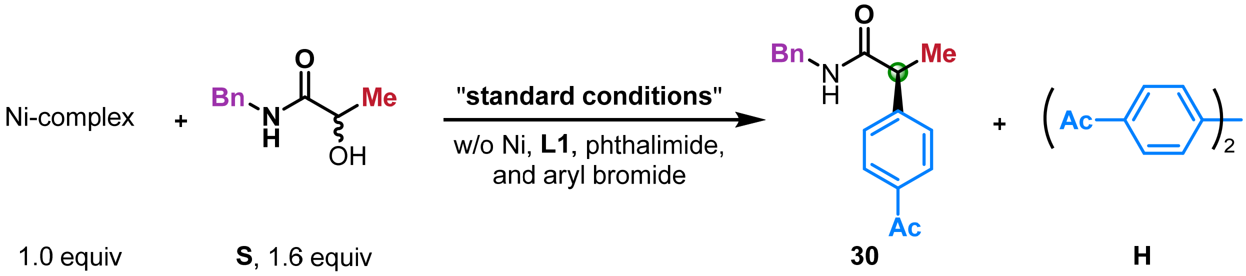
HRMS (ESI-MS) *m/z* $[M]^+$ calcd for $C_{54}H_{65}N_5NiO_3$: 889.4441, found: 889.4450.

Figure S10. Picture of Ni–aryl phthalimide complex **Ni²**



Ni²

6. The reactivity and selectivity of Ni¹ and Ni².



entry	Ni-complex	product **30** yield (%)[a]	product **30** ee (%)[b]	yield of **H** (%)[a]
1	**Ni¹**	15	71	23
2	**Ni²**	30	96	30

[a]Isolated yield. [b]Determined through HPLC analysis.

Stoichiometric experiments. In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with *N*-benzyl-2-hydroxypropanamide (28.6 mg, 0.16 mmol, 1.6 equiv), NHC (63.3 mg, 0.16 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (0.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (16.3 μL, 0.16 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). Then, an oven-dried 4 mL vial that contained a stir bar was charged with **Ni¹** (82.5 mg, 0.10 mmol, 1.0 equiv) or **Ni²** (89.1 mg, 0.10 mmol, 1.0 equiv), and $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (1.8 mg, 0.0015 mmol, 1.5 mol%). Anhydrous (trifluoromethyl)benzene (0.5 mL) was added, and NHC-alcohol adduct solution was transferred via syringe to the reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours. The reaction was stopped by ending the irradiation. The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel to afford the homocoupling product **H** and cross-coupling product **30**. The results are displayed in the table.

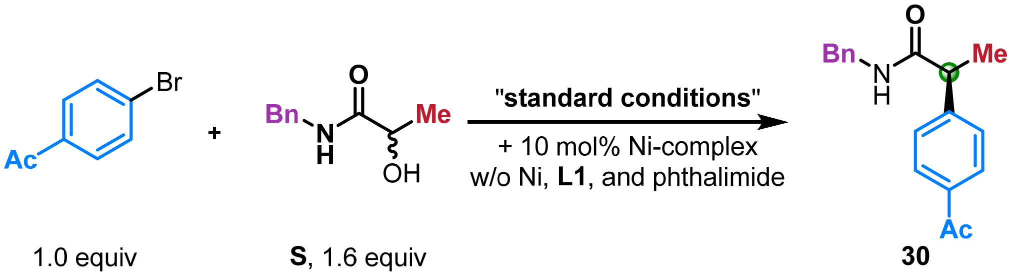
1,1'-([1,1'-Biphenyl]-4,4'-diyl)bis(ethan-1-one) (H). The product was purified by column chromatography on silica gel (1:15 EtOAc/hexanes). White solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 (d, *J* = 8.0 Hz, 4H), 7.70 (d, *J* = 8.0 Hz, 4H), 2.63 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 197.5, 144.2, 136.5, 128.9, 127.3, 26.6.

FT-IR (film): 1680, 1605, 1356, 1275, 952, 809, 607 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{16}H_{15}O_2$: 239.1067, found: 239.1069.



entry	Ni-complex	variation	yield (%)[a]	ee (%)[b]
1	**Ni[1]**	none	67	67
2	**Ni[1]**	+ 20 mol% phthalimide	94	93
3	**Ni[2]**	none	96	98

[a]Isolated yield. [b]Determined through HPLC analysis.

Catalytic experiments. In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with *N*-benzyl-2-hydroxypropanamide (28.6 mg, 0.16 mmol, 1.6 equiv), NHC (63.3 mg, 0.16 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (0.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (16.3 μL, 0.16 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). Then, an oven-dried 4 mL vial that contained a stir bar was charged with **Ni[1]** (8.3 mg, 0.010 mmol, 10 mol%) or **Ni[2]** (8.9 mg, 0.010 mmol, 10 mol%), 4-bromoacetophenone (19.8 mg, 0.10 mmol, 1.0 equiv), phthalimide (2.9 mg, 0.020 mmol, 20.0 mol%) (only for entry 2), and Ir[dF(CF_3)ppy]$_2$(dtbbpy)PF_6 (1.8 mg, 0.0015 mmol, 1.5 mol%). Anhydrous (trifluoromethyl)benzene (0.5 mL) was added, and NHC-alcohol adduct solution was transferred via syringe to the reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours. The reaction was stopped by ending the irradiation. The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel. The results are displayed in the table.

7. Kinetic studies.

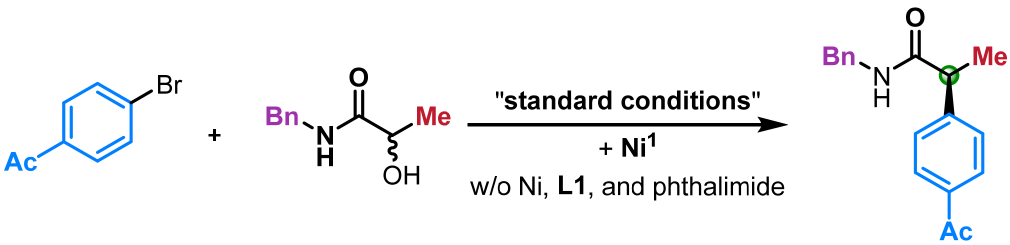
General Procedure 4 (GP-4).

Preparation of the NHC-alcohol adduct solution: In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with α-hydroxy amide (0.05-0.30 M), NHC (63.3 mg, 0.16 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (0.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (16.3 μL, 0.16 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution.

Cross-coupling: In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with **Ni**[1] or **Ni**[2] (0.004-0.02 M), the aryl bromide (0.04-0.30 M), quinuclidine (13.4 mg, 0.12 mmol, 1.2 equiv), and a stir bar. The NHC-alcohol adduct solution was transferred via syringe to the 4 mL reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C.

Work-up: The reaction was stopped by ending the irradiation. The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the yield was determined via GC analysis with n–tetradecane as an internal standard.

Figure S11–13: *N*-Benzyl-2-hydroxypropanamide was reacted with 1-(4-bromophenyl)ethan-1-one in the presence of **Ni**[1] according to **GP-4**. Run five reactions in parallel, stopping one reaction every 4 minutes. Rate constants were calculated for each reaction using the initial rates method (<10% conversion). Error analysis was conducted using standard equations and calculations. **Ni**[1] is first-order dependent; both alkyl alcohol and aryl bromide are zero-order dependent.



30

Figure S11. Rate on the concentration of **Ni**[1]

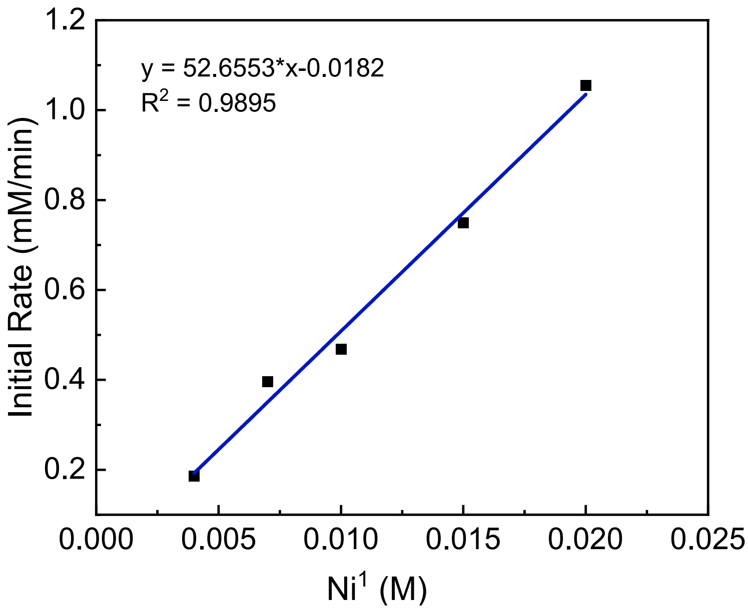


Figure S12. Rate on the concentration of alkyl alcohol

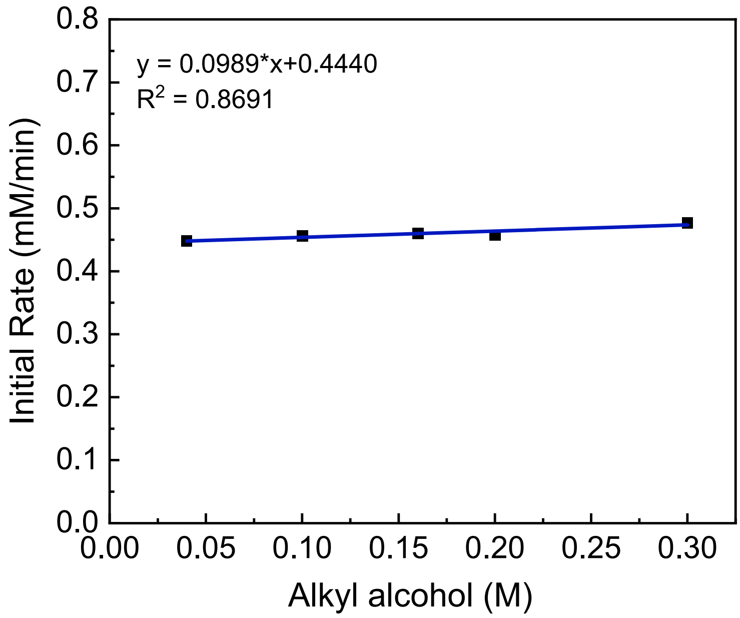


Figure S13. Rate on the concentration of aryl bromide

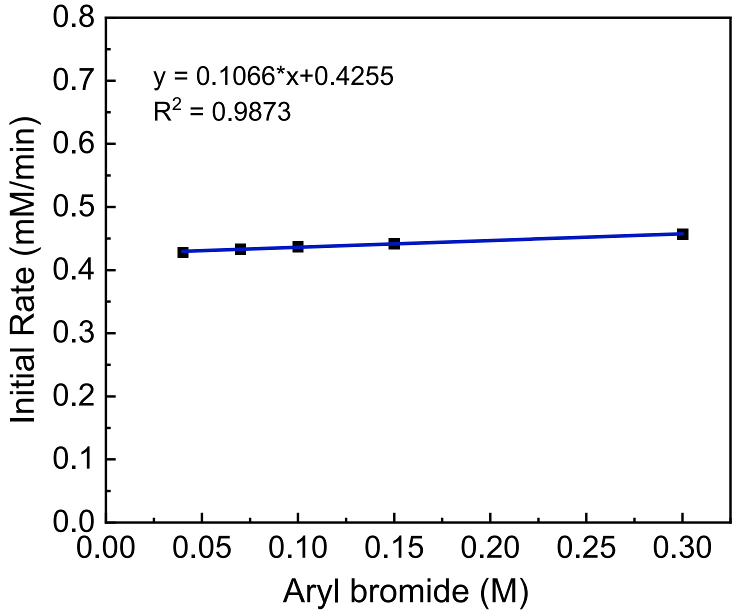


Figure S14–16: *N*-Benzyl-2-hydroxypropanamide was reacted with 1-(4-bromophenyl)ethan-1-one in the presence of **Ni²** according to **GP-4**. Run five or four reactions in parallel, stopping one reaction every 4 minutes. Rate constants were calculated for each reaction using the initial rates method (<10% conversion). Error analysis was conducted using standard equations and calculations. **Ni¹** and aryl bromide are first-order dependent; alkyl alcohol is zero-order dependent.

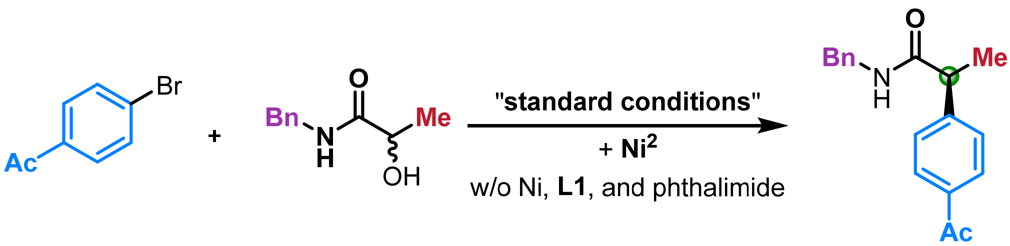


Figure S14. Rate on the concentration of **Ni²**

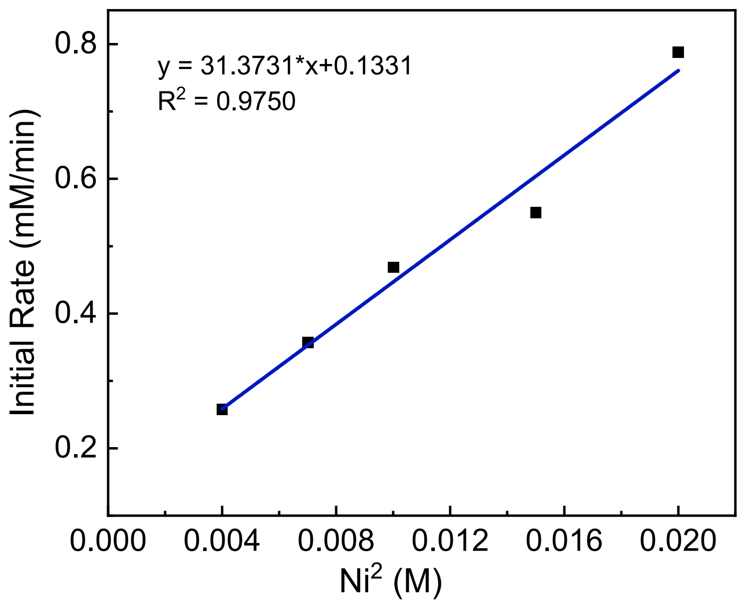


Figure S15. Rate on the concentration of alkyl alcohol

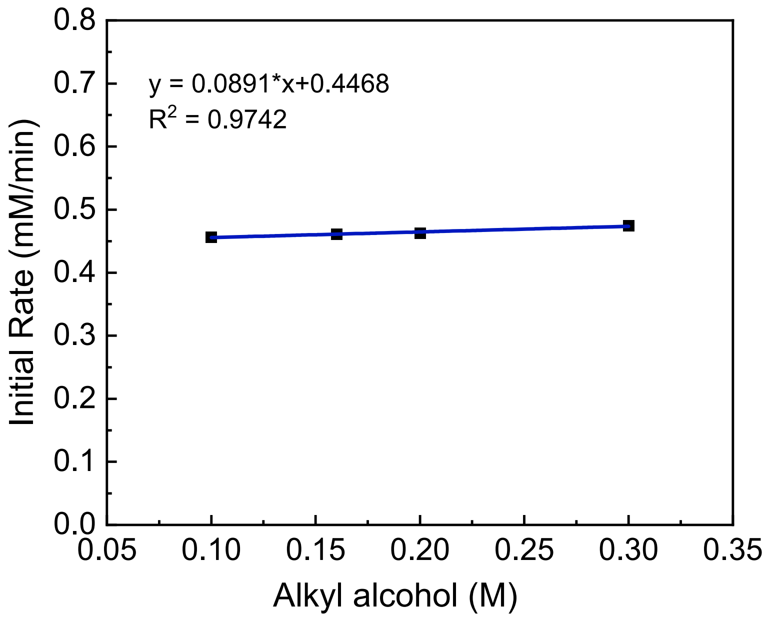


Figure S16. Rate on the concentration of aryl bromide

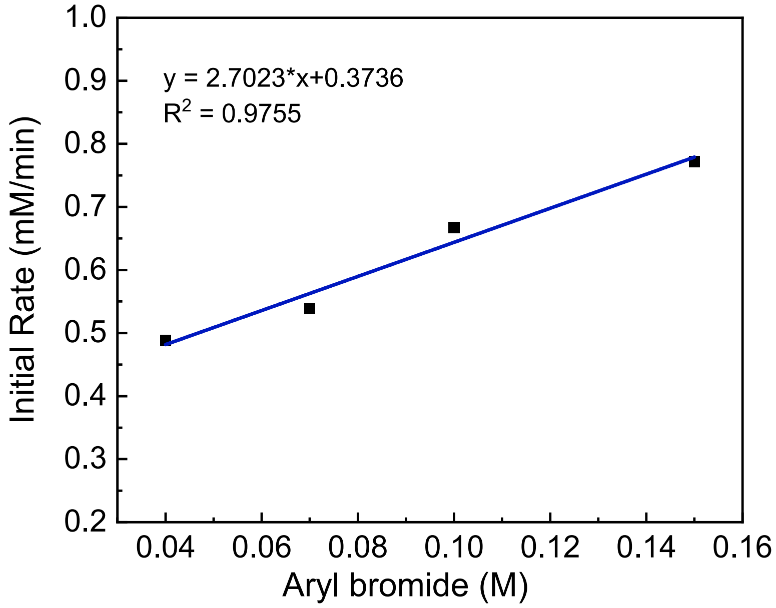
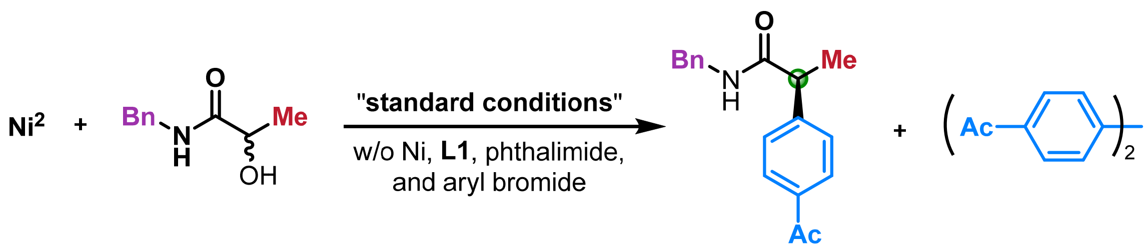
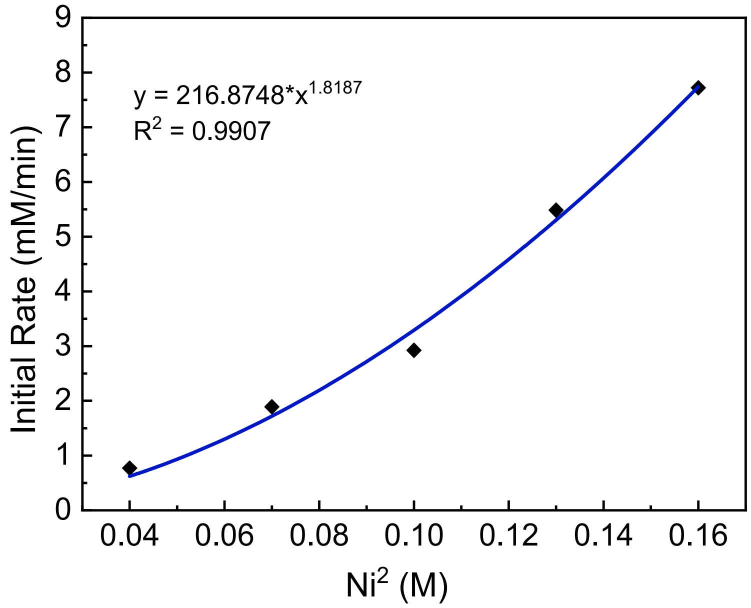


Figure S17: *N*-Benzyl-2-hydroxypropanamide was reacted with **Ni²** in the absence of aryl bromide according to **GP-4**. Run five reactions in parallel, stopping one reaction every 4 minutes. Rate constants were calculated for each reaction using the initial rates method (<15% conversion). Error analysis was conducted using standard equations and calculations. **Ni²** is second-order dependent.

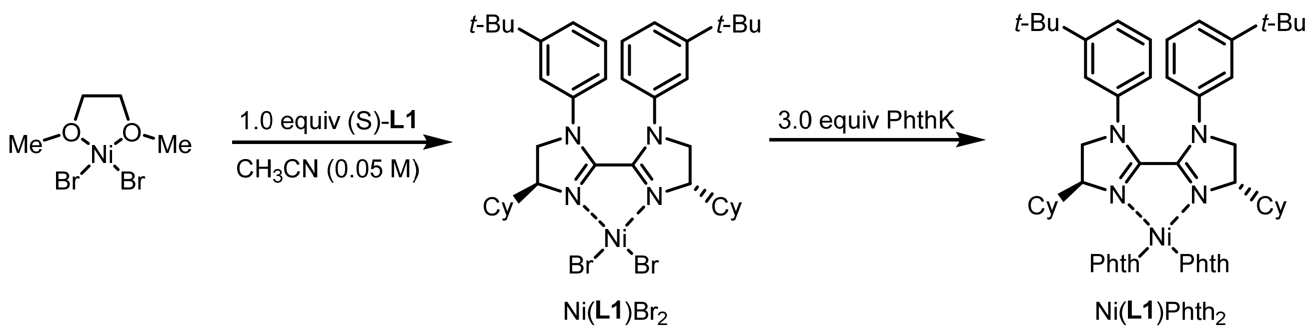


30 **H**

Figure S17. Rate on the concentration of **Ni²**



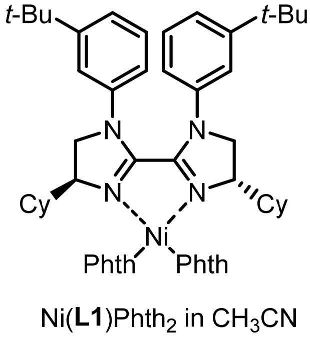
8. Preparation of Ni(L1)Phth₂ and measurement of its potential.



Preparation of Ni(L1)Phth$_2$: In a nitrogen-filled glovebox, an oven-dried 4 mL vial that contained a stir bar was charged with (*S*)-**L1** (28.3 mg, 0.050 mmol, 1.0 equiv), $NiBr_2$·DME (15.4 mg, 0.050 mmol, 1.0 equiv), and dry CH_3CN (1.0 mL). The reaction was stirred at room temperature for 2 hours, then potassium phthalimide (27.8 mg, 0.150 mmol, 3.0 equiv) was added. The reaction was stirred at room temperature for another 12 hours. The suspension was filtered to furnish a homogeneous green solution.

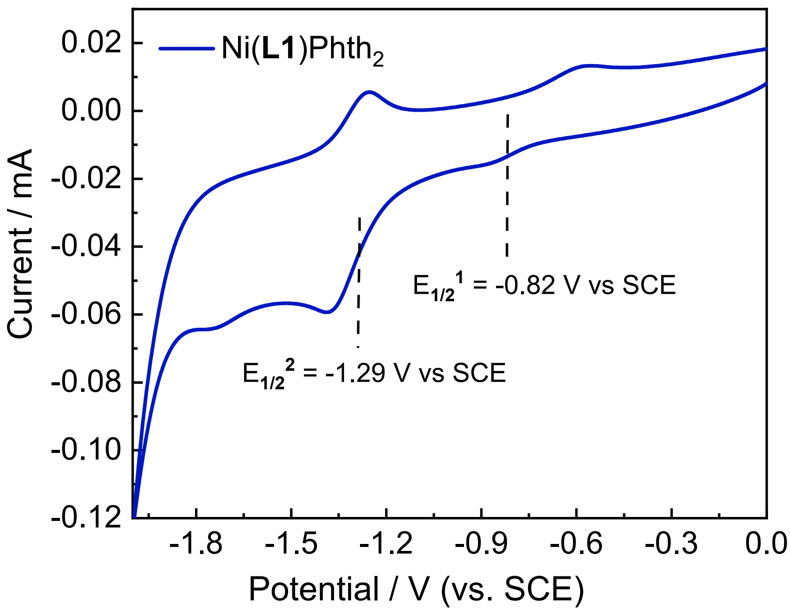
HRMS (ESI-MS) m/z [M-phthalimide]$^+$ calcd for $C_{46}H_{58}N_5NiO_2$: 770.3939, found: 770.3954.

Figure S18. Picture of Ni(**L1**)Phth$_2$ in CH_3CN

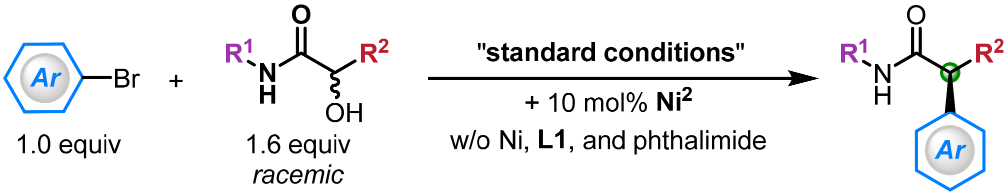


Cyclic voltammogram of Ni(L1)Phth$_2$. Cyclic voltammograms were collected with a CorrTest CS2350M electrochemical workstation. Samples were prepared by mixing 0.050 mmol of Ni(**L1**)Phth$_2$ (1.0 mL solution of Ni(**L1**)Phth$_2$) in 10 mL of 0.1 M *n*-Bu_4NPF_6 (387.4 mg, 1.0 mmol) in anhydrous CH_3CN. Measurements employed a glassy carbon working electrode, platinum wire counter electrode, saturated calomel electrode (SCE) reference electrode, and a scan rate of 100 mV/s. The glassy carbon electrode was polished between each scan. The samples were sparged with N_2 for at least 15 minutes prior to data collection.

Figure S19. Cyclic voltammogram of Ni(**L1**)Phth$_2$



VII. Catalytic Asymmetric Cross-Couplings using Ni² as the Catalyst

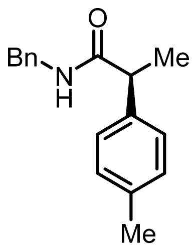


General Procedure 5 (GP-5).

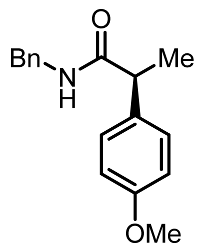
Preparation of the NHC-alcohol adduct solution: In a nitrogen-filled glovebox, an oven-dried 4 mL vial was charged with the α-hydroxy amide (0.80 mmol, 1.6 equiv), NHC (316.5 mg, 0.80 mmol, 1.6 equiv), and a stir bar. Methyl *tert*-butyl ether (2.5 mL) was added, and the mixture was stirred at room temperature for 5 min. Next, 4-methoxypyridine (81.2 µL, 0.80 mmol, 1.6 equiv) was added dropwise, and the resulting solution was stirred at room temperature for another 30 min (a white solid precipitated during this time). The suspension was filtered to furnish a homogeneous solution.

Cross-coupling: In a nitrogen-filled glovebox, an oven-dried 20 mL vial was charged with **Ni²** (44.5 mg, 0.050 mmol, 10.0 mol%), the aryl bromide (0.50 mmol, 1.0 equiv), quinuclidine (67 mg, 0.60 mmol, 1.2 equiv), and a stir bar. The NHC-alcohol adduct solution was transferred via syringe to the 20 mL reaction vial. The vial was transferred out of the glovebox and placed in an EtOH cooling bath at 0 °C for 5 min. Then the reaction was irradiated with blue LEDs (455 nm, 30 W) and was stirred at 0 °C for 36 hours.

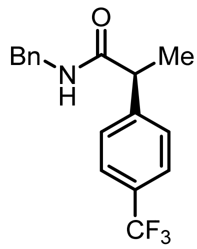
Work-up: The reaction mixture was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with EtOAc. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel.



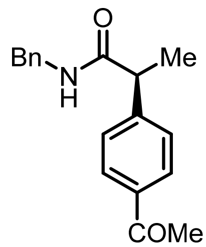
(*S*)-*N*-Benzyl-2-(*p*-tolyl)propanamide (26). The title compound was synthesized according to **GP-5** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-methylbenzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). White solid, 103.7 mg, 82% yield, 94% ee.



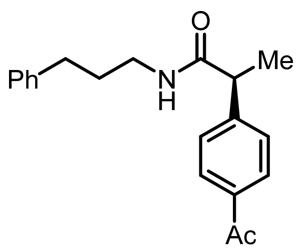
(*S*)-*N*-Benzyl-2-(4-methoxyphenyl)propanamide (27). The title compound was synthesized according to **GP-5** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-methoxybenzene. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 107.7 mg, 80% yield, 95% ee.



(*S*)-*N*-Benzyl-2-(4-(trifluoromethyl)phenyl)propanamide (28). The title compound was synthesized according to **GP-5** from *N*-benzyl-2-hydroxypropanamide and 1-bromo-4-(trifluoromethyl)benzene. The product was purified by column chromatography on silica gel (1:4 EtOAc/hexanes). Yellow oil, 142.2 mg, 93% yield, 96% ee.



(*S*)-2-(4-Acetylphenyl)-*N*-benzylpropanamide (30). The title compound was synthesized according to **GP-5** from *N*-benzyl-2-hydroxypropanamide and 1-(4-bromophenyl)ethan-1-one. The product was purified by column chromatography on silica gel (1:3 EtOAc/hexanes). White solid, 134.9 mg, 96% yield, 98% ee.



(*S*)-2-(4-Acetylphenyl)-*N*-(3-phenylpropyl)propanamide (58). The title compound was synthesized according to **GP-5** from 2-hydroxy-*N*-(3-phenylpropyl)propanamide and 1-(4-

bromophenyl)ethan-1-one. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). White solid, 139.1 mg, 90% yield, 95% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (20% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 29.8 min (minor), 32.0 min (major).

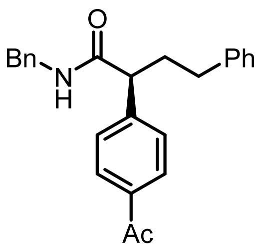
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.2 Hz, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.27 – 7.22 (m, 2H), 7.19 – 7.16 (m, 1H), 7.09 (d, *J* = 7.5 Hz, 2H), 5.38 (s, 1H), 3.53 (q, *J* = 7.1 Hz, 1H), 3.24 (q, *J* = 6.7 Hz, 2H), 2.58 (s, 3H), 2.55 (dd, *J* = 8.5, 6.8 Hz, 2H), 1.76 (p, *J* = 7.3 Hz, 2H), 1.50 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.6, 173.1, 147.0, 141.1, 135.7, 128.5, 128.2, 128.0, 127.5, 125.7, 46.7, 39.1, 32.9, 30.8, 26.4, 18.3.

FT-IR (film): 3291, 2926, 1724, 1680, 1638, 1537, 1263, 1069, 701 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+H]$^+$ calcd for $C_{20}H_{24}NO_2$: 310.1802, found: 310.1805.

[α]$^{15}_{D}$ = +6.7 (c 1.0, $CHCl_3$); 95% ee, from (*S*)-**L1**.



(*S*)-2-(4-Acetylphenyl)-*N*-benzyl-4-phenylbutanamide (59). The title compound was synthesized according to **GP-5** from *N*-benzyl-2-hydroxy-4-phenylbutanamide and 1-(4-bromophenyl)ethan-1-one. The product was purified by column chromatography on silica gel (1:2 EtOAc/hexanes). White solid, 139.1 mg, 75% yield, 91% ee.

HPLC analysis: The ee was determined via HPLC on a CHIRALPAK IC-3 column (30% *i*-PrOH in hexane, 1.0 mL/min); retention times for compound obtained using (*S*)-**L1**: 16.1 min (minor), 18.5 min (major).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.25 (m, 5H), 7.21 (d, *J* = 7.3 Hz, 1H), 7.18 – 7.11 (m, 4H), 5.93 (s, 1H), 4.46 (dd, *J* = 14.8, 5.8 Hz, 1H), 4.34 (dd, *J* = 14.8, 5.6 Hz, 1H), 3.41 (t, *J* = 6.9 Hz, 1H), 2.59 (s, 3H), 2.57 – 2.51 (m, 3H), 2.18 – 2.09 (m, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.7, 172.1, 145.2, 141.0, 138.0, 136.2, 128.8, 128.6, 128.4, 128.2, 127.6, 127.5, 126.0, 52.3, 43.7, 34.6, 33.4, 26.5.

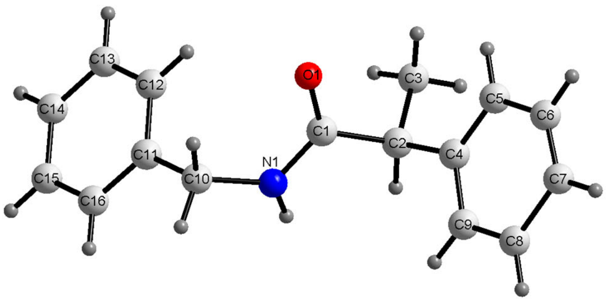
FT-IR (film): 3303, 2941, 1726, 1675, 1629, 1534, 1275, 726 cm^{-1}.

HRMS (ESI-MS) *m/z* [M+Na]$^+$ calcd for $C_{25}H_{25}NNaO_2$: 394.1778, found: 394.1781.

[α]$^{15}_{D}$ = +4.5 (c 1.0, $CHCl_3$); 91% ee, from (*S*)-**L1**.

VIII. Assignment of Absolute Configuration

The configuration of the coupling product illustrated in **Figure. 2c, entry 22**, using (*S*)-**L1**, was determined via X-ray crystallography.

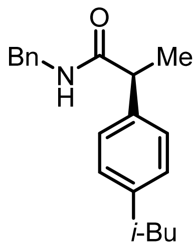


(*S*)-*N*-Benzyl-2-phenylpropanamide (Figure. 2c, entry 22). X-ray quality crystals were obtained by slow evaporation of a saturated solution in diethyl ether/hexanes of a sample synthesized using (*S*)-**L1**. A suitable crystal was selected and measured on a Bruker APEX-III CMOS diffractometer. The crystal was kept at 100.0 K during data collection. The absolute stereochemistry was determined on the basis of the absolute structure parameter.

Table 1. Crystal data for $C_{16}H_{17}NO$.

Identificationcode	cu_231121a_a
Empirical formula	$C_{16}H_{17}NO$
Formula weight	239.30
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1$
a/Å	4.93690(10)
b/Å	26.4029(6)
c/Å	10.0274(2)
α/°	90
β/°	94.5140(10)
γ/°	90
Volume/Å^3	1303.00(5)
Z	4
ρcalcg/cm^3	1.220

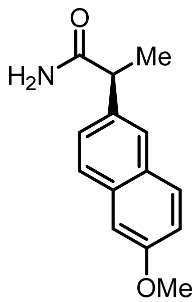
μ/mm^{-1}	0.591
F(000)	512.0
Crystal size/mm^3	0.28 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.696 to 154.766
Index ranges	$-6 \leq h \leq 5$, $-33 \leq k \leq 32$, $-11 \leq l \leq 12$
Reflections collected	18534
Independent reflections	5334 [Rint = 0.0569, Rsigma = 0.0493]
Data/restraints/parameters	5334/181/408
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R1 = 0.0502, wR2 = 0.1130
Final R indexes [all data]	R1 = 0.0587, wR2 = 0.1197
Largest diff. peak/hole / e $Å^{-3}$	0.25/-0.20
Flack parameter	-0.1(2)



(*S*)-*N*-Benzyl-2-(4-isobutylphenyl)propanamide (Figure. 2e, entry 49). The absolute configuration of this compound has been established by the literature.[3] It was obtained with (*S*)-**L1**. As shown below, the (*S*)-configuration was assigned by comparison with published optical rotation.

Optical rotation: $[\alpha]^{15}_{D}$ = +4.20 (*c* 1.0, $CHCl_3$); 93% ee, from (*S*)-**L1**.

Lit.: $[\alpha]^{20}_{D}$ = +1.68 (c 1.27, $CHCl_3$); 93% ee for (*S*)-configuration.



(*S*)-2-(6-Methoxynaphthalen-2-yl)propanamide (Figure. 2e, entry 54). The absolute configuration of this compound has been established by the literature.[4] It was obtained with (*S*)-**L1**. As shown below, the (*S*)-configuration was assigned by comparison with published optical rotation.

Optical rotation: $[\alpha]^{15}_{D}$ = +19.0 (c 1.0, $CHCl_3$); 80% ee, from (*S*)-**L1**.

Lit.: $[\alpha]^{25}_{D}$ = –16.3 (c 1.2, $CHCl_3$); 75% ee for (*R*)-configuration.

IX. DFT calculations

Density functional theory (DFT) calculations were carried out with Gaussian 16 program. Geometry optimization calculations were performed with B3LYP hybrid exchange correlation functional, and a mixed basis set denoted as BS1, which uses 6-31G(d) on C, H, O, N, Br atoms, and def2-SVP basis set on Ni atom. Frequency calculations were performed with B3LYP/BS1 method, and the imaginary frequencies were checked to confirm the structures of the stationery and saddle points. IRC calculations were also performed to make sure the transition states were the correct ones between the intermediate structures. Conformational search for the key structures was carried out with CREST prgrom,[5] and only the lowest-energy isomers were shown in the research paper. The electronic energies were obtained from single point calculations with PW6B95D3 functional with D3 dispersion correction and a larger mixed basis set denoted as BS2, which used triple-ζ basis set 6-311G(d,p) on C, H, O, N, Br atoms, and def2-TZVP basis set on Ni atom. Solvation energies were calculated on the same level of method PW6B95D3/BS2, adopting the implicit solvation model SMD with mixed solvent of 50% MTBE and 50% $PhCF_3$. Special SMD parameters for Br ion were used according to Engelage et al.[6] SMD Parameters for solvent were calculated by averaging the parameters of MTBE and $PhCF_3$, as shown below:

SMD parameters	MTBE	$PhCF_3$	1:1 solvent
n^2	1.874	1.999	1.936
alpha	0.000	0.000	0.000
beta	0.450	0.100	0.275
gamma	26.340	30.801	28.571
epsilon	4.500	9.180	6.840
phi	0.000	0.600	0.300
psi	0.000	0.300	0.150
n25	1.366	1.414	1.390

Zero-point energies and enthalpies were calculated from vibrational frequencies at 0 °C by using Shermo progrom. To avoid the problems caused by low vibrational frequencies for enthalpy, all vibrational frequencies less than 100 cm^{-1} were substituted with values of 100 cm^{-1}.

In conclusion, the final reported geometries were optimized with B3LYP/BS1; the thermal corrections were also calculated with B3LYP/BS1; the electronic energies and solvation energies calculated with PW6B95D3/BS2/SMD. The energies and thermal corrections are shown in the following table (unit: Hartree).

Species	Thermal correction for G	Thermal correction for H	Electronic energy with solvation energy correction
Alkyl radical	0.165310	0.209886	-519.0420456

dehydrogenated phthalimide (-1)	0.073967	0.109951	-513.3834357
Br (-1)	0.000000	0.000000	-2575.413542
L1-Ni-Br	0.801989	0.899363	-5786.821651
L1-Ni-Phthalimide	0.901845	1.010038	-3724.823806
product (R and S)	0.365706	0.426445	-908.6340718
IS	0.998824	1.111577	-6176.266233
TS1(b)	0.998475	1.110959	-6176.259690
IM1	1.001415	1.113733	-6176.330674
IM2	0.997757	1.112588	-6176.336070
TS2-R	1.188404	1.324591	-6695.386755
IM3-R	1.194282	1.327065	-6695.405237
TS3-R	1.193905	1.326191	-6695.394798
TS2-S	1.189575	1.325070	-6695.389439
IM3-S	1.193477	1.326724	-6695.406543
TS3-S	1.192841	1.325511	-6695.394050
TS4	1.094929	1.224561	-6689.737765
IM4	1.097719	1.222911	-4114.332930
TS5-R	1.288715	1.435057	-4633.393606
IM5-R	1.294543	1.437701	-4633.421729
TS6-R	1.292821	1.435724	-4633.412187
TS5-S	1.289463	1.435635	-4633.396386
IM5-S	1.293555	1.437362	-4633.414412
TS6-S	1.292590	1.436000	-4633.413000

Cartesion coordinates:

Alkyl radical

H	-2.593670	-2.841630	-0.534150
H	-1.045628	-1.206041	0.764551
C	-3.001515	-2.038372	0.098230
H	-3.281245	-2.513430	1.050473
C	-1.999574	-0.961321	0.307368
O	-3.295550	0.696739	-0.767143
C	-2.264446	0.397796	-0.151404
H	-3.897091	-1.634079	-0.378569
N	-1.307977	1.366343	0.105073
H	-0.435592	0.771928	1.926901
H	-1.593965	2.286028	-0.202134
C	-0.153983	1.258585	0.983014
H	0.129289	2.284002	1.251128

H	0.564535	0.960427	-1.657056
C	1.059616	0.546913	0.393409
C	1.291366	0.512319	-0.985843
C	1.991473	-0.051794	1.250914
C	2.435462	-0.103483	-1.496898
H	1.818672	-0.038650	2.325676
H	2.600405	-0.125151	-2.571028
C	3.137495	-0.665131	0.742744
C	3.363021	-0.692286	-0.635172
H	3.849169	-1.127507	1.421776
H	4.251868	-1.173559	-1.034122

phthalimide (-1)

C	2.533546	0.700413	-0.000001
C	2.533545	-0.700416	-0.000044
C	1.325438	-1.418163	-0.000027
C	0.141753	-0.695090	0.000041
C	0.141754	0.695088	0.000044
C	1.325440	1.418161	0.000038
C	-1.327242	1.114098	0.000001
N	-2.121906	0.000002	-0.000026
C	-1.327247	-1.114096	0.000182
O	-1.675739	2.300652	-0.000066
O	-1.675744	-2.300649	-0.000076
H	3.482977	1.234537	-0.000007
H	3.482976	-1.234542	-0.000086
H	1.308661	-2.506092	-0.000032
H	1.308663	2.506090	0.000039

L1–Ni–Br

N	0.271679	-1.725552	0.024892
N	0.672386	1.466911	-0.495290
N	-1.897068	-1.142493	-0.379622
N	-1.589319	1.397703	-0.313321
C	-2.748417	-3.333802	-1.273860
C	-2.234714	3.728552	0.268251
C	-1.932279	-2.605807	-0.183867
C	-1.273903	2.822520	-0.535782
C	-4.199757	-2.820179	-1.394340
C	-2.756588	-4.865438	-1.052122
C	-2.171321	5.211156	-0.162767

C	-2.179894	3.585020	1.809654
C	-0.431987	-3.013349	-0.165685
C	0.259543	2.880966	-0.305630
C	-5.094089	-3.243111	-0.218685
C	-3.644877	-5.301120	0.127204
C	-1.065430	6.021987	0.532280
C	-1.142565	4.466847	2.531606
C	-0.658183	-0.732243	-0.217635
C	-0.475212	0.709325	-0.361514
C	-5.078441	-4.766297	-0.020115
C	-1.195771	5.927587	2.059502
C	1.427047	-1.624106	0.836599
C	1.873447	1.108293	-1.146630
C	2.465618	-2.550024	0.641562
C	3.050360	1.804045	-0.820688
C	1.539702	-0.657839	1.842404
C	1.908578	0.110317	-2.127502
C	3.622256	-2.532882	1.426592
C	4.267462	1.523805	-1.448829
C	4.770172	-3.539861	1.226480
C	5.565801	2.277247	-1.104072
C	2.698211	-0.619328	2.617177
C	3.121830	-0.190528	-2.744484
C	3.723222	-1.541332	2.419158
C	4.284068	0.504027	-2.417395
C	6.067919	-2.773372	0.876170
C	4.983660	-4.341059	2.533072
C	4.485431	-4.541635	0.091197
C	6.618123	1.270282	-0.581632
C	6.108093	2.973802	-2.375043
C	5.354929	3.353106	-0.021625
H	-2.234080	-3.125806	-2.224104
H	-3.218128	3.342796	-0.032126
H	-2.387858	-2.789532	0.798469
H	-1.475725	3.028678	-1.599593
H	-4.211138	-1.730239	-1.497659
H	-4.620677	-3.226042	-2.325618
H	-3.138382	-5.334340	-1.969870
H	-1.735384	-5.248993	-0.920130
H	-2.071288	5.280611	-1.254764
H	-3.136589	5.675007	0.083391

H	-3.173876	3.857664	2.188776
H	-2.043244	2.529737	2.075377
H	-0.134379	-3.472122	-1.118707
H	-0.176777	-3.701415	0.643652
H	0.521012	3.207640	0.705285
H	0.776068	3.521099	-1.024292
H	-4.762782	-2.741063	0.700610
H	-6.115531	-2.887166	-0.394789
H	-3.218055	-4.940595	1.074517
H	-3.650670	-6.396726	0.194861
H	-0.072391	5.660313	0.226421
H	-1.120209	7.069671	0.209814
H	-0.125242	4.081402	2.378411
H	-1.320410	4.413941	3.613613
H	-5.678551	-5.046261	0.855060
H	-5.550551	-5.248158	-0.889653
H	-0.409334	6.514955	2.550805
H	-2.155027	6.372716	2.362671
H	2.355278	-3.277027	-0.154060
H	2.996516	2.562336	-0.048920
H	0.728022	0.036634	2.031048
H	1.000318	-0.406813	-2.417369
H	2.789585	0.127474	3.401659
H	3.153096	-0.963007	-3.508596
H	4.606036	-1.490034	3.049328
H	5.208932	0.252901	-2.927883
H	6.359636	-2.080979	1.672849
H	6.896884	-3.475848	0.725650
H	5.941457	-2.190872	-0.043407
H	4.081532	-4.903231	2.800546
H	5.806258	-5.056359	2.411266
H	5.232098	-3.688029	3.376118
H	3.588282	-5.139567	0.289135
H	4.357816	-4.038872	-0.874335
H	5.327775	-5.235502	-0.007277
H	6.857495	0.506833	-1.329311
H	7.549784	1.790112	-0.326492
H	6.255603	0.756986	0.316173
H	5.385550	3.701396	-2.762255
H	7.039635	3.507033	-2.149111
H	6.320337	2.256471	-3.174556

H	4.635060	4.116473	-0.338819
H	5.003826	2.919886	0.921957
H	6.304184	3.861099	0.182243
Ni	-3.233987	0.307488	-0.275563
Br	-5.436176	0.862390	0.067974

L1–Ni–Phth

N	1.588473	1.715994	-0.499467
N	1.313587	-1.406697	0.233253
N	-0.649630	1.638359	-0.071659
N	-0.848527	-0.955989	-0.316065
C	-0.824786	4.033793	0.893568
C	-1.396008	-3.174756	-1.363431
C	-0.358185	3.080346	-0.245041
C	-0.813066	-2.423482	-0.143870
C	-0.554337	3.504804	2.323249
C	-2.279404	4.538975	0.757878
C	-2.832661	-2.739945	-1.722852
C	-1.347188	-4.708524	-1.161420
C	1.191610	3.135696	-0.418741
C	0.694391	-2.743380	0.093007
C	-1.640517	2.555186	2.861205
C	-3.336409	3.565805	1.294345
C	-3.884101	-3.244964	-0.721654
C	-2.394560	-5.220445	-0.156688
C	0.463325	0.975678	-0.228127
C	0.344014	-0.485796	-0.088038
C	-3.043791	3.166535	2.746941
C	-3.811326	-4.769017	-0.544149
C	2.727687	1.307248	-1.238129
C	2.468739	-1.203790	1.027179
C	3.938764	1.984102	-1.022753
C	3.547100	-2.090878	0.876189
C	2.656681	0.296924	-2.202949
C	2.535625	-0.185469	1.984330
C	5.091928	1.674536	-1.750641
C	4.700011	-1.985456	1.660489
C	6.423573	2.420291	-1.544124
C	5.881675	-2.964277	1.526282
C	3.807760	-0.038185	-2.915052
C	3.692262	-0.054410	2.751775

C	5.005386	0.639398	-2.698705
C	4.756975	-0.939457	2.598754
C	7.520132	1.412813	-1.124770
C	6.835290	3.103882	-2.870234
C	6.329114	3.504850	-0.454026
C	7.164386	-2.180007	1.161917
C	6.093005	-3.694320	2.874569
C	5.646311	-4.027668	0.436592
H	-0.184999	4.918591	0.748178
H	-0.742843	-2.919506	-2.211894
H	-0.857152	3.399720	-1.169931
H	-1.404668	-2.656567	0.749661
H	0.432174	3.020712	2.371467
H	-0.492986	4.376052	2.991199
H	-2.353435	5.480132	1.322675
H	-2.484983	4.794281	-0.290858
H	-2.888459	-1.652173	-1.815785
H	-3.064218	-3.150710	-2.716091
H	-1.537883	-5.178821	-2.136233
H	-0.342384	-5.036655	-0.860666
H	1.672960	3.619983	0.439770
H	1.500626	3.661336	-1.326940
H	1.129850	-3.275263	-0.762535
H	0.879213	-3.333103	0.995016
H	-1.632126	1.614604	2.298732
H	-1.414982	2.304792	3.906182
H	-3.358008	2.661169	0.674982
H	-4.331152	4.021937	1.211665
H	-3.743714	-2.750374	0.249083
H	-4.882445	-2.950322	-1.066332
H	-2.160259	-4.853449	0.853275
H	-2.342701	-6.315583	-0.101265
H	-3.789049	2.441924	3.090219
H	-3.118258	4.053700	3.395596
H	-4.534646	-5.103484	0.210404
H	-4.095394	-5.257241	-1.488648
H	3.962782	2.754732	-0.261937
H	3.469375	-2.863771	0.121351
H	1.715255	-0.199192	-2.414015
H	1.689855	0.473715	2.148539
H	3.759704	-0.820805	-3.667636

H	3.749283	0.733342	3.498388
H	5.877576	0.364056	-3.284015
H	5.634663	-0.819313	3.226683
H	7.673092	0.637018	-1.882375
H	8.476823	1.929602	-0.980786
H	7.256038	0.916235	-0.184333
H	6.079392	3.831061	-3.188229
H	7.786729	3.635095	-2.745298
H	6.962354	2.378457	-3.680551
H	5.590197	4.274371	-0.705686
H	6.066316	3.080871	0.521963
H	7.298718	4.003718	-0.346510
H	7.417345	-1.434387	1.923040
H	8.016470	-2.864781	1.071784
H	7.045093	-1.657138	0.206320
H	5.201351	-4.266678	3.154962
H	6.936066	-4.392169	2.801647
H	6.309276	-2.993768	3.687841
H	4.767731	-4.646617	0.652086
H	5.514918	-3.575761	-0.553311
H	6.512886	-4.695947	0.381589
Ni	-2.279209	0.451309	-0.181609
C	-8.830498	0.023643	0.411126
C	-8.815141	0.109605	-0.987688
C	-7.606740	0.214980	-1.690926
C	-6.433356	0.230494	-0.950200
C	-6.448677	0.145414	0.440993
C	-7.637936	0.040610	1.148251
C	-5.017750	0.191026	0.902480
N	-4.210119	0.298267	-0.221736
C	-4.992101	0.330924	-1.370774
O	-4.634027	0.142785	2.066715
O	-4.579893	0.412412	-2.521583
H	-9.782804	-0.057144	0.929182
H	-9.755787	0.094424	-1.532434
H	-7.582050	0.282931	-2.774763
H	-7.637247	-0.025572	2.232478

(*R*)-product

C	0.874368	1.241500	0.360371
C	1.531404	1.129133	-0.876432

C	2.551612	0.200955	-1.063824
C	2.960939	-0.654065	-0.027247
C	1.276047	0.385240	1.392220
C	2.300820	-0.545995	1.201520
C	4.084876	-1.645421	-0.242930
C	5.502903	-1.019140	-0.261331
H	3.927169	-2.165778	-1.197756
H	4.051281	-2.416443	0.539140
H	0.785598	0.448583	2.361597
H	1.233565	1.769831	-1.703253
H	3.037060	0.131809	-2.035274
H	2.588881	-1.198733	2.022554
H	5.500686	-0.222154	-1.019822
C	6.542863	-2.068927	-0.678637
C	5.870972	-0.387052	1.087851
H	5.149317	0.381072	1.384698
H	6.861923	0.079878	1.043358
H	5.898036	-1.147134	1.880357
H	6.312544	-2.493986	-1.663087
H	6.576361	-2.896309	0.042402
H	7.547210	-1.632033	-0.727731
C	0.263091	3.712243	0.430400
H	-0.605567	2.134524	1.598703
C	-0.232372	2.264315	0.571995
O	-2.095584	2.957345	-0.832009
C	-1.464833	2.030318	-0.336643
N	-1.827775	0.721103	-0.488182
H	-2.650423	-0.178737	-2.204797
H	-1.223793	0.006659	-0.104723
C	-2.980336	0.305008	-1.275169
H	-3.492365	1.230850	-1.555298
H	-4.164195	0.708961	1.152727
C	-3.906700	-0.627429	-0.517503
C	-4.435713	-0.253501	0.726335
C	-4.262171	-1.869767	-1.053301
C	-5.301231	-1.102489	1.414285
H	-3.855909	-2.172758	-2.016098
H	-5.705696	-0.797547	2.376036
C	-5.131598	-2.722441	-0.367830
C	-5.652617	-2.340956	0.868519
H	-5.396528	-3.684350	-0.798988

H	-6.327357	-3.002486	1.405293
H	-0.559240	4.411404	0.598310
H	0.655335	3.899594	-0.574149
H	1.061261	3.909611	1.153253

(*S*)-product

C	-0.874370	1.241501	0.360370
C	-1.531400	1.129131	-0.876430
C	-2.551610	0.200951	-1.063820
C	-2.960940	-0.654069	-0.027250
C	-1.276050	0.385241	1.392220
C	-2.300820	-0.545999	1.201520
C	-4.084880	-1.645419	-0.242930
C	-5.502900	-1.019139	-0.261330
H	-3.927169	-2.165779	-1.197760
H	-4.051279	-2.416439	0.539140
H	-0.785600	0.448581	2.361600
H	-1.233570	1.769831	-1.703250
H	-3.037060	0.131811	-2.035270
H	-2.588880	-1.198729	2.022550
H	-5.500690	-0.222149	-1.019820
C	-6.542859	-2.068930	-0.678640
C	-5.870970	-0.387049	1.087850
H	-5.149320	0.381071	1.384700
H	-6.861920	0.079880	1.043360
H	-5.898040	-1.147129	1.880360
H	-6.312539	-2.493989	-1.663090
H	-6.576359	-2.896310	0.042400
H	-7.547210	-1.632030	-0.727730
C	-0.263090	3.712241	0.430400
H	0.605570	2.134521	1.598700
C	0.232370	2.264311	0.572000
O	2.095580	2.957351	-0.832010
C	1.464830	2.030321	-0.336640
N	1.827770	0.721101	-0.488180
H	2.650420	-0.178739	-2.204800
H	1.223790	0.006661	-0.104720
C	2.980340	0.305012	-1.275170
H	3.492360	1.230852	-1.555300
H	4.164200	0.708962	1.152730
C	3.906700	-0.627428	-0.517500

C	4.435710	-0.253498	0.726330
C	4.262171	-1.869768	-1.053300
C	5.301230	-1.102488	1.414290
H	3.855911	-2.172758	-2.016100
H	5.705700	-0.797548	2.376040
C	5.131601	-2.722438	-0.367830
C	5.652621	-2.340958	0.868520
H	5.396531	-3.684348	-0.798990
H	6.327361	-3.002488	1.405290
H	0.559240	4.411401	0.598310
H	-0.655340	3.899591	-0.574150
H	-1.061260	3.909611	1.153250

IS

N	-1.640325	1.309489	1.196093
N	-2.130318	-1.031994	-0.961185
N	0.357331	1.411686	0.094575
N	0.136884	-0.894320	-1.092163
C	0.125139	3.890954	0.046281
C	0.776839	-3.168384	-1.942255
C	0.324676	2.628520	0.934828
C	-0.233965	-2.003102	-2.007447
C	1.189329	4.024577	-1.067447
C	0.061283	5.201852	0.866981
C	0.591432	-4.189221	-3.089496
C	0.921999	-3.877595	-0.572940
C	-0.871448	2.372451	1.893554
C	-1.728504	-2.266564	-1.676072
C	2.554767	4.510269	-0.554242
C	1.429822	5.672061	1.387516
C	-0.438332	-5.293944	-2.801872
C	-0.041998	-5.051575	-0.310222
C	-0.775492	0.785565	0.256554
C	-0.964219	-0.388396	-0.611569
C	2.438844	5.818569	0.239912
C	-0.103447	-6.027497	-1.494869
C	-2.552433	0.525619	1.972836
C	-3.430551	-0.486667	-1.074622
C	-2.193469	-0.747364	2.439318
C	-3.626187	0.864874	-1.404068
C	-3.786192	1.078048	2.319388

C	-4.535984	-1.328883	-0.910138
C	-3.062518	-1.502151	3.237266
C	-4.910323	1.402513	-1.546455
C	-2.699158	-2.904197	3.761502
C	-5.150918	2.879031	-1.915026
C	-4.656438	0.343261	3.123048
C	-5.818375	-0.807170	-1.066296
C	-4.302582	-0.928676	3.568760
C	-6.006210	0.538903	-1.371859
C	-3.711958	-3.933340	3.204825
C	-1.284105	-3.342251	3.339054
C	-2.760707	-2.910279	5.307833
C	-5.913531	2.955080	-3.259537
C	-5.997490	3.553195	-0.809014
C	-3.838449	3.671655	-2.062656
H	-0.851409	3.754741	-0.442790
H	1.726871	-2.657690	-2.131434
H	1.267089	2.696292	1.484546
H	-0.158507	-1.592169	-3.025701
H	1.303749	3.066969	-1.584675
H	0.812406	4.746639	-1.806293
H	-0.347403	5.982969	0.210046
H	-0.646616	5.114309	1.701265
H	0.342931	-3.663093	-4.021129
H	1.562808	-4.671398	-3.266938
H	1.944632	-4.277220	-0.529007
H	0.861588	-3.137028	0.233986
H	-1.498255	3.252274	2.055457
H	-0.543562	1.997013	2.871922
H	-1.869148	-3.132750	-1.023835
H	-2.346489	-2.400114	-2.567414
H	3.001612	3.738324	0.084499
H	3.238370	4.637960	-1.403029
H	1.819798	4.955753	2.125280
H	1.310800	6.624698	1.919602
H	-1.451876	-4.871603	-2.735455
H	-0.459376	-6.002639	-3.639772
H	-1.056602	-4.687652	-0.097169
H	0.278750	-5.580618	0.596844
H	3.419845	6.118925	0.629605
H	2.106735	6.625779	-0.430288

H	-0.837213	-6.819669	-1.297269
H	0.871781	-6.524524	-1.605901
H	-1.214450	-1.132593	2.177534
H	-2.753378	1.483786	-1.570539
H	-4.060139	2.060071	1.946956
H	-4.390814	-2.372611	-0.649171
H	-5.622096	0.761020	3.394406
H	-6.680066	-1.456974	-0.938568
H	-5.004696	-1.480077	4.187252
H	-7.018294	0.915998	-1.484035
H	-3.683198	-3.957696	2.109191
H	-3.475255	-4.938984	3.572975
H	-4.738404	-3.699783	3.506898
H	-0.513741	-2.664924	3.724880
H	-1.073757	-4.340815	3.737932
H	-1.178168	-3.395907	2.249677
H	-2.049743	-2.191744	5.731295
H	-3.757906	-2.653569	5.680168
H	-2.507914	-3.905369	5.693330
H	-6.882430	2.447553	-3.208282
H	-6.098270	4.000826	-3.534058
H	-5.334257	2.489575	-4.064988
H	-5.476186	3.526640	0.155213
H	-6.187918	4.603331	-1.061871
H	-6.966688	3.061037	-0.677928
H	-3.254731	3.667851	-1.134820
H	-3.207670	3.274036	-2.865762
H	-4.063543	4.715557	-2.308170
Ni	1.737389	0.244189	-0.753363
Br	3.696585	-0.863225	-3.069413
C	3.432013	-0.478015	-1.076925
C	3.581129	0.912103	-0.649156
C	4.234720	1.151204	0.614126
C	4.646426	0.139180	1.449673
C	3.943852	-1.516955	-0.223088
C	4.470583	-1.215290	1.005326
C	5.316640	0.426304	2.779617
C	6.872252	0.458639	2.785426
H	4.993505	-0.324022	3.516173
H	4.963609	1.396095	3.156035
H	3.887532	-2.549416	-0.556262

H	3.680487	1.695436	-1.400367
H	4.440847	2.183498	0.896955
H	4.782760	-2.026218	1.660358
H	7.160023	0.680881	3.824785
C	7.430331	1.582046	1.900682
C	7.498742	-0.893329	2.414646
H	7.134675	-1.696663	3.067688
H	8.590754	-0.854584	2.511444
H	7.264061	-1.170095	1.380811
H	7.036318	2.561135	2.201590
H	7.164294	1.424177	0.849476
H	8.524182	1.626855	1.969132

TS1

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C	0.219014	3.878557	0.548305
C	0.827275	-3.181096	-1.738457
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C	-0.132115	-1.976877	-1.831572
C	1.444460	4.022577	-0.381738
C	0.127304	5.113273	1.477652
C	0.677735	-4.158913	-2.928574
C	0.859683	-3.934534	-0.386158
C	-1.127568	2.304703	2.108331
C	-1.659176	-2.202540	-1.675287
C	2.750024	4.316830	0.376082
C	1.430507	5.405539	2.240873
C	-0.404278	-5.235130	-2.741480
C	-0.166666	-5.073046	-0.223657
C	-0.855461	0.755459	0.446965
C	-0.963984	-0.388558	-0.468286
C	2.619056	5.551126	1.279782
C	-0.182878	-6.014628	-1.436974
C	-2.812687	0.458595	1.952383
C	-3.352286	-0.360903	-1.238776
C	-2.536358	-0.840675	2.402372
C	-3.448856	1.007885	-1.539752
C	-4.066790	1.028081	2.177780

C	-4.504206	-1.155474	-1.238255
C	-3.507111	-1.603735	3.063436
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C	-3.235863	-3.033910	3.566948
C	-4.812527	3.105962	-2.155202
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C	-5.735041	-0.569546	-1.526345
C	-4.765310	-1.012709	3.274025
C	-5.827259	0.792948	-1.801693
C	-4.189567	-4.015896	2.845092
C	-1.786948	-3.485740	3.303881
C	-3.488907	-3.102781	5.092165
C	-5.407795	3.259167	-3.575508
C	-5.752536	3.785948	-1.131278
C	-3.458075	3.838853	-2.121846
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H	1.801919	-2.698446	-1.860361
H	1.061908	2.500269	2.015052
H	0.071450	-1.505340	-2.802565
H	1.553700	3.121096	-0.992608
H	1.244350	4.851485	-1.075513
H	-0.111487	5.983045	0.849409
H	-0.707060	5.017868	2.184560
H	0.508440	-3.593785	-3.854363
H	1.640642	-4.671604	-3.062330
H	1.860554	-4.378668	-0.288282
H	0.772588	-3.215293	0.437592
H	-1.754821	3.198271	2.163182
H	-0.959259	1.941370	3.129914
H	-1.898937	-3.073000	-1.057232
H	-2.175722	-2.302300	-2.632886
H	3.028204	3.446076	0.984939
H	3.565528	4.458678	-0.344456
H	1.638713	4.596867	2.956548
H	1.306845	6.317410	2.839050
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H	-0.391101	-5.920116	-3.599085
H	-1.177605	-4.669373	-0.073595
H	0.065791	-5.637940	0.688823
H	3.546824	5.715032	1.842586
H	2.469056	6.444561	0.655364

H	-0.955195	-6.784553	-1.310815
H	0.779893	-6.543860	-1.497218
H	-1.542286	-1.240312	2.236829
H	-2.536096	1.589015	-1.583116
H	-4.277074	2.029830	1.816691
H	-4.435944	-2.212615	-1.000895
H	-6.020997	0.715011	3.019694
H	-6.632746	-1.182110	-1.526461
H	-5.545573	-1.570209	3.783759
H	-6.801458	1.220406	-2.019271
H	-4.024301	-3.997240	1.761543
H	-4.019496	-5.040759	3.196682
H	-5.241215	-3.770121	3.026897
H	-1.059556	-2.841257	3.810681
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H	-2.824196	-2.418195	5.631292
H	-4.520148	-2.840386	5.350095
H	-3.302272	-4.118344	5.461517
H	-6.397483	2.797444	-3.655145
H	-5.512689	4.320418	-3.832066
H	-4.758916	2.791071	-4.324284
H	-5.348887	3.706330	-0.114825
H	-5.866685	4.850959	-1.367408
H	-6.750719	3.336053	-1.130061
H	-2.988800	3.780904	-1.132697
H	-2.754816	3.434709	-2.858587
H	-3.606494	4.898941	-2.356123
Ni	1.731715	0.307535	-0.450758
Br	2.817052	-0.219387	-3.079154
C	3.352953	-0.409567	-0.732351
C	3.787343	0.862956	-0.253823
C	4.779164	0.901198	0.760084
C	5.377017	-0.256199	1.239880
C	4.024848	-1.583118	-0.328653
C	4.983974	-1.495808	0.664478
C	6.453408	-0.207433	2.306992
C	7.925535	-0.145300	1.807095
H	6.355526	-1.088519	2.956920
H	6.280934	0.667458	2.948246
H	3.746149	-2.548291	-0.739057

H	3.602120	1.771296	-0.819306
H	5.128794	1.868636	1.118288
H	5.437926	-2.412280	1.037180
H	8.544009	-0.112289	2.717159
C	8.214713	1.131197	1.004909
C	8.336871	-1.395403	1.016270
H	8.171525	-2.310917	1.598290
H	9.401029	-1.355402	0.753852
H	7.767000	-1.482622	0.084325
H	7.974673	2.031531	1.584620
H	7.625363	1.160522	0.081478
H	9.274554	1.185510	0.728114

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C	1.764701	2.702532	-0.326732
C	-1.391187	-3.734184	-1.240068
C	1.492859	1.572351	0.715156
C	-1.357020	-2.335178	-1.917683
C	2.807779	2.302992	-1.396713
C	2.179012	4.052572	0.309847
C	-2.014032	-4.826955	-2.143728
C	-1.975334	-3.800013	0.190035
C	0.380915	1.940412	1.720348
C	-2.668259	-1.508503	-2.026008
C	4.258250	2.348501	-0.887582
C	3.621117	4.074060	0.840420
C	-3.544945	-4.952496	-2.060363
C	-3.505903	-3.954126	0.275105
C	-0.395850	0.467903	0.181010
C	-1.172609	-0.467718	-0.659504
C	4.614858	3.706675	-0.269484
C	-4.012224	-5.107375	-0.605202
C	-2.047033	1.375486	1.817768
C	-3.328193	0.705327	-1.086377
C	-2.377127	0.214961	2.531626
C	-2.836178	1.858384	-1.714857
C	-2.827677	2.524766	1.935451

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C	-3.503058	0.171133	3.364562
C	-3.643756	2.988227	-1.897853
C	-3.888091	-1.078496	4.178749
C	-3.136767	4.268282	-2.588855
C	-3.953638	2.494603	2.756576
C	-5.470924	1.764062	-0.835521
C	-4.286493	1.335420	3.454461
C	-4.972801	2.914395	-1.444395
C	-5.258541	-1.602662	3.686934
C	-2.854613	-2.211981	4.039318
C	-3.989490	-0.708882	5.678319
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C	-3.265684	5.464177	-1.615372
C	-1.662676	4.158940	-3.022280
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H	-0.324753	-3.970264	-1.163657
H	2.412909	1.270628	1.216429
H	-0.911235	-2.490817	-2.904039
H	2.582383	1.304806	-1.784577
H	2.703749	3.004169	-2.237845
H	2.089518	4.817476	-0.475180
H	1.481208	4.359746	1.098519
H	-1.694933	-4.675783	-3.183065
H	-1.582239	-5.789349	-1.835280
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H	-1.643666	-2.931023	0.772539
H	0.291196	3.007742	1.922264
H	0.500018	1.411814	2.677162
H	-3.577415	-2.084318	-1.864545
H	-2.745723	-1.005572	-2.999268
H	4.413866	1.556809	-0.146074
H	4.936546	2.115582	-1.717272
H	3.728821	3.366288	1.675415
H	3.845739	5.068054	1.248673
H	-4.033498	-4.077805	-2.512593
H	-3.871378	-5.816542	-2.653507
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H	-3.794097	-4.130372	1.320005
H	5.638776	3.688497	0.124636
H	4.589674	4.487141	-1.045405

H	-5.107050	-5.171925	-0.557362
H	-3.625665	-6.057104	-0.206447
H	-1.726157	-0.647563	2.440462
H	-1.812753	1.852079	-2.072840
H	-2.562307	3.414929	1.374583
H	-5.020270	-0.243829	-0.158954
H	-4.577470	3.379157	2.849975
H	-6.502878	1.736658	-0.496611
H	-5.169493	1.342663	4.086621
H	-5.634737	3.765756	-1.573385
H	-5.210989	-1.894401	2.631419
H	-5.560784	-2.482356	4.267941
H	-6.044338	-0.846760	3.792172
H	-1.862969	-1.905323	4.391676
H	-3.167088	-3.070547	4.643927
H	-2.759491	-2.557993	3.004610
H	-3.032734	-0.329741	6.055054
H	-4.750069	0.056207	5.864955
H	-4.259036	-1.593832	6.266928
H	-5.049708	4.676980	-3.606264
H	-3.645315	5.453325	-4.352390
H	-3.914720	3.712326	-4.562726
H	-2.654738	5.308188	-0.718307
H	-2.923902	6.386903	-2.099413
H	-4.300535	5.621011	-1.293498
H	-0.996582	3.988675	-2.168377
H	-1.506427	3.350701	-3.745650
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Ni	1.526360	-1.239080	-0.874199
Br	2.039436	-3.037403	-2.265483
C	3.309960	-1.125736	-0.237801
C	4.480021	-1.142717	-1.014994
C	5.748367	-1.139983	-0.429624
C	5.915876	-1.134574	0.963830
C	3.483729	-1.127872	1.157798
C	4.754131	-1.136968	1.746624
C	7.294105	-1.153366	1.596146
C	7.944244	0.229422	1.886281
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H	7.245969	-1.706279	2.544426
H	2.615363	-1.143478	1.816838

H	4.403896	-1.191105	-2.097361
H	6.628848	-1.167940	-1.070079
H	4.841194	-1.165785	2.832169
H	8.921805	0.007966	2.341309
C	7.141040	1.053242	2.902734
C	8.205108	1.035736	0.606263
H	8.825716	0.472333	-0.101551
H	8.726669	1.973473	0.834924
H	7.267028	1.286737	0.098089
H	6.999462	0.502718	3.841313
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H	7.656963	1.991853	3.140067

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C	-0.789877	-2.483986	0.710356
C	0.844359	1.728795	-2.467251
C	-2.044211	-3.932877	-1.020229
C	-1.407988	-4.907758	1.223169
C	0.468879	3.756051	-4.005471
C	-0.669463	3.743534	-1.716563
C	0.374109	-2.419742	1.744607
C	2.190465	2.017247	-1.748171
C	-3.490933	-3.740897	-0.535107
C	-2.851575	-4.716221	1.721662
C	1.391666	4.888219	-3.524946
C	0.210564	4.931234	-1.281931
C	0.620888	-0.825479	0.119381
C	1.083393	0.277326	-0.758147
C	-3.856557	-4.755002	0.559673
C	0.686999	5.766142	-2.480100
C	1.855794	-0.422584	2.260554
C	3.577722	0.260409	-0.518051
C	1.550552	0.935556	2.438469
C	3.787450	-1.118677	-0.677243
C	2.837435	-1.030585	3.047156

C	4.622441	1.081619	-0.084224
C	2.231648	1.716009	3.380411
C	5.021108	-1.707156	-0.378011
C	1.912885	3.206060	3.605117
C	5.277274	-3.216813	-0.545976
C	3.512651	-0.266572	3.997221
C	5.861252	0.508454	0.197567
C	3.220961	1.086328	4.156076
C	6.056927	-0.864162	0.062295
C	3.178808	4.046879	3.313100
C	0.777926	3.710339	2.694257
C	1.481079	3.424456	5.075232
C	6.410306	-3.433852	-1.577657
C	5.702655	-3.817829	0.815004
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H	-1.722164	-2.117508	1.156122
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H	-1.962064	-4.916066	-1.505911
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H	-0.706563	-4.869719	2.068379
H	0.982140	3.125718	-4.744159
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H	2.165613	2.933527	-1.151210
H	3.041164	2.064981	-2.431324
H	-3.629533	-2.718094	-0.159680
H	-4.172849	-3.841842	-1.388081
H	-2.944979	-3.756935	2.250859
H	-3.089006	-5.494261	2.458658
H	2.316349	4.476973	-3.093479
H	1.703100	5.496065	-4.384074
H	1.088235	4.583941	-0.718794
H	-0.357710	5.561177	-0.585401
H	-4.871741	-4.567923	0.931642
H	-3.862558	-5.767225	0.127626

H	1.351303	6.572492	-2.143233
H	-0.181025	6.251473	-2.950398
H	0.750757	1.365491	1.846832
H	2.975581	-1.720572	-1.067313
H	3.075688	-2.080110	2.905648
H	4.462245	2.147755	0.042968
H	4.279750	-0.729453	4.611941
H	6.678730	1.139264	0.535924
H	3.766723	1.655609	4.902477
H	7.032896	-1.279955	0.293818
H	3.503300	3.918901	2.273670
H	2.974129	5.111925	3.475555
H	4.015395	3.765015	3.961136
H	-0.161066	3.173804	2.870561
H	0.591720	4.771673	2.892030
H	1.030821	3.615297	1.632179
H	0.582428	2.842990	5.310159
H	2.264655	3.130255	5.781208
H	1.255675	4.483249	5.250328
H	7.344419	-2.955664	-1.265019
H	6.609526	-4.504901	-1.703621
H	6.134188	-3.022628	-2.555147
H	4.914300	-3.686605	1.565672
H	5.897321	-4.892158	0.712287
H	6.613361	-3.349751	1.202745
H	3.190721	-3.880425	-0.338629
H	3.697629	-3.627402	-2.021473
H	4.261582	-5.043260	-1.129076
Ni	-1.500997	-0.395234	-1.723055
Br	-1.841670	-0.709069	-4.058837
C	-2.904667	0.304480	-0.505895
C	-4.219134	0.452140	-0.989547
C	-5.252127	0.955294	-0.192440
C	-5.025925	1.338353	1.137706
C	-2.693199	0.703024	0.825880
C	-3.719304	1.210302	1.629889
C	-6.146714	1.874831	2.006480
C	-6.948851	0.820087	2.821494
H	-6.858924	2.424664	1.376188
H	-5.734606	2.605181	2.716599
H	-1.695824	0.629853	1.264882

H	-4.445051	0.178720	-2.019338
H	-6.250684	1.063201	-0.614109
H	-3.502533	1.520335	2.651920
H	-7.705351	1.390913	3.381455
C	-6.075012	0.084312	3.847302
C	-7.694945	-0.174369	1.920749
H	-8.361748	0.343219	1.220016
H	-8.307141	-0.859355	2.520211
H	-6.995444	-0.777047	1.330554
H	-5.580732	0.787279	4.529792
H	-5.294409	-0.504047	3.351624
H	-6.679416	-0.601251	4.453938

TS2-R

N	-2.172969	-1.037095	-1.876533
N	-2.357280	-1.453185	1.270476
N	-0.127259	-0.268751	-1.295214
N	-0.882027	0.271038	1.245823
C	1.152370	-1.108671	-3.294501
C	-1.125977	1.270799	3.535913
C	-0.079468	-0.334128	-2.771736
C	-1.091232	-0.019400	2.686353
C	2.497724	-0.512700	-2.826865
C	1.146063	-1.220236	-4.838916
C	-0.965711	0.990871	5.049324
C	-2.293807	2.252979	3.266613
C	-1.428955	-1.017854	-3.154066
C	-2.306147	-0.989867	2.684305
C	2.860621	0.806652	-3.526474
C	1.506440	0.097630	-5.547325
C	-2.280950	0.660515	5.772738
C	-3.587959	1.998791	4.065095
C	-1.302894	-0.643702	-0.899507
C	-1.543998	-0.609061	0.564501
C	2.853219	0.649348	-5.053732
C	-3.315413	1.774923	5.559795
C	-3.587211	-1.129011	-1.815444
C	-2.580396	-2.824036	0.933393
C	-4.334751	-0.179934	-1.101164
C	-1.517906	-3.605274	0.454619
C	-4.235843	-2.143071	-2.525219

C	-3.841415	-3.386257	1.135259
C	-5.732326	-0.239876	-1.054948
C	-1.698413	-4.958526	0.143258
C	-6.579194	0.790545	-0.284374
C	-0.549721	-5.843709	-0.375074
C	-5.628067	-2.203464	-2.498609
C	-4.026742	-4.738511	0.849561
C	-6.364898	-1.273500	-1.768789
C	-2.975142	-5.508827	0.355709
C	-7.544490	1.500339	-1.263965
C	-7.400727	0.062133	0.806163
C	-5.717355	1.867751	0.400769
C	-0.265602	-6.961934	0.656580
C	-0.959741	-6.483694	-1.722987
C	0.750662	-5.047925	-0.598252
H	1.067005	-2.123195	-2.876767
H	-0.212074	1.787677	3.213405
H	-0.051916	0.701129	-3.131954
H	-0.190815	-0.571261	2.992073
H	2.500638	-0.393795	-1.738495
H	3.278614	-1.255525	-3.047161
H	1.888304	-1.981137	-5.118100
H	0.180381	-1.595476	-5.205119
H	-0.227994	0.192516	5.204384
H	-0.542791	1.891779	5.515756
H	-1.934259	3.257221	3.529601
H	-2.507296	2.289307	2.191668
H	-1.271298	-2.042708	-3.513569
H	-1.999388	-0.469707	-3.908656
H	-3.248865	-0.498105	2.936454
H	-2.167505	-1.844513	3.349958
H	2.151159	1.592934	-3.236945
H	3.838718	1.145868	-3.167946
H	0.721531	0.847760	-5.371311
H	1.531899	-0.067757	-6.632303
H	-2.690255	-0.294666	5.412377
H	-2.084873	0.522566	6.843581
H	-4.128304	1.128210	3.669305
H	-4.262855	2.853654	3.928464
H	3.069876	1.609143	-5.539465
H	3.655012	-0.042177	-5.354561

H	-4.250126	1.540237	6.084869
H	-2.932316	2.706057	6.003154
H	-3.803479	0.623471	-0.605087
H	-0.540719	-3.142006	0.365540
H	-3.658700	-2.881707	-3.072327
H	-4.660760	-2.769792	1.491675
H	-6.141258	-2.990055	-3.045023
H	-5.002241	-5.192215	1.002351
H	-7.448079	-1.349641	-1.765324
H	-3.153387	-6.558352	0.140344
H	-8.224062	0.794885	-1.753187
H	-8.157016	2.234749	-0.727248
H	-6.989317	2.028813	-2.047144
H	-6.741591	-0.438420	1.525399
H	-8.021010	0.778711	1.357993
H	-8.066253	-0.695309	0.378902
H	-5.027138	1.435319	1.134198
H	-5.131123	2.445014	-0.323169
H	-6.364665	2.571764	0.935272
H	-1.146400	-7.589551	0.830829
H	0.543050	-7.611233	0.299835
H	0.040446	-6.537255	1.619204
H	-1.164796	-5.714214	-2.476597
H	-0.150469	-7.119715	-2.101162
H	-1.855006	-7.107444	-1.628861
H	0.618096	-4.250084	-1.338421
H	1.126655	-4.589084	0.322153
H	1.530496	-5.719709	-0.974247
Ni	0.902276	0.758480	0.196960
Br	2.071159	-1.174968	1.238604
C	0.595794	2.604514	-0.474071
C	-0.702473	3.147367	-0.430050
C	-1.010344	4.403225	-0.960784
C	-0.026944	5.191837	-1.574684
C	1.570645	3.400325	-1.110030
C	1.266698	4.657899	-1.645331
C	-0.351072	6.559675	-2.142129
C	-0.194256	7.762048	-1.167474
H	-1.385659	6.560641	-2.512743
H	0.290231	6.748606	-3.013835
H	2.597779	3.051230	-1.195858

H	-1.508654	2.577266	0.029729
H	-2.033233	4.775037	-0.905571
H	2.053995	5.230335	-2.133927
H	-0.468913	8.653937	-1.751277
C	1.254314	7.948169	-0.694393
C	-1.156501	7.678627	0.026010
H	-2.199510	7.597628	-0.305490
H	-1.074613	8.573324	0.655362
H	-0.936441	6.806204	0.651729
H	1.940990	8.060667	-1.542526
H	1.592442	7.088761	-0.104635
H	1.347249	8.843943	-0.068106
C	3.593317	1.817272	2.876943
H	3.138473	3.071740	1.076241
C	3.635699	2.175545	1.426970
O	4.705462	2.058728	-0.675533
C	4.517006	1.546873	0.440268
N	5.165183	0.395340	0.841323
H	6.294926	0.328239	-0.869735
H	4.676167	-0.154909	1.539904
C	5.925625	-0.384775	-0.126135
H	5.267093	-1.086882	-0.658494
H	6.616528	-2.996851	-0.480661
C	7.071202	-1.143450	0.515029
C	7.294788	-2.488722	0.201486
C	7.946535	-0.507329	1.406727
C	8.372062	-3.184468	0.755773
H	7.772271	0.533579	1.665294
H	8.528165	-4.229872	0.501544
C	9.020724	-1.199382	1.964908
C	9.238844	-2.541336	1.639815
H	9.690371	-0.691200	2.654414
H	10.075633	-3.080777	2.075992
H	2.937166	2.496483	3.429741
H	4.595617	1.867886	3.329343
H	3.225071	0.793066	3.030972

IM3-R

N	-2.188496	-1.062271	-1.504333
N	-1.302766	-2.066201	1.386191
N	-0.101807	-0.183848	-1.386632

N	-0.334113	-0.002119	1.373025
C	0.393857	-1.182750	-3.635231
C	-0.866694	0.507578	3.752230
C	-0.441498	-0.146245	-2.831392
C	-0.180076	-0.476696	2.768764
C	1.920842	-0.984058	-3.501700
C	0.013461	-1.216530	-5.136865
C	-0.434929	0.306824	5.226258
C	-2.406105	0.630470	3.635149
C	-1.963208	-0.467316	-2.842884
C	-0.648443	-1.961218	2.716911
C	2.449777	0.219626	-4.299006
C	0.533815	-0.007661	-5.932706
C	-1.240872	-0.751052	5.998676
C	-3.218522	-0.395790	4.447843
C	-1.093758	-0.724682	-0.753757
C	-0.932903	-0.930531	0.706158
C	2.053961	0.144411	-5.780021
C	-2.748860	-0.473479	5.908391
C	-3.535324	-1.154291	-1.017034
C	-1.399150	-3.369136	0.786728
C	-4.136942	-0.052965	-0.389627
C	-0.339706	-3.872522	0.017247
C	-4.266877	-2.313508	-1.270495
C	-2.522650	-4.151128	1.052575
C	-5.481900	-0.089172	0.002892
C	-0.393683	-5.165800	-0.520750
C	-6.193146	1.110426	0.657047
C	0.755610	-5.763545	-1.353869
C	-5.605455	-2.364911	-0.880510
C	-2.584303	-5.442603	0.528181
C	-6.199618	-1.270961	-0.255166
C	-1.538564	-5.936823	-0.249493
C	-7.348976	1.575749	-0.261832
C	-6.770724	0.687945	2.028735
C	-5.247234	2.305340	0.879733
C	1.315287	-7.009694	-0.625910
C	0.221332	-6.181763	-2.744638
C	1.910641	-4.766228	-1.561267
H	0.141665	-2.163206	-3.203712
H	-0.458039	1.478884	3.441861

H	-0.252213	0.865844	-3.197995
H	0.892089	-0.452865	2.987893
H	2.207090	-0.901207	-2.450048
H	2.402622	-1.895985	-3.885717
H	0.453694	-2.128763	-5.564280
H	-1.070495	-1.316940	-5.276878
H	0.638176	0.078122	5.270987
H	-0.563430	1.267912	5.744908
H	-2.682030	1.632682	3.994319
H	-2.699991	0.594070	2.579171
H	-2.253081	-1.176070	-3.621385
H	-2.580768	0.434525	-2.946327
H	-1.343305	-2.248660	3.504894
H	0.211556	-2.639855	2.738366
H	2.068035	1.150564	-3.862701
H	3.539847	0.270768	-4.192606
H	0.039818	0.912342	-5.587201
H	0.261508	-0.121843	-6.990244
H	-1.026941	-1.757325	5.613576
H	-0.920399	-0.755507	7.048492
H	-3.153938	-1.389453	3.987116
H	-4.280795	-0.119545	4.412210
H	2.403571	1.034543	-6.319535
H	2.548497	-0.720256	-6.248544
H	-3.314144	-1.242941	6.449766
H	-2.965686	0.482891	6.407821
H	-3.537159	0.838226	-0.236307
H	0.533567	-3.241234	-0.120848
H	-3.785112	-3.157257	-1.753077
H	-3.332945	-3.743585	1.648883
H	-6.188473	-3.262816	-1.066715
H	-3.453064	-6.065601	0.724428
H	-7.245702	-1.338047	0.029380
H	-1.613856	-6.946581	-0.643148
H	-8.084169	0.781179	-0.427906
H	-7.873301	2.426900	0.189344
H	-6.969322	1.890810	-1.240472
H	-5.974737	0.354235	2.704013
H	-7.284131	1.534383	2.500647
H	-7.494618	-0.128511	1.935596
H	-4.414849	2.049472	1.544552

H	-4.828543	2.680178	-0.060767
H	-5.800636	3.128731	1.345342
H	0.549019	-7.779204	-0.481103
H	2.130297	-7.455216	-1.209280
H	1.711872	-6.740685	0.359589
H	-0.177622	-5.316694	-3.287194
H	1.029752	-6.614501	-3.346380
H	-0.576025	-6.929580	-2.672972
H	1.587121	-3.871643	-2.103930
H	2.352697	-4.433223	-0.616876
H	2.702756	-5.242357	-2.150735
Ni	1.194613	0.901432	-0.156631
Br	2.545840	-1.209287	0.521495
C	0.180780	2.517719	-0.573351
C	-0.913114	2.926510	0.200958
C	-1.706108	4.012603	-0.186823
C	-1.435462	4.738751	-1.355574
C	0.464280	3.248065	-1.736704
C	-0.337591	4.327939	-2.123735
C	-2.290365	5.921528	-1.766954
C	-1.844309	7.311893	-1.230228
H	-3.324368	5.750397	-1.437238
H	-2.321365	5.978775	-2.863608
H	1.322447	2.982290	-2.346476
H	-1.161784	2.390134	1.111412
H	-2.552915	4.300025	0.434976
H	-0.101851	4.860009	-3.044241
H	-2.576680	8.030374	-1.628745
C	-0.461127	7.726460	-1.751623
C	-1.902737	7.395702	0.301619
H	-2.903435	7.149497	0.678524
H	-1.656513	8.407679	0.645397
H	-1.191436	6.702179	0.764420
H	-0.426997	7.717107	-2.848235
H	0.319783	7.049272	-1.387483
H	-0.208075	8.740334	-1.418558
C	2.741151	1.859138	2.245182
H	2.143282	3.162244	0.624835
C	2.483584	2.135405	0.771722
O	2.952510	1.458334	-1.404412
C	3.469835	1.820259	-0.317446

N	4.817069	1.888783	-0.234747
H	5.025971	2.756576	1.629838
H	5.280962	1.528845	-1.062680
C	5.671448	2.375051	0.837339
H	6.251591	3.233676	0.472146
H	8.211982	2.741323	1.714136
C	6.622954	1.320948	1.382776
C	7.901039	1.702474	1.809436
C	6.237148	-0.021486	1.495218
C	8.780076	0.764756	2.353257
H	5.253102	-0.339389	1.157057
H	9.769521	1.075904	2.678535
C	7.120488	-0.959109	2.034492
C	8.390554	-0.571344	2.466617
H	6.810262	-1.997610	2.114683
H	9.074706	-1.305767	2.883776
H	1.784061	1.854177	2.778645
H	3.348122	2.640173	2.727309
H	3.215101	0.888097	2.404156

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N	-2.168709	0.958461	-0.773359
N	-1.600092	-1.699338	0.889232
N	0.017714	0.587221	-1.258585
N	0.379712	-0.610525	1.230747
C	-0.439158	0.719054	-3.713223
C	0.648537	-1.317785	3.617602
C	-0.455517	1.467231	-2.349658
C	0.430726	-1.775487	2.150634
C	0.946662	0.152556	-4.094672
C	-0.976004	1.592840	-4.874212
C	0.947930	-2.487360	4.589846
C	-0.412877	-0.365544	4.215898
C	-1.899110	1.860113	-1.914960
C	-0.835555	-2.607601	1.783353
C	1.935971	1.231942	-4.563837
C	0.011663	2.676642	-5.338582
C	-0.292710	-3.170848	5.193401
C	-1.653774	-1.057997	4.806147
C	-0.984590	0.325389	-0.483166
C	-0.741559	-0.666024	0.593931

C	1.367496	2.065541	-5.720329
C	-1.258039	-2.148668	5.813889
C	-3.271354	1.190740	0.086119
C	-2.448437	-2.294761	-0.111067
C	-4.514802	1.502072	-0.490664
C	-3.804995	-2.476811	0.175243
C	-3.142247	1.178651	1.479141
C	-1.902047	-2.742177	-1.317613
C	-5.634839	1.806923	0.290948
C	-4.659145	-3.107845	-0.738239
C	-6.986549	2.215069	-0.326283
C	-6.154251	-3.340267	-0.452724
C	-4.260560	1.445242	2.267563
C	-2.748616	-3.355796	-2.242257
C	-5.487690	1.760010	1.688473
C	-4.100682	-3.536779	-1.955436
C	-8.111369	1.294089	0.201850
C	-7.296273	3.677679	0.076585
C	-6.983510	2.130958	-1.864661
C	-7.001768	-2.639461	-1.540921
C	-6.450415	-4.859070	-0.474772
C	-6.580808	-2.787618	0.920643
H	-1.125195	-0.131844	-3.585896
H	1.576409	-0.734323	3.551293
H	0.196734	2.345029	-2.386938
H	1.316920	-2.350630	1.863798
H	1.368902	-0.418803	-3.264120
H	0.791544	-0.560498	-4.918166
H	-1.179573	0.922563	-5.721393
H	-1.940842	2.051854	-4.620980
H	1.588092	-3.229550	4.094718
H	1.541165	-2.080931	5.421701
H	0.071930	0.196614	5.027786
H	-0.700941	0.380792	3.466547
H	-2.627161	1.694812	-2.712470
H	-1.982711	2.901302	-1.580971
H	-1.450376	-2.902199	2.632954
H	-0.555849	-3.504482	1.220269
H	2.189473	1.892652	-3.725341
H	2.877893	0.754074	-4.857722
H	0.159908	3.418768	-4.540178

H	-0.418427	3.223760	-6.187858
H	-0.820222	-3.758286	4.430857
H	0.030097	-3.891909	5.955584
H	-2.268499	-1.492200	4.007336
H	-2.286252	-0.307255	5.298773
H	2.072348	2.855562	-6.011660
H	1.234178	1.423214	-6.604186
H	-2.151549	-2.654989	6.201249
H	-0.769241	-1.673891	6.678051
H	-4.593510	1.498972	-1.570356
H	-4.173187	-2.105473	1.124184
H	-2.180401	0.995630	1.942042
H	-0.834812	-2.636591	-1.505046
H	-4.161594	1.433909	3.349789
H	-2.344415	-3.710401	-3.186668
H	-6.330700	1.988703	2.333416
H	-4.728979	-4.028756	-2.692852
H	-8.202239	1.339581	1.291908
H	-9.076795	1.594203	-0.223358
H	-7.929414	0.249877	-0.075727
H	-6.519938	4.358453	-0.290948
H	-8.256658	3.995364	-0.347770
H	-7.355109	3.794349	1.163882
H	-6.246348	2.808268	-2.310770
H	-6.774177	1.114574	-2.218234
H	-7.967764	2.418608	-2.250840
H	-6.783121	-3.026379	-2.541771
H	-8.071189	-2.793390	-1.350965
H	-6.808437	-1.560491	-1.550848
H	-5.869168	-5.382532	0.292924
H	-7.514328	-5.043317	-0.280763
H	-6.205119	-5.308224	-1.442885
H	-6.041951	-3.276102	1.740674
H	-6.413012	-1.707464	0.997718
H	-7.650363	-2.970428	1.075329
Ni	1.873698	0.144978	-0.332251
Br	2.063640	-2.420469	-0.920734
C	2.365163	1.871126	0.467715
C	1.924527	2.172000	1.771582
C	1.622781	3.479081	2.152695
C	1.771990	4.559722	1.270386

C	2.538851	2.961560	-0.414035
C	2.231816	4.263856	-0.022658
C	1.456787	5.979453	1.694560
C	2.629562	6.788544	2.320277
H	0.634143	5.963344	2.422646
H	1.088316	6.541043	0.825066
H	2.909645	2.783691	-1.418346
H	1.785490	1.372445	2.491041
H	1.254875	3.661823	3.160966
H	2.347946	5.071494	-0.743754
H	2.211263	7.778400	2.558000
C	3.786648	7.001380	1.334121
C	3.131619	6.172569	3.633752
H	2.318177	6.064017	4.362069
H	3.904930	6.803194	4.088907
H	3.564698	5.179758	3.466286
H	3.443332	7.487839	0.412529
H	4.250894	6.048413	1.055508
H	4.563739	7.636190	1.776851
C	4.034476	-0.510352	1.517932
H	4.462092	1.435458	0.733066
C	3.881391	0.561023	0.432229
O	3.396424	0.449616	-1.885473
C	4.258837	0.245262	-1.007160
N	5.486010	-0.188710	-1.371884
H	6.474633	-0.040485	0.437945
H	5.543184	-0.430318	-2.356125
C	6.654248	-0.467573	-0.552108
H	7.509629	0.081155	-0.967773
H	9.102376	-1.536389	-0.132883
C	7.006578	-1.945254	-0.447000
C	8.338666	-2.308695	-0.208088
C	6.033865	-2.946566	-0.558408
C	8.696451	-3.649448	-0.067846
H	4.994006	-2.694162	-0.755457
H	9.734137	-3.915890	0.116012
C	6.396333	-4.289398	-0.423312
C	7.722866	-4.645531	-0.176132
H	5.631142	-5.055504	-0.514349
H	7.999163	-5.691762	-0.074032
H	3.463765	-0.202994	2.400657

H	5.075242	-0.624955	1.849693
H	3.663214	-1.481195	1.184870

TS2-S

N	-1.988989	-1.214970	-1.521372
N	-2.467050	-1.105762	1.613219
N	0.170549	-0.875914	-0.881631
N	-0.633242	0.208870	1.481350
C	0.808295	-2.767911	-2.362757
C	-0.951899	1.789047	3.409610
C	0.235830	-1.314076	-2.308426
C	-1.076080	0.337775	2.891837
C	2.346823	-2.758965	-2.210764
C	0.436169	-3.586384	-3.621639
C	-1.117450	1.886126	4.945146
C	-1.797775	2.860887	2.679012
C	-1.226506	-1.154007	-2.789890
C	-2.467148	-0.357276	2.894279
C	3.076771	-2.299198	-3.485604
C	1.136746	-3.102316	-4.900274
C	-2.572075	2.021665	5.423756
C	-3.227878	3.075684	3.213529
C	-1.084011	-0.921870	-0.536258
C	-1.417726	-0.623367	0.878005
C	2.661169	-3.115538	-4.716589
C	-3.262613	3.212525	4.743107
C	-3.365219	-0.801949	-1.534427
C	-3.212802	-2.297078	1.435985
C	-4.342262	-1.735159	-1.877422
C	-4.546682	-2.328417	1.866408
C	-3.706374	0.537319	-1.296127
C	-2.625096	-3.452054	0.907399
C	-5.669462	-1.317382	-1.969187
C	-5.267909	-3.510639	1.749985
C	-5.036782	0.969479	-1.381733
C	-3.348754	-4.648688	0.772490
C	-6.008245	0.011273	-1.722651
C	-4.682205	-4.656324	1.204905
H	0.380552	-3.290192	-1.495186
H	0.097667	2.017691	3.196031
H	0.894650	-0.635669	-2.854376

H	-0.362457	-0.255421	3.478717
H	2.639013	-2.131869	-1.362639
H	2.668956	-3.781569	-1.966566
H	0.750209	-4.622355	-3.428562
H	-0.649615	-3.636193	-3.766992
H	-0.627755	1.030297	5.428314
H	-0.568978	2.776370	5.283016
H	-1.259916	3.812955	2.780186
H	-1.810038	2.651673	1.602818
H	-1.564433	-1.927496	-3.478789
H	-1.397112	-0.175712	-3.260120
H	-3.296021	0.354454	2.900854
H	-2.596106	-1.050777	3.729013
H	2.871548	-1.236120	-3.671147
H	4.155754	-2.351446	-3.318829
H	0.806170	-2.082753	-5.150468
H	0.842854	-3.737156	-5.746191
H	-3.137389	1.101279	5.215004
H	-2.588677	2.145936	6.514146
H	-3.888823	2.249218	2.915938
H	-3.651351	3.974376	2.746410
H	3.158886	-2.729620	-5.615241
H	2.995348	-4.157426	-4.597072
H	-4.298434	3.310600	5.093049
H	-2.744383	4.137908	5.035298
H	-4.062559	-2.769122	-2.050482
H	-5.009240	-1.434265	2.271822
H	-2.911575	1.237953	-1.062079
H	-1.577465	-3.419496	0.626077
H	-7.050145	0.307095	-1.803258
H	-5.276205	-5.559656	1.132504
Ni	1.175383	0.551967	0.491012
Br	2.443128	0.418648	2.615170
C	0.787441	2.318840	-0.307829
C	1.190495	3.470030	0.393359
C	0.859546	4.756864	-0.042927
C	0.109131	4.961066	-1.210448
C	0.026388	2.535077	-1.468243
C	-0.306321	3.820677	-1.912020
C	-0.236938	6.355790	-1.693669
C	0.787430	7.024266	-2.655022

H	-0.362767	7.016080	-0.824728
H	-1.209197	6.328770	-2.204807
H	-0.314404	1.688987	-2.064486
H	1.779832	3.366927	1.303623
H	1.185629	5.618971	0.537249
H	-0.897091	3.939696	-2.819836
H	0.367043	8.013667	-2.891382
C	0.936280	6.258960	-3.977567
C	2.153896	7.250090	-1.992790
H	2.060385	7.839792	-1.072319
H	2.828599	7.790103	-2.668049
H	2.631566	6.298801	-1.732492
H	-0.030930	6.138432	-4.481807
H	1.354304	5.259343	-3.812854
H	1.605534	6.793045	-4.662869
C	3.589187	1.854781	-1.961762
H	3.651642	1.623312	0.252336
C	3.692113	1.081759	-0.687938
O	5.012719	-0.556770	-1.790380
C	4.516513	-0.151832	-0.726911
N	4.730683	-0.776004	0.466320
H	5.527884	-2.473180	-0.385402
H	4.276251	-0.405748	1.298998
C	5.558144	-1.968491	0.584732
H	5.097035	-2.626802	1.329507
H	6.821030	-2.504770	2.956218
C	7.000076	-1.682169	0.973689
C	7.485177	-2.025324	2.239783
C	7.866604	-1.063057	0.059987
C	8.810377	-1.757871	2.593855
H	7.489878	-0.795652	-0.923582
H	9.171833	-2.030475	3.582265
C	9.188533	-0.793760	0.412260
C	9.665110	-1.140746	1.680251
H	9.850870	-0.315049	-0.304837
H	10.696518	-0.931405	1.952378
H	4.580935	2.257232	-2.225982
H	2.890085	2.686297	-1.875348
H	3.299258	1.210838	-2.798754
H	-6.444126	-2.033340	-2.229324
H	-6.302174	-3.542111	2.081538

C	-5.453263	2.433199	-1.144436
C	-4.256924	3.336085	-0.791635
C	-6.467436	2.495128	0.022896
C	-6.116159	2.989266	-2.427936
H	-5.418123	2.963452	-3.272401
H	-6.423591	4.030529	-2.273926
H	-7.006473	2.417890	-2.711386
H	-3.757691	3.015281	0.128889
H	-4.606404	4.362494	-0.633808
H	-3.506550	3.364319	-1.589045
H	-6.020818	2.119667	0.950903
H	-7.365847	1.902862	-0.181291
H	-6.783391	3.530888	0.195447
C	-2.656953	-5.895875	0.188812
C	-3.574935	-7.133446	0.200912
C	-1.394060	-6.229891	1.018596
C	-2.248410	-5.613489	-1.276201
H	-3.887496	-7.399698	1.217008
H	-3.037491	-7.992745	-0.215215
H	-4.474406	-6.983279	-0.407012
H	-3.130168	-5.411252	-1.896280
H	-1.728239	-6.479785	-1.702460
H	-1.579193	-4.750385	-1.352039
H	-1.653340	-6.429713	2.064411
H	-0.662594	-5.415345	1.005041
H	-0.901502	-7.122215	0.614266

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N	-2.275002	-0.982228	-1.571741
N	-1.608387	-1.868214	1.381611
N	-0.147421	-0.209777	-1.440398
N	-0.392633	0.052007	1.306049
C	0.348634	-1.243599	-3.677485
C	-0.285463	0.718470	3.728123
C	-0.463405	-0.177437	-2.889765
C	-0.250314	-0.435453	2.701604
C	1.878604	-1.113716	-3.504896
C	0.003178	-1.246882	-5.187944
C	0.240389	0.297884	5.121903
C	-1.616191	1.505318	3.845395
C	-1.996579	-0.451288	-2.926739

C	-1.287635	-1.590680	2.804458
C	2.477644	0.075536	-4.272856
C	0.598062	-0.056160	-5.959175
C	-0.821530	-0.333821	6.035925
C	-2.651540	0.946202	4.842175
C	-1.176271	-0.681078	-0.811787
C	-1.070761	-0.837762	0.658797
C	2.118870	0.029879	-5.764489
C	-2.025381	0.604448	6.202114
C	-3.625343	-1.005310	-1.094810
C	-1.823986	-3.198721	0.908789
C	-4.135294	0.071280	-0.354693
C	-0.847795	-3.833926	0.126437
C	-4.445688	-2.078616	-1.440723
C	-2.984130	-3.876432	1.288714
C	-5.469811	0.091062	0.070663
C	-1.022905	-5.153953	-0.310266
C	-6.067019	1.257403	0.880072
C	0.036603	-5.892313	-1.149755
C	-5.779111	-2.067649	-1.031664
C	-3.160210	-5.195450	0.872530
C	-6.279254	-1.002720	-0.285017
C	-2.198437	-5.820124	0.080129
C	-7.252944	1.871854	0.098135
C	-6.571581	0.728785	2.244159
C	-5.040264	2.374168	1.146677
C	0.566127	-7.103946	-0.345123
C	-0.605229	-6.394028	-2.465424
C	1.232778	-4.991974	-1.511253
H	0.043700	-2.215459	-3.260950
H	0.450108	1.422612	3.317650
H	-0.236109	0.825535	-3.260641
H	0.760088	-0.866881	2.740056
H	2.142672	-1.060716	-2.445607
H	2.328805	-2.041052	-3.890119
H	0.410163	-2.175000	-5.613859
H	-1.081050	-1.294316	-5.353781
H	1.099383	-0.375958	5.005626
H	0.623259	1.197276	5.625294
H	-1.362765	2.524552	4.169285
H	-2.068757	1.610223	2.851429

H	-2.284933	-1.182899	-3.684837
H	-2.584001	0.462437	-3.084377
H	-2.200753	-1.308744	3.335275
H	-0.874026	-2.486990	3.272960
H	2.119467	1.016920	-3.838599
H	3.565046	0.082872	-4.135074
H	0.134948	0.882033	-5.619977
H	0.349909	-0.151090	-7.024538
H	-1.159501	-1.296626	5.626363
H	-0.376365	-0.558026	7.013674
H	-3.135006	0.046839	4.438377
H	-3.454699	1.683593	4.971414
H	2.519538	0.908954	-6.286271
H	2.589328	-0.850887	-6.227774
H	-2.777736	0.155556	6.863229
H	-1.690439	1.530887	6.692287
H	-3.470073	0.898654	-0.132494
H	0.064956	-3.287481	-0.090617
H	-4.034449	-2.910511	-2.003342
H	-3.736802	-3.370538	1.885574
H	-6.429796	-2.898690	-1.289866
H	-4.057356	-5.737056	1.160844
H	-7.321168	-1.024052	0.021223
H	-2.364159	-6.848387	-0.228358
H	-8.046139	1.139720	-0.086074
H	-7.691427	2.701905	0.665158
H	-6.923429	2.260196	-0.872259
H	-5.748282	0.300605	2.827697
H	-7.012590	1.545184	2.828897
H	-7.336262	-0.046123	2.124714
H	-4.187277	2.013403	1.732381
H	-4.655746	2.809931	0.217631
H	-5.514159	3.179929	1.718444
H	-0.234648	-7.805925	-0.087675
H	1.315031	-7.650648	-0.931121
H	1.038804	-6.776291	0.587594
H	-0.988012	-5.555523	-3.058958
H	0.139221	-6.924671	-3.071288
H	-1.436899	-7.083352	-2.283298
H	0.926237	-4.128739	-2.112259
H	1.753941	-4.607728	-0.628714

H	1.956106	-5.565620	-2.102257
Ni	1.203869	0.765646	-0.183490
Br	2.352568	-1.468278	0.454533
C	0.382786	2.462613	-0.669890
C	-0.729408	2.962440	0.019568
C	-1.410145	4.098627	-0.431139
C	-1.005972	4.785278	-1.584934
C	0.794160	3.146982	-1.822403
C	0.106203	4.280363	-2.272192
C	-1.738414	6.022588	-2.065919
C	-1.226799	7.383252	-1.511889
H	-2.802747	5.933859	-1.807941
H	-1.688988	6.066338	-3.162506
H	1.667759	2.807889	-2.370040
H	-1.076853	2.462562	0.918219
H	-2.274643	4.456224	0.126966
H	0.443793	4.779171	-3.179512
H	-1.874297	8.148629	-1.966180
C	0.215901	7.686431	-1.940400
C	-1.382740	7.492362	0.011498
H	-2.422358	7.326084	0.320816
H	-1.085452	8.488004	0.362569
H	-0.758311	6.754526	0.527961
H	0.323575	7.659842	-3.031960
H	0.917041	6.957774	-1.517951
H	0.521538	8.682946	-1.599118
H	1.532152	3.323724	1.973987
H	2.743576	1.088254	1.735842
C	2.428793	3.202309	1.357216
H	3.292012	3.508178	1.968604
C	2.563638	1.754502	0.887390
O	3.149578	1.263361	-1.341311
C	3.583437	1.538782	-0.202262
H	2.344794	3.901873	0.521949
N	4.917588	1.640217	0.007404
H	4.855768	1.770825	2.069685
H	5.479162	1.399363	-0.803091
C	5.615958	1.751059	1.284214
H	6.152721	2.707837	1.334394
H	8.257145	1.908024	1.932920
C	6.588694	0.608147	1.518636

C	7.919598	0.876174	1.856997
C	6.162976	-0.724729	1.414606
C	8.817500	-0.166744	2.097225
H	5.132220	-0.949245	1.145277
H	9.848888	0.056442	2.357883
C	7.061842	-1.764734	1.651422
C	8.389234	-1.490559	1.993935
H	6.721752	-2.793600	1.568380
H	9.085650	-2.305002	2.176187

TS3-S

N	2.269912	0.864305	-1.525958
N	1.491111	1.855279	1.352329
N	0.163749	0.027860	-1.429985
N	0.273398	-0.072529	1.330364
C	-0.309169	0.997297	-3.690080
C	0.071773	-0.599854	3.786713
C	0.521872	-0.026896	-2.867018
C	0.074206	0.491514	2.693359
C	-1.836045	0.809594	-3.544621
C	0.067763	0.994832	-5.192531
C	-0.502781	-0.095219	5.132934
C	1.393365	-1.381929	3.999672
C	2.045218	0.295426	-2.874399
C	1.101336	1.656207	2.772944
C	-2.370508	-0.412934	-4.308487
C	-0.463277	-0.228332	-5.959324
C	0.527797	0.588906	6.044997
C	2.394981	-0.762901	4.995364
C	1.157501	0.553156	-0.786941
C	0.983249	0.779670	0.667144
C	-1.982971	-0.372569	-5.793185
C	1.722750	-0.338195	6.309178
C	3.602142	1.018456	-1.038016
C	1.596106	3.173368	0.799263
C	4.130474	0.138383	-0.082068
C	0.531940	3.707243	0.056529
C	4.399576	2.026842	-1.582682
C	2.735736	3.934316	1.062056
C	5.453867	0.258320	0.362266
C	0.594252	5.011032	-0.453923

C	6.069444	-0.690994	1.407536
C	-0.562852	5.639862	-1.252915
C	5.722041	2.148658	-1.159558
C	2.800592	5.238691	0.572703
C	6.238149	1.281879	-0.198402
C	1.749130	5.764409	-0.176400
C	7.293336	-1.410949	0.791913
C	6.523190	0.129732	2.638590
C	5.074777	-1.764990	1.885534
C	-1.141832	6.828867	-0.448514
C	-0.035396	6.153414	-2.614017
C	-1.700504	4.638343	-1.527211
H	-0.049387	1.984762	-3.279390
H	-0.654737	-1.326079	3.396962
H	0.334395	-1.042910	-3.226116
H	-0.940417	0.911834	2.665223
H	-2.118344	0.755784	-2.489902
H	-2.316470	1.712803	-3.949726
H	-0.365842	1.900509	-5.639956
H	1.152702	1.082905	-5.335980
H	-1.354534	0.570943	4.944299
H	-0.906206	-0.962249	5.675762
H	1.123836	-2.377300	4.381213
H	1.879067	-1.552559	3.030834
H	2.328523	1.016910	-3.644029
H	2.666498	-0.601719	-2.996302
H	1.990501	1.413444	3.360350
H	0.662292	2.574851	3.169399
H	-1.984189	-1.333341	-3.852820
H	-3.459240	-0.462436	-4.192598
H	0.029994	-1.142891	-5.598417
H	-0.197710	-0.137487	-7.020831
H	0.882099	1.525813	5.592001
H	0.048609	0.870237	6.991399
H	2.894433	0.109370	4.553713
H	3.191391	-1.491129	5.197397
H	-2.338085	-1.273541	-6.310697
H	-2.478416	0.482616	-6.277761
H	2.453108	0.149672	6.967345
H	1.368823	-1.232961	6.843048
H	3.490562	-0.650086	0.297767

H	-0.355964	3.095279	-0.076299
H	3.977993	2.712804	-2.310587
H	3.555941	3.502465	1.627085
H	6.350959	2.931729	-1.574364
H	3.680008	5.846323	0.769624
H	7.270816	1.403942	0.115052
H	1.829085	6.783796	-0.543182
H	8.065629	-0.704735	0.469625
H	7.746014	-2.086032	1.528276
H	6.999227	-2.007088	-0.079385
H	5.672279	0.640279	3.104436
H	6.975719	-0.529175	3.389592
H	7.264862	0.890206	2.372206
H	4.192974	-1.321874	2.361265
H	4.735830	-2.405165	1.063235
H	5.559061	-2.410274	2.627136
H	-0.384235	7.595410	-0.250508
H	-1.960194	7.301673	-1.005286
H	-1.538789	6.490990	0.515305
H	0.383214	5.331871	-3.207099
H	-0.853234	6.603014	-3.190032
H	0.744158	6.914052	-2.497319
H	-1.355536	3.782871	-2.118602
H	-2.148480	4.240789	-0.611195
H	-2.494005	5.135474	-2.097337
Ni	-1.222174	-0.885752	-0.153812
Br	-2.649075	1.212561	0.562192
C	-0.715186	-2.765714	-0.206180
C	0.293085	-3.214526	0.672428
C	1.157148	-4.250219	0.320619
C	1.052421	-4.913083	-0.912414
C	-0.849736	-3.462613	-1.426337
C	0.020788	-4.499006	-1.767517
C	1.993753	-6.038064	-1.290985
C	3.278428	-5.629760	-2.067823
H	1.451073	-6.771349	-1.903059
H	2.306237	-6.567656	-0.380587
H	-1.642534	-3.188861	-2.113102
H	0.409800	-2.741002	1.640640
H	1.925069	-4.559024	1.028337
H	-0.114799	-5.004615	-2.722267

H	3.828102	-6.566677	-2.244307
C	4.191273	-4.708253	-1.246393
C	2.965484	-5.013707	-3.438610
H	2.355466	-5.688921	-4.051343
H	3.889004	-4.803728	-3.991802
H	2.415203	-4.071476	-3.333040
H	4.457869	-5.163137	-0.284179
H	3.700216	-3.750038	-1.039190
H	5.122494	-4.498806	-1.786884
H	-1.901576	-4.125419	1.886903
H	-2.533676	-1.725217	1.593711
C	-2.698175	-3.836352	1.196535
H	-3.653603	-3.949879	1.724108
C	-2.497520	-2.390486	0.722005
O	-3.051984	-1.489655	-1.405589
C	-3.493914	-1.926280	-0.325509
H	-2.683754	-4.541489	0.360554
N	-4.830565	-1.995630	-0.117515
H	-4.813663	-1.974491	1.964243
H	-5.365574	-1.593064	-0.880378
C	-5.539194	-2.126626	1.159450
H	-5.943395	-3.141507	1.268725
H	-8.196224	-2.604908	1.543833
C	-6.662605	-1.114050	1.275833
C	-7.979549	-1.540476	1.479657
C	-6.389674	0.259848	1.186975
C	-9.016268	-0.612046	1.601243
H	-5.367996	0.601581	1.024547
H	-10.035083	-0.956211	1.759300
C	-7.427615	1.184262	1.304497
C	-8.741080	0.752987	1.512808
H	-7.206924	2.246127	1.235466
H	-9.545747	1.478087	1.603917

TS4

N	-2.203550	0.254267	1.906323
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N	-0.077603	-0.050710	1.138468
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C	1.345119	0.269654	3.187734
C	-2.193168	-1.734255	-3.317664

C	0.020215	-0.260953	2.603248
C	-1.594817	-0.420714	-2.747111
C	1.567002	-0.168833	4.654332
C	1.634301	1.778155	2.995168
C	-1.241683	-2.948233	-3.249236
C	-2.685443	-1.543510	-4.773704
C	-1.339390	0.278084	3.122681
C	-2.678721	0.691413	-2.574702
C	0.935004	0.763399	5.701286
C	1.077030	2.710965	4.087836
C	-0.095264	-2.889999	-4.271707
C	-1.539201	-1.471074	-5.798604
C	-1.319418	0.121082	0.847579
C	-1.712375	0.131789	-0.578835
C	1.408553	2.210756	5.502105
C	-0.621574	-2.699591	-5.702480
C	-3.440022	-0.474126	1.928501
C	-3.271999	2.084301	-0.584941
C	-3.484894	-1.798656	1.481590
C	-2.404662	3.102631	-0.178082
C	-4.585671	0.136729	2.450756
C	-4.657297	2.286761	-0.566604
C	-4.673724	-2.545979	1.537841
C	-2.898640	4.344033	0.261200
C	-4.661507	-4.010445	1.062510
C	-1.907699	5.444526	0.684288
C	-5.766686	-0.596637	2.518093
C	-5.156607	3.512852	-0.139583
C	-5.812387	-1.919401	2.064479
C	-4.288369	4.529218	0.271119
C	-6.051666	-4.665994	1.166830
C	-4.196330	-4.075097	-0.412055
C	-3.667460	-4.820265	1.931745
C	-2.620486	6.750061	1.085323
C	-1.079370	4.949116	1.892452
C	-0.945281	5.752980	-0.488949
H	2.091710	-0.258723	2.585560
H	-3.067390	-1.962443	-2.689641
H	0.045820	-1.355337	2.716597
H	-0.781866	-0.076758	-3.394426
H	1.213690	-1.199534	4.793477

H	2.650914	-0.193049	4.836707
H	2.727877	1.891774	2.986211
H	1.294890	2.093489	2.001465
H	-0.847776	-3.062436	-2.234938
H	-1.847946	-3.845371	-3.452494
H	-3.324577	-2.402427	-5.026286
H	-3.325414	-0.654518	-4.864872
H	-1.274244	1.306569	3.488560
H	-1.776572	-0.347022	3.904444
H	-3.650421	0.402991	-2.988887
H	-2.381914	1.646013	-3.027357
H	-0.162339	0.728251	5.636766
H	1.192646	0.414142	6.710846
H	-0.012461	2.812790	3.994892
H	1.483198	3.721188	3.941532
H	0.602487	-2.082488	-4.018479
H	0.489818	-3.816333	-4.206868
H	-0.943072	-0.562603	-5.632107
H	-1.958149	-1.380405	-6.810819
H	0.959907	2.871376	6.257220
H	2.497835	2.252380	5.656040
H	0.212068	-2.604869	-6.411355
H	-1.192080	-3.592504	-6.004974
H	-2.565508	-2.253324	1.113534
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H	-4.540107	1.170583	2.779010
H	-5.319188	1.481877	-0.871330
H	-6.666351	-0.135747	2.919593
H	-6.230707	3.681863	-0.118269
H	-6.751536	-2.458147	2.132243
H	-4.712478	5.472936	0.596517
H	-6.797753	-4.144246	0.554704
H	-5.996460	-5.701125	0.810315
H	-6.416430	-4.692966	2.200960
H	-3.169296	-3.714183	-0.524988
H	-4.221094	-5.113074	-0.767935
H	-4.852581	-3.479108	-1.058689
H	-2.642111	-4.453102	1.818751
H	-3.943140	-4.770922	2.992612
H	-3.676601	-5.874906	1.627248
H	-3.291266	6.605826	1.940945

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H	-3.206814	7.167242	0.257651
H	-0.500687	4.056615	1.639206
H	-0.372359	5.725129	2.212848
H	-1.728919	4.709752	2.743225
H	-0.341517	4.879324	-0.752862
H	-1.501754	6.076156	-1.377417
H	-0.258899	6.562186	-0.206439
Ni	1.037403	-0.977541	-0.388288
C	2.905344	-1.309187	0.330953
C	3.862053	-0.275943	0.407878
C	5.163188	-0.468198	0.887923
C	5.595059	-1.731755	1.313812
C	3.360982	-2.567940	0.773684
C	4.662644	-2.776192	1.240033
C	6.990005	-2.007562	1.857028
C	8.175406	-1.285623	1.158271
H	7.155419	-3.091833	1.797598
H	7.033478	-1.770280	2.933522
H	2.675904	-3.412492	0.752627
H	3.593484	0.727598	0.079514
H	5.843495	0.381464	0.914628
H	4.964641	-3.776587	1.555592
H	7.871778	-1.067415	0.125645
C	9.413147	-2.195878	1.103019
C	8.538332	0.042465	1.844057
H	7.679756	0.717338	1.913288
H	9.335459	0.566536	1.300505
H	8.897430	-0.139464	2.866734
H	9.205216	-3.115516	0.543012
H	9.731432	-2.486690	2.113892
H	10.261608	-1.692118	0.621322
C	3.206487	4.314904	-4.039636
C	3.718965	3.290059	-4.845297
C	3.479475	1.942624	-4.535473
C	2.725159	1.669580	-3.404636
C	2.213754	2.686900	-2.604616
C	2.439451	4.023098	-2.901102
C	1.445953	2.015108	-1.487349
N	1.547348	0.656351	-1.640698
C	2.270311	0.371121	-2.785475

O	0.826222	2.631624	-0.611661
O	2.483762	-0.744859	-3.248682
H	3.408065	5.351027	-4.302440
H	4.310703	3.545558	-5.721486
H	3.869772	1.136833	-5.151035
H	2.037724	4.811729	-2.270707
Br	-0.086004	-3.297781	0.428398

IM4

N	0.821071	-1.203707	-1.929052
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N	-0.439147	0.484489	-1.107262
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C	-1.055791	1.636470	-3.261968
C	0.090857	-0.192232	3.930956
C	-0.921403	0.305505	-2.493579
C	0.994214	0.059876	2.703553
C	-2.032251	2.629760	-2.593913
C	-1.479572	1.406156	-4.732752
C	0.810306	0.092799	5.270691
C	-0.663256	-1.544411	3.972621
C	0.123063	-0.664145	-3.115866
C	2.206303	-0.868582	2.409607
C	-3.509504	2.227394	-2.736414
C	-2.952728	0.985889	-4.879622
C	1.621919	-1.093629	5.816961
C	0.111948	-2.722391	4.592862
C	0.470919	-0.410777	-0.870112
C	0.997699	-0.456951	0.515472
C	-3.892575	1.998127	-4.206216
C	0.746349	-2.349364	5.941242
C	1.427547	-2.486507	-1.919923
C	3.419110	-0.838758	0.167932
C	1.083445	-3.434308	-0.943768
C	3.682845	0.332533	-0.556159
C	2.324290	-2.821770	-2.937753
C	4.348251	-1.879747	0.201242
C	1.644117	-4.716686	-0.945937
C	4.869288	0.477697	-1.285758
C	1.280111	-5.780295	0.107306
C	5.193844	1.761013	-2.072791

C	2.877748	-4.100718	-2.958238
C	5.542069	-1.736309	-0.504654
C	2.550169	-5.031089	-1.974673
C	5.794361	-0.580397	-1.242381
C	2.558214	-6.201814	0.871108
C	0.253407	-5.266585	1.134150
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C	6.426743	2.445936	-1.435313
C	5.512186	1.402916	-3.543830
C	4.023462	2.763703	-2.064805
H	-0.053259	2.089739	-3.259364
H	-0.680910	0.581509	3.817696
H	-1.900973	-0.183766	-2.418584
H	1.361312	1.092301	2.783882
H	-1.776659	2.765635	-1.538492
H	-1.884302	3.609415	-3.070942
H	-1.329037	2.350307	-5.274759
H	-0.824121	0.672001	-5.221017
H	1.447131	0.982347	5.172238
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H	-1.565836	-1.386706	4.579051
H	-1.024313	-1.798443	2.969300
H	0.833670	-0.127966	-3.759844
H	-0.322107	-1.479512	-3.690886
H	2.088722	-1.873205	2.823839
H	3.151937	-0.451181	2.761138
H	-3.709770	1.320121	-2.151349
H	-4.138437	3.010311	-2.296086
H	-3.108758	-0.007298	-4.434024
H	-3.199271	0.884108	-5.944411
H	2.479947	-1.307808	5.163618
H	2.044335	-0.827091	6.794247
H	0.899279	-3.075073	3.912666
H	-0.572102	-3.571340	4.720614
H	-4.933058	1.657926	-4.282159
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H	1.333524	-3.190396	6.332020
H	-0.050717	-2.156627	6.674735
H	0.350463	-3.158015	-0.195307
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H	2.597102	-2.086396	-3.688050

H	4.129016	-2.787753	0.754286
H	3.578722	-4.369343	-3.743825
H	6.276367	-2.537272	-0.489051
H	3.000301	-6.018417	-2.016386
H	6.733255	-0.500828	-1.782831
H	3.000599	-5.347727	1.397537
H	2.320445	-6.971126	1.615712
H	3.319732	-6.611773	0.199434
H	-0.693277	-4.982384	0.660977
H	0.033101	-6.056314	1.860886
H	0.629536	-4.402067	1.692974
H	-0.236243	-6.749841	-1.145539
H	1.374481	-7.464862	-1.312710
H	0.415051	-7.786054	0.139046
H	7.304649	1.790549	-1.441414
H	6.684839	3.357474	-1.988340
H	6.223174	2.725314	-0.395530
H	4.655942	0.913095	-4.022488
H	5.743216	2.311413	-4.113098
H	6.372948	0.731128	-3.629425
H	3.127179	2.340809	-2.534591
H	3.750558	3.081578	-1.053389
H	4.303909	3.657085	-2.634711
Ni	-1.297231	1.208025	0.647453
C	-2.942923	0.105096	0.682169
C	-4.176629	0.730426	0.957298
C	-5.376984	0.013550	1.011188
C	-5.410281	-1.369485	0.783416
C	-2.995578	-1.283170	0.462242
C	-4.190104	-2.007163	0.513659
C	-6.711564	-2.146149	0.831592
C	-7.487253	-2.271568	-0.511073
H	-7.382856	-1.677953	1.564389
H	-6.511950	-3.161971	1.200059
H	-2.075376	-1.833004	0.253882
H	-4.206039	1.804127	1.139516
H	-6.303992	0.536896	1.242381
H	-4.177389	-3.084852	0.352767
H	-8.389539	-2.857708	-0.278623
C	-6.696405	-3.046425	-1.574714
C	-7.947958	-0.910490	-1.051615

H	-8.558761	-0.373626	-0.315225
H	-8.551726	-1.035659	-1.958927
H	-7.092300	-0.273100	-1.301631
H	-6.409102	-4.042054	-1.213680
H	-5.778896	-2.514221	-1.850541
H	-7.294507	-3.180581	-2.484471
C	-1.297212	4.080770	1.104370
C	-0.484541	5.333471	1.263425
C	-0.853510	6.659668	1.433894
C	0.174605	7.606861	1.547584
H	-0.073346	8.656323	1.683501
C	1.520343	7.221432	1.488776
H	2.295231	7.978179	1.580307
C	1.879945	5.876996	1.314296
H	2.920290	5.568141	1.267672
H	-1.899936	6.947130	1.477854
C	0.854421	4.949565	1.203117
C	0.877661	3.455171	1.014756
O	1.895742	2.767276	0.915203
O	-2.521118	3.996790	1.070243
N	-0.426259	3.007320	0.981951

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N	3.101123	0.088871	-1.406201
N	0.865910	-0.567192	1.346016
N	0.846402	0.265762	-1.242669
C	0.618052	-1.925114	3.450721
C	0.214550	1.142597	-3.518663
C	0.996176	-0.564684	2.823308
C	1.109883	0.184723	-2.701774
C	-0.866869	-2.294603	3.237348
C	0.956688	-1.996566	4.959870
C	0.208288	0.808465	-5.030231
C	0.411370	2.661274	-3.279139
C	2.484364	-0.173541	3.057571
C	2.656942	0.313642	-2.803872
C	-1.834188	-1.497148	4.129380
C	0.001331	-1.174998	5.841533
C	1.347666	1.460844	-5.829453
C	1.478411	3.353537	-4.150654

C	1.935185	-0.030724	0.845128
C	1.978827	0.118782	-0.629919
C	-1.457790	-1.596140	5.614538
C	1.347105	2.983906	-5.635424
C	3.941611	1.288705	1.577830
C	4.311604	-0.605030	-1.105402
C	3.702146	2.486565	0.887203
C	4.257763	-1.887744	-0.542763
C	5.183698	1.057414	2.174383
C	5.537396	-0.021241	-1.429302
C	4.699342	3.459672	0.753128
C	5.428485	-2.603414	-0.264809
C	4.463205	4.788792	0.011319
C	5.397352	-4.021654	0.334285
C	6.179524	2.025667	2.059132
C	6.708696	-0.733509	-1.174051
C	5.945351	3.203555	1.353131
C	6.655335	-1.999903	-0.593637
C	4.695632	5.969631	0.984476
C	5.455636	4.897134	-1.171037
C	3.032783	4.905381	-0.547888
C	5.998618	-5.016949	-0.687134
C	6.235460	-4.055070	1.634246
C	3.965929	-4.481288	0.673029
H	1.233934	-2.673552	2.930117
H	-0.788033	0.905970	-3.143889
H	0.328288	0.222553	3.194575
H	0.827114	-0.837842	-2.985659
H	-1.139092	-2.173997	2.184420
H	-0.979712	-3.364928	3.462236
H	0.890070	-3.050942	5.263367
H	1.996653	-1.698090	5.146389
H	0.213244	-0.280784	-5.171675
H	-0.742646	1.165788	-5.449668
H	-0.551825	3.145497	-3.490757
H	0.605056	2.846404	-2.216112
H	3.090552	-1.045755	3.336439
H	2.619467	0.601147	3.816305
H	2.985044	1.301119	-3.137019
H	3.097948	-0.441501	-3.458463
H	-1.842717	-0.442629	3.824484

H	-2.855185	-1.865613	3.969497
H	0.109363	-0.103000	5.620608
H	0.277832	-1.299902	6.896366
H	2.320436	1.050458	-5.521654
H	1.235898	1.212921	-6.892624
H	2.490713	3.098099	-3.809259
H	1.388339	4.440022	-4.023448
H	-2.131948	-0.978661	6.221388
H	-1.588043	-2.633789	5.957342
H	2.155853	3.447328	-6.214767
H	0.405086	3.392782	-6.029916
H	2.710205	2.656710	0.485822
H	3.281024	-2.326696	-0.379598
H	5.371518	0.126945	2.700711
H	5.570514	0.977323	-1.853853
H	7.150129	1.854207	2.516540
H	7.671062	-0.292372	-1.419175
H	6.742399	3.937372	1.279365
H	7.585875	-2.527935	-0.405790
H	5.714813	5.976673	1.384743
H	4.533921	6.923554	0.468247
H	4.002793	5.920768	1.832056
H	5.302929	4.081432	-1.887734
H	5.311966	5.845391	-1.702889
H	6.497364	4.857416	-0.835610
H	2.809466	4.111766	-1.269985
H	2.277805	4.869172	0.245590
H	2.917771	5.863134	-1.067348
H	7.032680	-4.762165	-0.943394
H	5.996448	-6.033656	-0.275386
H	5.415346	-5.024298	-1.614781
H	5.831232	-3.360007	2.379735
H	6.222037	-5.061922	2.068847
H	7.281821	-3.784480	1.457308
H	3.499345	-3.831319	1.423082
H	3.314336	-4.496066	-0.206902
H	3.994689	-5.495480	1.087501
Ni	-0.757388	-0.362272	-0.003165
C	-1.461693	1.301006	0.805462
C	-0.870842	2.567325	0.652334
C	-1.387547	3.713134	1.263796

C	-2.531428	3.650687	2.072202
C	-2.589120	1.250358	1.648529
C	-3.109419	2.389776	2.269125
C	-3.137718	4.896029	2.684606
C	-4.199454	5.628266	1.813018
H	-2.338898	5.613834	2.918695
H	-3.610668	4.634343	3.641175
H	-3.102377	0.303424	1.811711
H	0.015251	2.676171	0.026909
H	-0.900124	4.674886	1.106312
H	-3.988087	2.300625	2.906193
H	-4.538591	6.481278	2.421181
C	-5.425013	4.752446	1.512258
C	-3.603217	6.193665	0.515944
H	-2.750964	6.855129	0.719525
H	-4.353795	6.775033	-0.033328
H	-3.258382	5.388856	-0.142529
H	-5.869529	4.358367	2.435462
H	-5.169302	3.903942	0.867771
H	-6.196958	5.338301	0.997980
C	-3.306337	-0.756636	-2.831686
H	-2.795278	1.327300	-2.219748
C	-3.354233	0.441086	-1.934749
O	-4.973553	1.888144	-1.014891
C	-4.502619	0.742929	-1.055156
N	-5.030531	-0.306597	-0.357511
H	-6.118388	0.930924	0.891115
H	-4.473987	-1.152839	-0.274125
C	-6.138509	-0.116242	0.572687
H	-5.954019	-0.744785	1.450518
H	-7.803633	-2.205144	1.188494
C	-7.498017	-0.449102	-0.020164
C	-8.220928	-1.565192	0.413309
C	-8.049253	0.368505	-1.018555
C	-9.470366	-1.866340	-0.135954
H	-7.489009	1.237373	-1.353272
H	-10.019556	-2.737365	0.213287
C	-9.294492	0.068580	-1.569599
C	-10.009763	-1.049849	-1.130188
H	-9.711726	0.711481	-2.340869
H	-10.981708	-1.280379	-1.559187

H	-2.279255	-1.020853	-3.106972
H	-3.845883	-0.549983	-3.772506
H	-3.775510	-1.633984	-2.380226
C	-2.082903	-3.006848	-0.410824
C	-1.871759	-4.437502	-0.810216
C	-0.556741	-4.534843	-1.258313
C	-0.030463	-5.736978	-1.707015
C	-0.874438	-6.857441	-1.690190
C	-2.716709	-5.537133	-0.785997
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C	-2.196375	-6.759268	-1.236706
N	-0.923259	-2.298253	-0.653314
O	-3.119922	-2.544576	0.070437
O	1.205168	-2.870631	-1.434352
H	0.995162	-5.803385	-2.058332
H	-0.499983	-7.817949	-2.034315
H	-3.739868	-5.449734	-0.432580
H	-2.826179	-7.644910	-1.235785

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N	-2.801453	0.223332	-1.515188
N	-0.453585	0.536599	1.192785
N	-0.568731	-0.179693	-1.445385
C	-0.137770	1.886448	3.296685
C	-0.465862	-1.336929	-3.667482
C	-0.582551	0.538119	2.675564
C	-0.872650	-0.055822	-2.892519
C	1.389480	2.105490	3.209833
C	-0.598005	2.077215	4.763773
C	-0.368434	-1.117280	-5.198312
C	-1.266568	-2.621657	-3.337474
C	-2.085609	0.213635	2.914168
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C	2.191503	1.291949	4.241607
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C	-1.561465	0.077831	0.696635
C	-1.662985	0.016258	-0.783886
C	1.695013	1.522086	5.675176

C	-2.323862	-2.659947	-5.659965
C	-3.635703	-1.141351	1.440456
C	-3.968530	0.931397	-1.077344
C	-3.448629	-2.398812	0.846190
C	-3.848231	2.172484	-0.437941
C	-4.878471	-0.790127	1.973048
C	-5.225457	0.403097	-1.371259
C	-4.501081	-3.319410	0.754145
C	-4.982068	2.898439	-0.051985
C	-4.330309	-4.720617	0.136925
C	-4.882127	4.271346	0.638513
C	-5.930943	-1.699094	1.889923
C	-6.362303	1.124107	-1.006982
C	-5.747332	-2.939770	1.283529
C	-6.241339	2.348233	-0.351471
C	-4.719487	-5.795479	1.180591
C	-5.253219	-4.848585	-1.098626
C	-2.882506	-4.996329	-0.308698
C	-5.522206	5.346212	-0.272851
C	-5.637353	4.231026	1.988198
C	-3.422966	4.680621	0.916564
H	-0.628537	2.662937	2.691953
H	0.558155	-1.517588	-3.320561
H	0.048332	-0.277033	3.051022
H	-0.246560	0.756251	-3.275163
H	1.749499	1.887605	2.200965
H	1.586828	3.173882	3.376726
H	-0.455184	3.138410	5.012807
H	-1.673508	1.890991	4.872859
H	0.065087	-0.129708	-5.404950
H	0.348090	-1.851036	-5.593630
H	-0.602029	-3.476048	-3.527368
H	-1.491296	-2.649123	-2.264498
H	-2.652254	1.105629	3.209975
H	-2.250241	-0.565308	3.663051
H	-2.994089	-0.174822	-3.592442
H	-2.440051	1.463472	-3.177453
H	2.120046	0.220946	4.010954
H	3.253874	1.552684	4.156345
H	0.012295	0.162699	5.601510
H	-0.173346	1.443431	6.791955

H	-2.397116	-0.493634	-5.710774
H	-1.498976	-1.199435	-7.041560
H	-3.347348	-2.158825	-3.820698
H	-2.933445	-3.854456	-3.951965
H	2.255693	0.894819	6.379823
H	1.881382	2.566652	5.966488
H	-3.268321	-2.776674	-6.206687
H	-1.653003	-3.453651	-6.021137
H	-2.454707	-2.656379	0.497956
H	-2.851462	2.569719	-0.292406
H	-5.021455	0.188465	2.419905
H	-5.304584	-0.563511	-1.859046
H	-6.903990	-1.433972	2.294385
H	-7.348474	0.724213	-1.226839
H	-6.586692	-3.626969	1.234378
H	-7.144965	2.886282	-0.079015
H	-5.759812	-5.696267	1.507023
H	-4.600436	-6.797889	0.752161
H	-4.081246	-5.728246	2.068911
H	-4.988282	-4.109849	-1.864031
H	-5.157874	-5.846577	-1.543470
H	-6.306474	-4.698660	-0.837899
H	-2.554052	-4.299543	-1.087007
H	-2.176965	-4.931771	0.527303
H	-2.812209	-6.007974	-0.723835
H	-6.576352	5.130844	-0.478112
H	-5.468972	6.332175	0.204884
H	-4.999144	5.405065	-1.233985
H	-5.200543	3.482598	2.660236
H	-5.578669	5.206424	2.486204
H	-6.697351	3.987519	1.859840
H	-2.923488	3.971708	1.587727
H	-2.829829	4.747375	-0.001564
H	-3.402159	5.663637	1.400490
Ni	1.171160	0.256774	-0.244350
C	1.471125	-1.478016	0.579756
C	0.843219	-2.657716	0.168139
C	1.018527	-3.851734	0.874257
C	1.837986	-3.916366	2.010015
C	2.284019	-1.534538	1.718795
C	2.455443	-2.729544	2.425528

C	2.082932	-5.223368	2.735755
C	3.267105	-6.079733	2.199681
H	1.173963	-5.839469	2.695408
H	2.270417	-5.015644	3.798039
H	2.829285	-0.654361	2.050656
H	0.222366	-2.661282	-0.722901
H	0.522072	-4.754897	0.523046
H	3.096576	-2.740106	3.305312
H	3.315313	-6.958722	2.860581
C	4.613249	-5.347549	2.297860
C	3.026442	-6.587170	0.770629
H	2.083718	-7.144412	0.695565
H	3.835698	-7.257886	0.457685
H	2.988031	-5.757341	0.056218
H	4.810877	-5.005475	3.321777
H	4.638585	-4.473207	1.637774
H	5.435491	-6.011149	2.004232
C	2.891675	0.679364	-2.593089
H	2.159040	-1.253234	-1.957419
C	2.622708	-0.373682	-1.510886
O	4.329574	-2.018479	-1.131163
C	3.920595	-0.877293	-0.899293
N	4.617058	0.015262	-0.142704
H	5.900563	-1.405034	0.614852
H	4.231862	0.946910	0.003784
C	5.901484	-0.322278	0.457380
H	5.959094	0.166127	1.436815
H	7.750353	1.640253	0.948758
C	7.103113	0.077373	-0.383868
C	7.952836	1.113076	0.018387
C	7.376400	-0.593667	-1.586007
C	9.055238	1.478070	-0.759360
H	6.716993	-1.399132	-1.897439
H	9.705591	2.285436	-0.431486
C	8.474678	-0.229838	-2.364257
C	9.318428	0.807075	-1.953753
H	8.677004	-0.759409	-3.292161
H	10.175547	1.087447	-2.560939
H	1.970807	1.023545	-3.072074
H	3.526162	0.229710	-3.372487
H	3.419751	1.553615	-2.207183

C	2.328204	3.040507	-0.221672
C	2.059314	4.491378	-0.489051
C	0.785999	4.559190	-1.044619
C	0.223127	5.768358	-1.424285
C	0.987403	6.927367	-1.220986
C	2.826779	5.627593	-0.281279
C	0.266905	3.147877	-1.114039
C	2.268308	6.858218	-0.657829
N	1.241544	2.293453	-0.624575
O	3.361767	2.601949	0.291749
O	-0.845741	2.837870	-1.539829
H	-0.768516	5.811632	-1.865506
H	0.583019	7.895120	-1.506012
H	3.820192	5.561332	0.152351
H	2.836864	7.773201	-0.514124

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N	0.316839	-1.740222	-2.316135
N	0.869899	-3.031903	0.522640
N	0.887334	0.109595	-1.123547
N	-0.216699	-1.137572	1.164318
C	2.653130	0.469734	-2.852777
C	-1.552048	-2.507304	2.806554
C	1.128211	0.463755	-2.545704
C	-0.155010	-1.978937	2.383722
C	3.470917	1.360841	-1.891854
C	2.956404	0.868384	-4.317336
C	-2.637607	-1.412668	2.874051
C	-1.494456	-3.261024	4.157516
C	0.382392	-0.652893	-3.320933
C	0.814113	-3.134599	1.998061
C	3.298868	2.864383	-2.160879
C	2.786263	2.372380	-4.590405
C	-2.480362	-0.467964	4.078449
C	-1.337476	-2.326050	5.370002
C	0.512829	-1.131422	-1.103785
C	0.367207	-1.791669	0.216887
C	3.627168	3.214183	-3.620194
C	-2.434774	-1.251642	5.399058
C	-0.569838	-2.841483	-2.539948
C	1.922906	-3.710811	-0.180982

C	-1.840257	-2.865707	-1.946065
C	3.186941	-3.117009	-0.310198
C	-0.174009	-3.854408	-3.414435
C	1.686542	-5.000078	-0.657211
C	-2.732085	-3.917600	-2.197513
C	4.240555	-3.803555	-0.930480
C	-4.138718	-3.976296	-1.572998
C	5.651189	-3.201150	-1.071365
C	-1.059661	-4.896684	-3.684949
C	2.727522	-5.691434	-1.277510
C	-2.315413	-4.929150	-3.080795
C	3.981762	-5.099454	-1.412062
C	-5.198695	-3.916065	-2.699105
C	-4.301513	-5.299603	-0.787634
C	-4.397323	-2.809041	-0.602470
C	6.666143	-4.100671	-0.325212
C	6.035945	-3.131560	-2.568522
C	5.742827	-1.780990	-0.483276
H	2.988156	-0.568463	-2.708546
H	-1.852644	-3.225163	2.028130
H	0.696117	1.446743	-2.743771
H	0.267939	-1.368878	3.186884
H	3.222097	1.114312	-0.856327
H	4.532327	1.104715	-2.029457
H	4.000028	0.592594	-4.526492
H	2.347733	0.288761	-5.023940
H	-2.649379	-0.854534	1.932867
H	-3.613286	-1.915524	2.952949
H	-2.431689	-3.824932	4.269024
H	-0.691069	-4.009499	4.155911
H	0.906921	-0.990028	-4.217439
H	-0.639682	-0.360519	-3.597356
H	0.452624	-4.122542	2.297816
H	1.821912	-2.991046	2.407259
H	2.270525	3.173282	-1.931085
H	3.946891	3.431181	-1.480115
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H	3.065953	2.589547	-5.629785
H	-1.567263	0.134845	3.980990
H	-3.313306	0.247114	4.094940
H	-0.353401	-1.837254	5.345289

H	-1.359584	-2.919085	6.293457
H	3.465969	4.282769	-3.807749
H	4.694077	3.019471	-3.809013
H	-2.276044	-0.568817	6.243102
H	-3.408524	-1.737232	5.565518
H	-2.122026	-2.035447	-1.307439
H	3.325676	-2.122461	0.100407
H	0.817231	-3.827685	-3.855836
H	0.700146	-5.440067	-0.550606
H	-0.765699	-5.693247	-4.363309
H	2.559462	-6.695400	-1.658396
H	-2.982976	-5.755230	-3.308676
H	4.774790	-5.662924	-1.895854
H	-5.091123	-4.745999	-3.405864
H	-6.208653	-3.966511	-2.274308
H	-5.115367	-2.981192	-3.264898
H	-3.562969	-5.369540	0.019414
H	-5.300704	-5.353296	-0.338487
H	-4.179322	-6.177971	-1.430289
H	-3.695859	-2.817952	0.239171
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H	-5.411029	-2.888478	-0.193625
H	6.681832	-5.120988	-0.723522
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H	5.337744	-2.493374	-3.122523
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Ni	0.049406	1.098113	0.623548
C	-0.343915	2.943648	0.085280
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C	0.449858	5.248488	0.224056
C	0.038796	5.526469	-1.090216
C	-0.751685	3.218080	-1.233728
C	-0.547266	4.476902	-1.808550
C	0.132269	6.923353	-1.676157
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H	-0.592589	7.571235	-1.159352

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H	-1.249182	2.448881	-1.817635
H	0.549523	3.842657	1.836075
H	0.906818	6.033753	0.823133
H	-0.880175	4.651243	-2.830764
H	1.832187	7.629219	-0.553395
C	1.408802	9.066932	-2.084375
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H	3.556817	7.331660	-2.326600
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H	0.681015	9.633203	-1.490370
H	1.089558	9.112560	-3.134134
H	2.375212	9.579604	-2.009870
C	4.821013	0.572700	5.319947
C	3.966204	1.372525	6.089949
C	2.746674	1.832896	5.571646
C	2.427743	1.466874	4.272418
C	3.275130	0.672473	3.507936
C	4.482454	0.207842	4.008337
C	2.599341	0.477159	2.176595
N	1.405050	1.177741	2.174695
C	1.230381	1.769380	3.413579
O	3.047797	-0.217996	1.265022
O	0.258664	2.429599	3.781442
H	5.760128	0.231601	5.748141
H	4.255475	1.638767	7.103359
H	2.074883	2.452605	6.158547
H	5.138770	-0.411499	3.403545
C	-2.708523	1.449800	0.065755
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N	-3.887125	2.099098	-0.149626
H	-4.118105	2.885575	0.439970
C	-4.812189	1.748743	-1.215776
C	-6.214365	1.440570	-0.721297
C	-6.421300	0.607076	0.386715
C	-7.713631	0.303529	0.814712
H	-7.858142	-0.342907	1.676549
C	-8.819800	0.827821	0.140287
H	-9.826304	0.592571	0.475757
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H	-9.477060	2.077970	-1.489915
H	-5.563740	0.201691	0.917097
C	-7.328191	1.965290	-1.386294
H	-7.180829	2.620034	-2.242757
H	-4.370910	0.879835	-1.713723
H	-4.853959	2.560009	-1.955238
C	-1.827514	1.959982	1.166745
H	-1.629180	1.113444	1.836145
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H	-2.486607	4.033890	1.430953
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H	-3.263825	2.847750	2.518168

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C	1.044908	-3.717226	1.055910
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C	1.205001	-2.209226	1.381075
C	2.480008	3.996555	-1.044550
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C	-1.469276	-4.050395	1.509974
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C	2.029936	-0.727521	-0.098199
C	1.060063	4.633583	0.965113
C	-1.154191	-4.943659	2.718668
C	3.666224	-0.512798	-2.787228
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C	4.508721	0.719508	1.633541
C	4.888353	-0.110348	-3.331330

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C	4.076955	-2.821081	-3.475491
C	5.745726	1.343943	1.842054
C	3.659944	-4.299105	-3.594996
C	5.938292	2.484119	2.859665
C	5.703873	-1.061668	-3.940827
C	6.717869	-0.169106	0.186864
C	5.309486	-2.397031	-4.002929
C	6.841435	0.885388	1.087949
C	3.672324	-4.721200	-5.084104
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C	4.656464	2.772128	3.664863
H	1.367959	4.047332	-2.873582
H	1.807218	-3.947254	0.295607
H	0.136728	2.019307	-2.777672
H	0.513432	-1.932205	2.180341
H	3.355747	3.414689	-1.363826
H	2.715092	5.044443	-1.282031
H	0.008167	5.346070	-1.535679
H	-0.933184	3.879702	-1.791353
H	-0.560625	-3.435570	-0.374525
H	-0.263006	-5.107682	0.069202
H	1.441836	-5.641067	1.936576
H	2.282867	-4.345329	2.763245
H	3.025679	2.331047	-3.235825
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H	3.310572	-2.730721	1.891168
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H	3.201423	4.259613	0.971834
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H	-1.078193	4.697752	0.556899
H	-1.641203	-3.021248	1.854831
H	-2.406292	-4.368250	1.036999
H	0.132886	-3.574791	3.792491
H	0.445752	-5.262702	4.159825
H	0.945219	4.501697	2.048260
H	1.190313	5.712890	0.787966

H	-1.951902	-4.867549	3.467797
H	-1.126453	-5.994963	2.394721
H	2.289366	-2.125503	-2.478789
H	3.621554	1.032656	2.172126
H	5.200832	0.926199	-3.255759
H	5.383052	-1.648010	-0.664429
H	6.658824	-0.760558	-4.362746
H	7.585586	-0.508119	-0.372452
H	5.968637	-3.115676	-4.480351
H	7.814461	1.351651	1.213584
H	4.664350	-4.614543	-5.534908
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H	4.664461	-4.908141	-1.742139
H	4.392046	-6.233396	-2.889665
H	5.685895	-5.060634	-3.180648
H	2.174072	-4.319695	-1.973001
H	1.484166	-3.982211	-3.573641
H	1.997197	-5.619951	-3.154525
H	8.014770	1.929146	3.367615
H	7.193269	2.898291	4.597184
H	6.790688	1.181200	4.405496
H	5.578089	4.083370	1.402753
H	6.509253	4.593401	2.824265
H	7.285138	3.636515	1.552328
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H	4.336159	1.895313	4.239576
H	4.846486	3.584089	4.376107
Ni	-0.696392	0.210420	-0.144099
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C	-3.045127	2.034102	-0.358142
C	-4.009345	2.810282	-1.005993
C	-4.143968	2.789815	-2.402343
C	-2.311043	1.186590	-2.462646
C	-3.276600	1.957878	-3.119562
C	-5.191675	3.636586	-3.094553
C	-4.851892	5.145816	-3.187219
H	-6.147228	3.534641	-2.561317
H	-5.363863	3.253017	-4.110107
H	-1.683256	0.539552	-3.076848
H	-2.993272	2.083098	0.726714

H	-4.676604	3.438396	-0.415994
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H	-6.940382	5.793696	-3.082788
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H	-5.841697	7.010302	-3.758892
C	-0.591489	1.336525	6.451091
C	-1.908253	0.860509	6.400850
C	-2.481453	0.445507	5.189659
C	-1.695402	0.533263	4.050478
C	-0.386090	1.004469	4.100016
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C	0.151742	0.937987	2.697909
N	-0.854836	0.483548	1.862580
C	-1.973245	0.176558	2.617834
O	1.305265	1.209383	2.364946
O	-3.013902	-0.335604	2.209055
H	-0.175320	1.651015	7.404533
H	-2.492238	0.812737	7.316099
H	-3.499613	0.071149	5.139584
H	1.217176	1.777388	5.320917
C	-4.193575	-1.535231	-1.248453
O	-4.837873	-1.681089	-2.298907
N	-4.752791	-1.082847	-0.087254
H	-4.141570	-0.866689	0.695887
C	-6.118729	-0.578279	-0.052898
C	-7.135131	-1.591409	0.449429
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C	-8.358699	-3.665873	0.137657
H	-8.577769	-4.544290	-0.464793
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H	-9.744304	-4.201722	1.706384
C	-8.733929	-2.341408	2.121178
H	-9.240339	-2.182750	3.070306
H	-6.914145	-2.872059	-1.262044
C	-7.797705	-1.407934	1.667257

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H	-6.373503	-0.272685	-1.072685
H	-6.134630	0.312613	0.583896
C	-2.768863	-1.884624	-1.168194
C	-2.080855	-2.398549	-2.386192
H	-2.551205	-1.984137	-3.281728
H	-2.167206	-3.495833	-2.459480
H	-1.009309	-2.164525	-2.384000
H	-2.318124	-2.005273	-0.187859

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C	0.949537	-3.623291	1.230077
C	0.945664	1.887377	-2.540029
C	1.018503	-2.089103	1.467058
C	2.544268	3.779023	-1.630902
C	0.036197	4.204205	-1.757190
C	-0.388099	-4.121252	0.644718
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C	2.084850	1.180025	-3.330798
C	2.450677	-1.640357	1.868904
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C	-0.025398	4.218024	-0.222332
C	-1.549894	-4.098096	1.654050
C	0.102590	-4.401652	3.545228
C	1.774294	0.217329	-1.280554
C	1.832007	-0.704437	-0.111317
C	1.298171	4.695503	0.385725
C	-1.208986	-4.897477	2.919662
C	3.502930	-0.813476	-2.777576
C	4.181745	-0.239166	0.718804
C	3.080072	-2.150724	-2.757345
C	4.298197	0.884925	1.550369
C	4.752291	-0.479134	-3.306295
C	5.297030	-0.764251	0.068009
C	3.902168	-3.180134	-3.237656
C	5.538712	1.505317	1.750126

C	3.465928	-4.657599	-3.242633
C	5.727944	2.698010	2.706764
C	5.576287	-1.491935	-3.792445
C	6.530332	-0.130817	0.229605
C	5.161700	-2.822026	-3.749539
C	6.647006	0.980472	1.060484
C	3.548588	-5.217078	-4.683456
C	4.411273	-5.467744	-2.323313
C	2.021511	-4.847486	-2.743495
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C	6.272063	3.915595	1.922750
C	4.413890	3.108208	3.398850
H	1.328797	3.742211	-3.391354
H	1.743241	-3.852457	0.502321
H	0.002934	1.824251	-3.090373
H	0.293469	-1.804190	2.231762
H	3.361150	3.113974	-1.941760
H	2.827488	4.783665	-1.978099
H	0.135887	5.242749	-2.107133
H	-0.906165	3.825388	-2.167560
H	-0.640921	-3.547950	-0.249574
H	-0.238339	-5.159537	0.313354
H	1.440292	-5.464750	2.230892
H	2.179830	-4.075964	2.999962
H	2.847610	1.877227	-3.687760
H	1.713384	0.606661	-4.189533
H	3.118679	-2.473318	2.102183
H	2.453731	-0.942786	2.713728
H	2.296139	2.798698	0.293571
H	3.407252	4.167873	0.306586
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H	-1.795905	-3.065657	1.936713
H	-2.452652	-4.502838	1.180185
H	-0.041903	-3.383006	3.932723
H	0.373392	-5.020964	4.410067
H	1.242020	4.671474	1.481185
H	1.486138	5.742076	0.097742
H	-2.028310	-4.829910	3.645941
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H	2.090273	-2.373275	-2.376345

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H	5.076613	0.556592	-3.312130
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X. References

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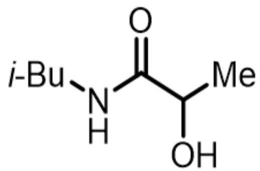
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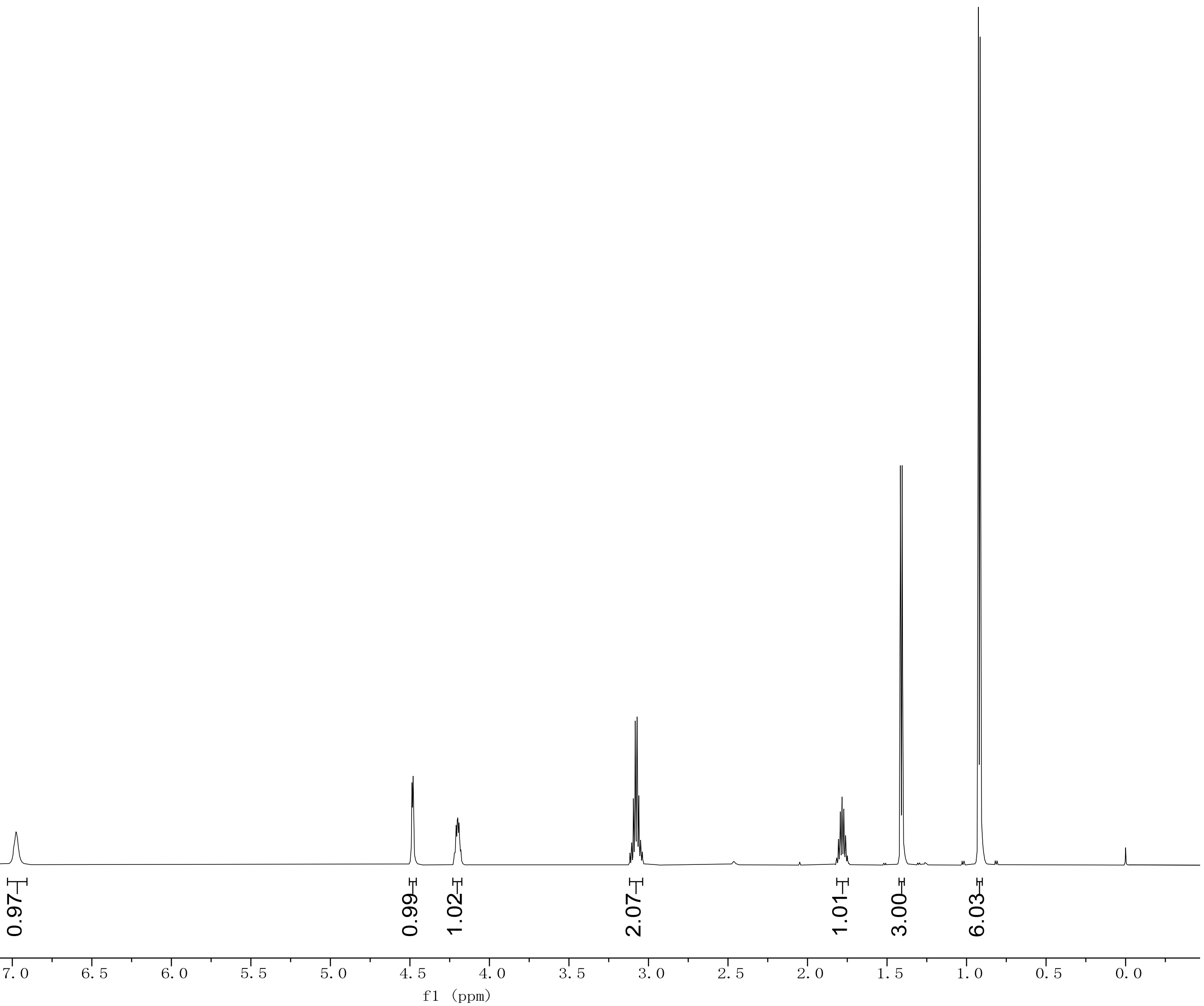
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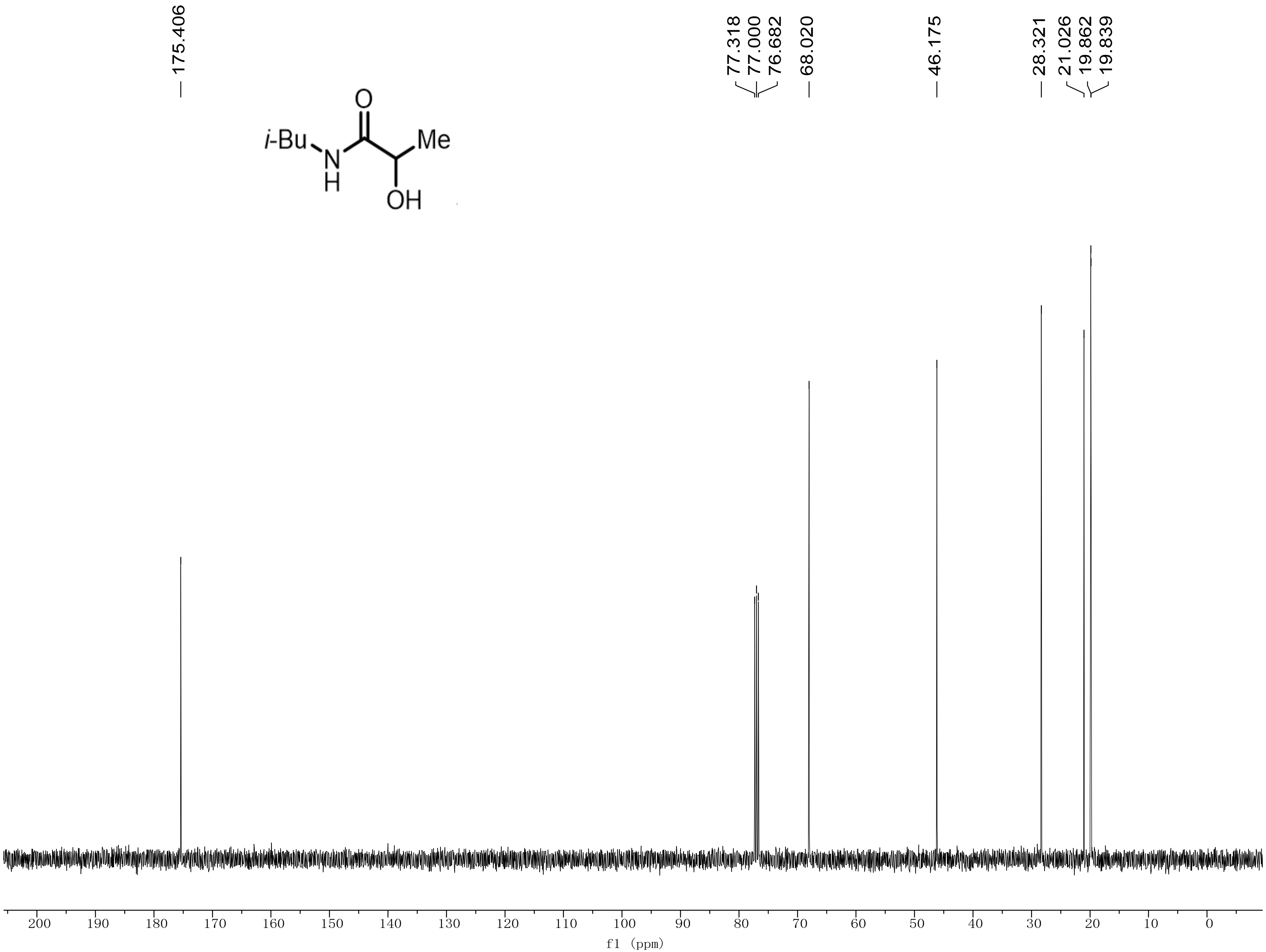
f1 (ppm)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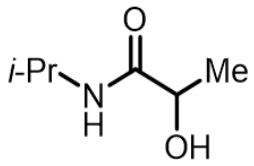

i-Pr
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Me
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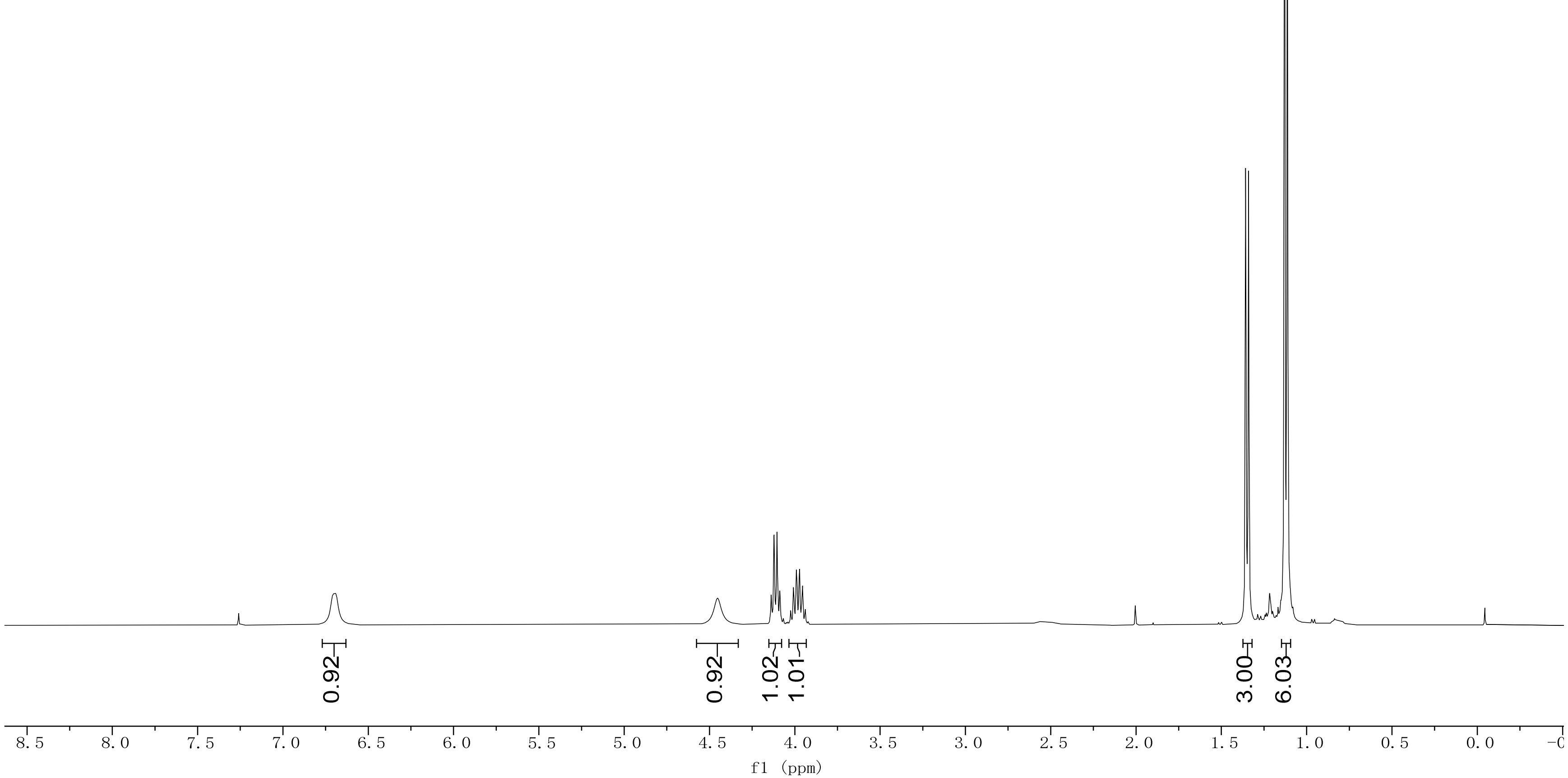

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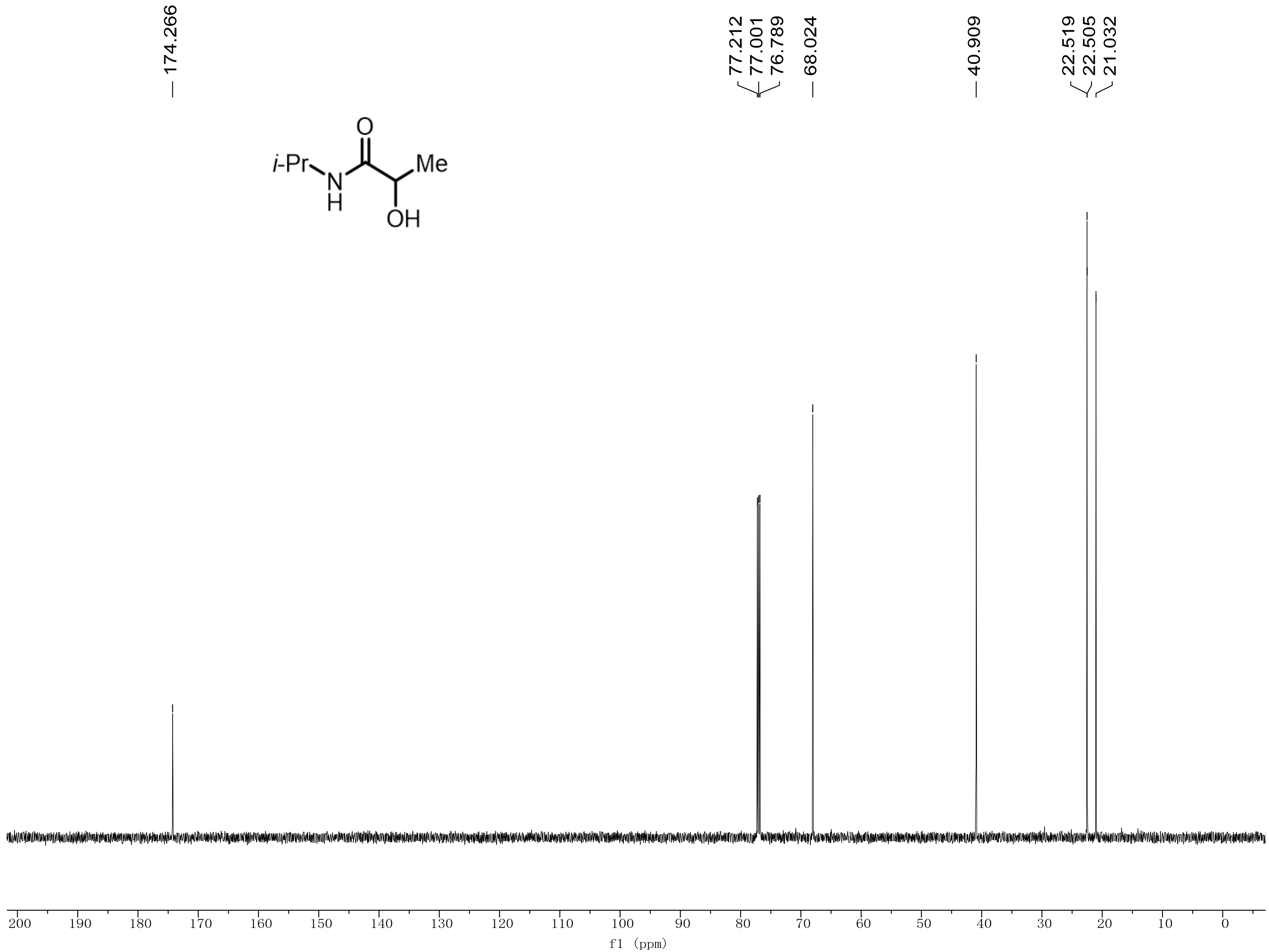
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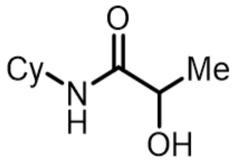
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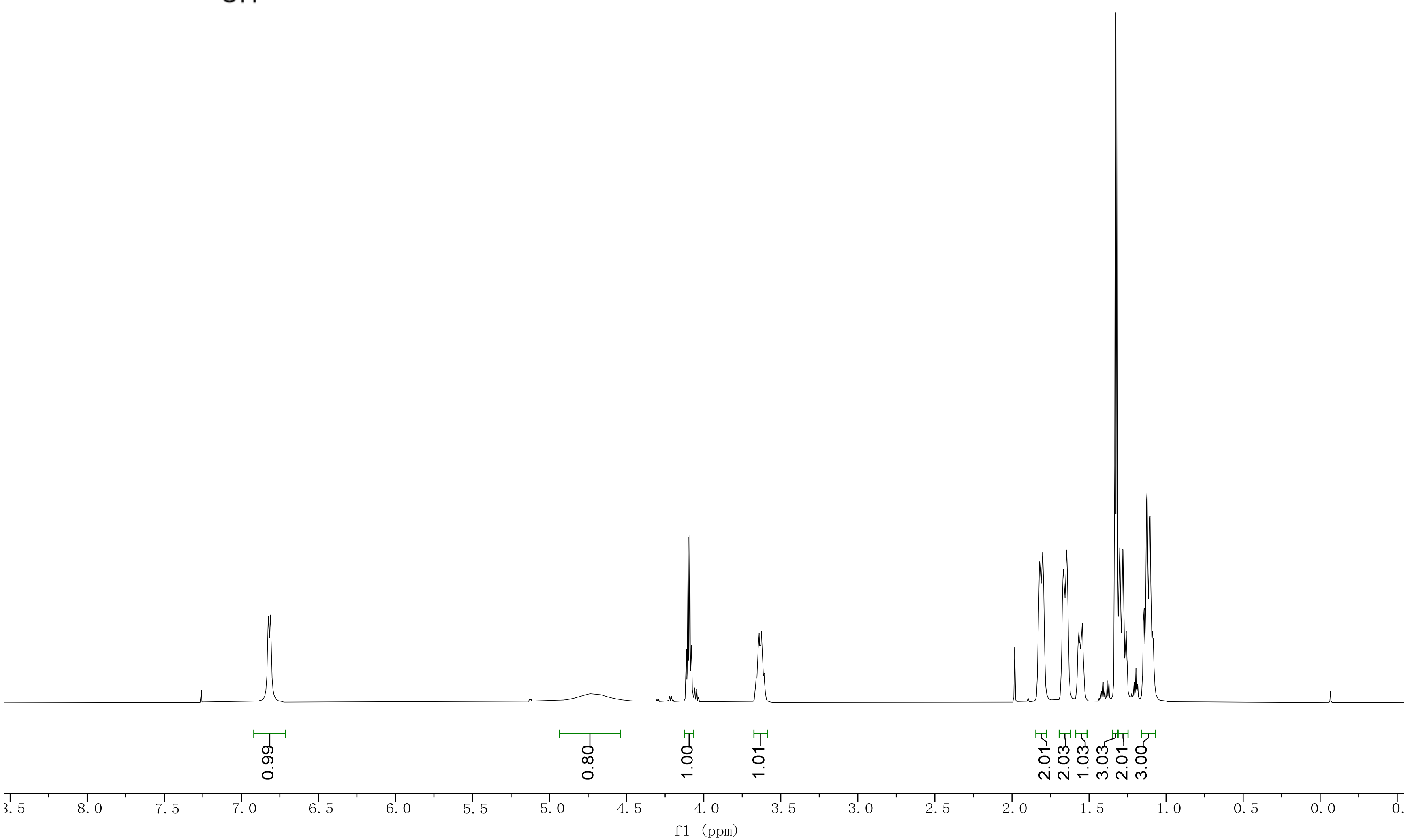
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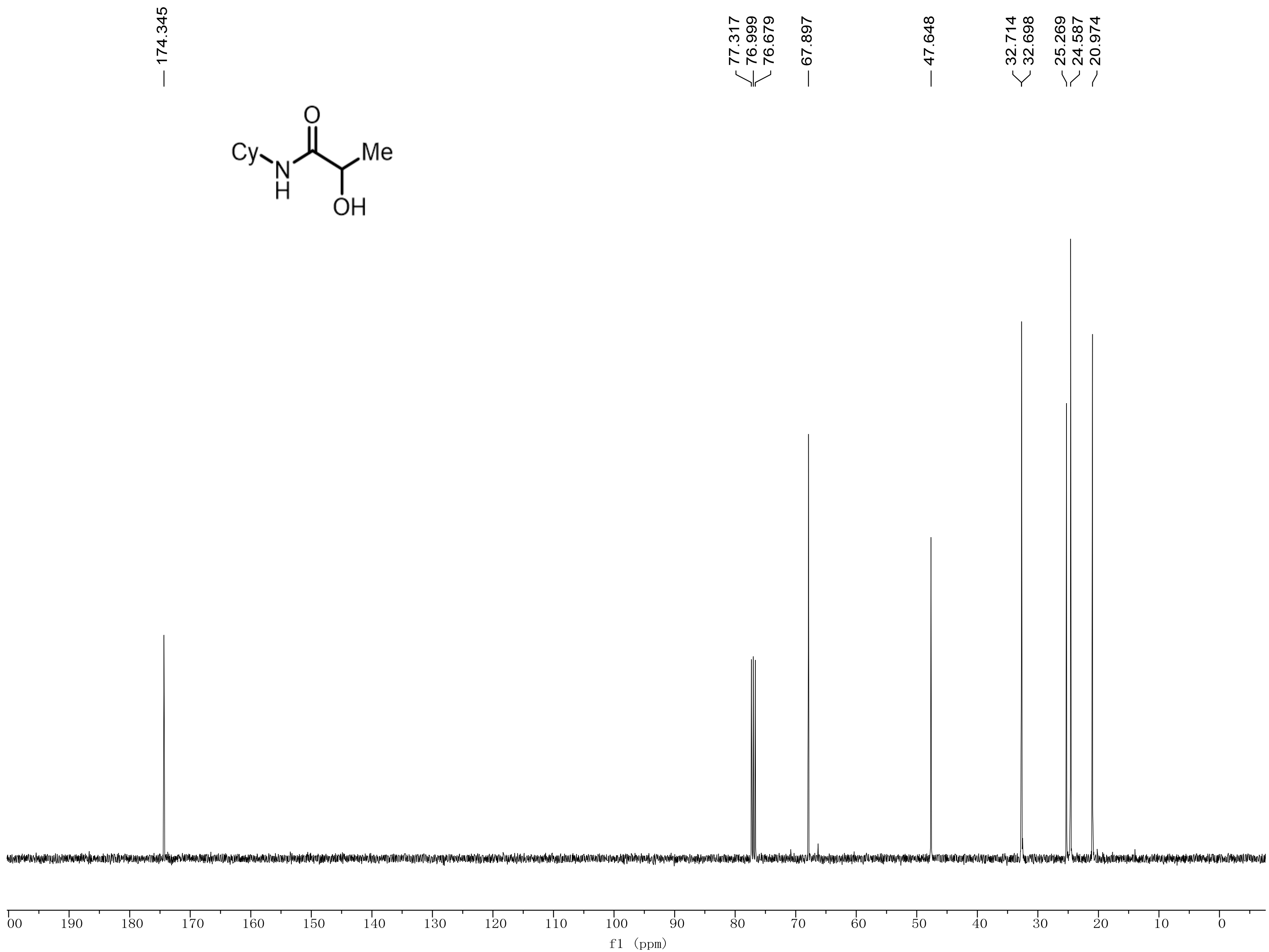
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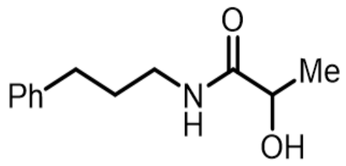
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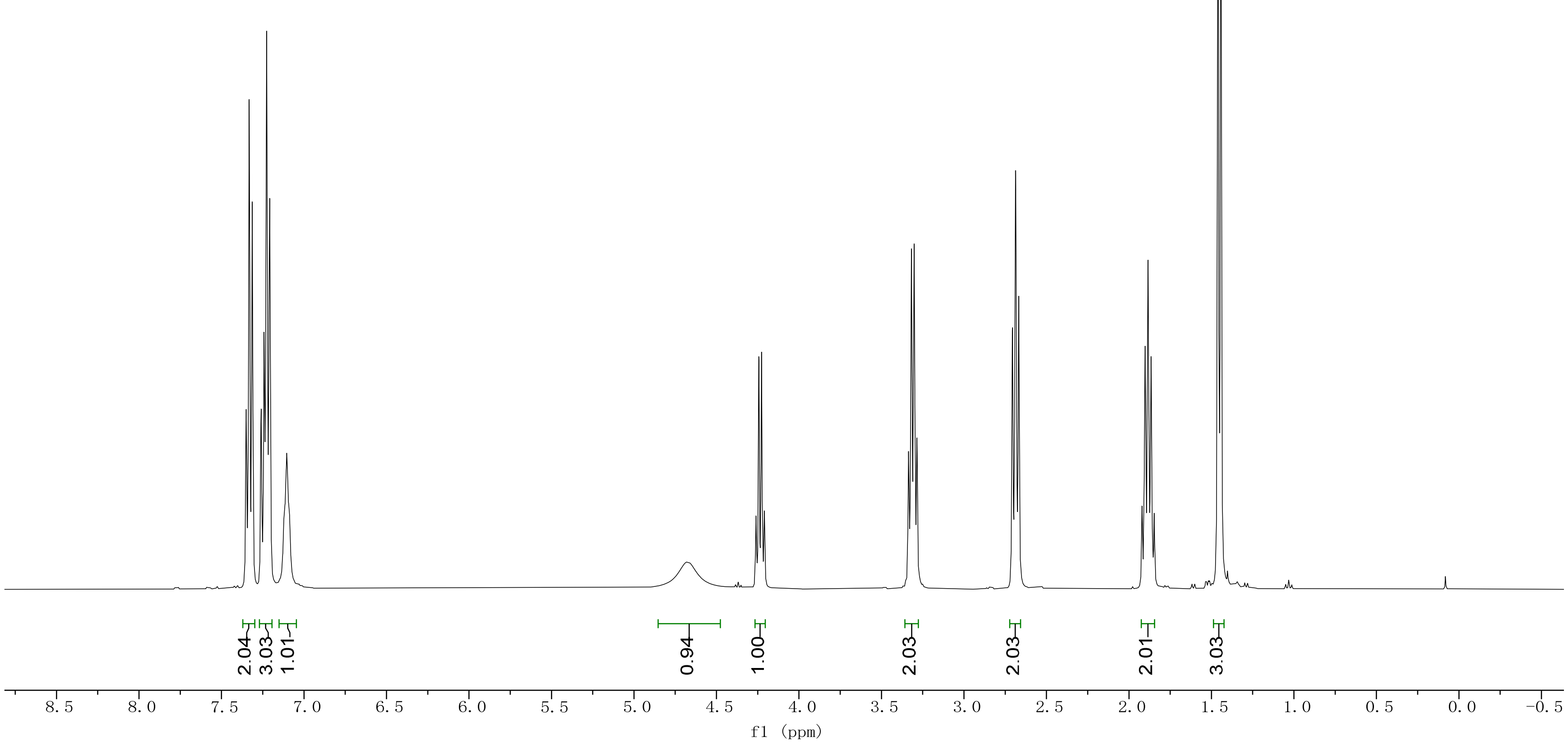
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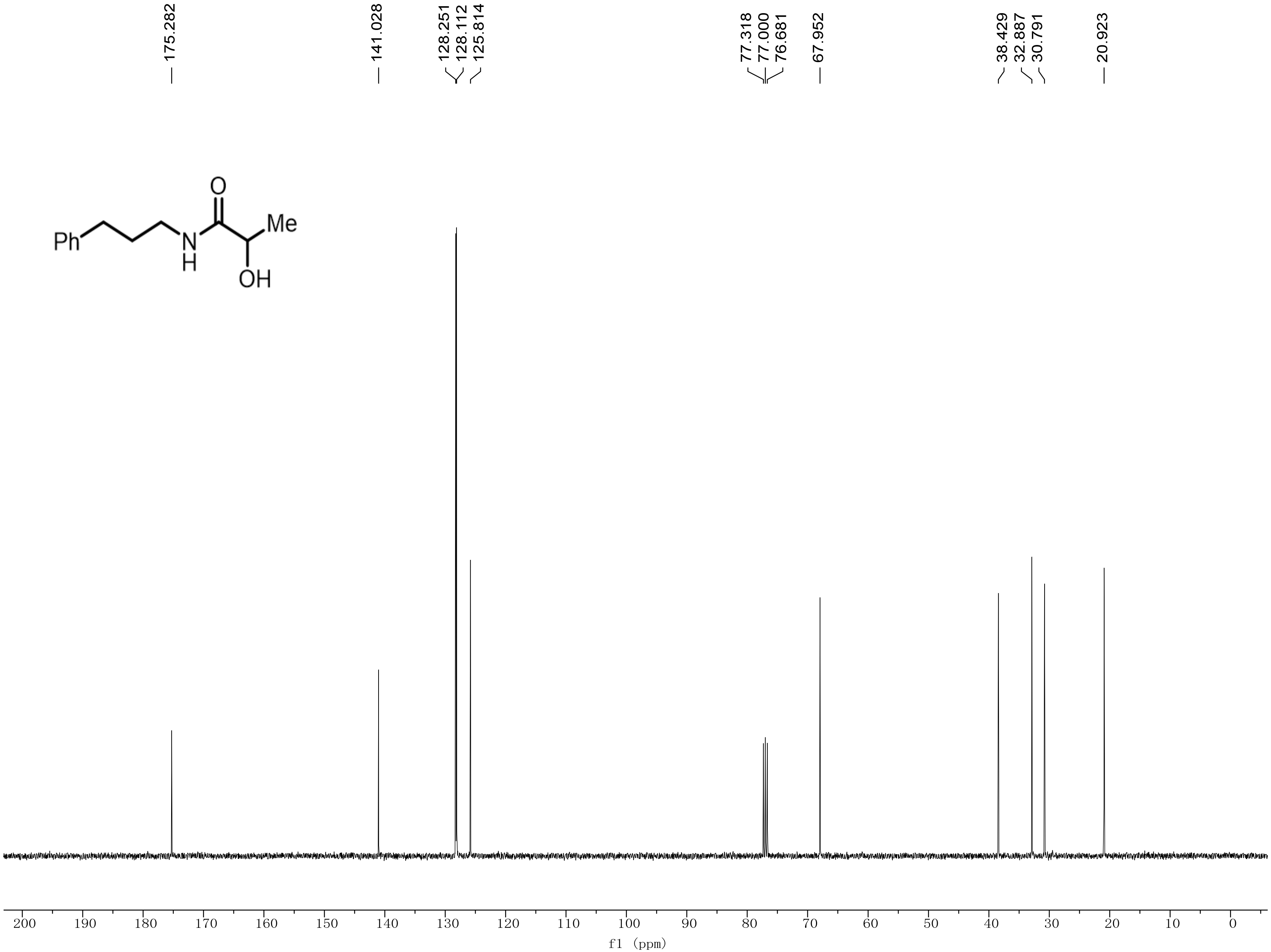
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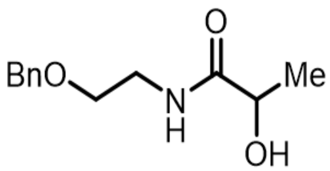
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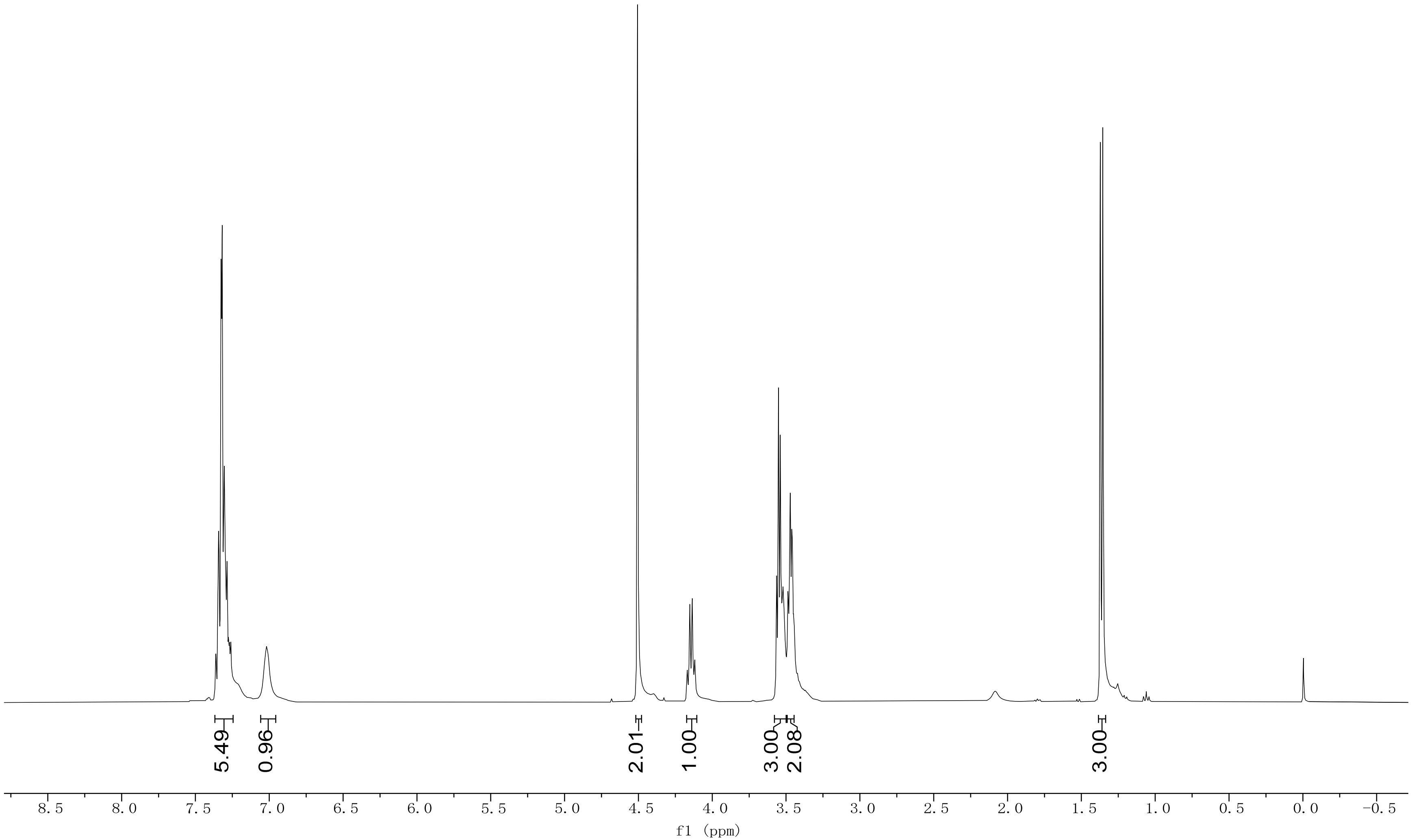
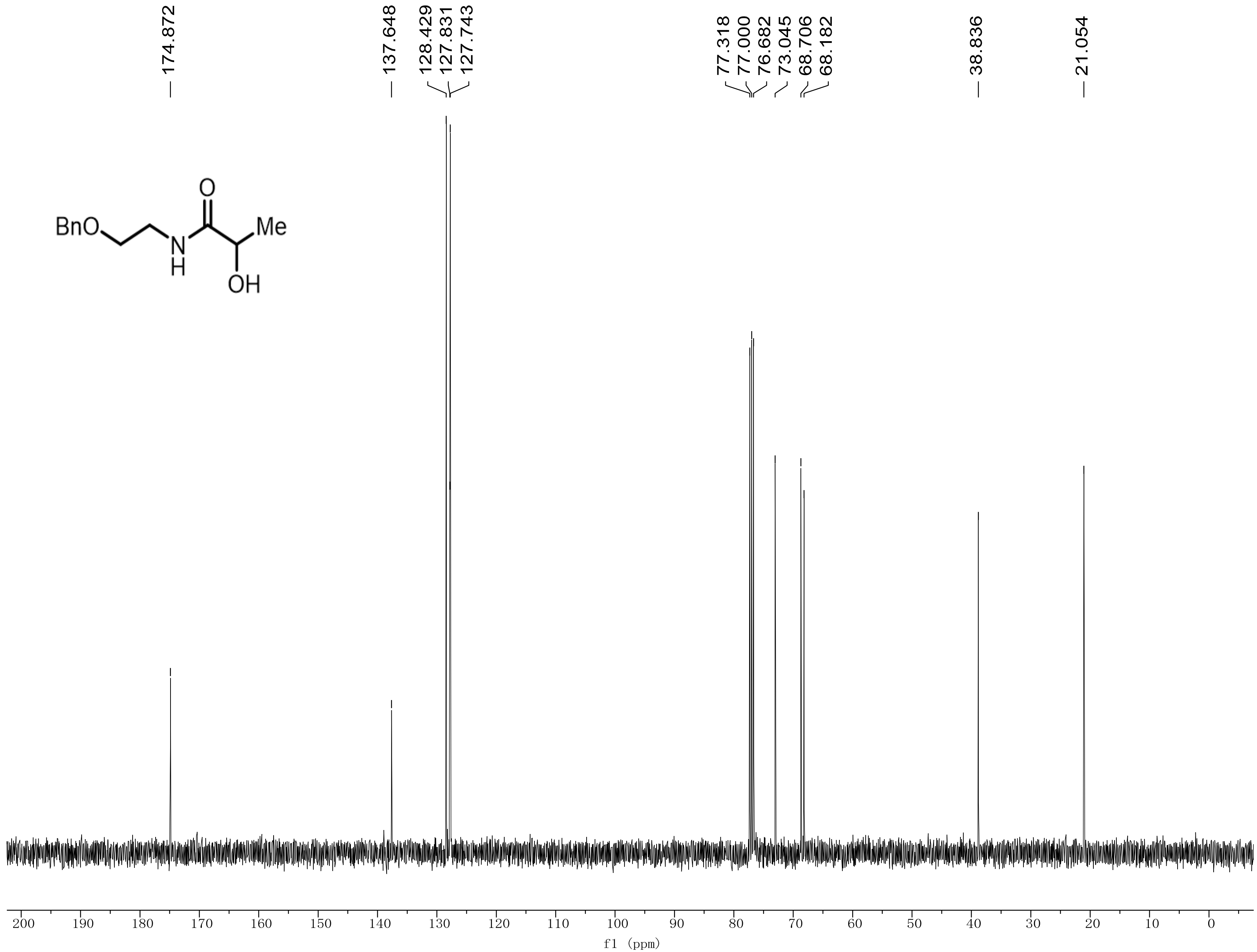
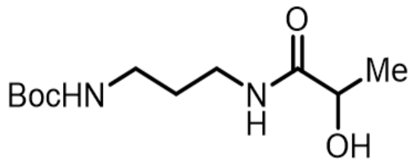
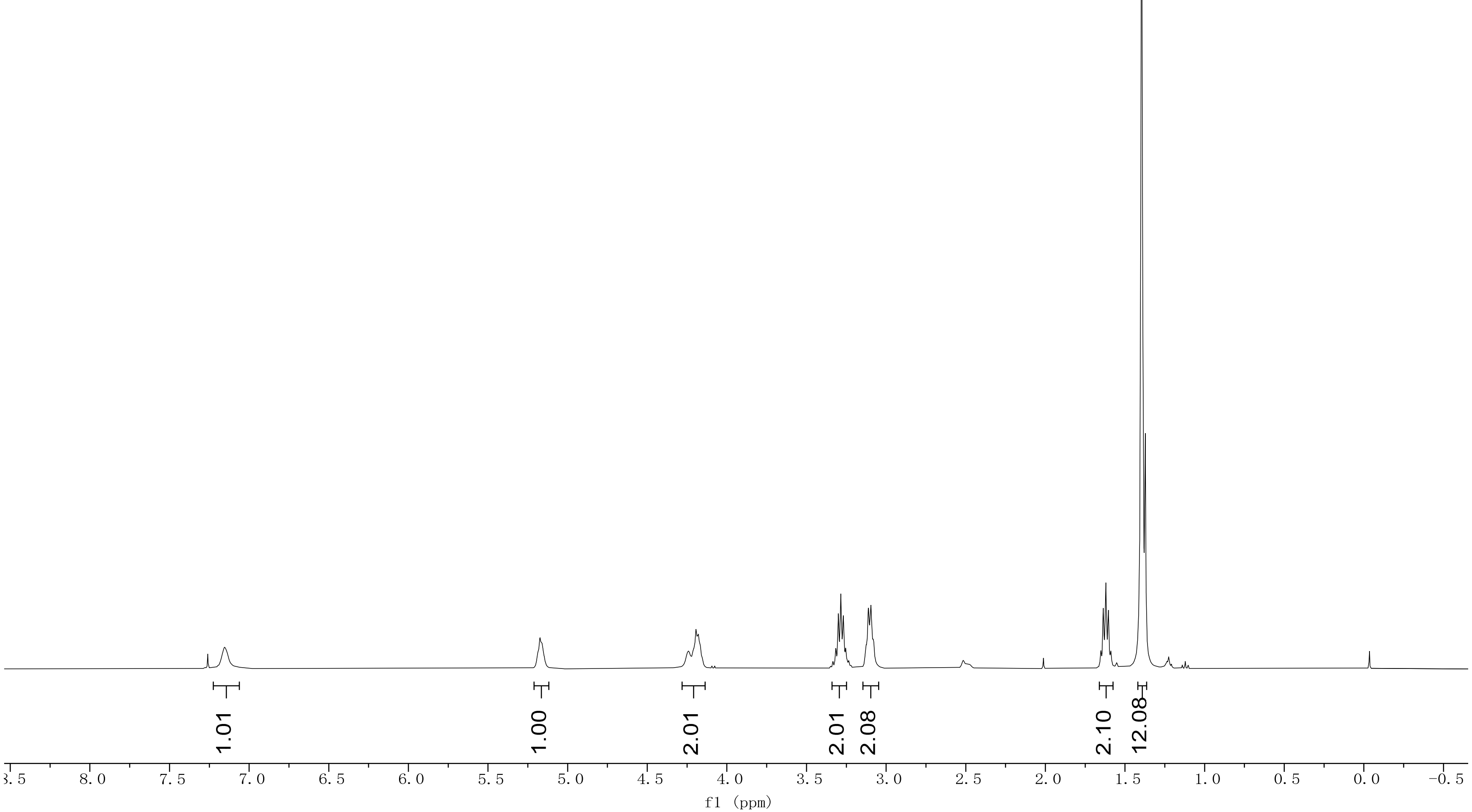
Me
OH


5.49
0.96
2.01
1.00
3.00
2.08
3.00
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
-0.5
f1 (ppm)

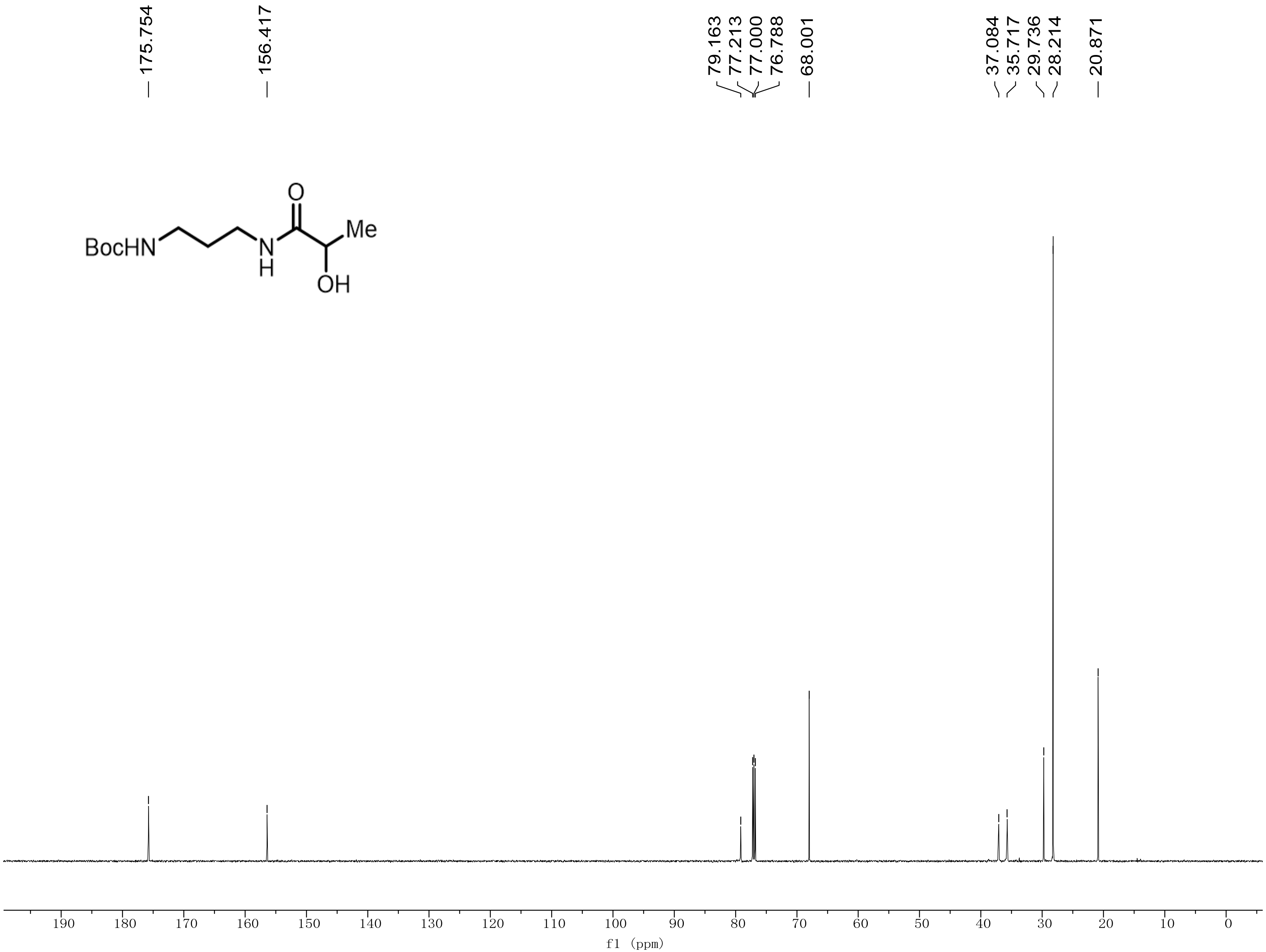


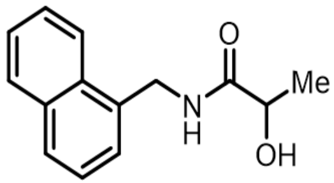
174.872
137.648
128.429
127.831
127.743
77.318
77.000
76.682
73.045
68.706
68.182
38.836
21.054
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

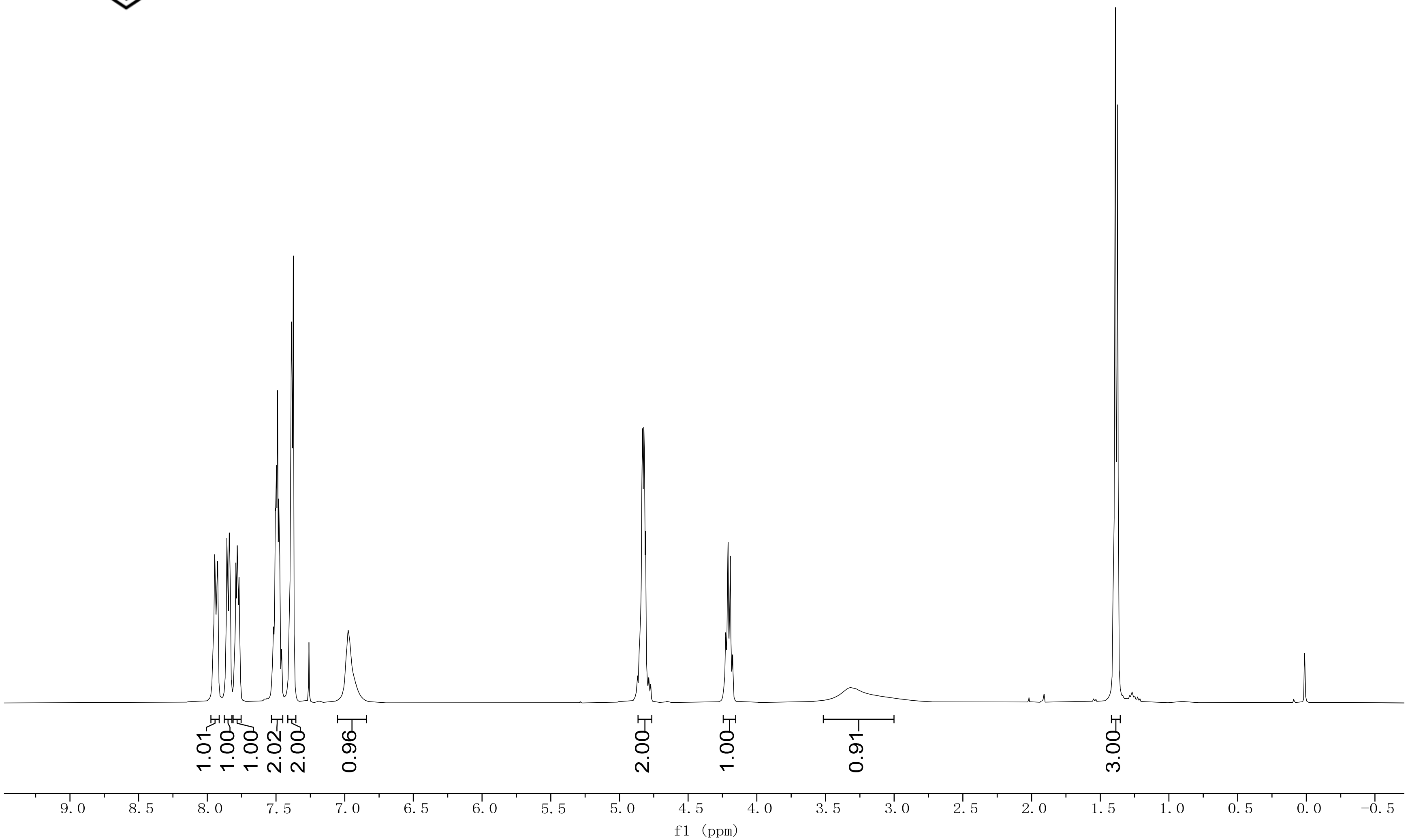


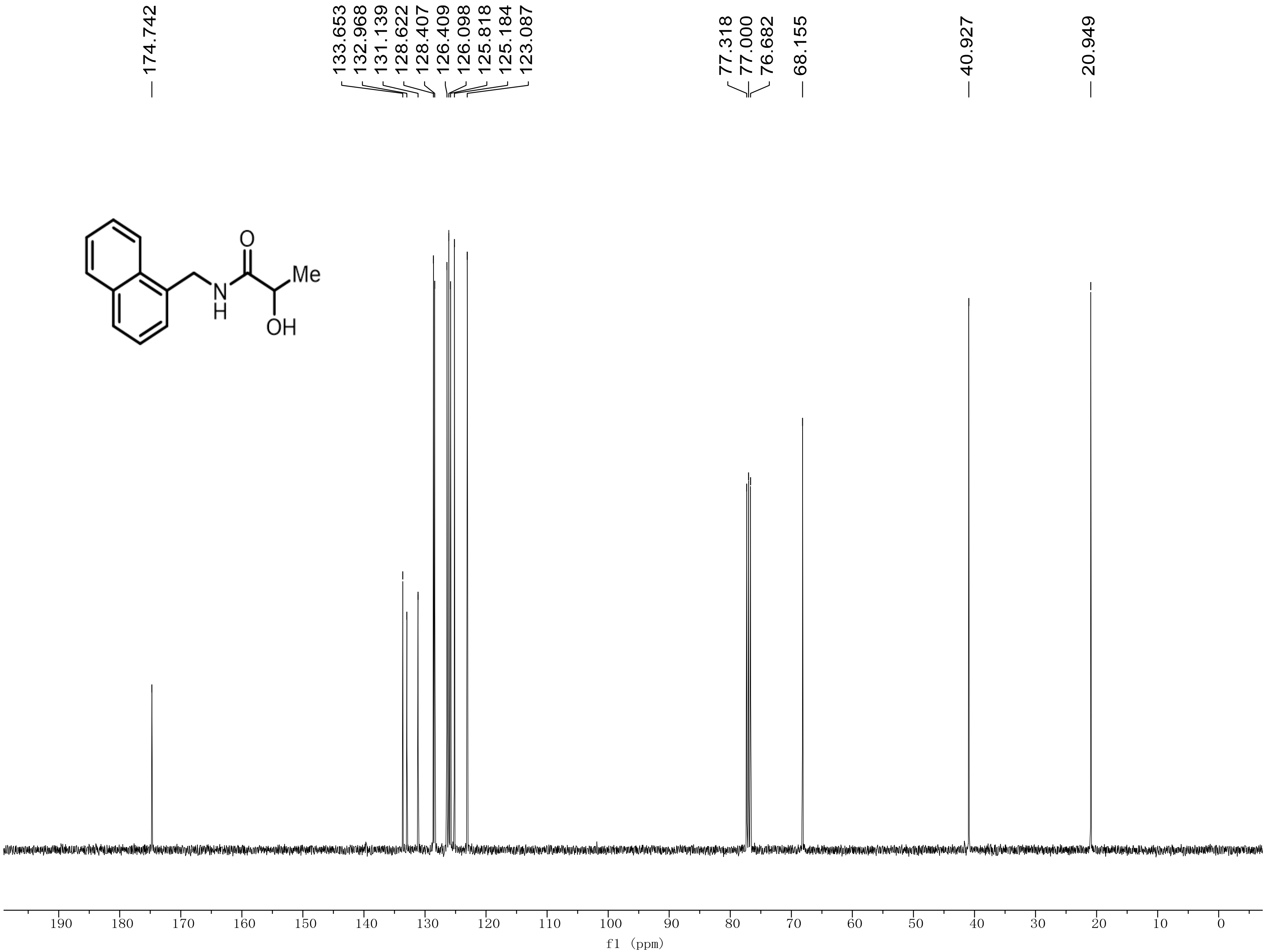


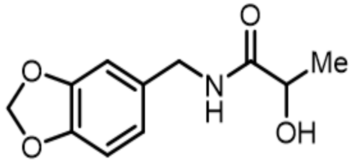
1.01
1.00
2.01
2.01
2.08
2.10
12.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

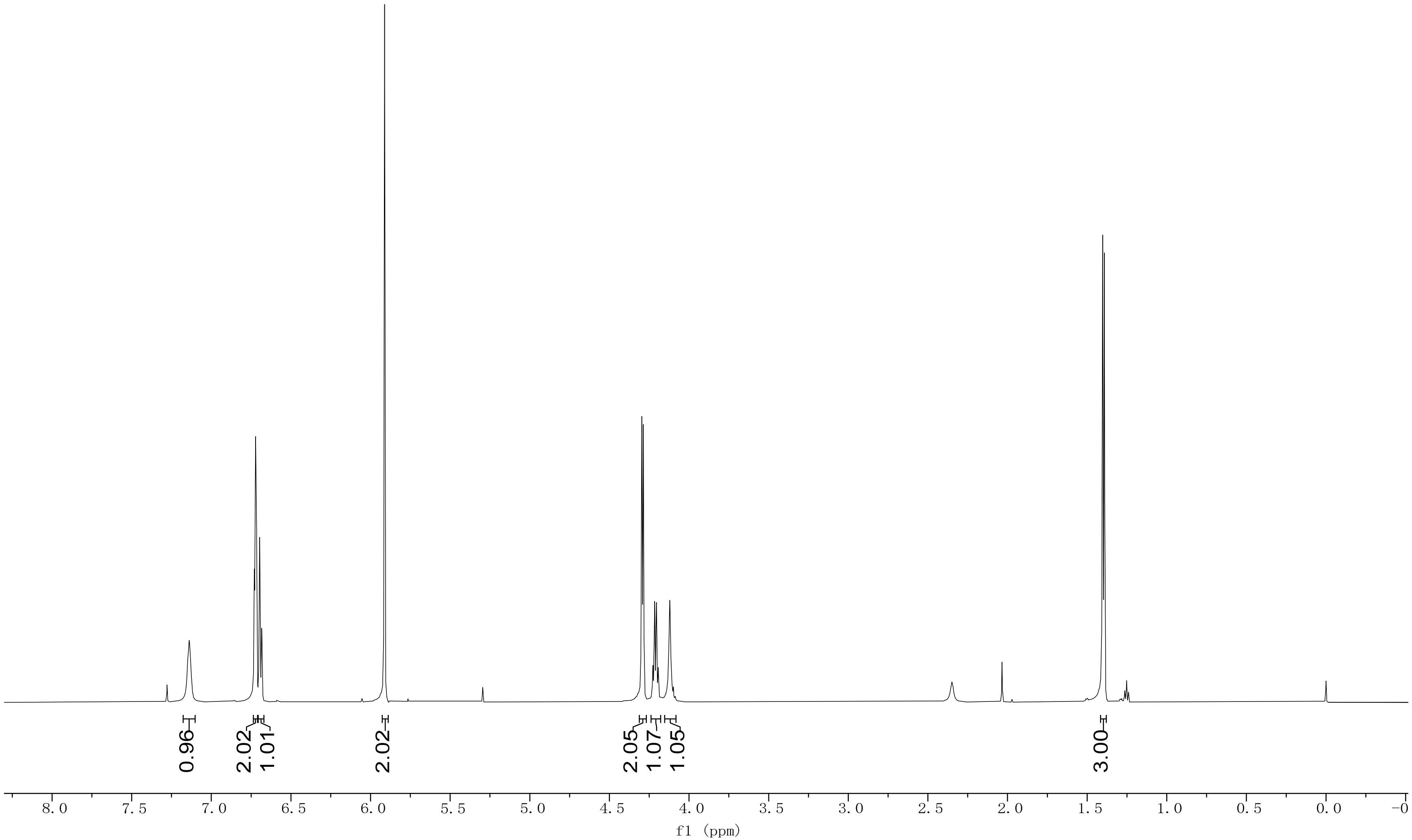

175.754
156.417
79.163
77.213
77.000
76.788
68.001
37.084
35.717
29.736
28.214
20.871
BocHN
N
H
O
Me
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
Me
N
H
OH

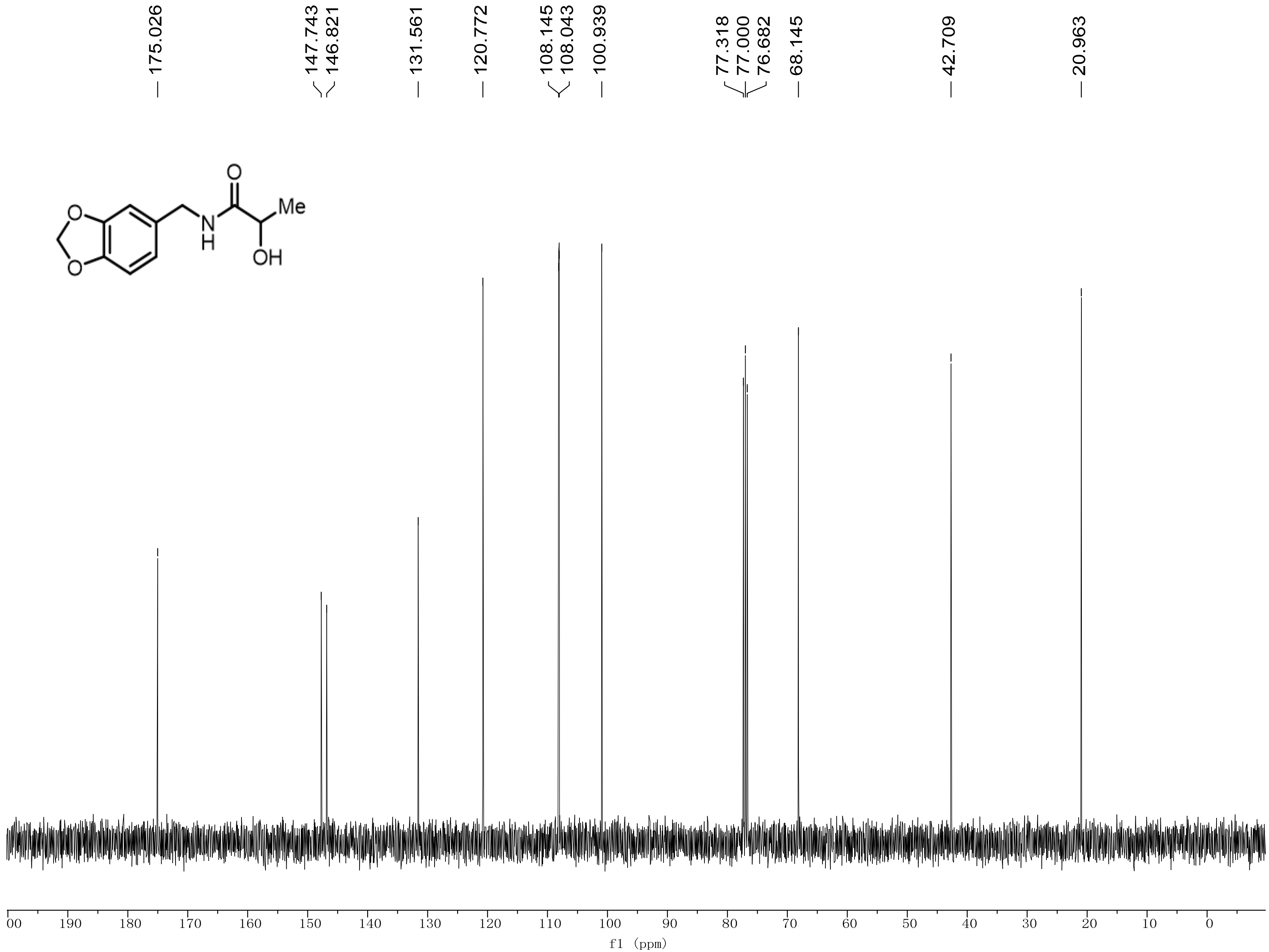

1.01
1.00
1.00
2.02
2.00
0.96
2.00
1.00
0.91
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


174.742
133.653
132.968
131.139
128.622
128.407
126.409
126.098
125.818
125.184
123.087
77.318
77.000
76.682
68.155
40.927
20.949
O
Me
N
H
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

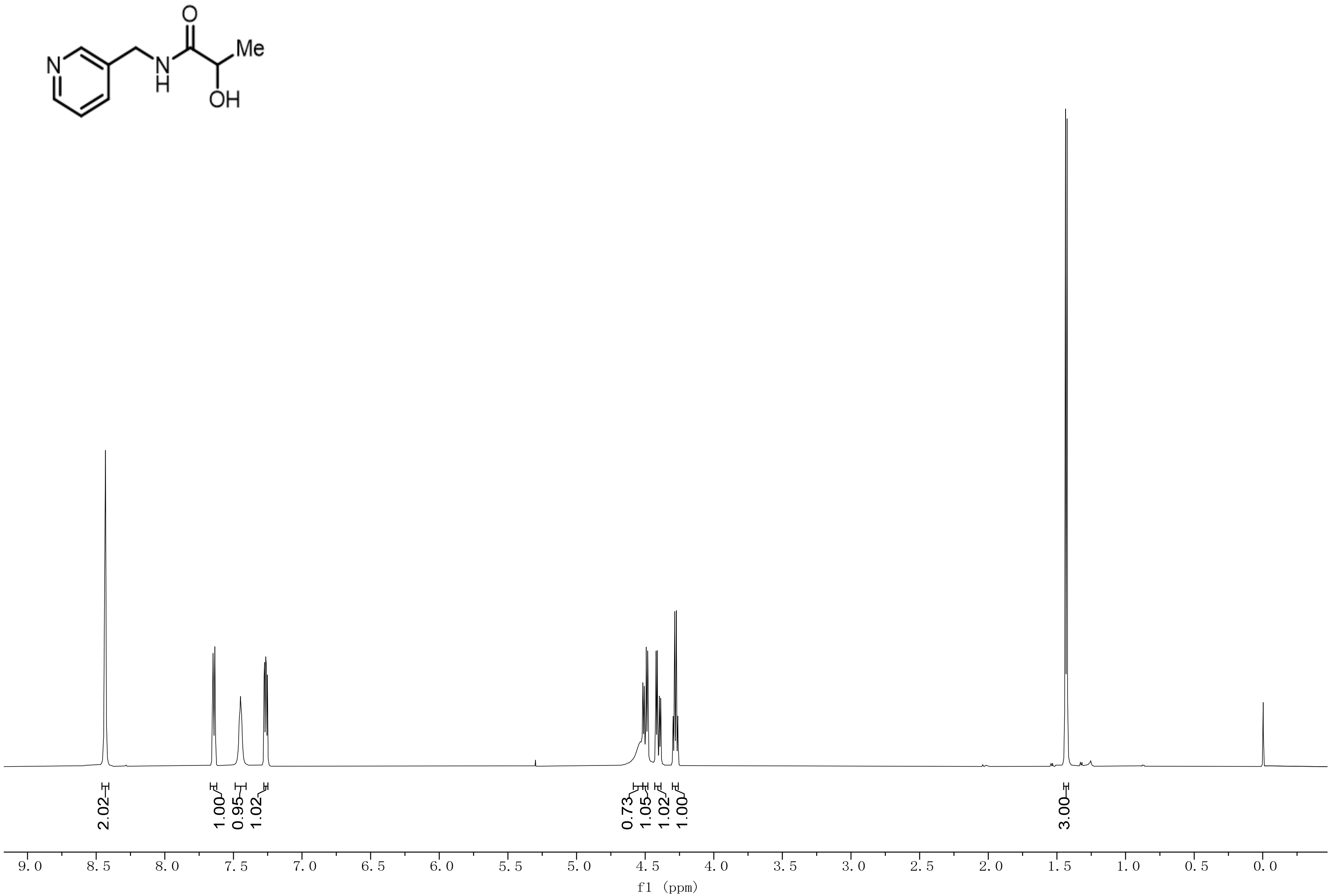




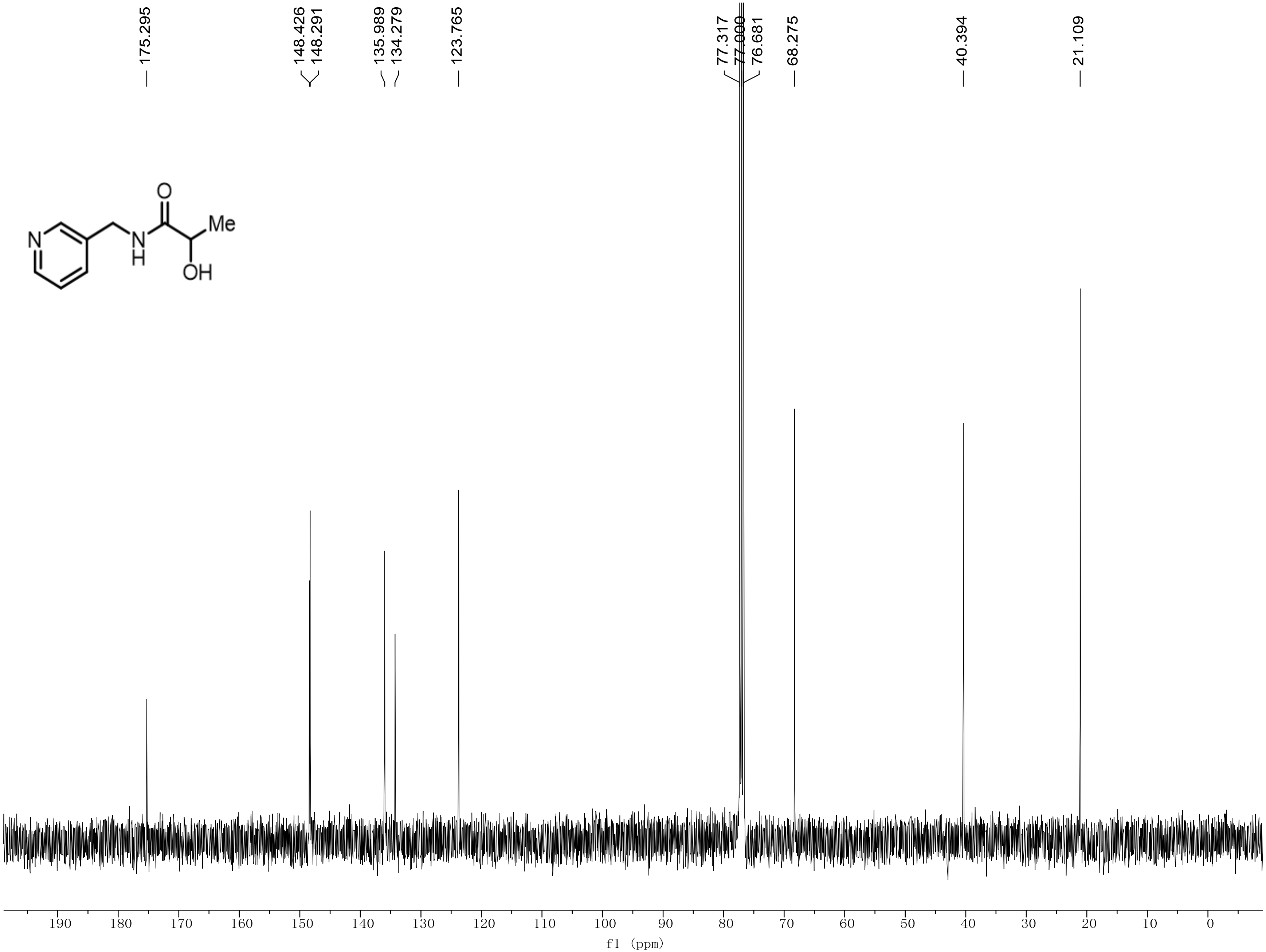
0.96
2.02
1.01
2.02
2.05
1.07
1.05
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

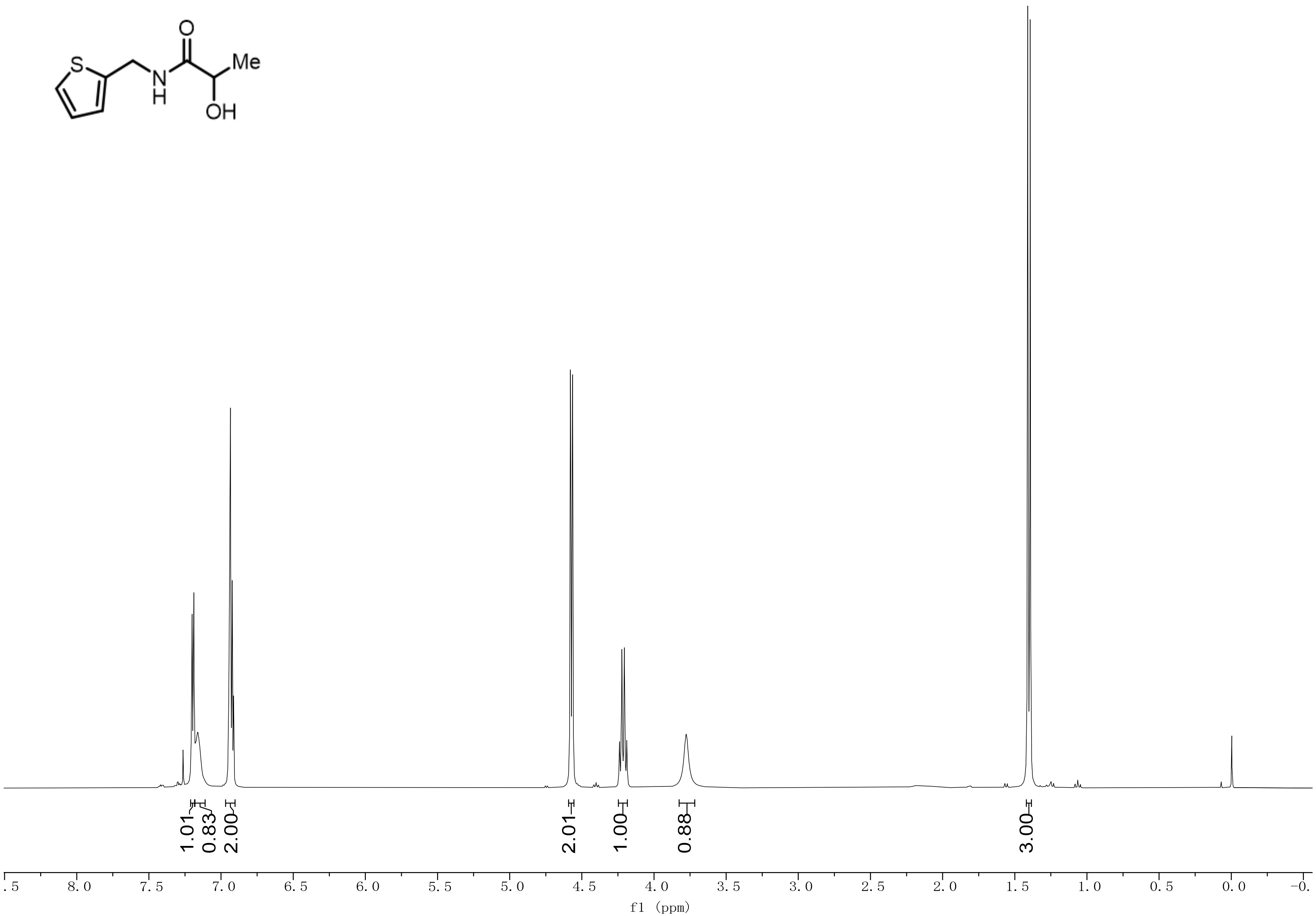


175.026
147.743
146.821
131.561
120.772
108.145
108.043
100.939
77.318
77.000
76.682
68.145
42.709
20.963
O
N
H
Me
OH
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

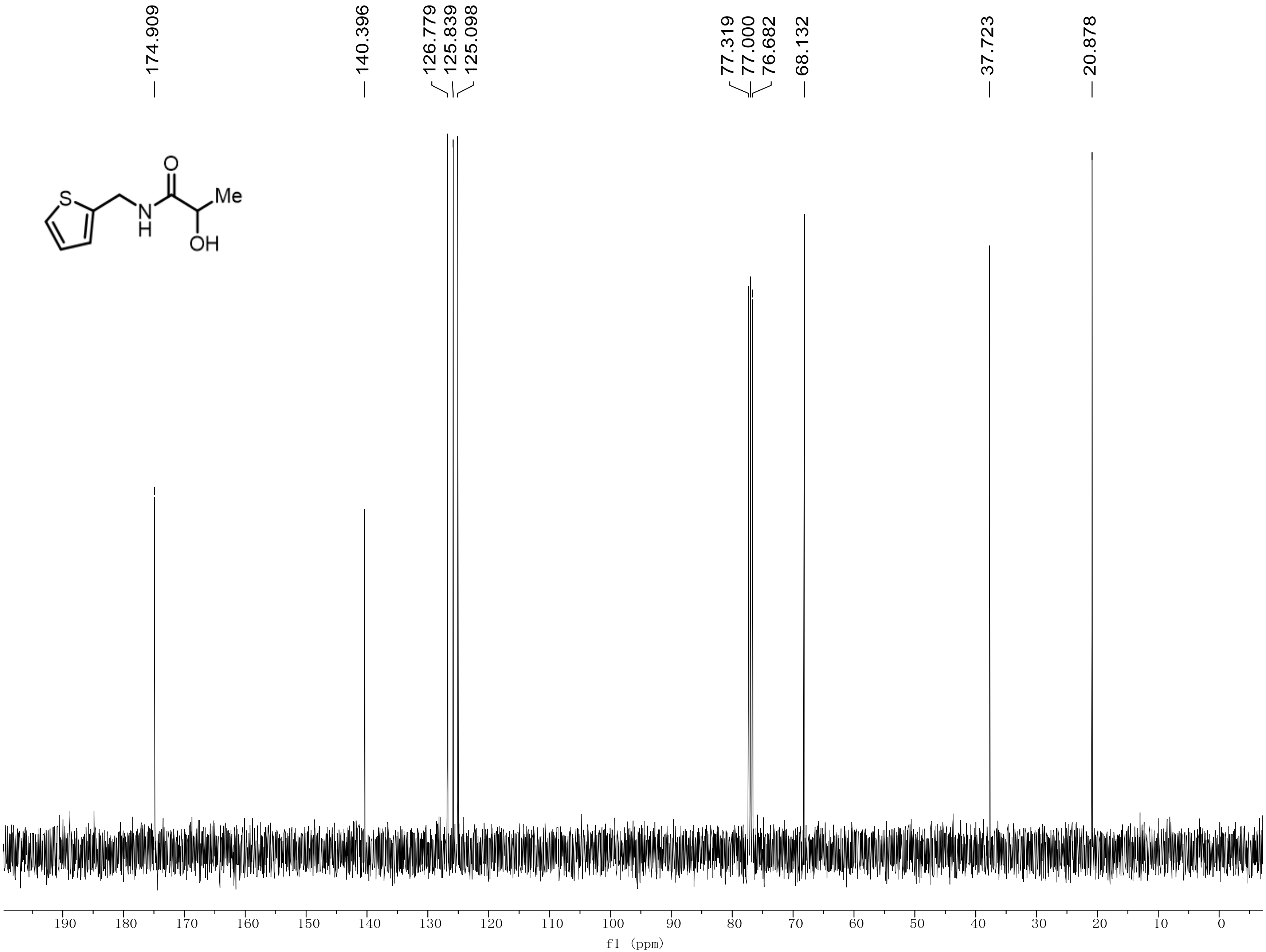


Me
O
N
H
OH
2.02
1.00
0.95
1.02
0.73
1.05
1.02
1.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

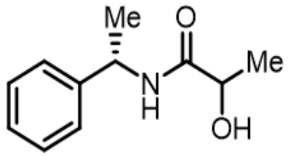

175.295
148.426
148.291
135.989
134.279
123.765
77.317
77.000
76.681
68.275
40.394
21.109
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

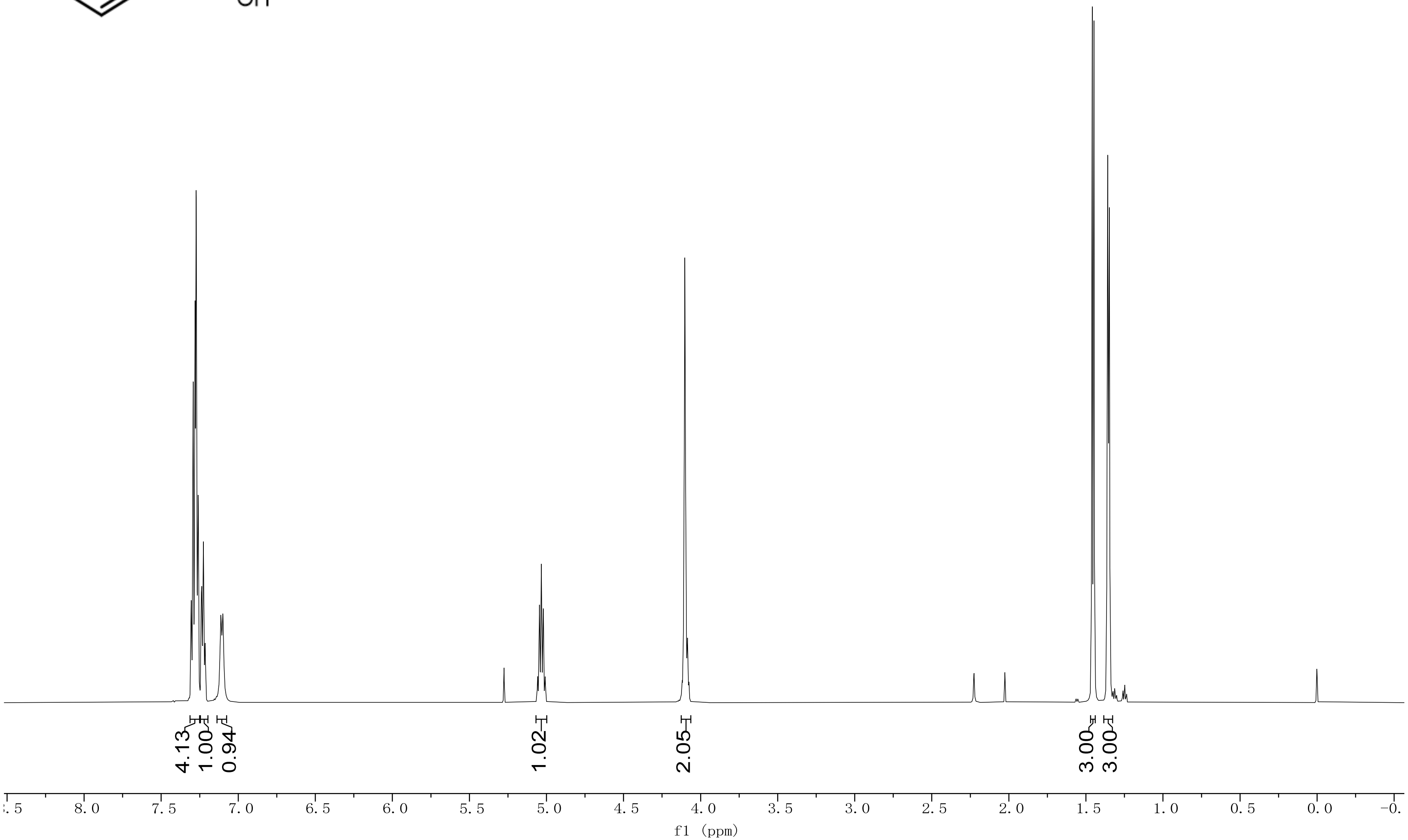


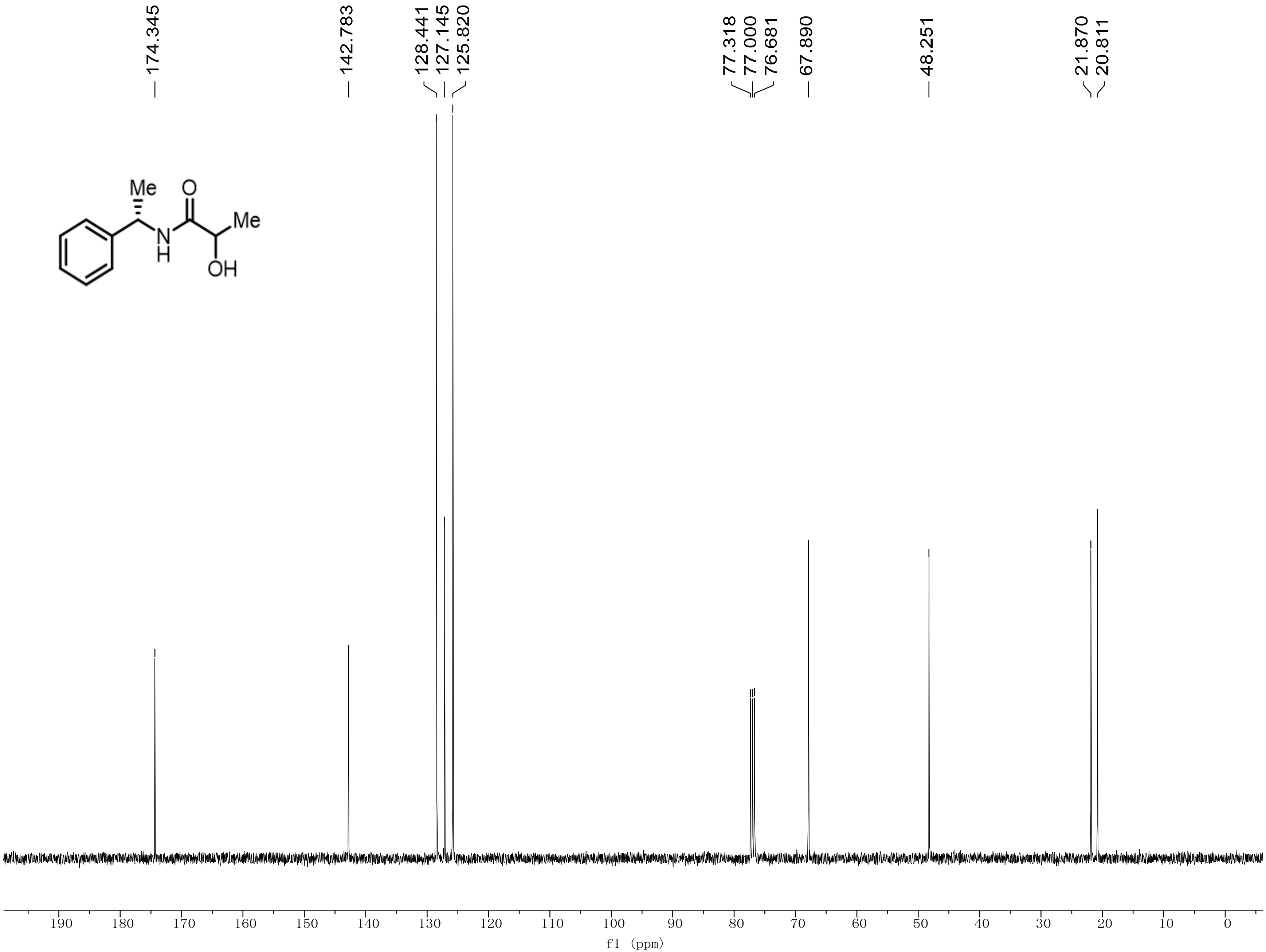
1.01
0.83
2.00
2.01
1.00
0.88
3.00
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)



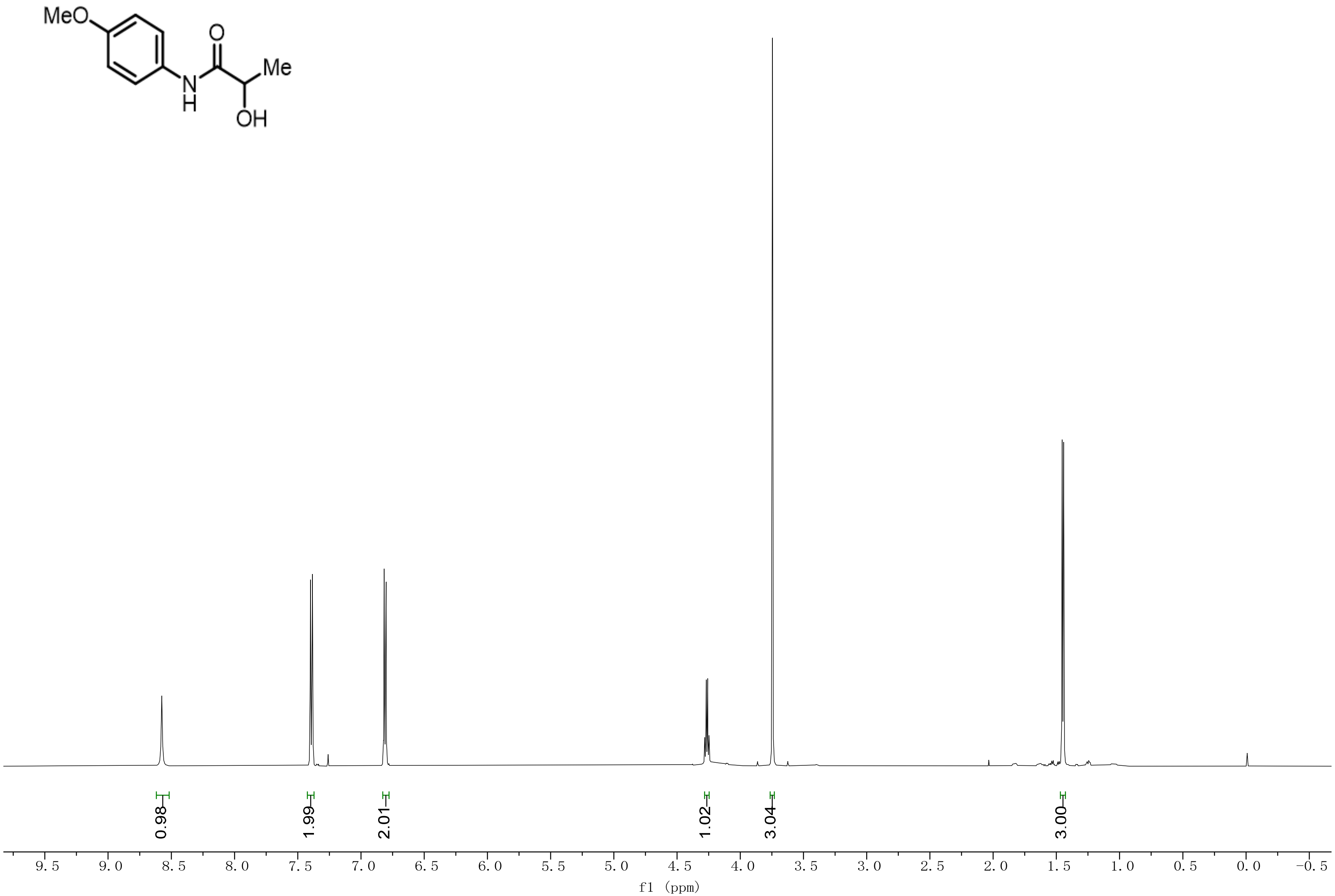
174.909
140.396
126.779
125.839
125.098
77.319
77.000
76.682
68.132
37.723
20.878
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

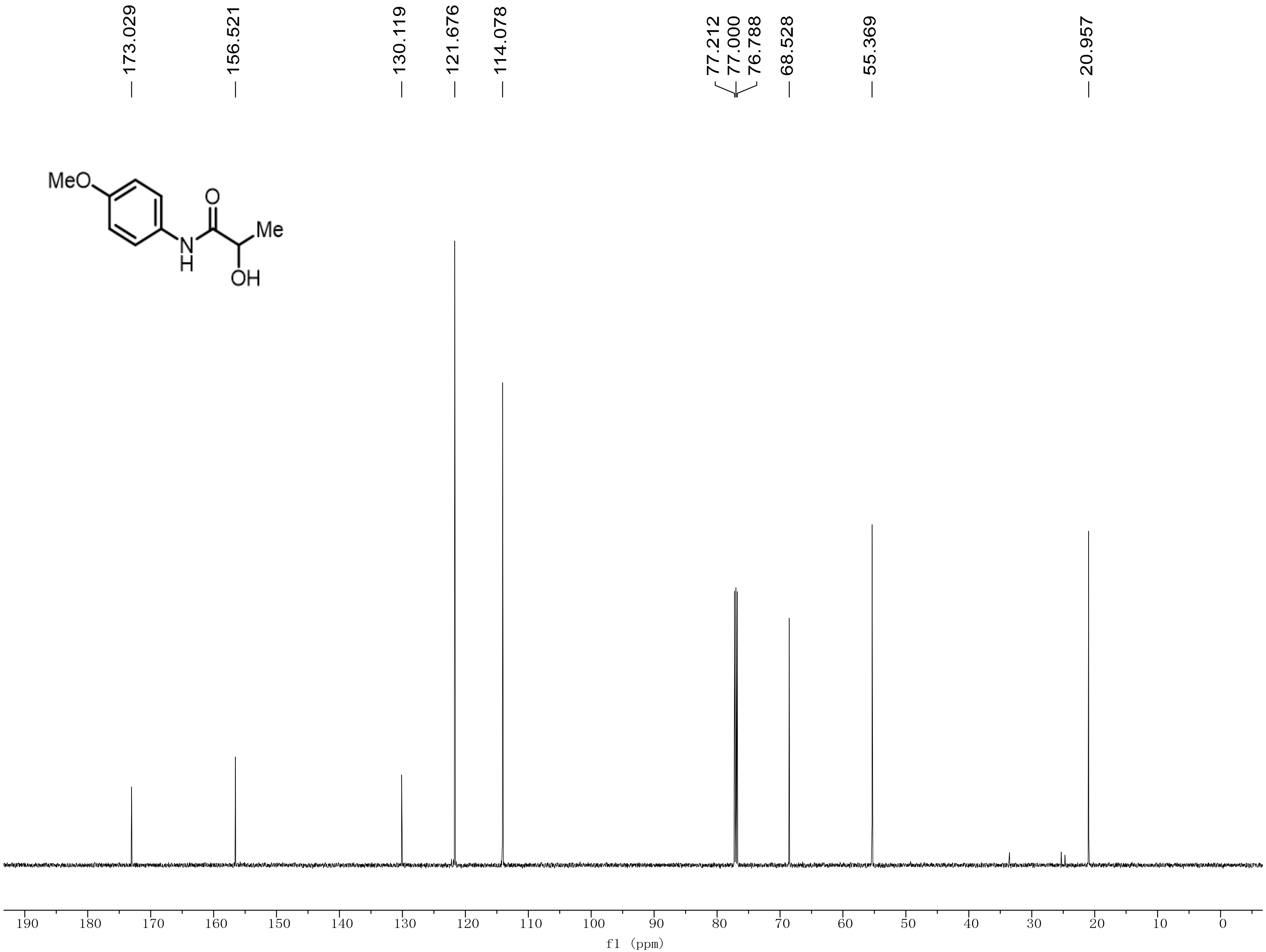

Me
O
Me
N
H
OH

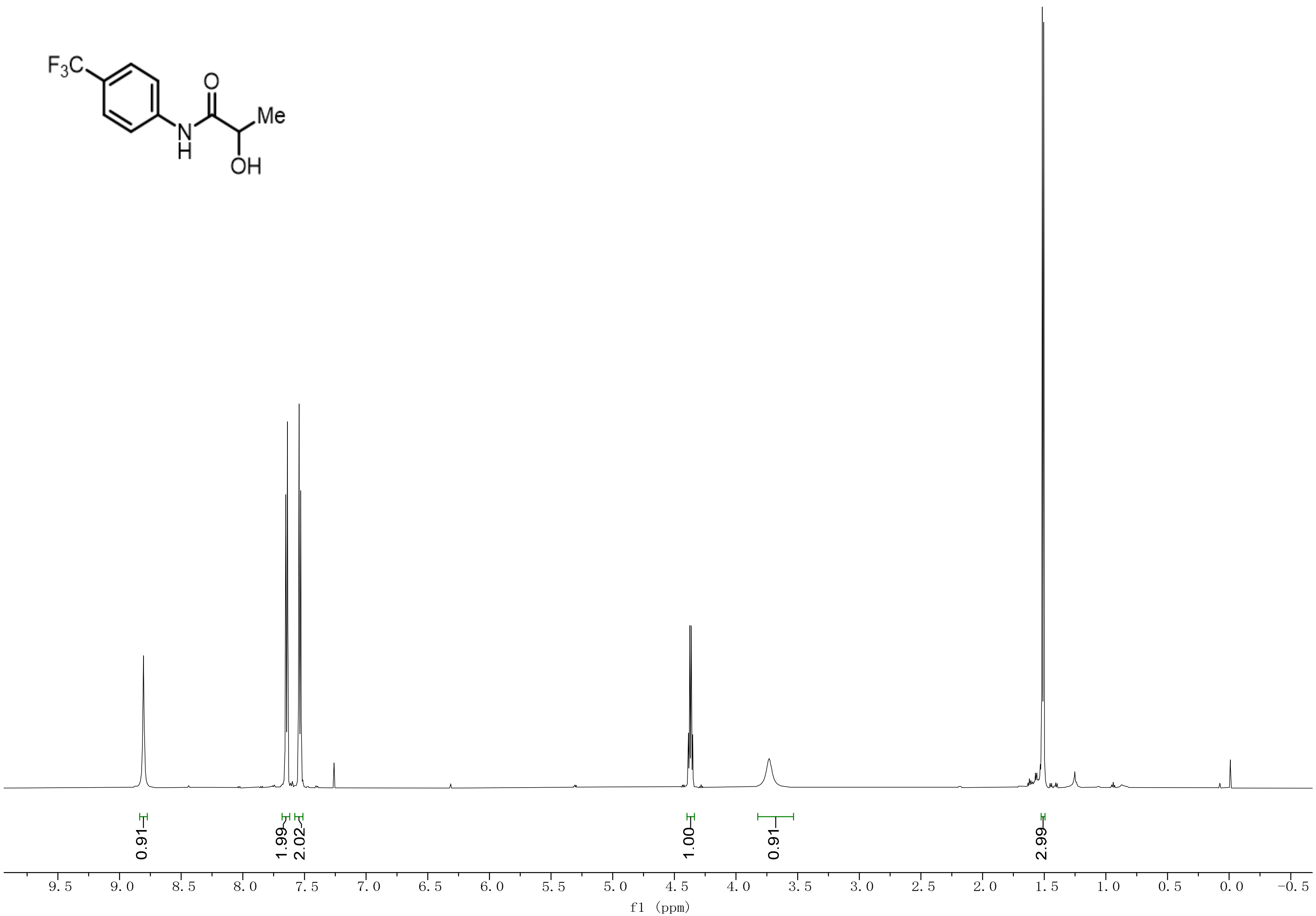

4.13
1.00
0.94
1.02
2.05
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

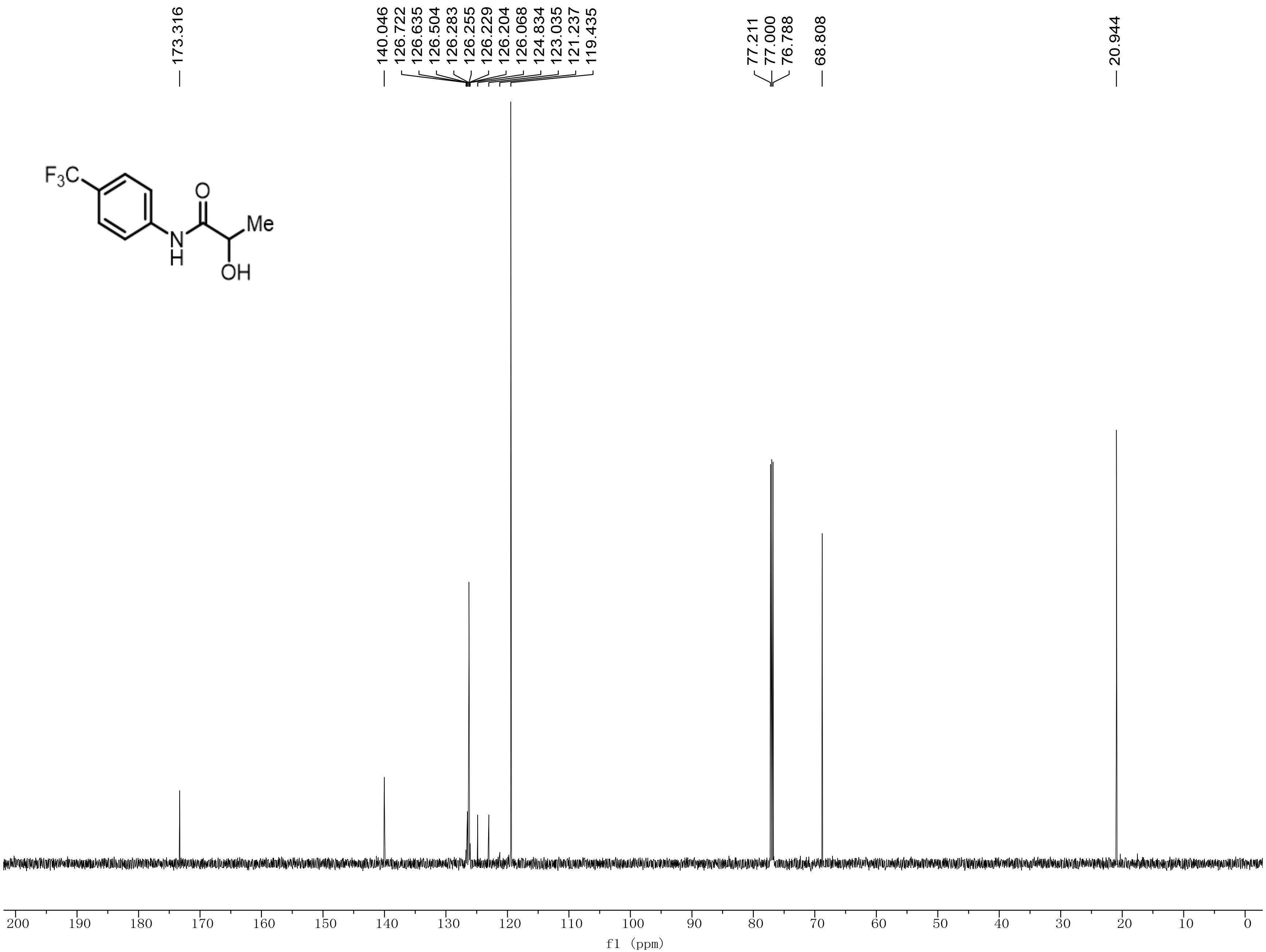


174.345
142.783
128.441
127.145
125.820
77.318
77.000
76.681
67.890
48.251
21.870
20.811
Me
O
Me
N
H
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

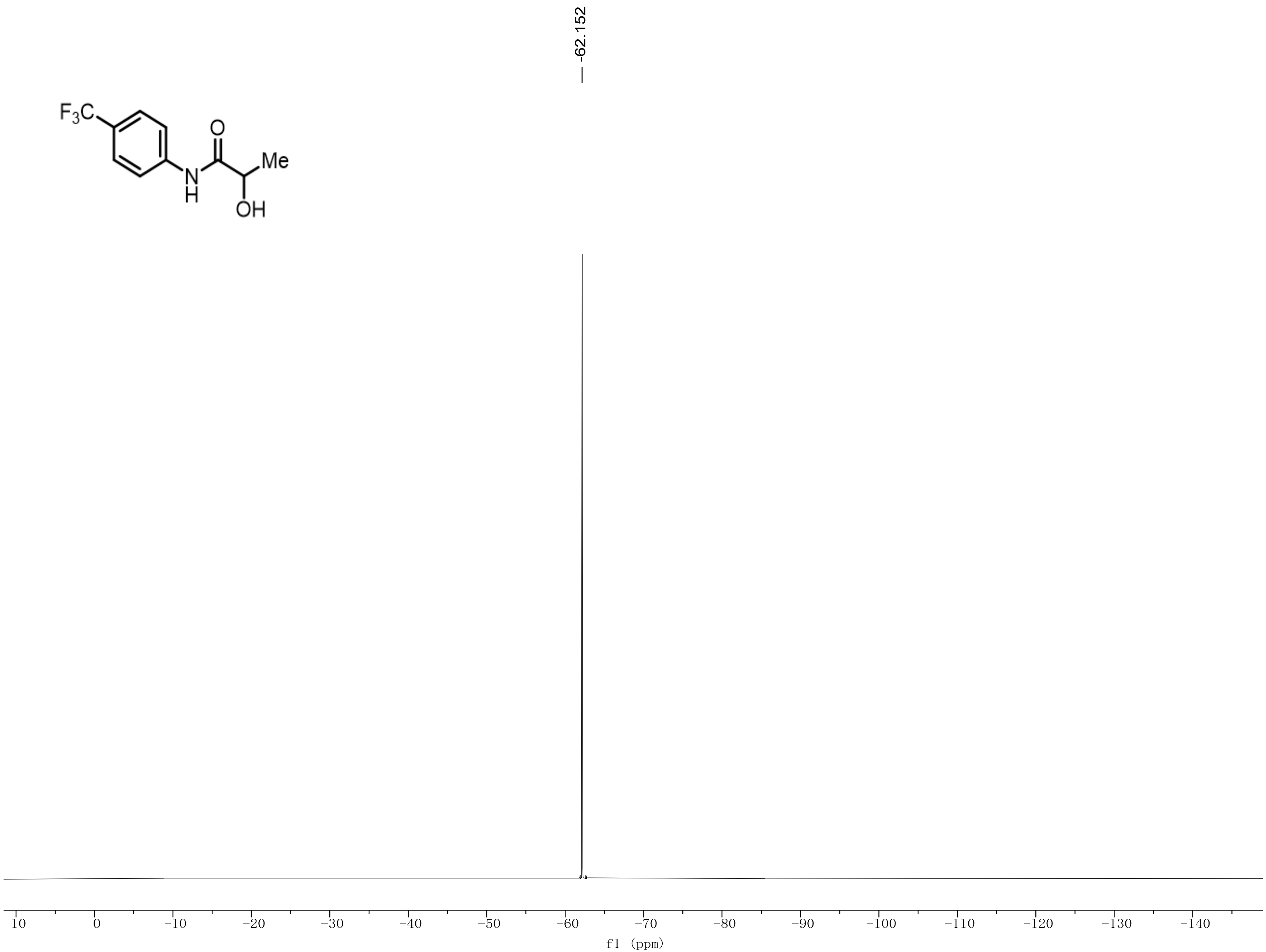

MeO
O
N
H
Me
OH
0.98
1.99
2.01
1.02
3.04
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)


173.029
156.521
130.119
121.676
114.078
77.212
77.000
76.788
68.528
55.369
20.957
MeO
O
Me
N
H
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


F3C
O
Me
N
H
OH
0.91
1.99
2.02
1.00
0.91
2.99
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
−0.5
f1 (ppm)



173.316
140.046
126.722
126.635
126.504
126.283
126.255
126.229
126.204
126.068
124.834
123.035
121.237
119.435
77.211
77.000
76.788
68.808
20.944
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-62.152
F3C
O
Me
N
H
OH
10
0
−10
−20
−30
−40
−50
−60
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−80
−90
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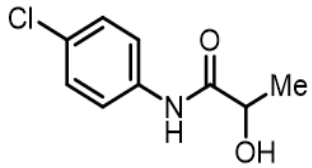
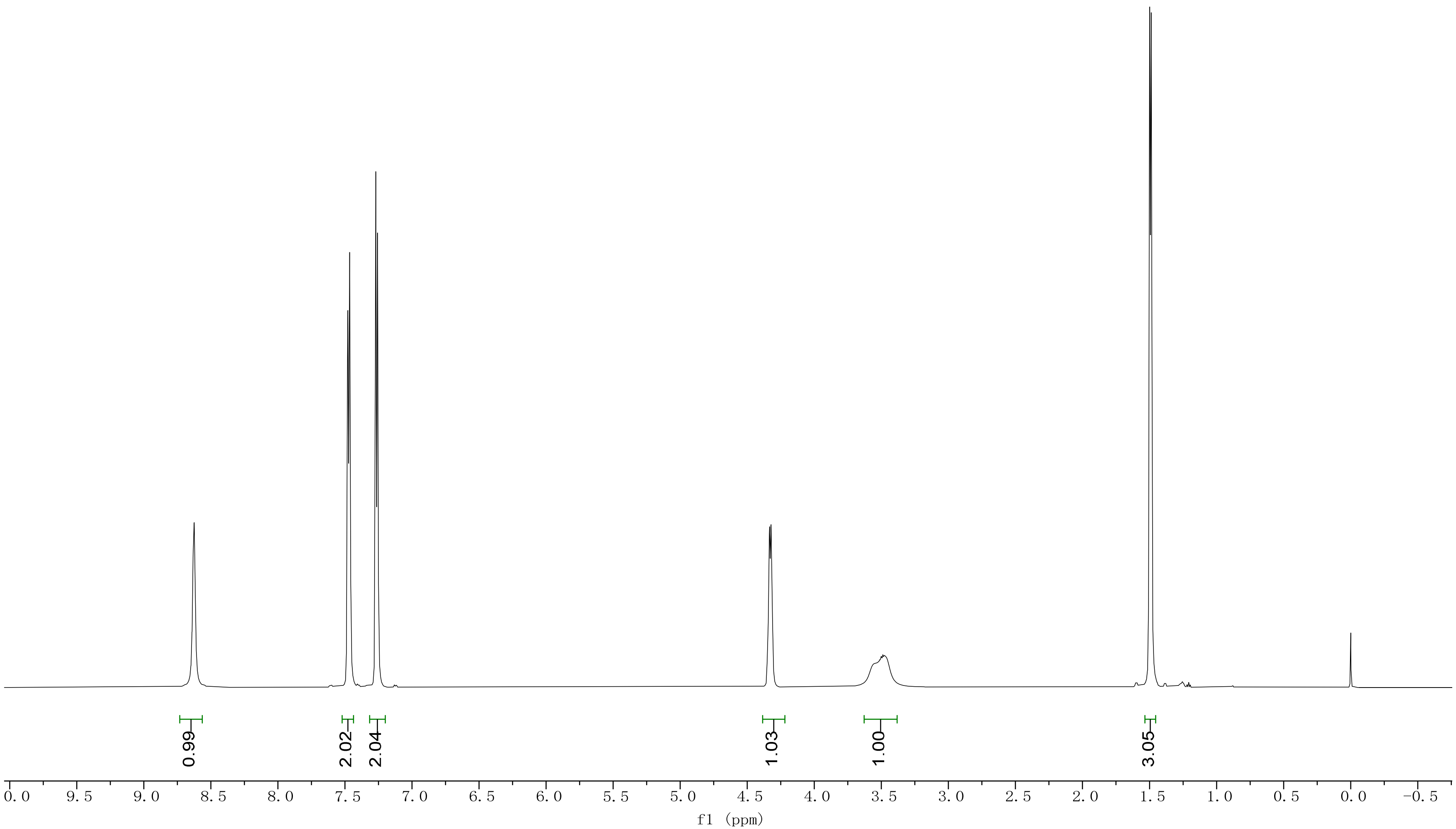
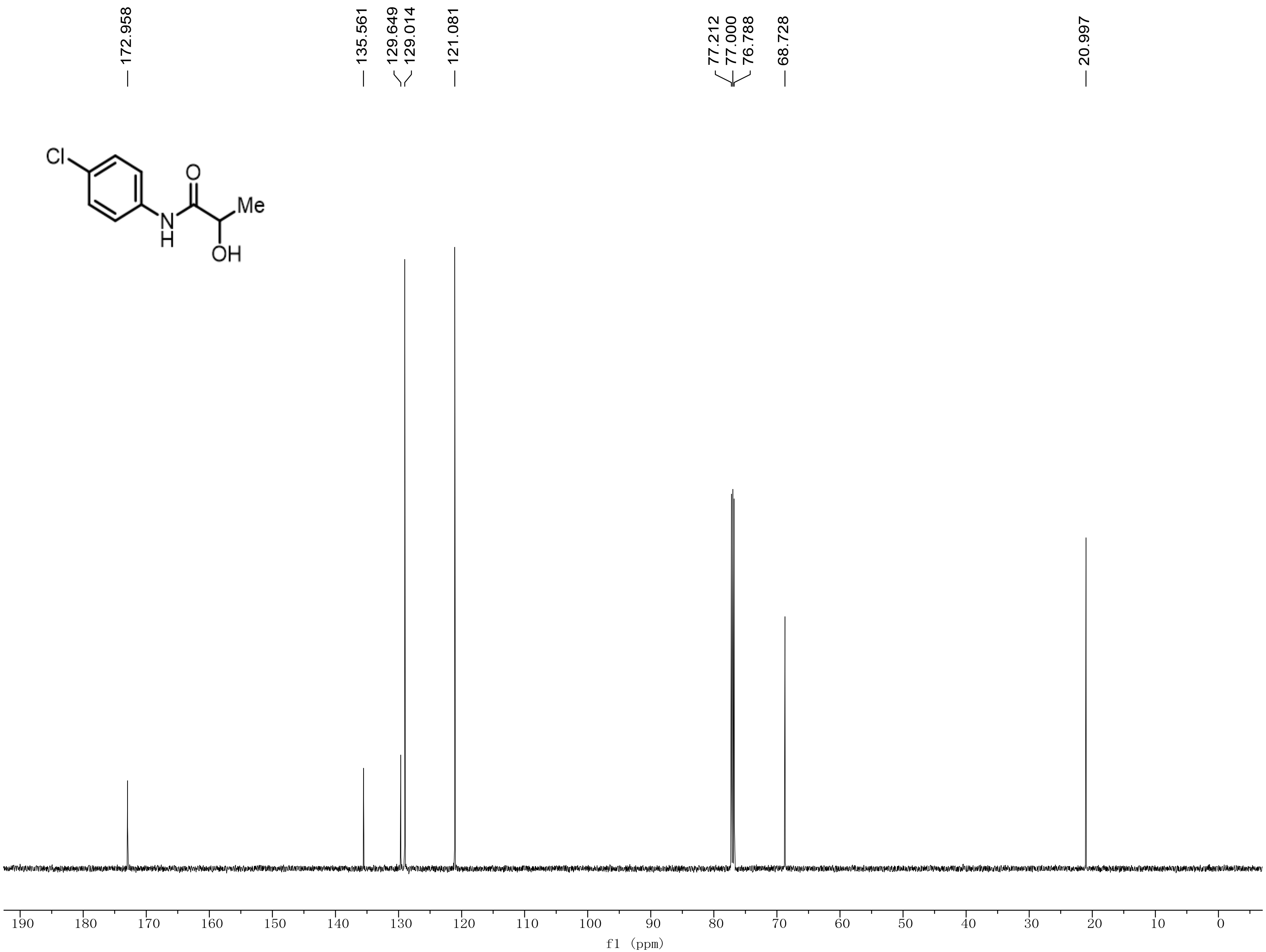
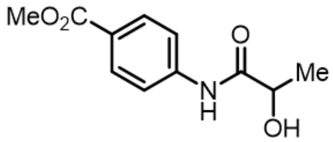
−110
−120
−130
−140
f1 (ppm)

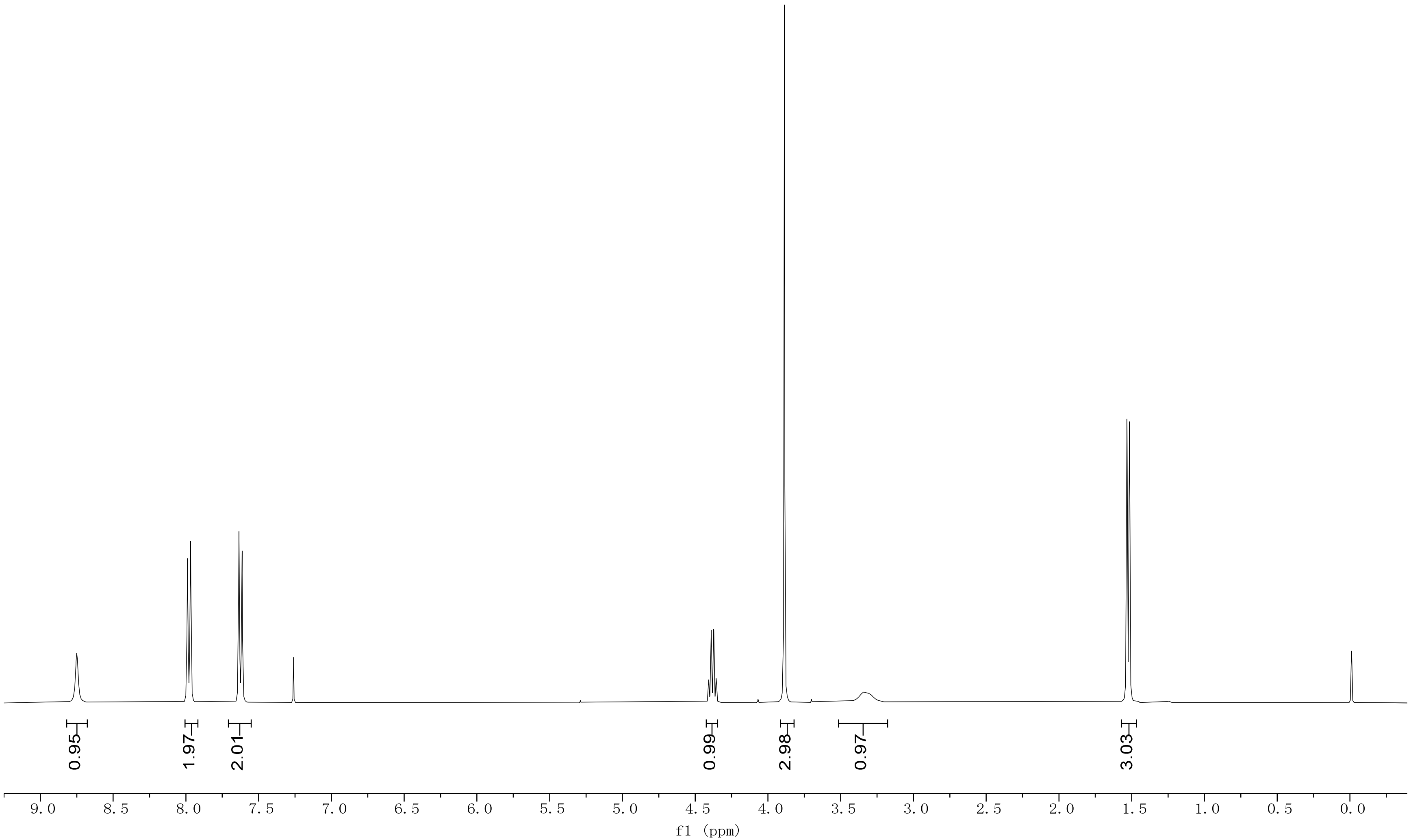

Cl
O
Me
N
H
OH


0.99
2.02
2.04
1.03
1.00
3.05
0.0
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
-0.5
f1 (ppm)

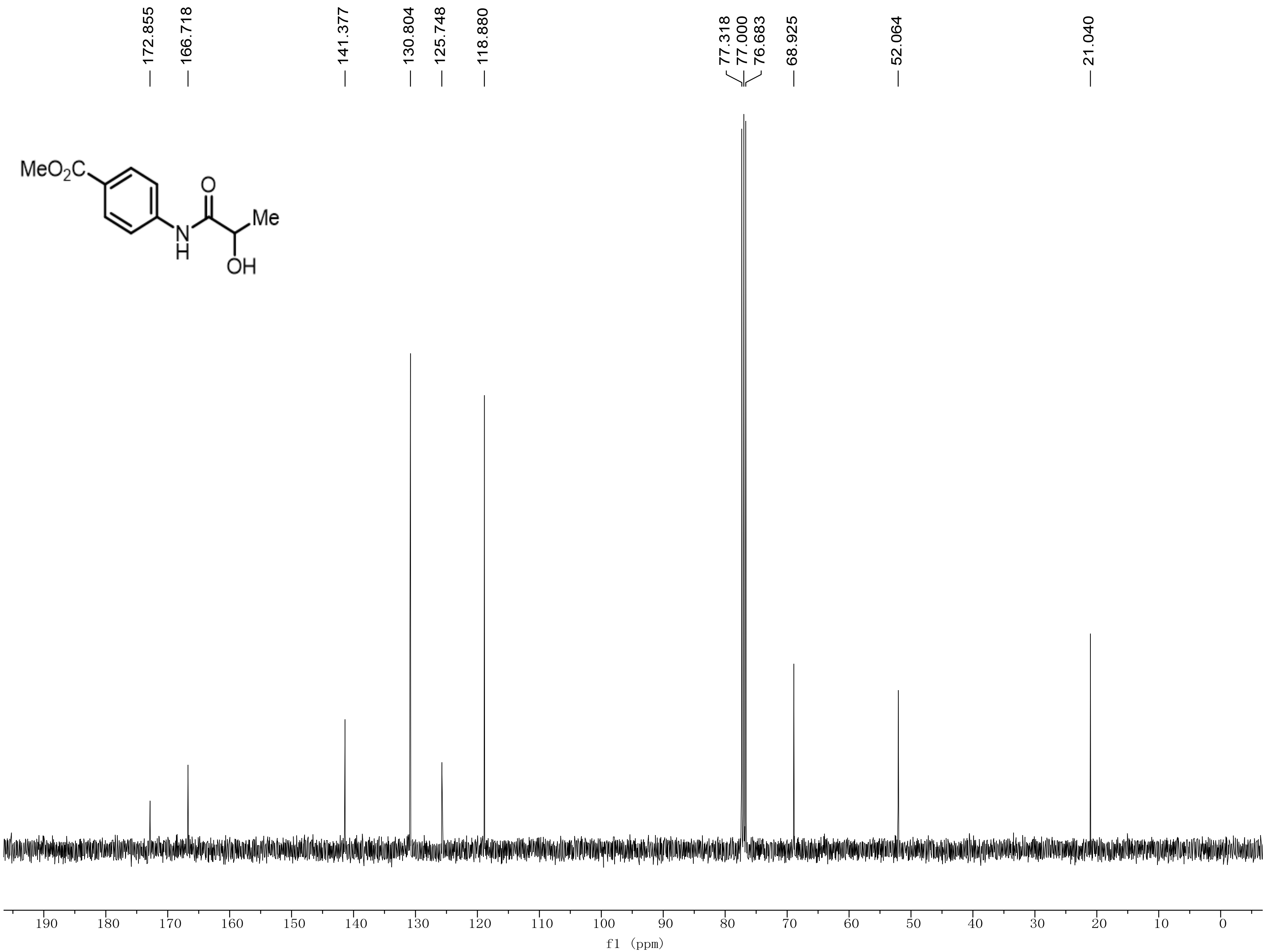

172.958
135.561
129.649
129.014
121.081
77.212
77.000
76.788
68.728
20.997
Cl
O
N
H
Me
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



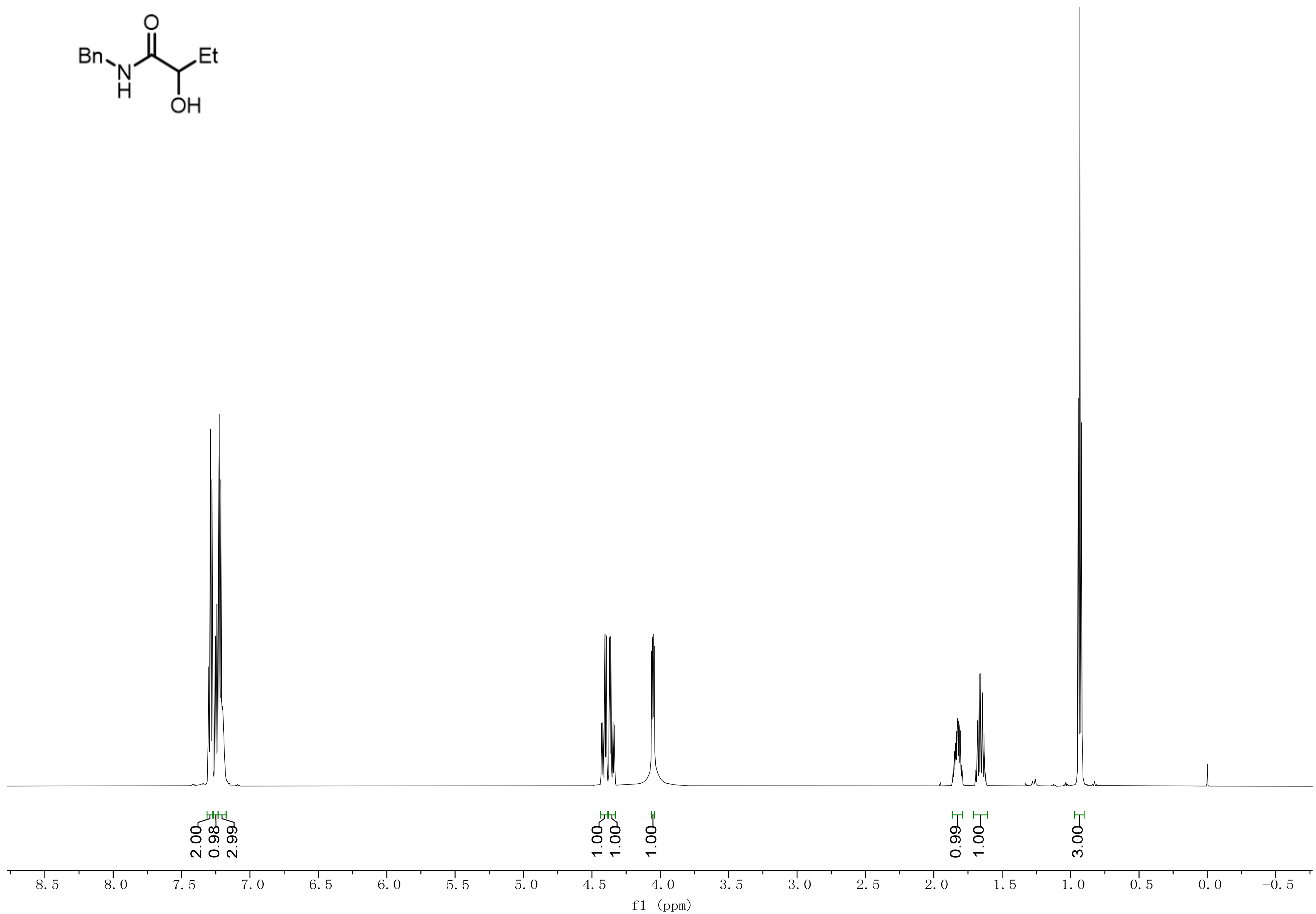
MeO2C
O
N
H
Me
OH

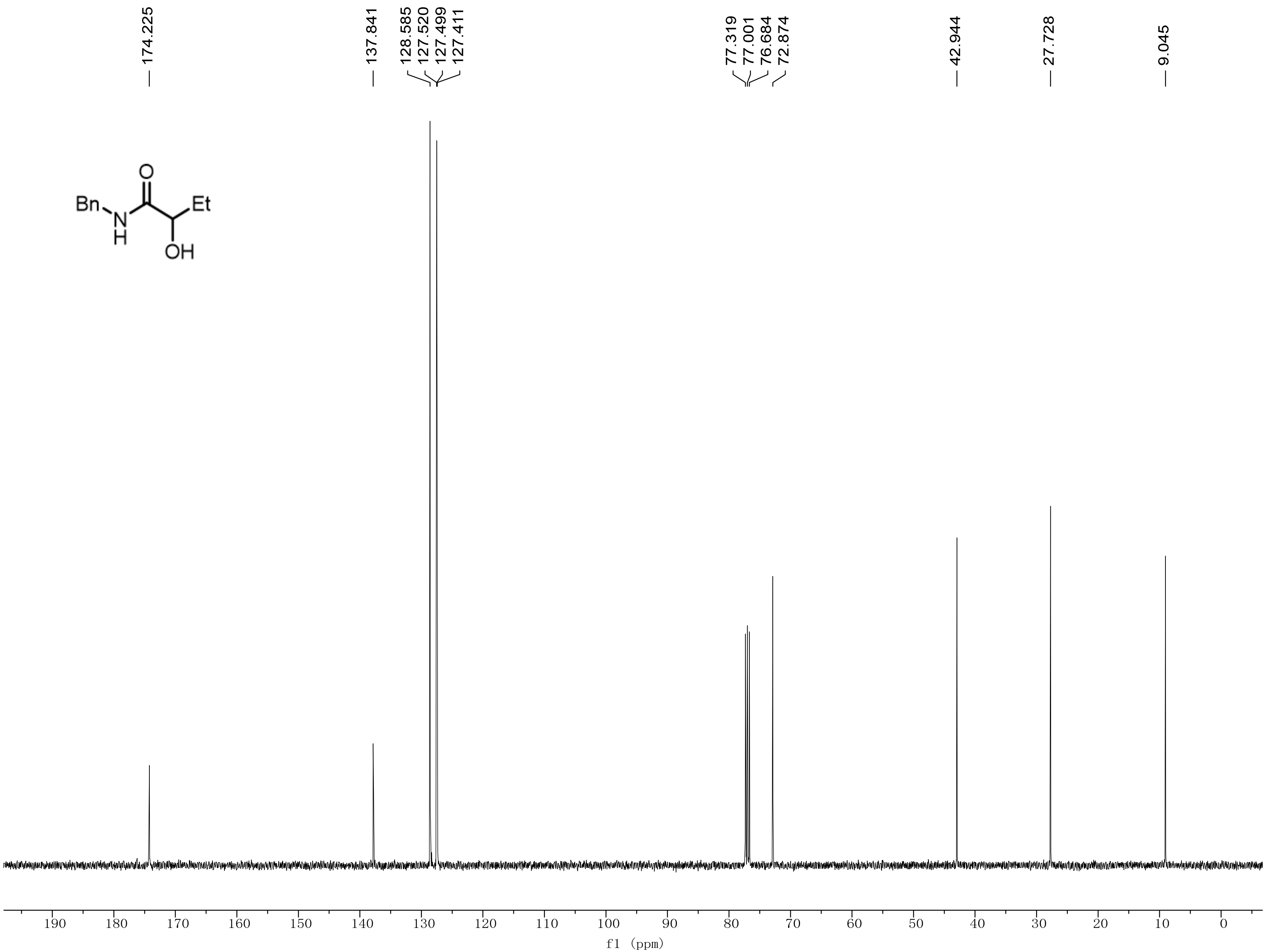


0.95
1.97
2.01
0.99
2.98
0.97
3.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

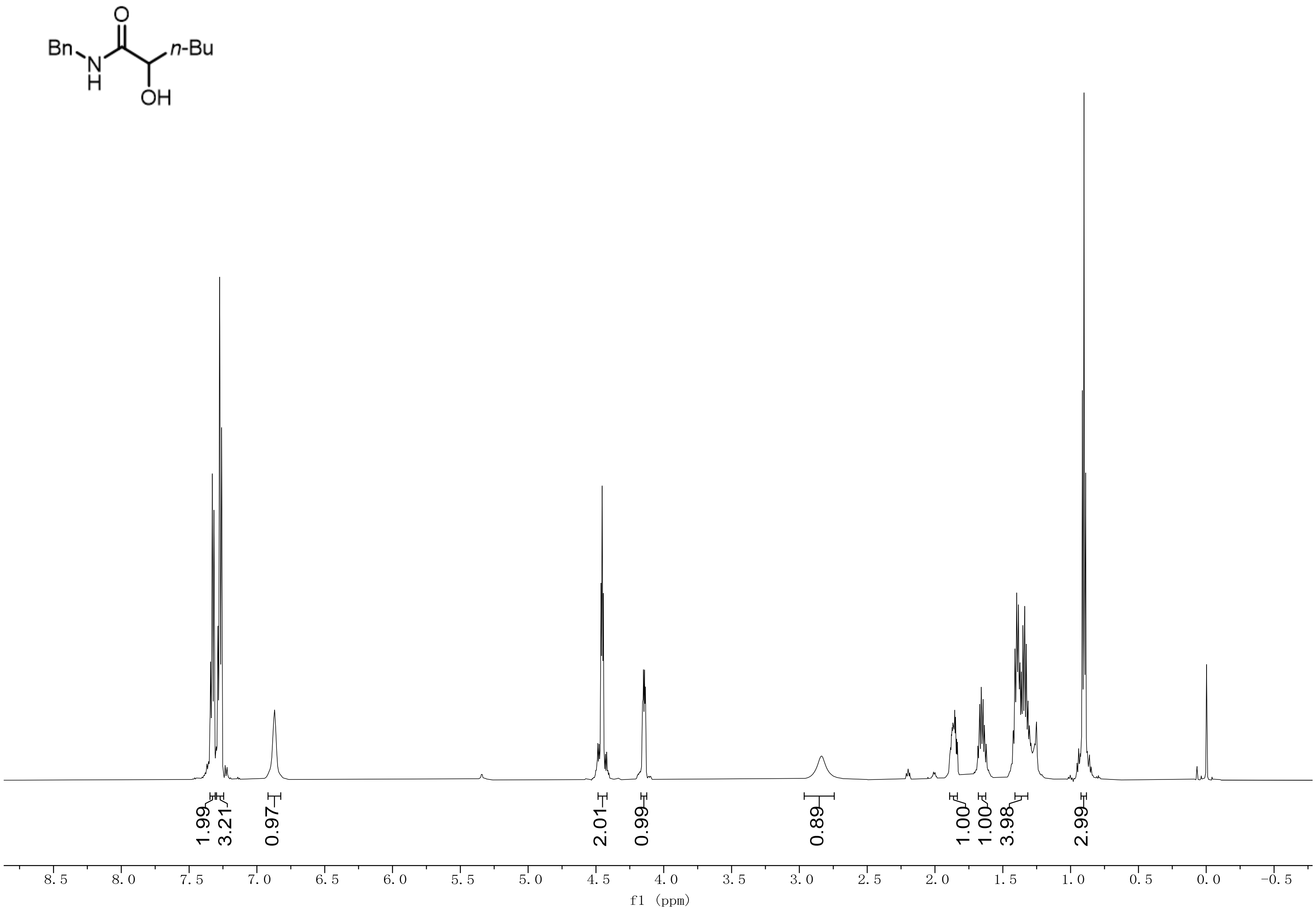


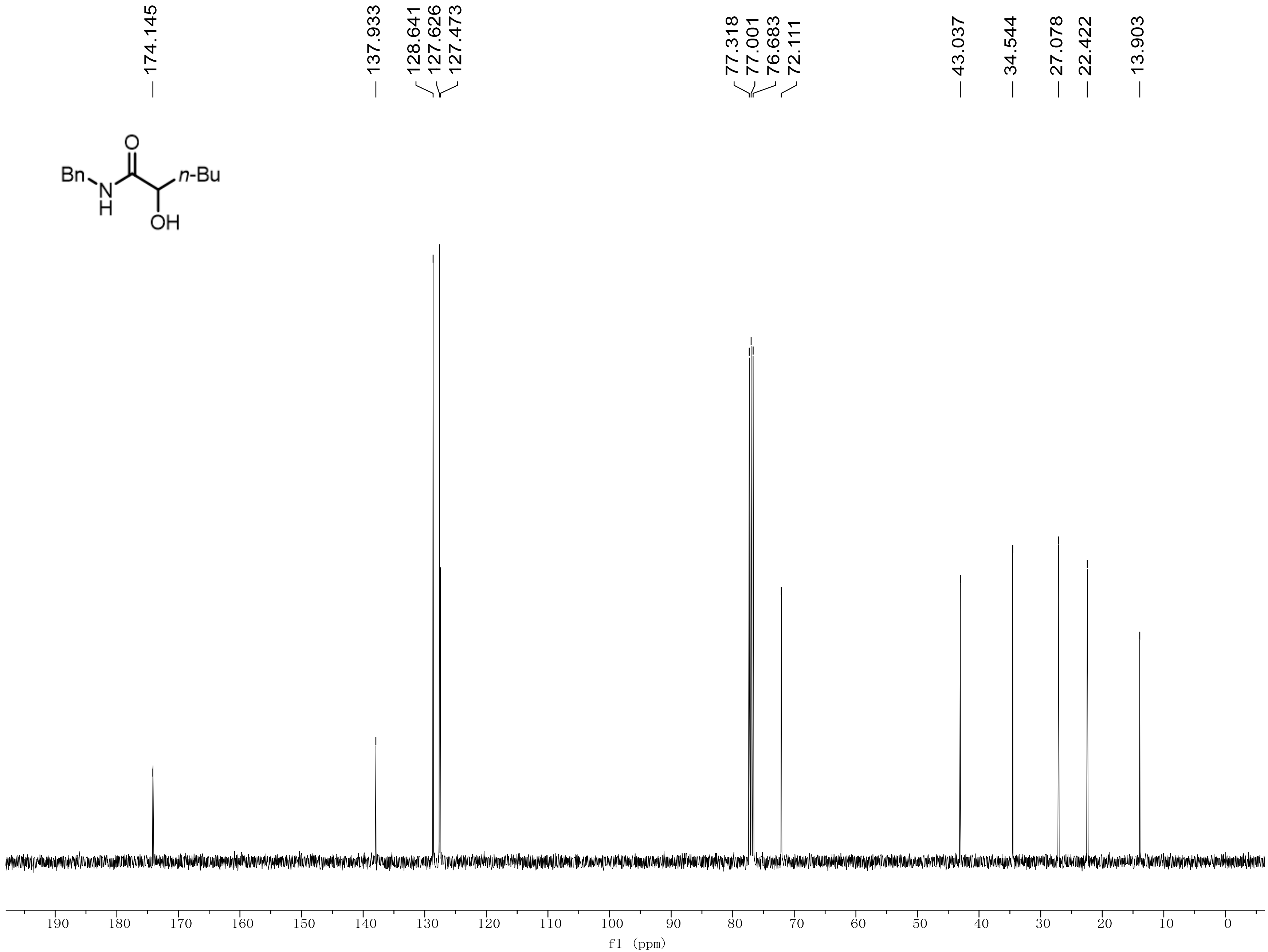
172.855
166.718
141.377
130.804
125.748
118.880
77.318
77.000
76.683
68.925
52.064
21.040
MeO2C
O
N
H
Me
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

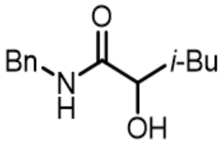

Bn
N
H
O
Et
OH
2.00
0.98
2.99
1.00
1.00
1.00
0.99
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

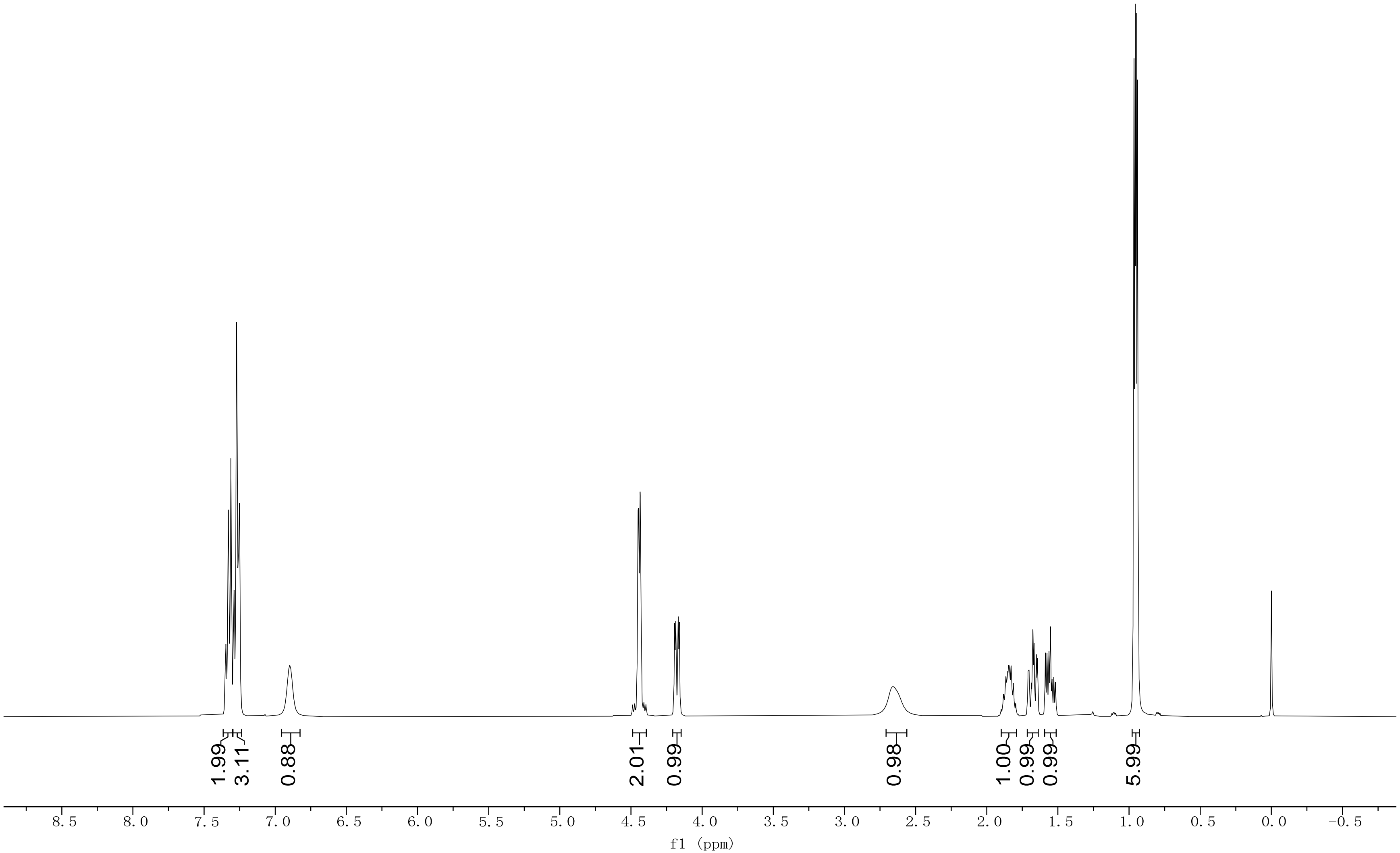


174.225
137.841
128.585
127.520
127.499
127.411
77.319
77.001
76.684
72.874
42.944
27.728
9.045
Bn
N
H
O
Et
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

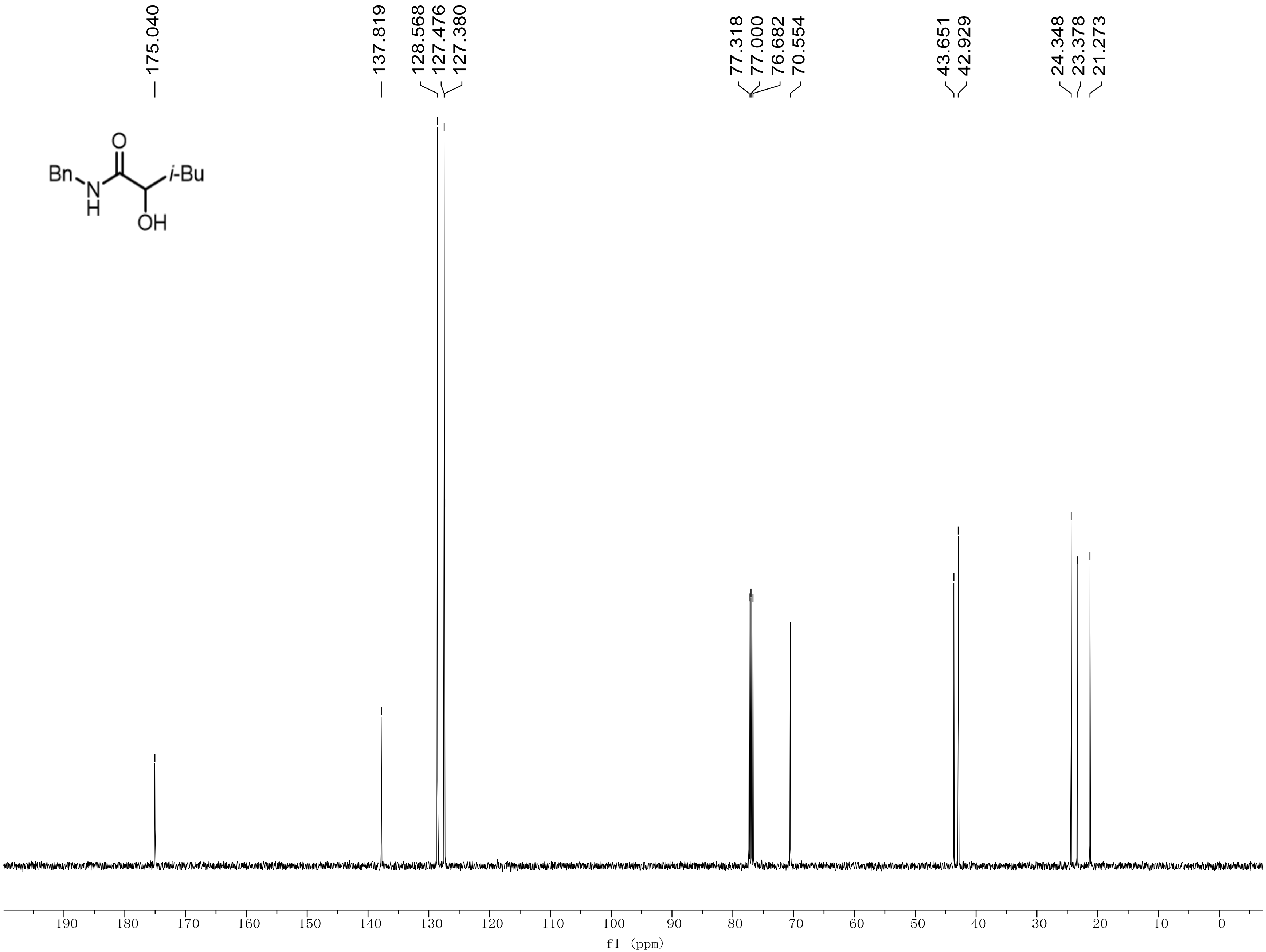

Bn
N
H
O
OH
n-Bu
1.99
3.21
0.97
2.01
0.99
0.89
1.00
1.00
3.98
2.99
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

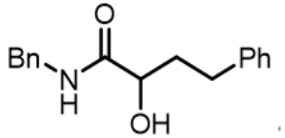

174.145
137.933
128.641
127.626
127.473
77.318
77.001
76.683
72.111
43.037
34.544
27.078
22.422
13.903
Bn
N
H
O
OH
n-Bu
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



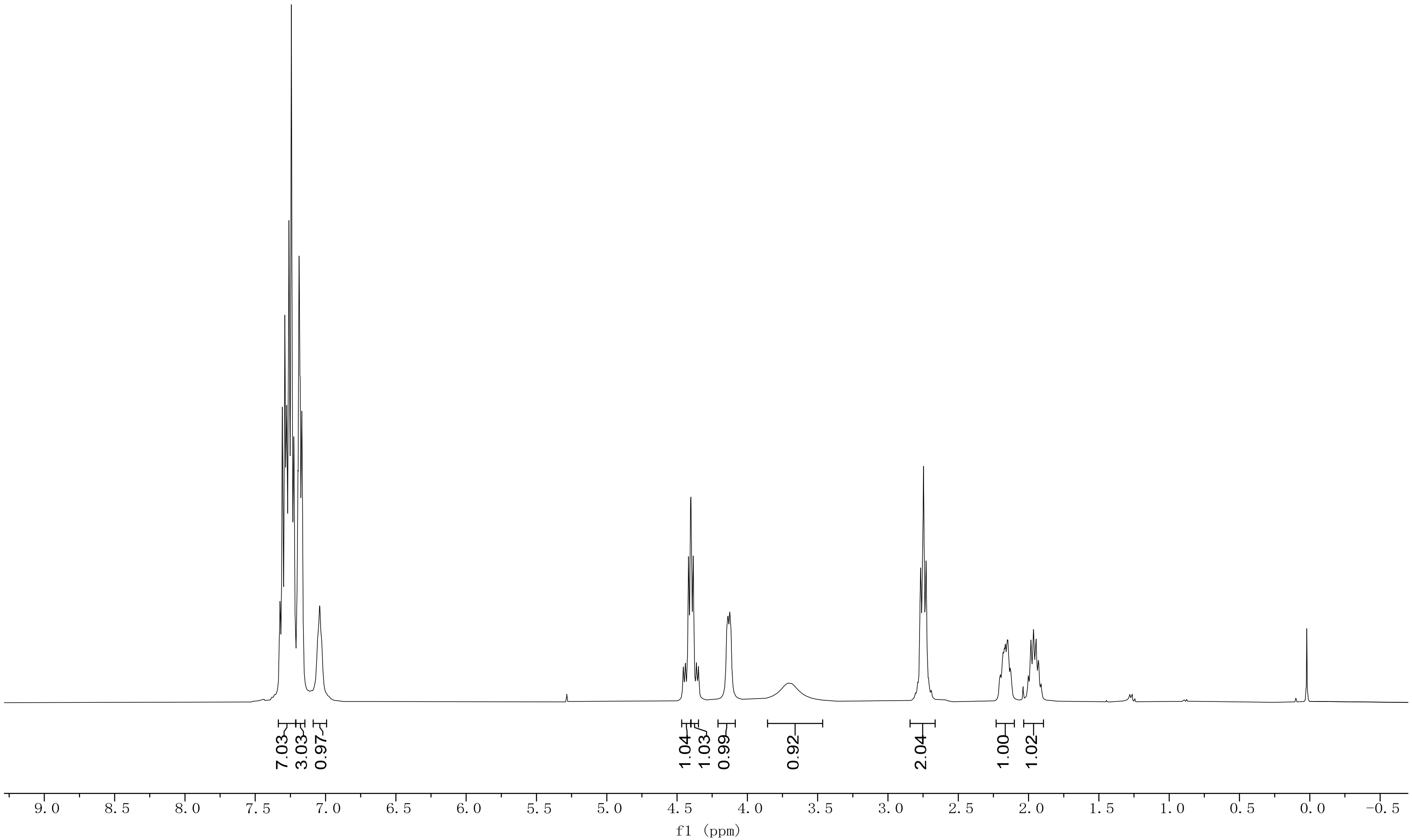


1.99
3.11
0.88
2.01
0.99
0.98
1.00
0.99
0.99
5.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

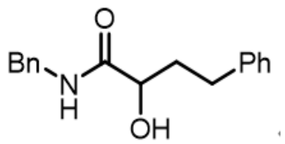

175.040
137.819
128.568
127.476
127.380
77.318
77.000
76.682
70.554
43.651
42.929
24.348
23.378
21.273
Bn
N
H
O
OH
i-Bu
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



Bn
N
H
O
OH
Ph



7.03
3.03
0.97
1.04
1.03
0.99
0.92
2.04
1.00
1.02
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
-0.5
f1 (ppm)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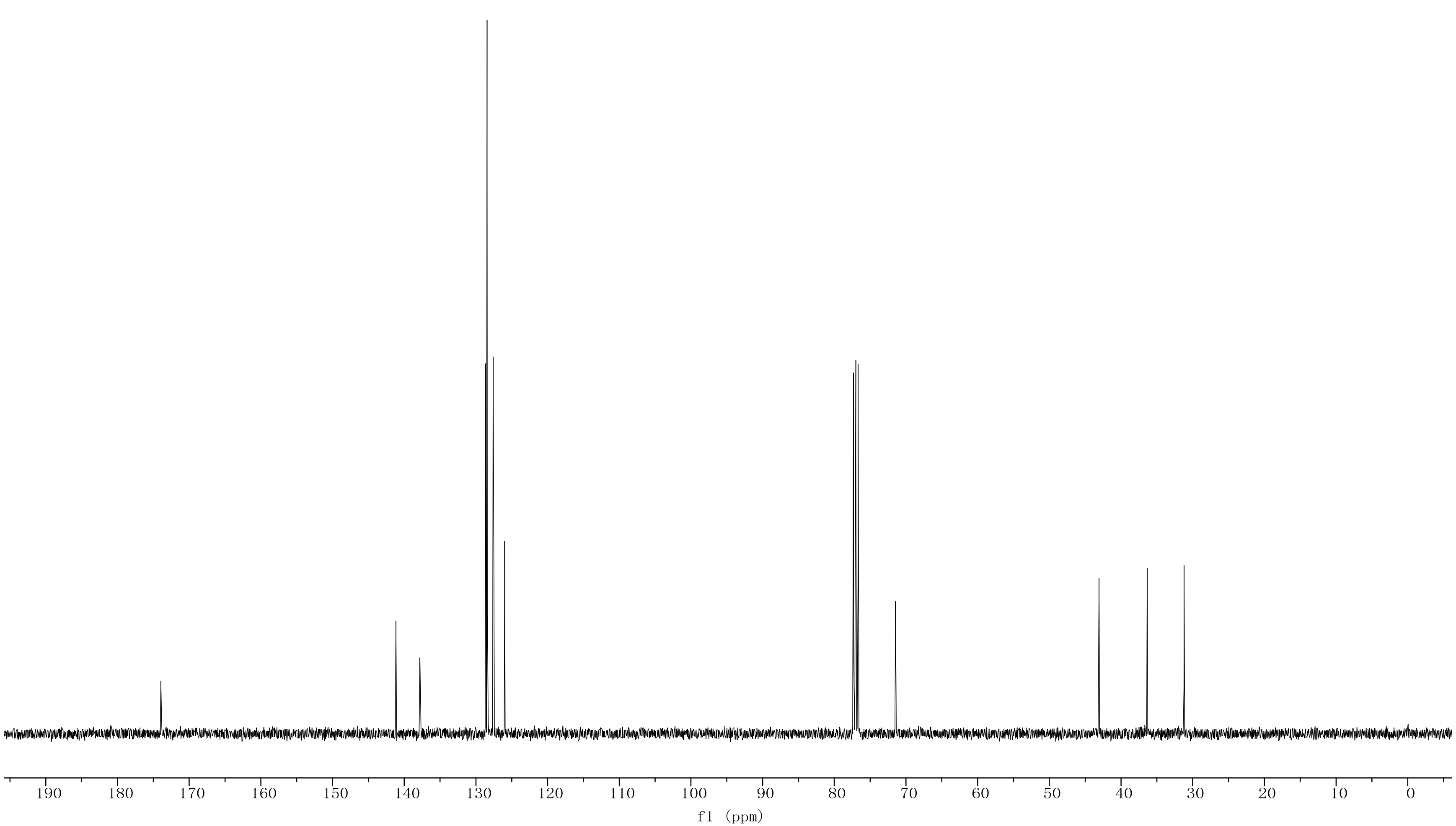
N
H
O
OH
Ph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128.666
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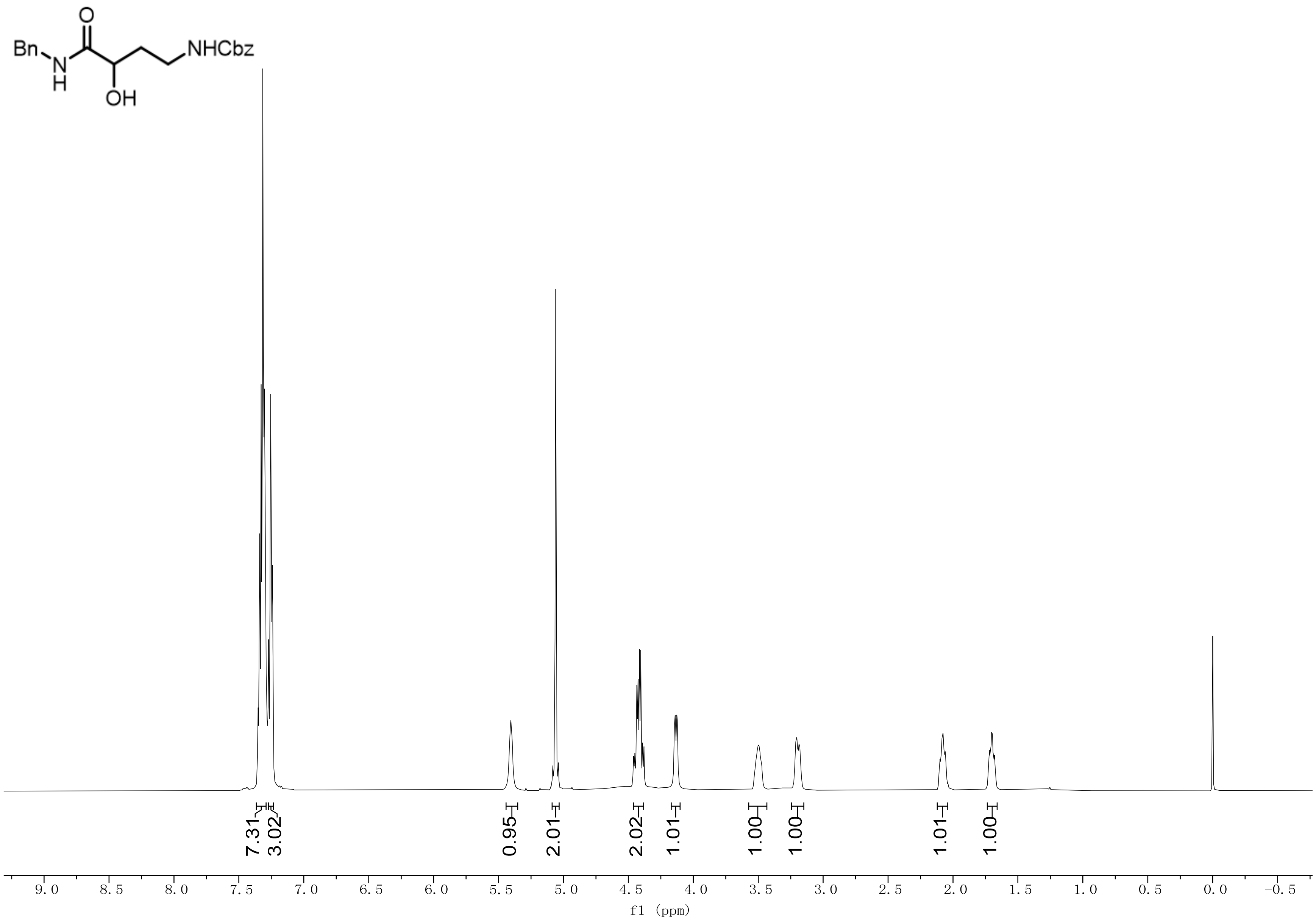
127.604
127.507
125.993
77.320
77.002
76.683
71.452
43.059
36.350
31.209
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
Bn N H
NHCbz
OH
7.31
3.02
0.95
2.01
2.02
1.01
1.00
1.00
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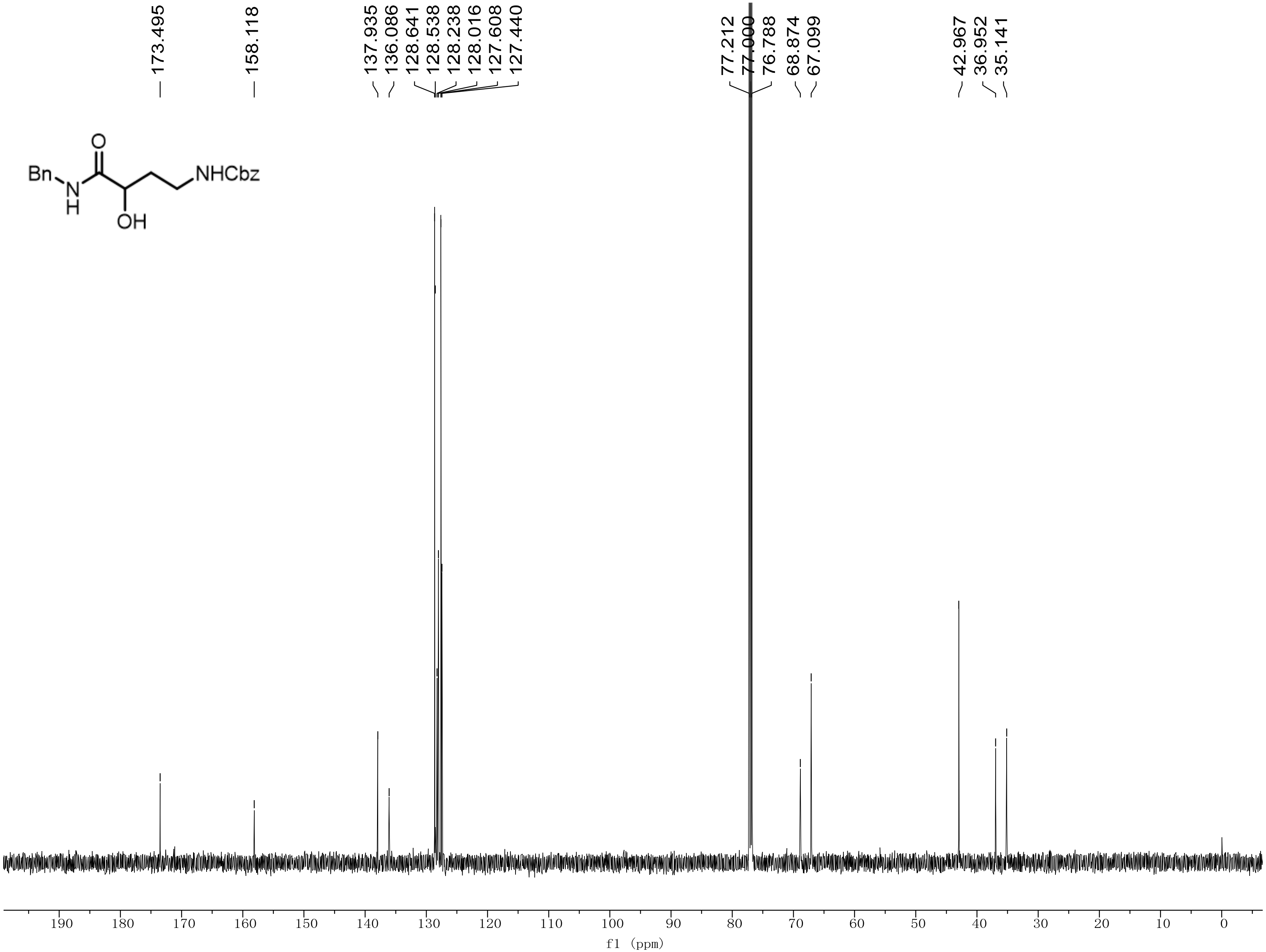
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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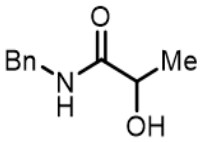
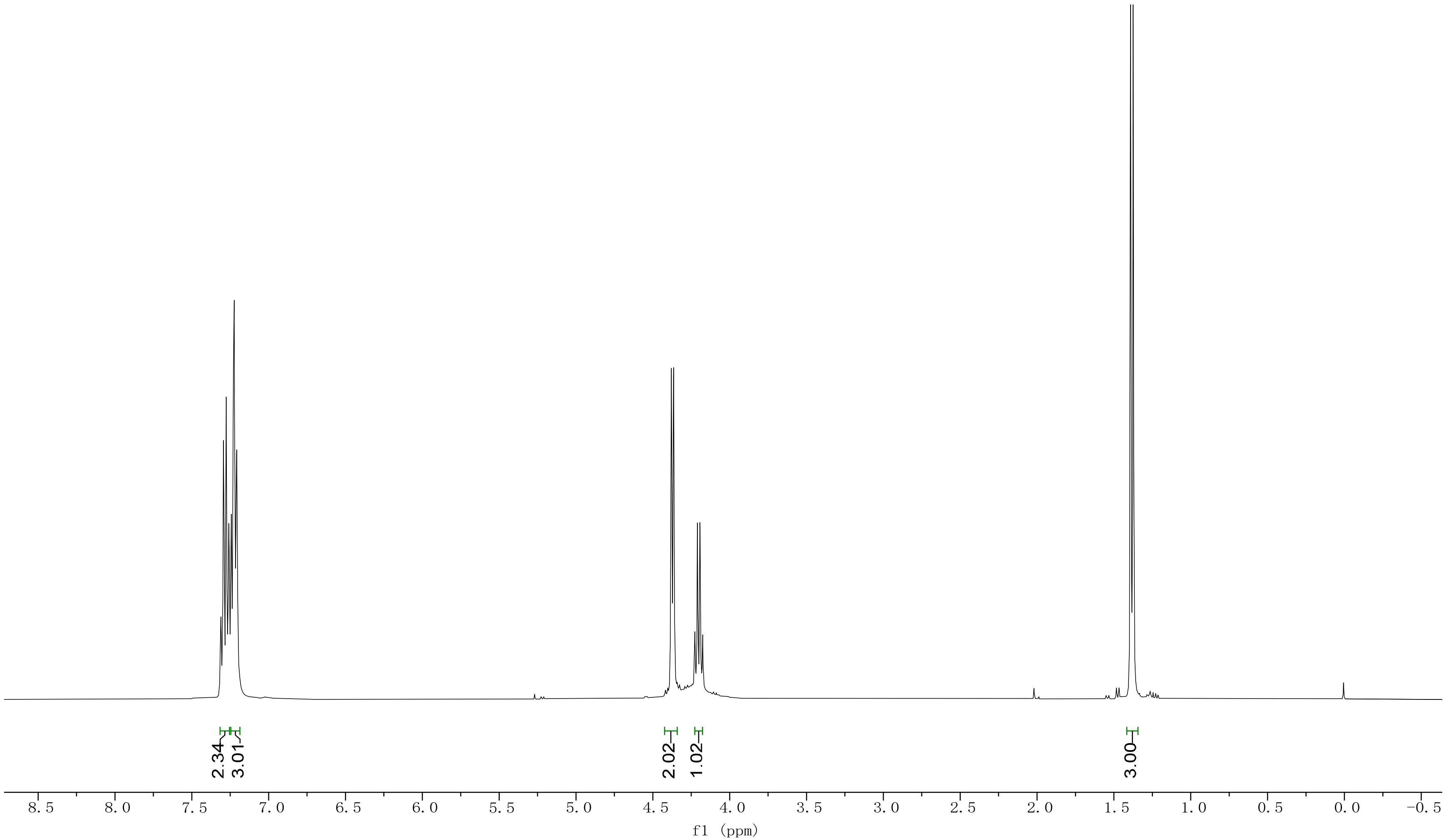
128.641
128.538
128.238
128.016
127.608
127.440
77.212
77.000
76.788
68.874
67.099
42.967
36.952
35.141
Bn
N
H
O
OH
NHCbz
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Bn
N
H
O
Me
OH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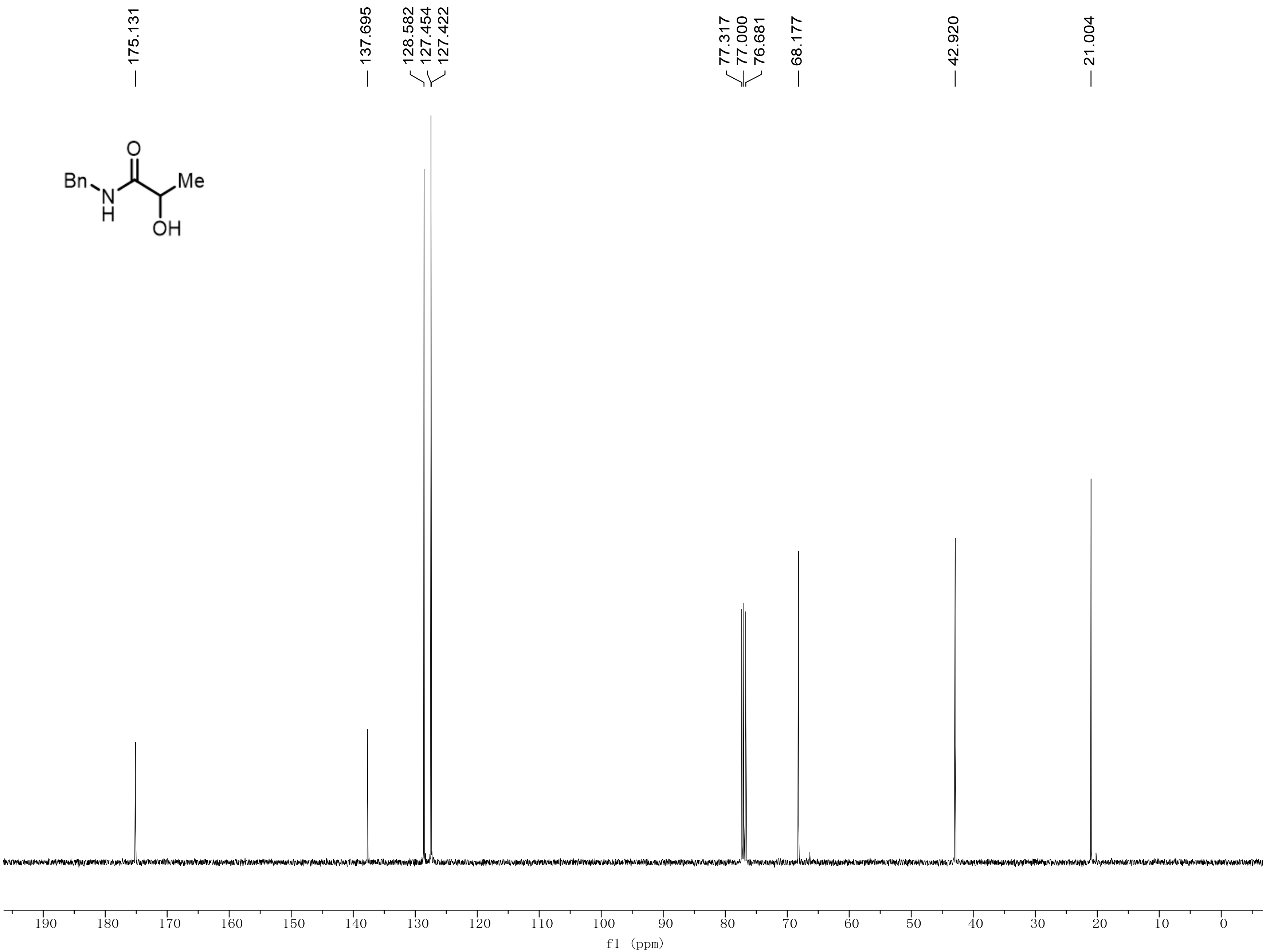
2.02
1.02
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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128.582
127.454
127.422
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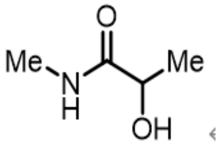
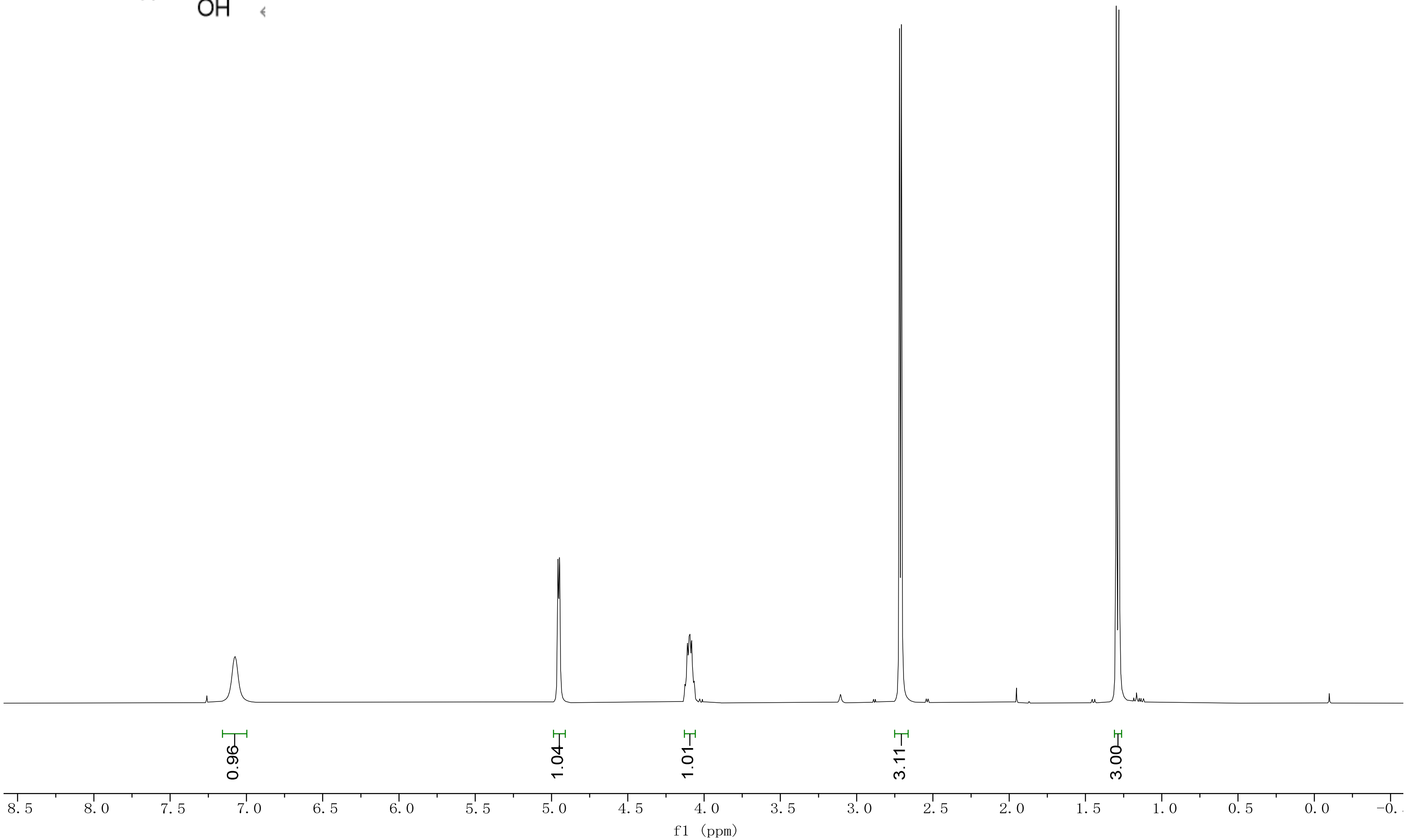
77.000
76.681
68.177
42.920
21.004
Bn
N
H
O
Me
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)





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1.04
1.01
3.11
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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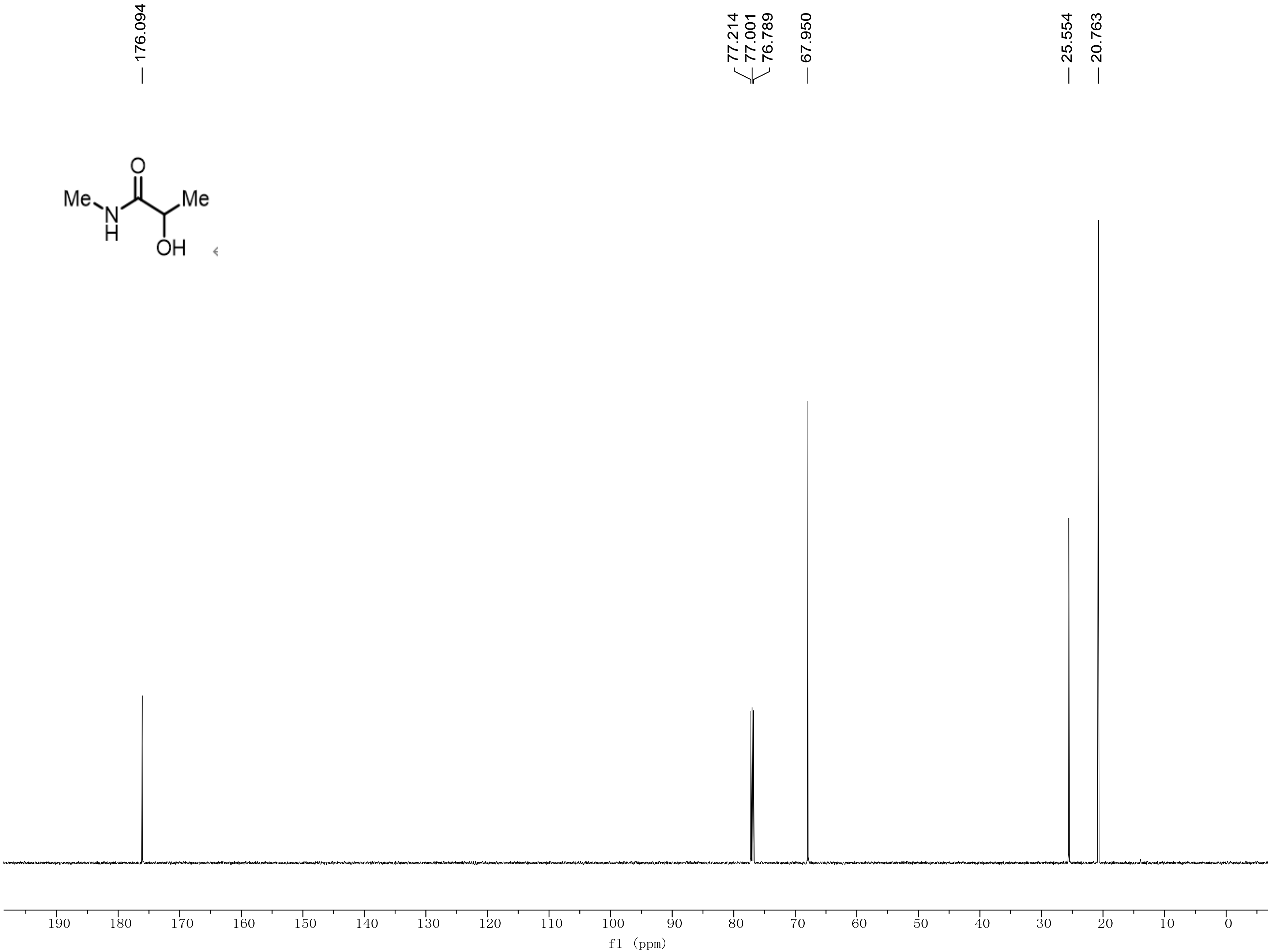
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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25.554
20.763
Me
N
H
O
Me
OH
190
180
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50
40
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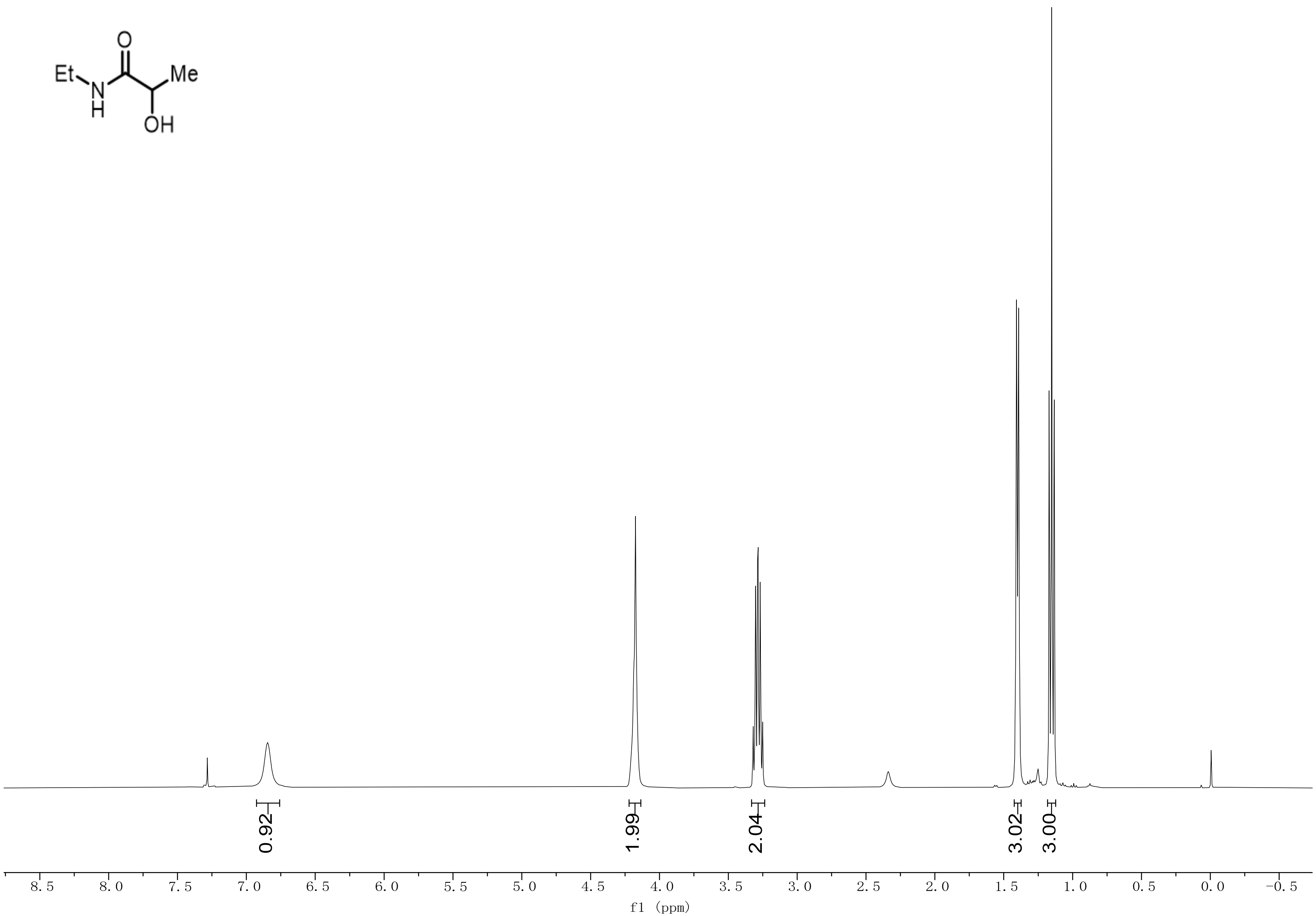
10
0
f1 (ppm)



Et
N
H
O
Me
OH
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1.99
2.04
3.02
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
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0.5
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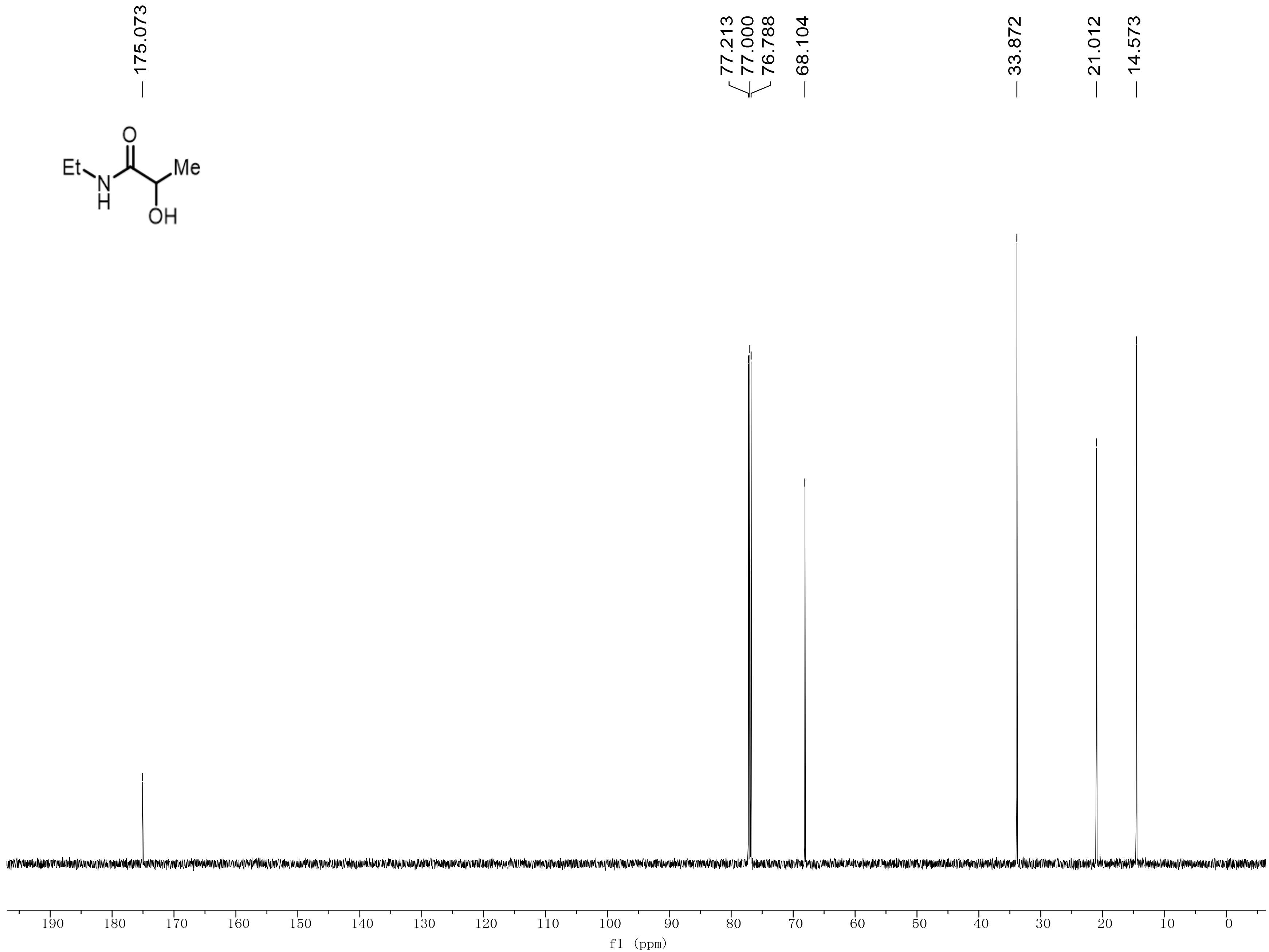
-0.5
f1 (ppm)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76.788
68.104
33.872
21.012
14.573
Et
N
H
O
Me
OH
190
180
170
160
150
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130
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110
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90
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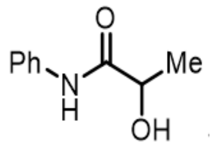
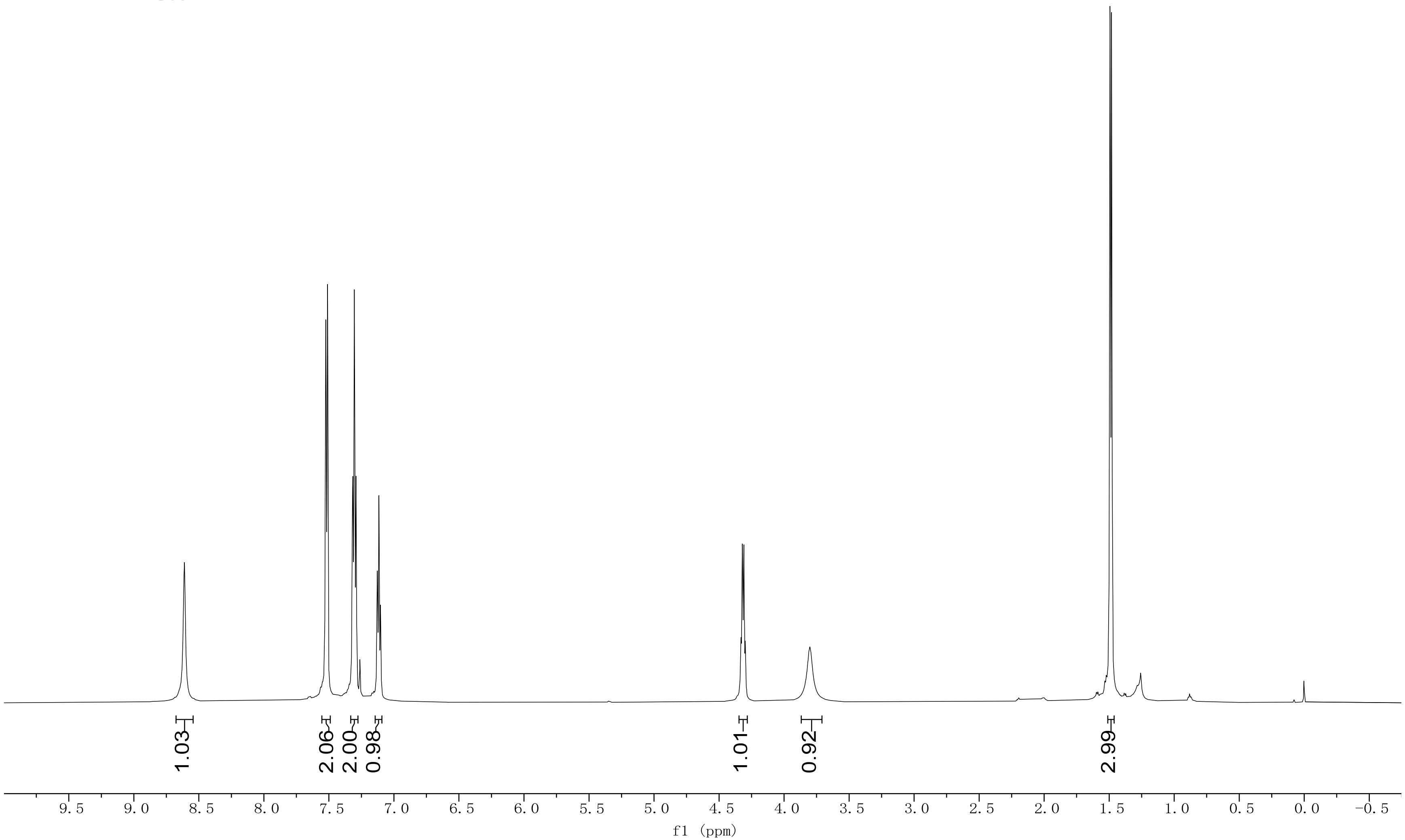
50
40
30
20
10
0
f1 (ppm)





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0.98
1.01
0.92
2.99
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
2.0
1.5
1.0
0.5
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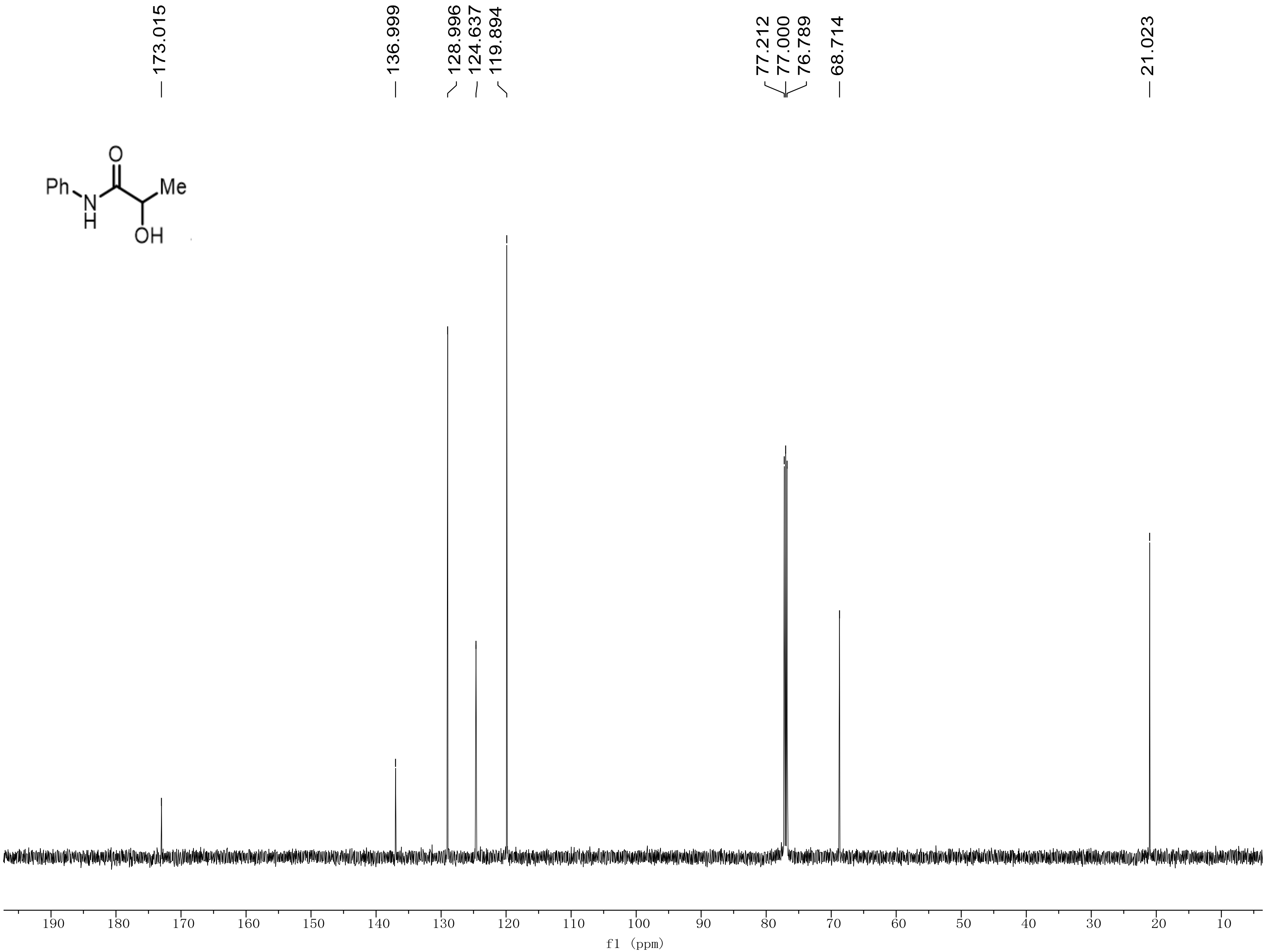
-0.5
f1 (ppm)



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119.894
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77.000
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68.714
21.023
Ph
N
H
O
Me
OH
190
180
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140
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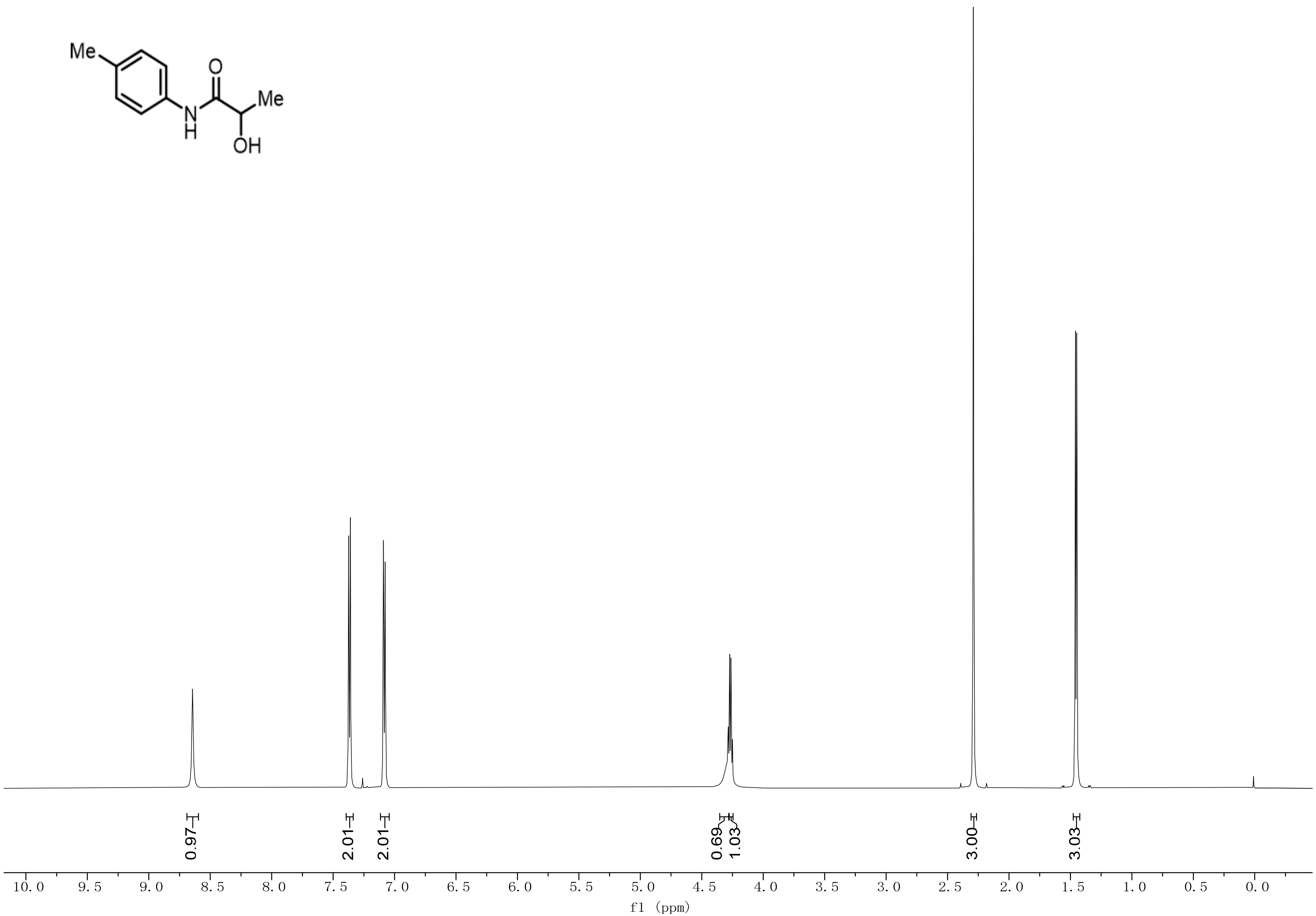
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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O
Me
N
H
OH
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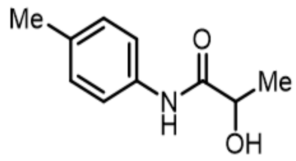
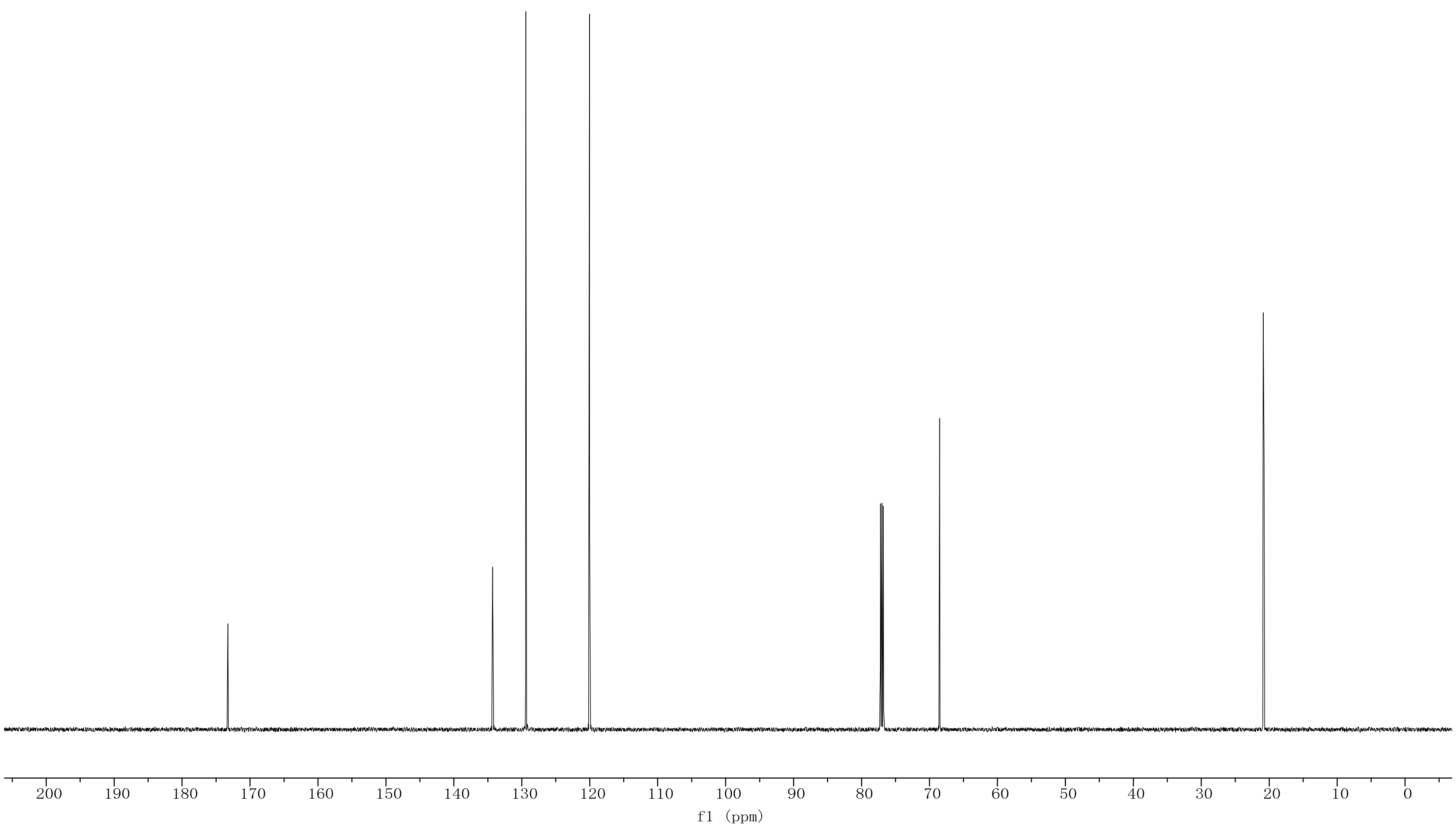
2.01
0.69
1.03
3.00
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

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20.887
20.759
200
190
180
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150
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130
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110
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90
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70
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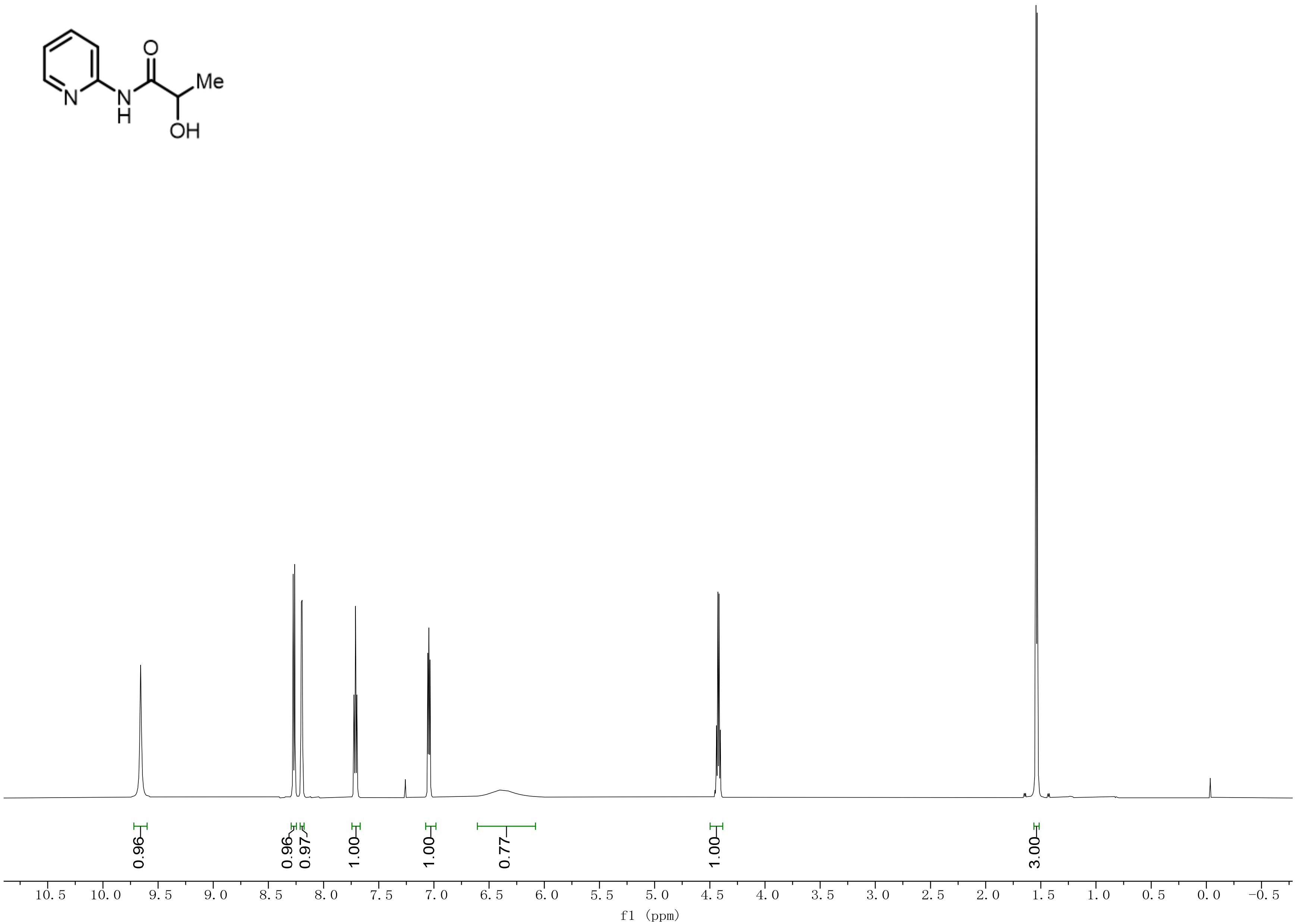
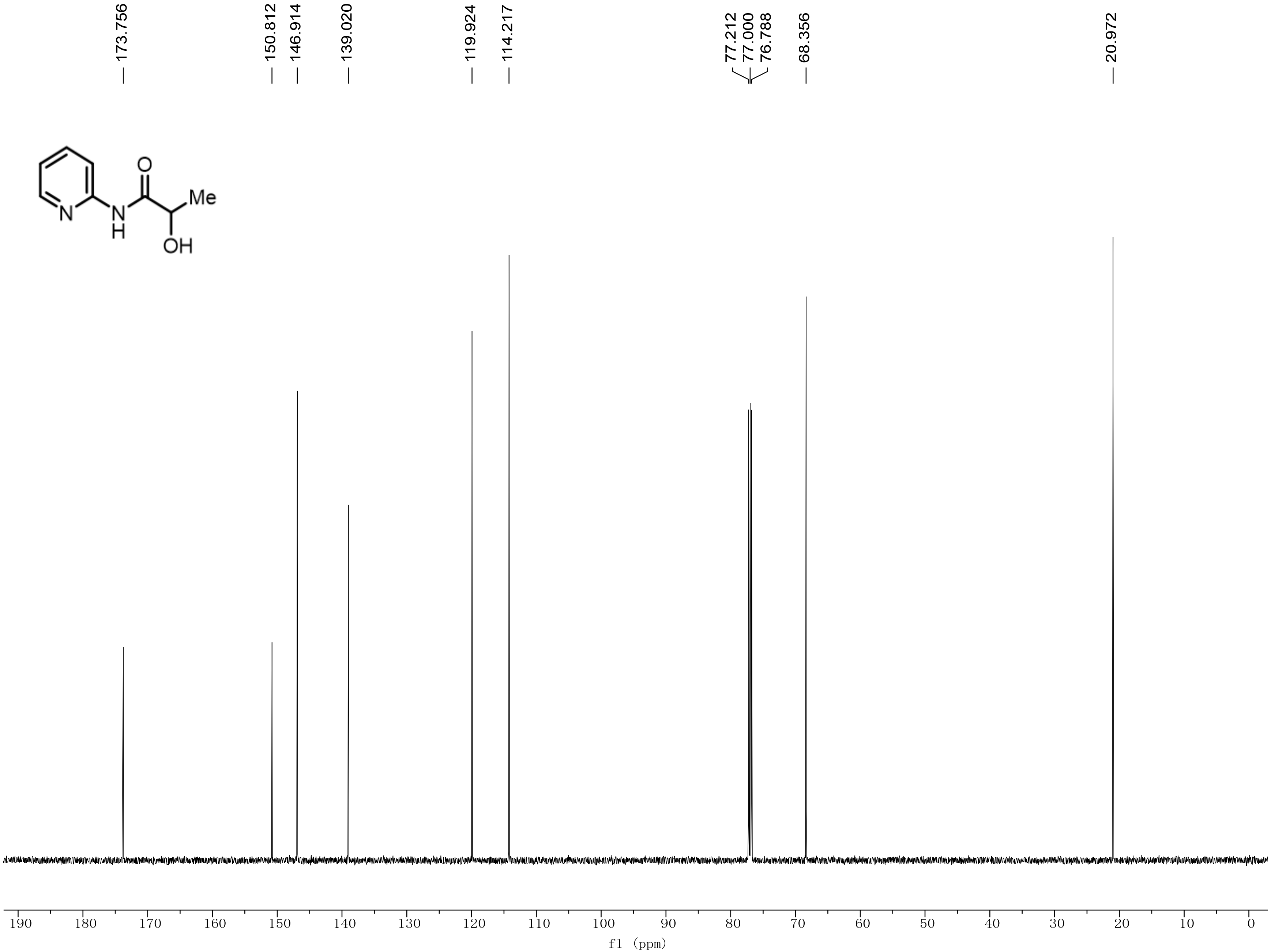
50
40
30
20
10
0
f1 (ppm)



O
Me
N
N
H
OH
0.96
0.96
0.97
1.00
1.00
0.77
1.00
3.00
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 -0.5
f1 (ppm)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77.000
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N
N
H
O
Me
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

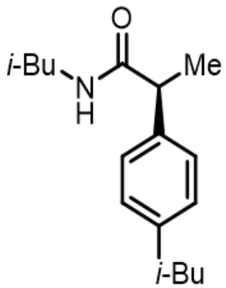
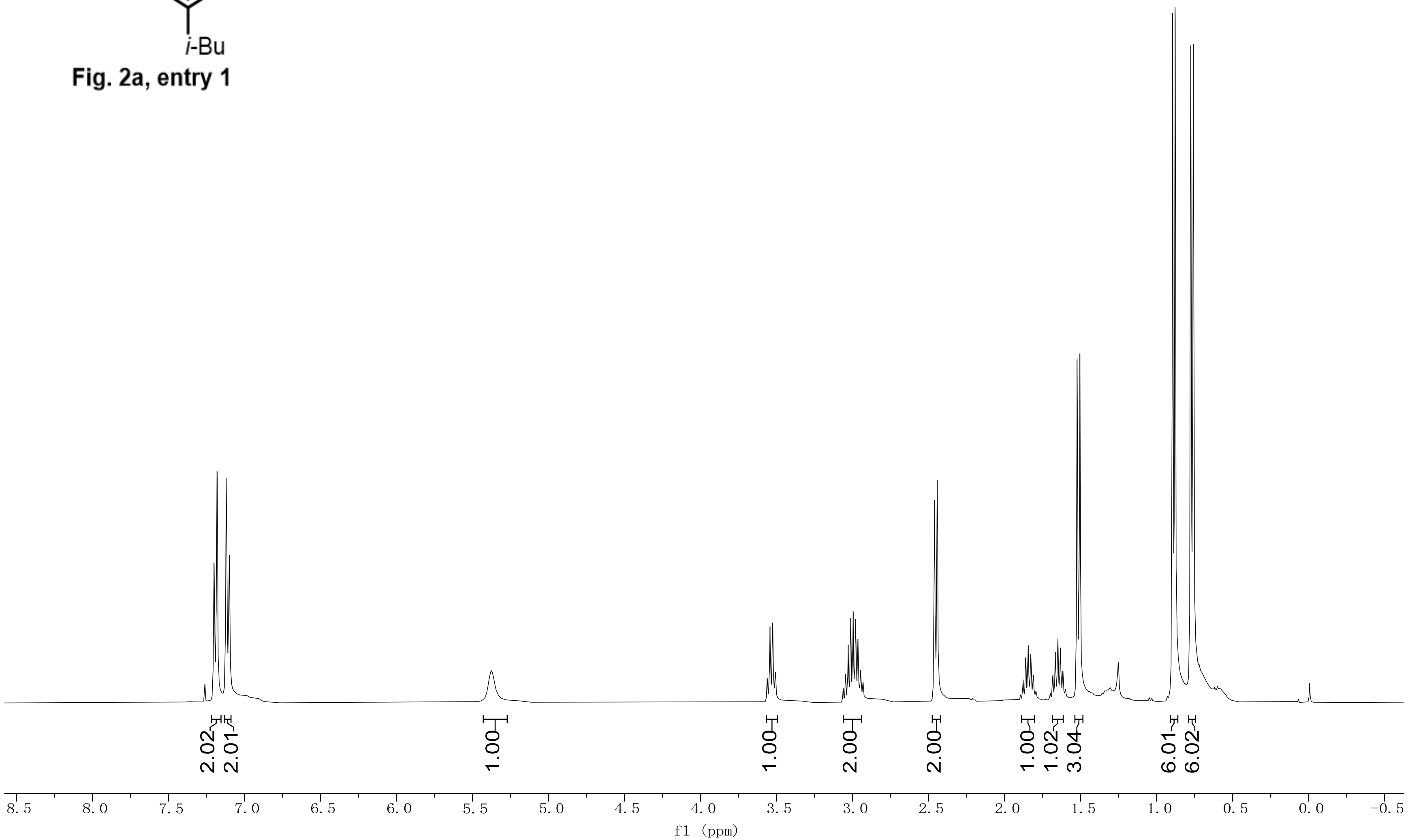


Fig. 2a, entry 1



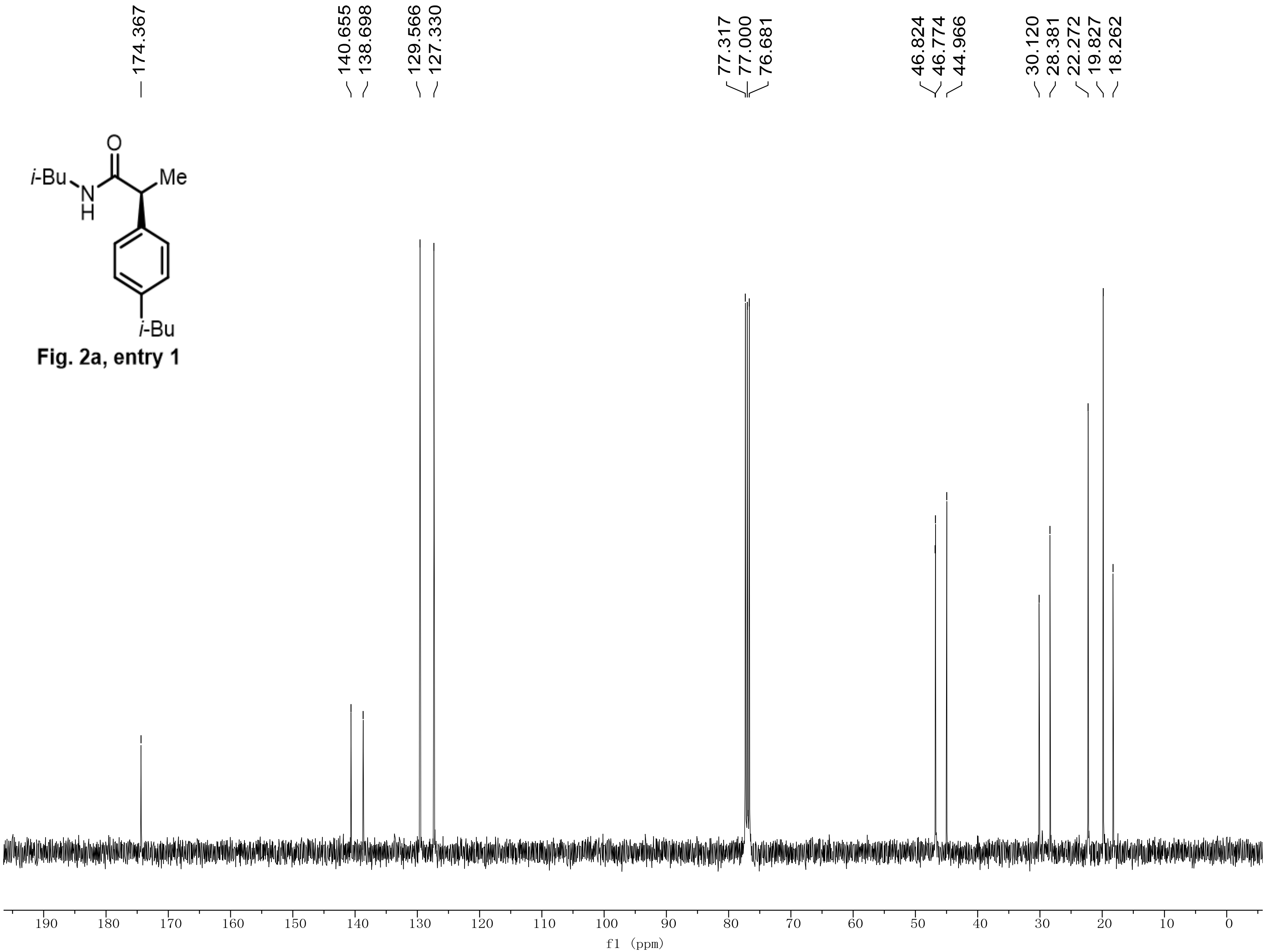


Fig. 2a, entry 1

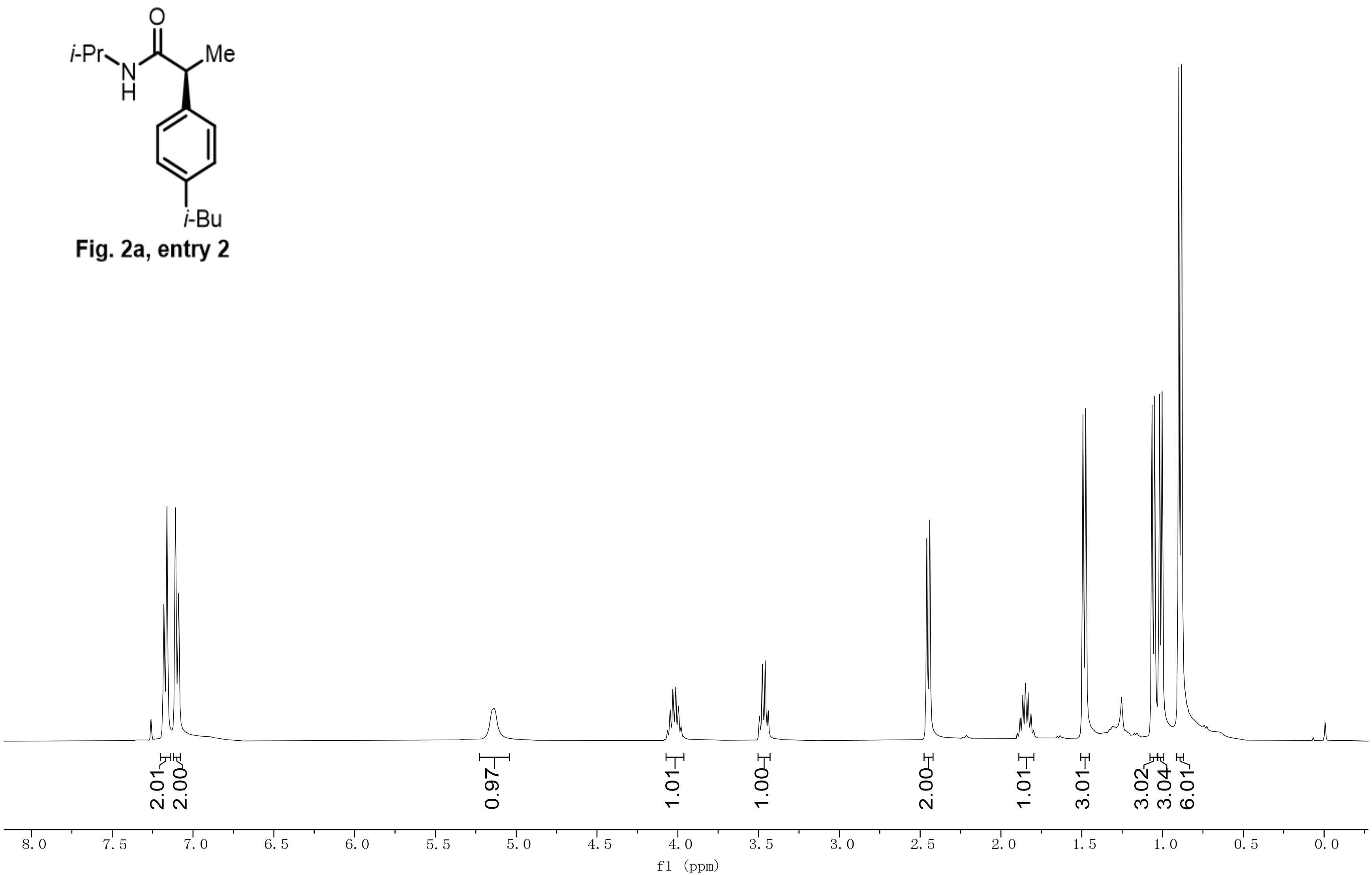


Fig. 2a, entry 2

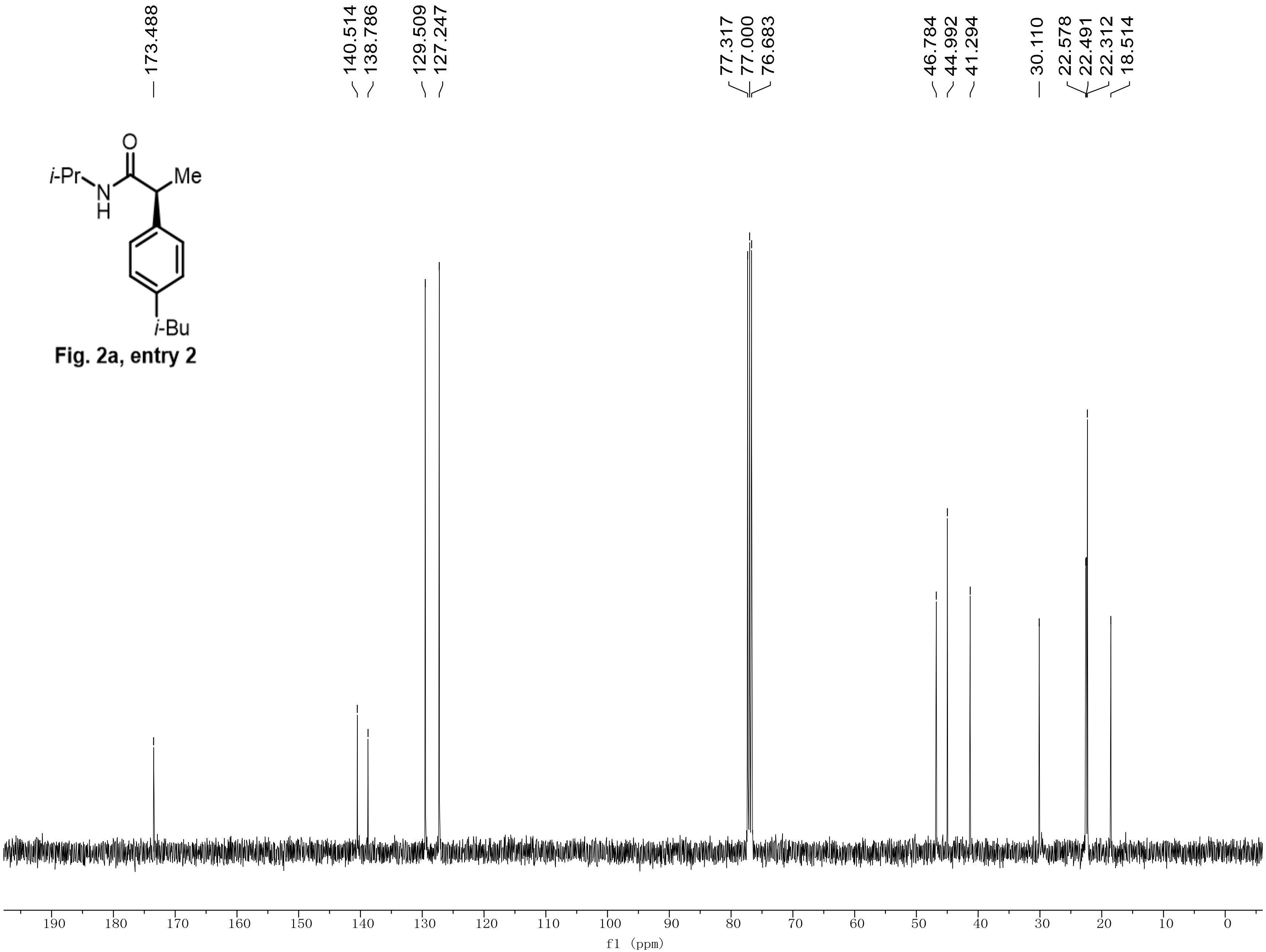


Fig. 2a, entry 2

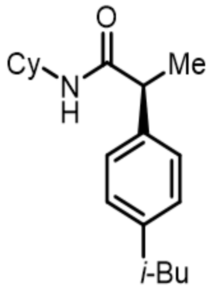
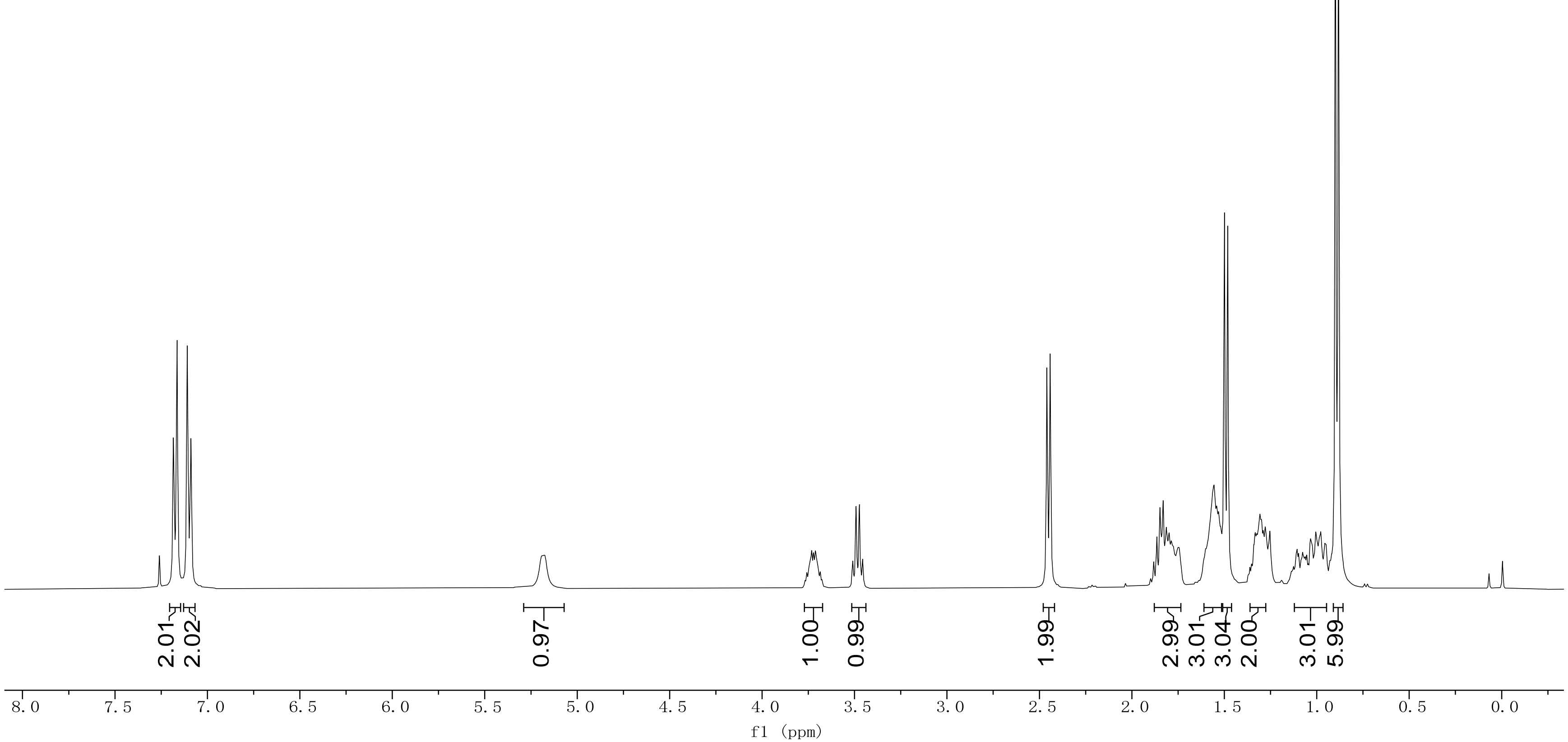


Fig. 2a, entry 3



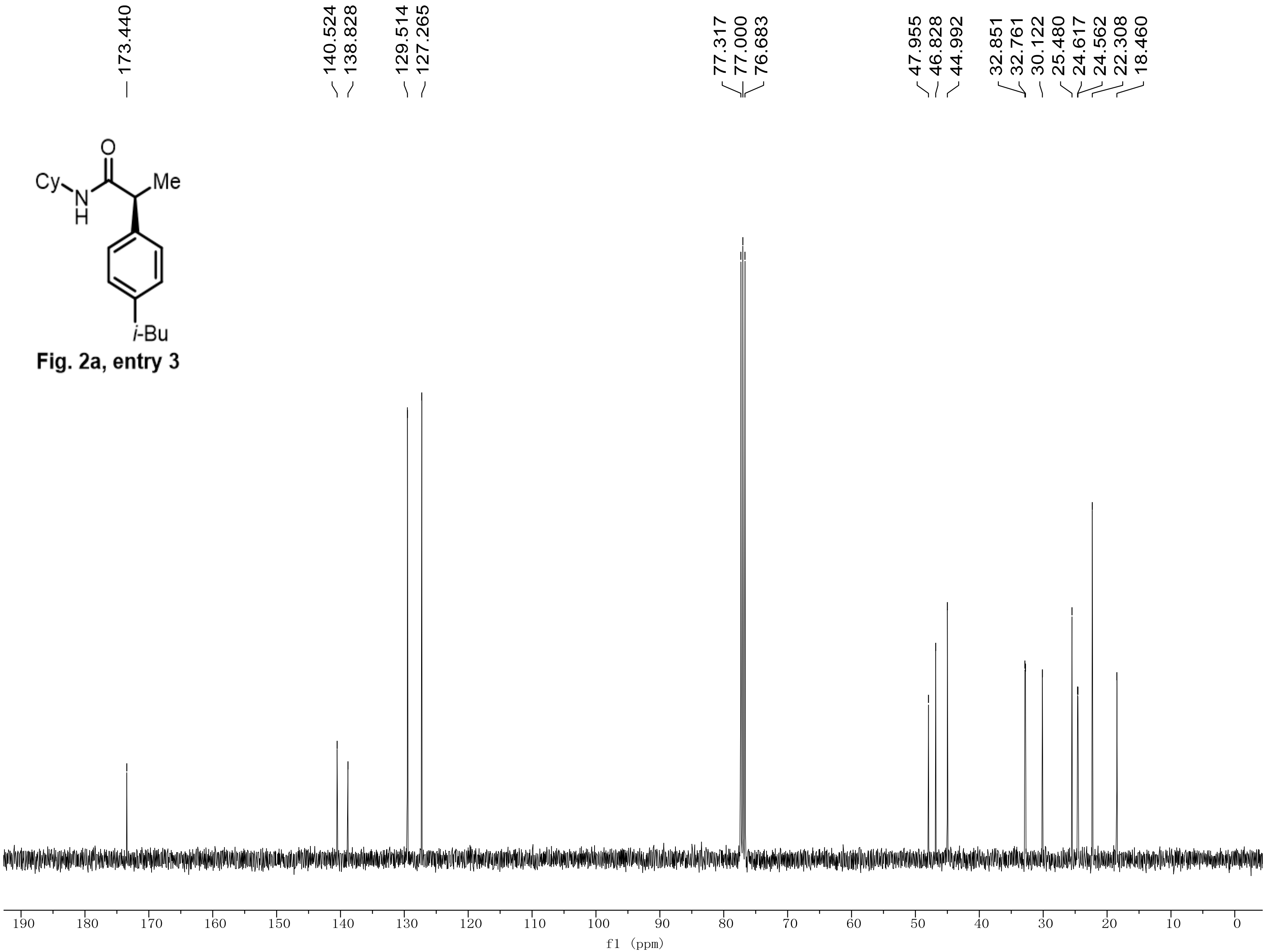


Fig. 2a, entry 3

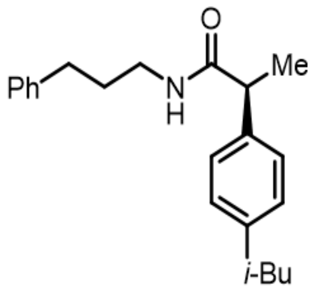
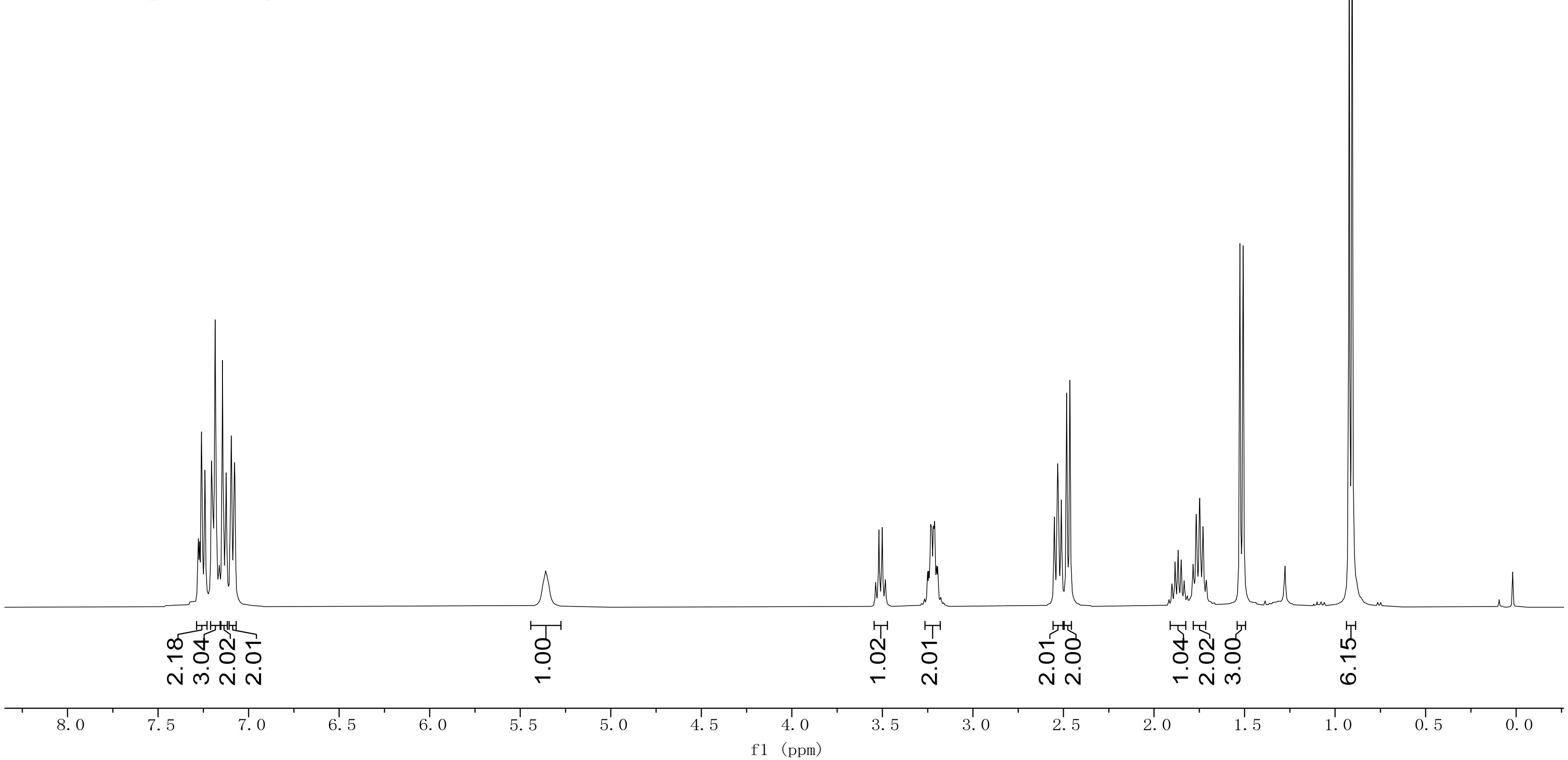


Fig. 2a, entry 4



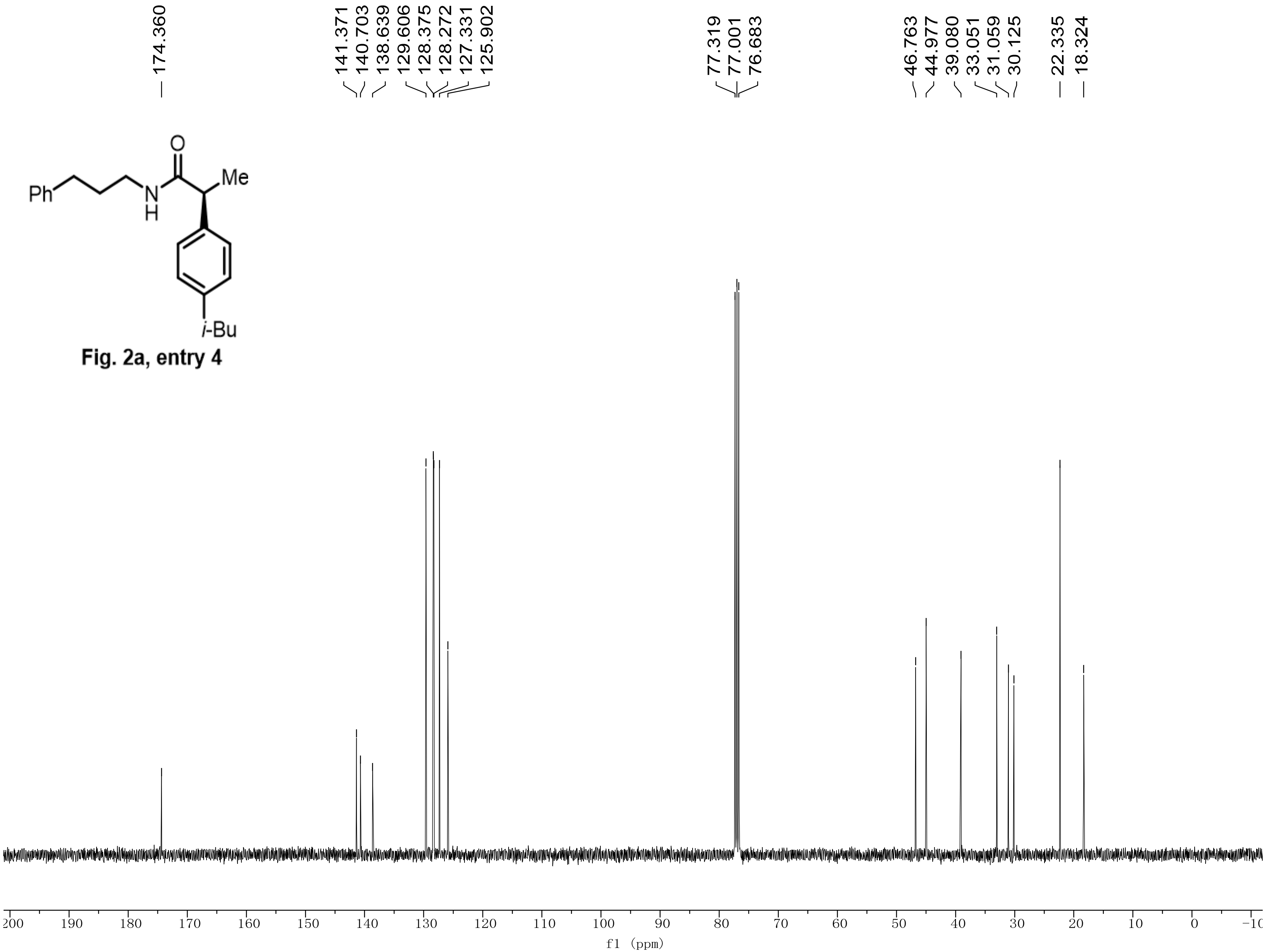


Fig. 2a, entry 4

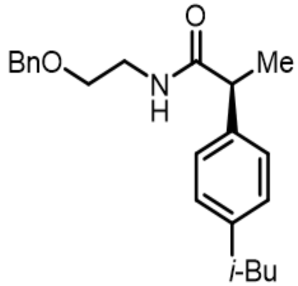
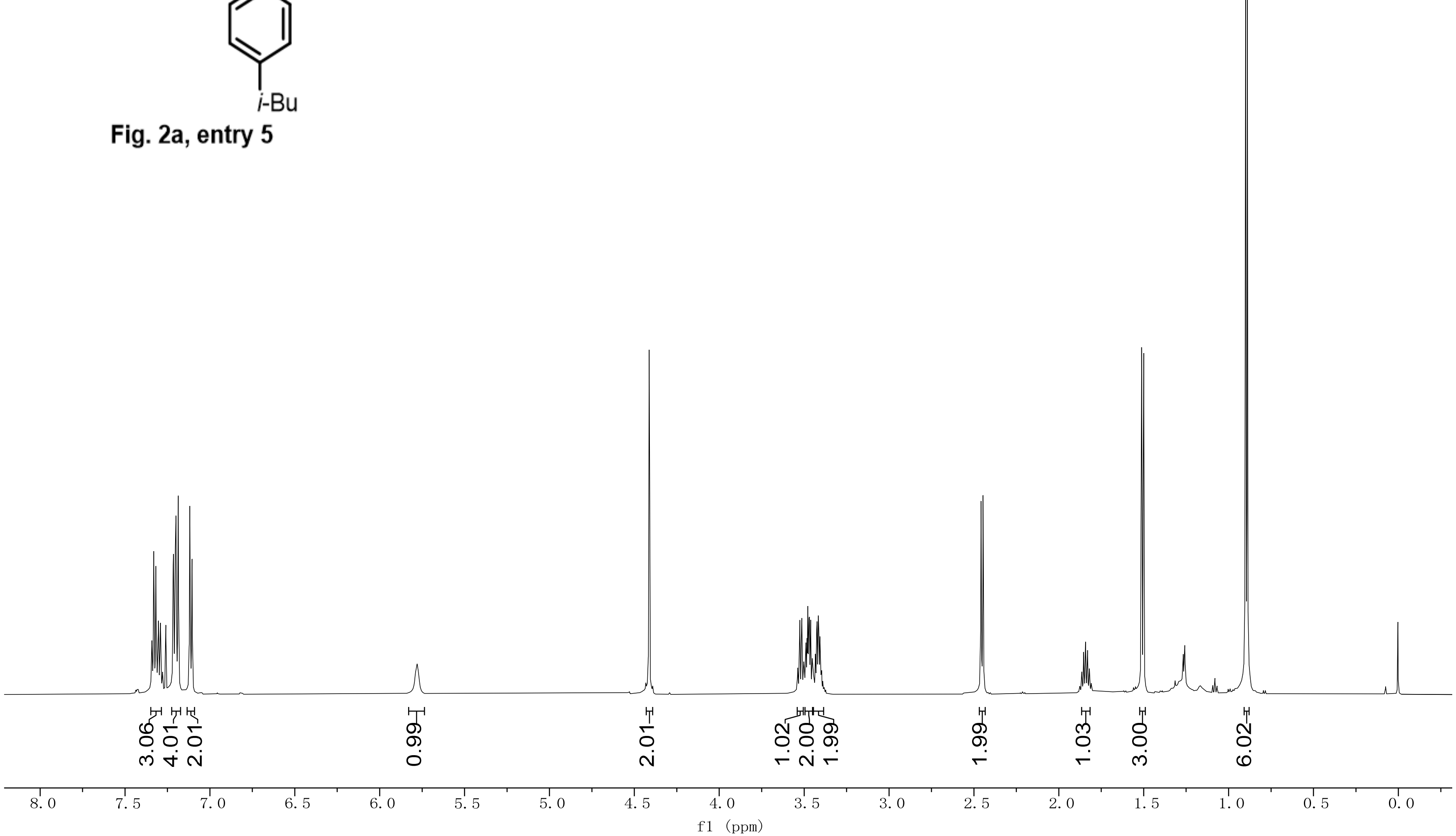
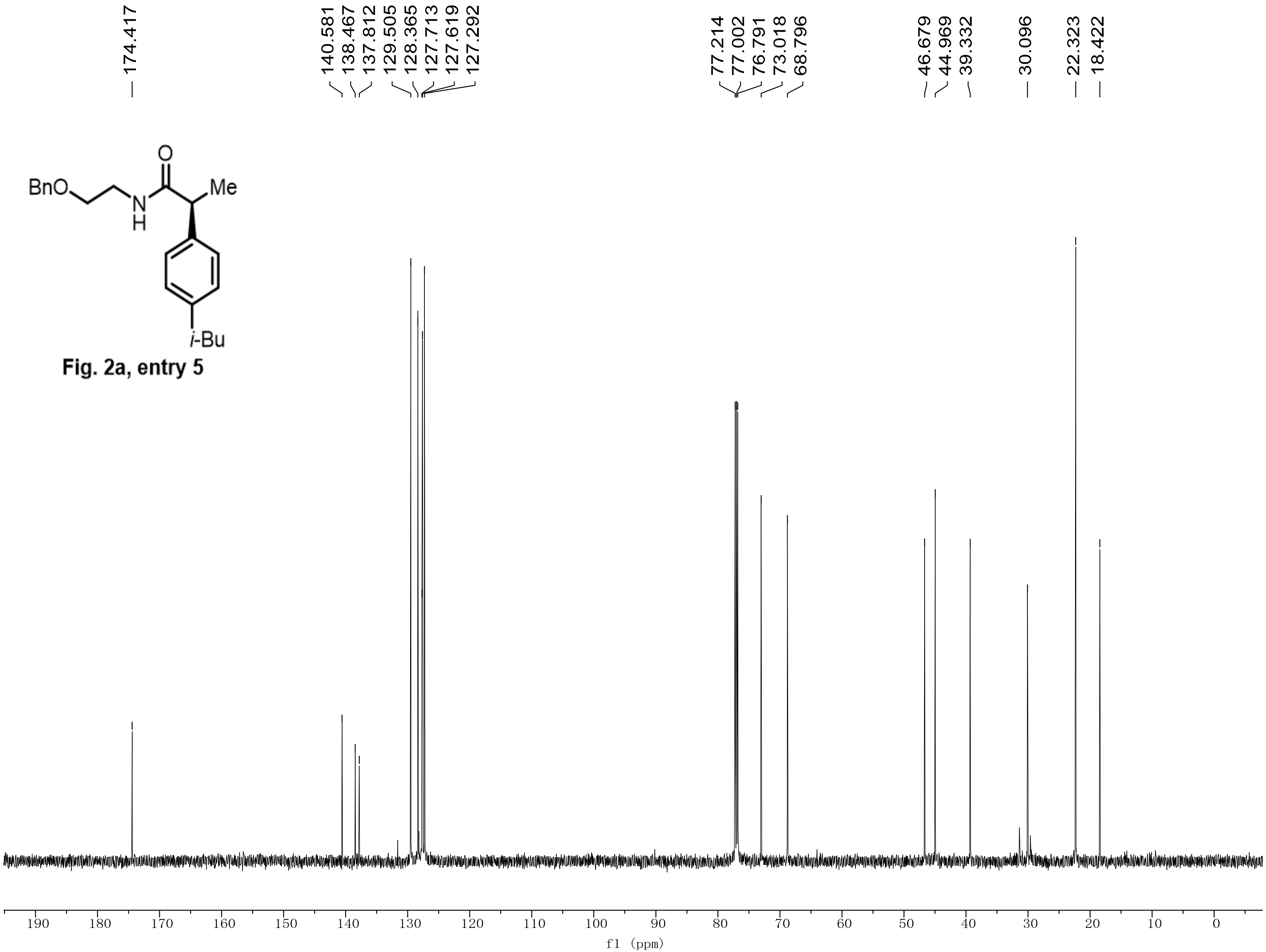


Fig. 2a, entry 5

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77.214
77.002
76.791
73.018
68.796
46.679
44.969
39.332
30.096
22.323
18.422
BnO
O
Me
N
H
i-Bu
Fig. 2a, entry 5
f1 (ppm)

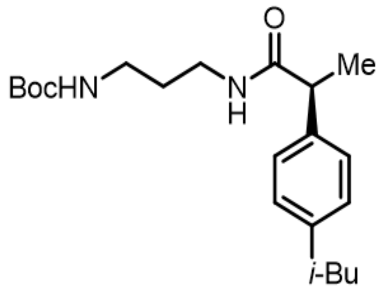
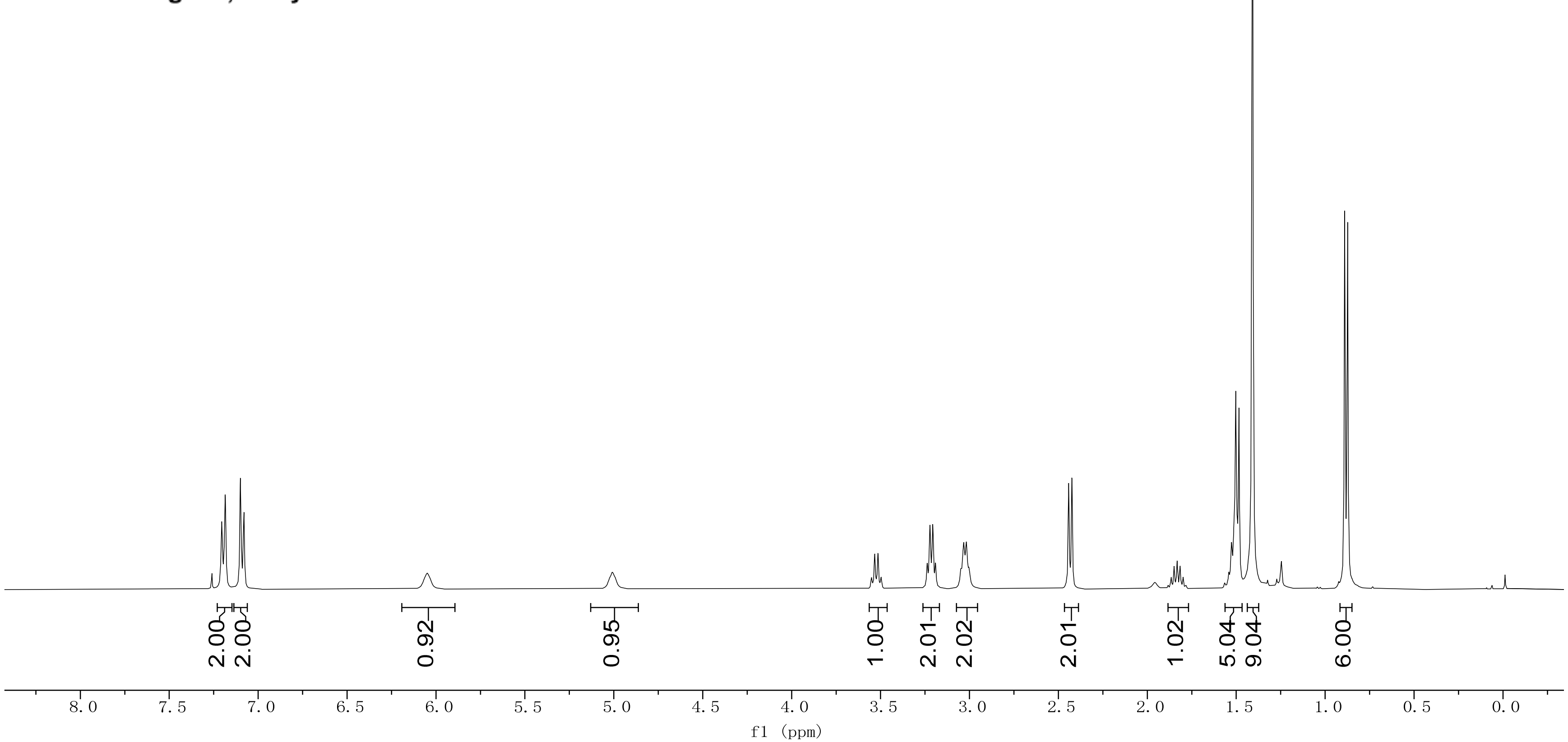


Fig. 2a, entry 6



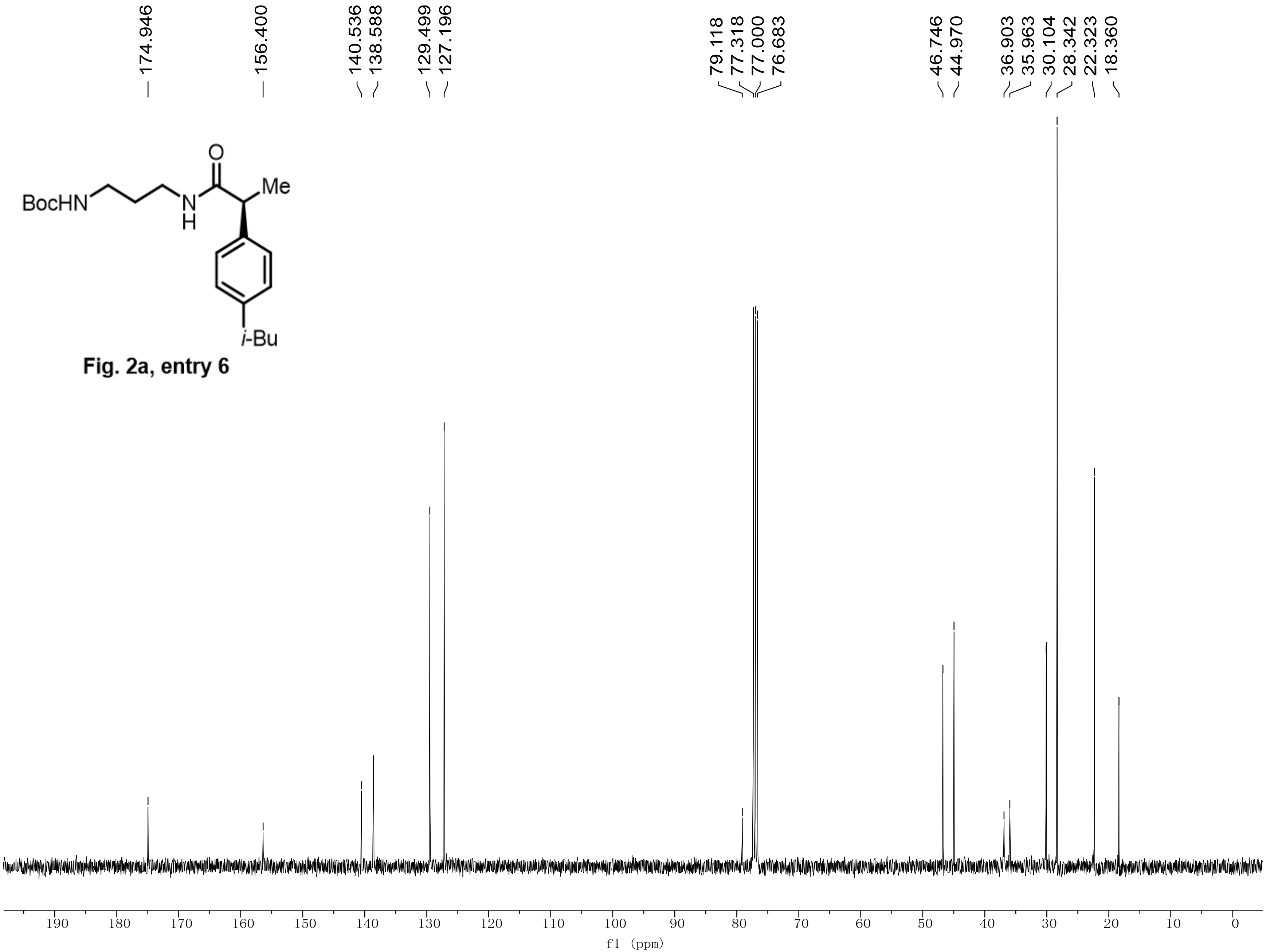


Fig. 2a, entry 6

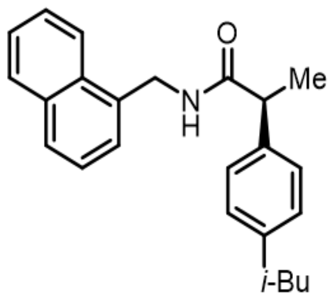
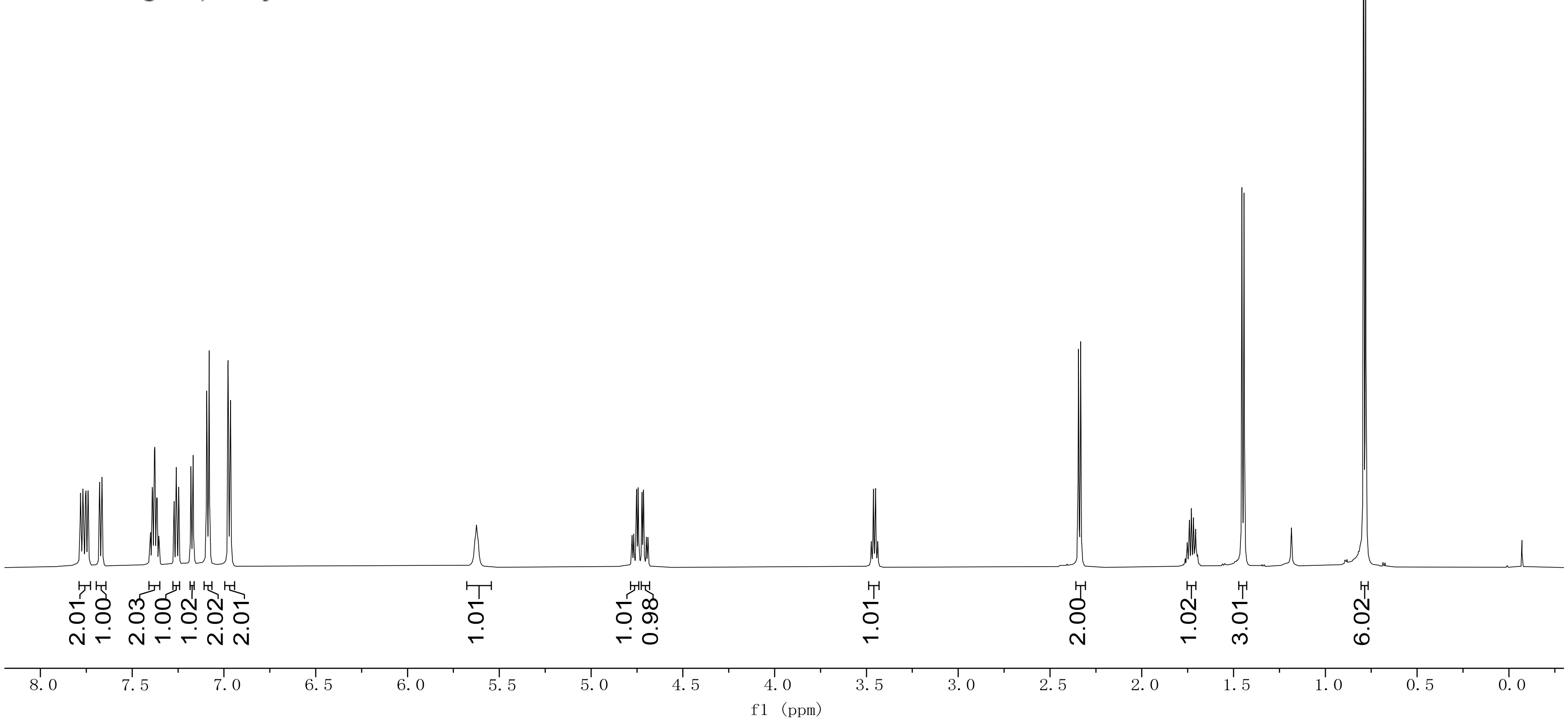


Fig. 2a, entry 7



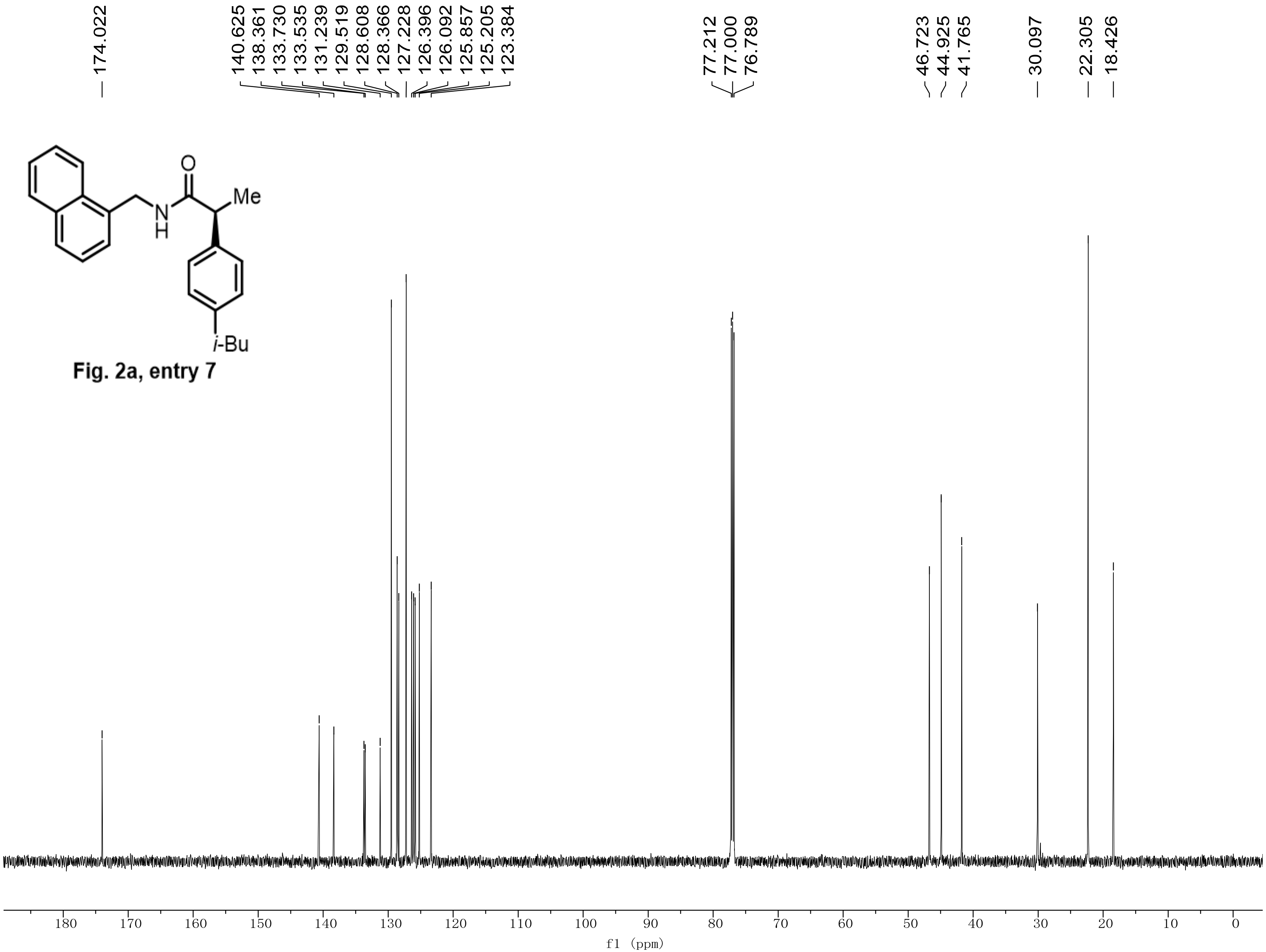


Fig. 2a, entry 7

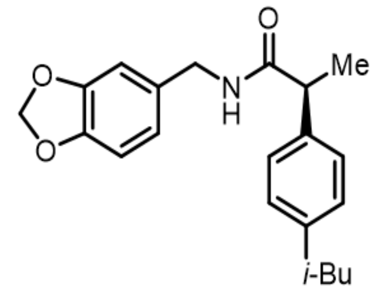
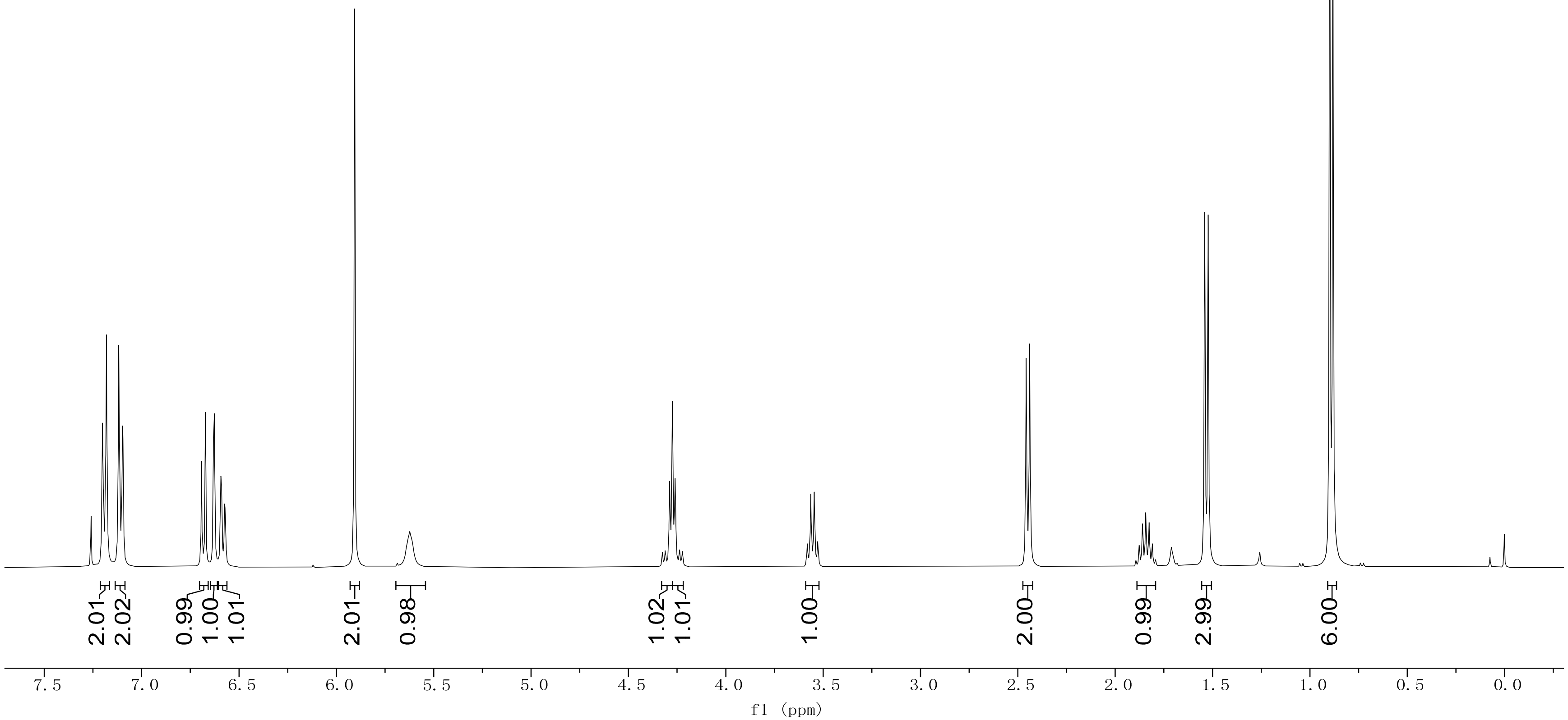


Fig. 2a, entry 8



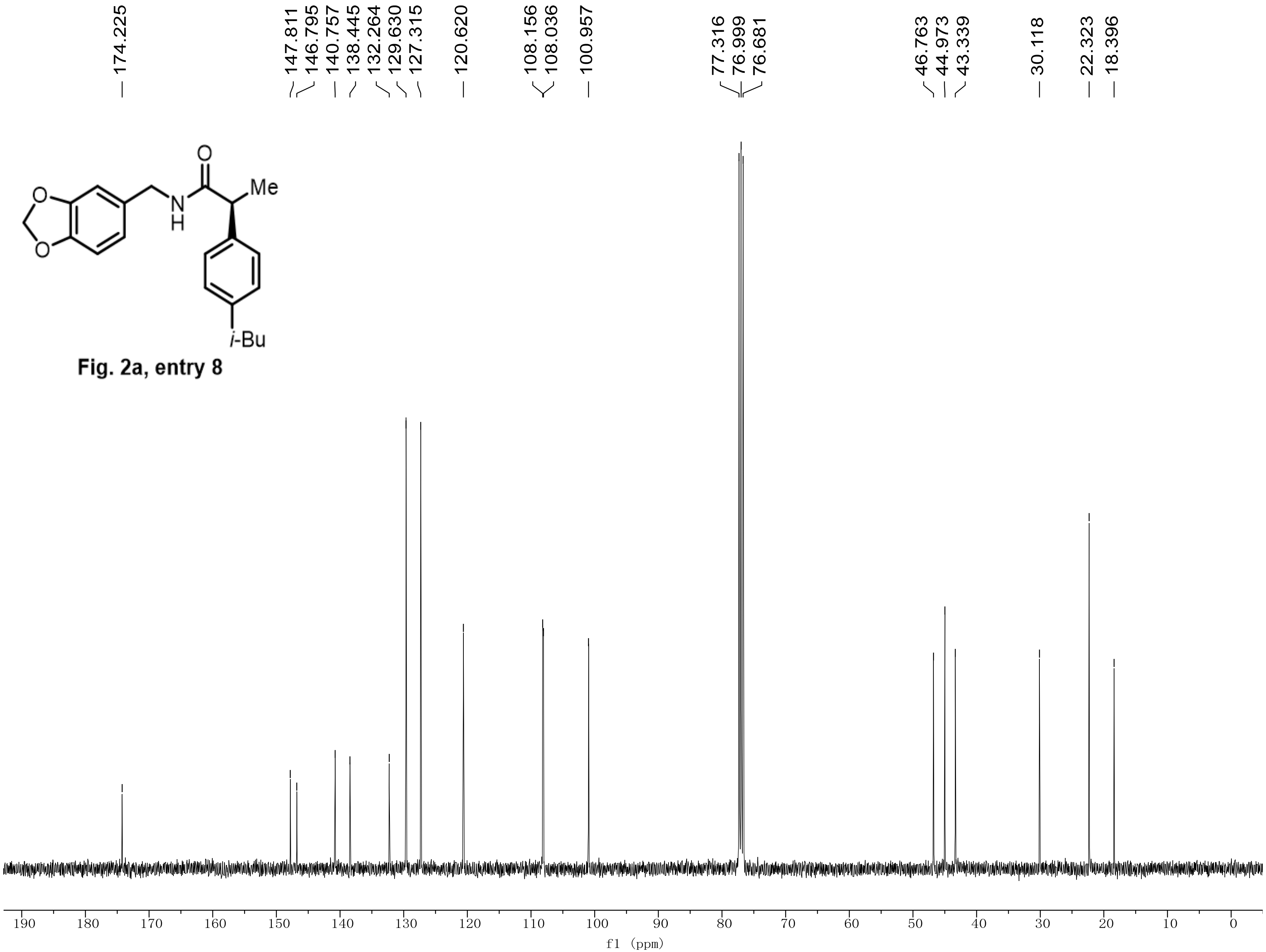


Fig. 2a, entry 8

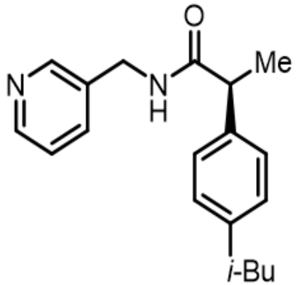
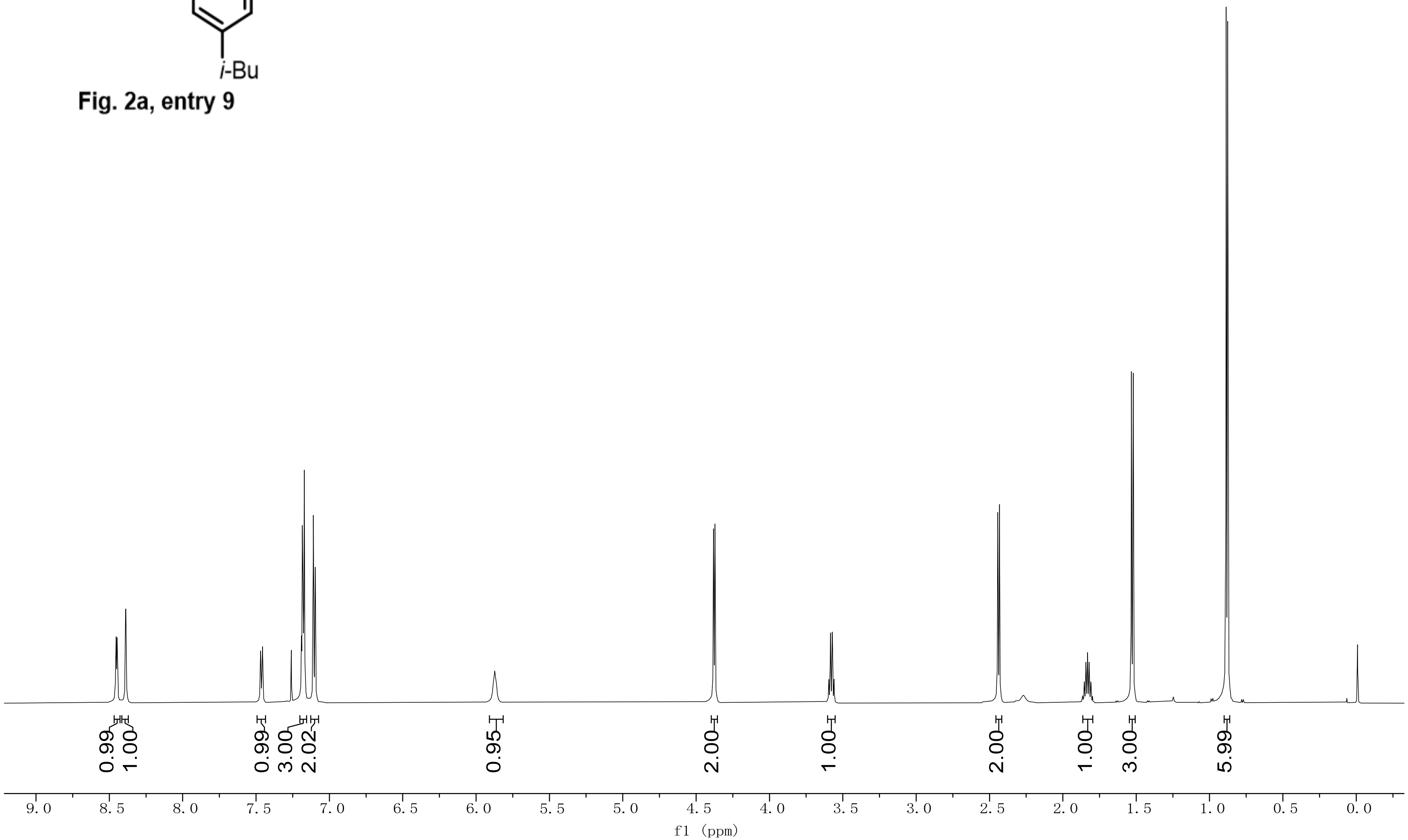
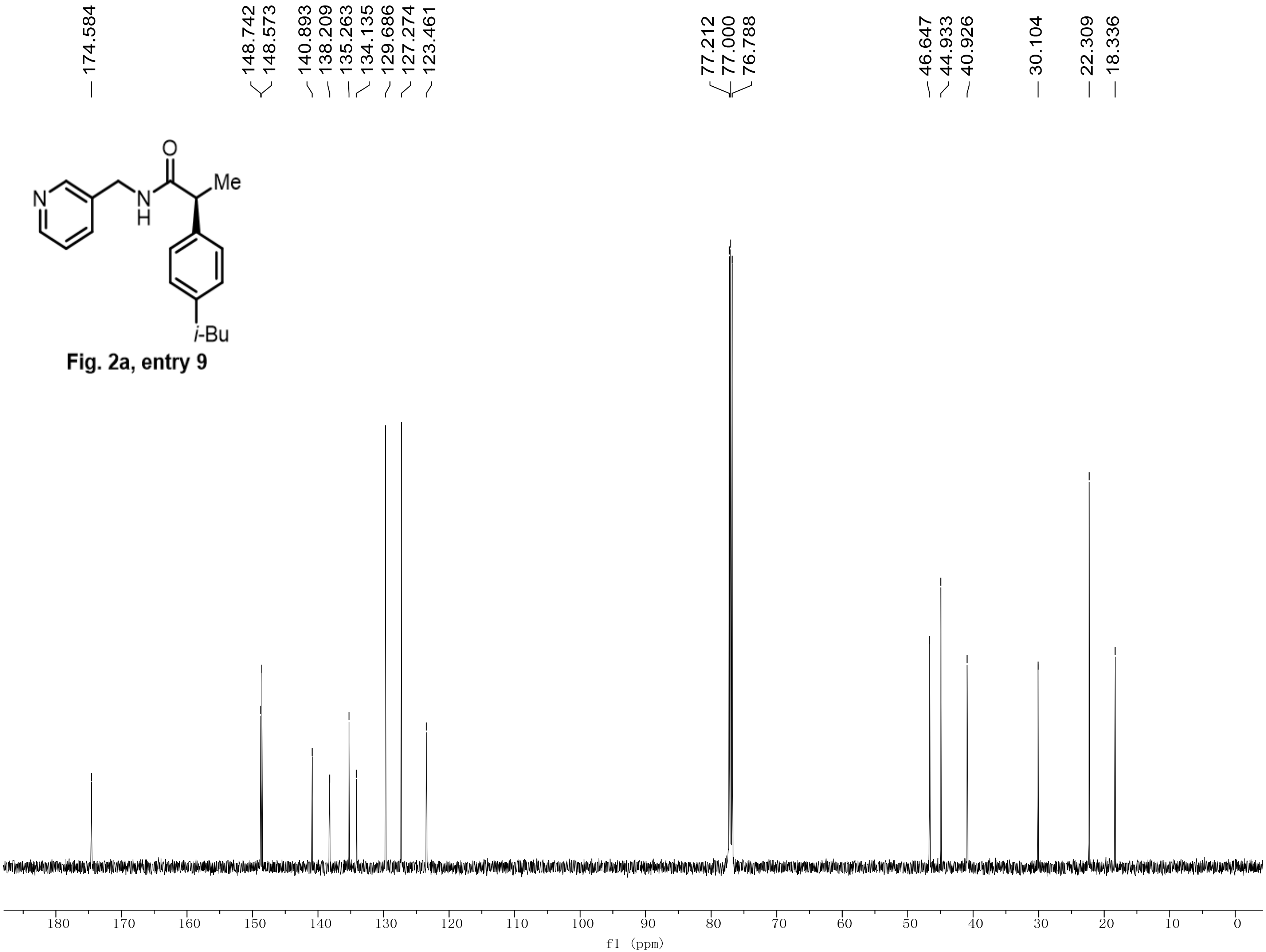


Fig. 2a, entry 9





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148.742
148.573
140.893
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135.263
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129.686
127.274
123.461
77.212
77.000
76.788
46.647
44.933
40.926
30.104
22.309
18.336
O
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N
H
Me
i-Bu
Fig. 2a, entry 9
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f1 (ppm)

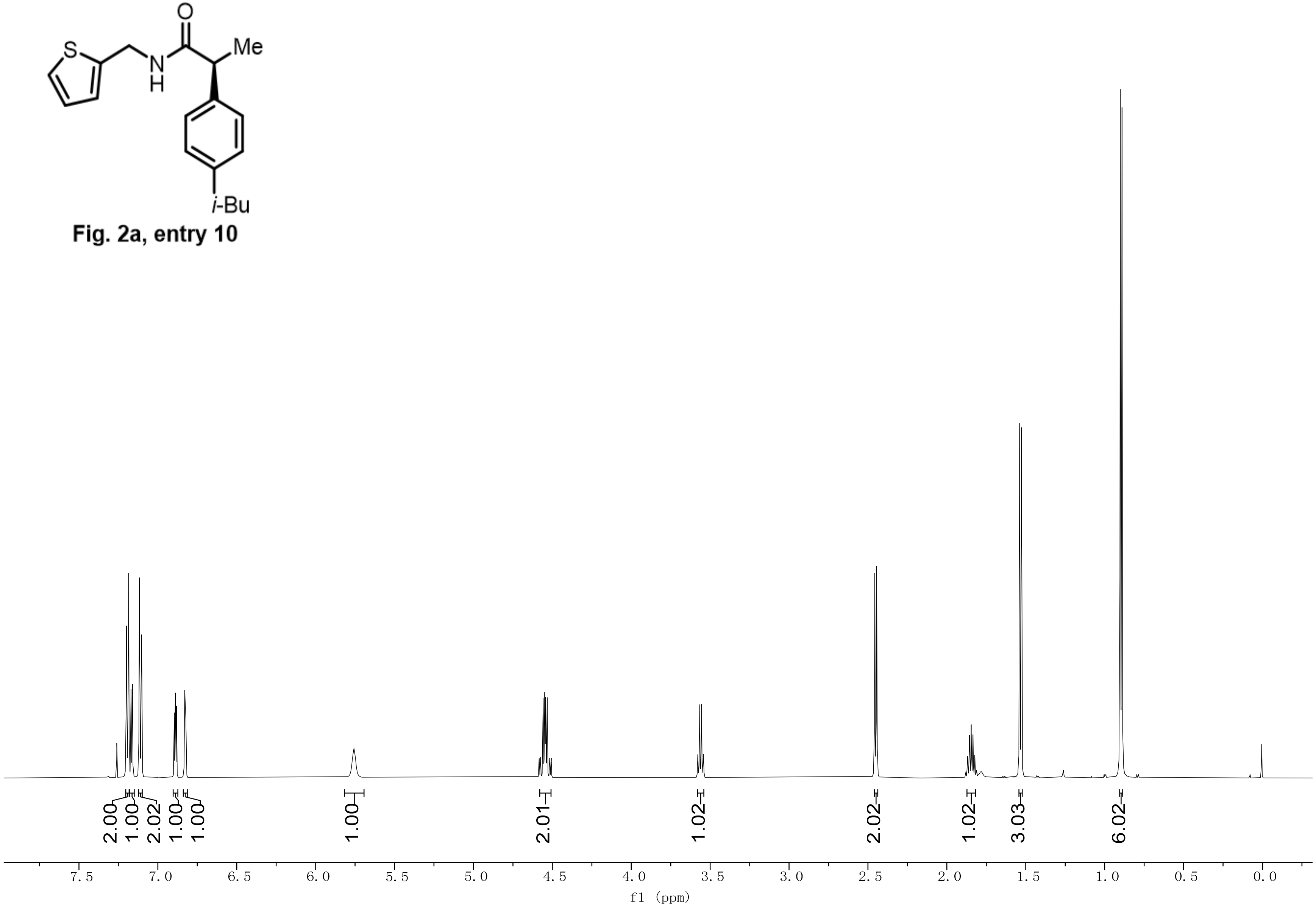


Fig. 2a, entry 10

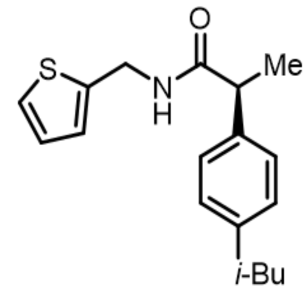
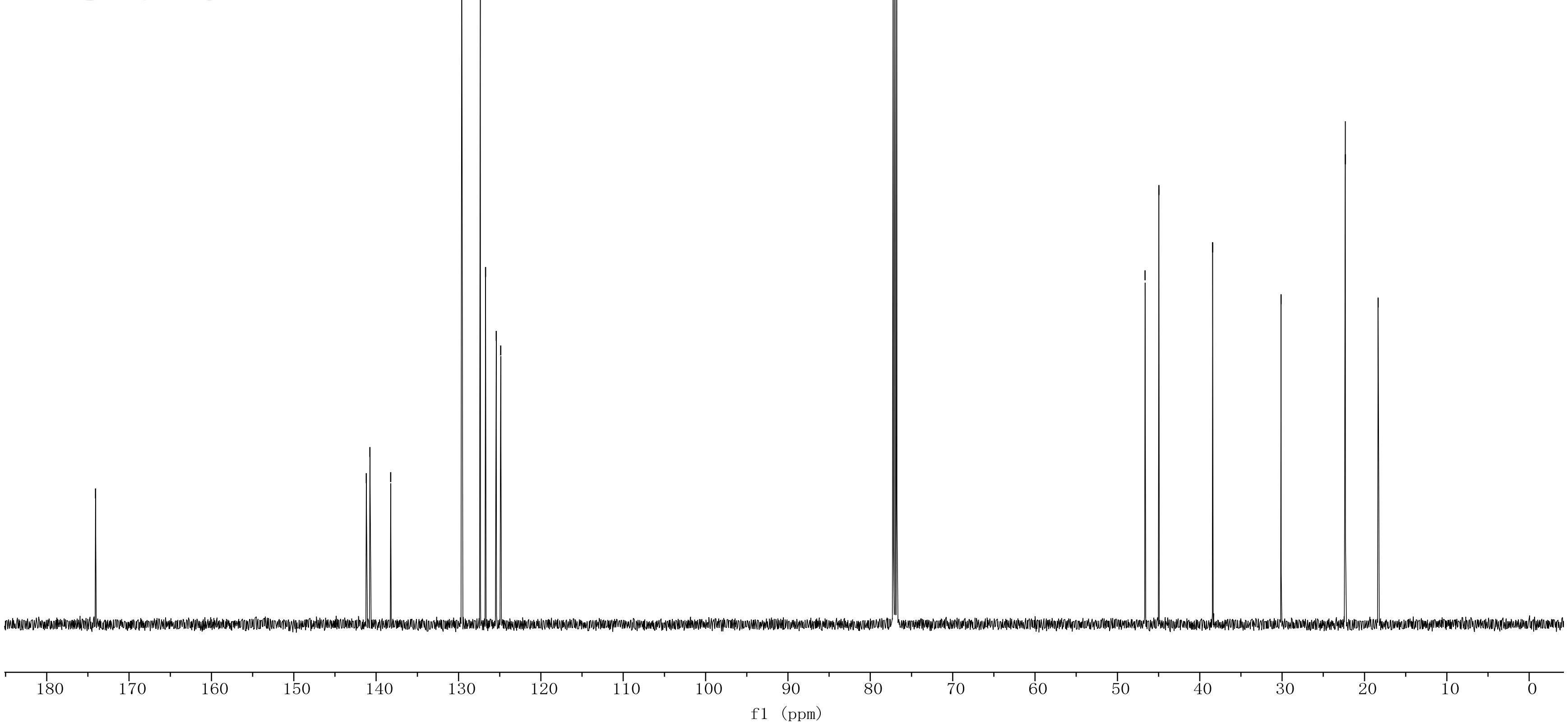


Fig. 2a, entry 10



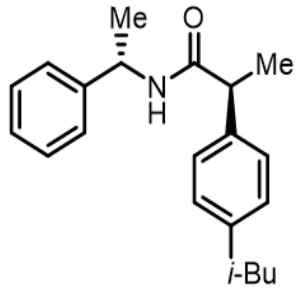
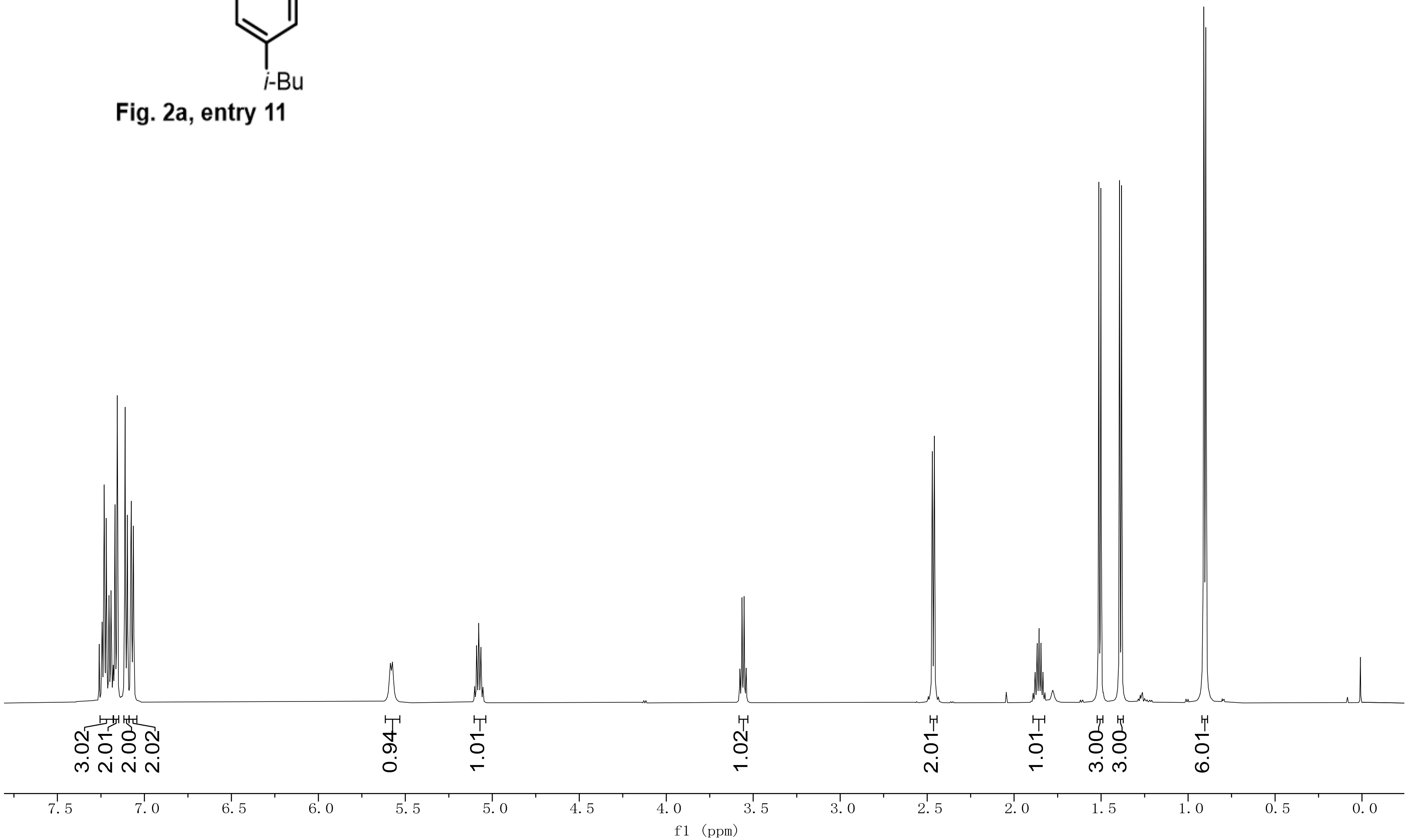


Fig. 2a, entry 11



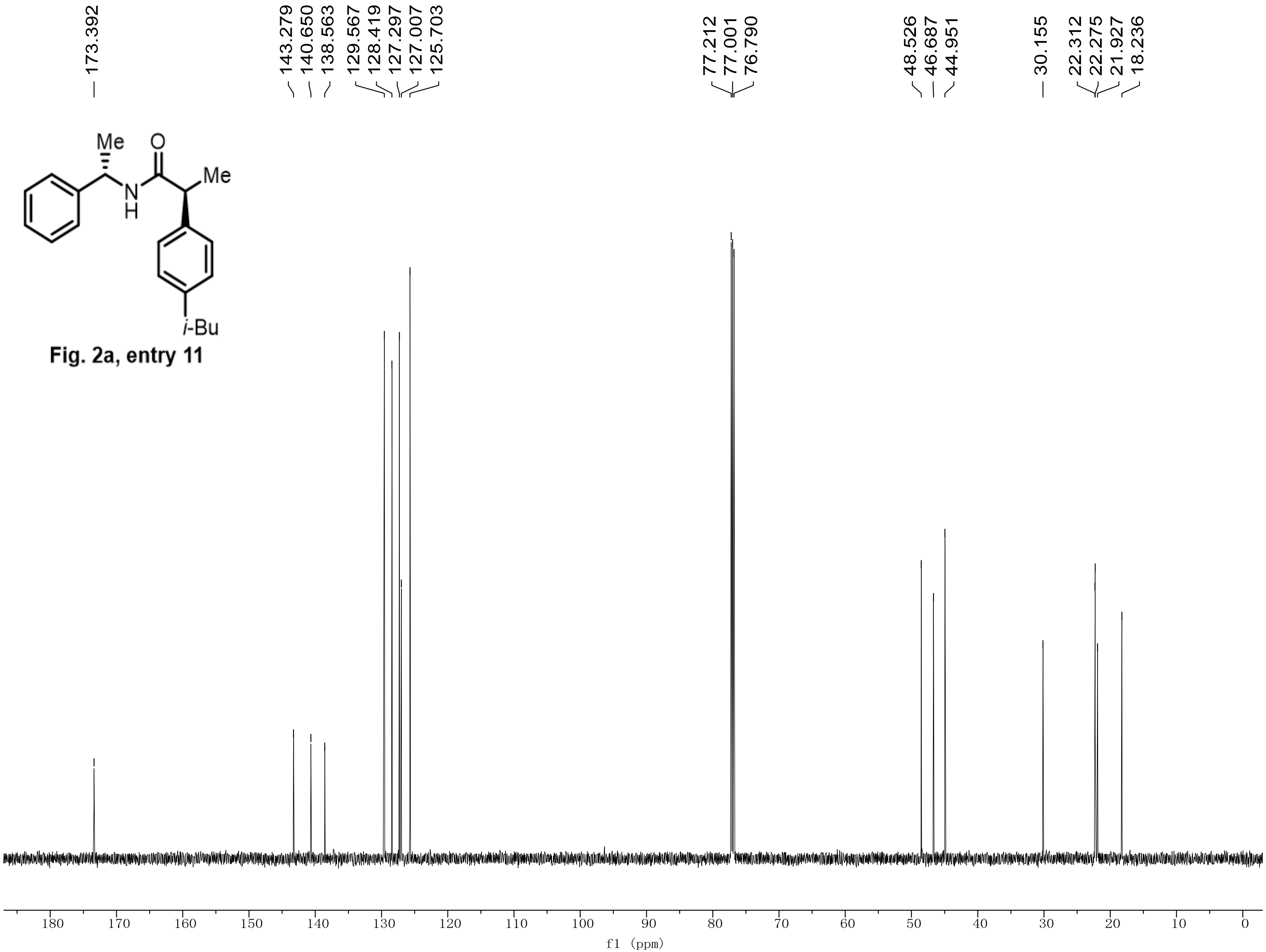


Fig. 2a, entry 11

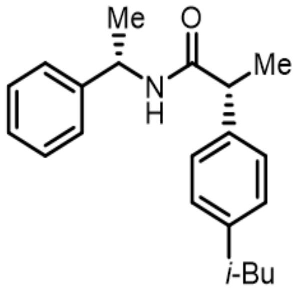
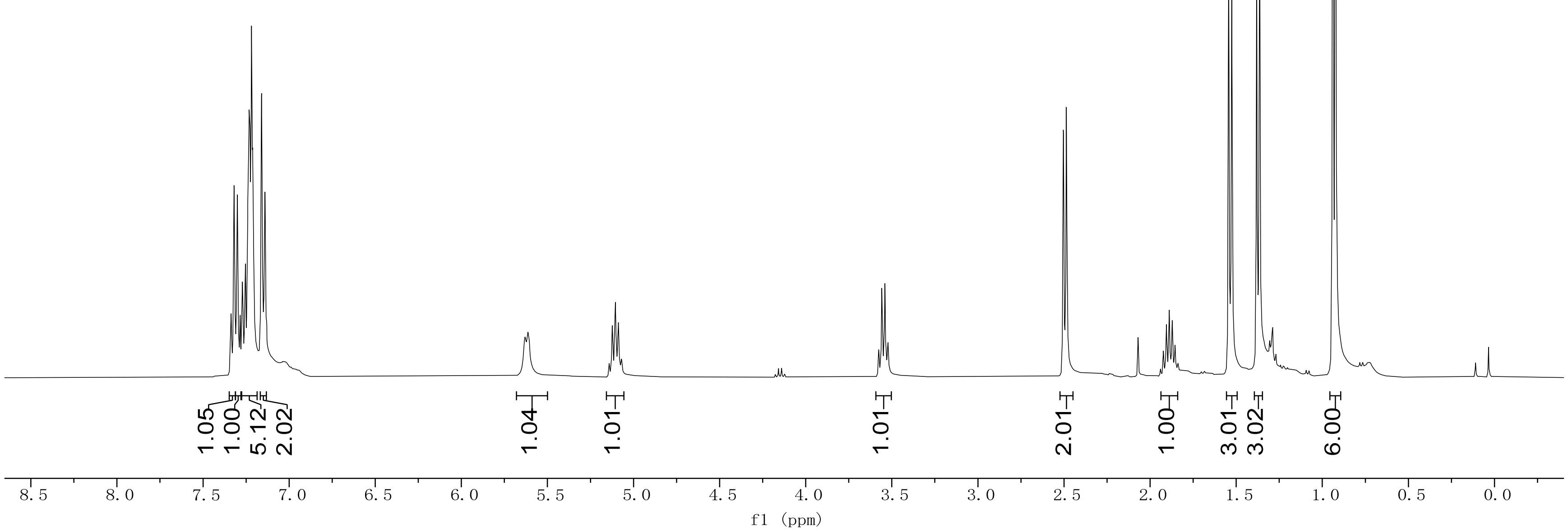


Fig. 2a, entry 12



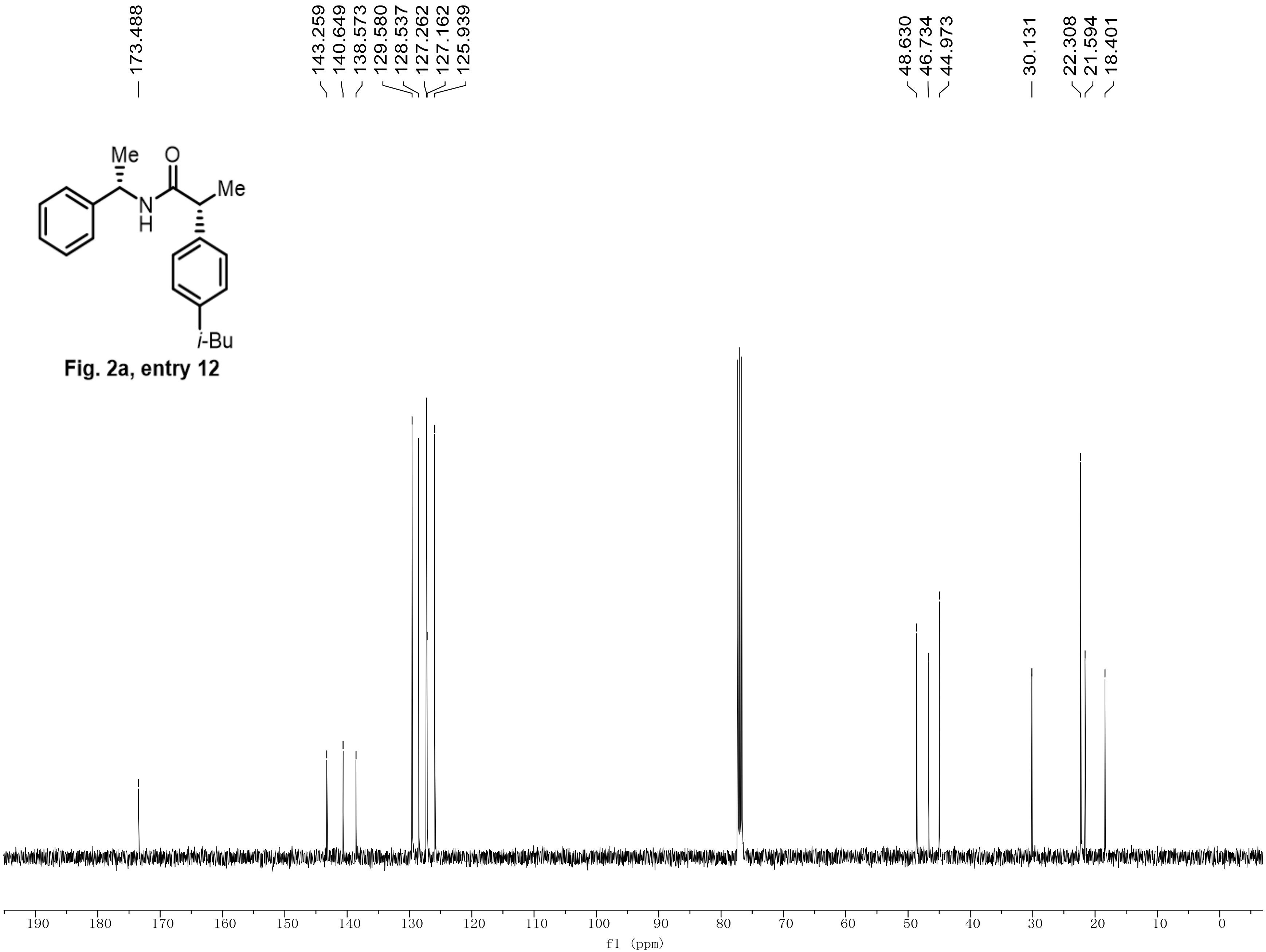


Fig. 2a, entry 12

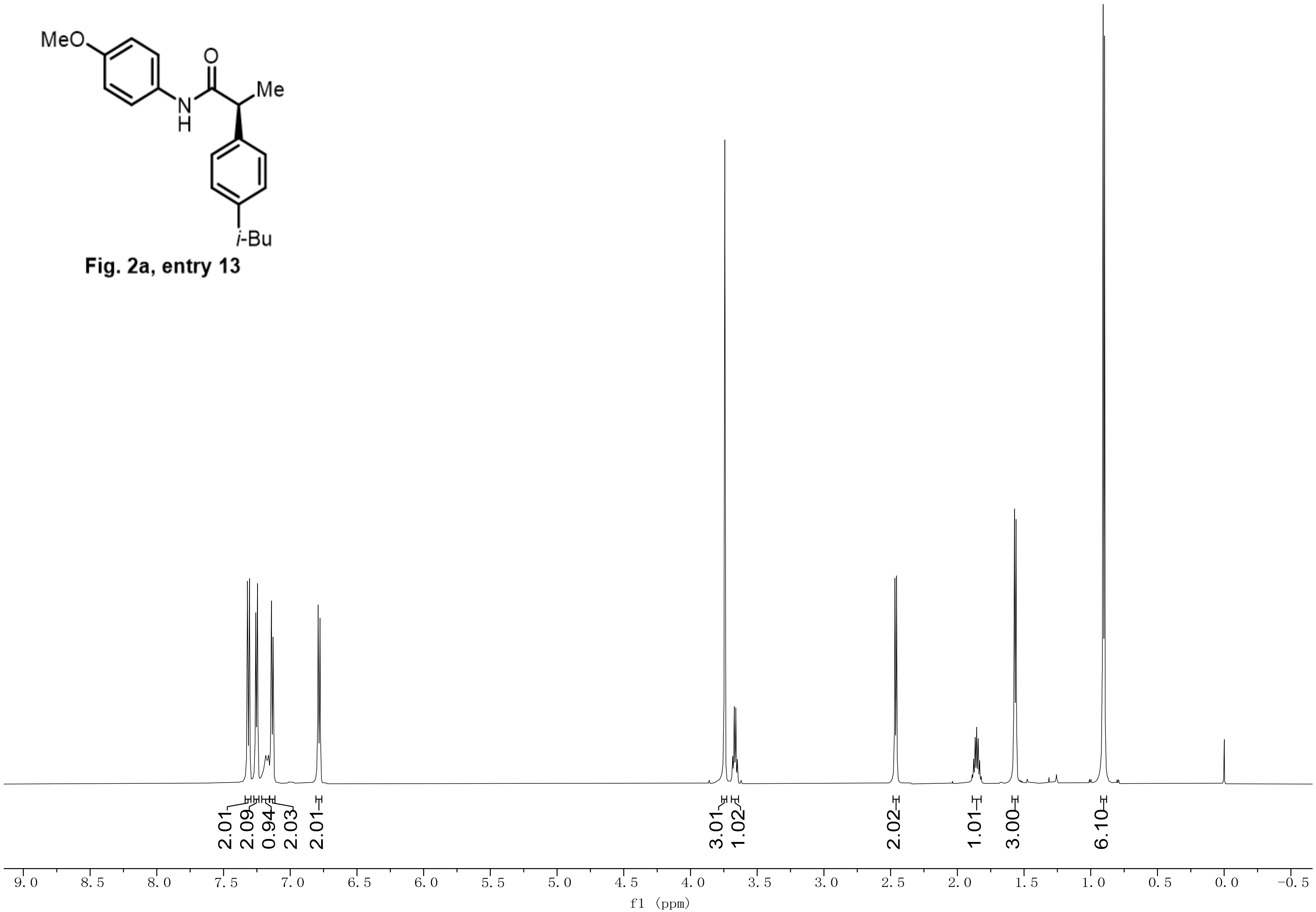


Fig. 2a, entry 13

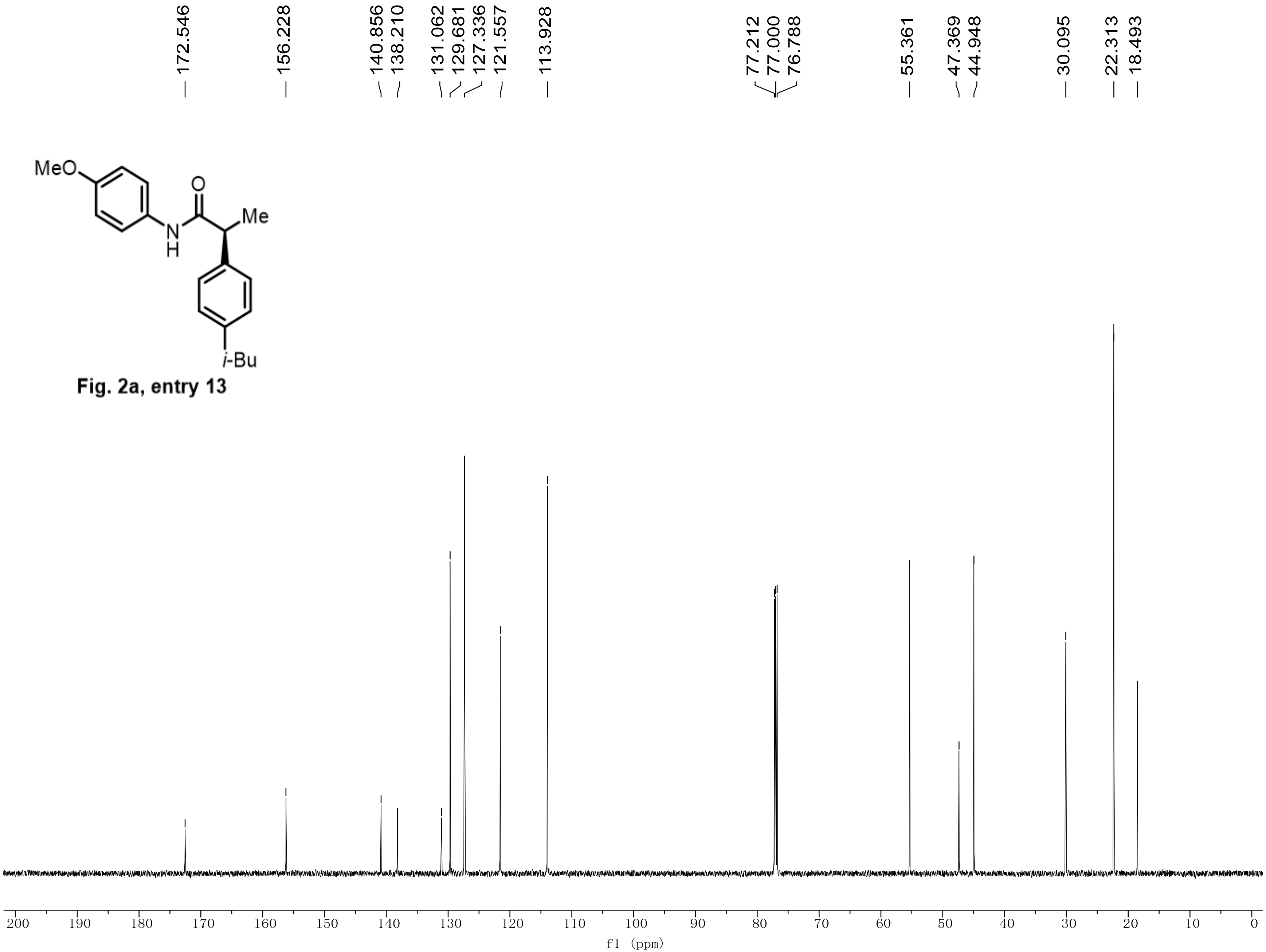


Fig. 2a, entry 13

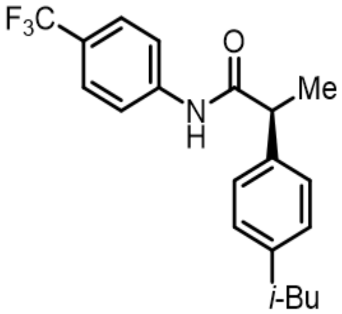
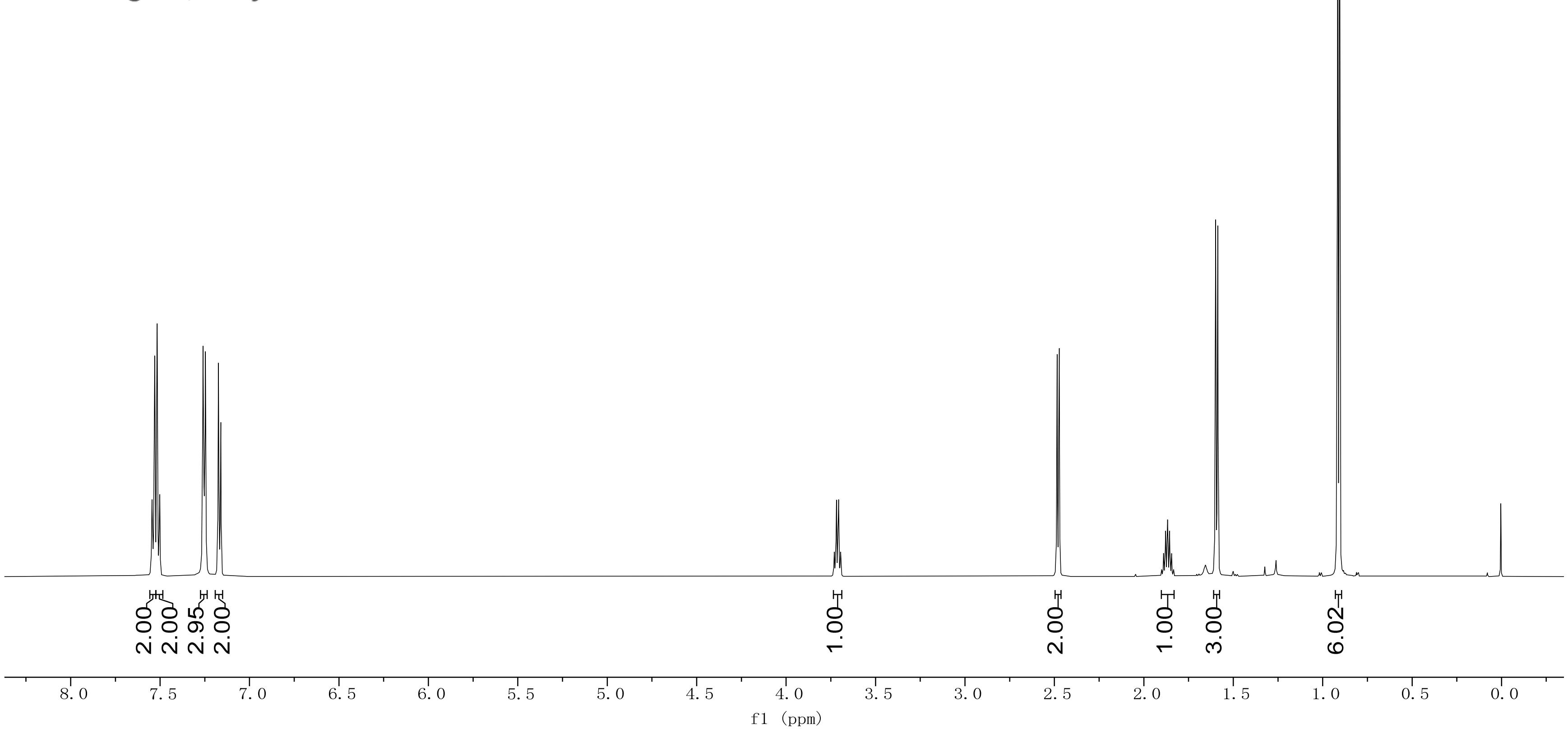


Fig. 2a, entry 14



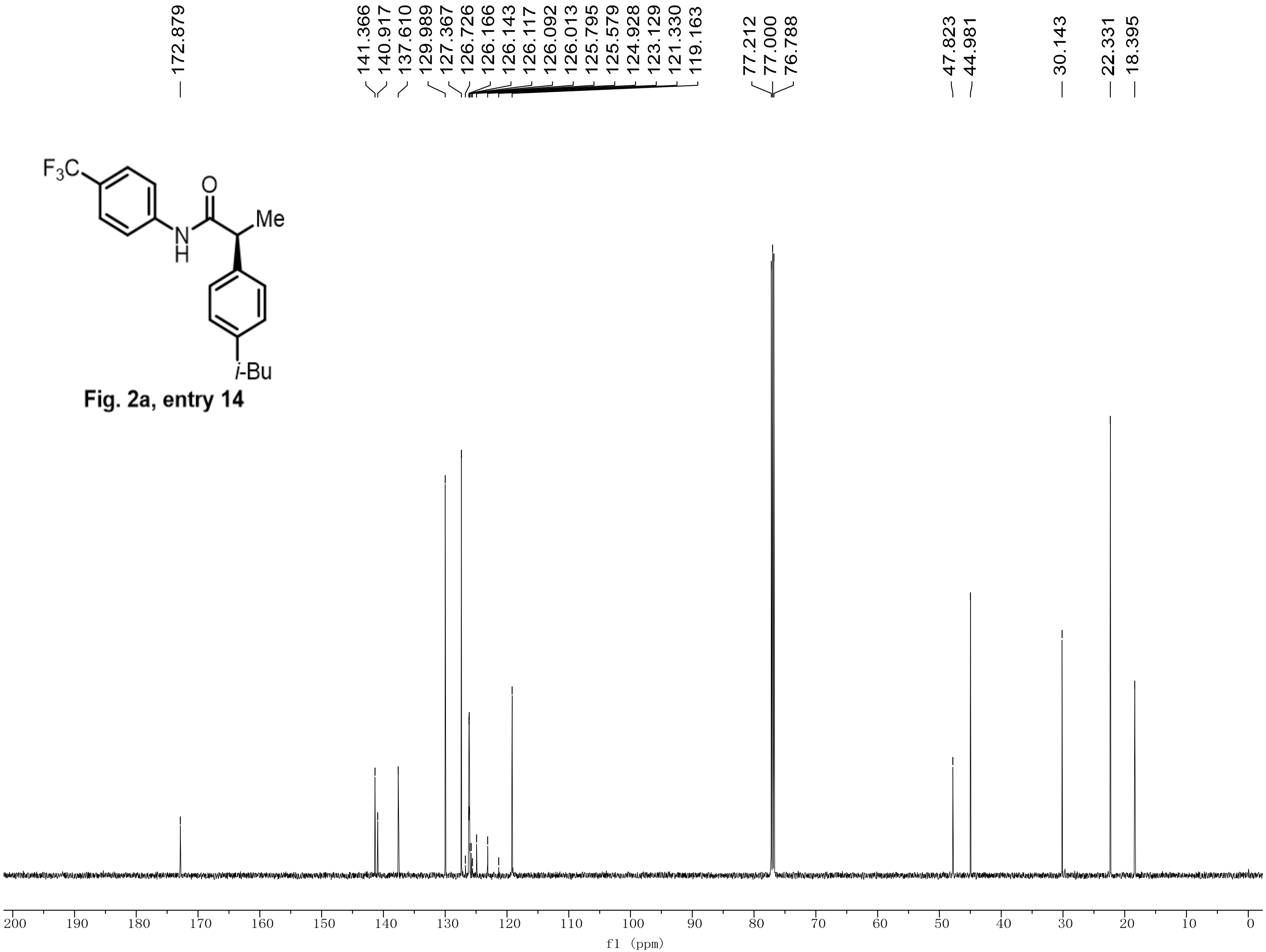


Fig. 2a, entry 14

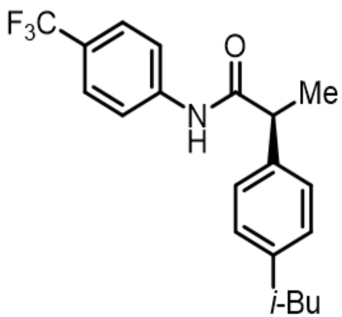
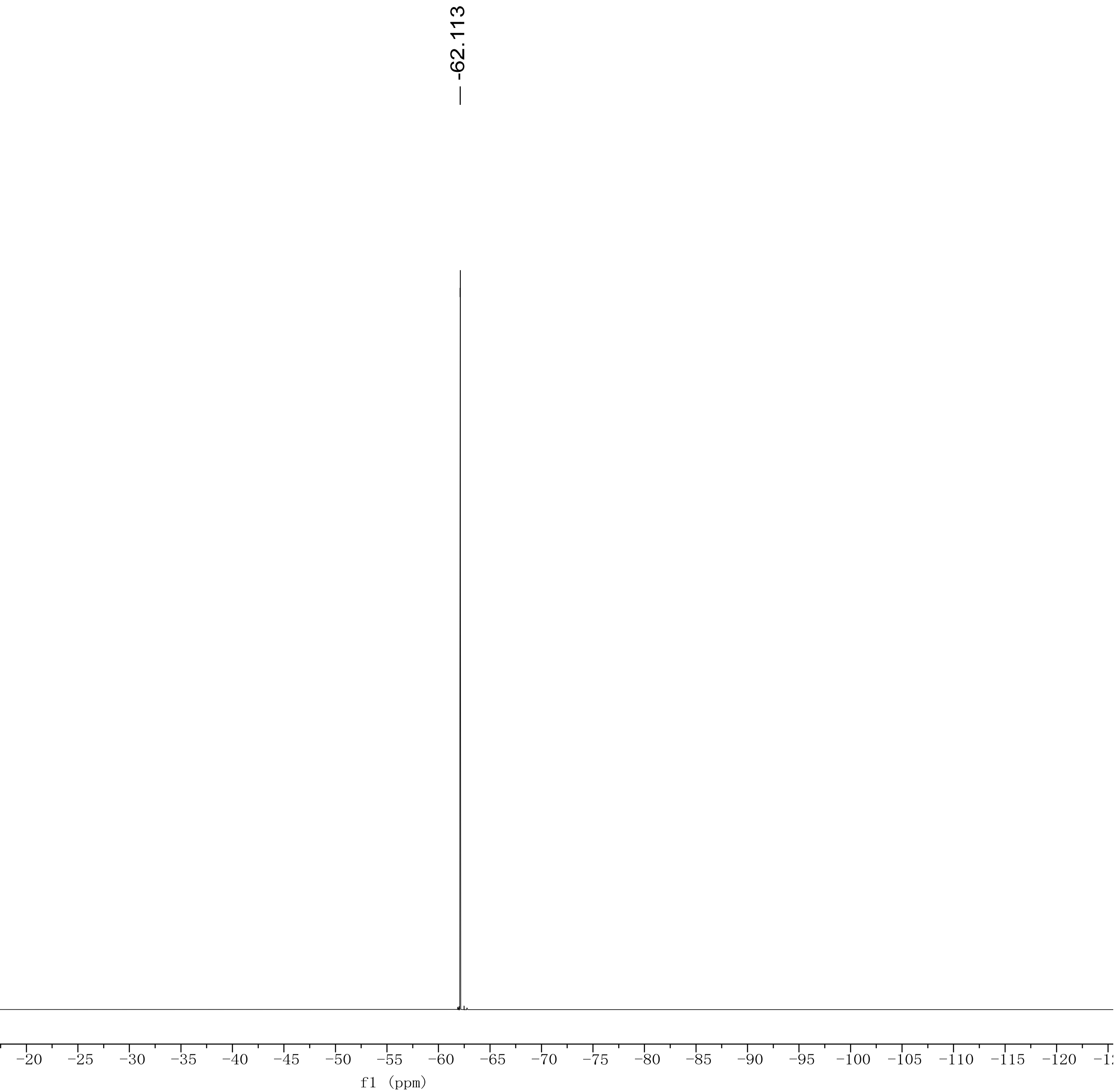


Fig. 2a, entry 14



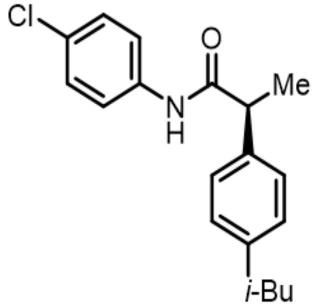
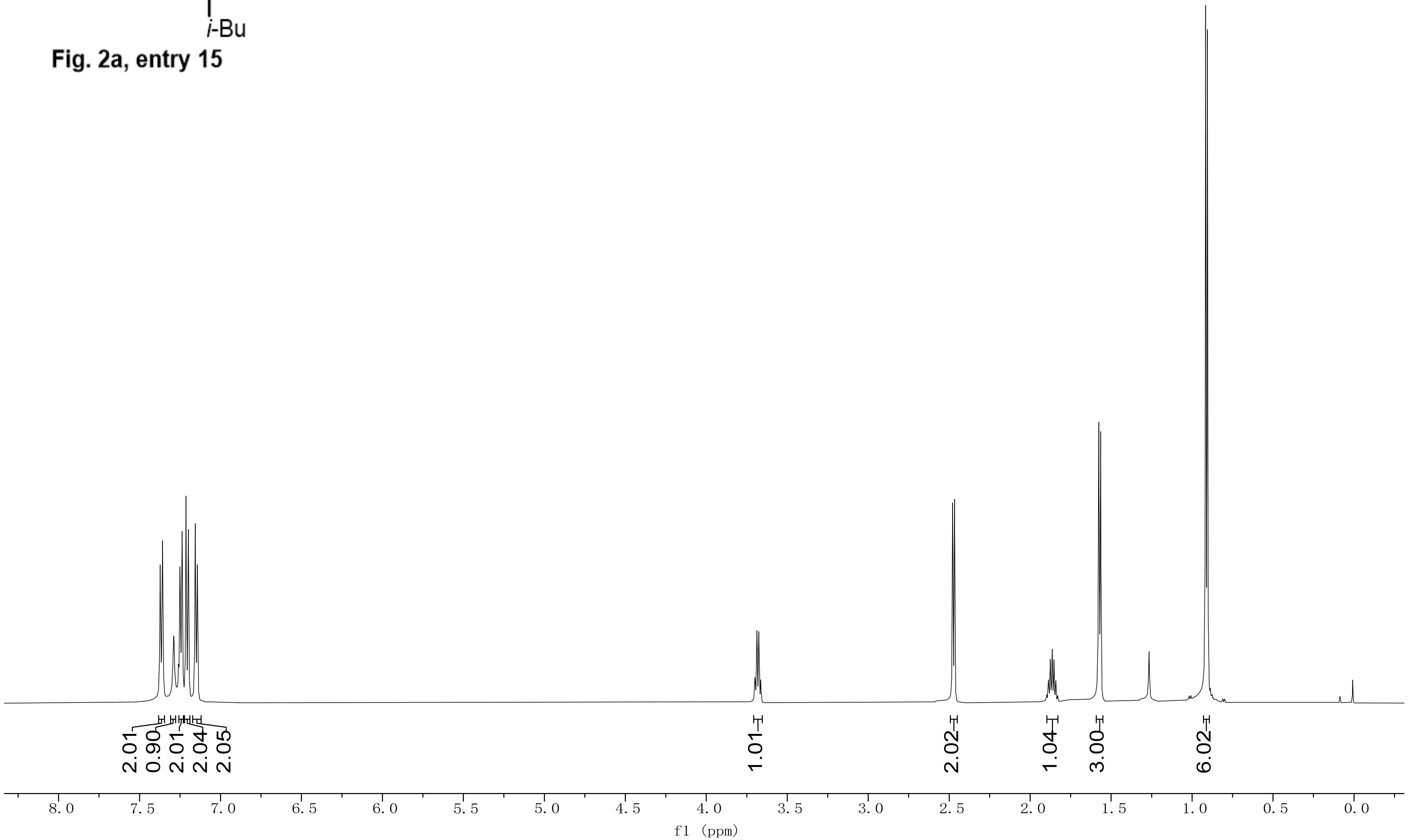
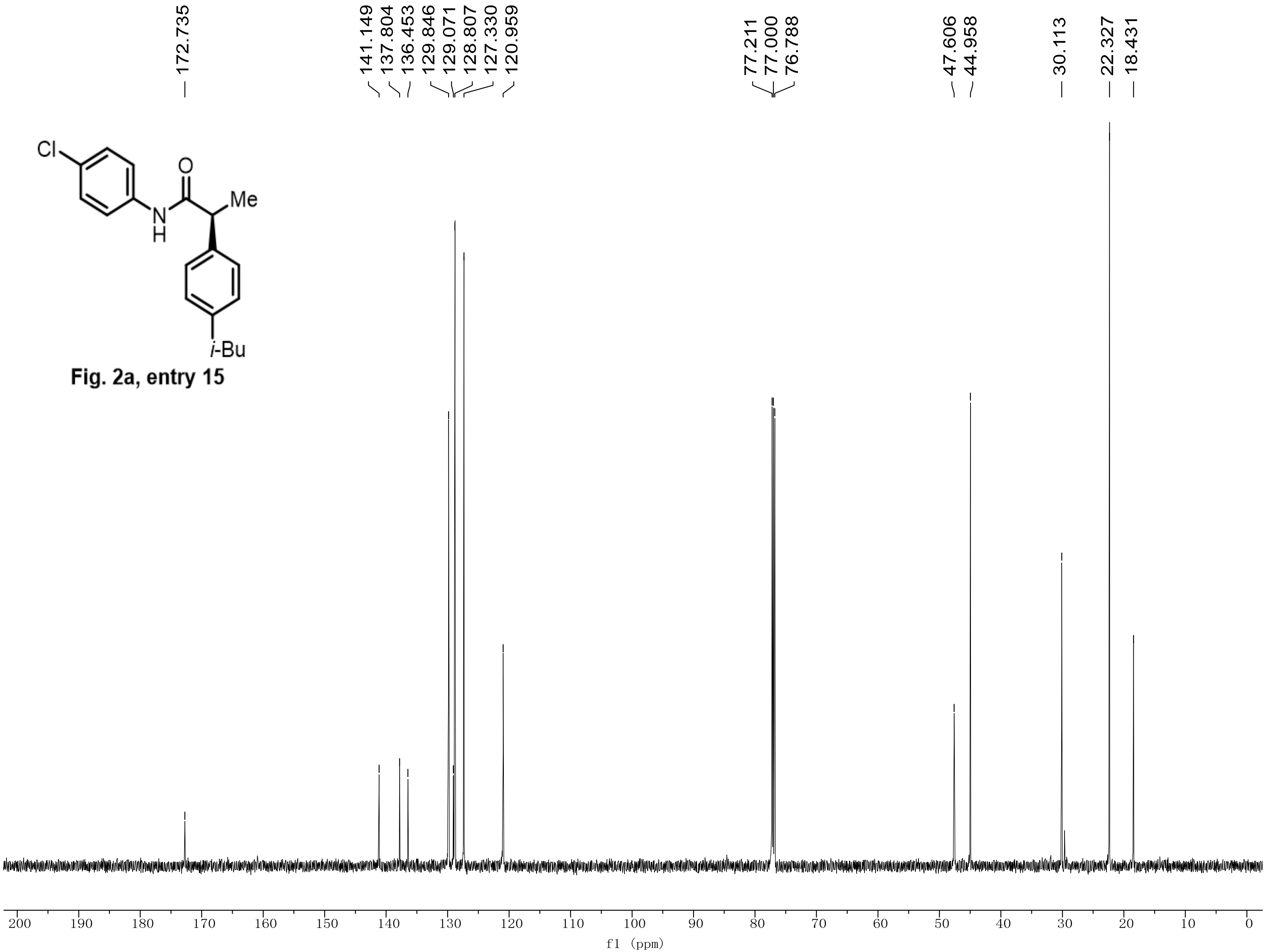


Fig. 2a, entry 15




Cl
O
Me
N
H
i-Bu
Fig. 2a, entry 15
172.735
141.149
137.804
136.453
129.846
129.071
128.807
127.330
120.959
77.211
77.000
76.788
47.606
44.958
30.113
22.327
18.431
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

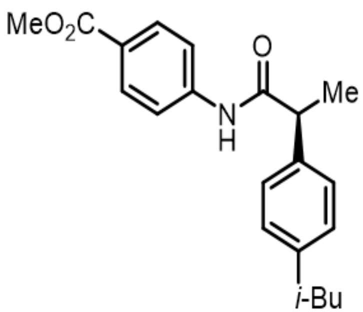
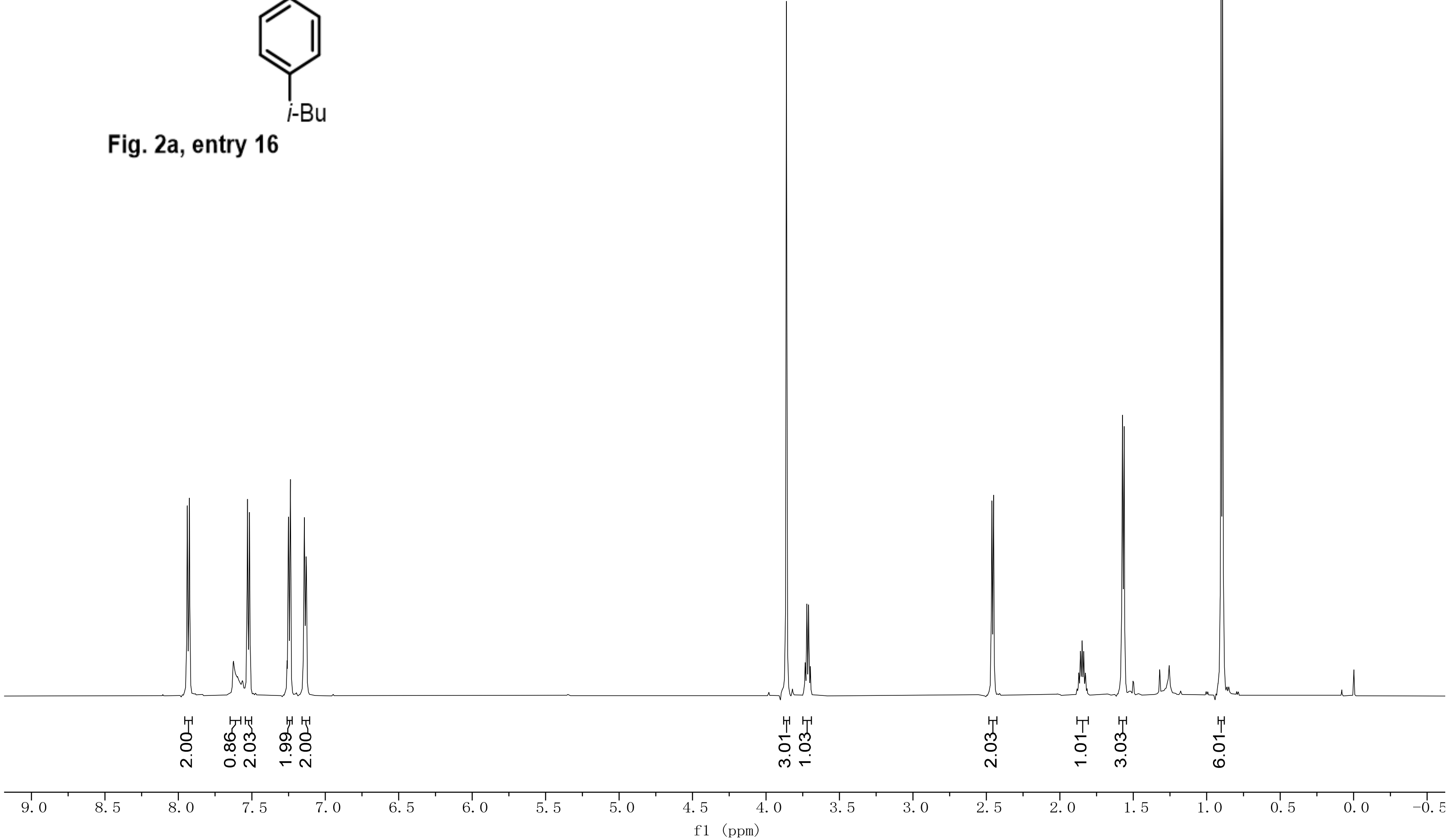


Fig. 2a, entry 16



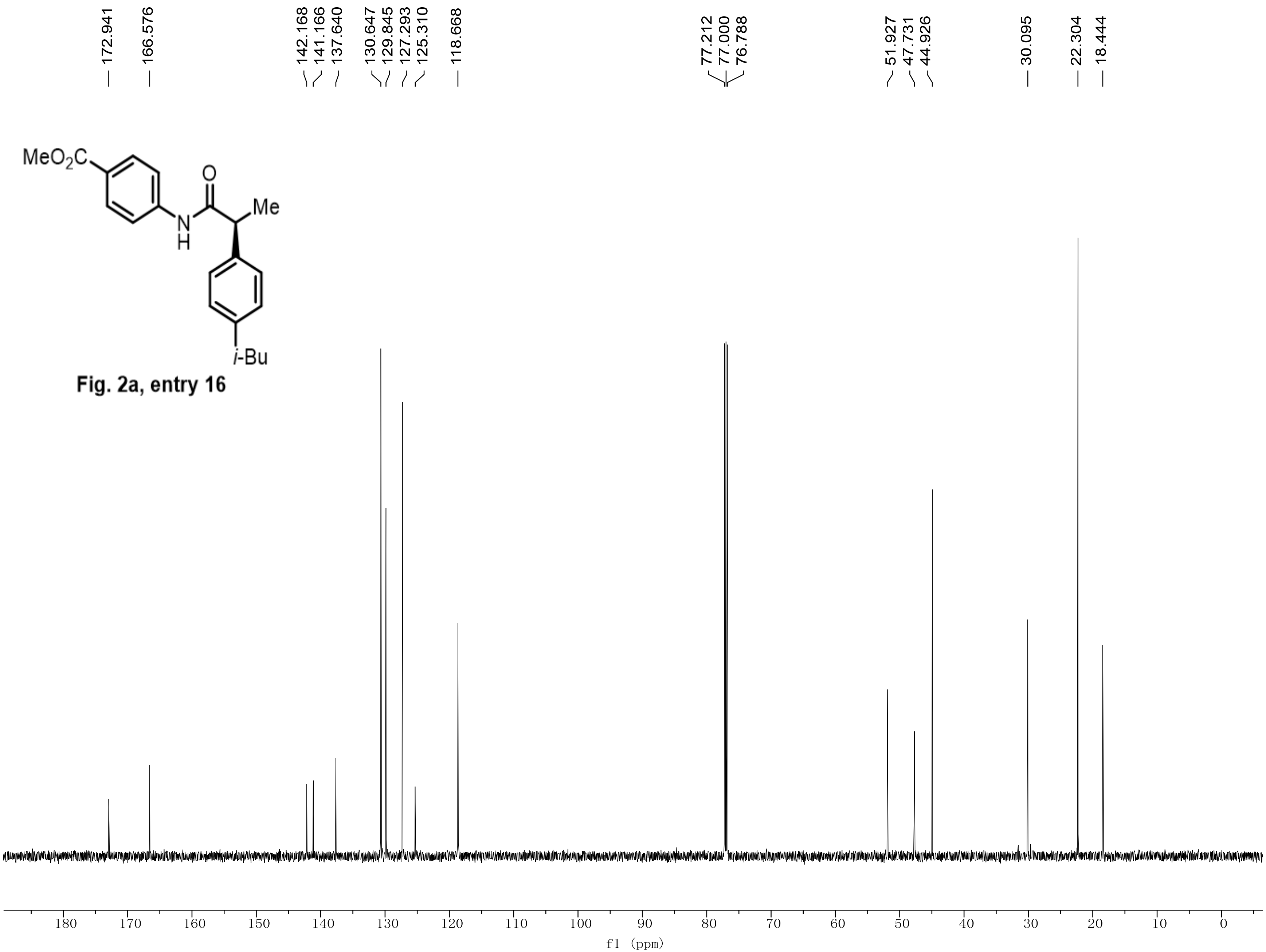


Fig. 2a, entry 16

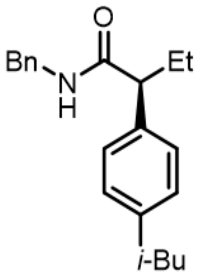
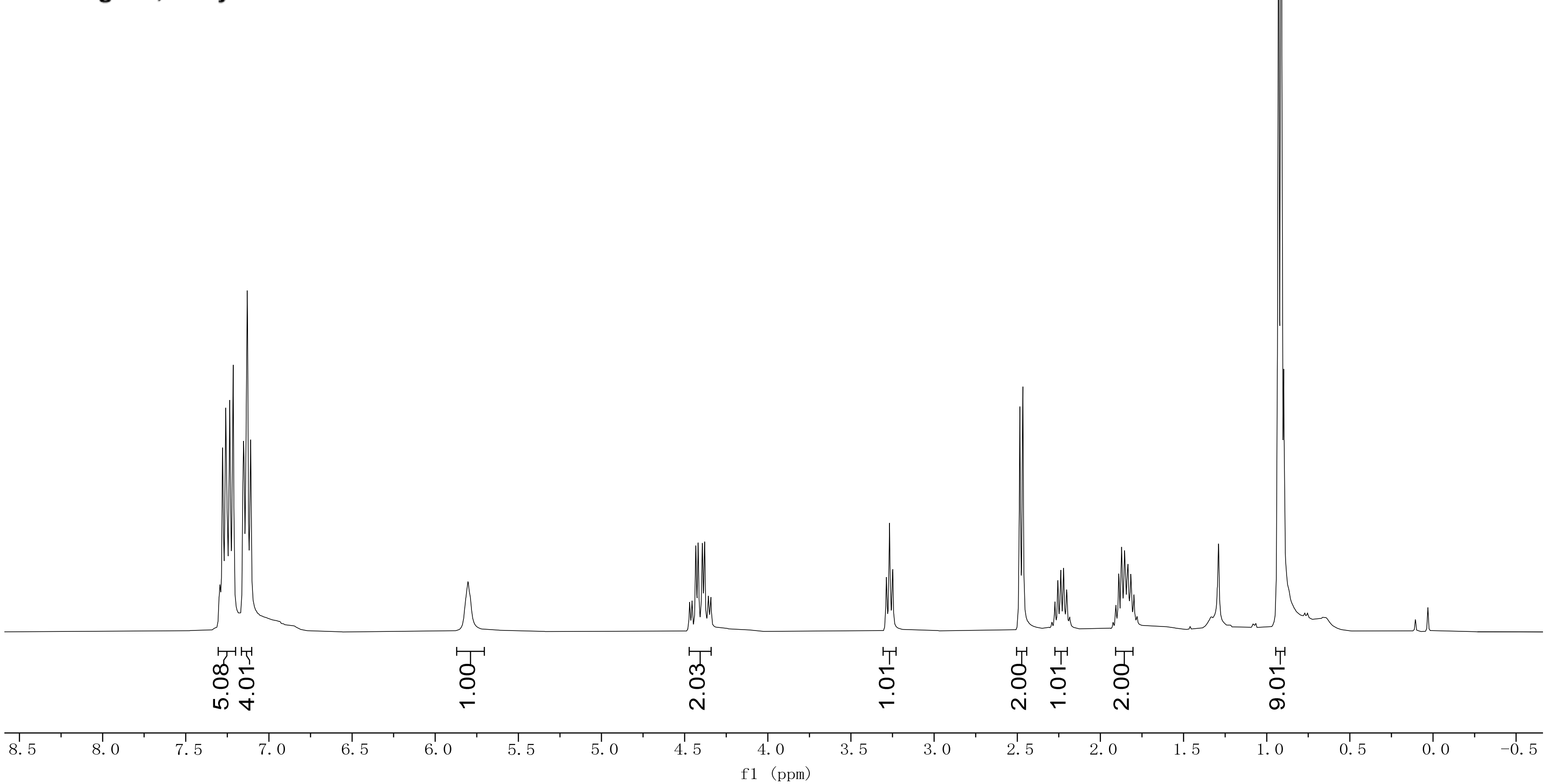


Fig. 2b, entry 17



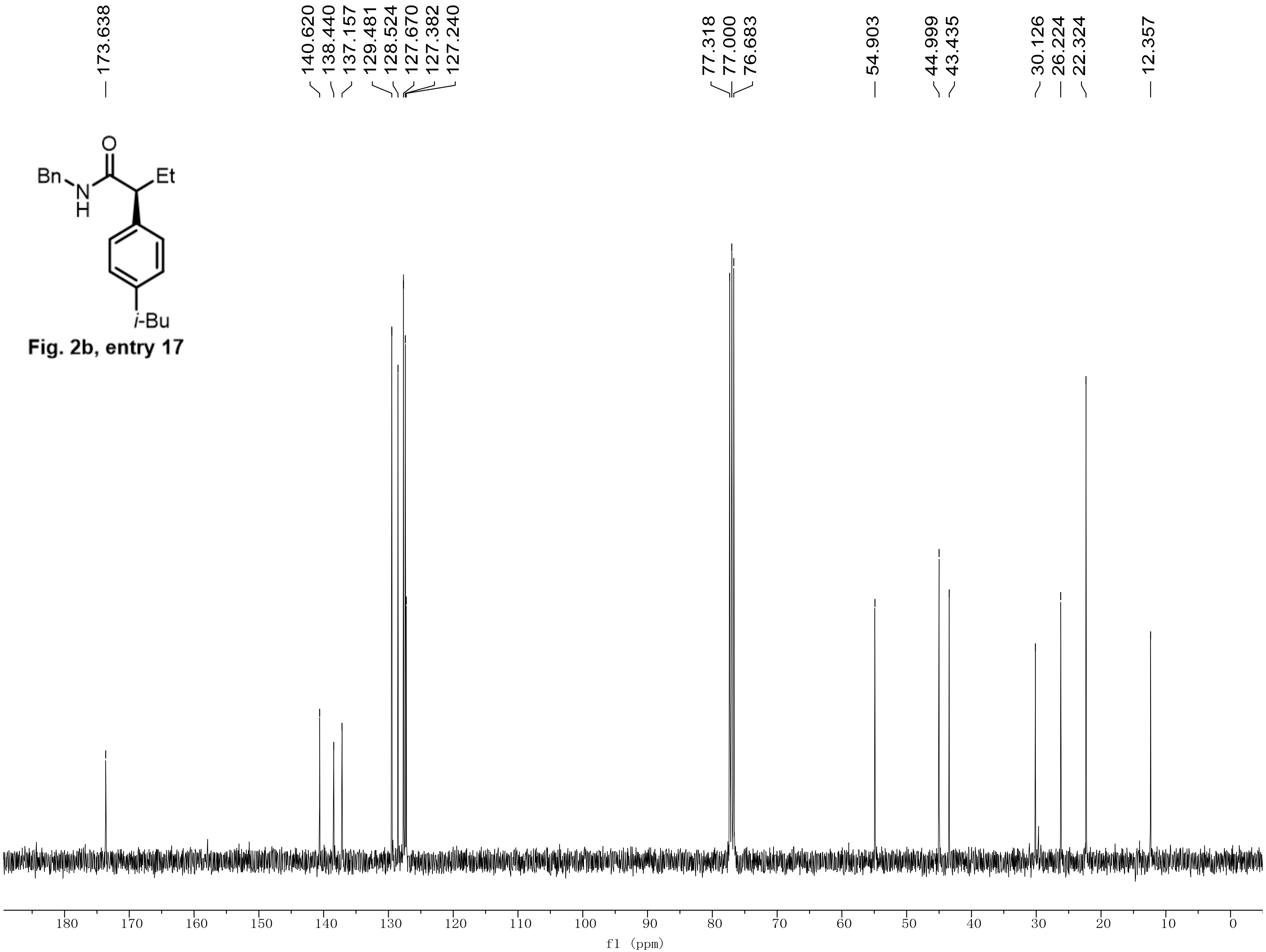


Fig. 2b, entry 17

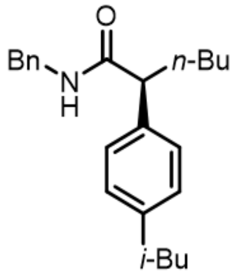
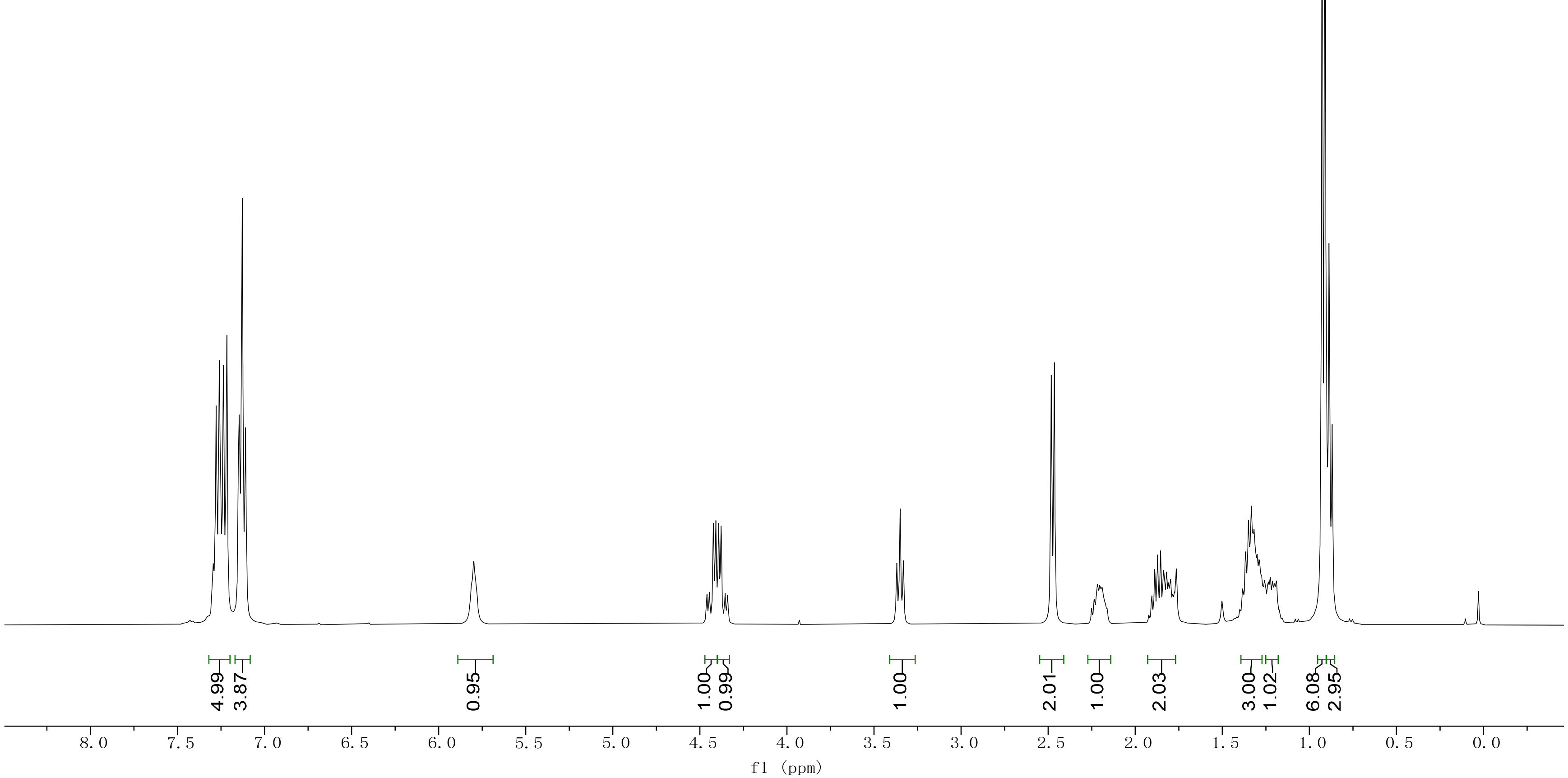
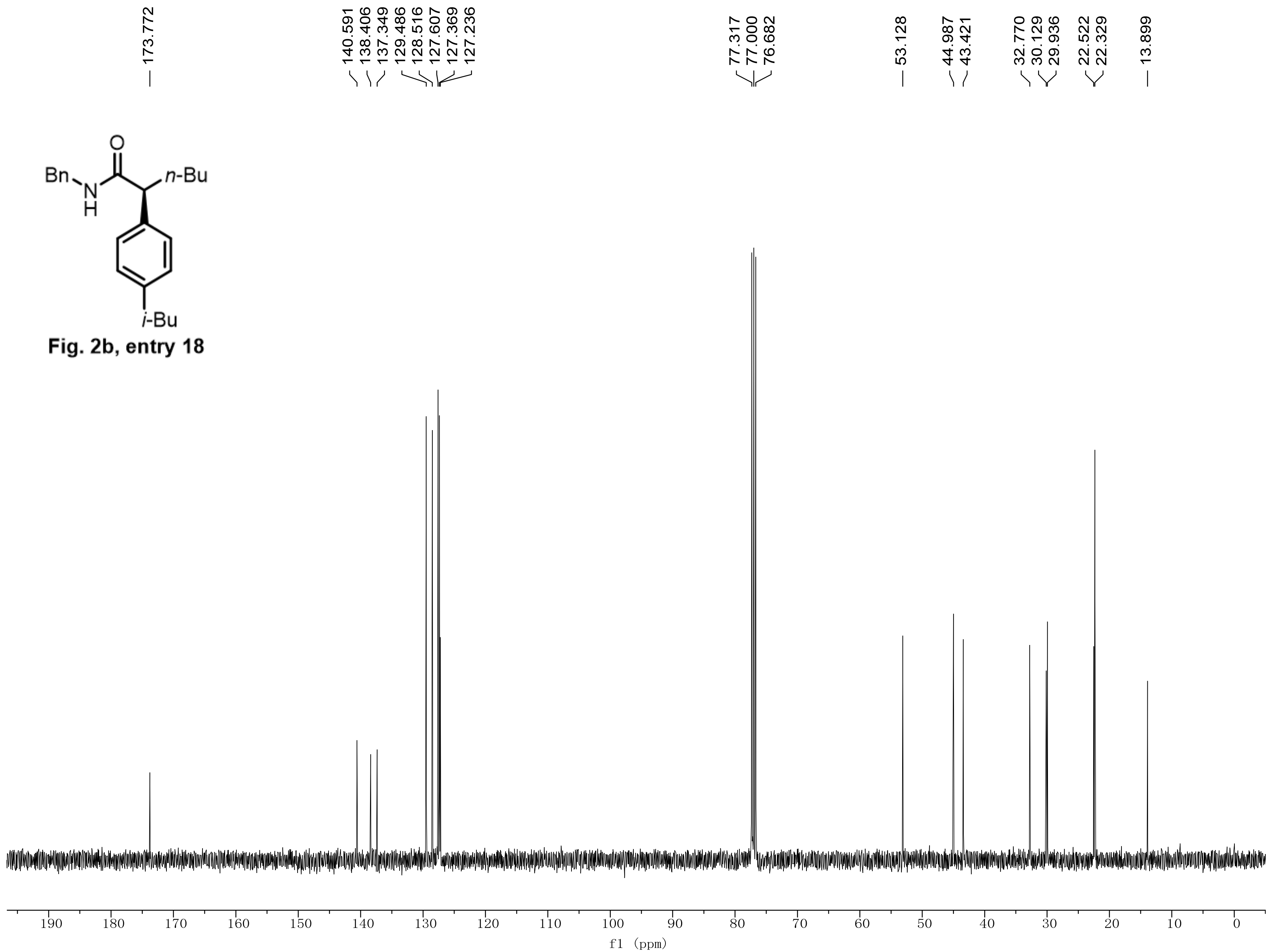


Fig. 2b, entry 18

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127.369
127.236
77.317
77.000
76.682
53.128
44.987
43.421
32.770
30.129
29.936
22.522
22.329
13.899
O
Bn
N
H
n-Bu
i-Bu
Fig. 2b, entry 18
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

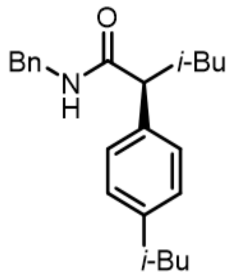
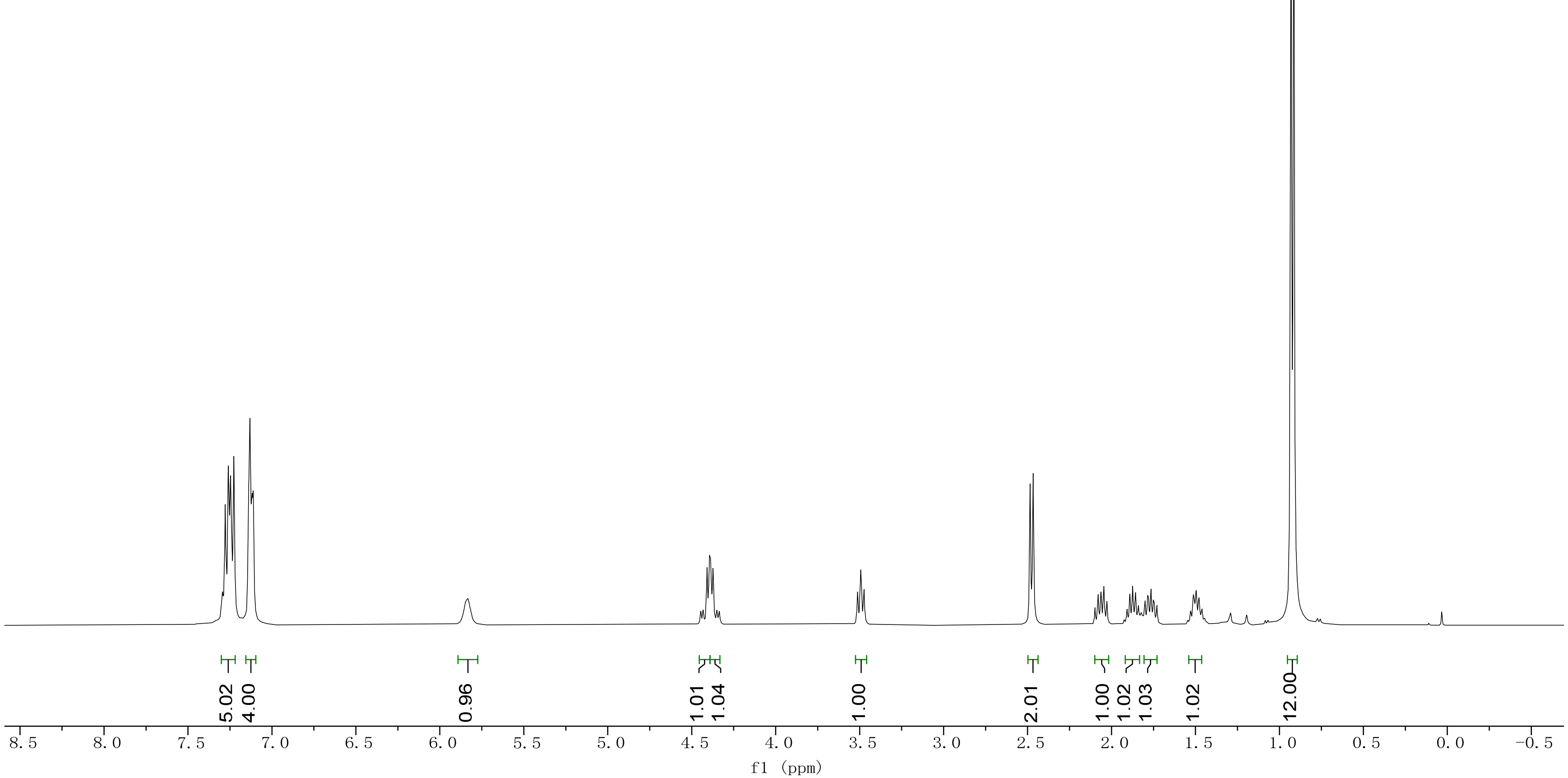


Fig. 2b, entry 19



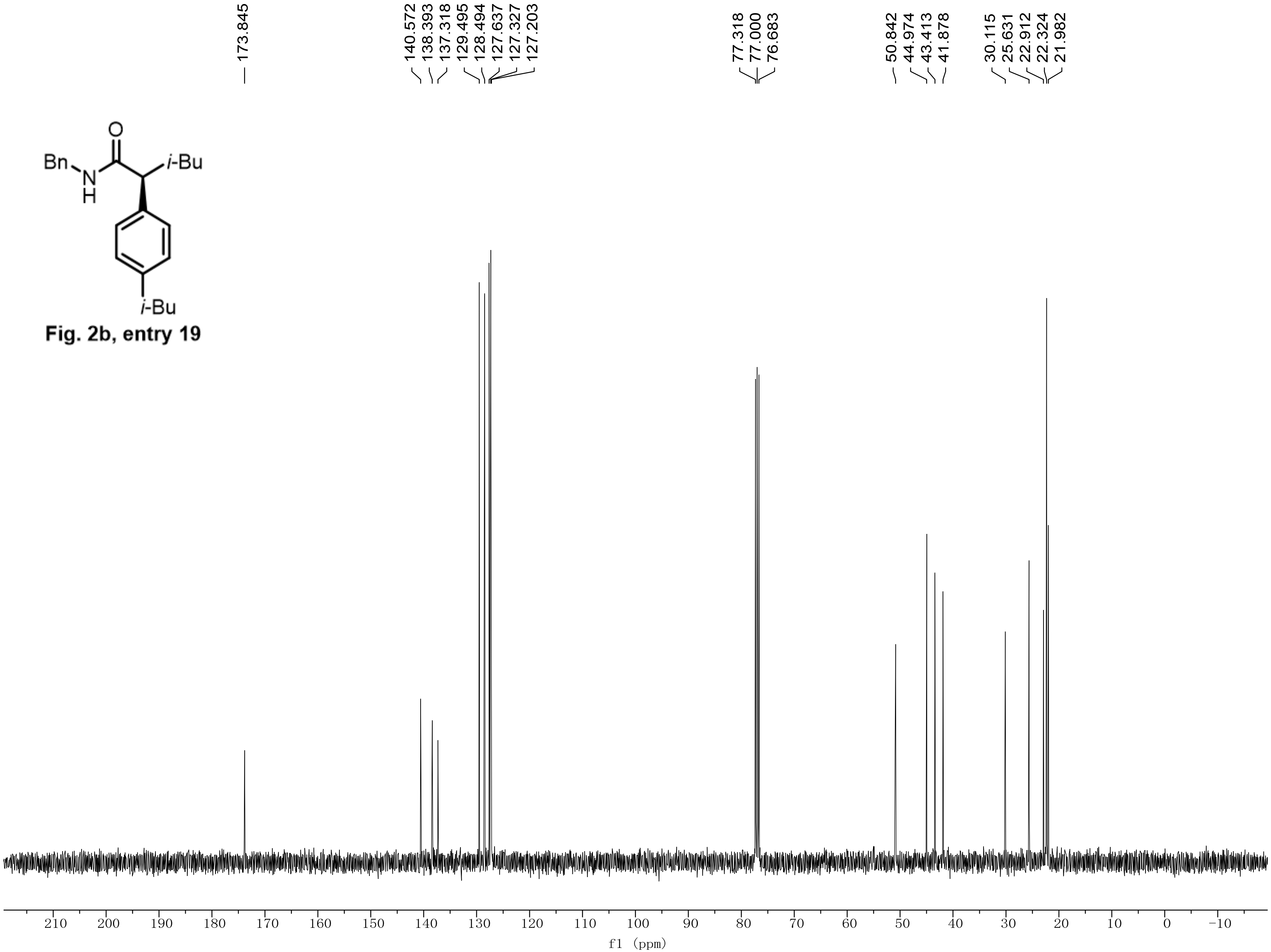


Fig. 2b, entry 19

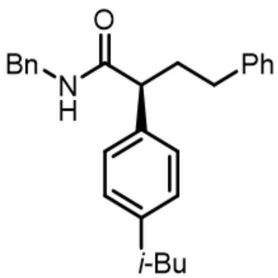
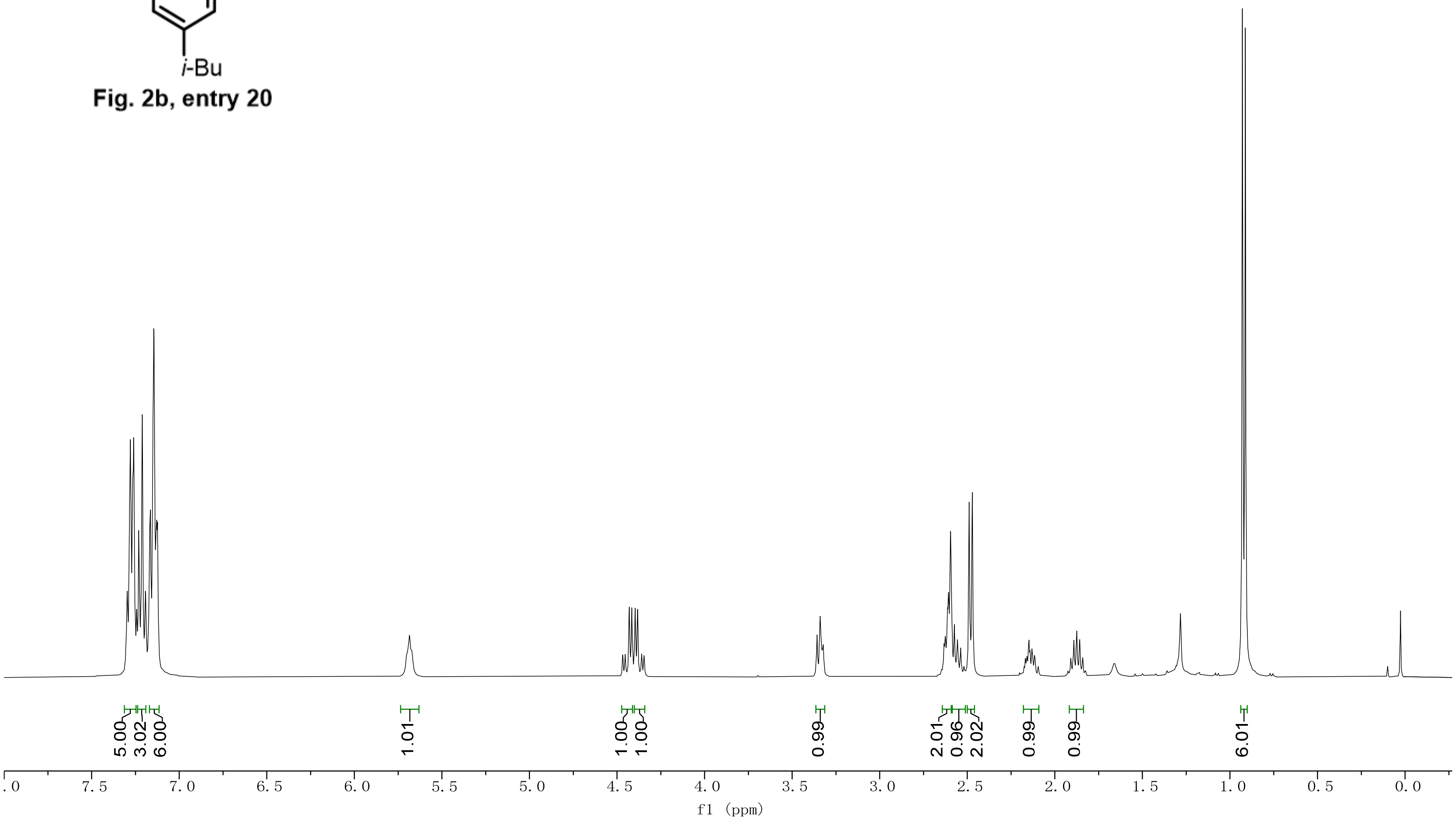


Fig. 2b, entry 20



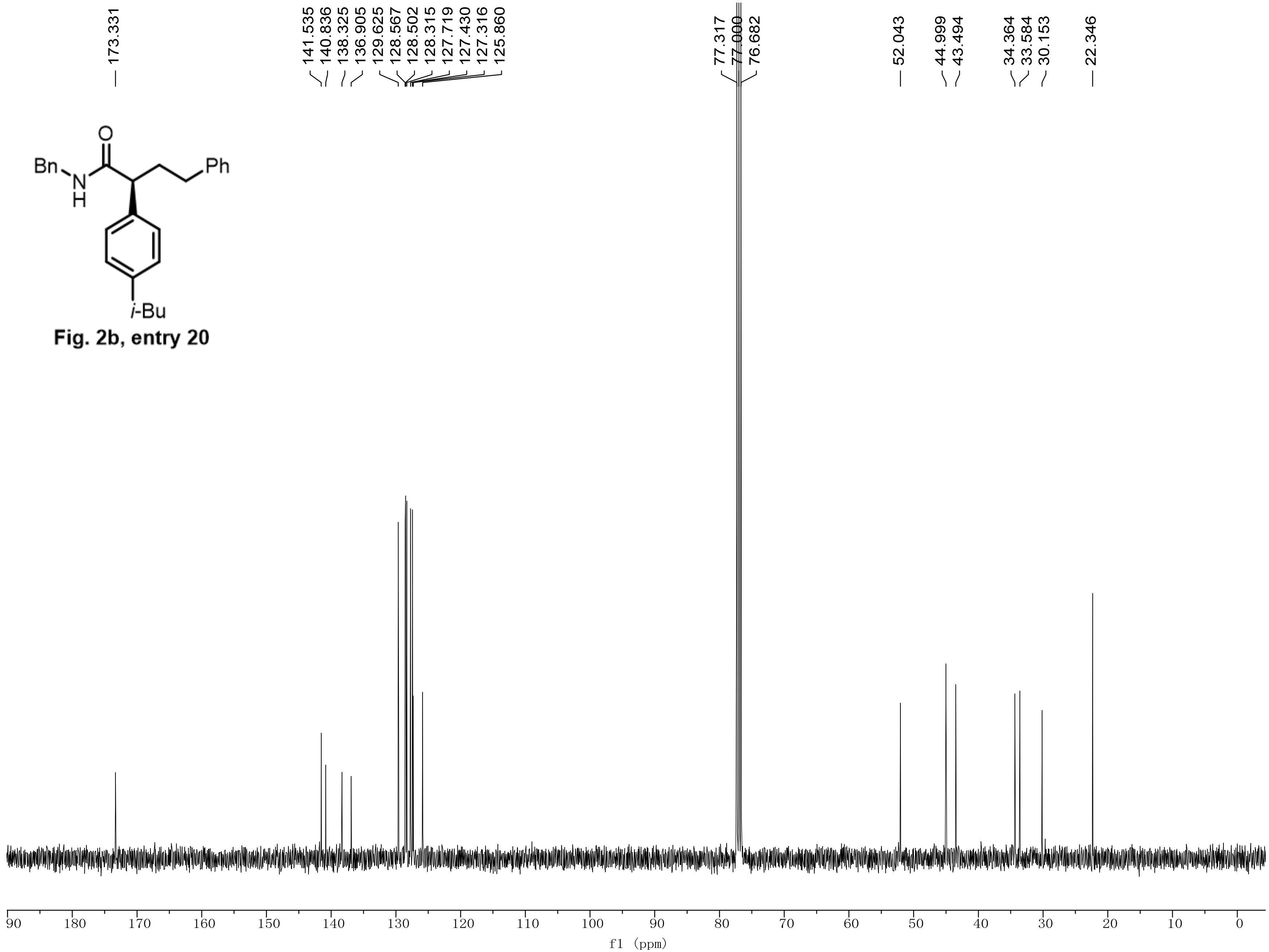


Fig. 2b, entry 20

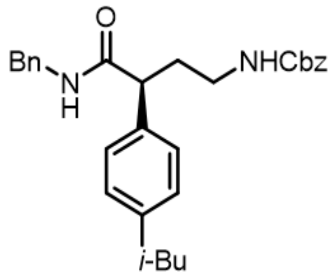
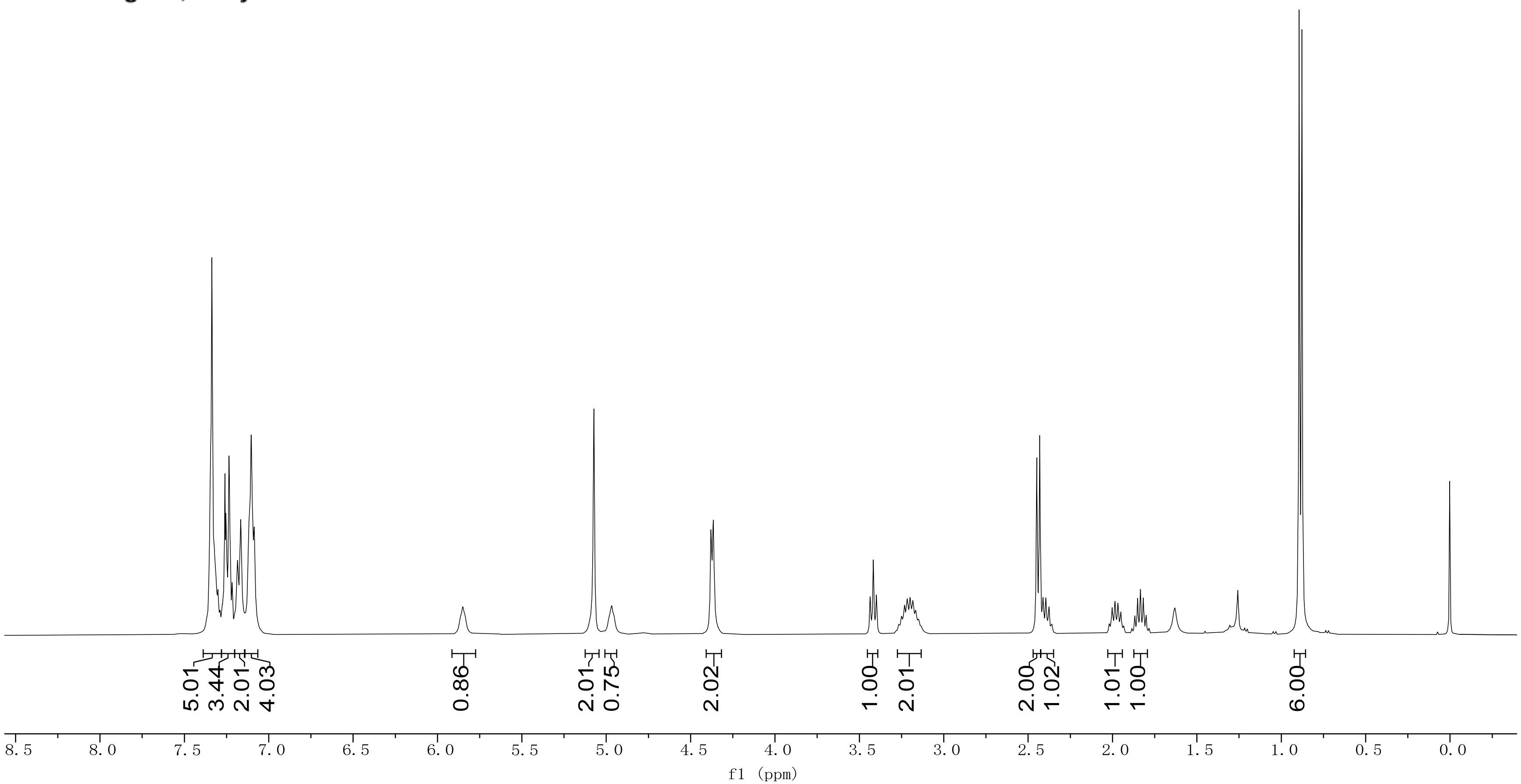


Fig. 2b, entry 21



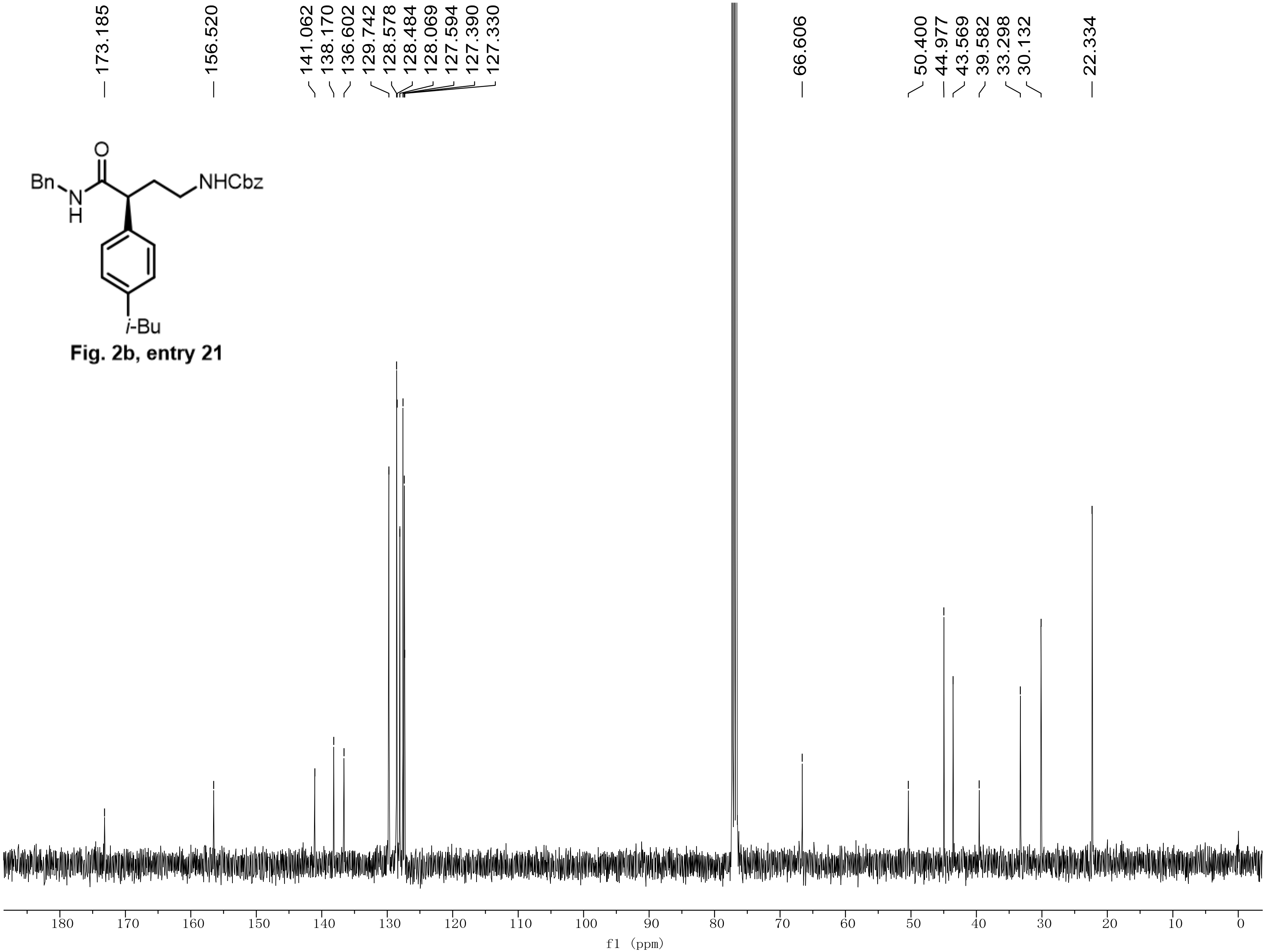


Fig. 2b, entry 21

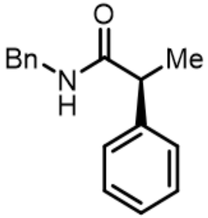
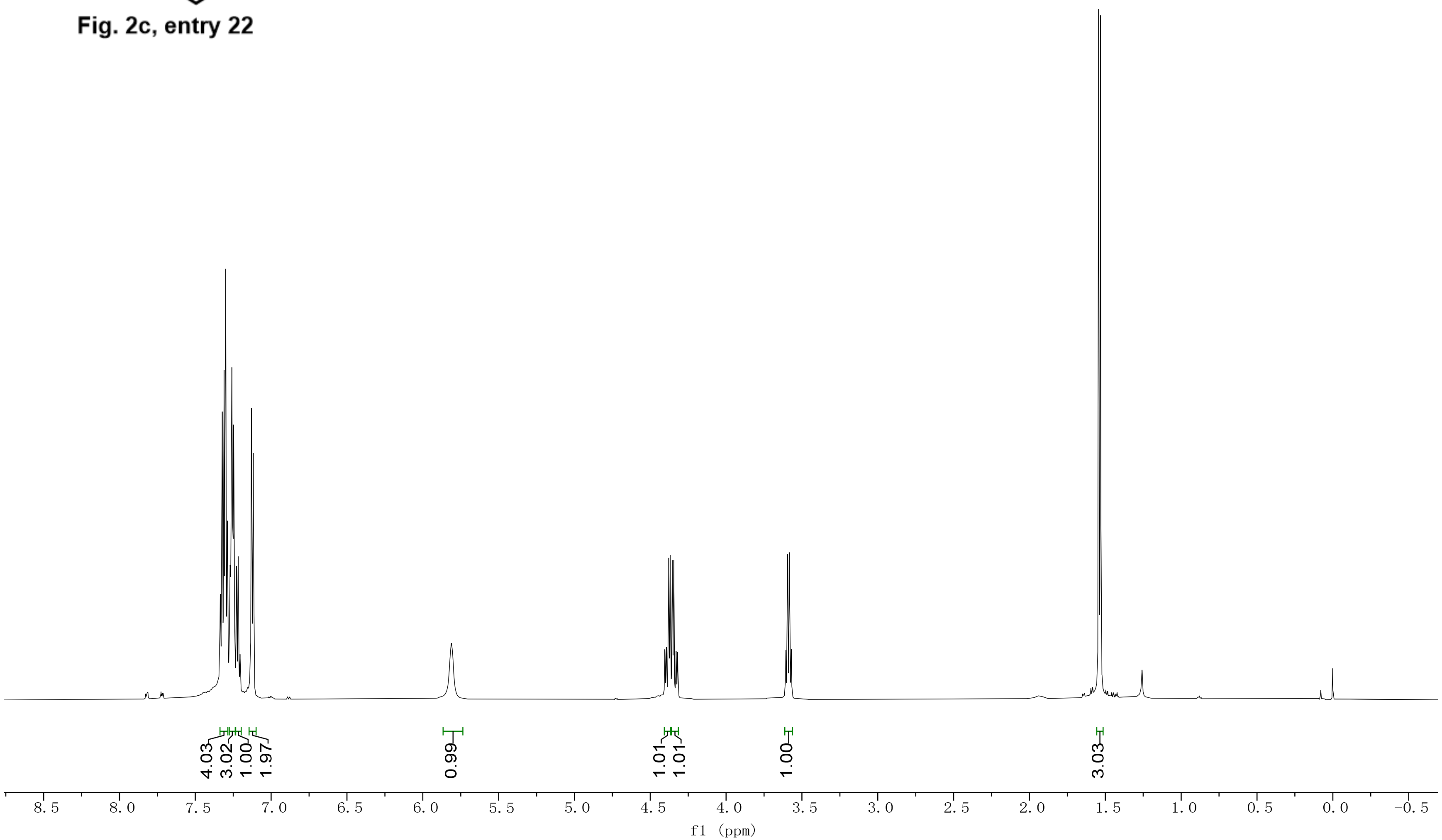


Fig. 2c, entry 22



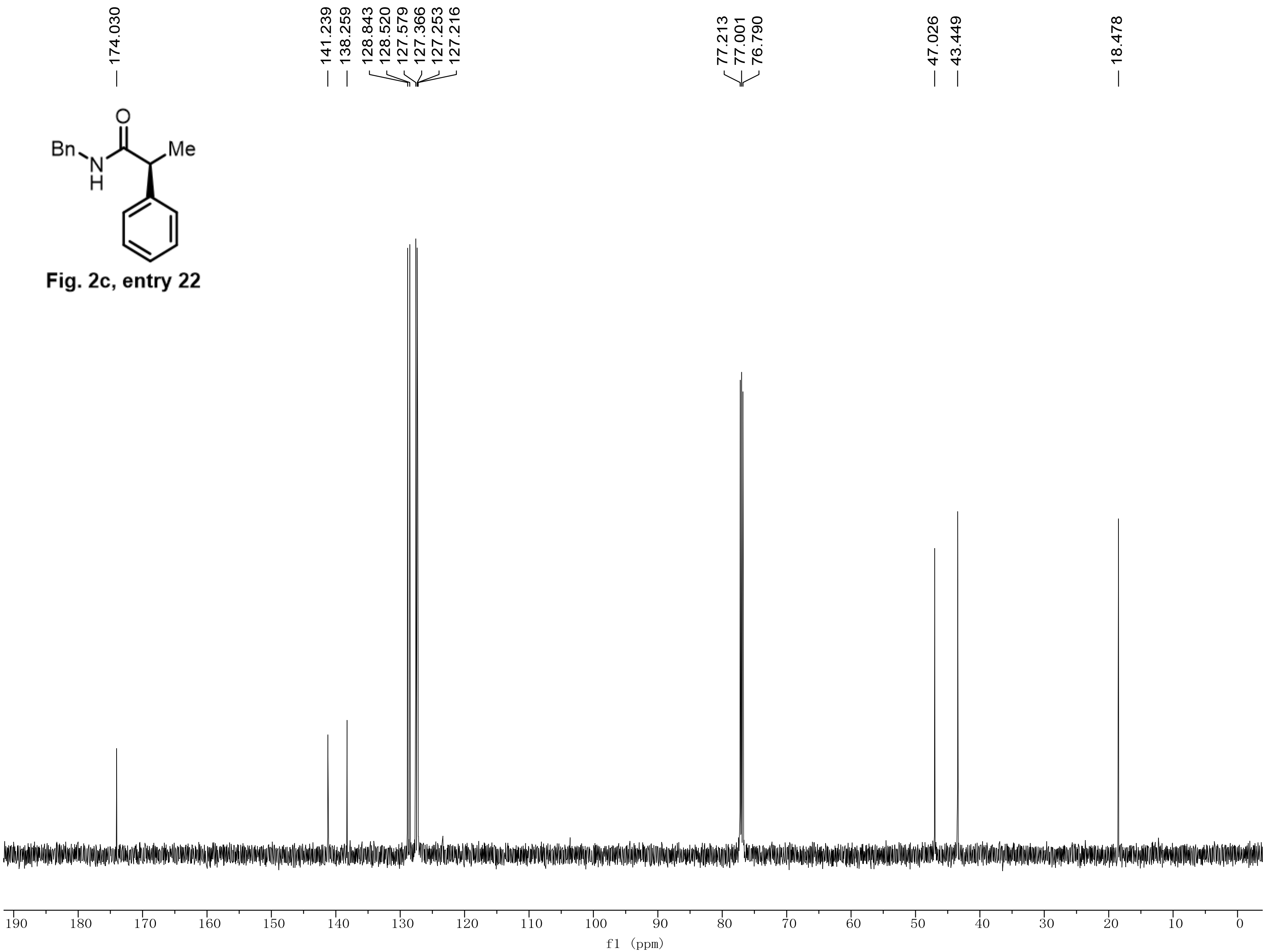


Fig. 2c, entry 22

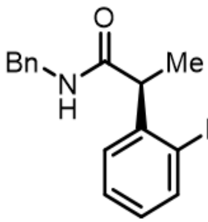
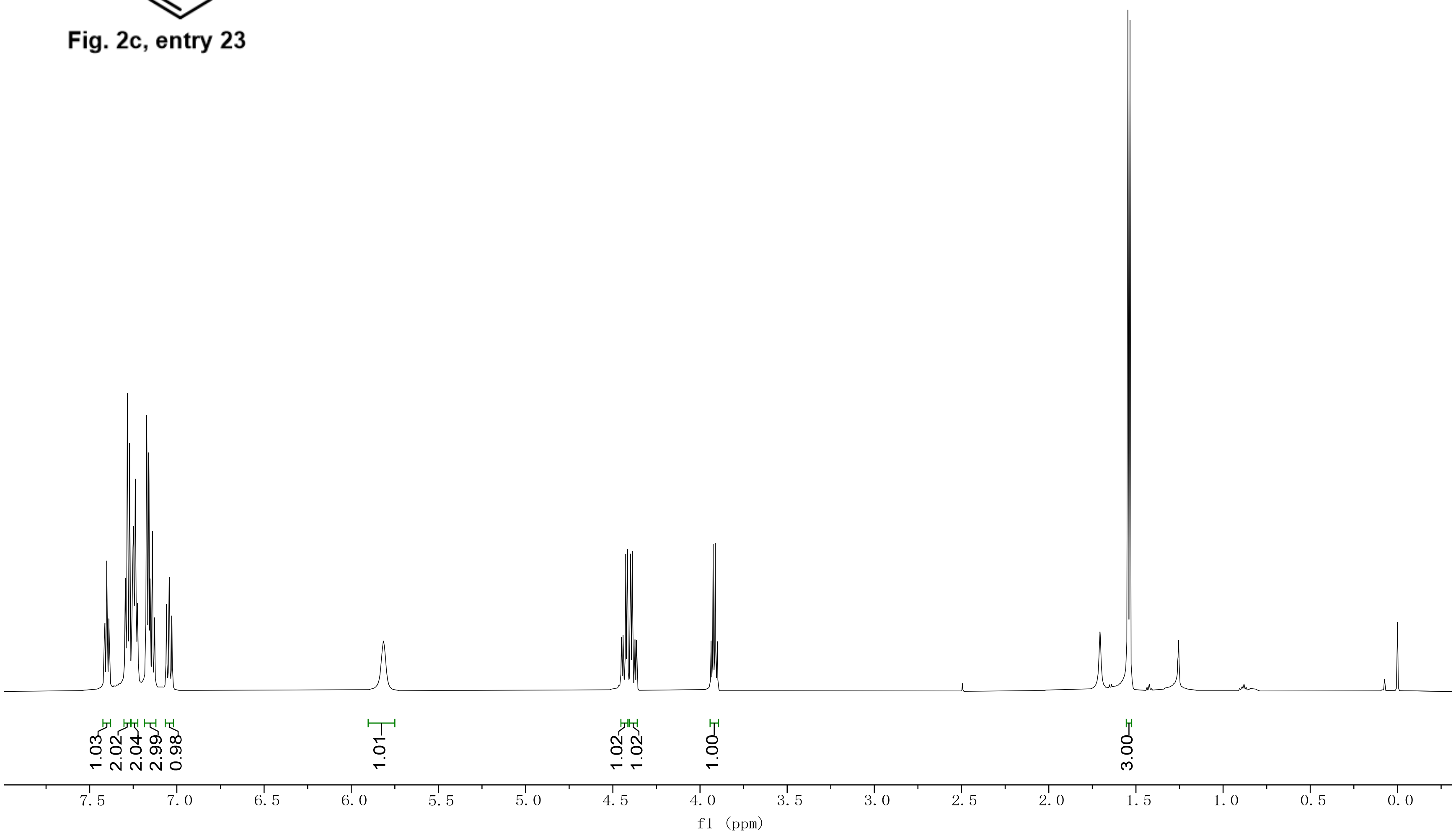


Fig. 2c, entry 23



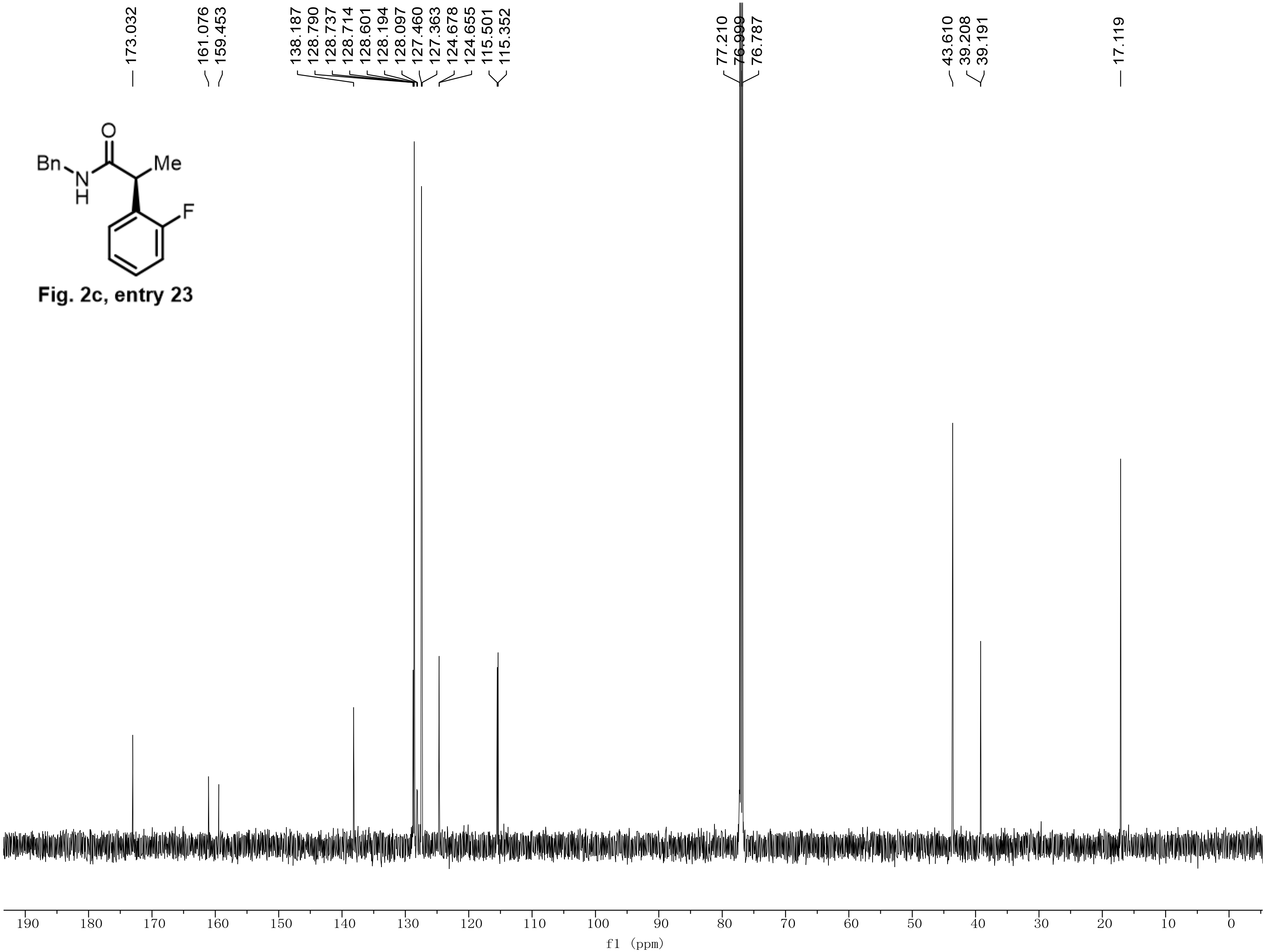


Fig. 2c, entry 23

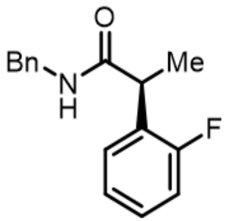
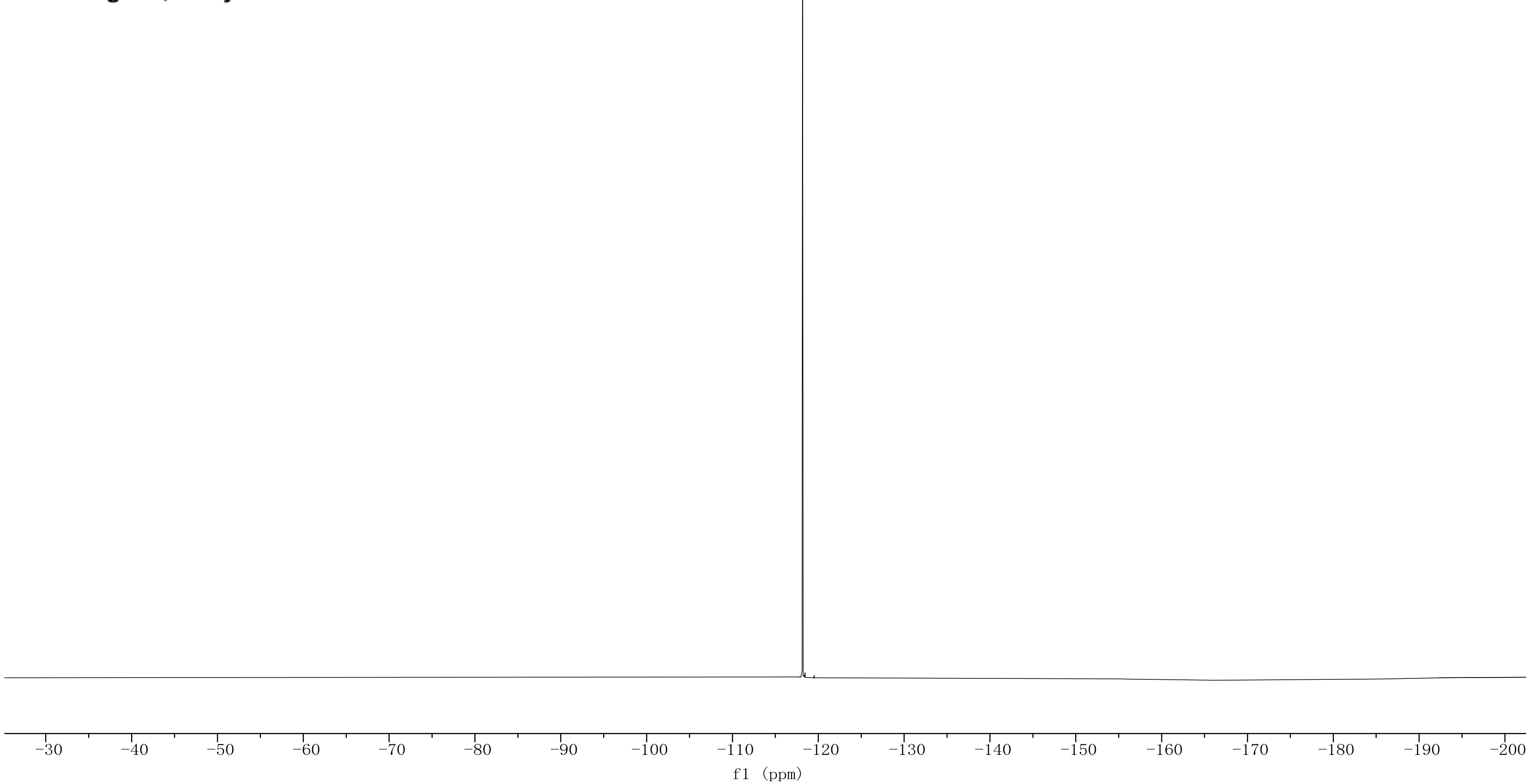


Fig. 2c, entry 23



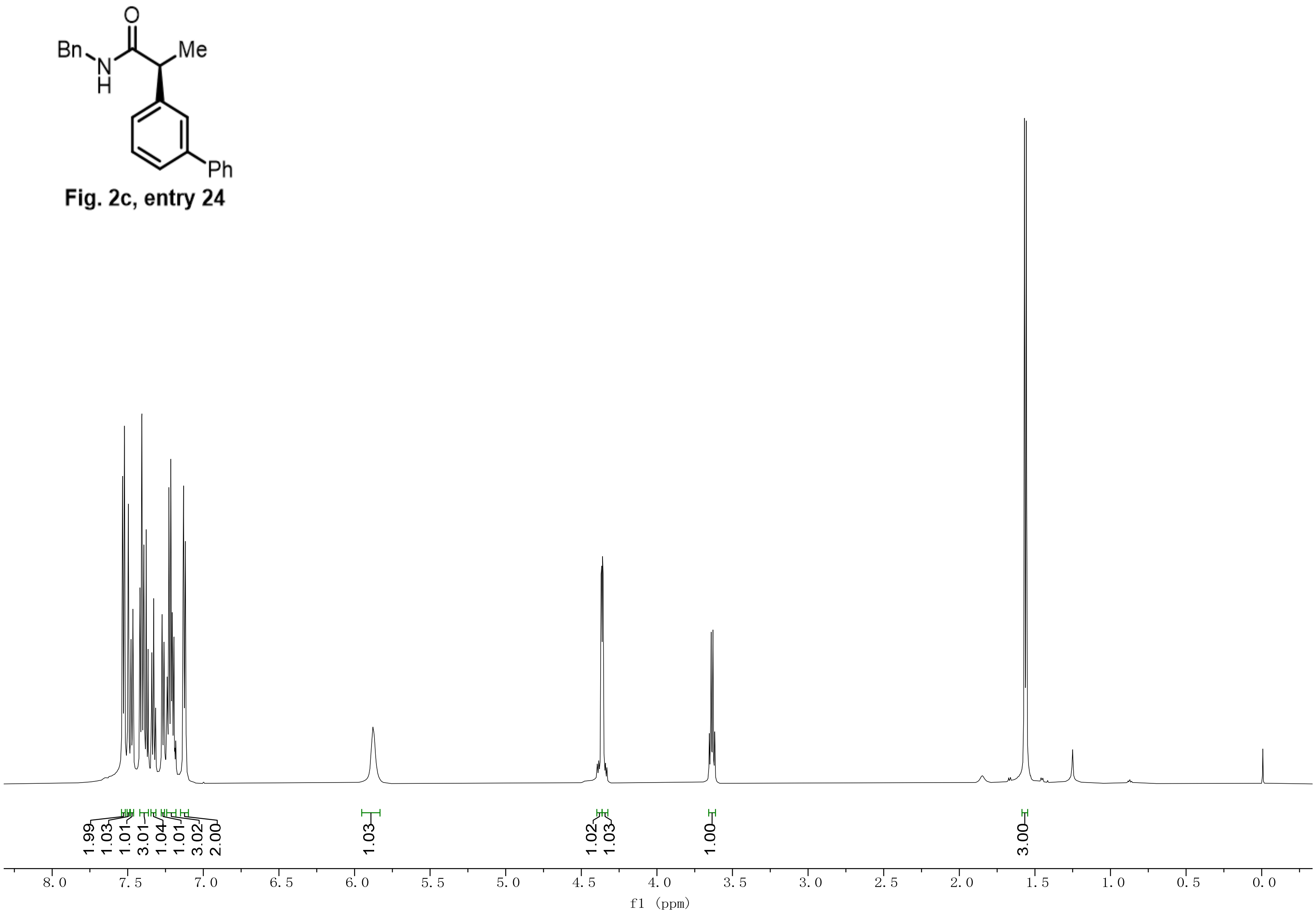


Fig. 2c, entry 24

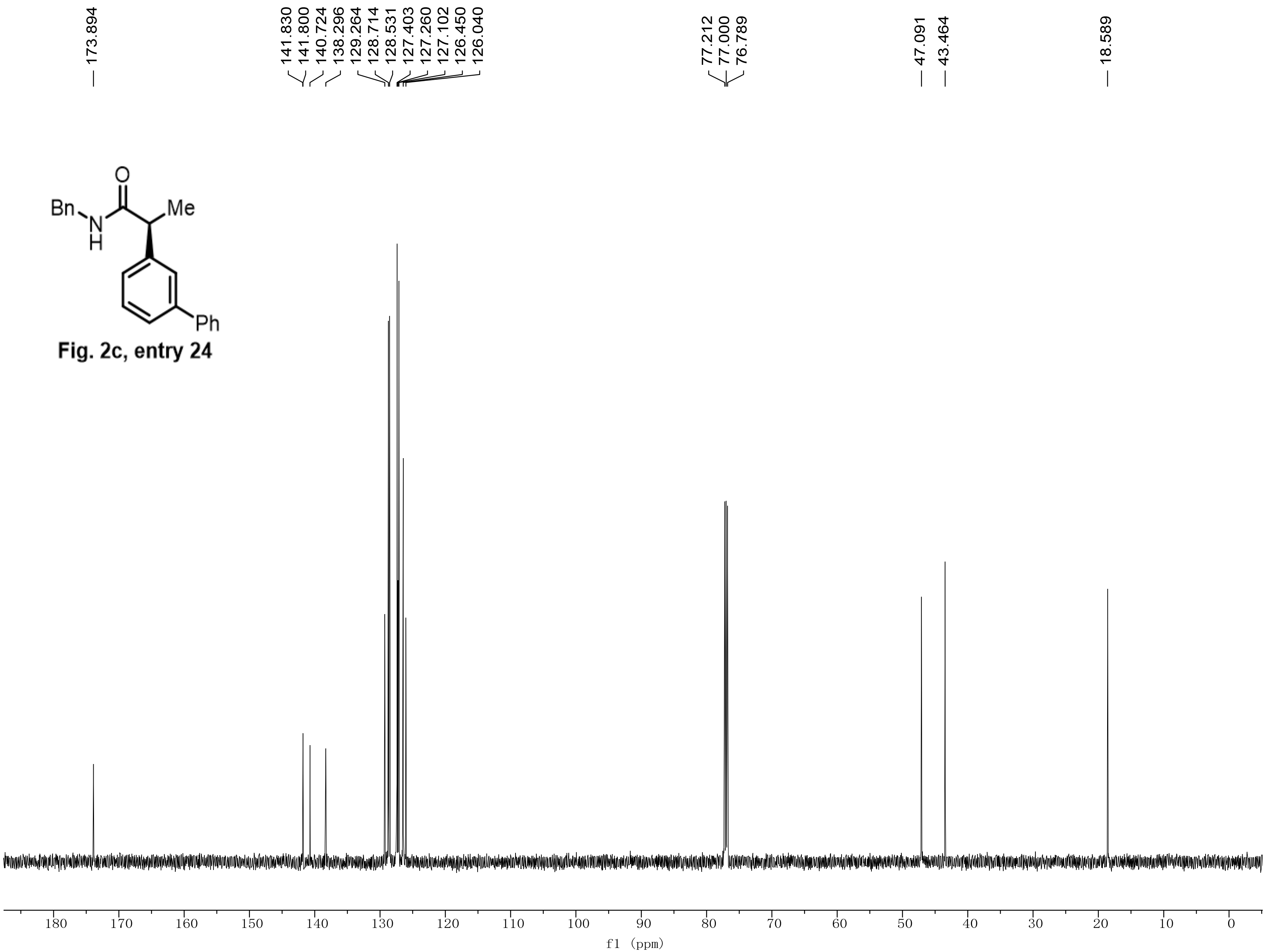


Fig. 2c, entry 24

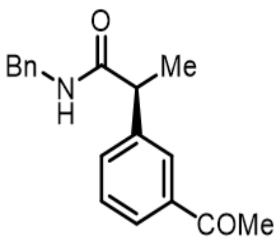
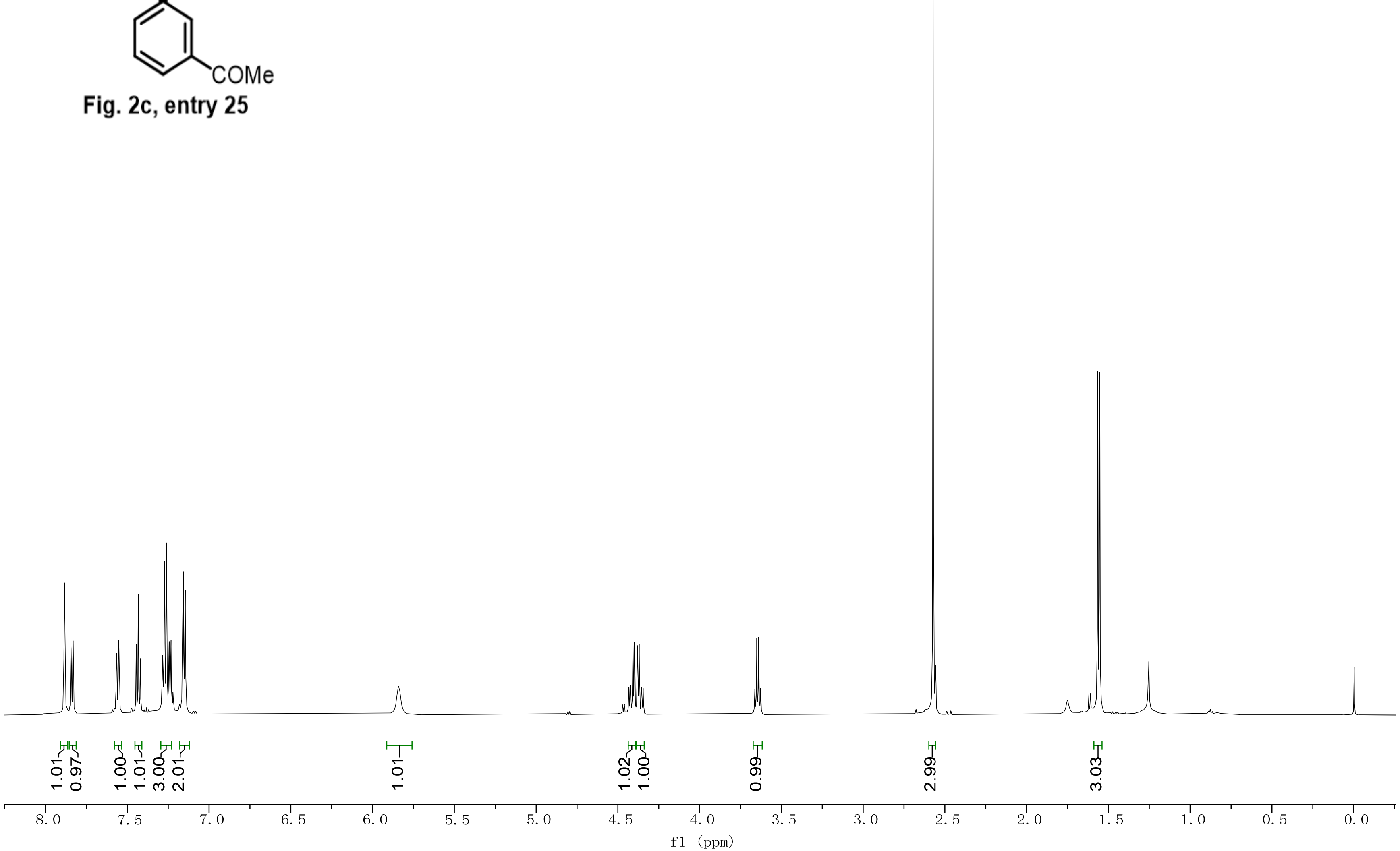


Fig. 2c, entry 25



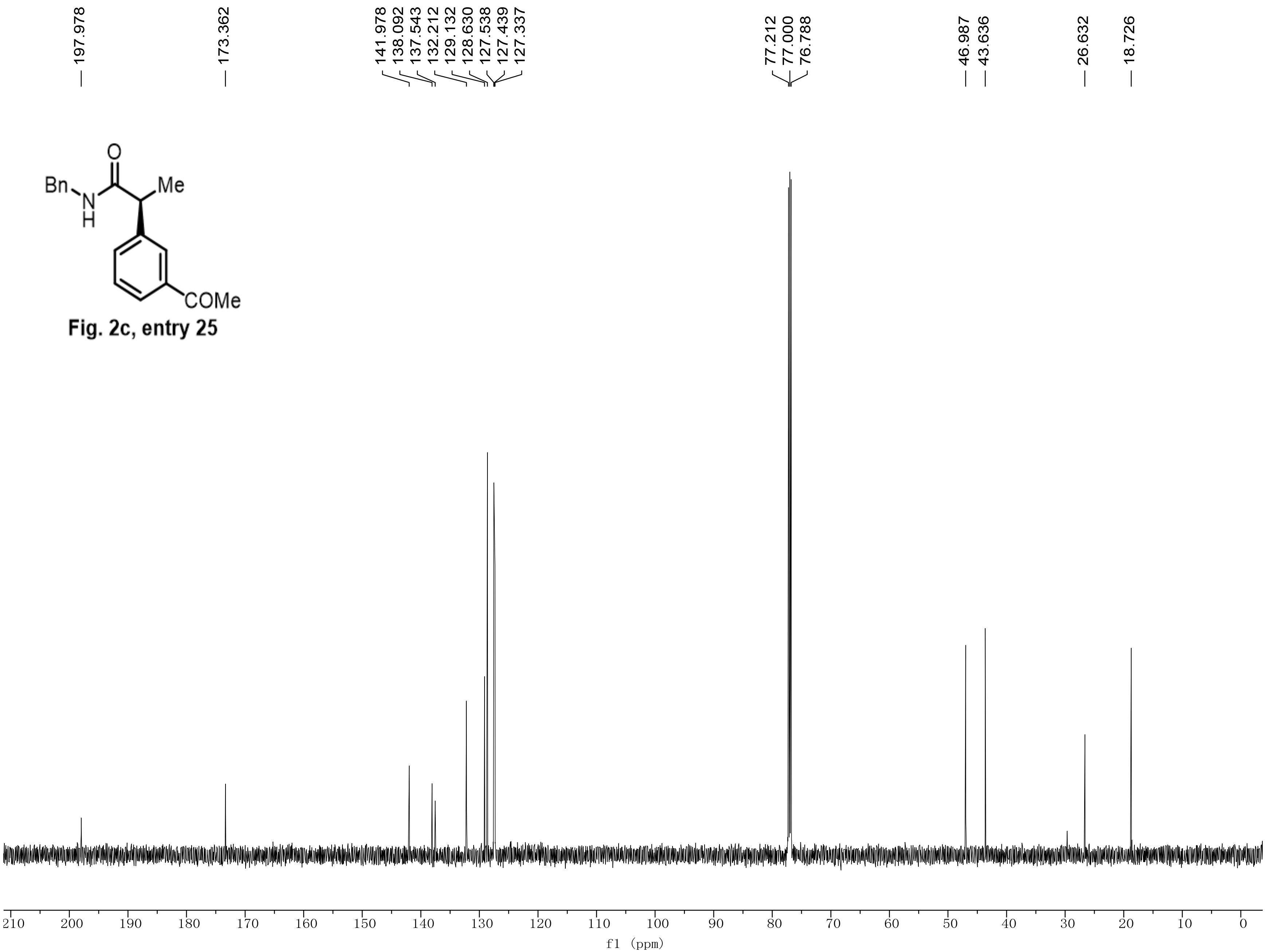


Fig. 2c, entry 25

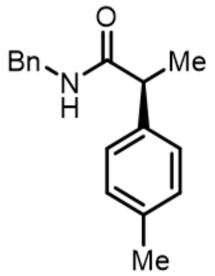
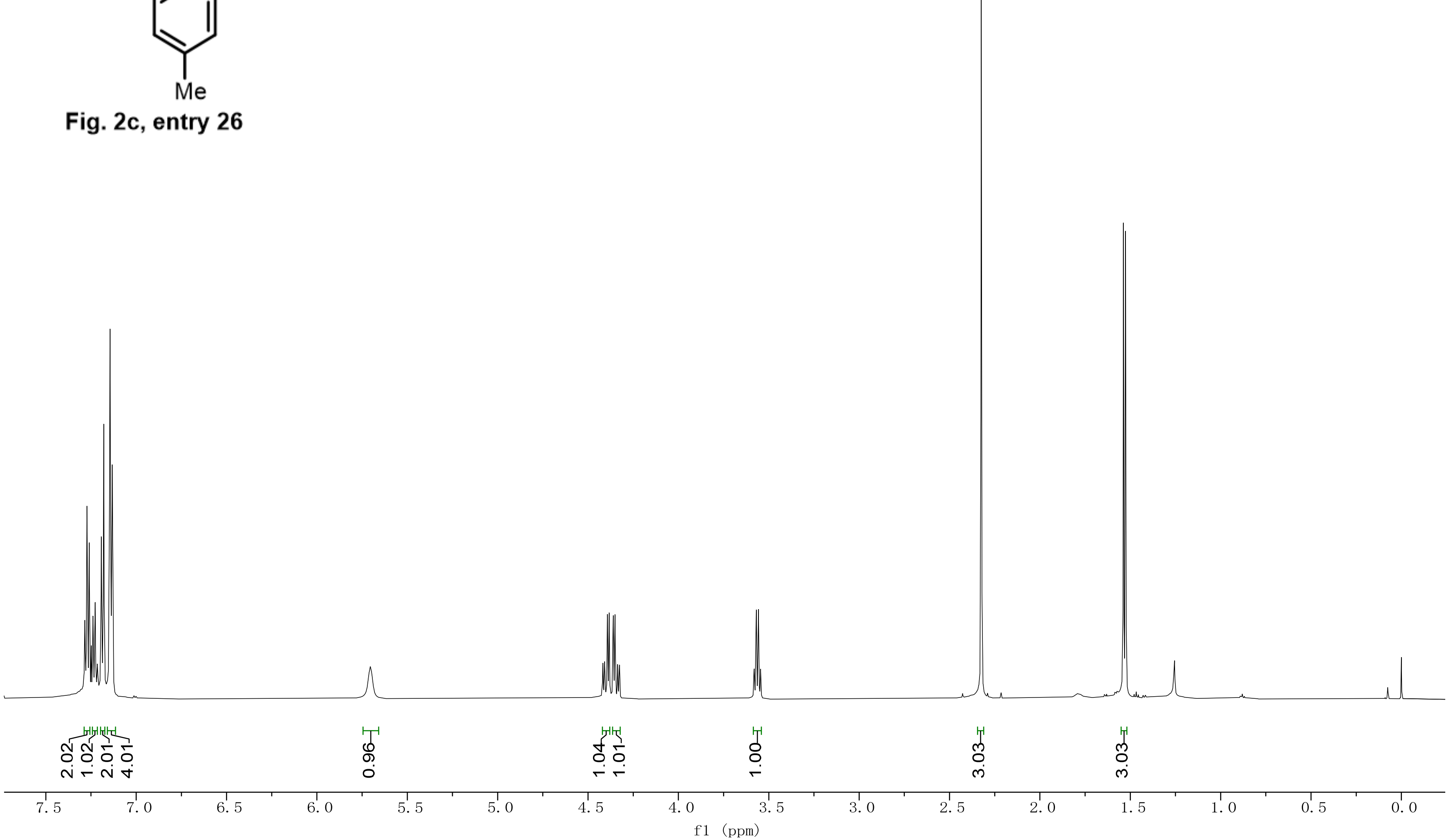


Fig. 2c, entry 26



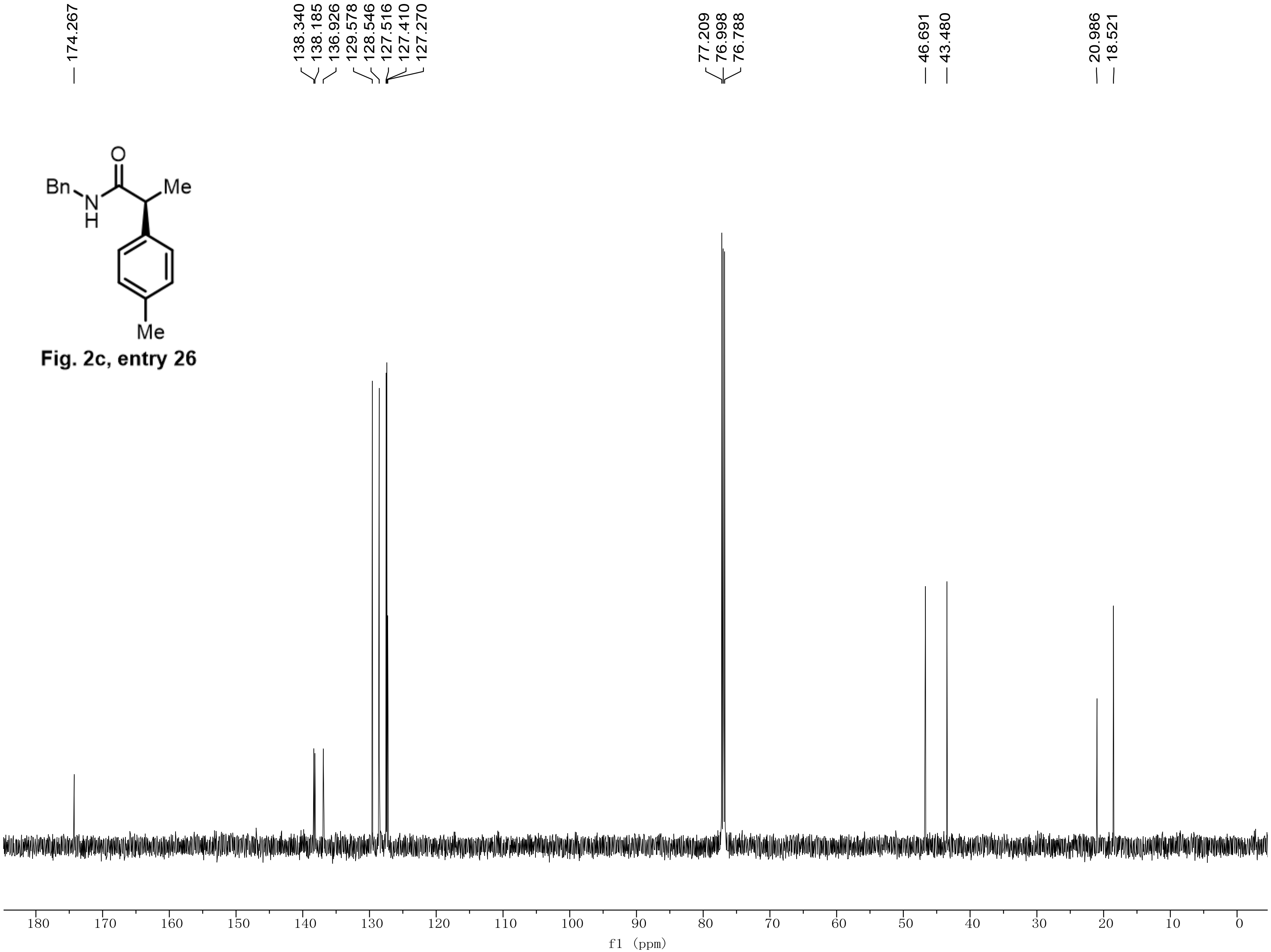


Fig. 2c, entry 26

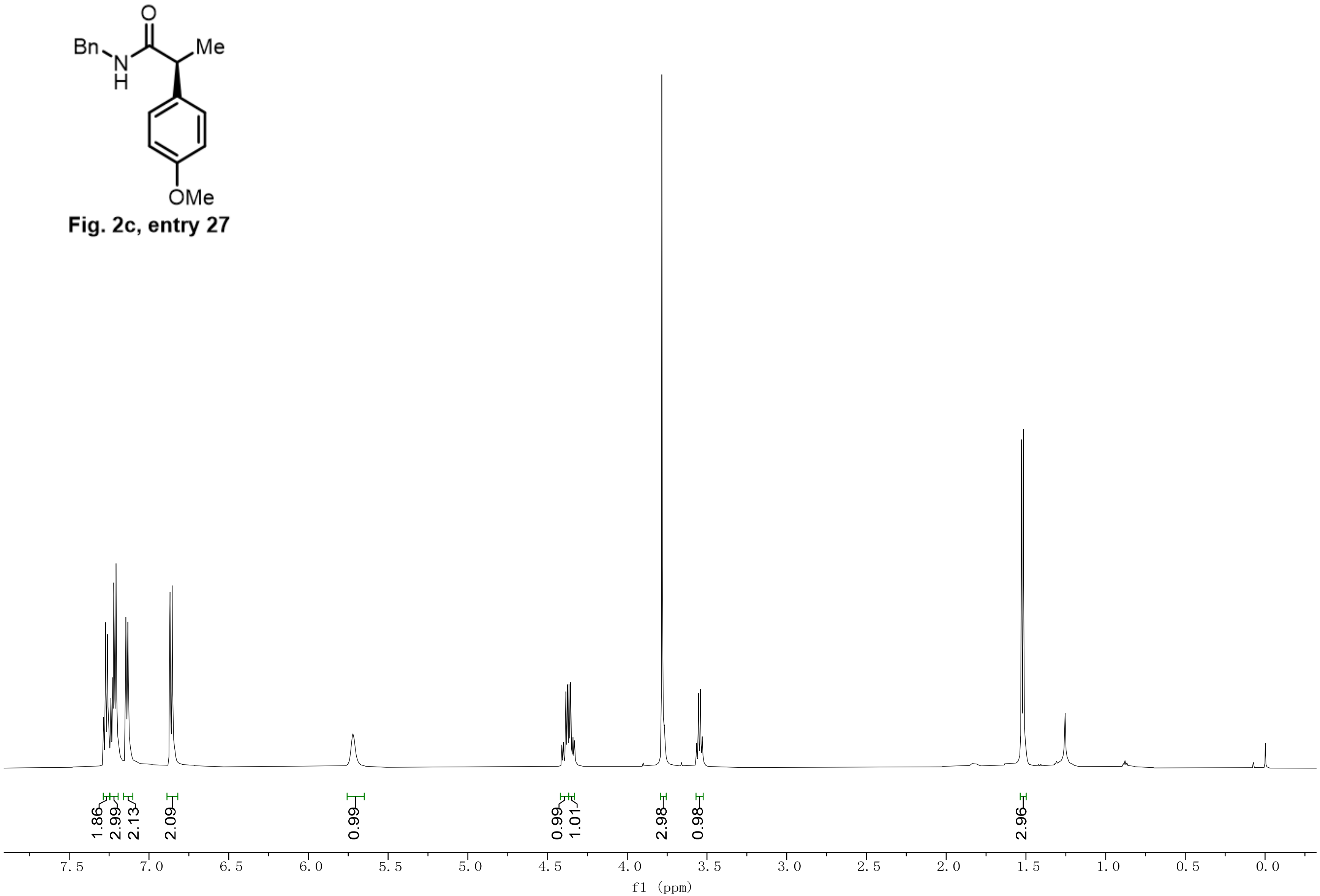
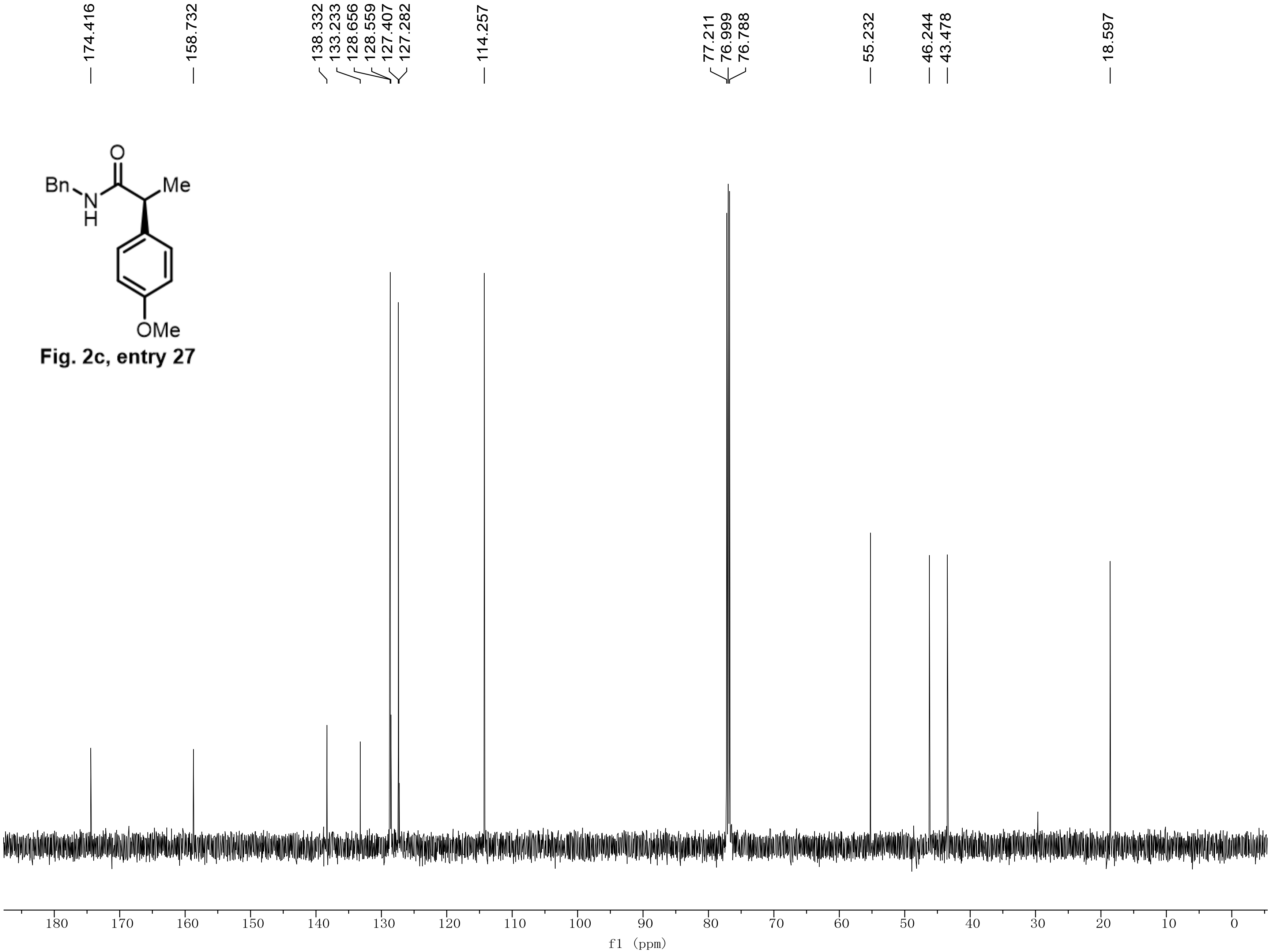


Fig. 2c, entry 27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133.233
128.656
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127.282
114.257
77.211
76.999
76.788
55.232
46.244
43.478
18.597
Bn
N
H
O
Me
OMe
Fig. 2c, entry 27
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

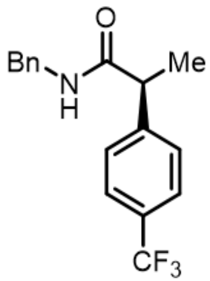
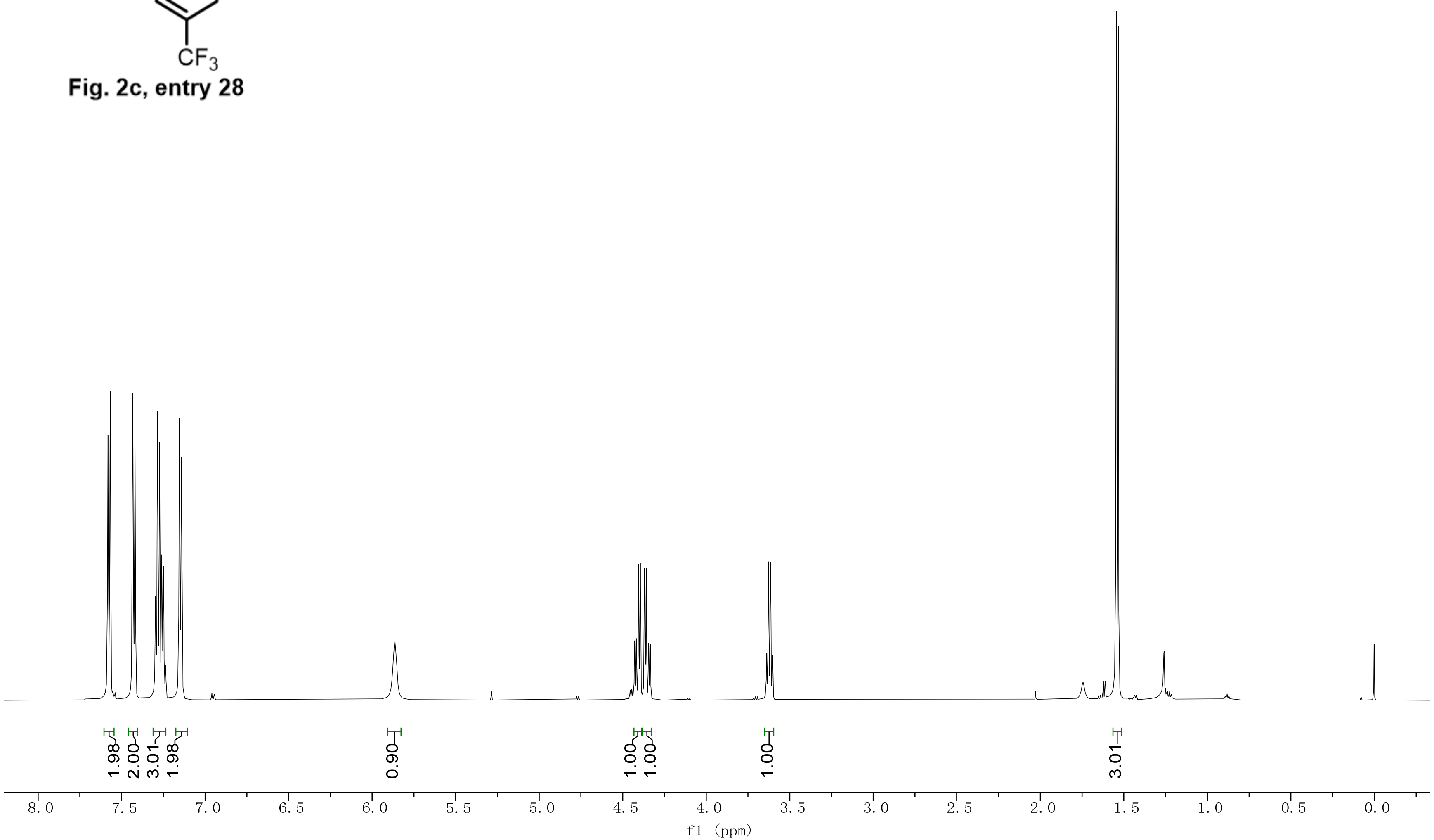
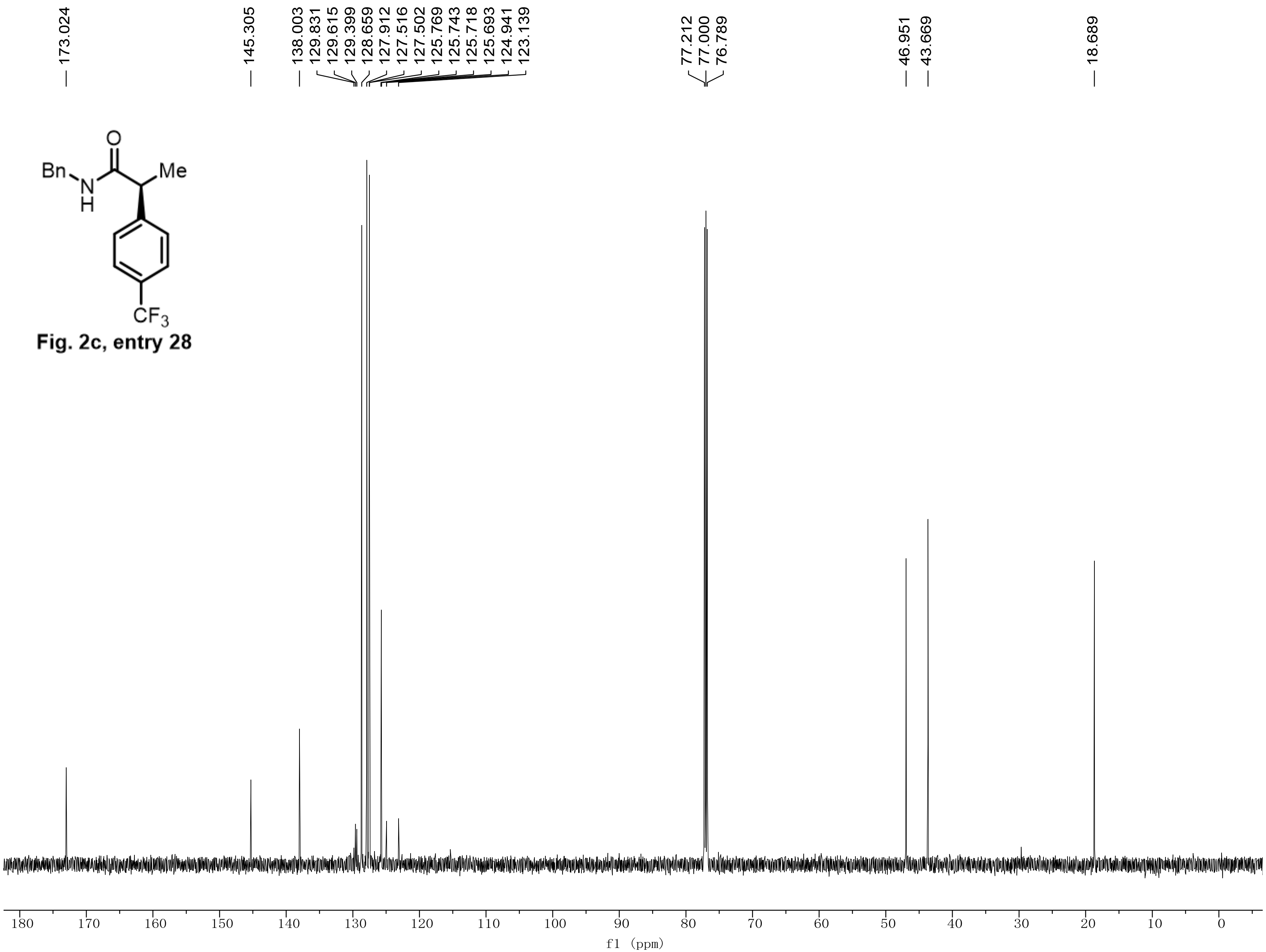


Fig. 2c, entry 28





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125.693
124.941
123.139
77.212
77.000
76.789
46.951
43.669
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O
Bn
N
H
Me
CF_3
Fig. 2c, entry 28
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

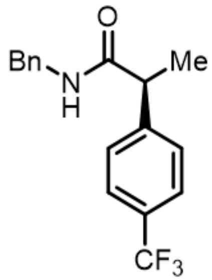
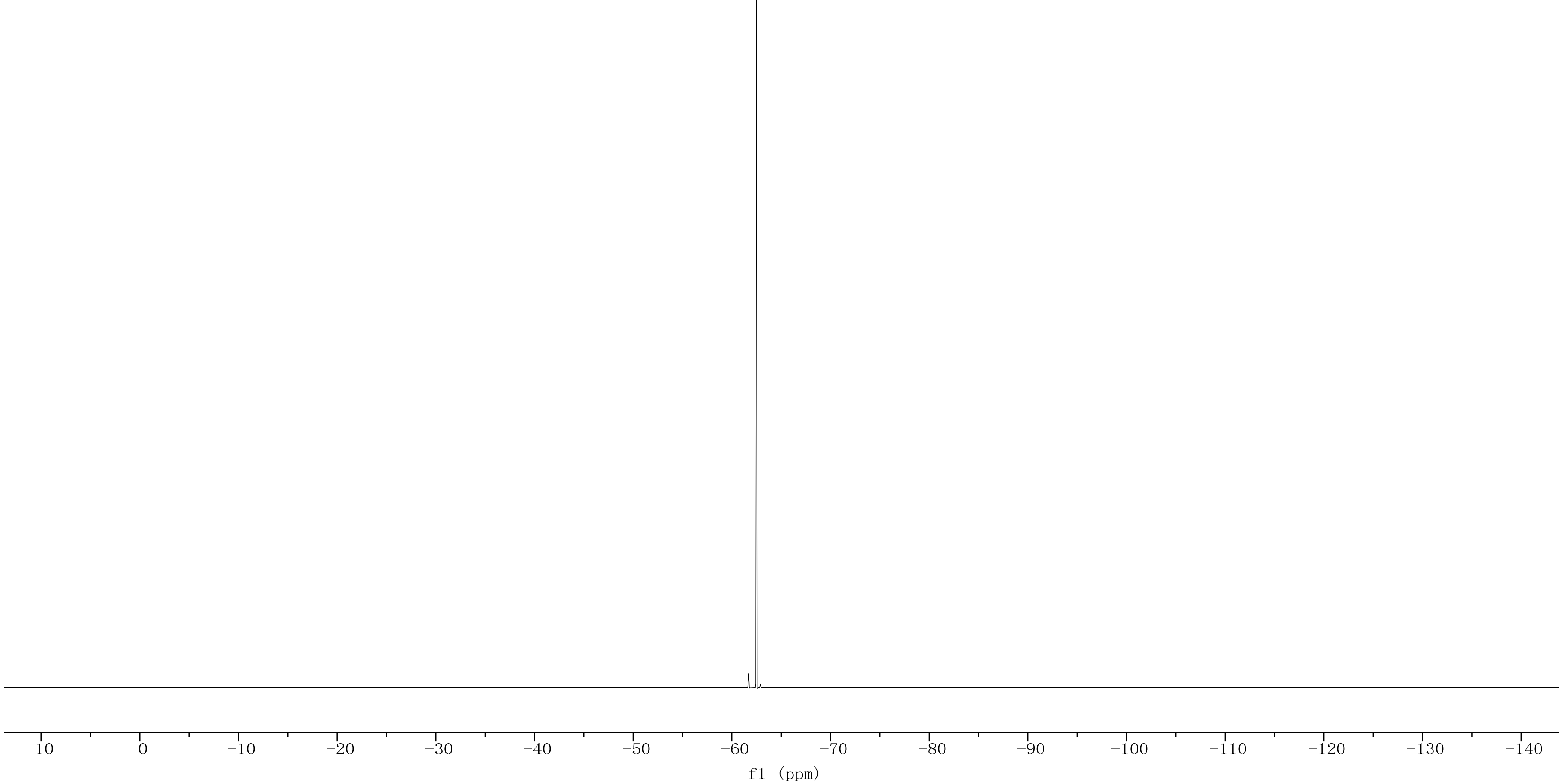


Fig. 2c, entry 28



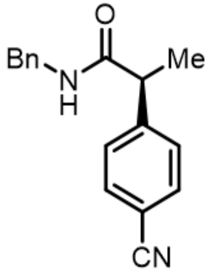
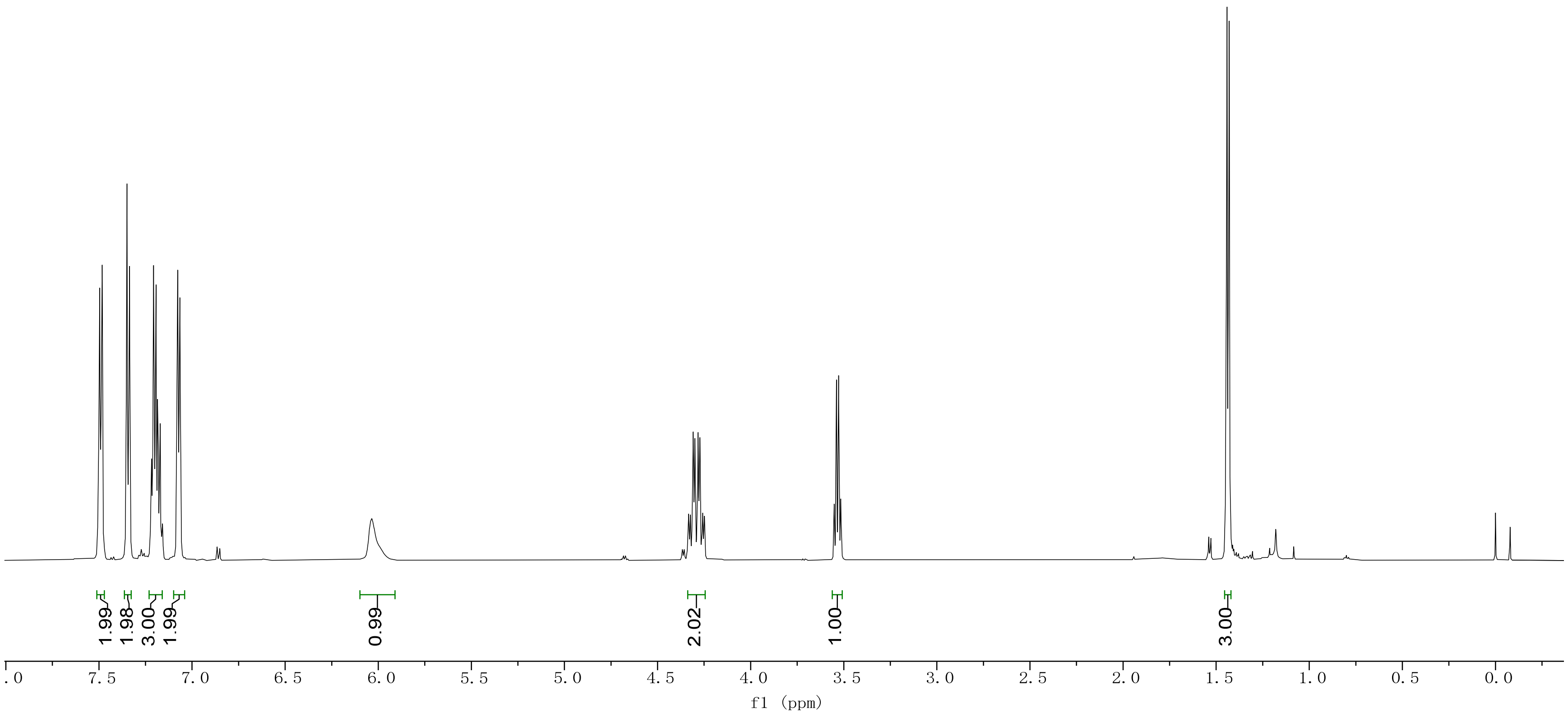
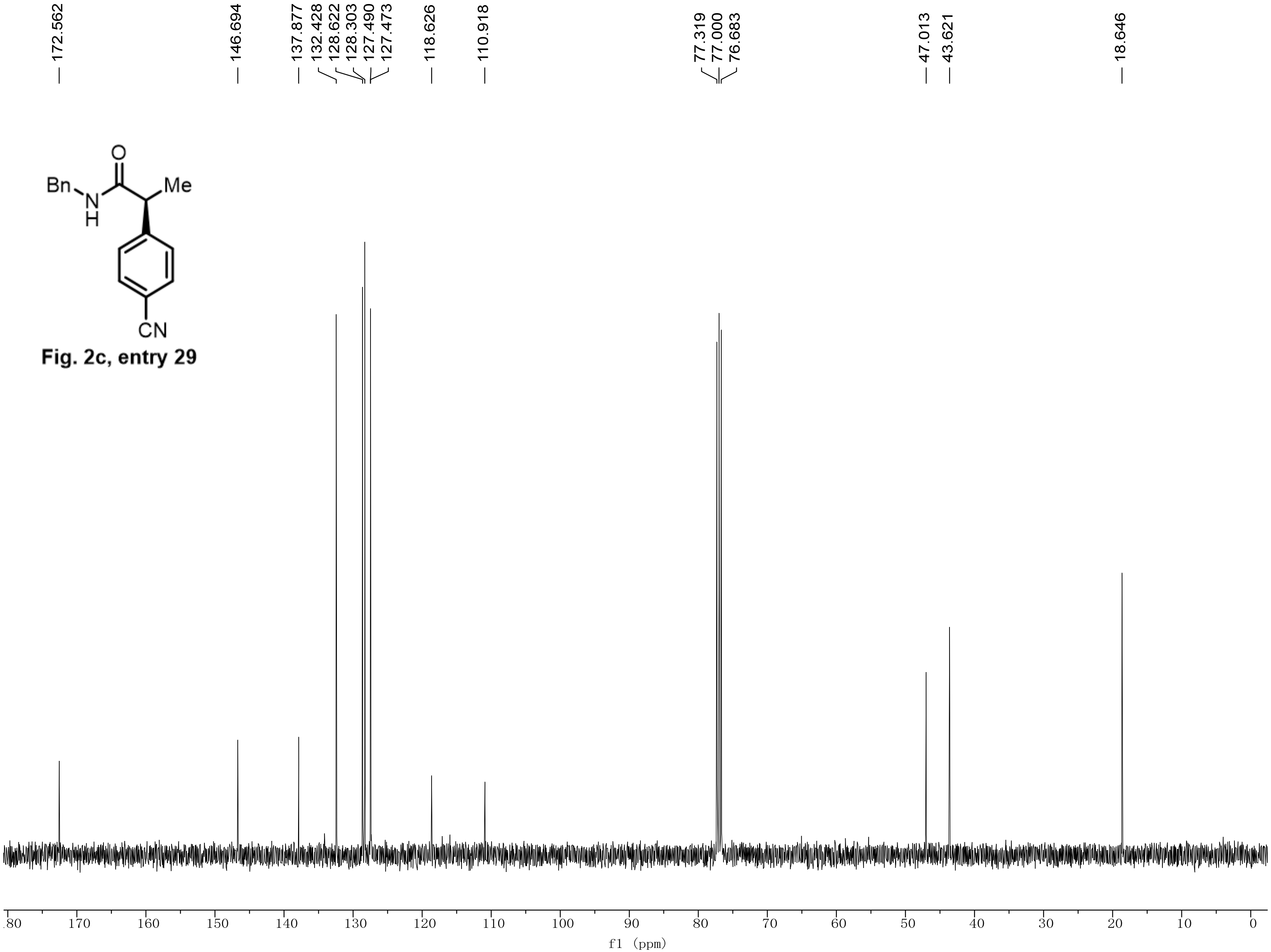


Fig. 2c, entry 29





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137.877
132.428
128.622
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127.473
118.626
110.918
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77.000
76.683
47.013
43.621
18.646
O
Bn
N
H
Me
CN
Fig. 2c, entry 29
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

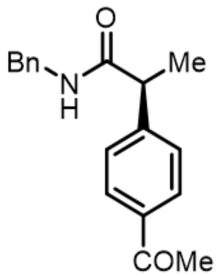
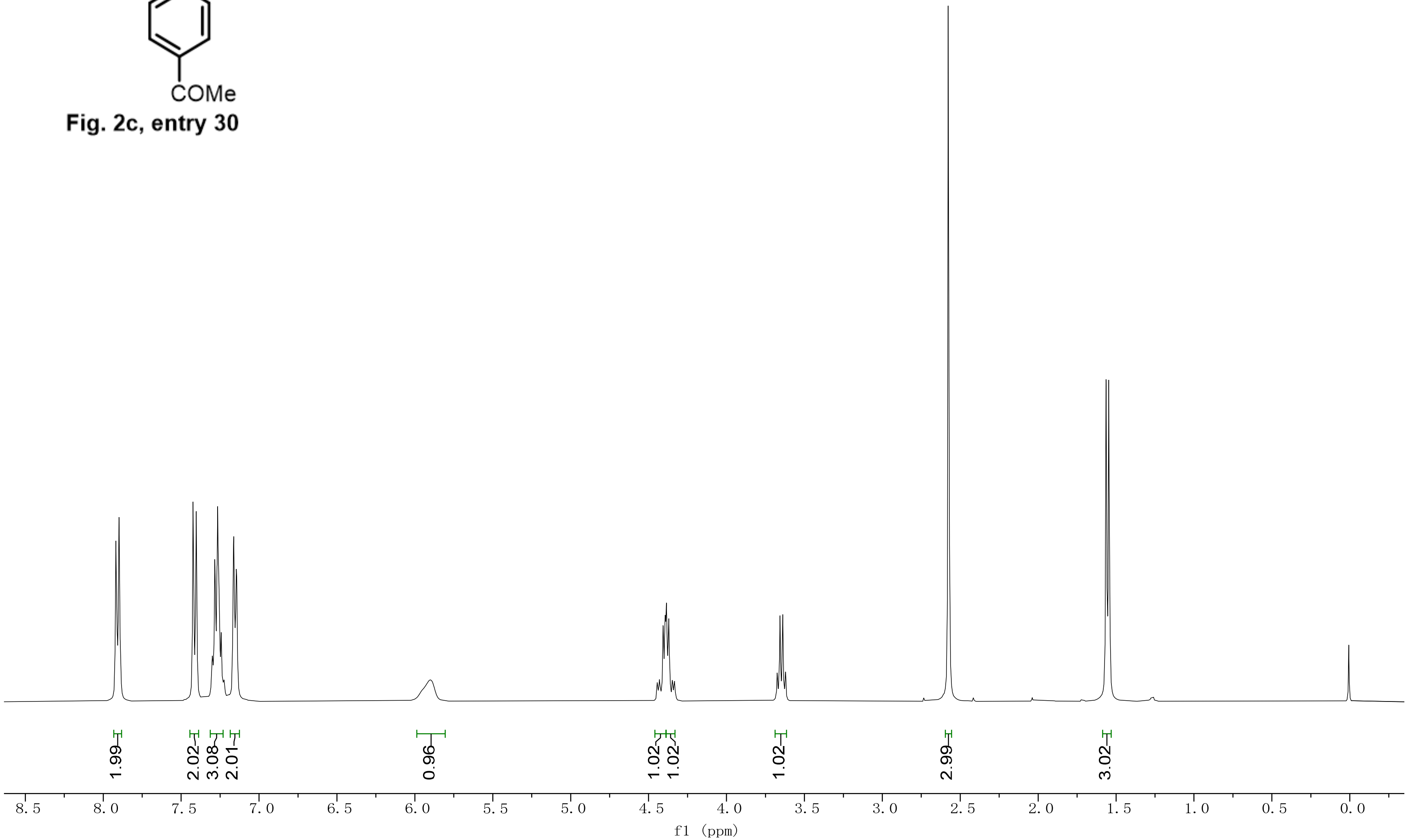


Fig. 2c, entry 30



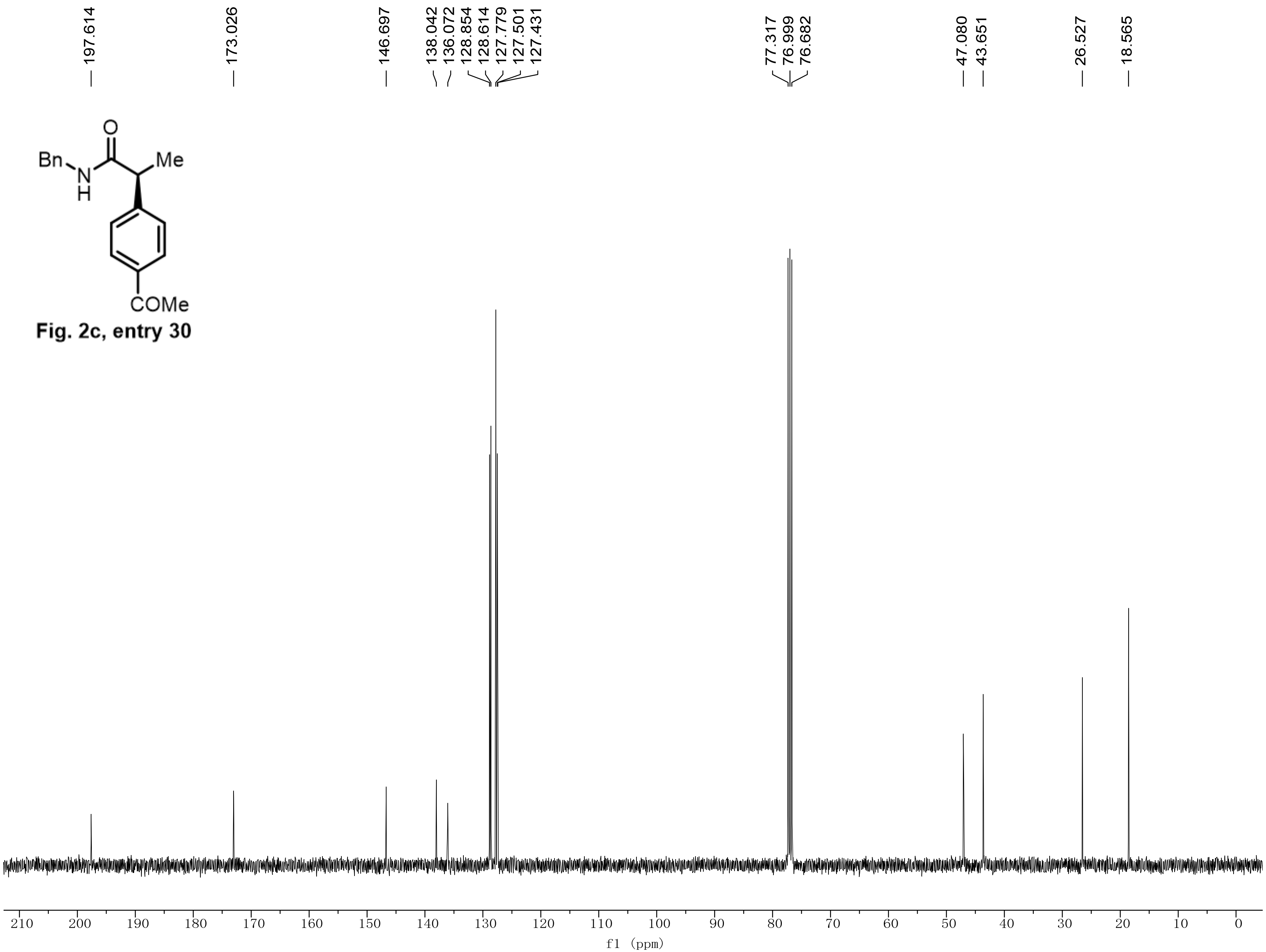


Fig. 2c, entry 30

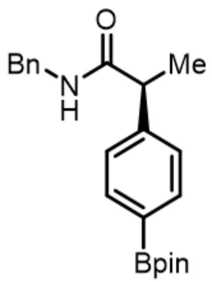
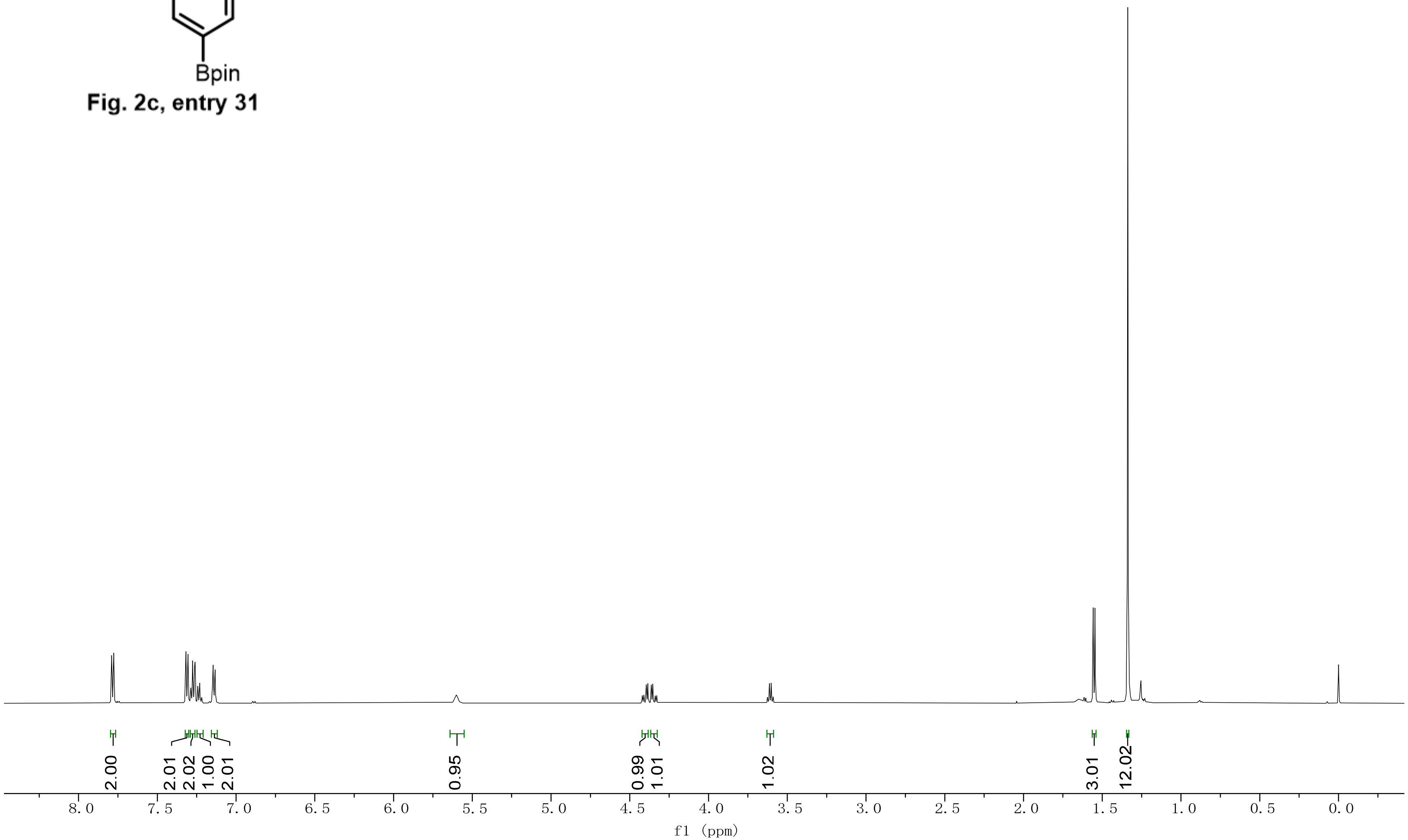


Fig. 2c, entry 31



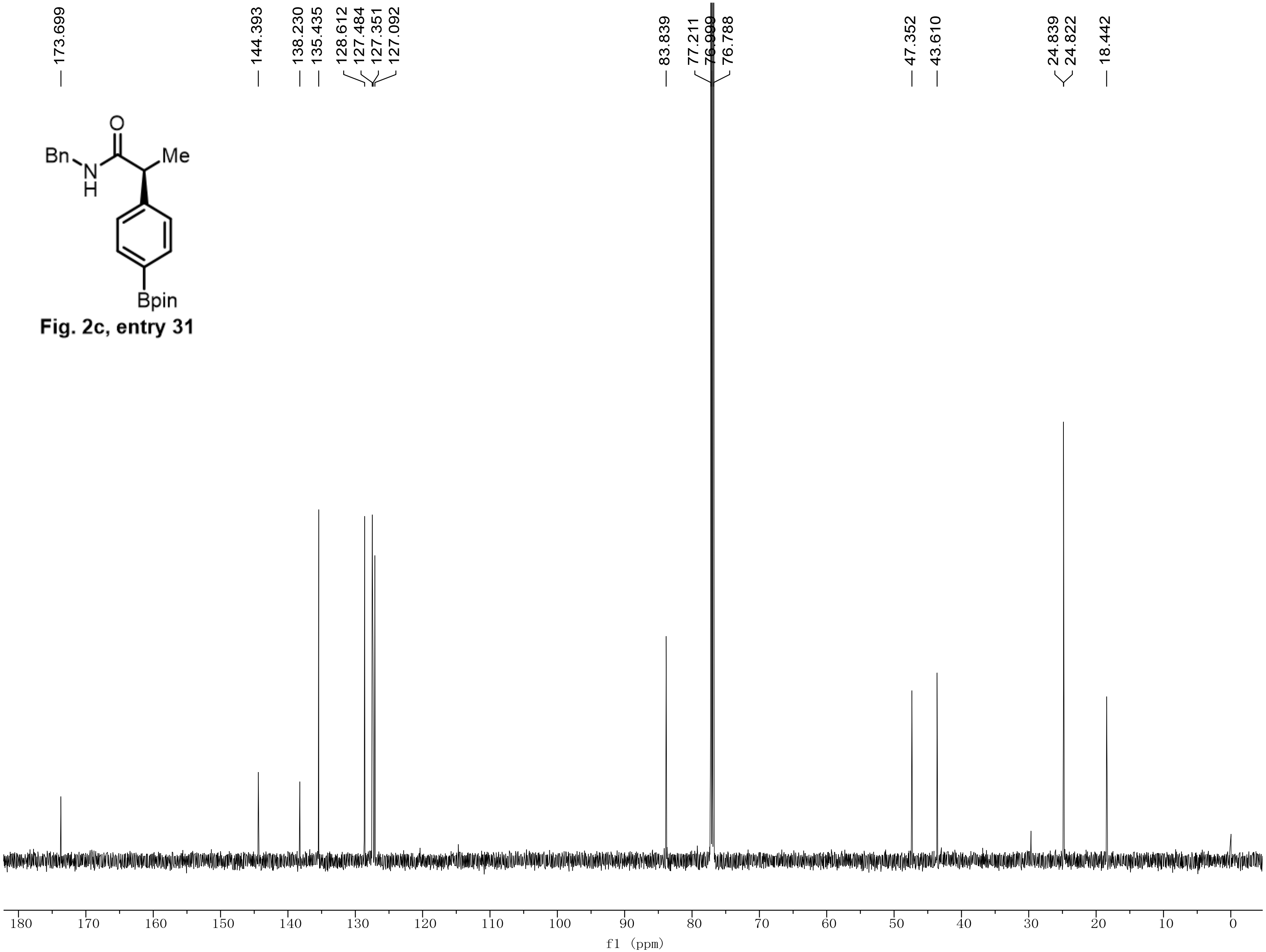


Fig. 2c, entry 31

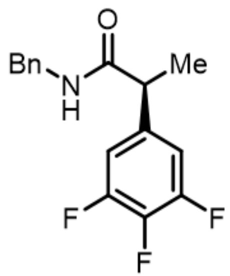
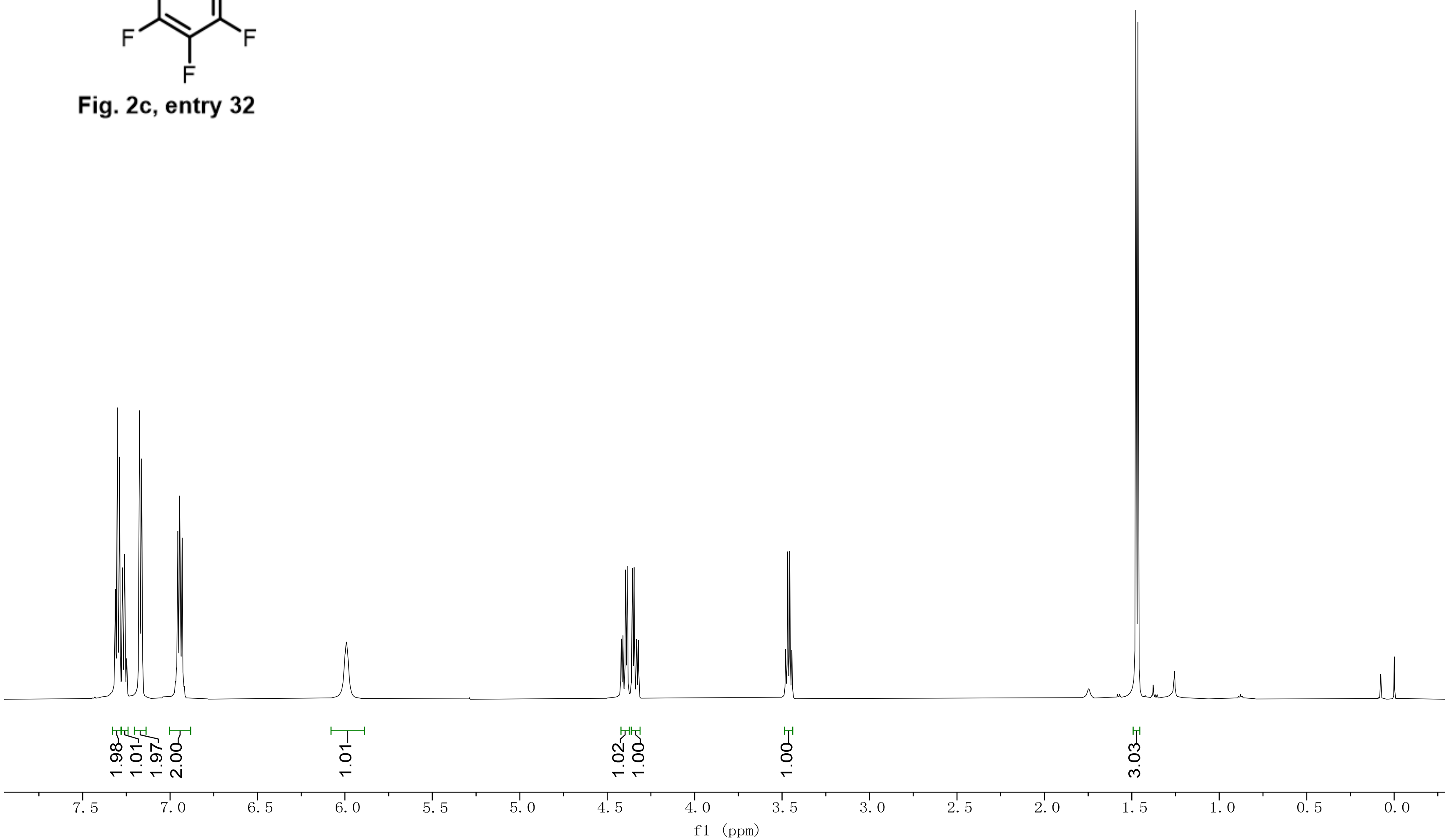


Fig. 2c, entry 32



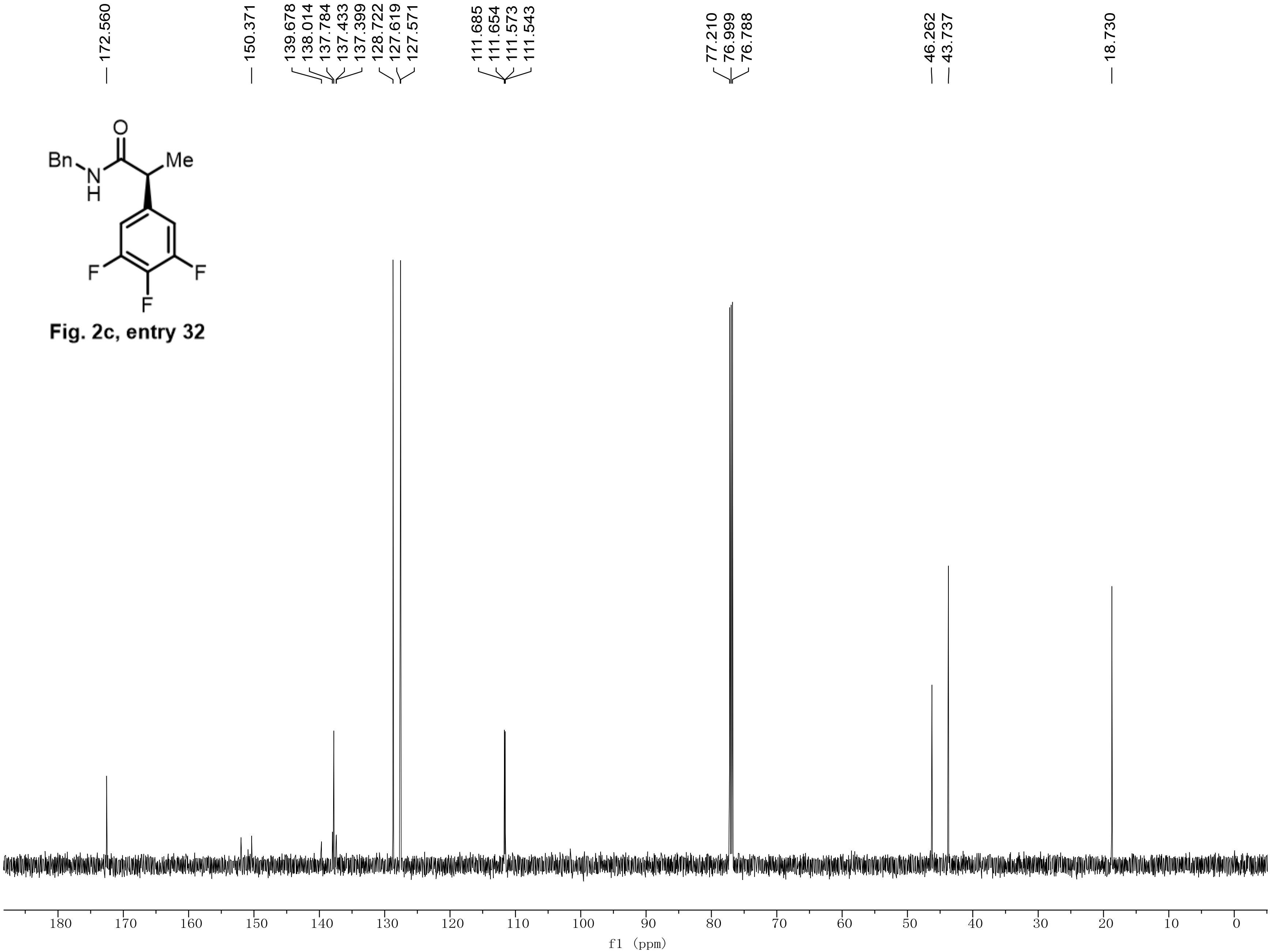


Fig. 2c, entry 32

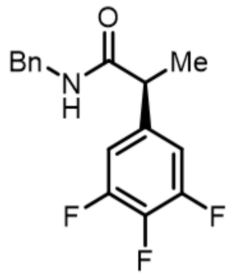
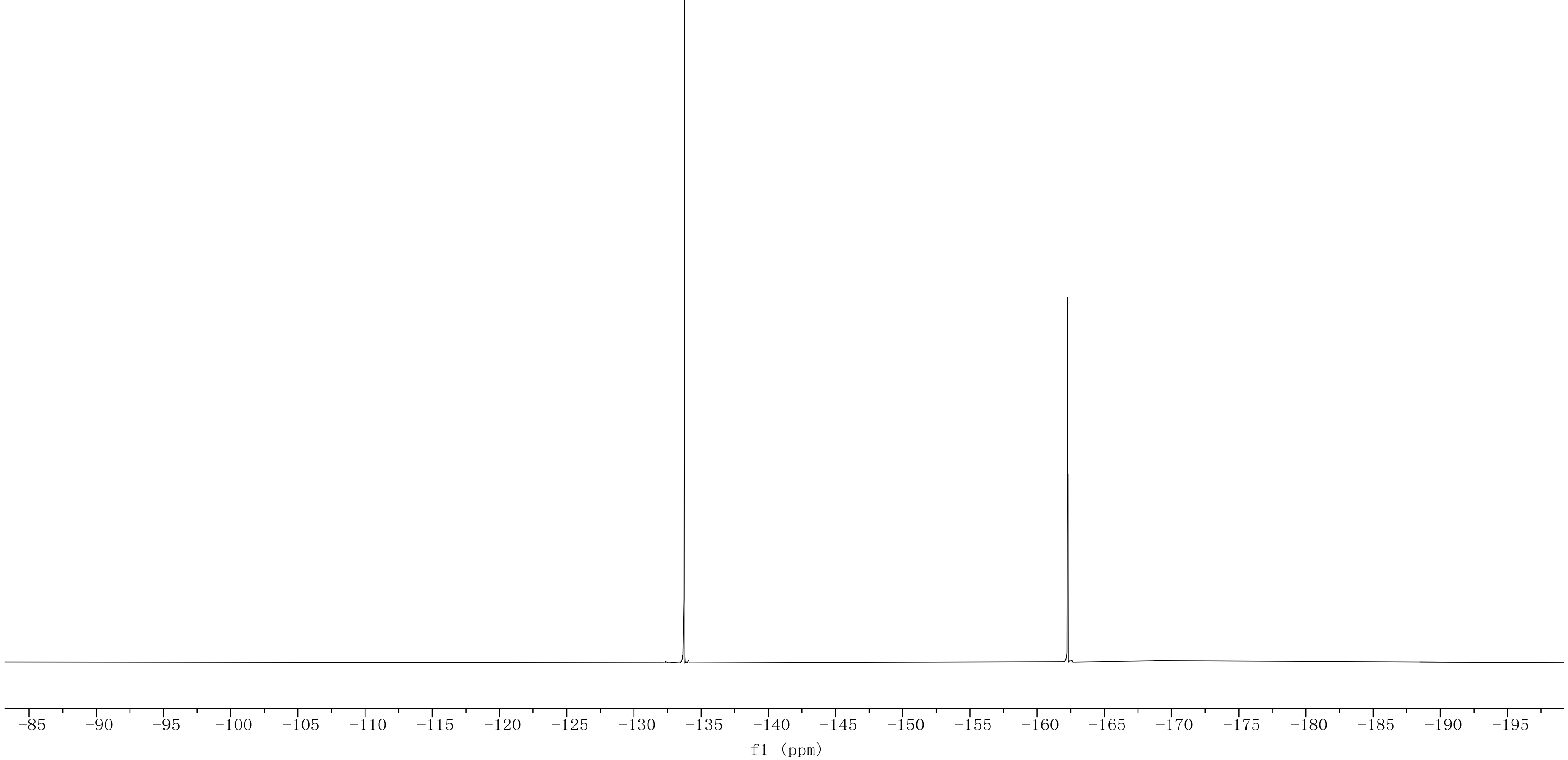


Fig. 2c, entry 32



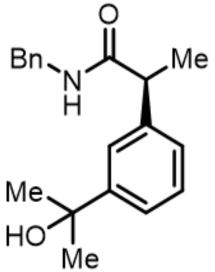
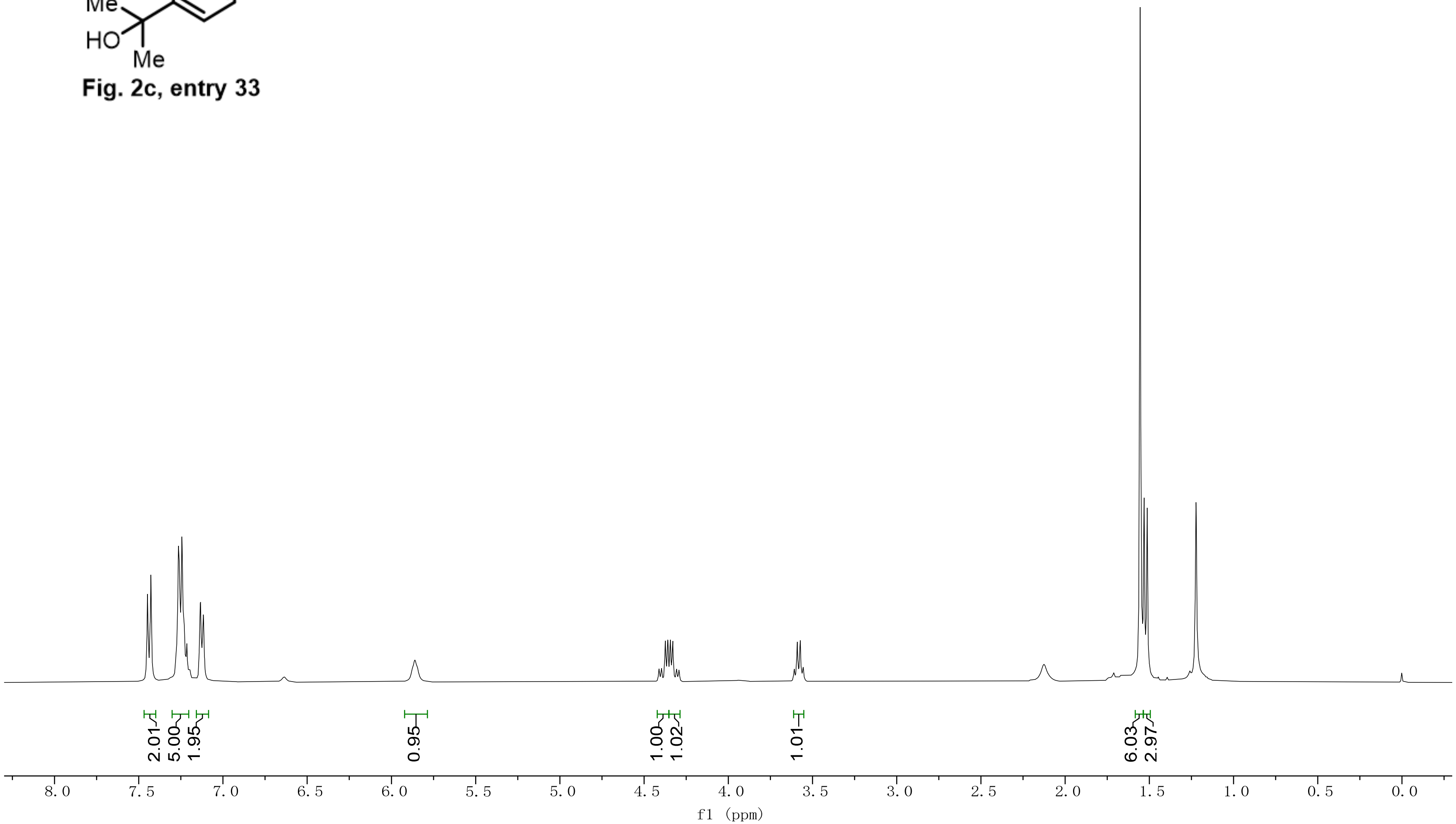
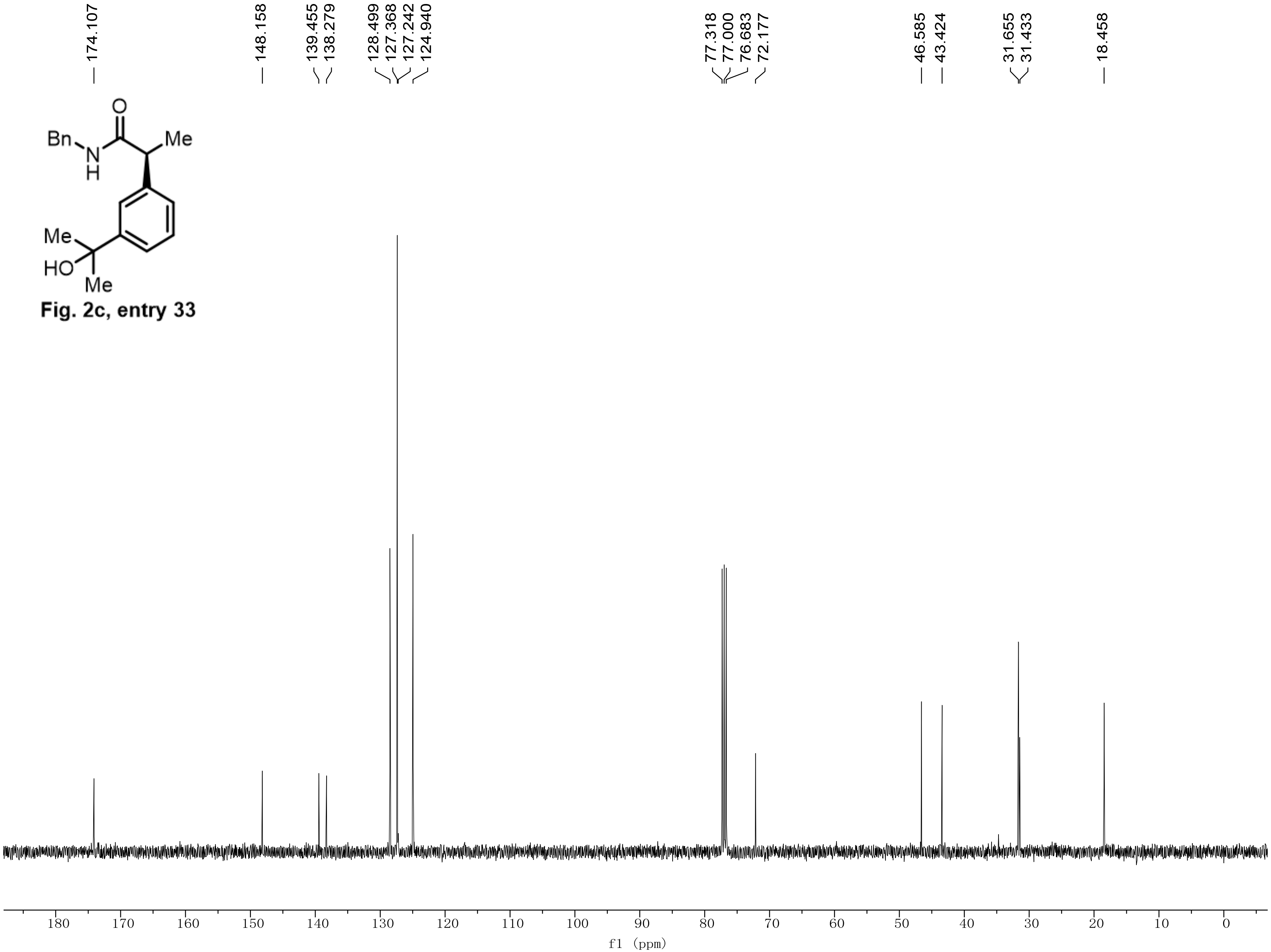


Fig. 2c, entry 33




174.107
148.158
139.455
138.279
128.499
127.368
127.242
124.940
77.318
77.000
76.683
72.177
46.585
43.424
31.655
31.433
18.458
Bn
N
H
O
Me
Me
HO
Me
Fig. 2c, entry 33
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

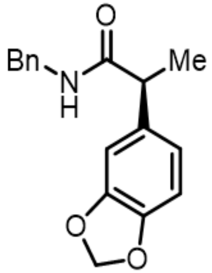
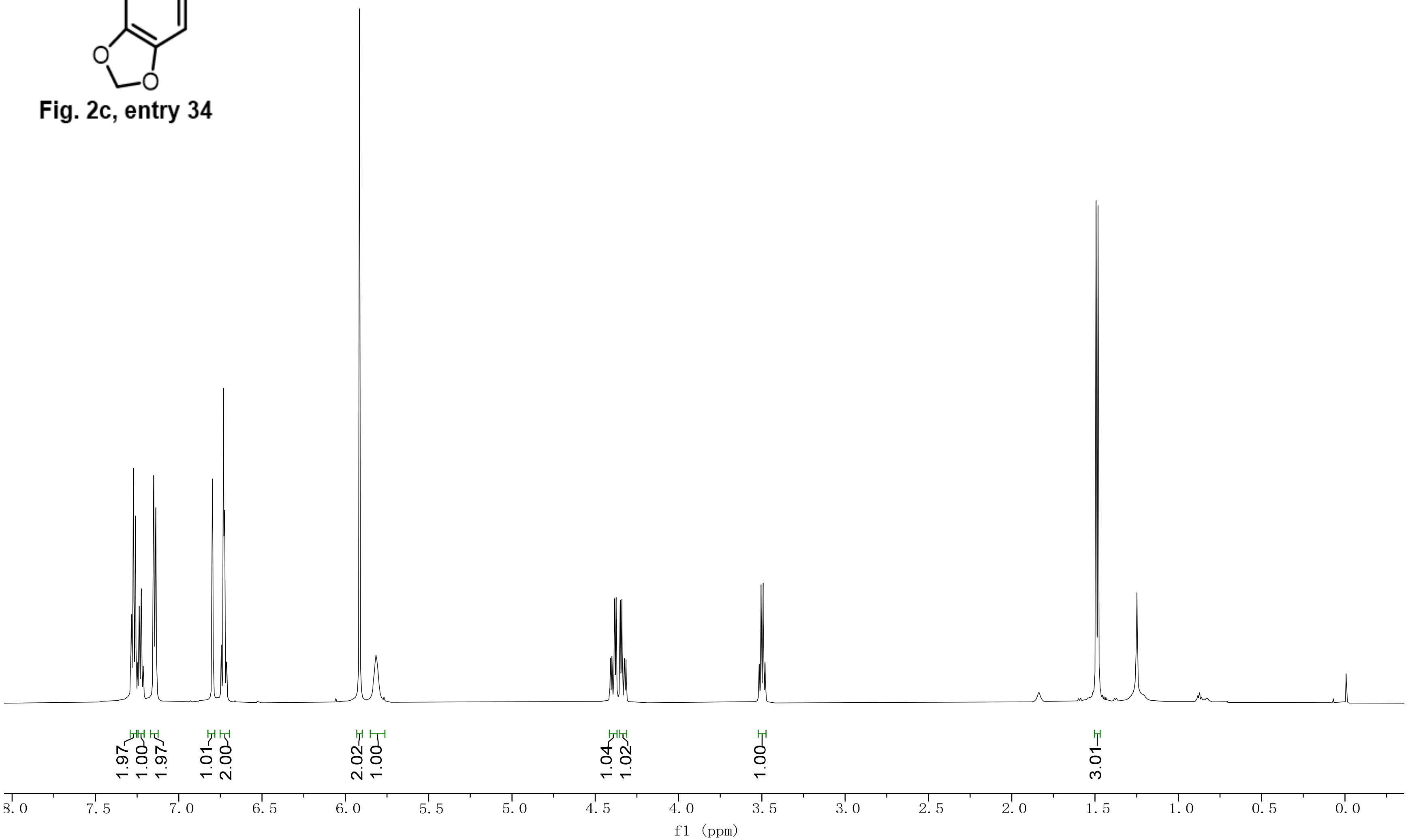


Fig. 2c, entry 34



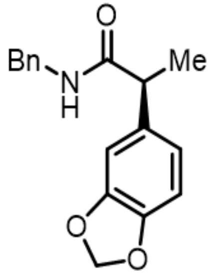
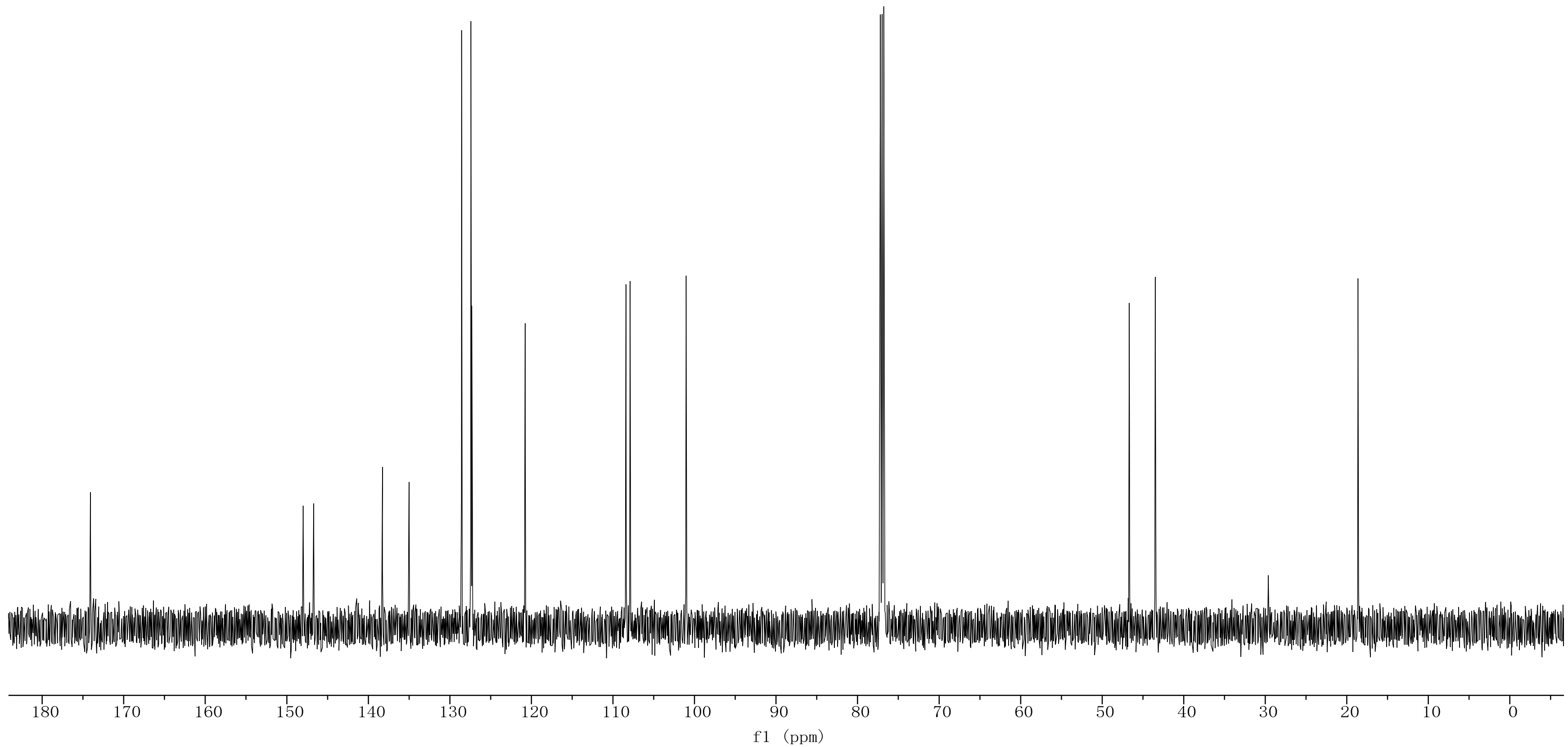


Fig. 2c, entry 34



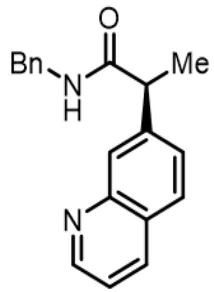
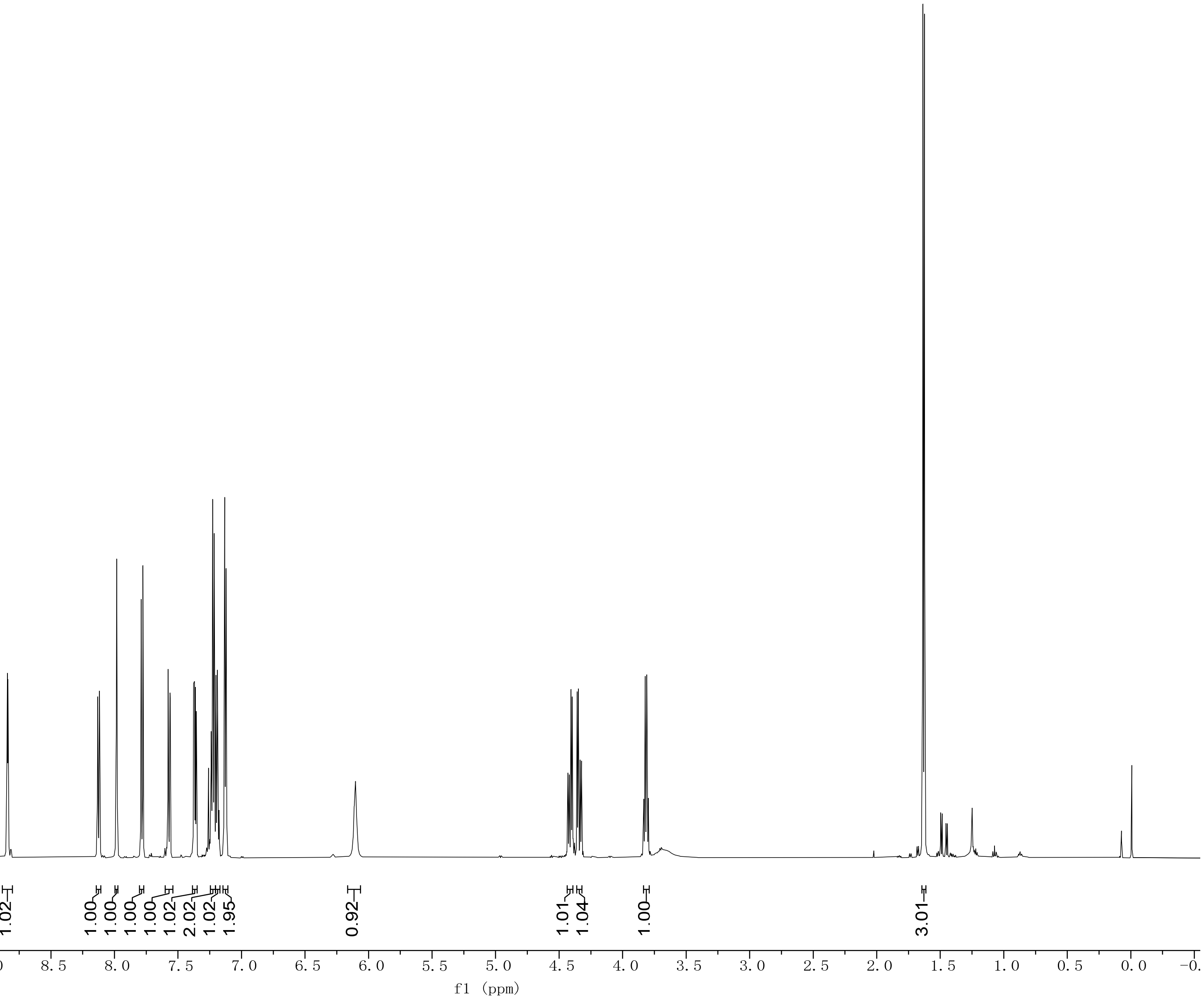


Fig. 2c, entry 35



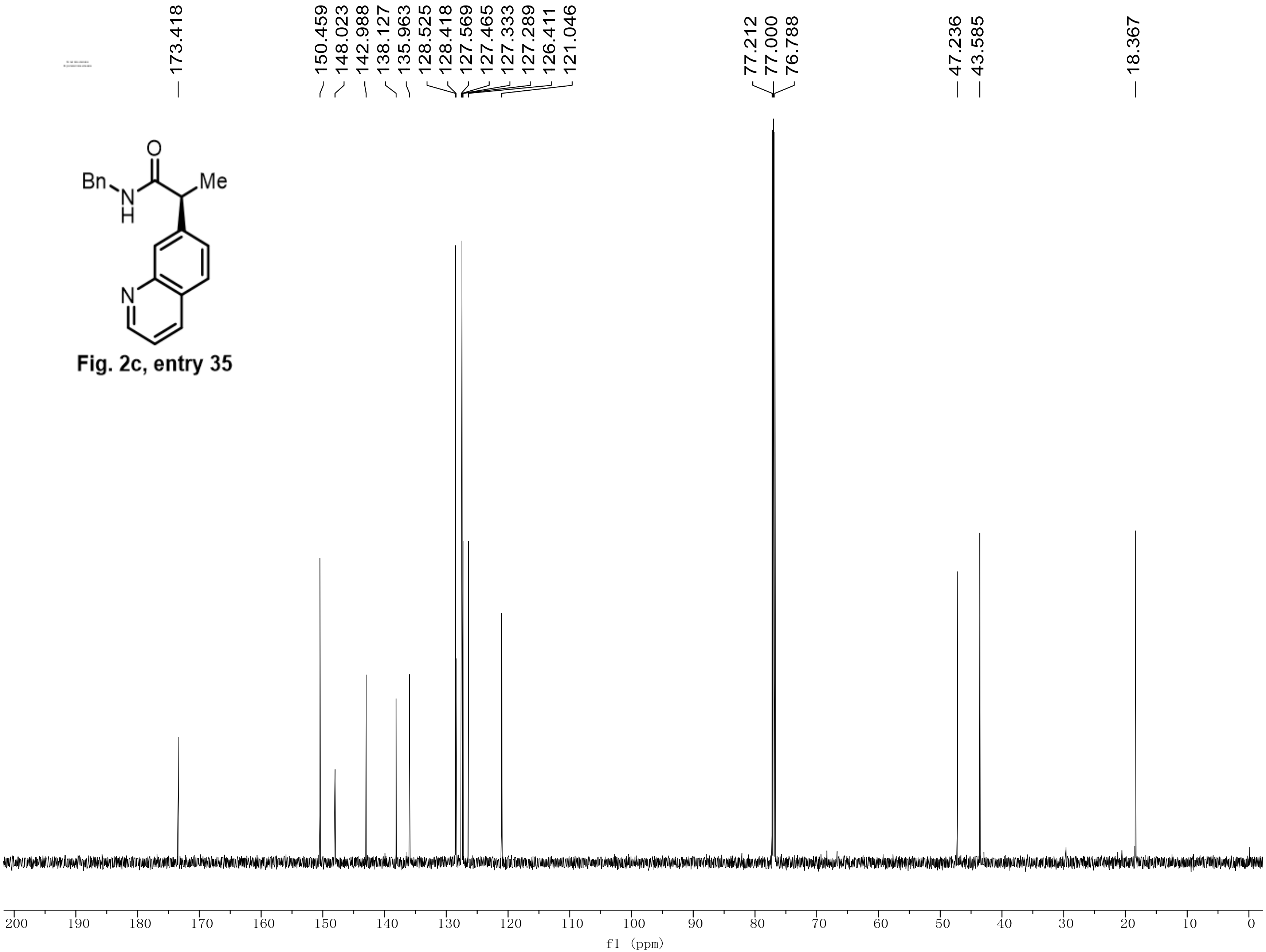


Fig. 2c, entry 35

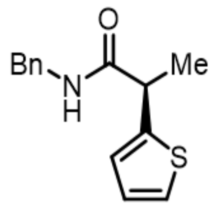
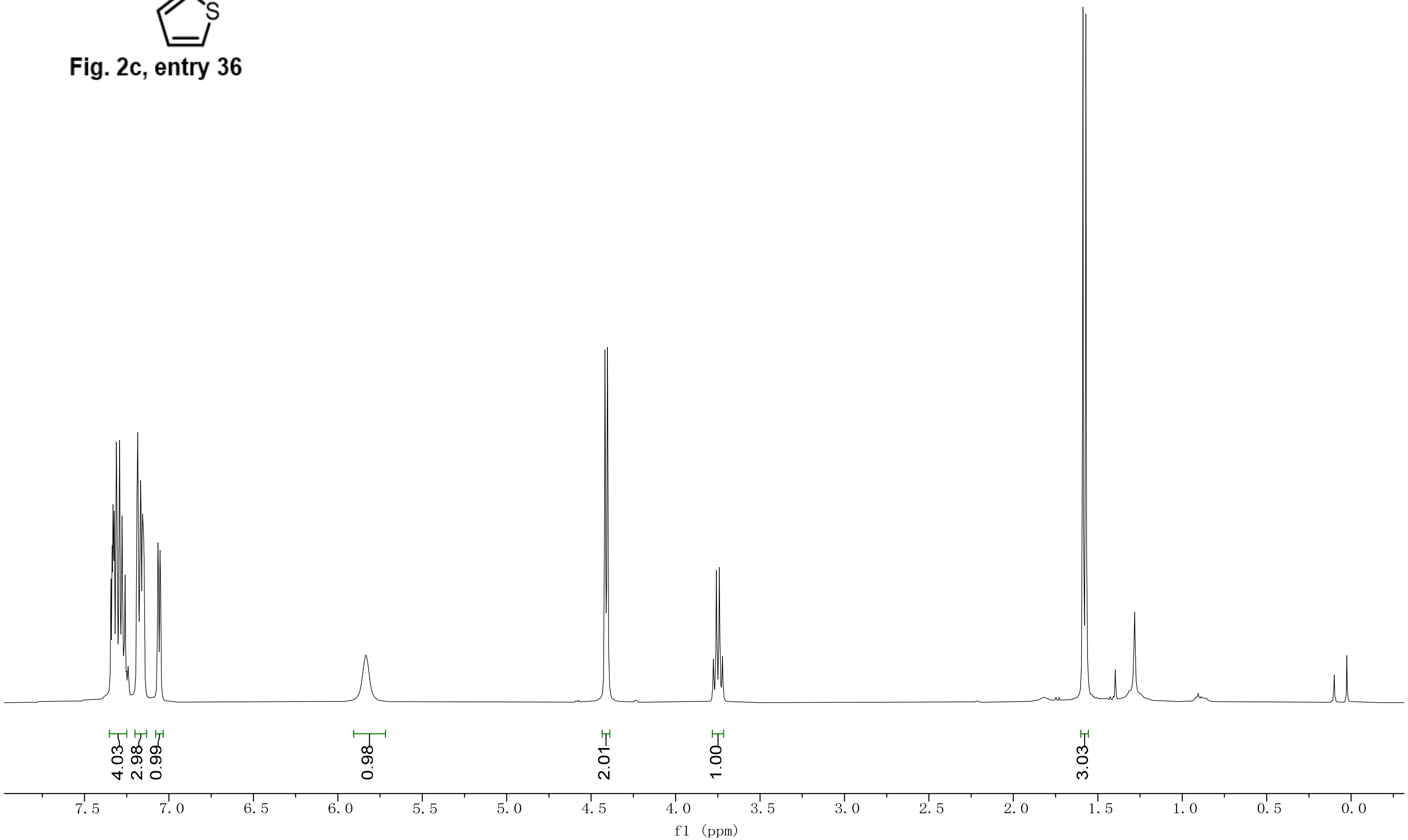


Fig. 2c, entry 36



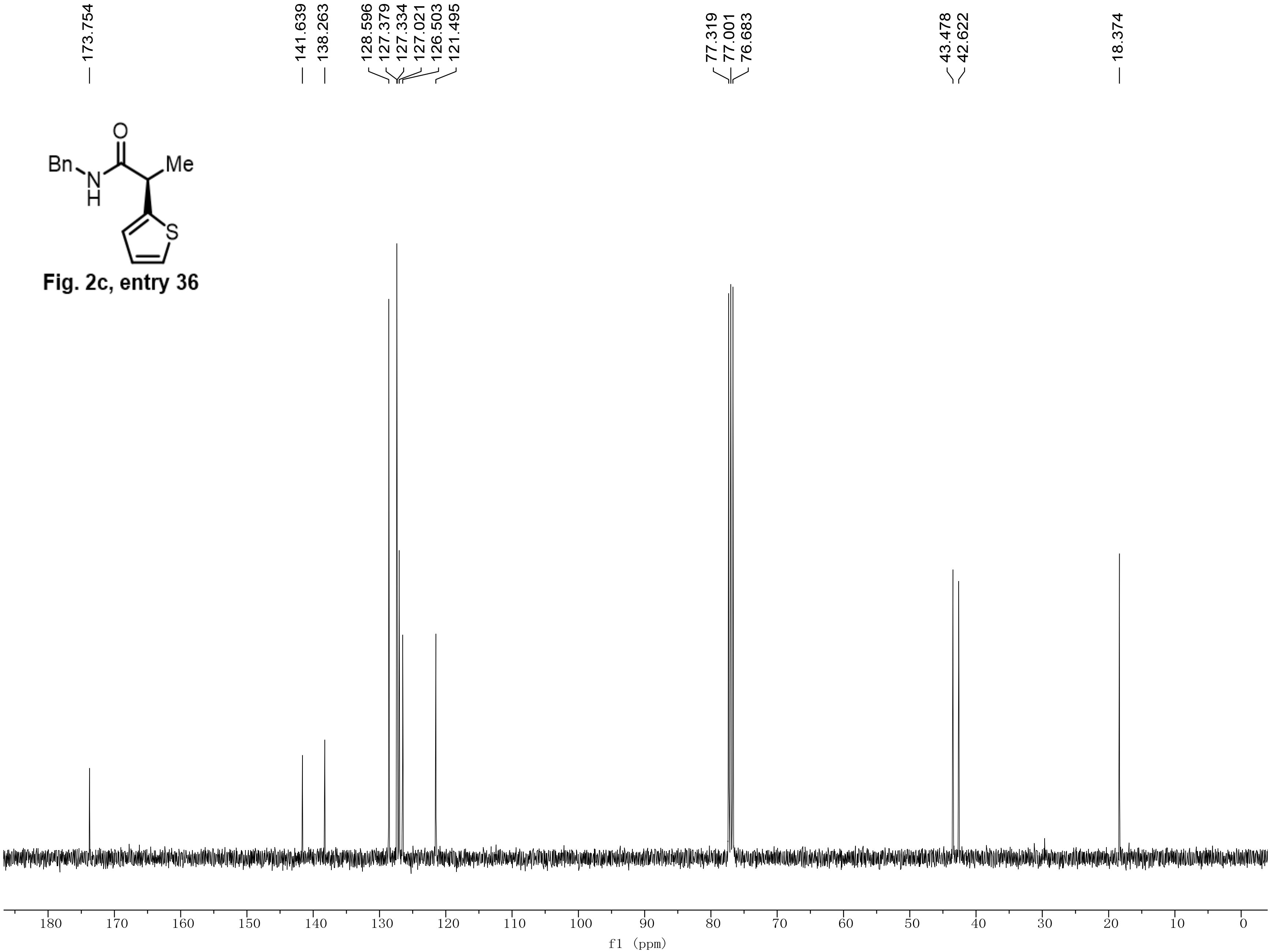


Fig. 2c, entry 36

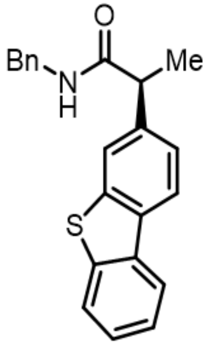
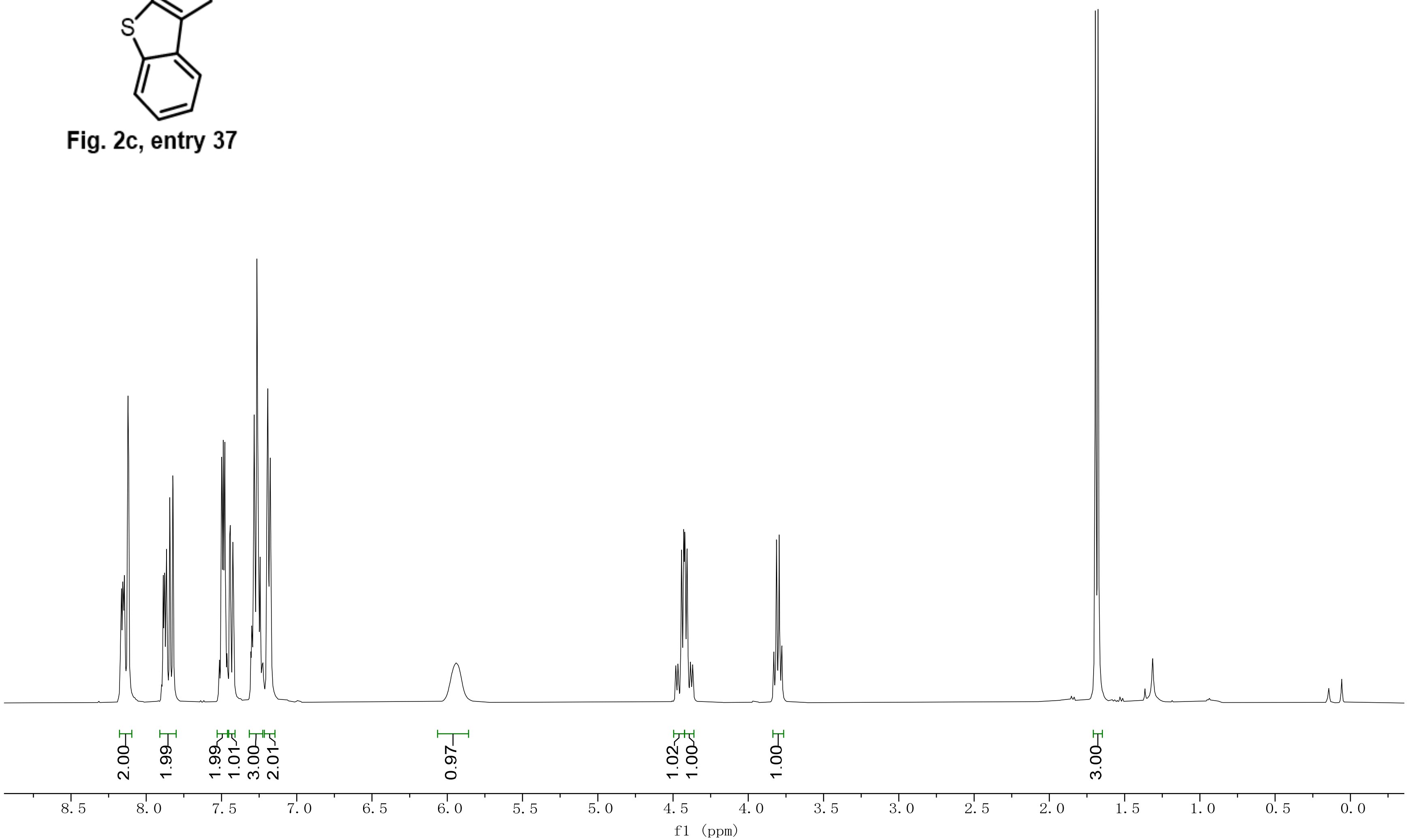


Fig. 2c, entry 37



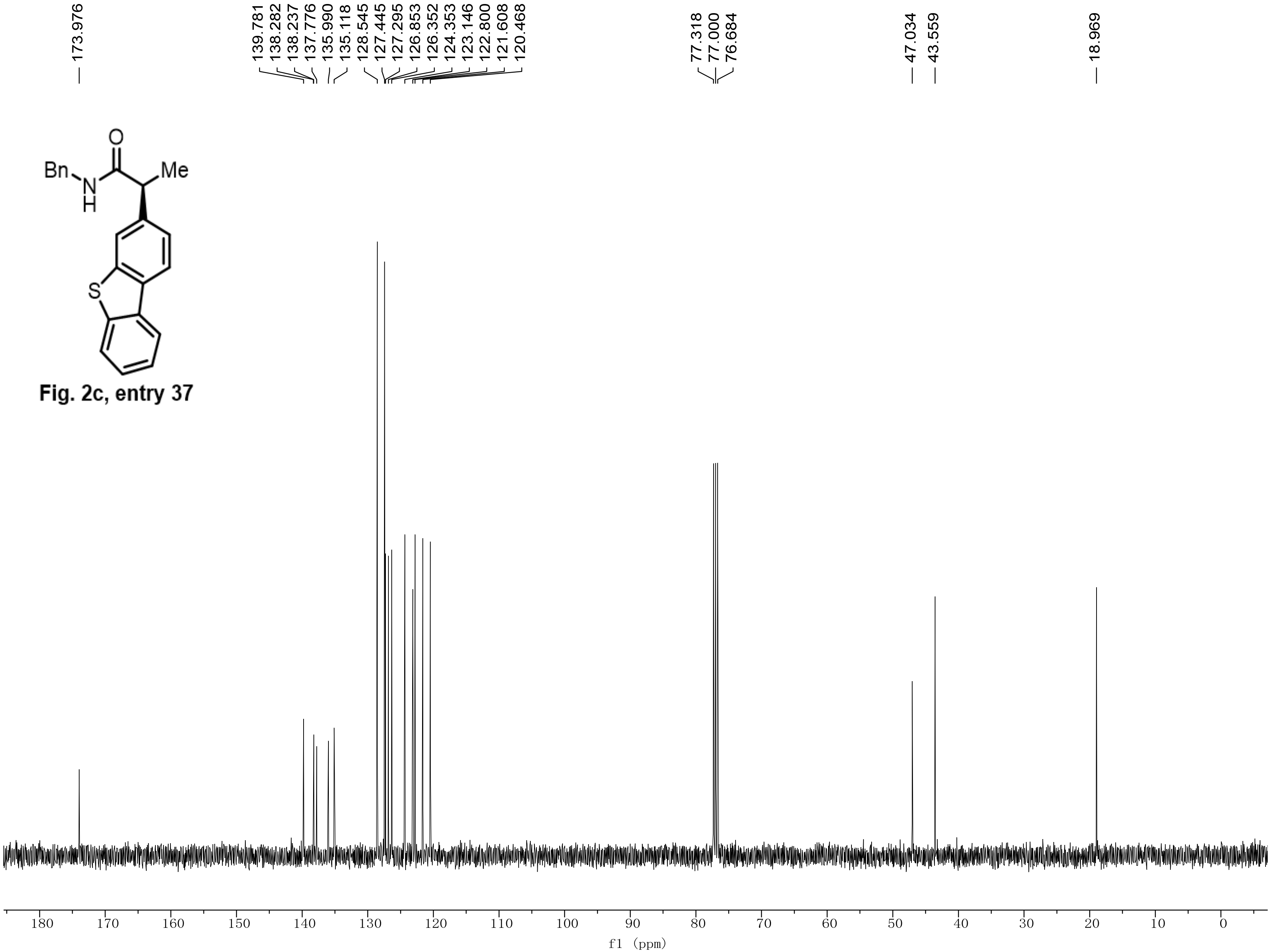


Fig. 2c, entry 37

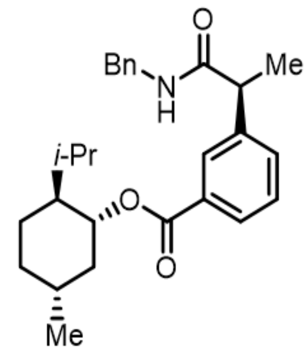
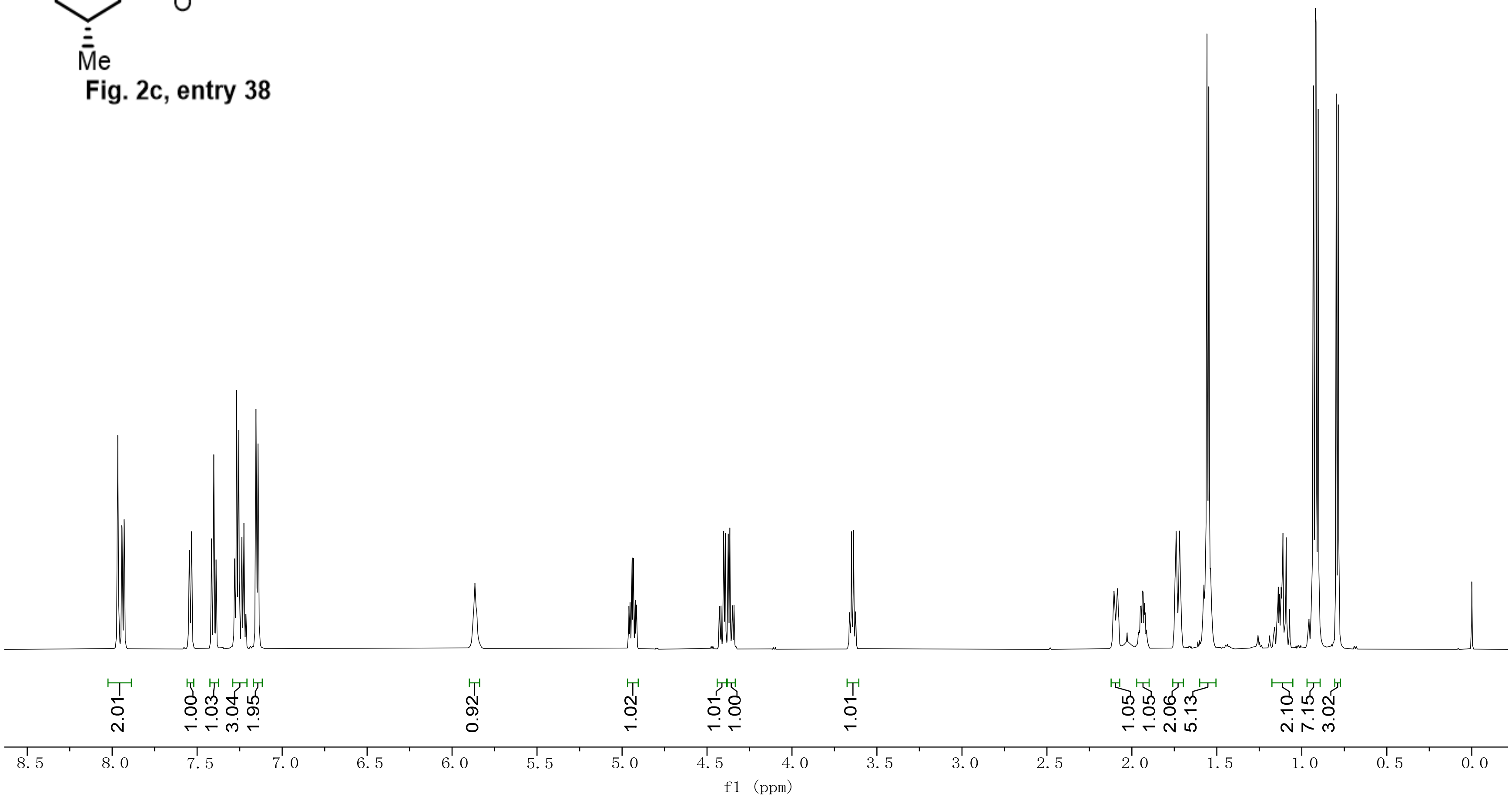


Fig. 2c, entry 38



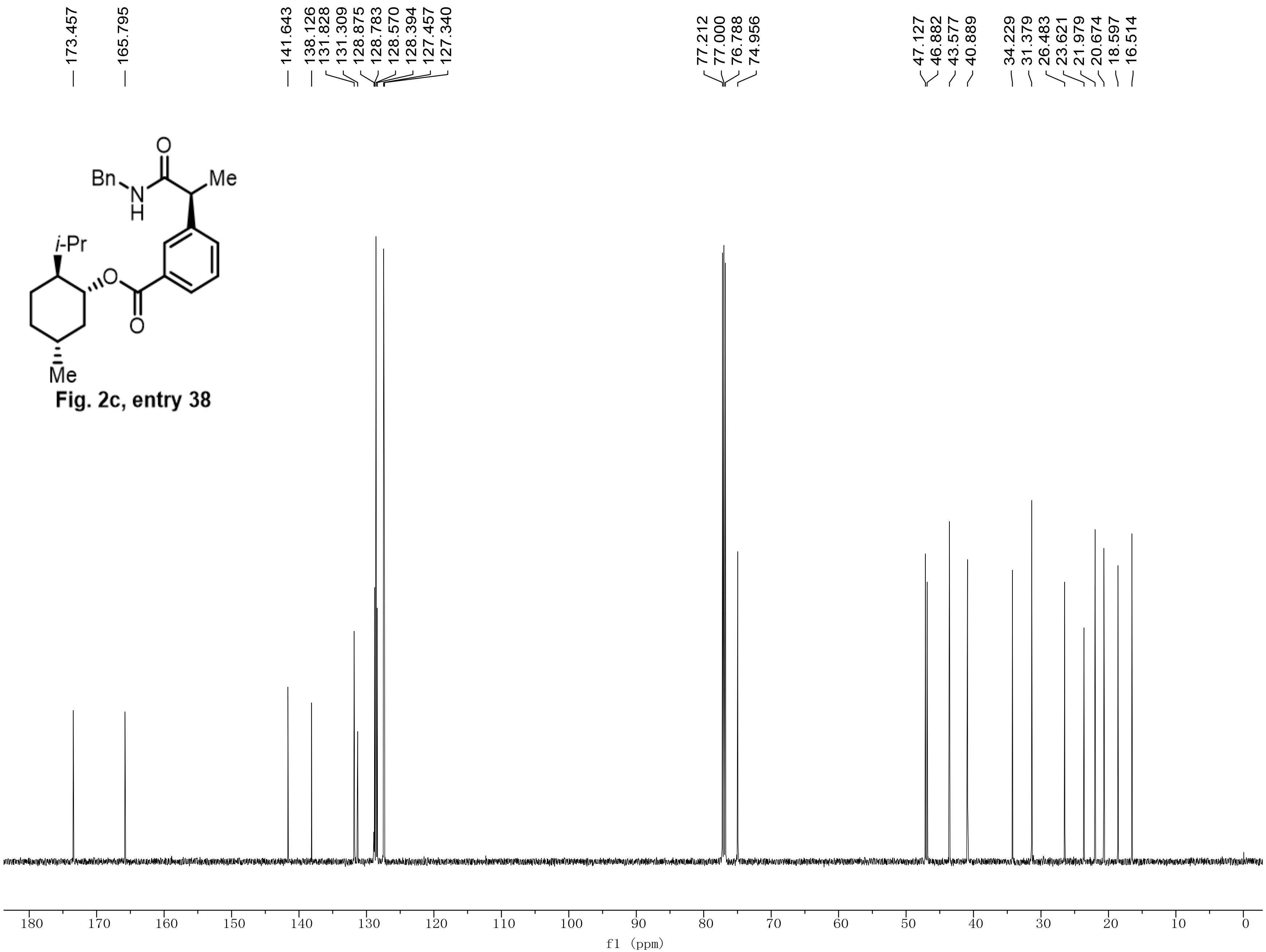


Fig. 2c, entry 38

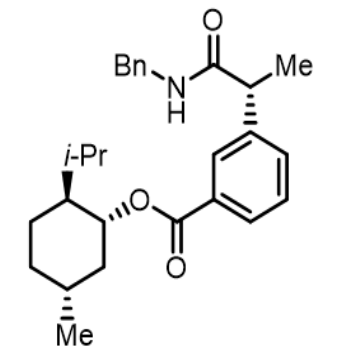
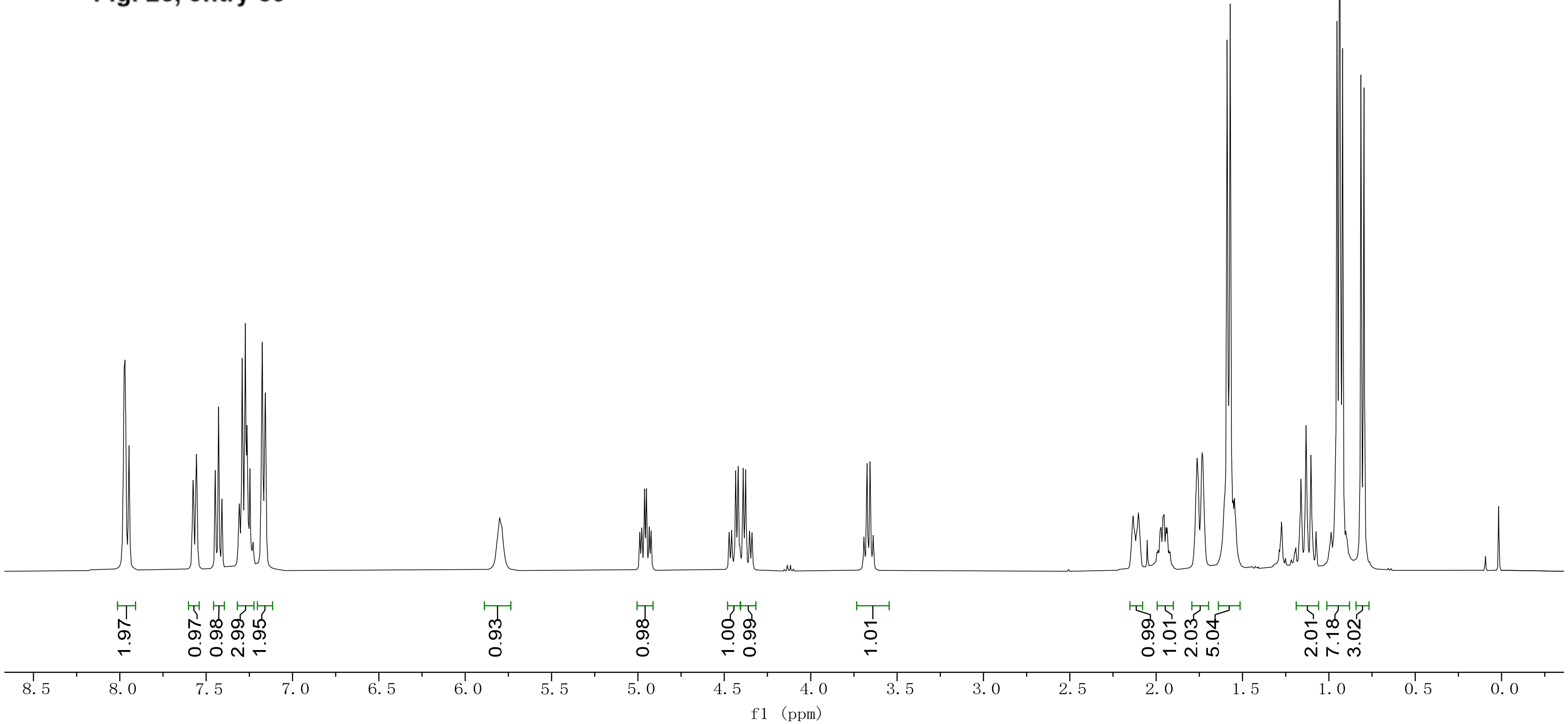


Fig. 2c, entry 39



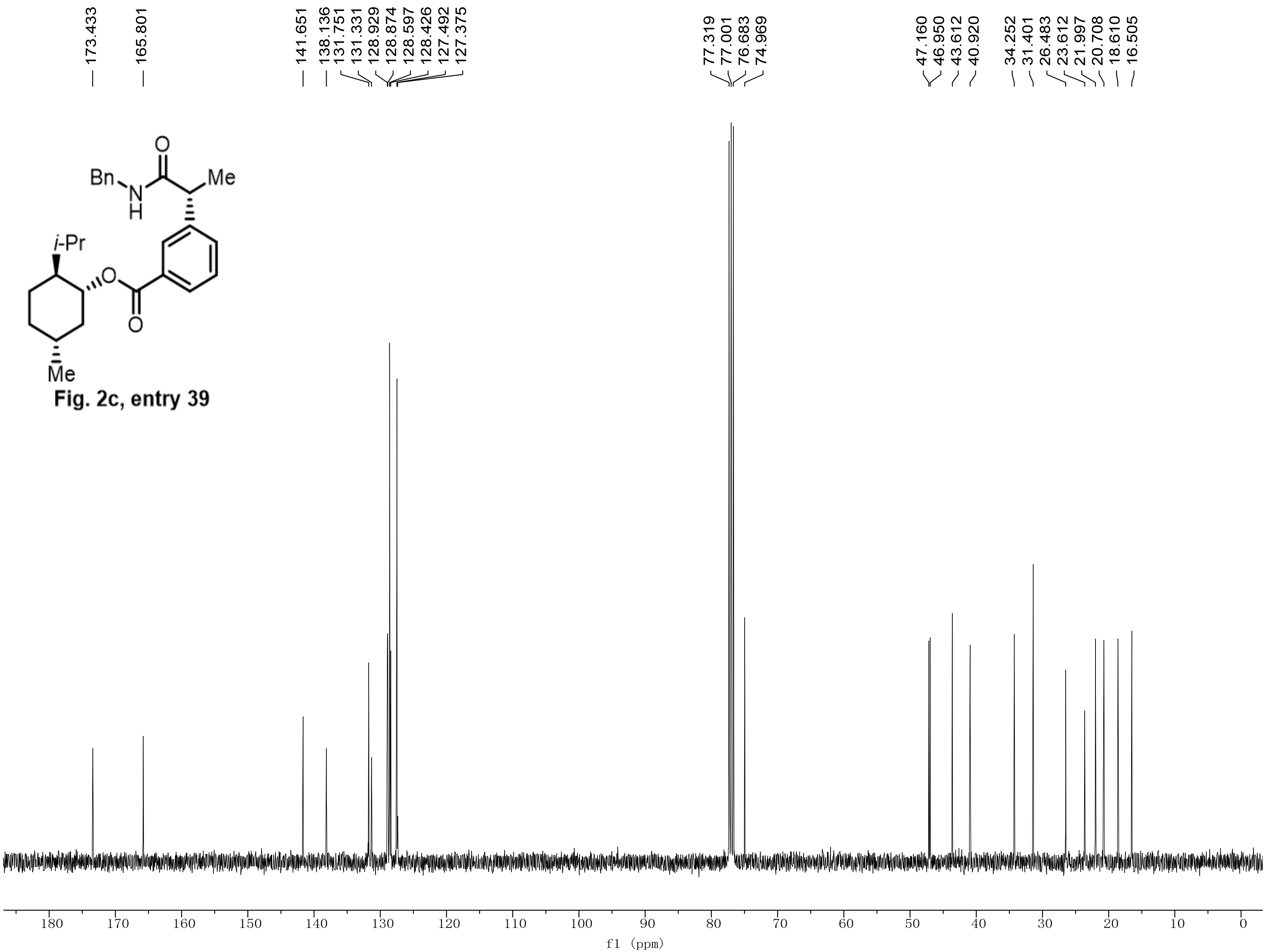


Fig. 2c, entry 39

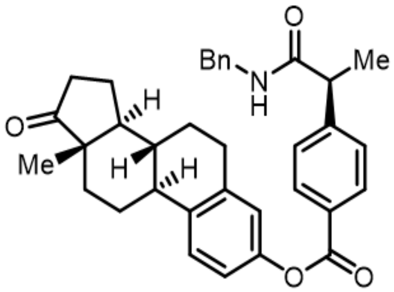
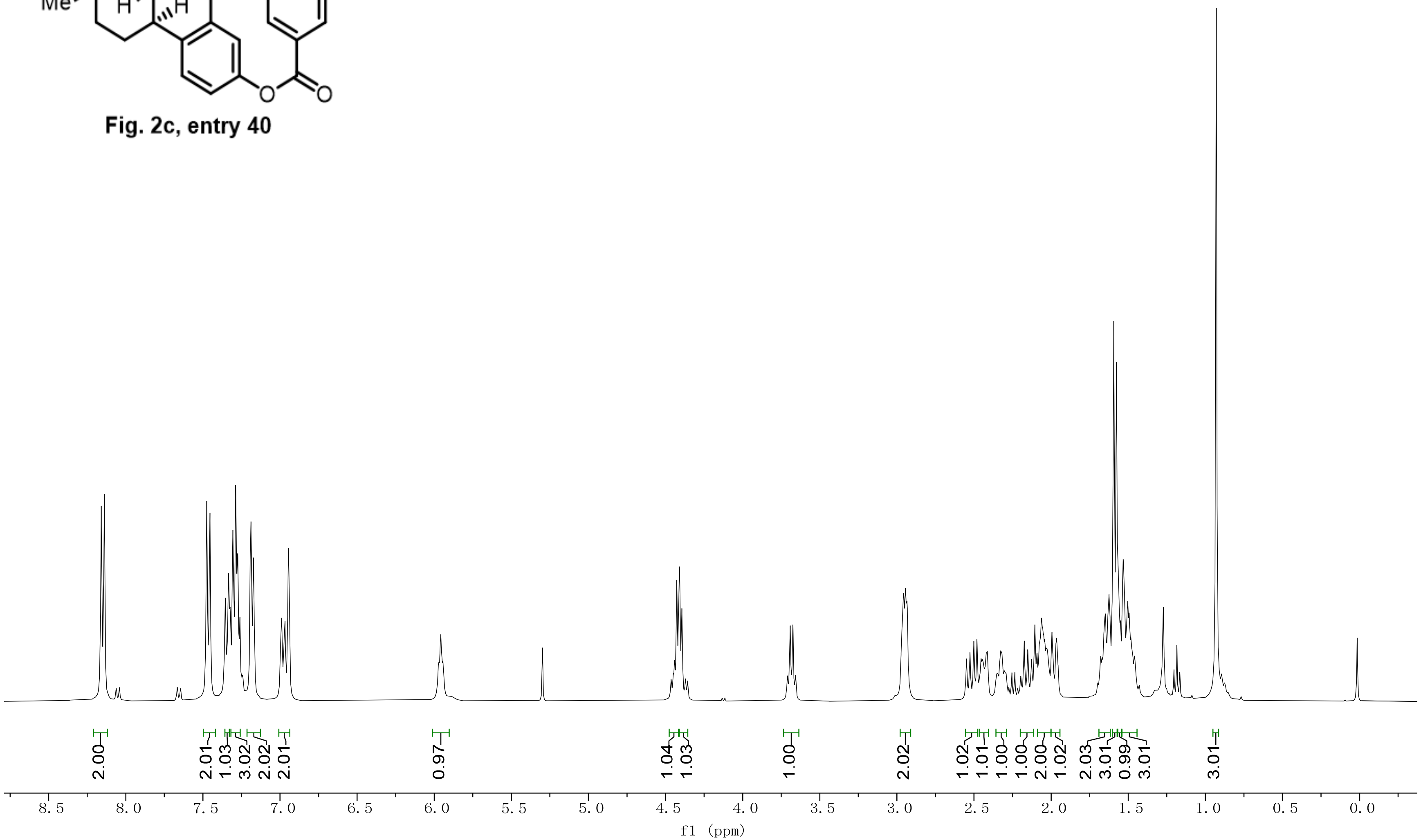


Fig. 2c, entry 40



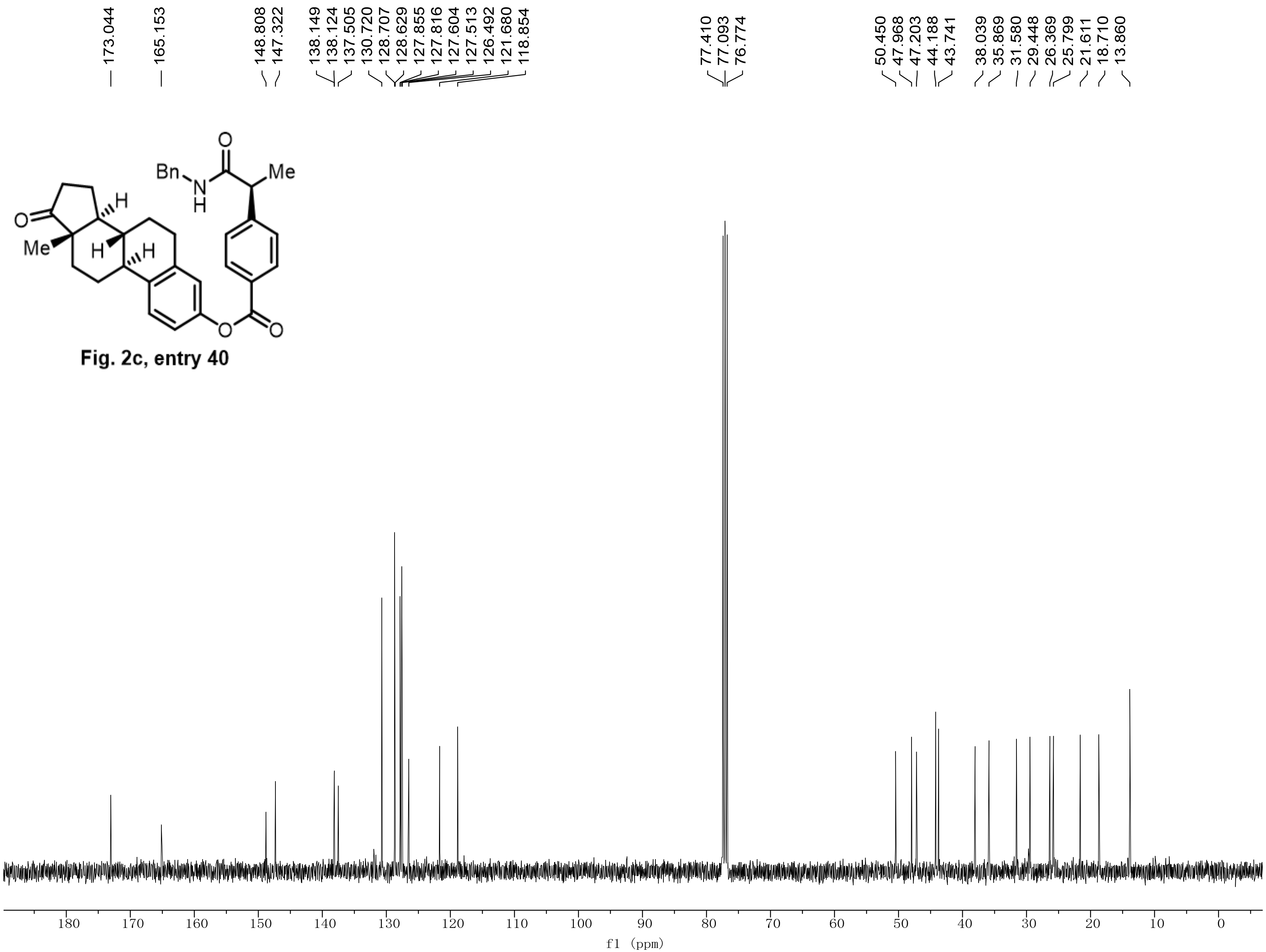


Fig. 2c, entry 40

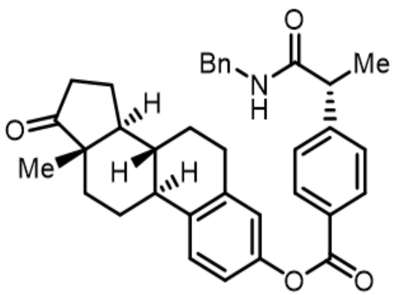
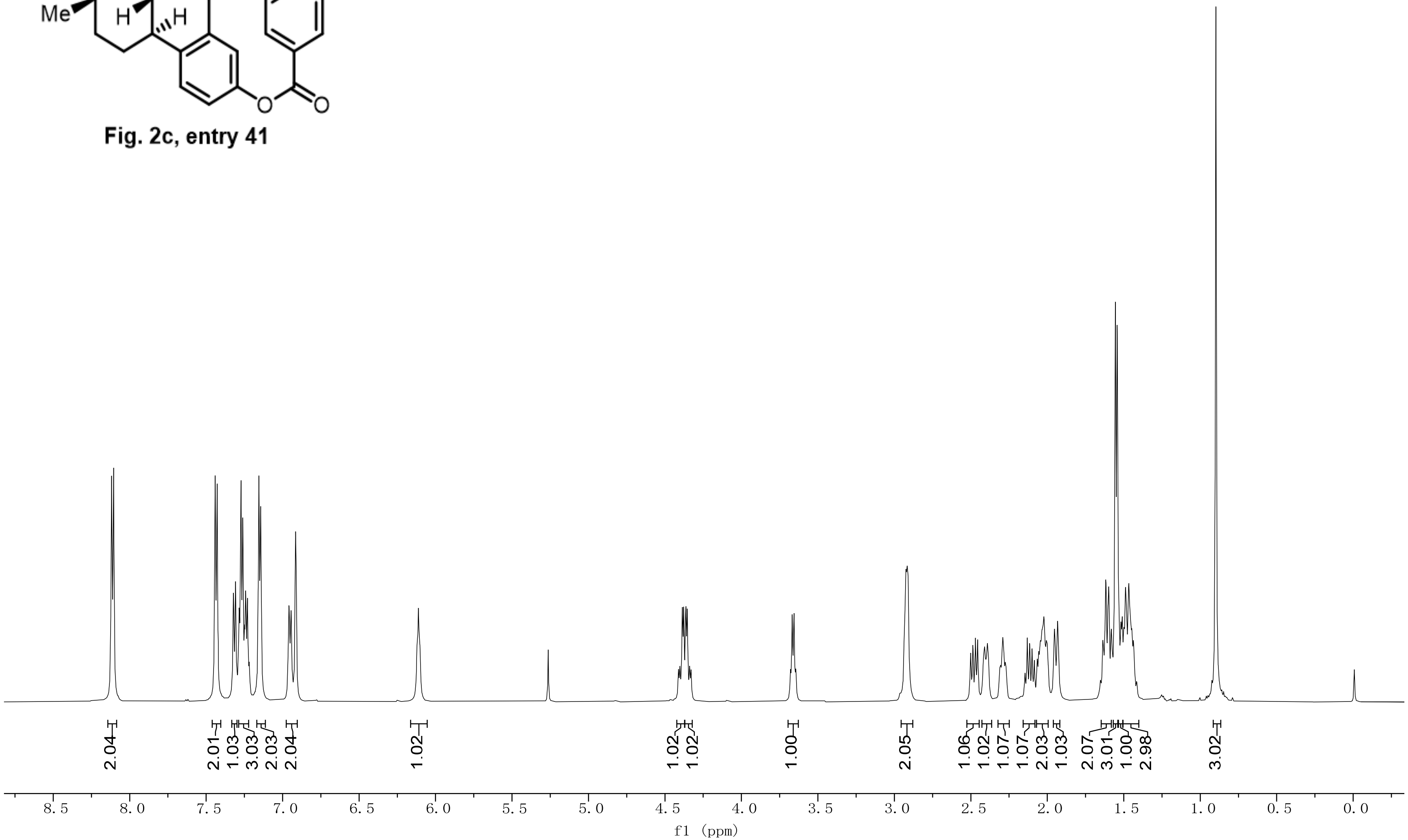


Fig. 2c, entry 41



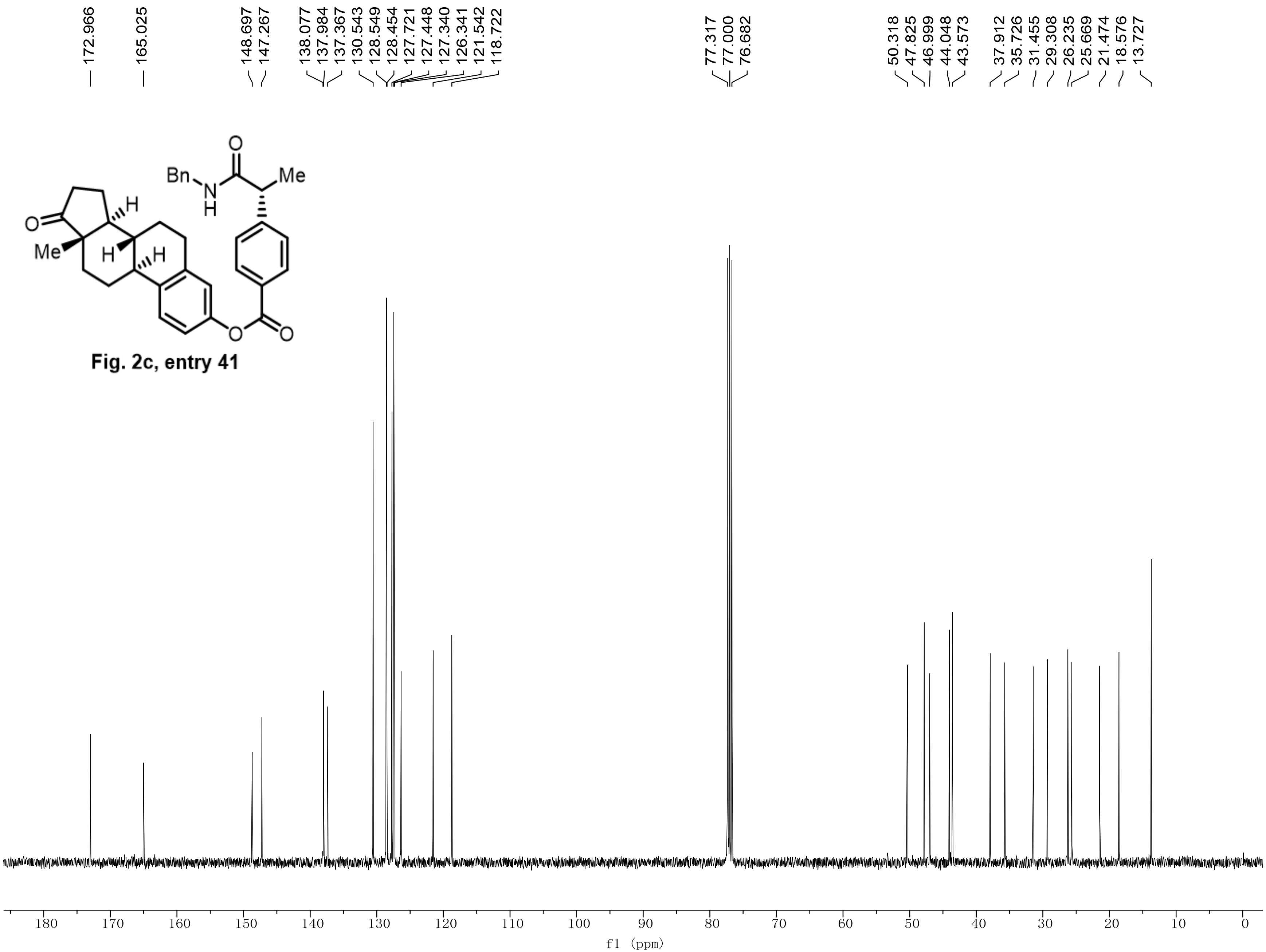


Fig. 2c, entry 41

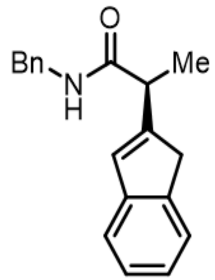
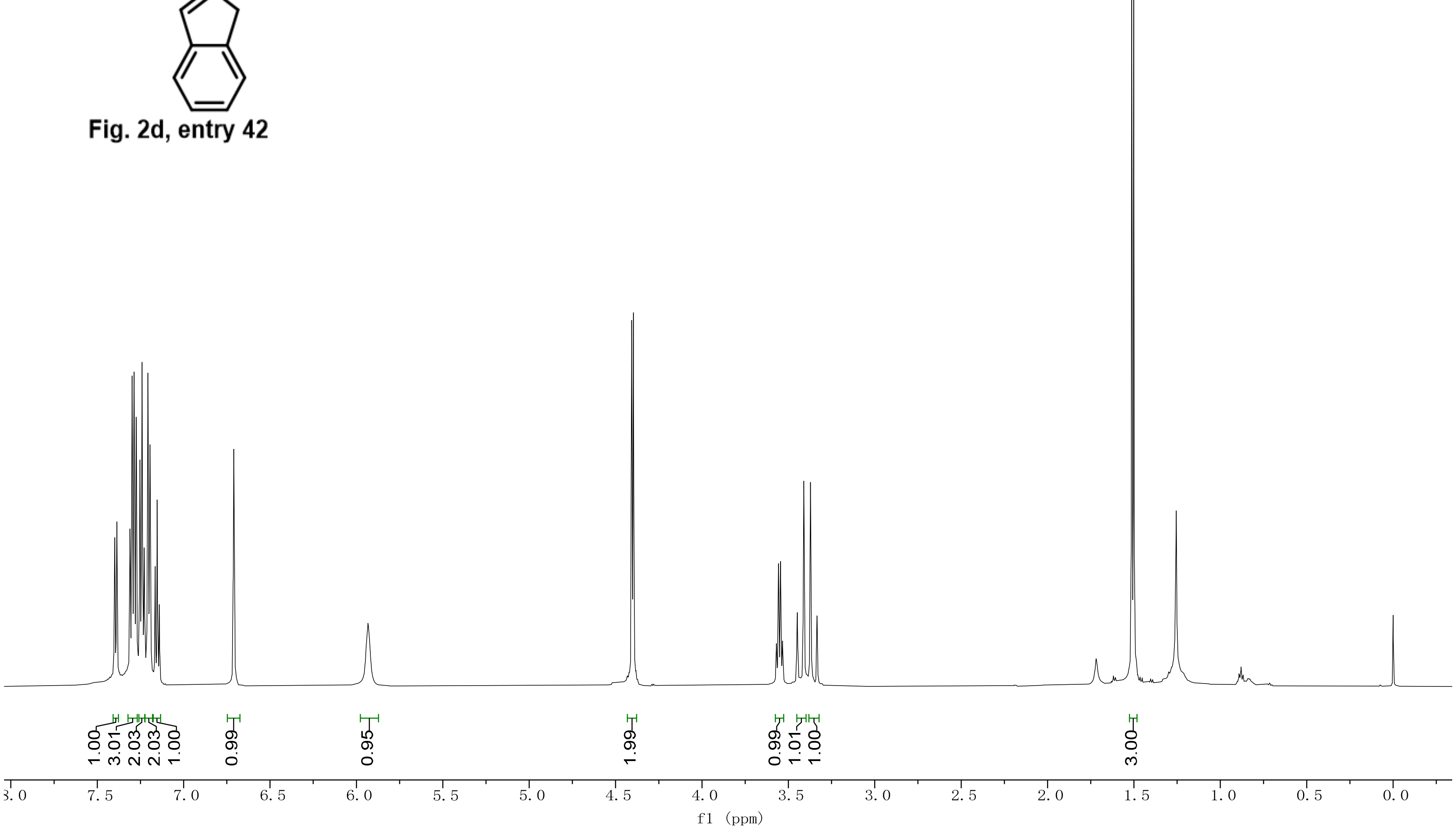
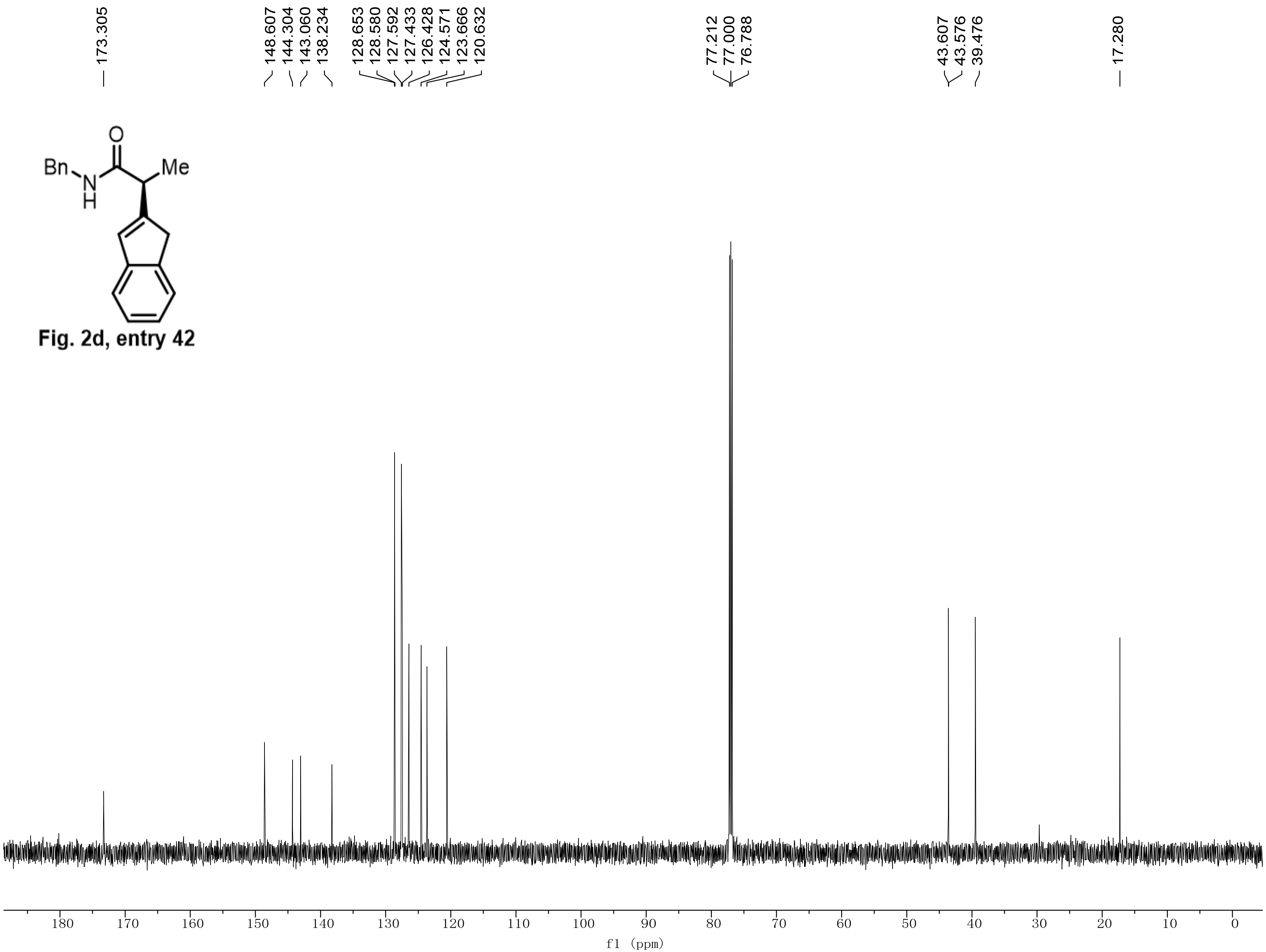


Fig. 2d, entry 42





Bn
N
H
O
Me
Fig. 2d, entry 42
173.305
148.607
144.304
143.060
138.234
128.653
128.580
127.592
127.433
126.428
124.571
123.666
120.632
77.212
77.000
76.788
43.607
43.576
39.476
17.280
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

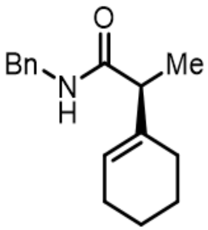
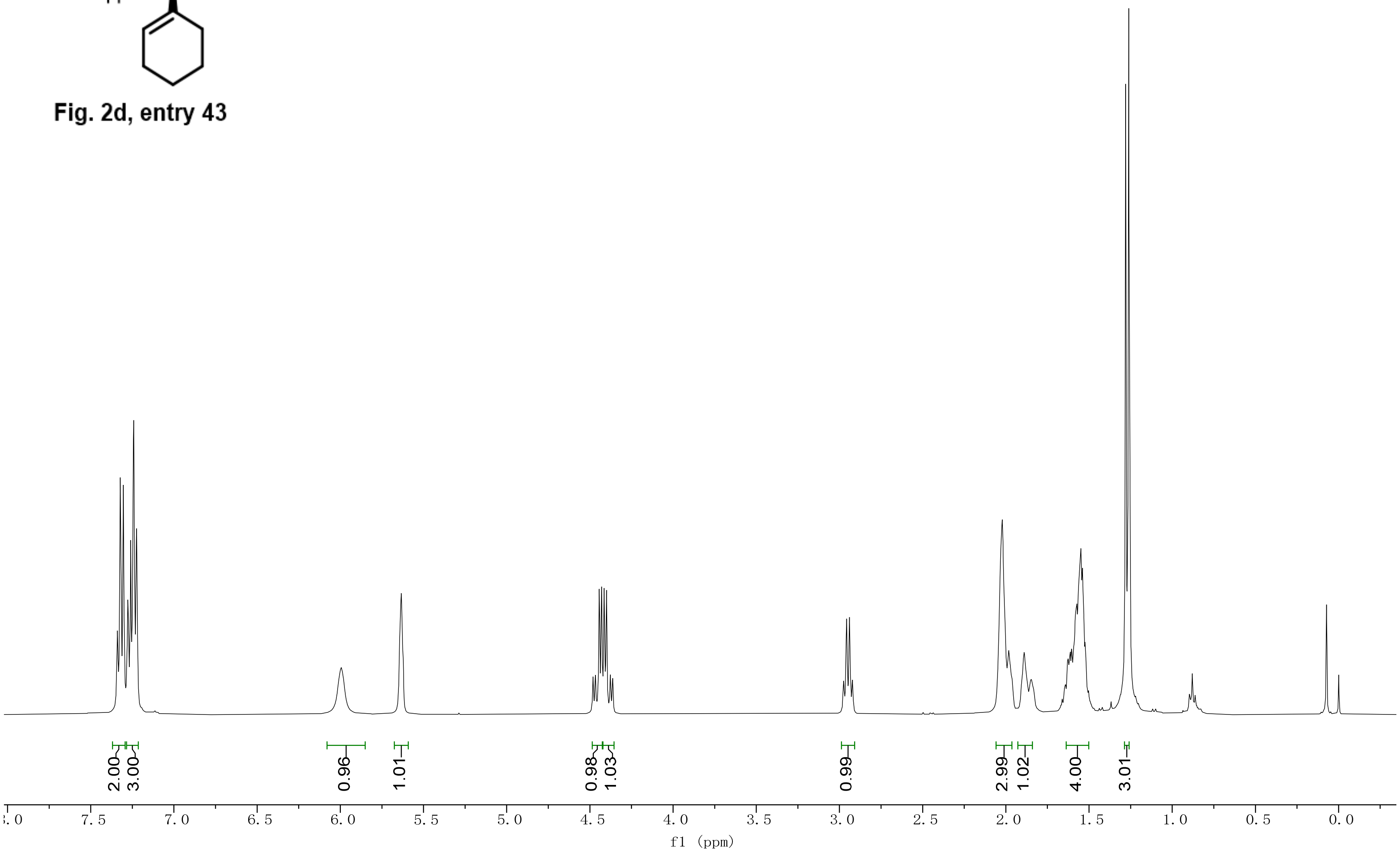


Fig. 2d, entry 43



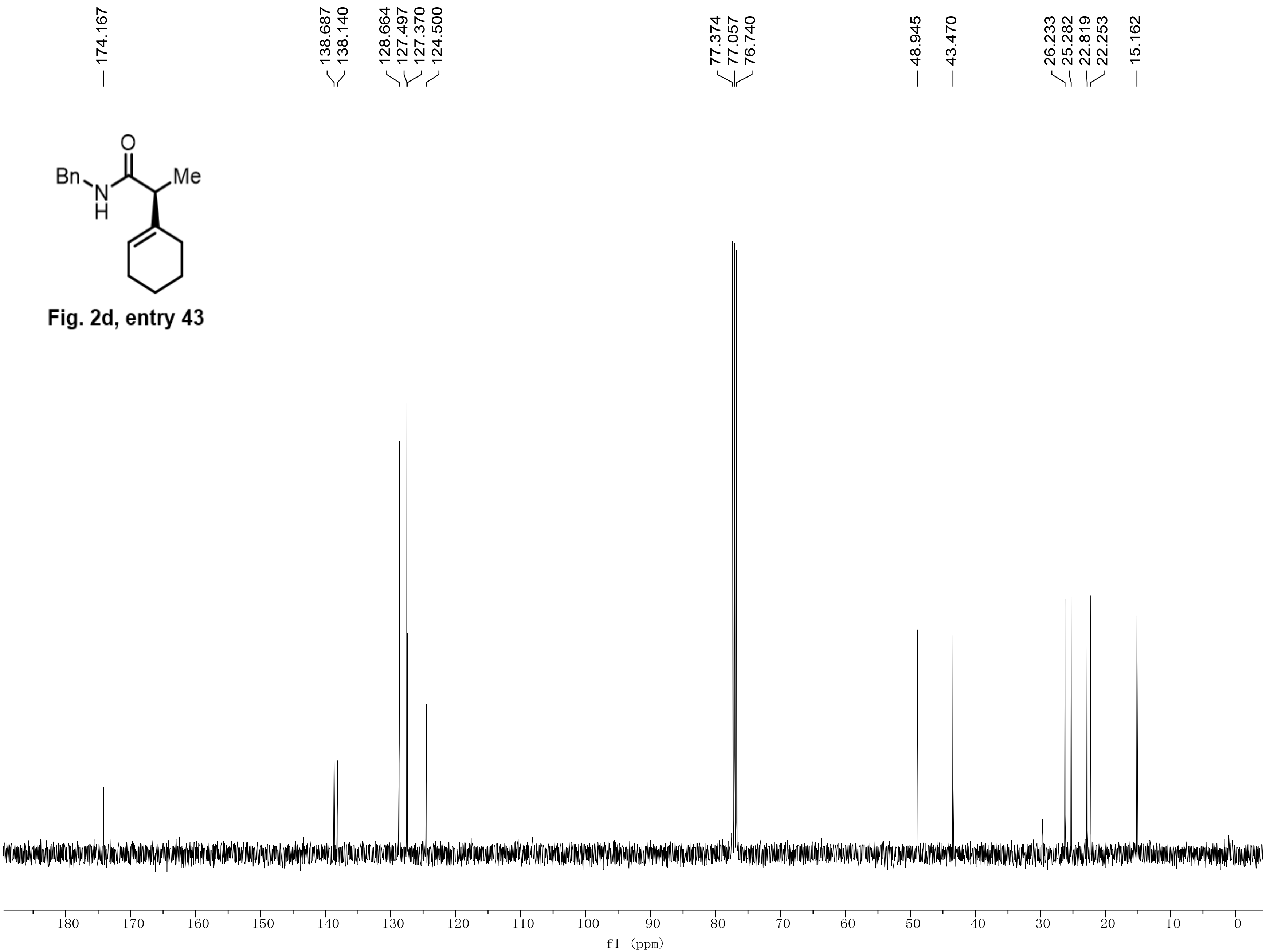


Fig. 2d, entry 43

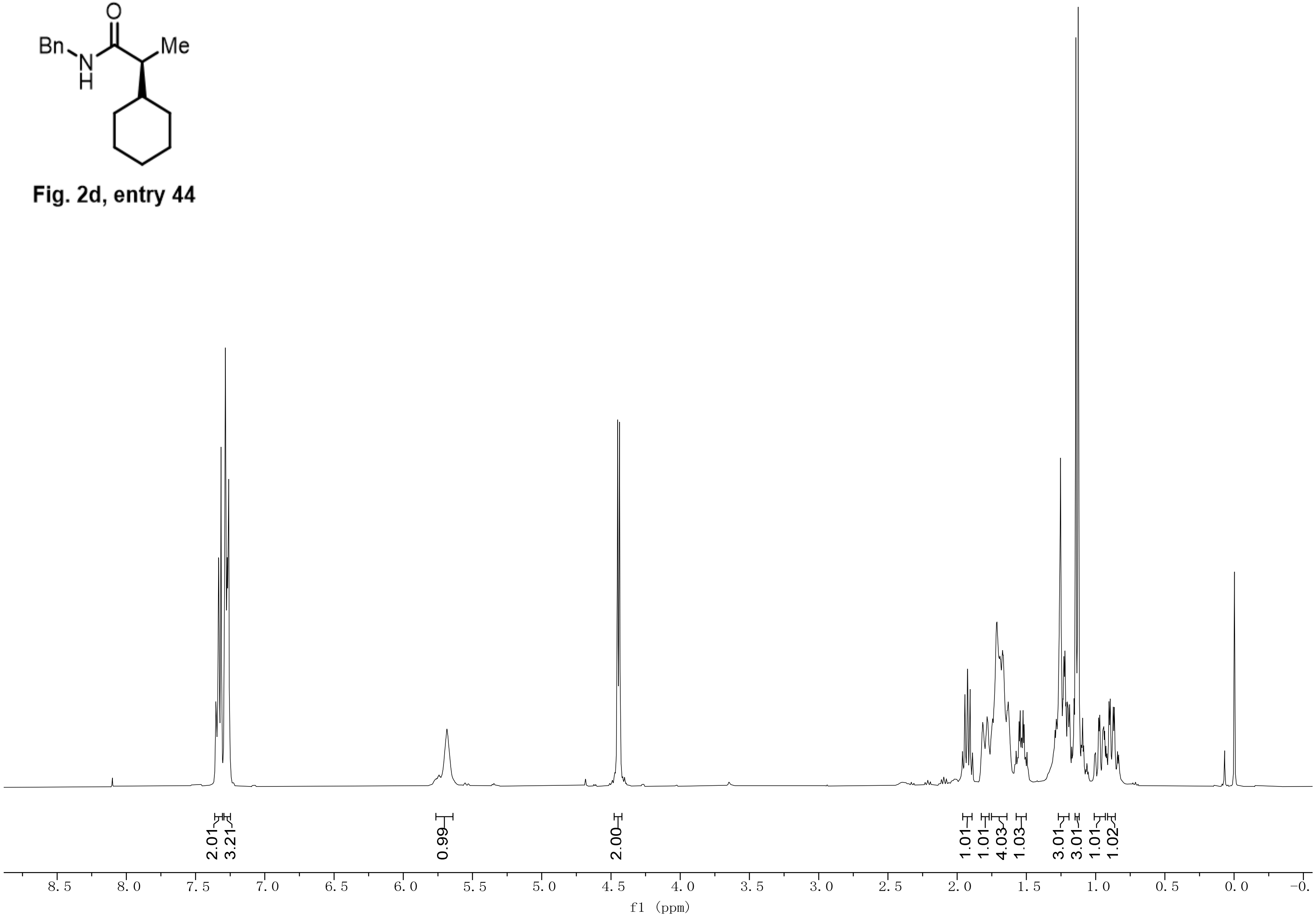


Fig. 2d, entry 44

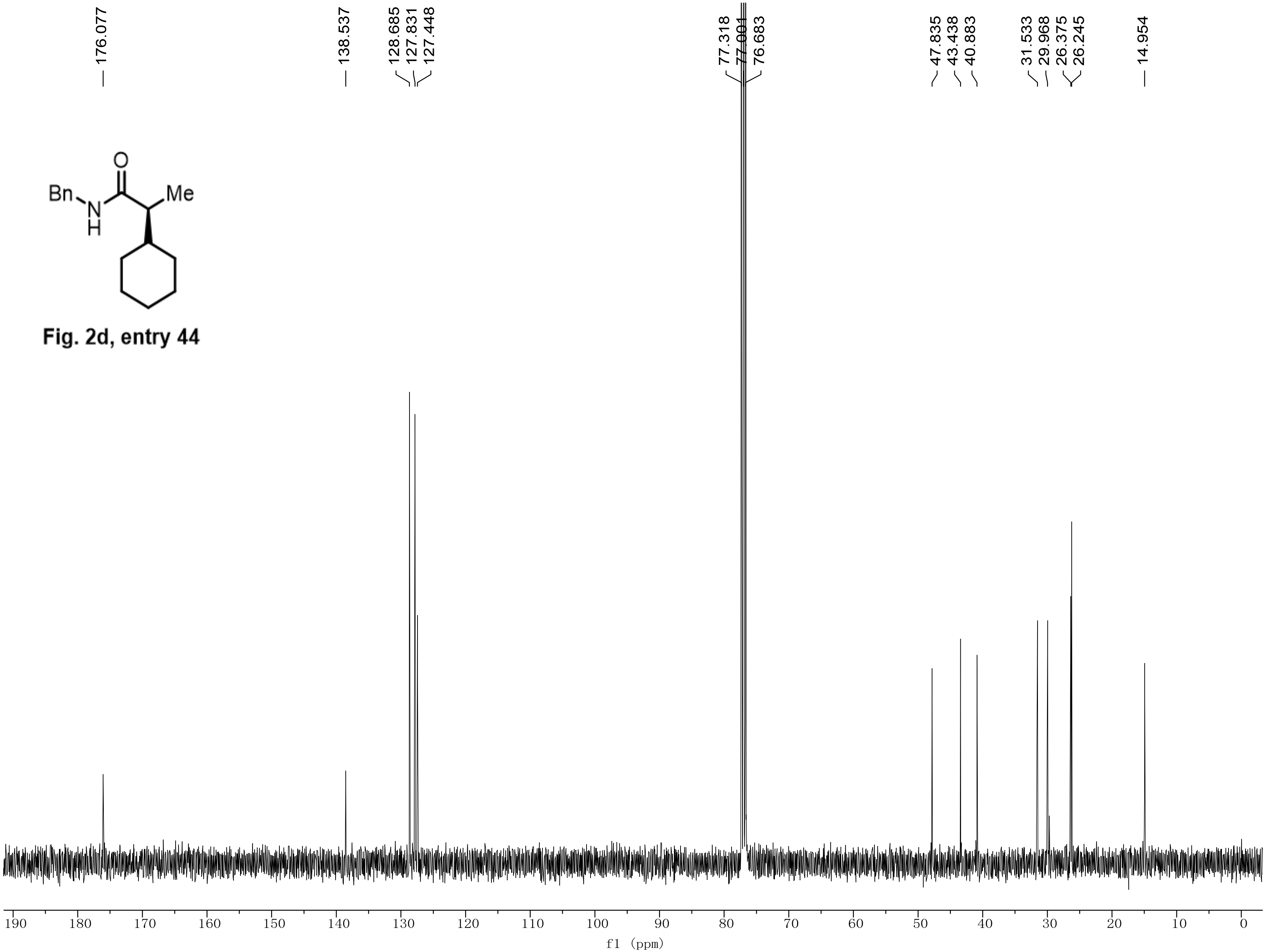


Fig. 2d, entry 44

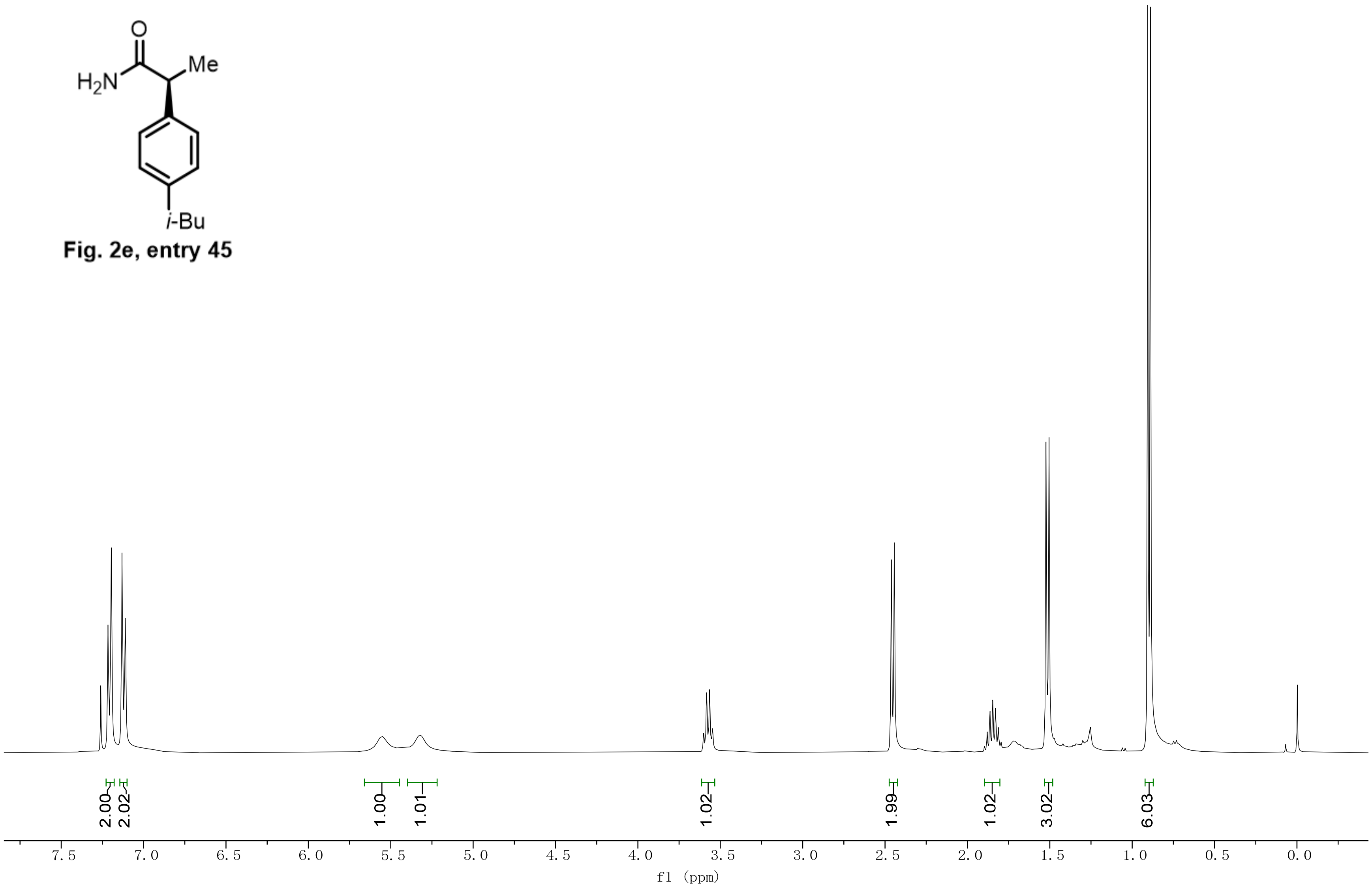
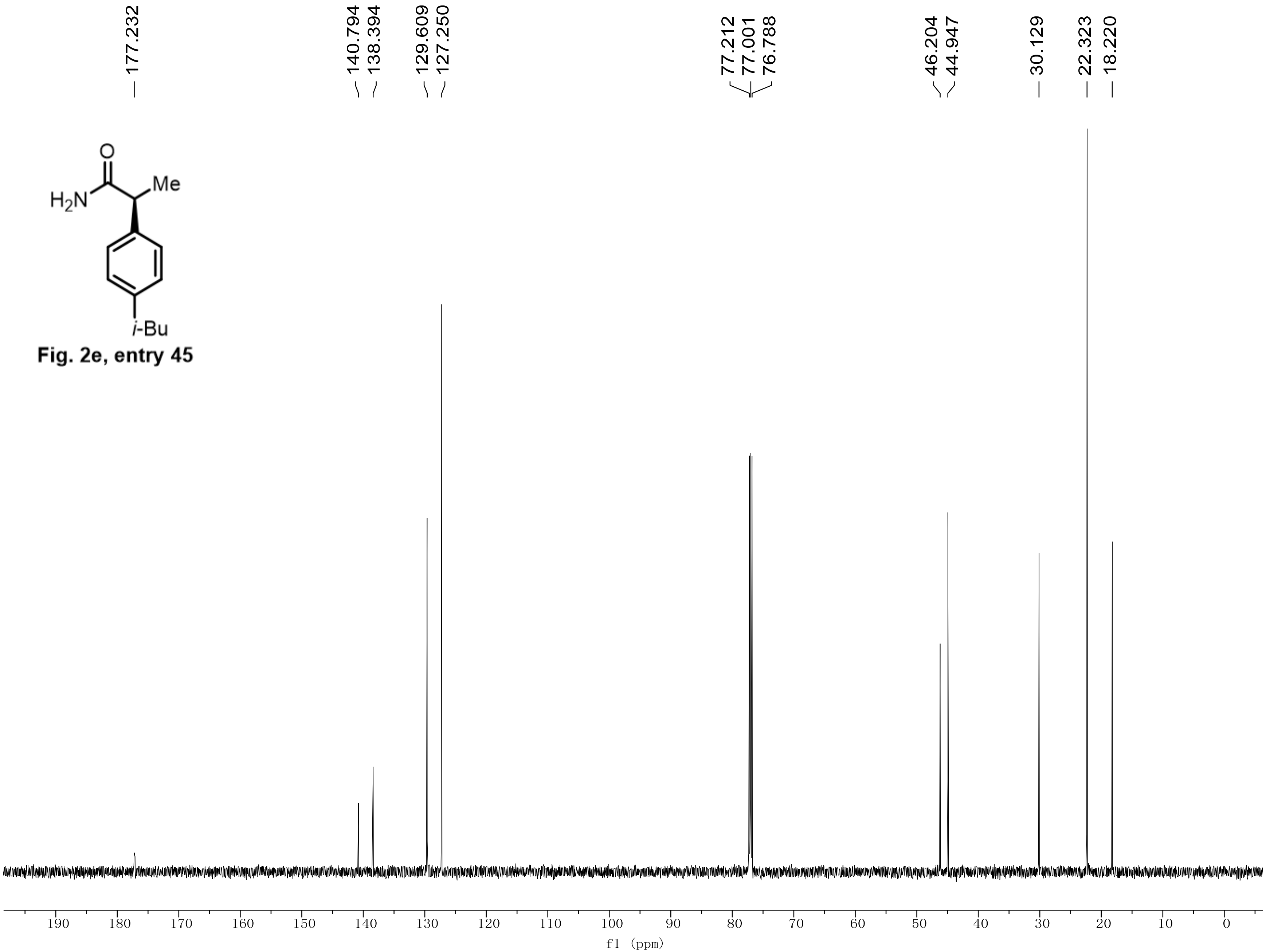


Fig. 2e, entry 45



177.232
140.794
138.394
129.609
127.250
77.212
77.001
76.788
46.204
44.947
30.129
22.323
18.220
O
H2N
Me
i-Bu
Fig. 2e, entry 45
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

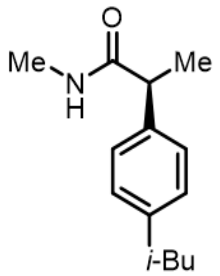
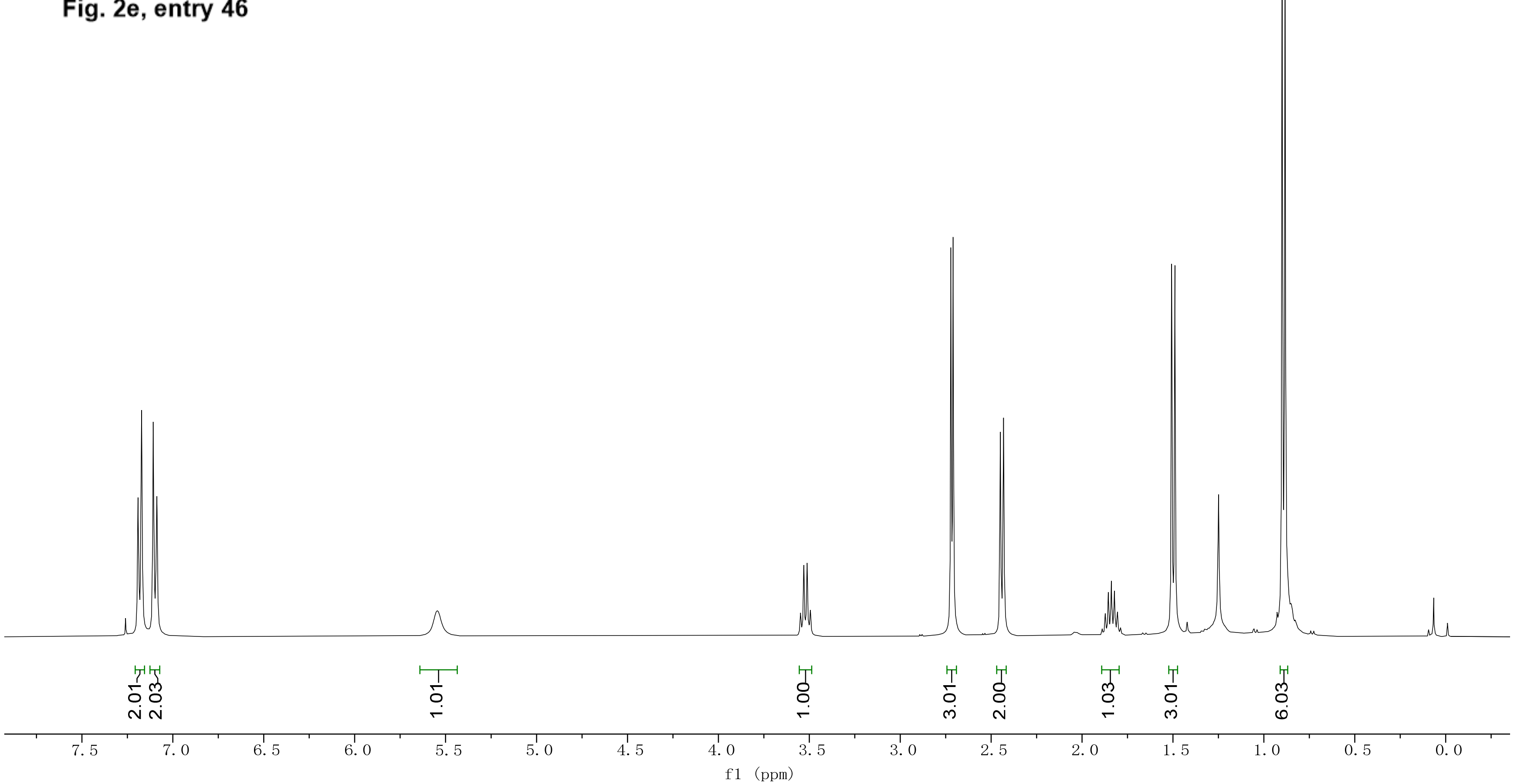
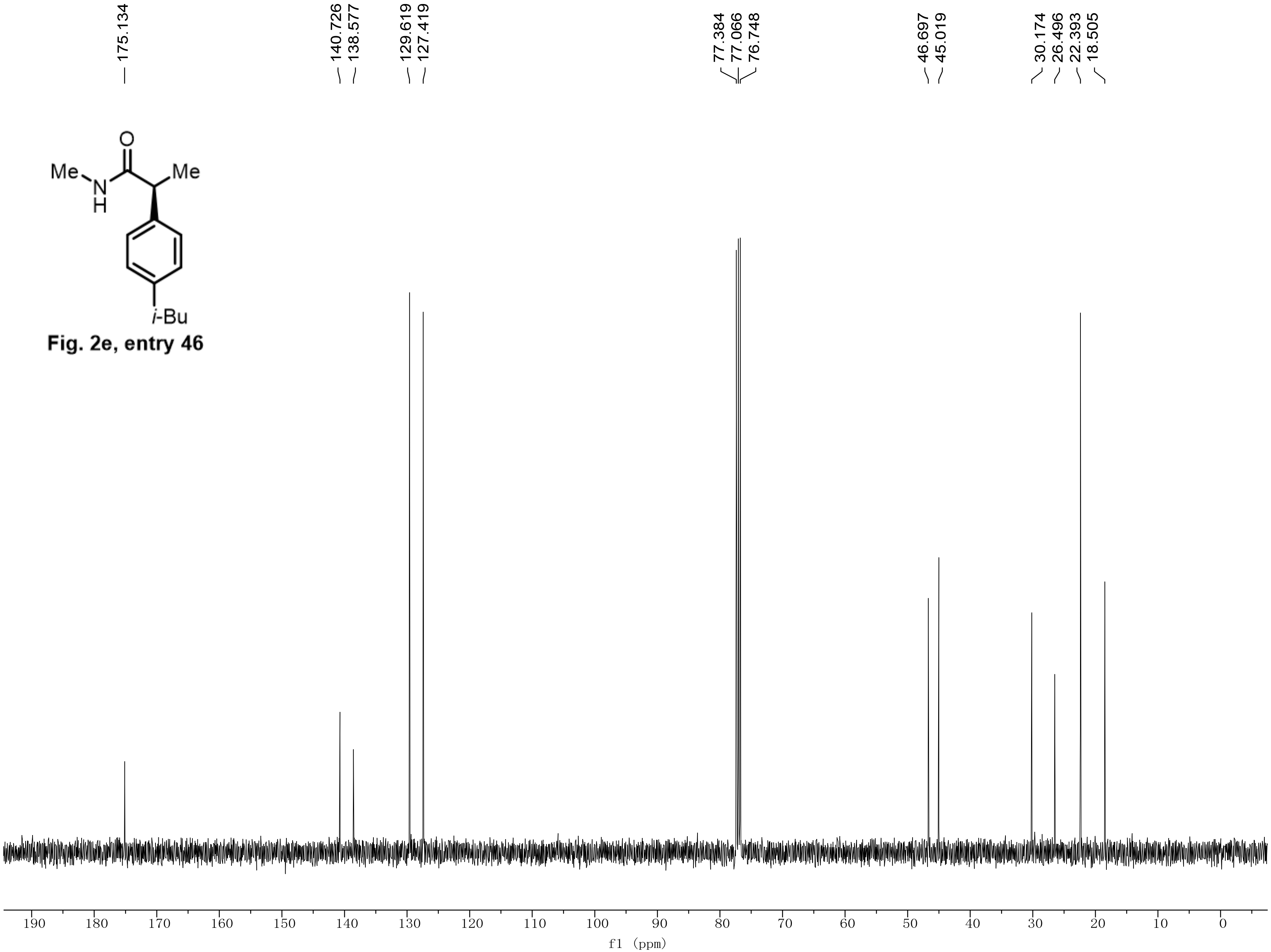


Fig. 2e, entry 46




O
Me
N
H
Me
i-Bu
Fig. 2e, entry 46
175.134
140.726
138.577
129.619
127.419
77.384
77.066
76.748
46.697
45.019
30.174
26.496
22.393
18.505
190
180
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20
10
0
f1 (ppm)

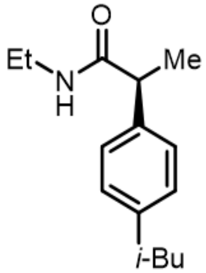
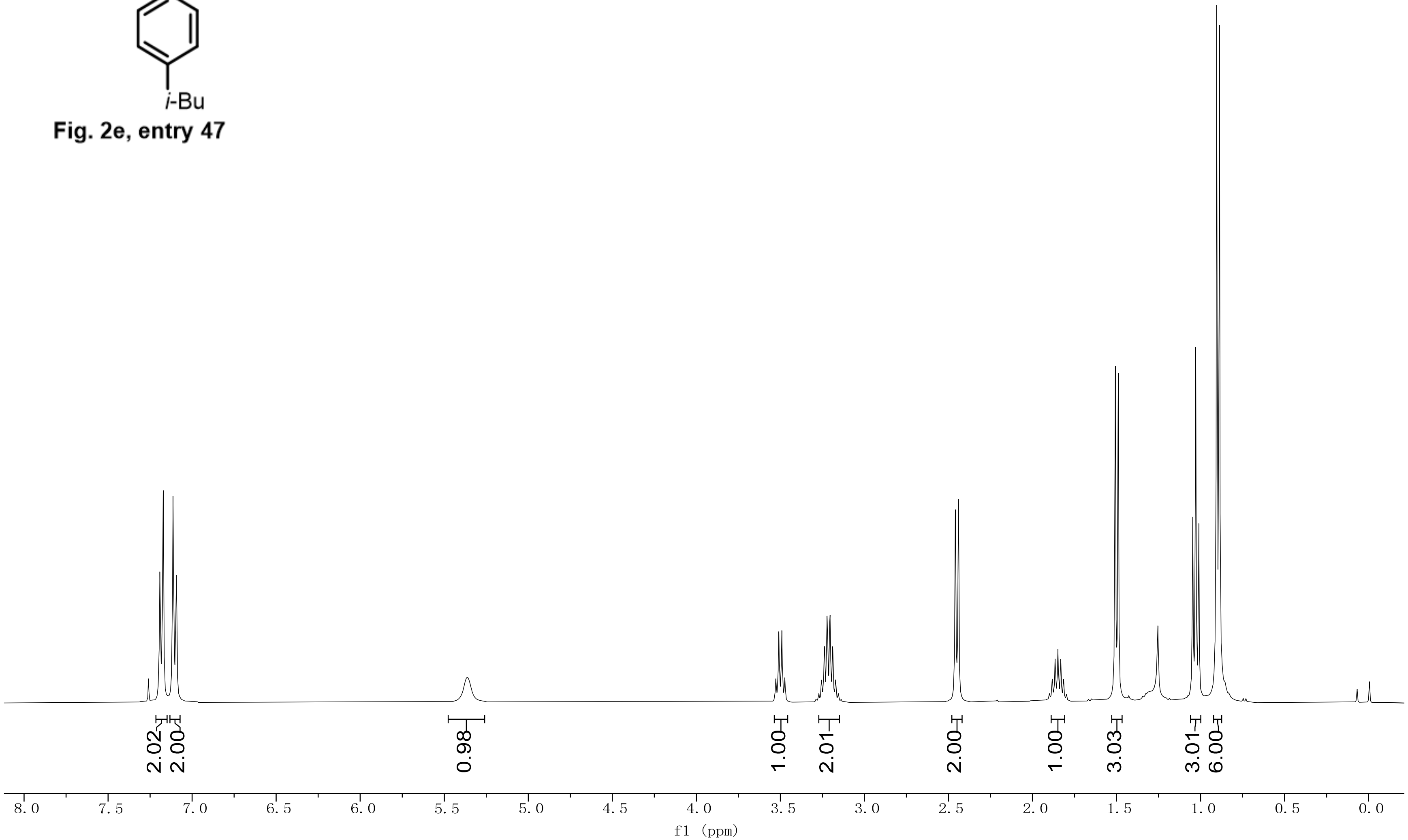


Fig. 2e, entry 47



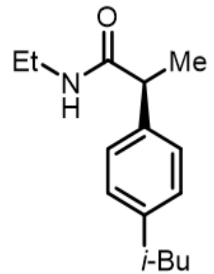
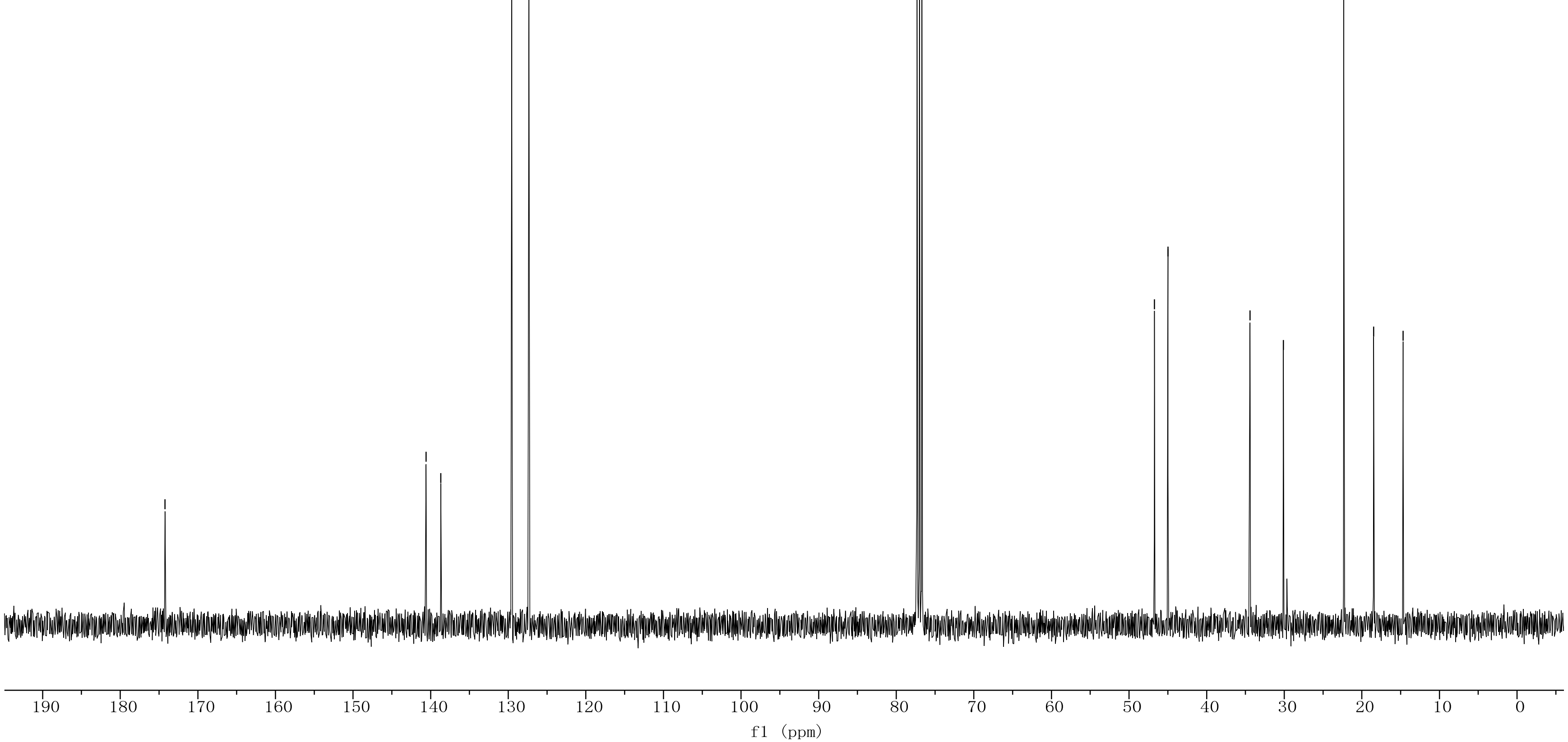


Fig. 2e, entry 47



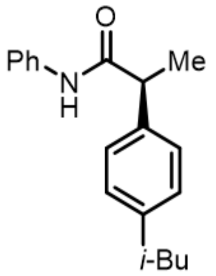
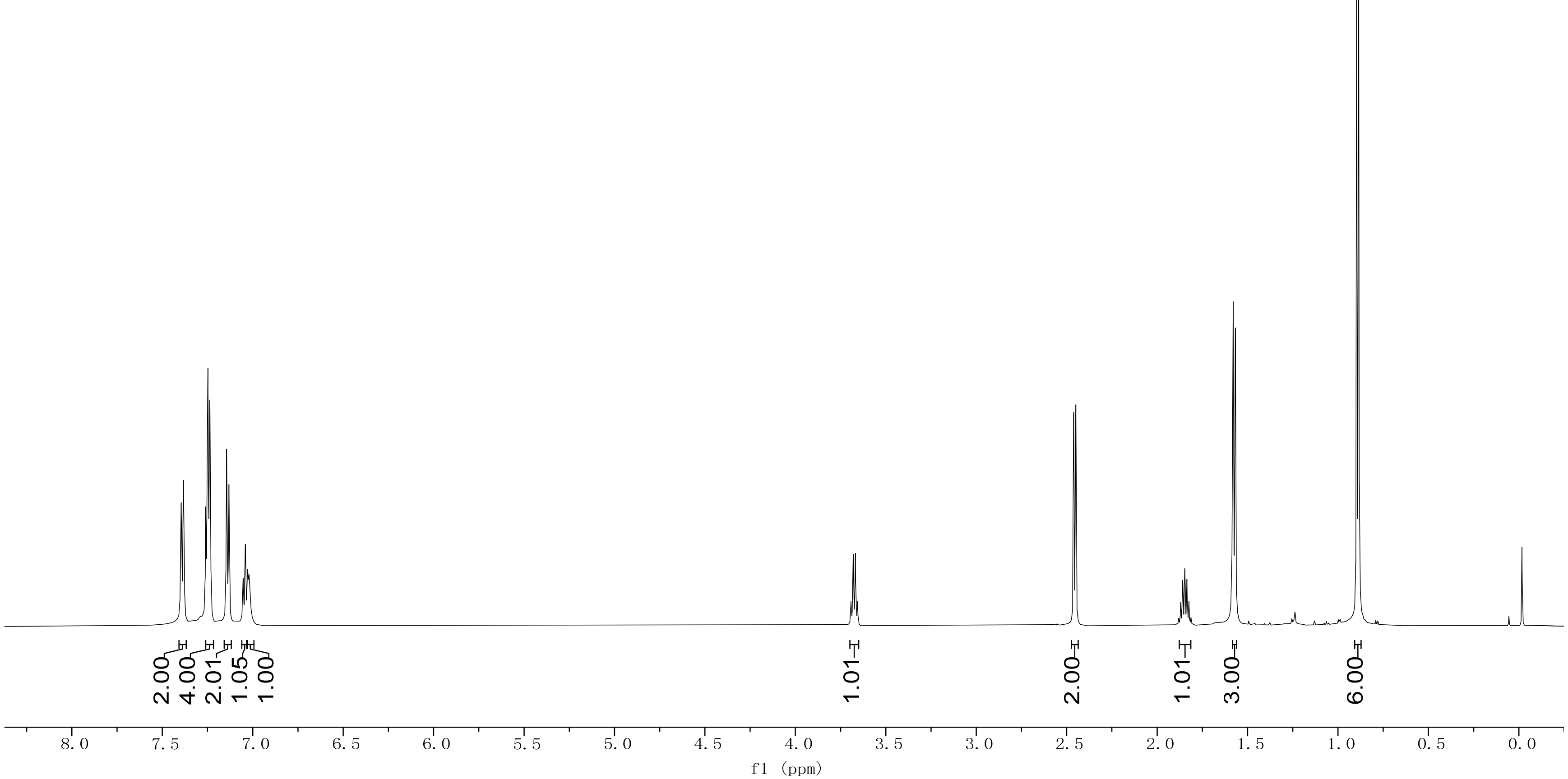


Fig. 2e, entry 48



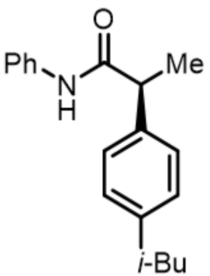
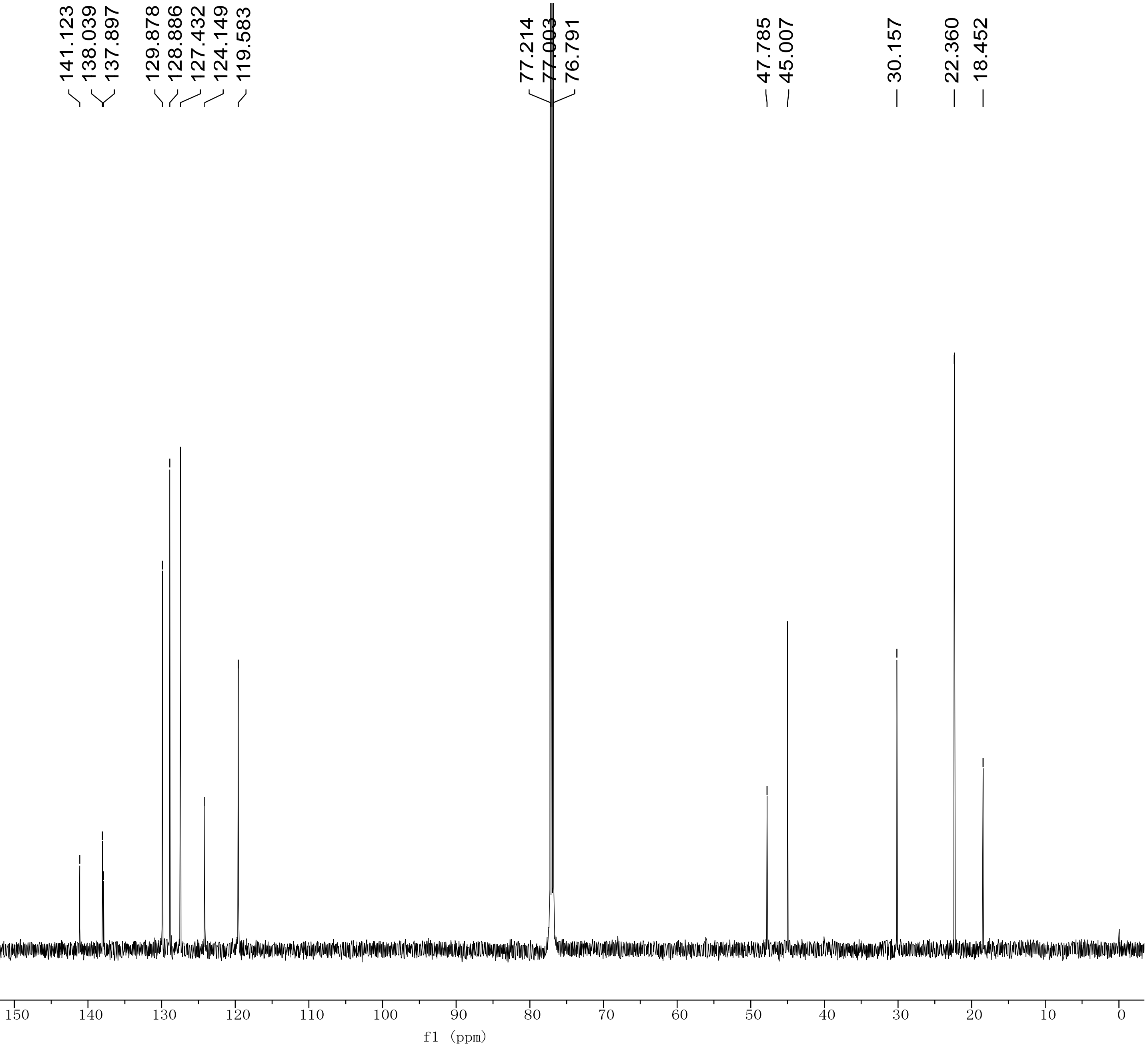


Fig. 2e, entry 48



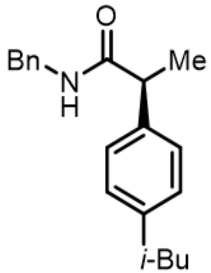
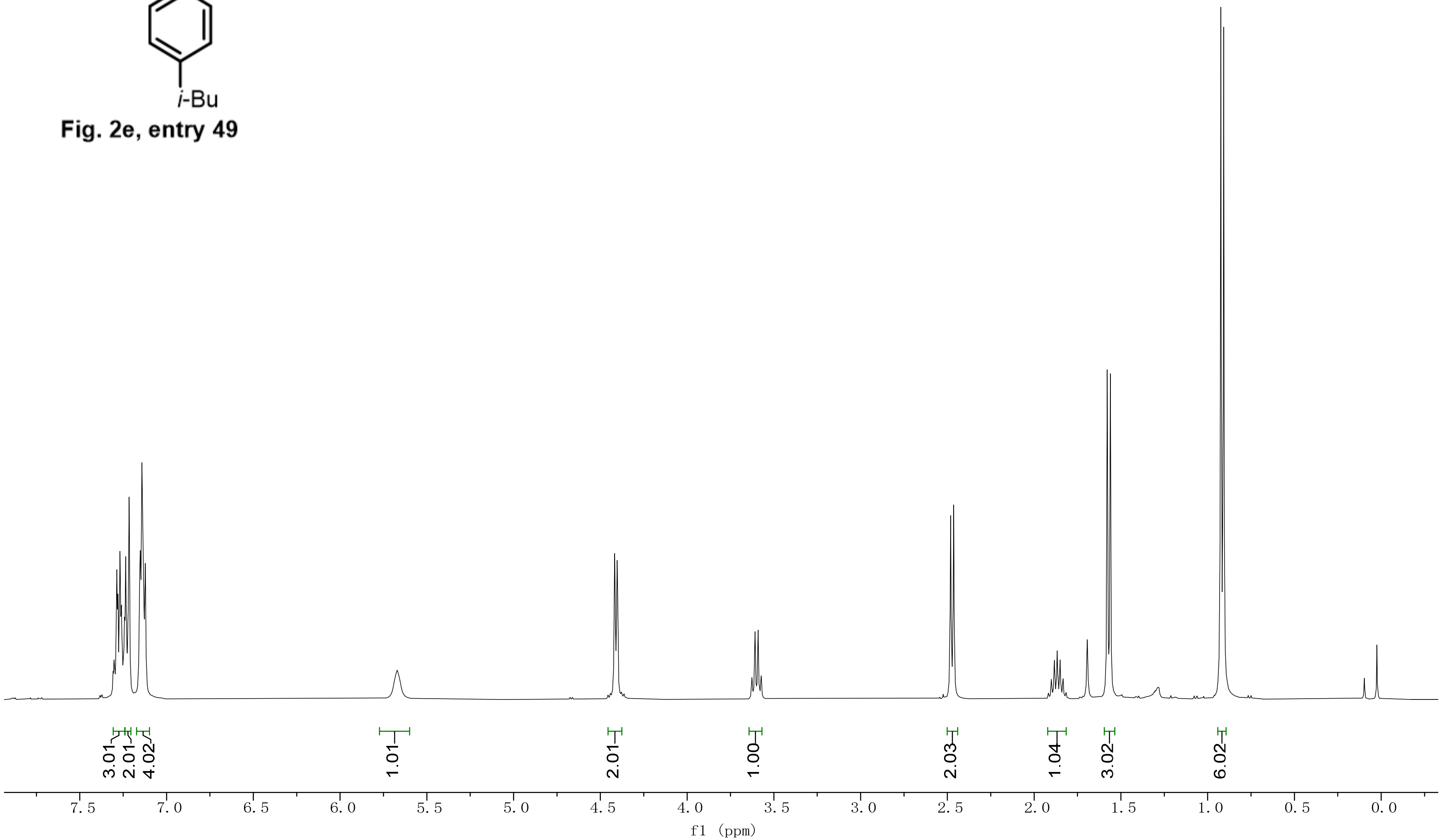


Fig. 2e, entry 49



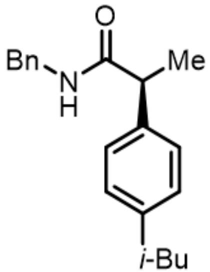
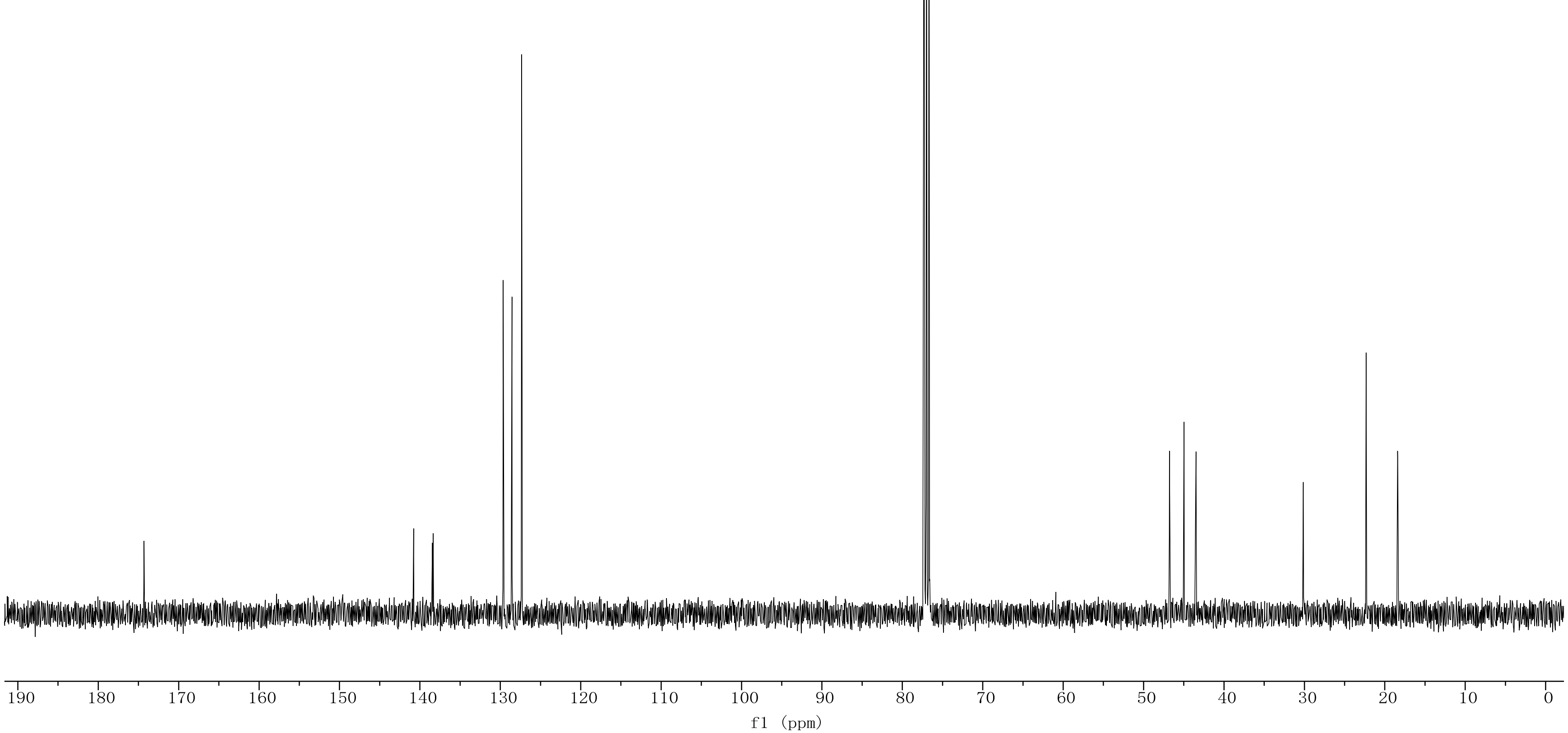


Fig. 2e, entry 49



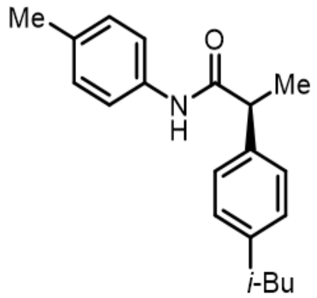
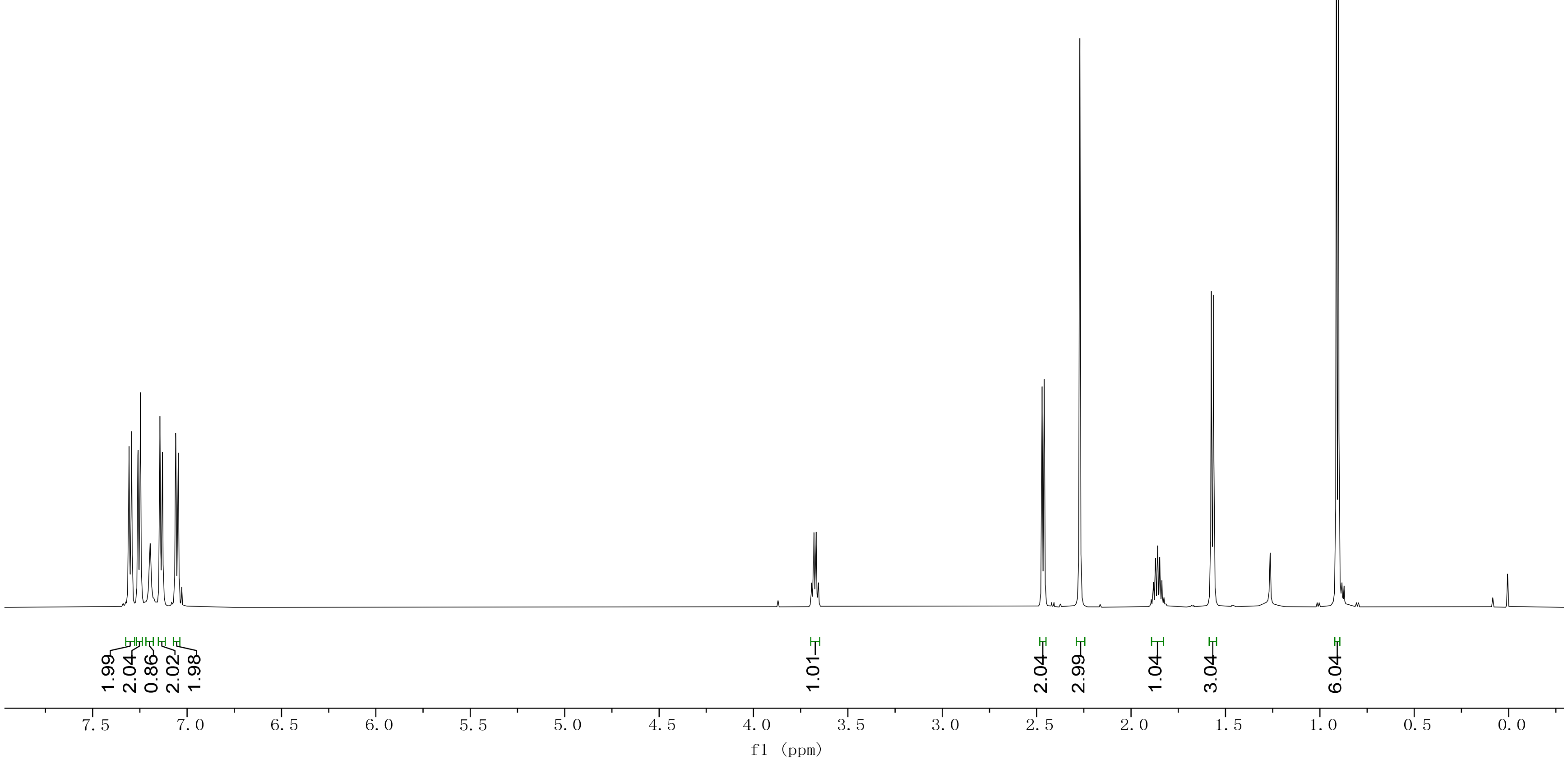


Fig. 2e, entry 50



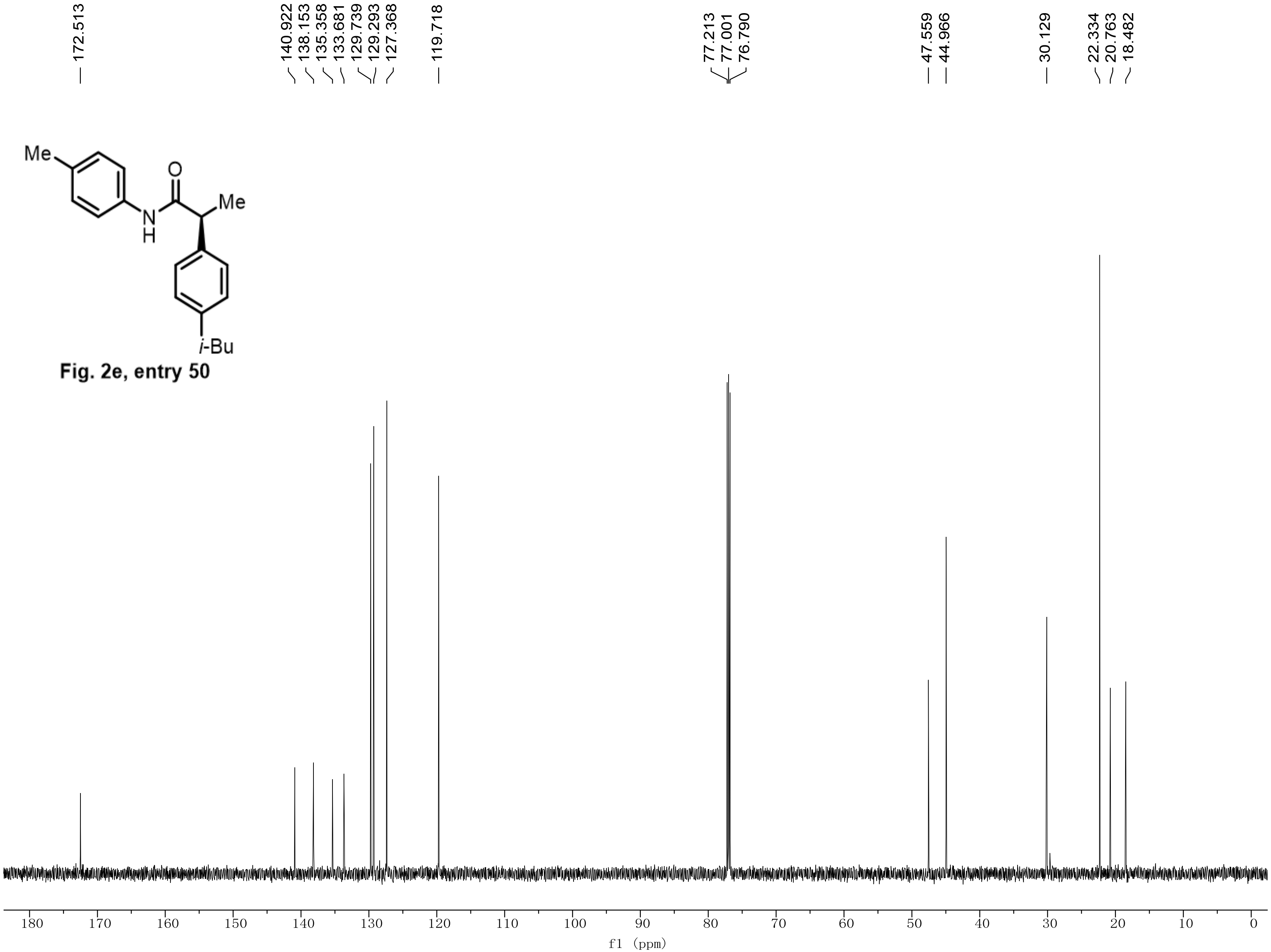


Fig. 2e, entry 50

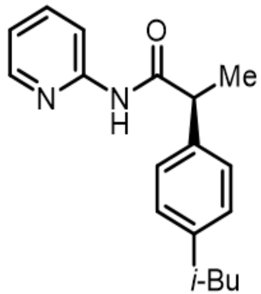
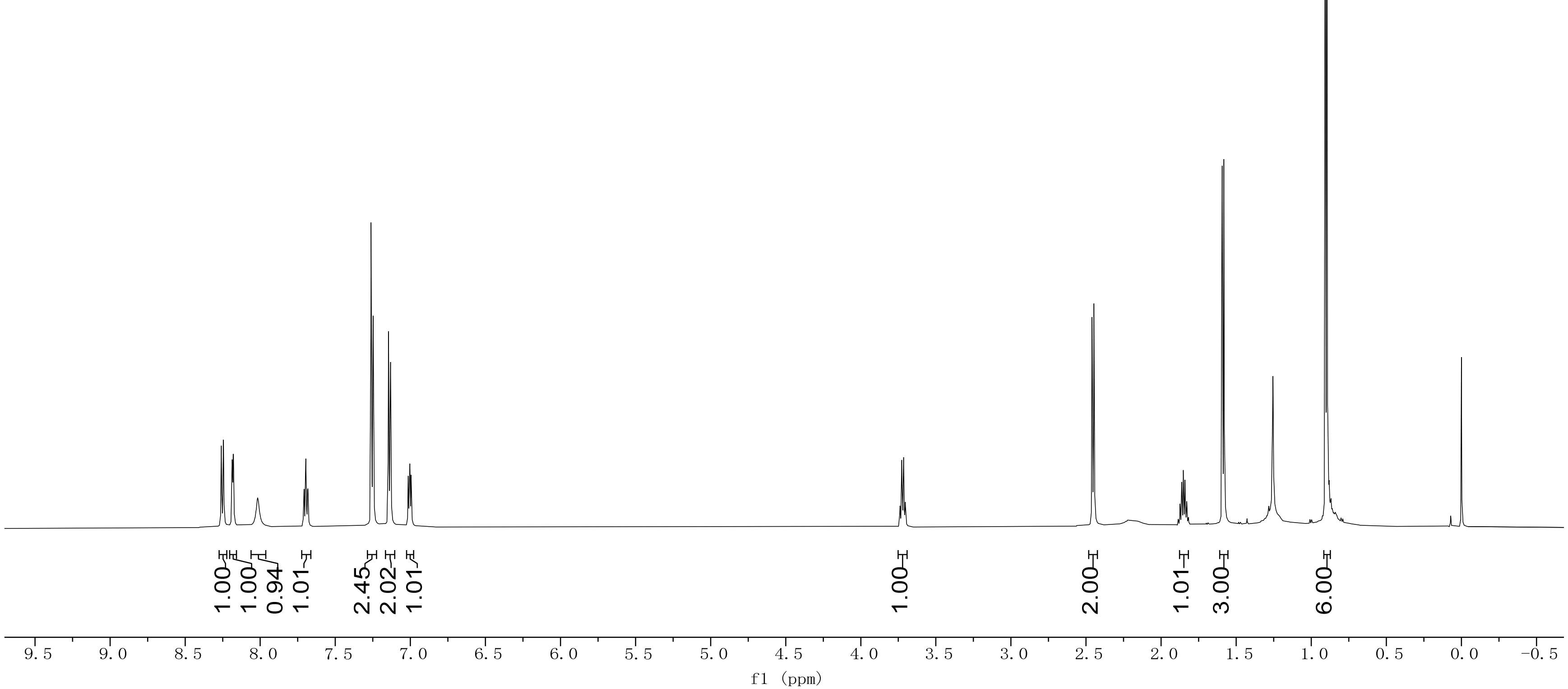


Fig. 2e, entry 51



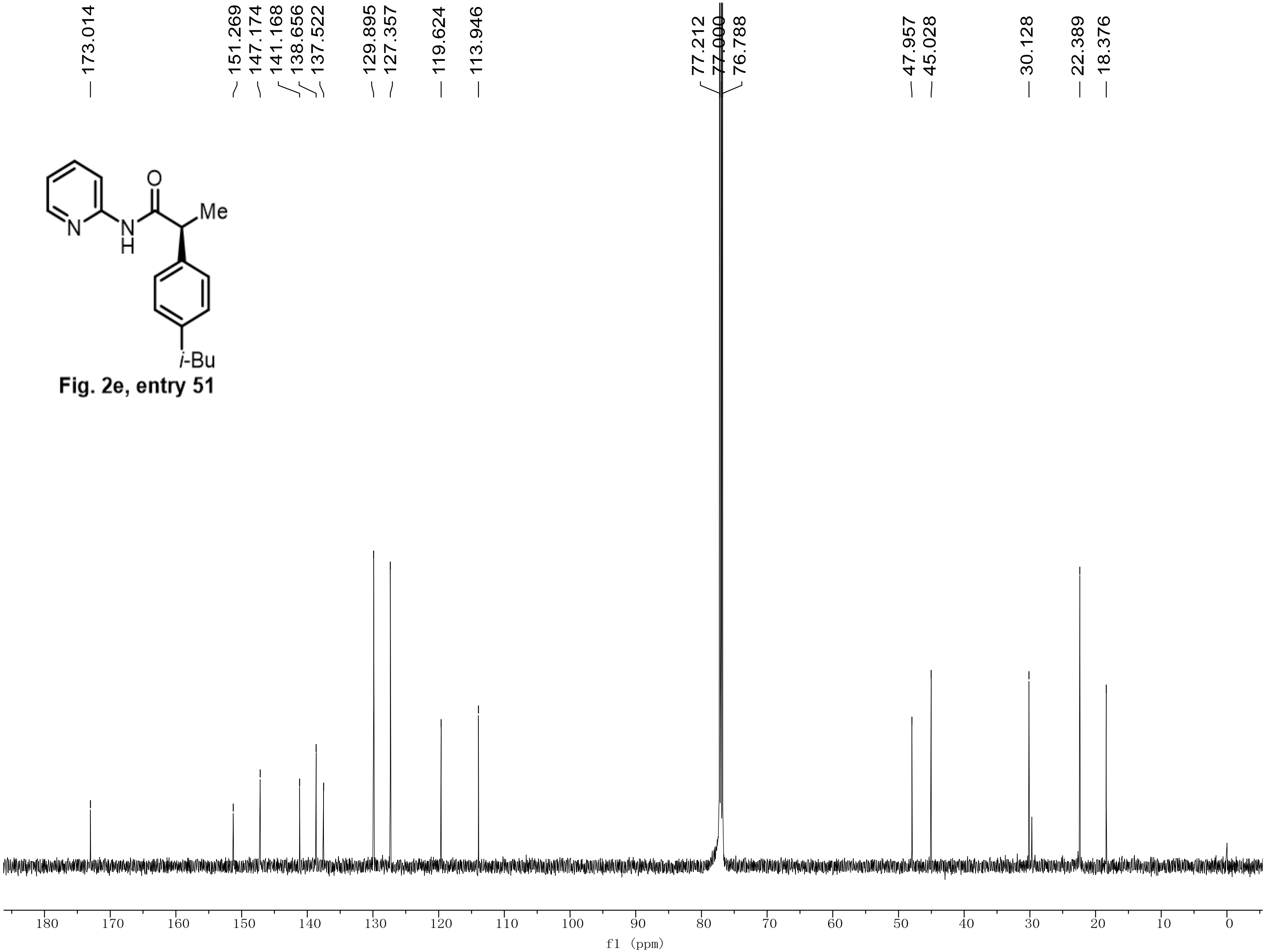


Fig. 2e, entry 51

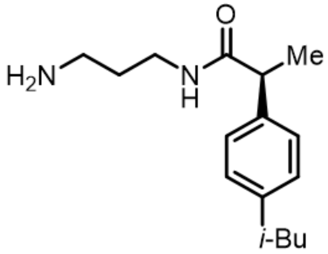
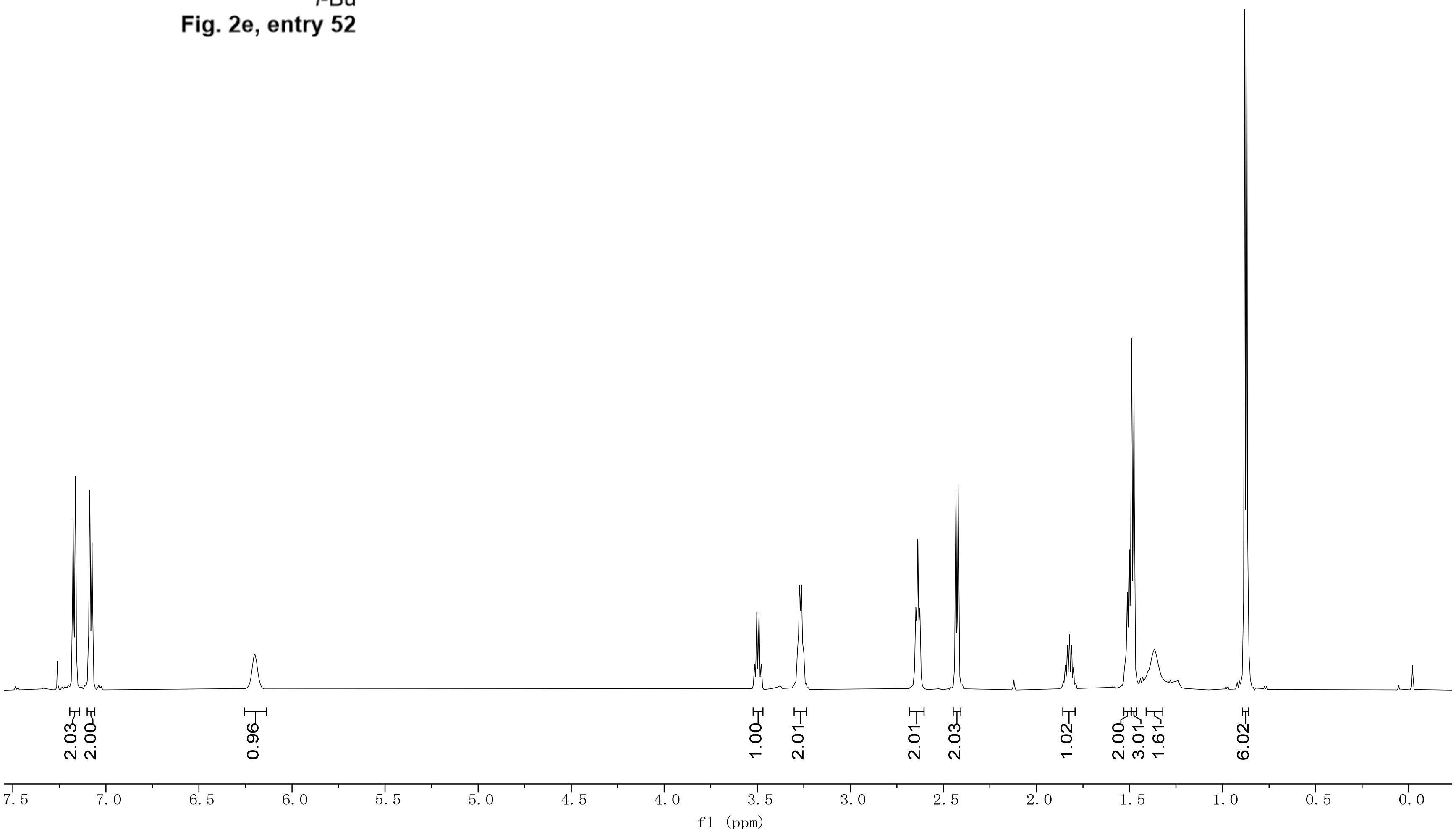


Fig. 2e, entry 52



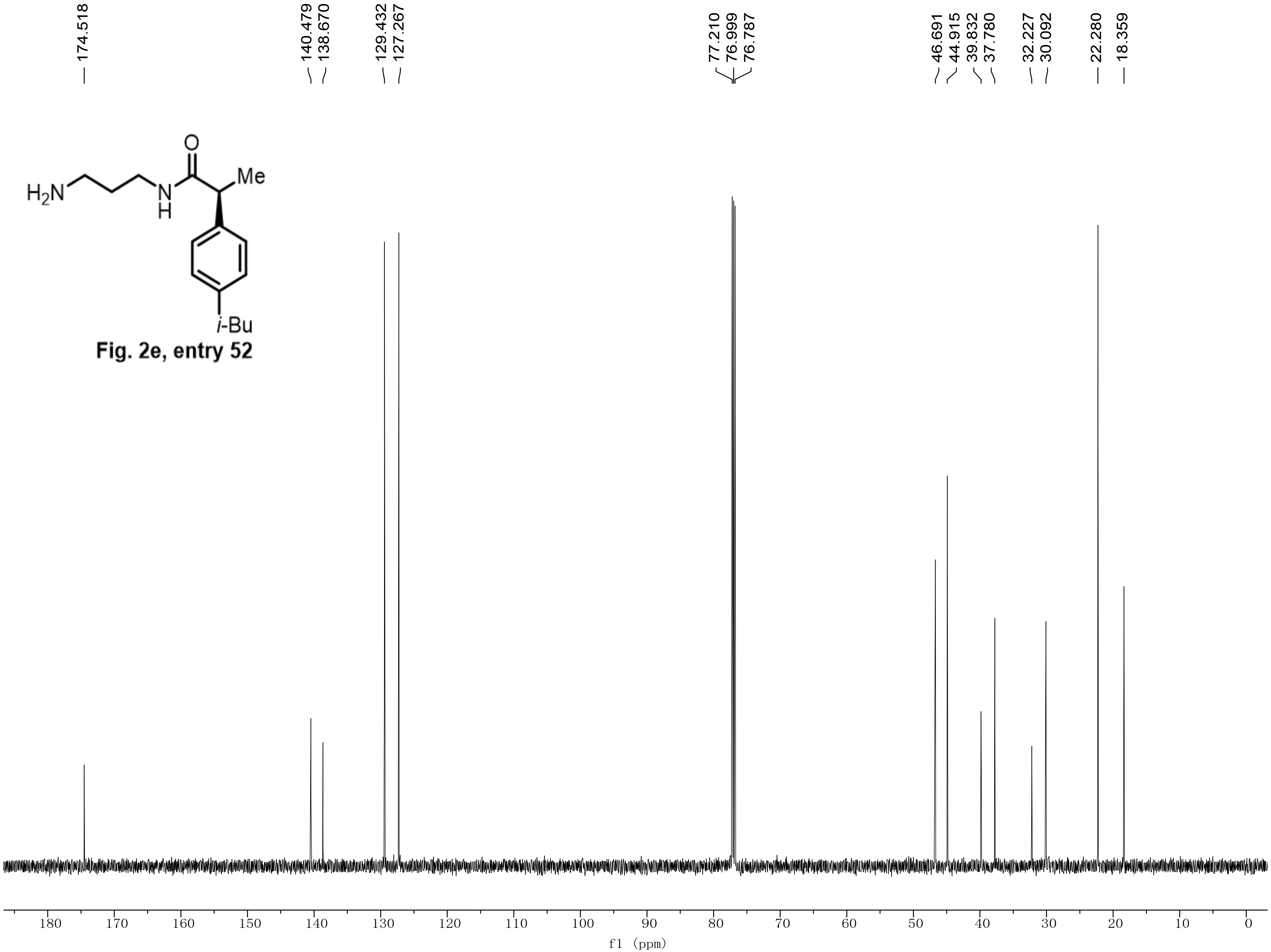


Fig. 2e, entry 52

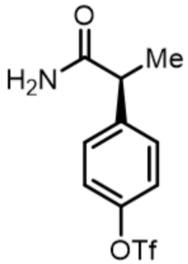
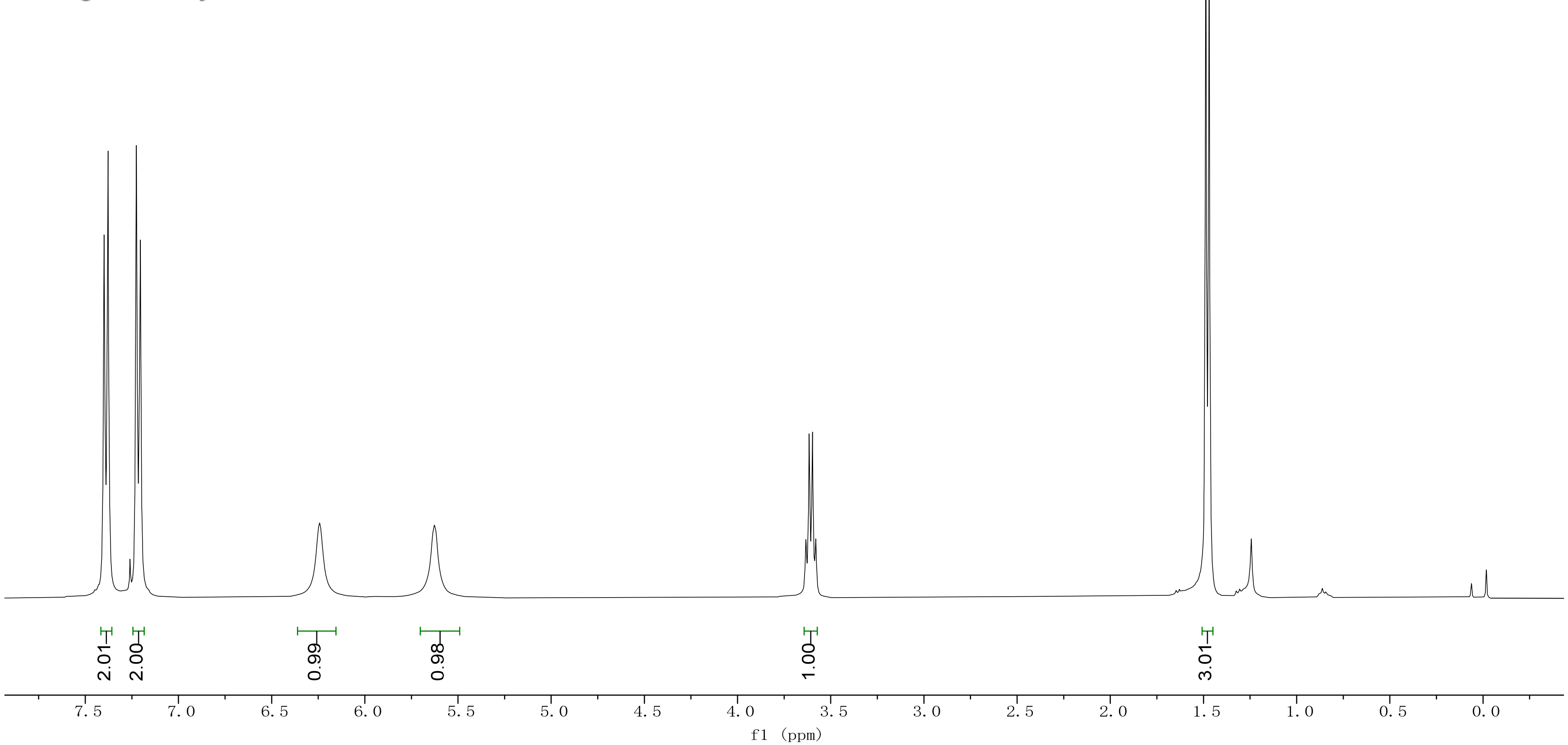


Fig. 2e, entry 53



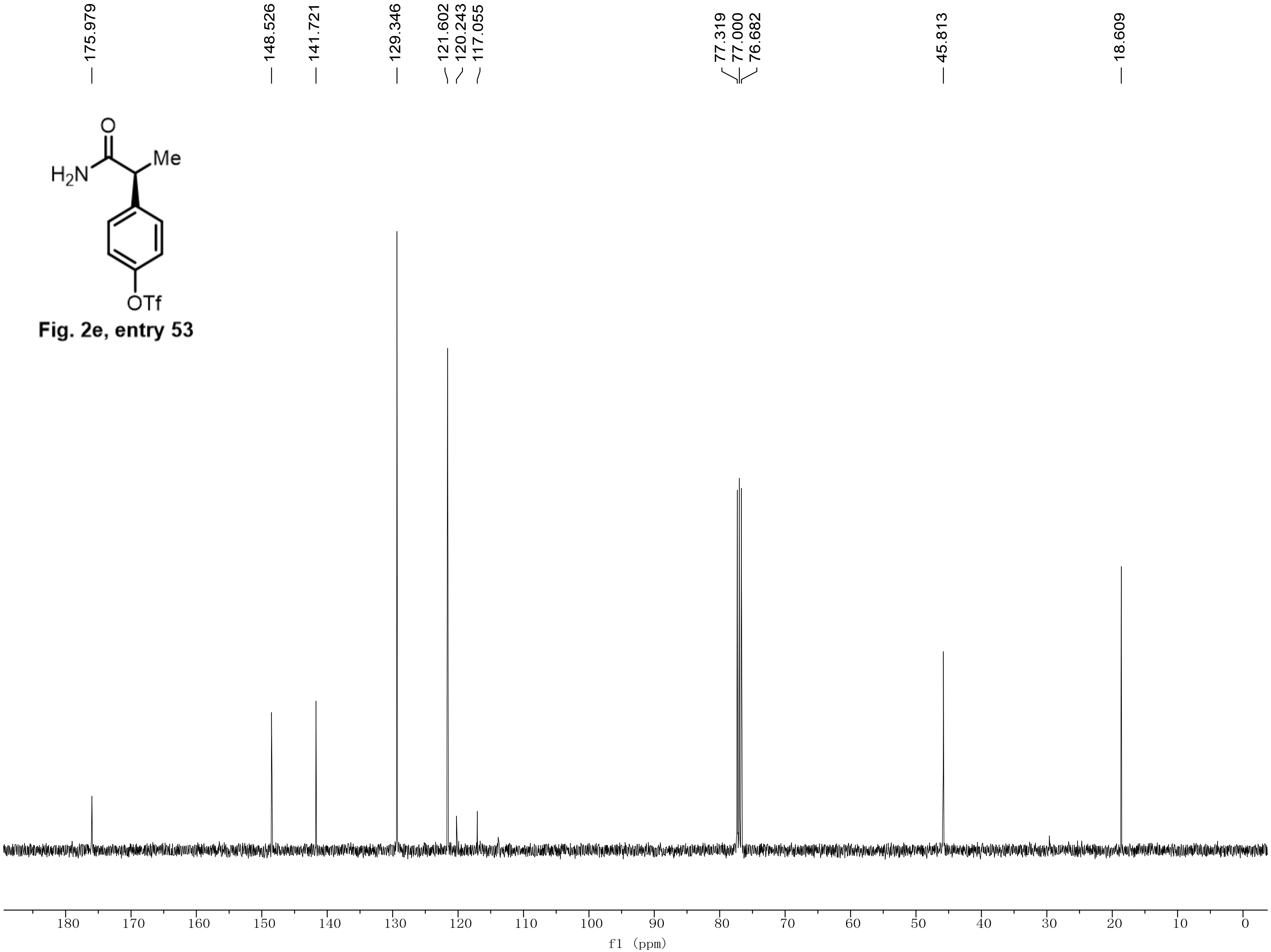


Fig. 2e, entry 53

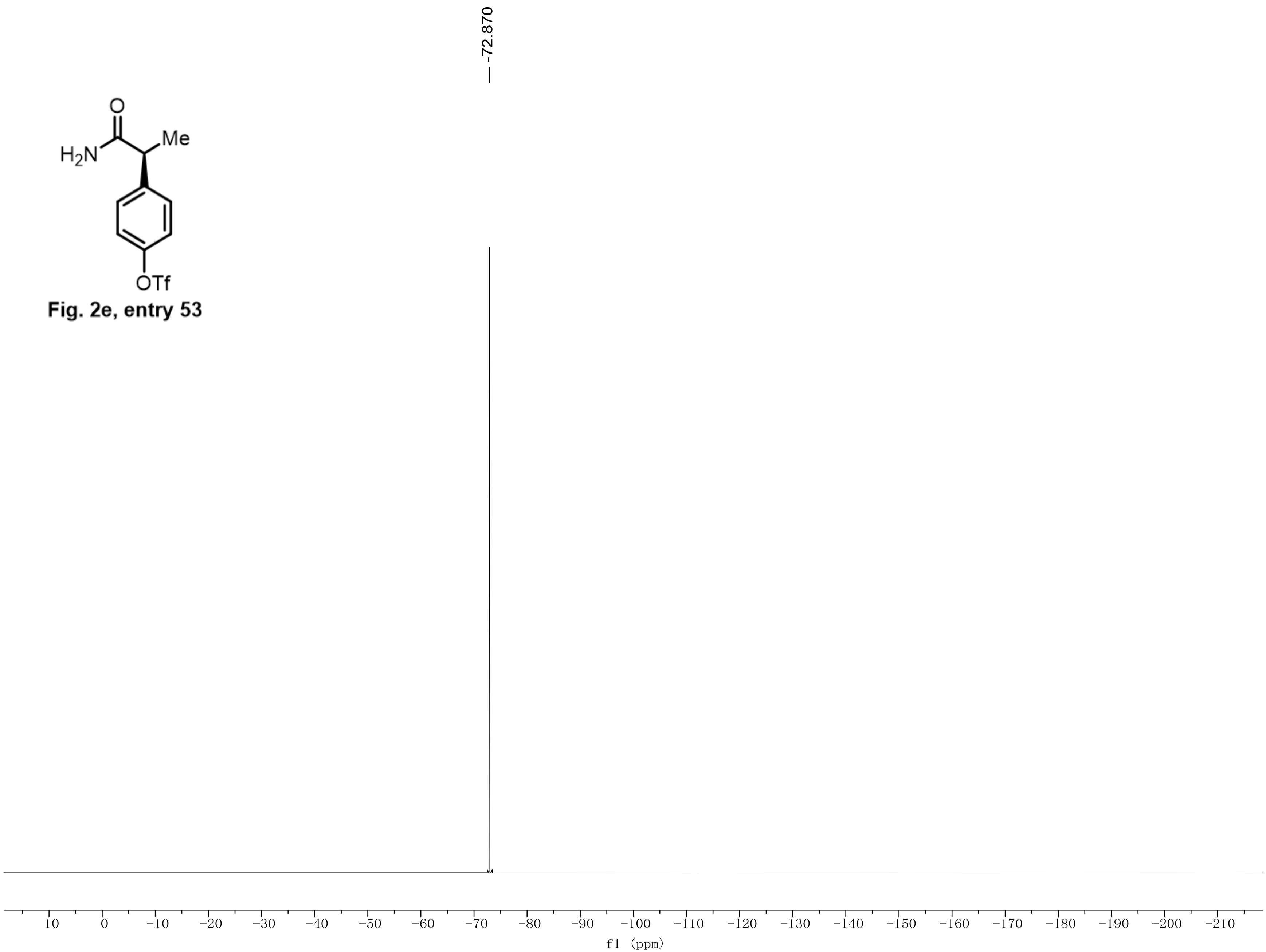


Fig. 2e, entry 53

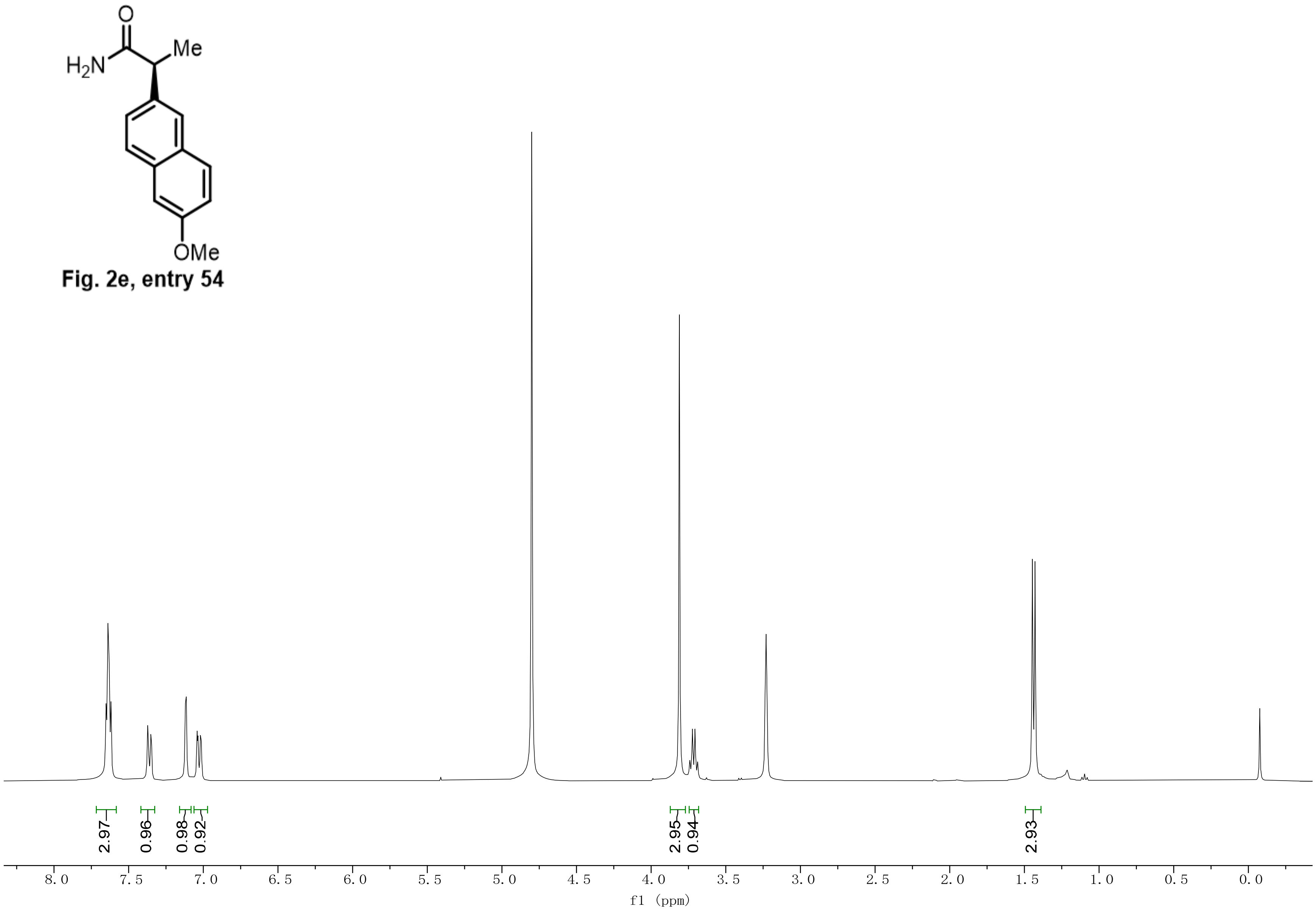


Fig. 2e, entry 54

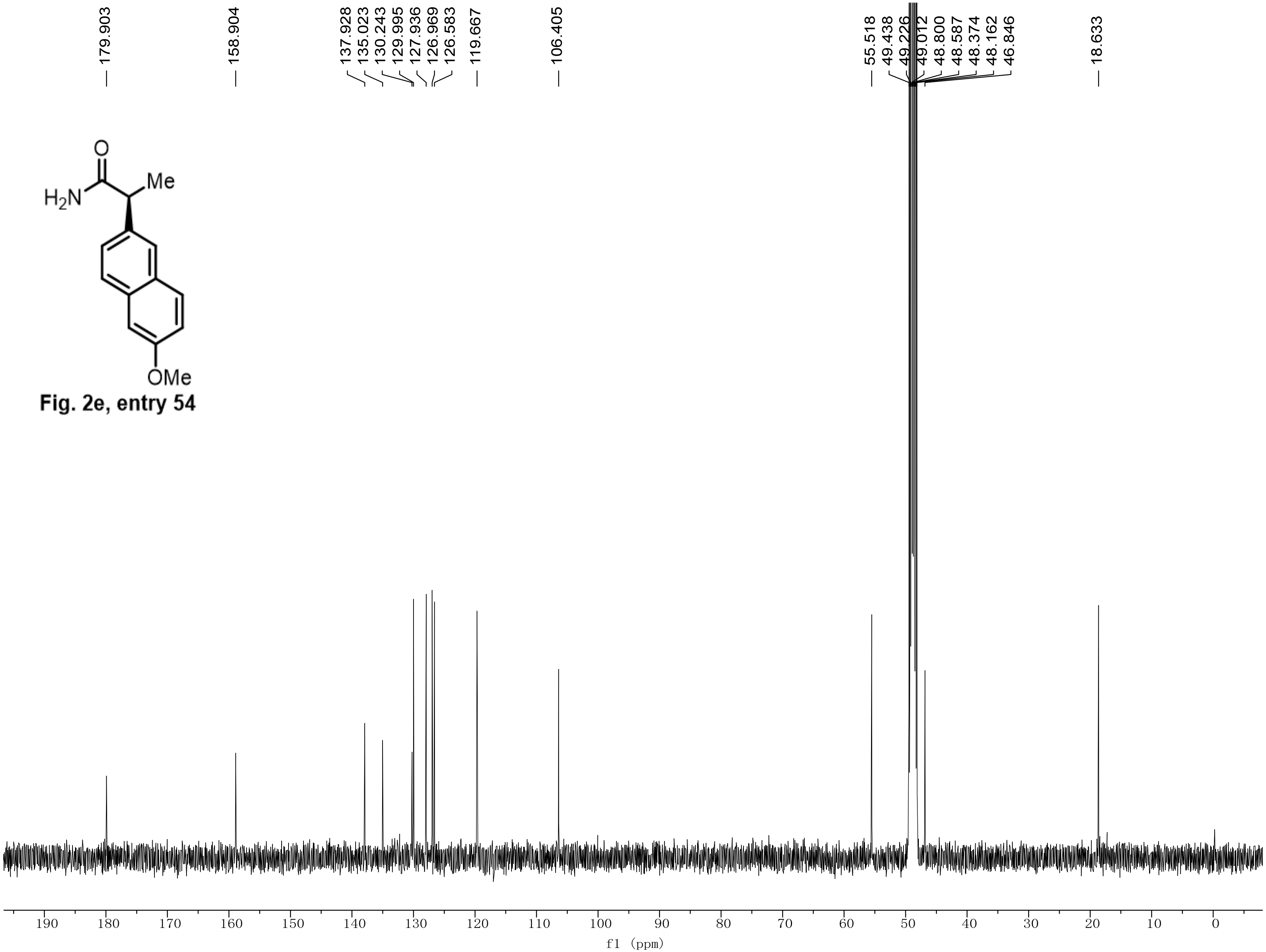


Fig. 2e, entry 54

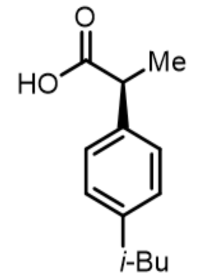
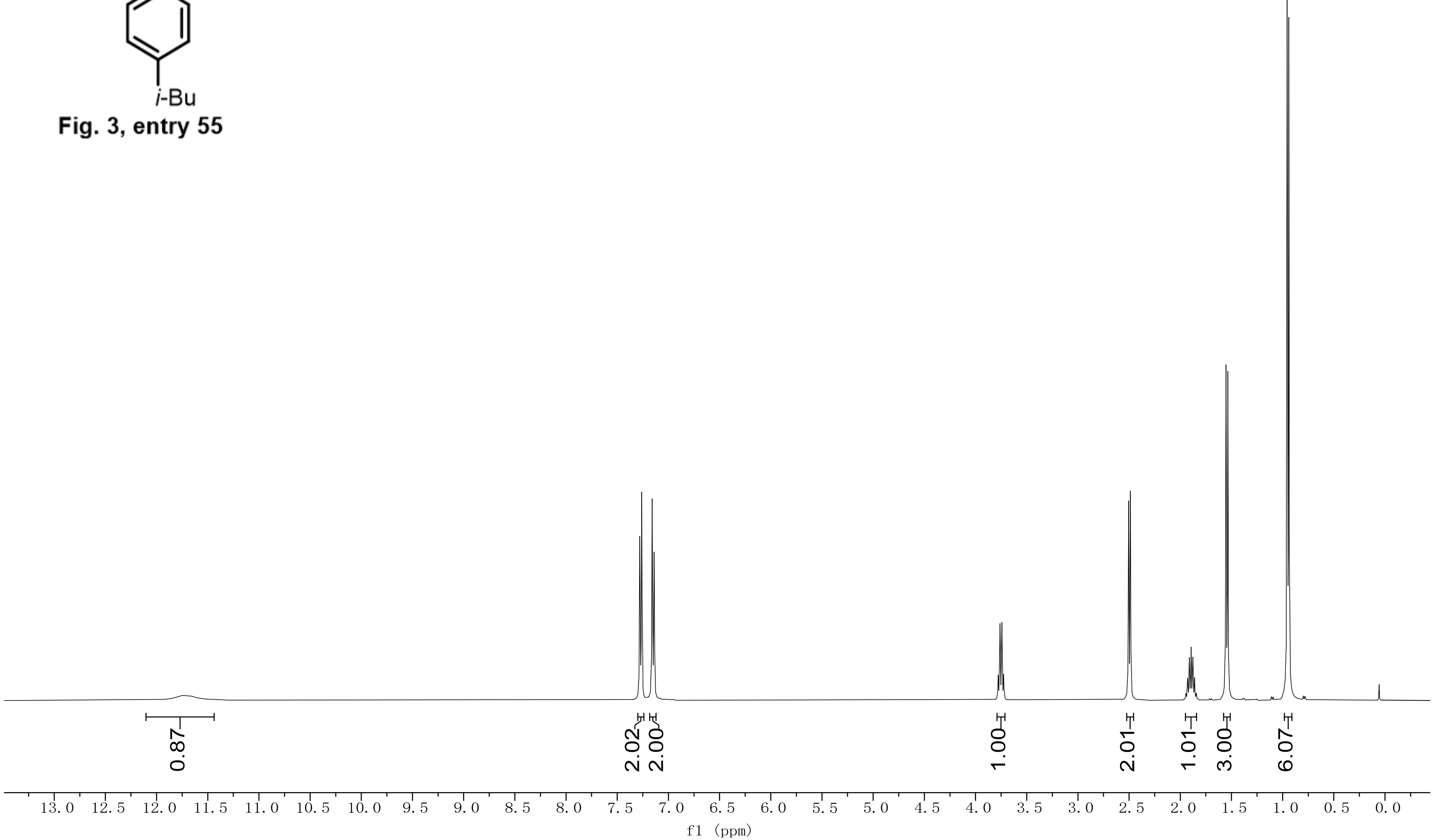
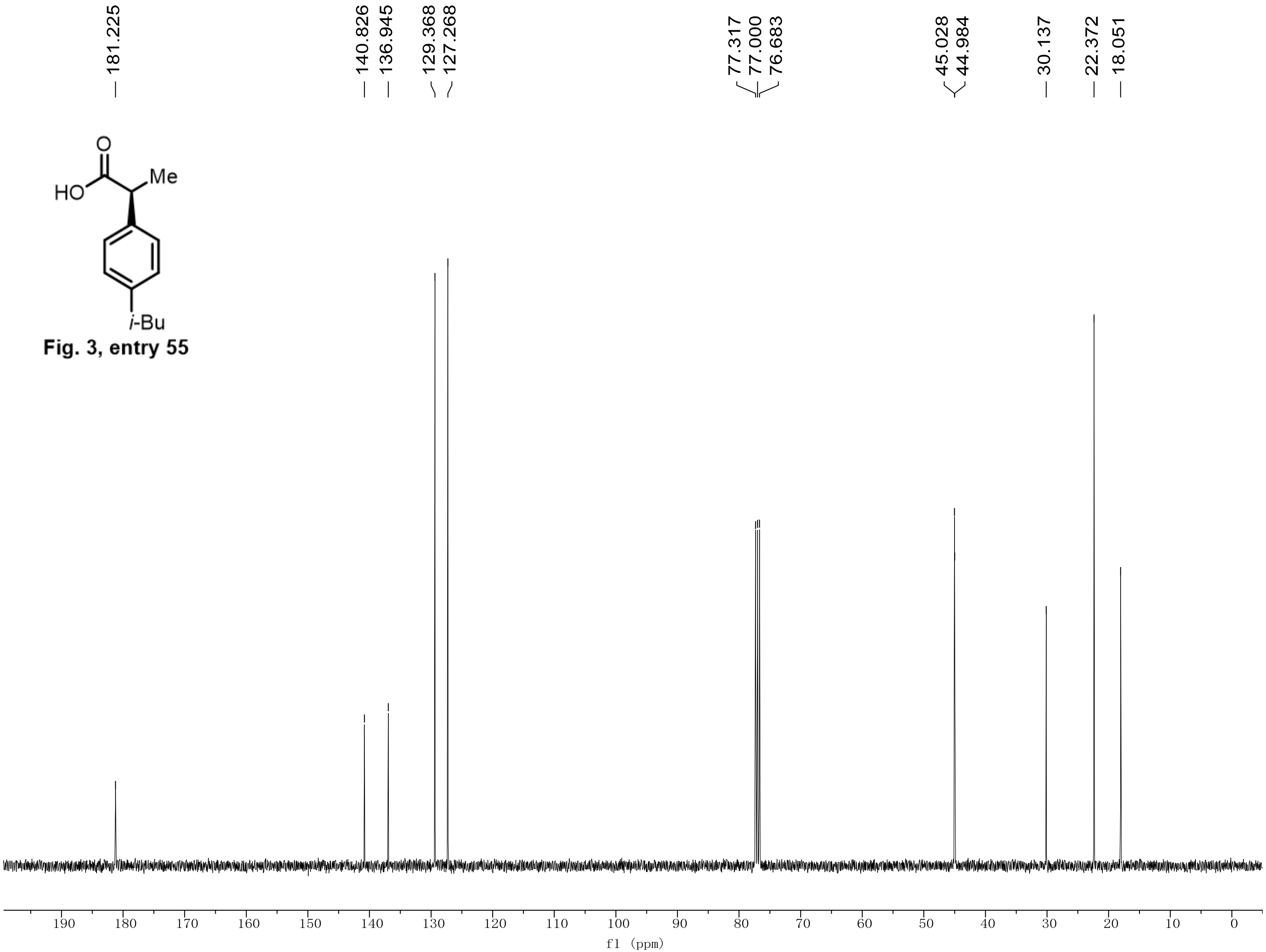


Fig. 3, entry 55




O
Me
HO
i-Bu
Fig. 3, entry 55
181.225
140.826
136.945
129.368
127.268
77.317
77.000
76.683
45.028
44.984
30.137
22.372
18.051
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

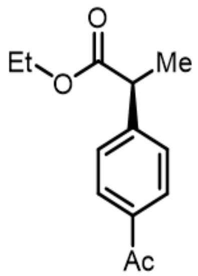
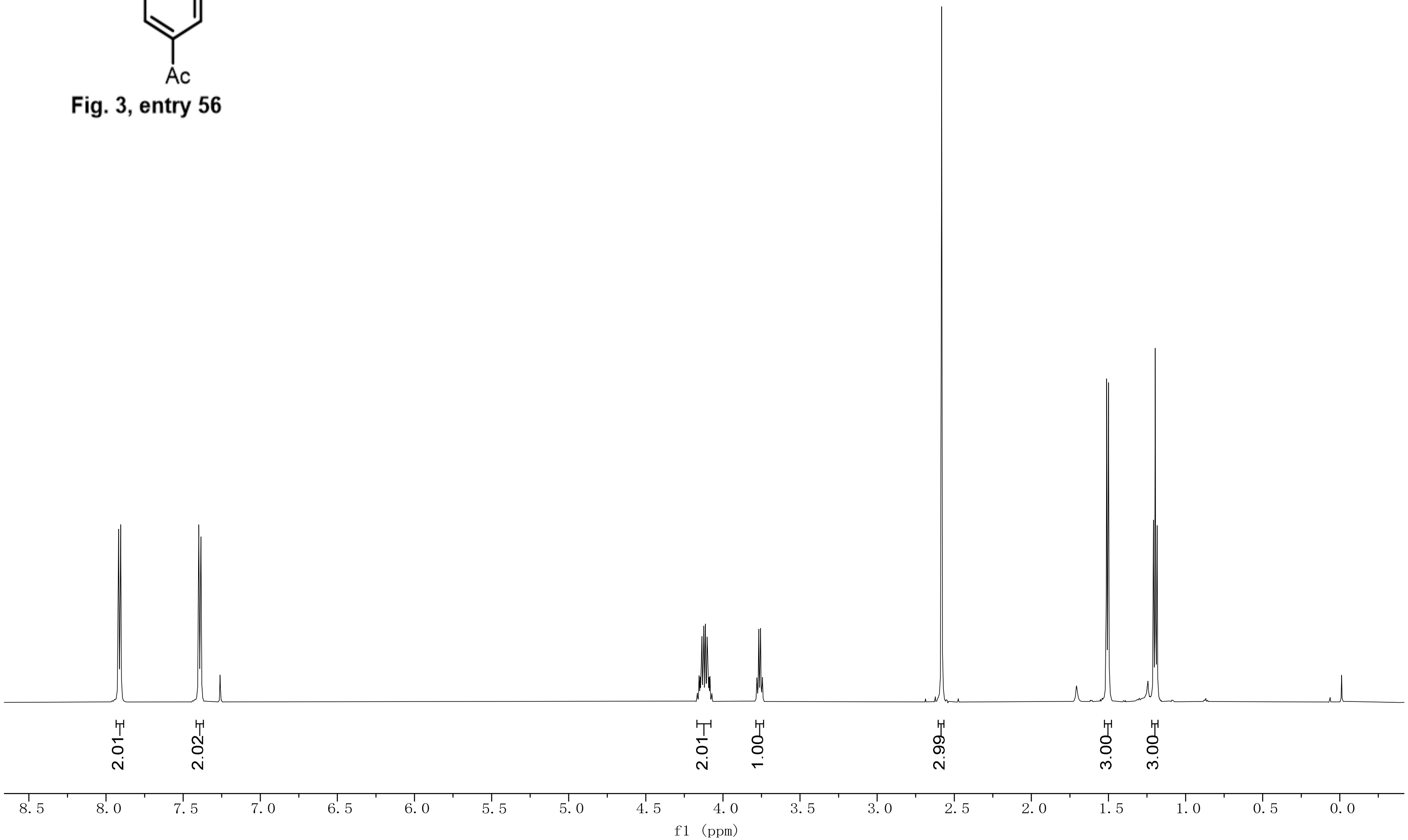
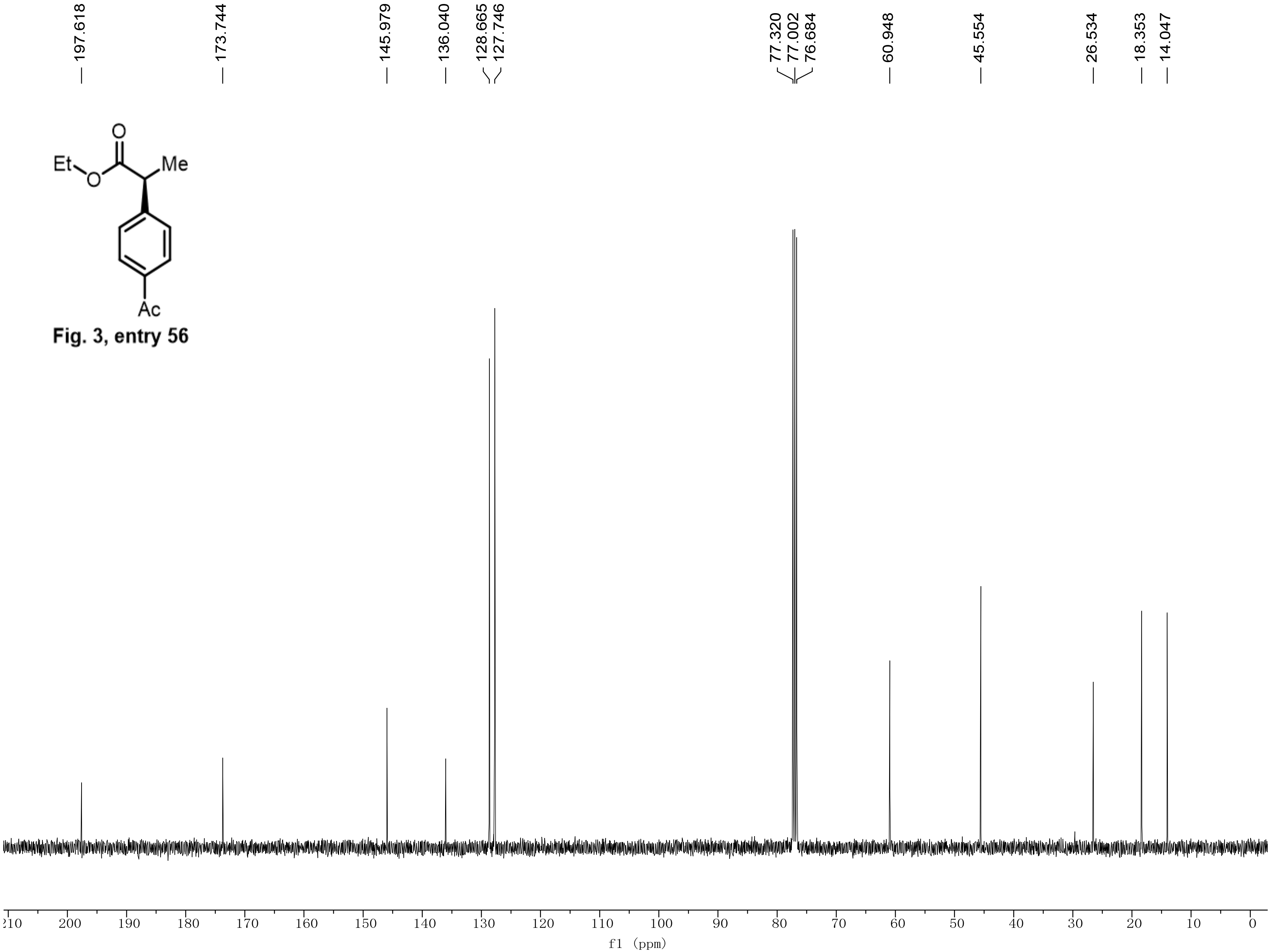


Fig. 3, entry 56




197.618
173.744
145.979
136.040
128.665
127.746
77.320
77.002
76.684
60.948
45.554
26.534
18.353
14.047
O
Et
O
Me
Ac
Fig. 3, entry 56
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

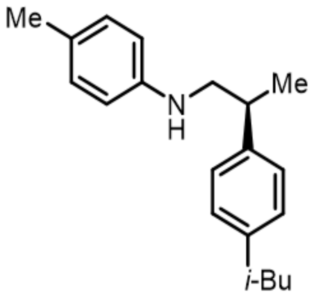
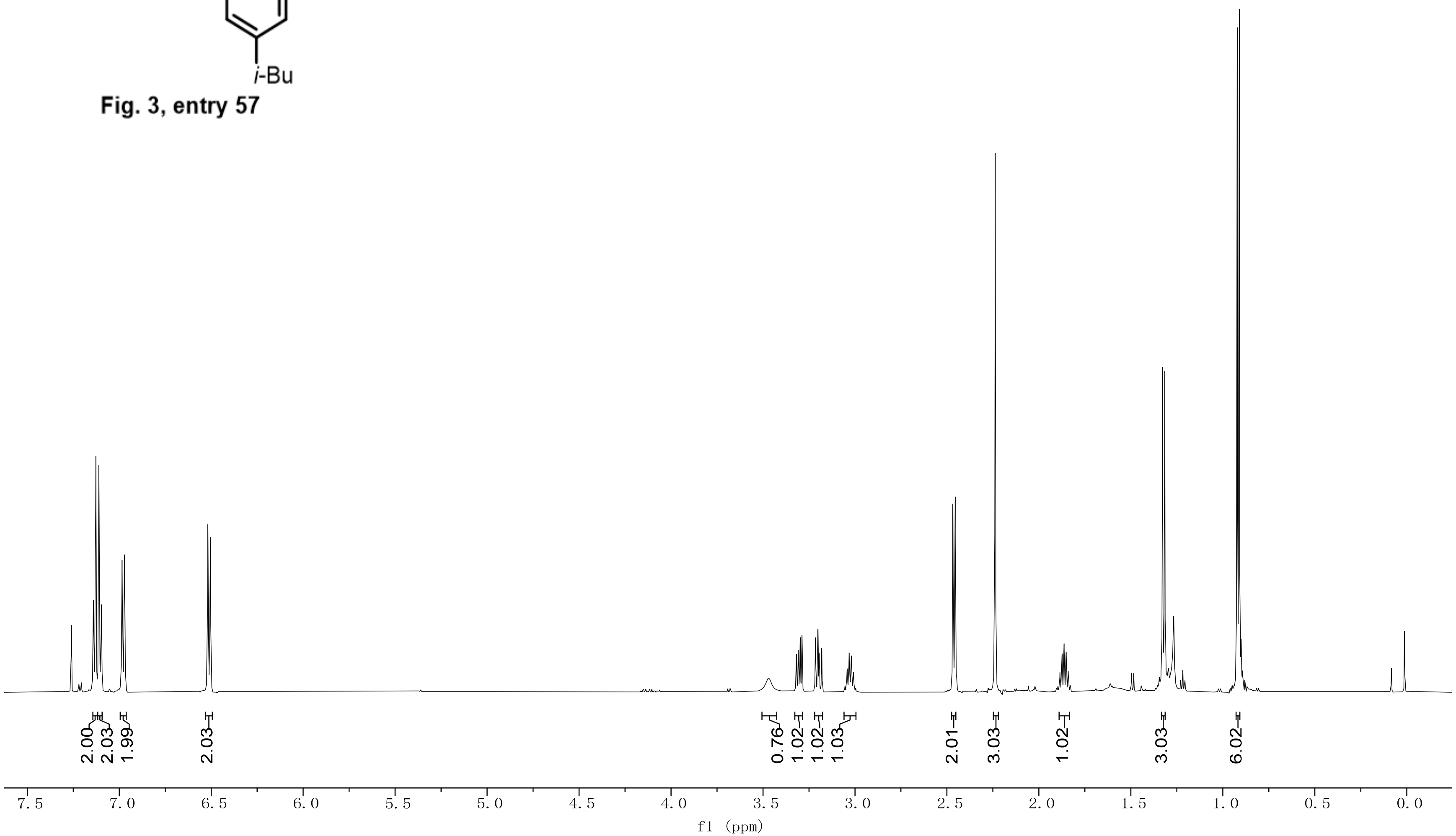


Fig. 3, entry 57



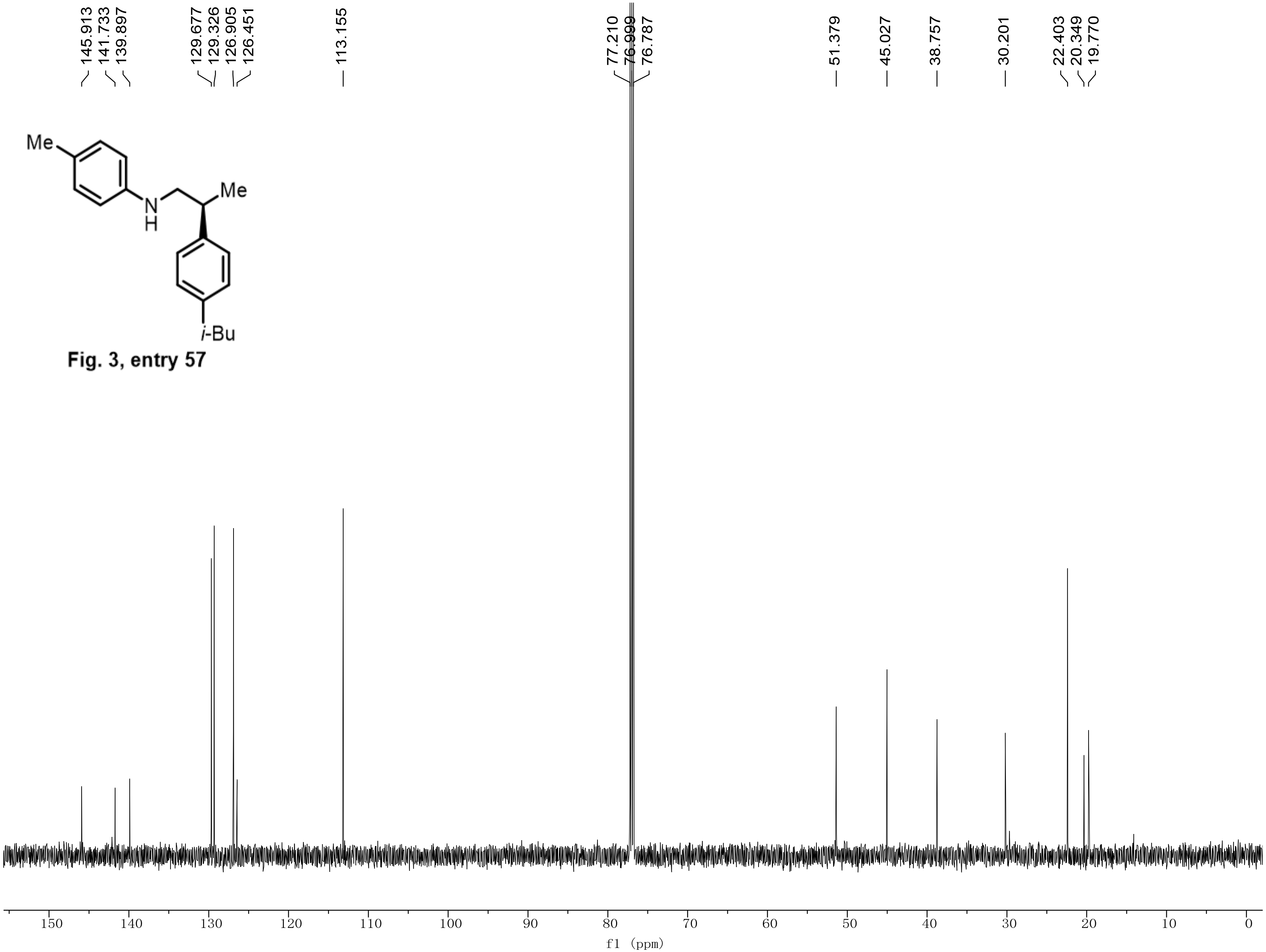


Fig. 3, entry 57

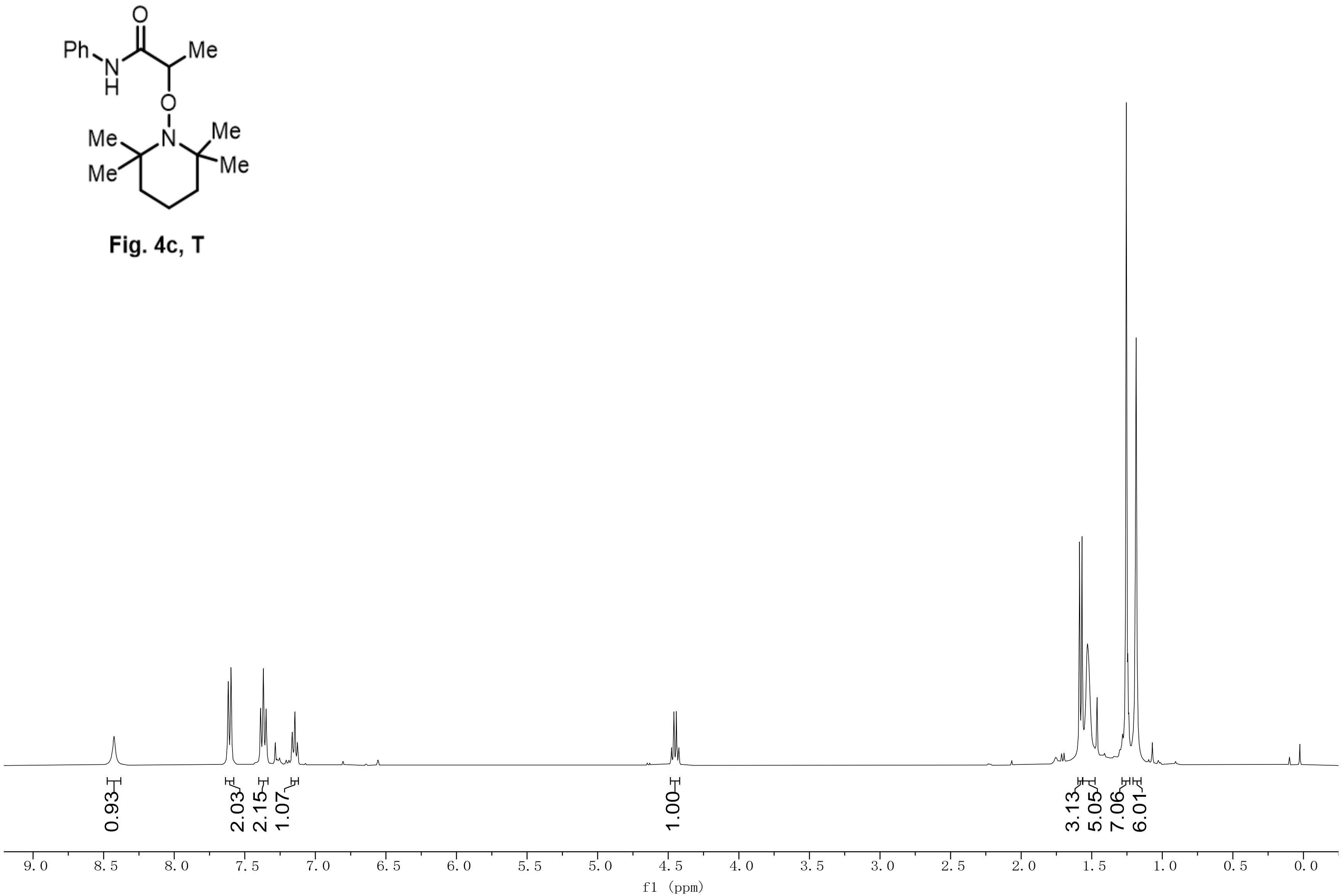


Fig. 4c, T

0.93
2.03
2.15
1.07
1.00
3.13
5.05
7.06
6.01
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)

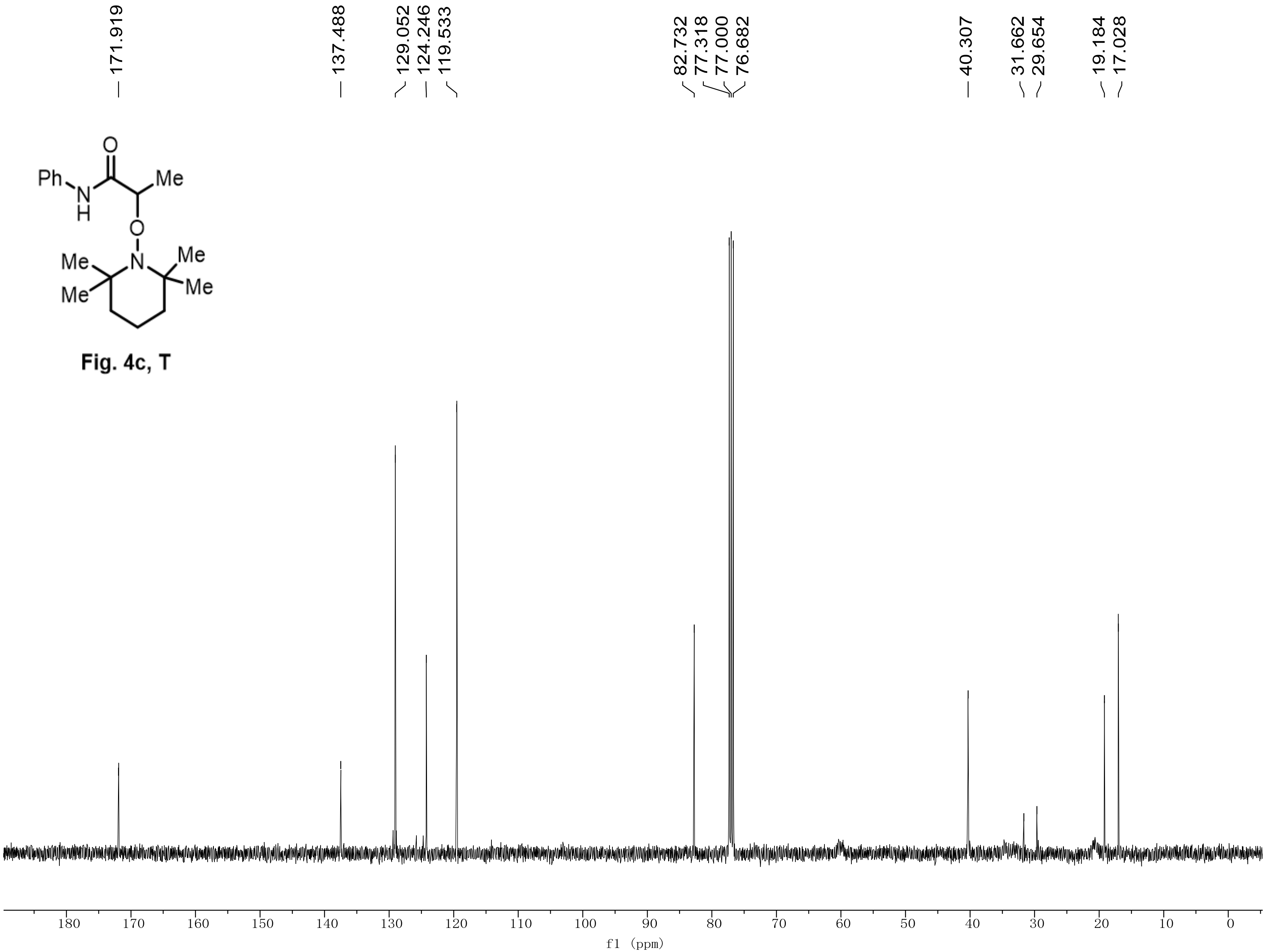

Ph
N
H
O
Me
O
N
Me
Me
Me
Me
171.919
137.488
129.052
124.246
119.533
82.732
77.318
77.000
76.682
40.307
31.662
29.654
19.184
17.028
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Fig. 4c, T

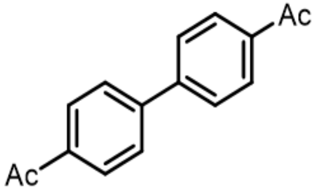
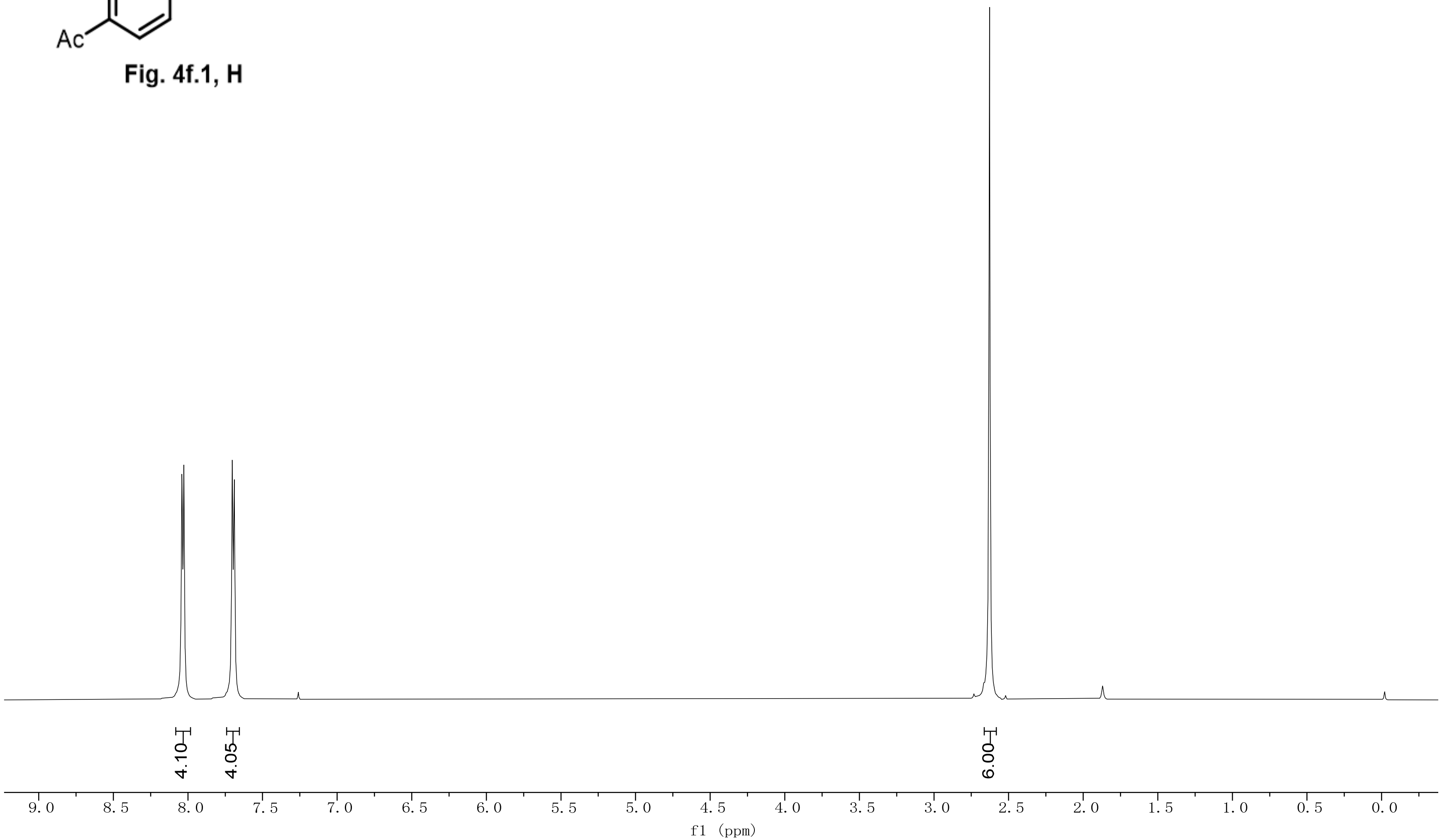

Ac
Ac

Fig. 4f.1, H


4.10
4.05
6.00
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)

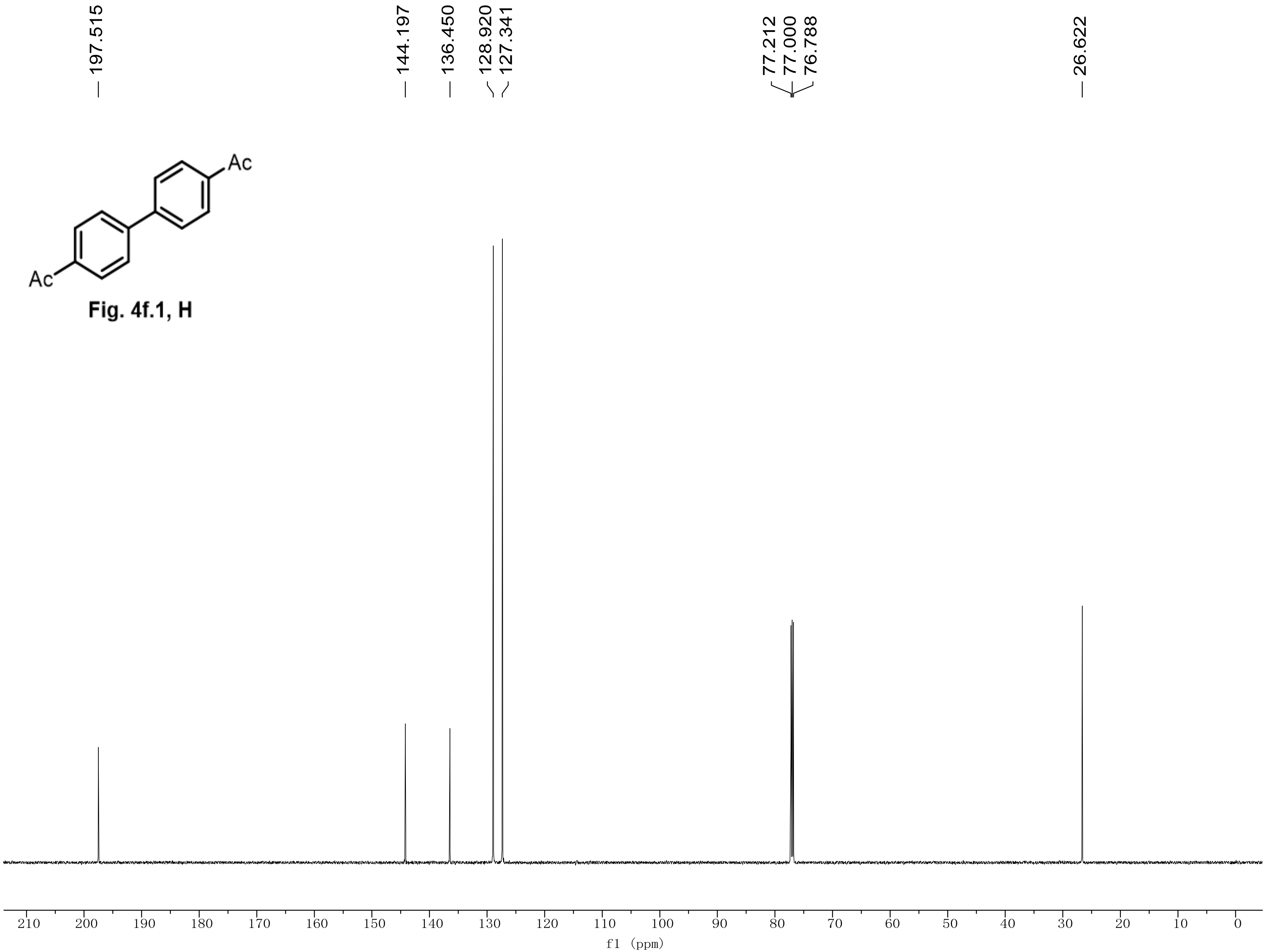

197.515
144.197
136.450
128.920
127.341
77.212
77.000
76.788
26.622
Ac
Ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Fig. 4f.1, H

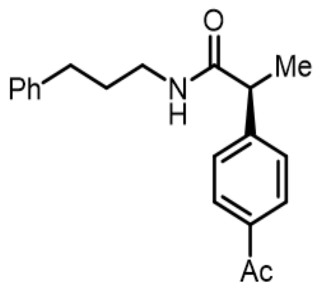
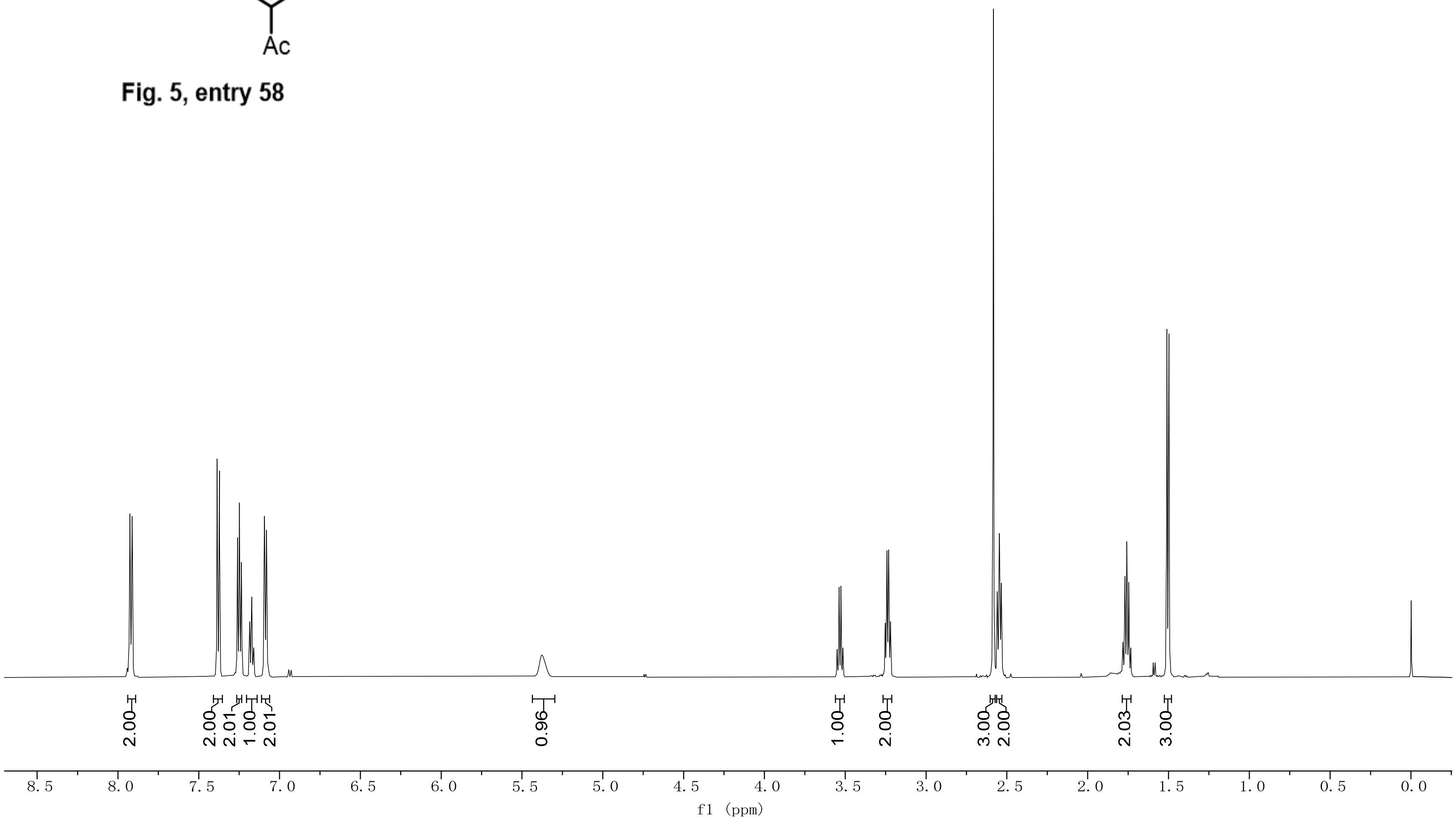


Fig. 5, entry 58



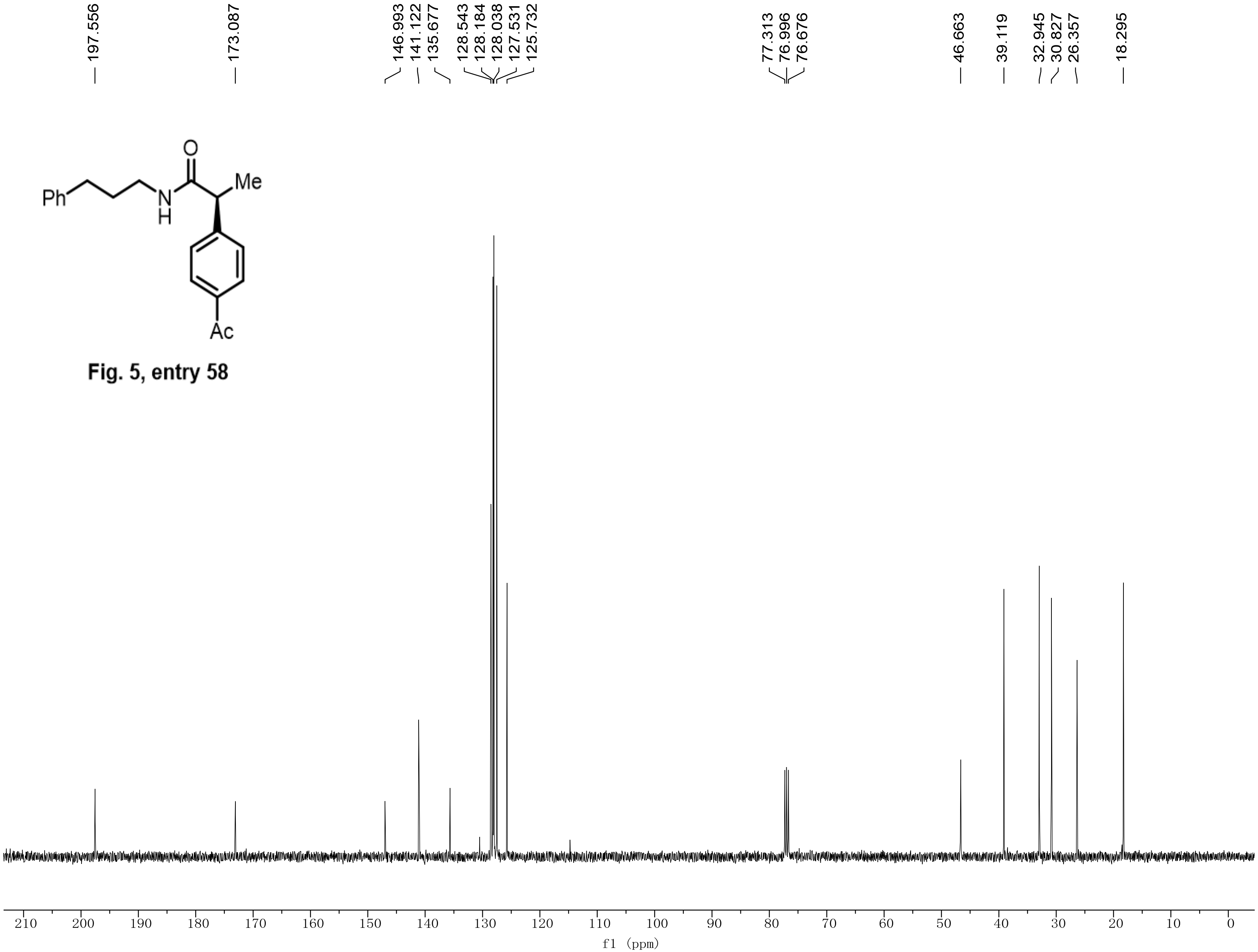
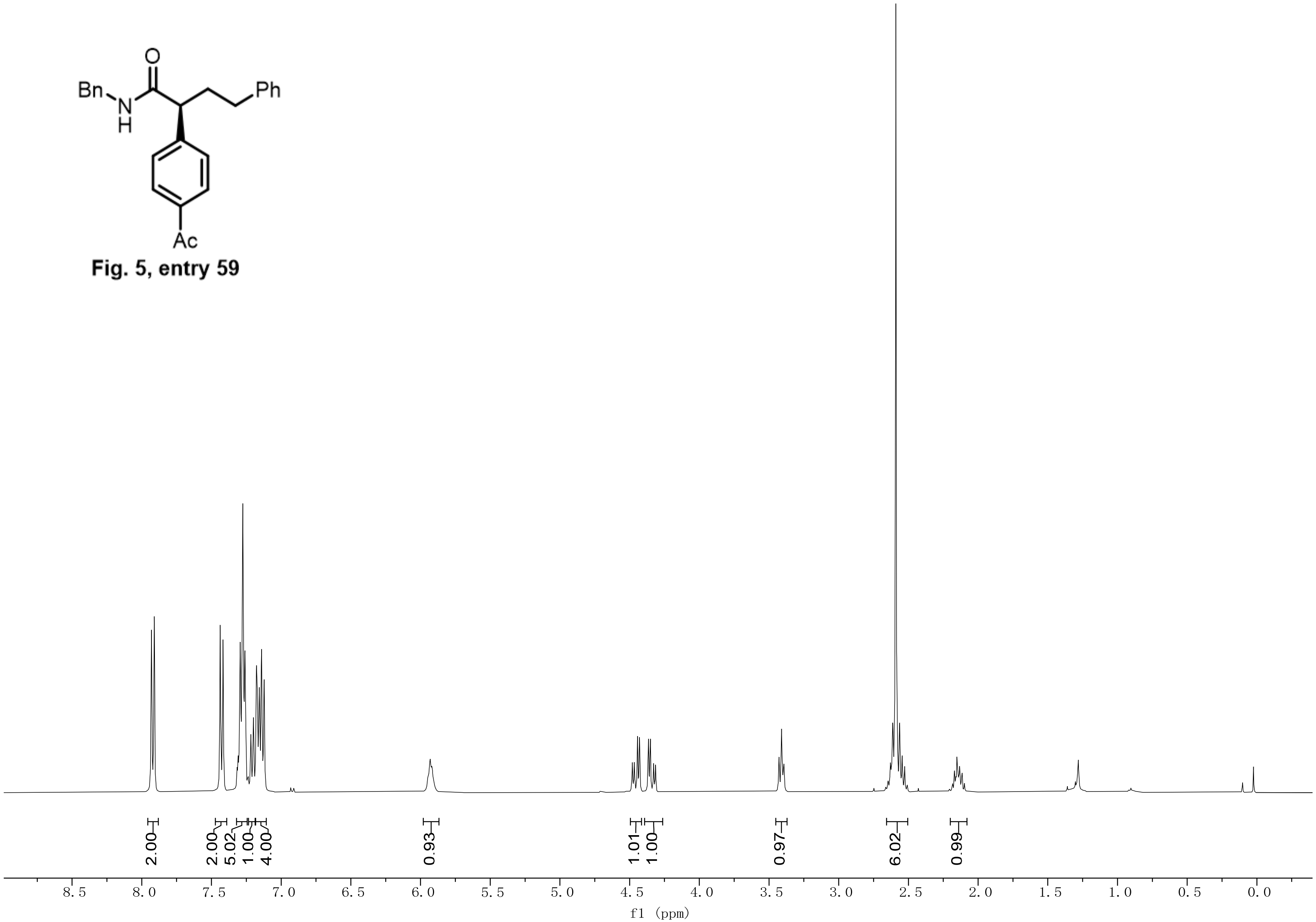


Fig. 5, entry 58


O
Bn
N
H
Ph
Ac
Fig. 5, entry 59
2.00
2.00
5.02
1.00
4.00
0.93
1.01
1.00
0.97
6.02
0.99
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)

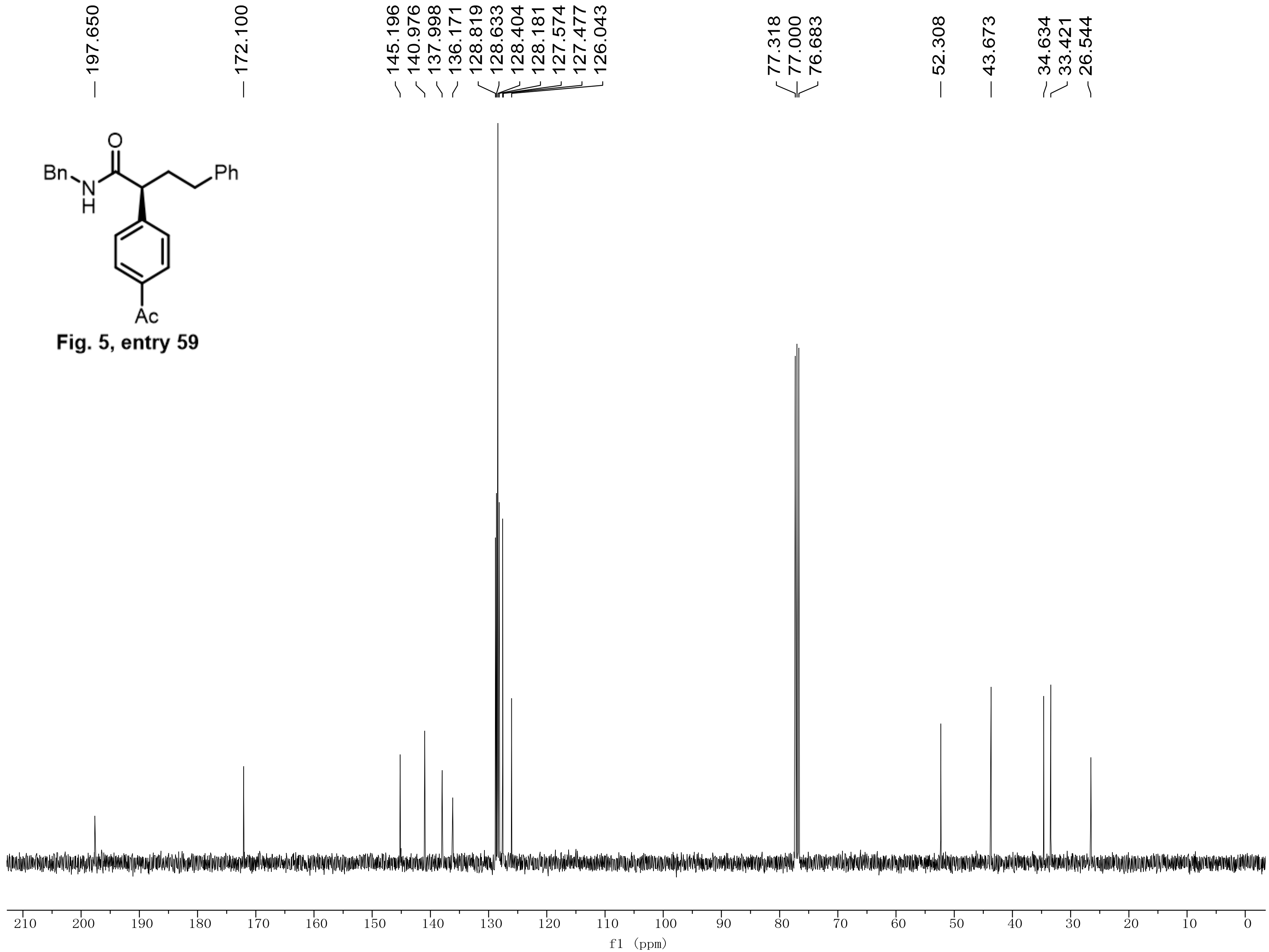


Fig. 5, entry 59

Determination of Stereoselectivity

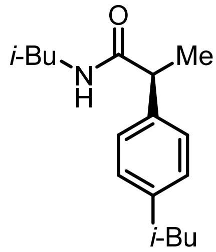
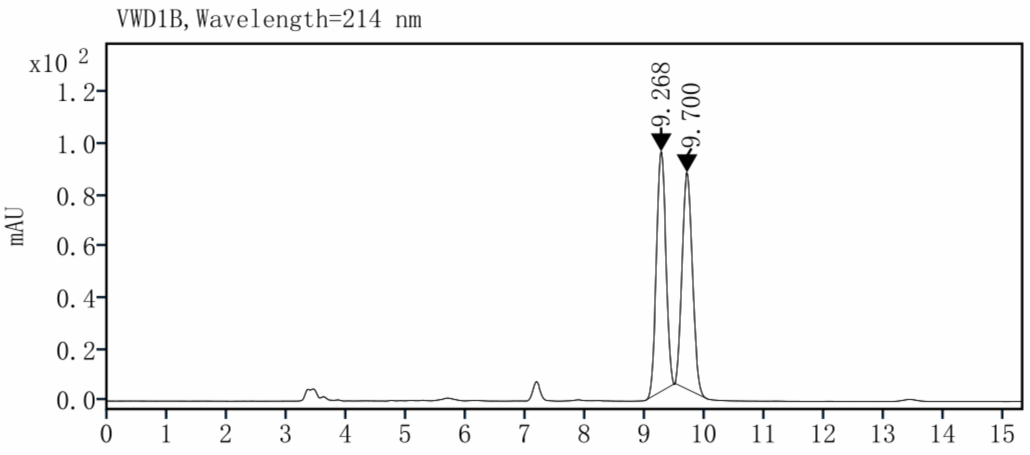
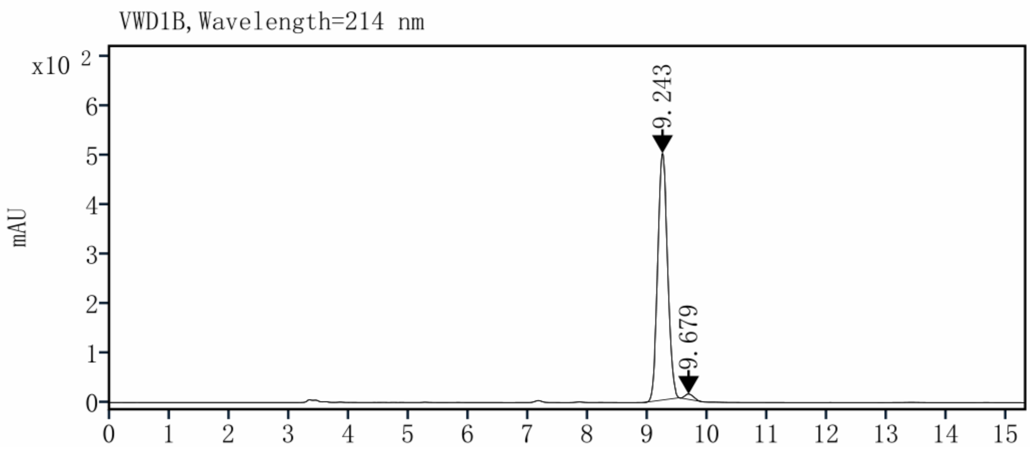


Fig. 2a, entry 1
(*S*)-**L1**: 96% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.268	MM m	1024.44	50.29
	9.700	MM m	1012.55	49.71



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.243	MM m	5726.00	98.14
	9.679	MM m	108.48	1.86

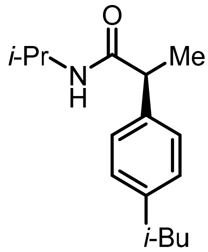
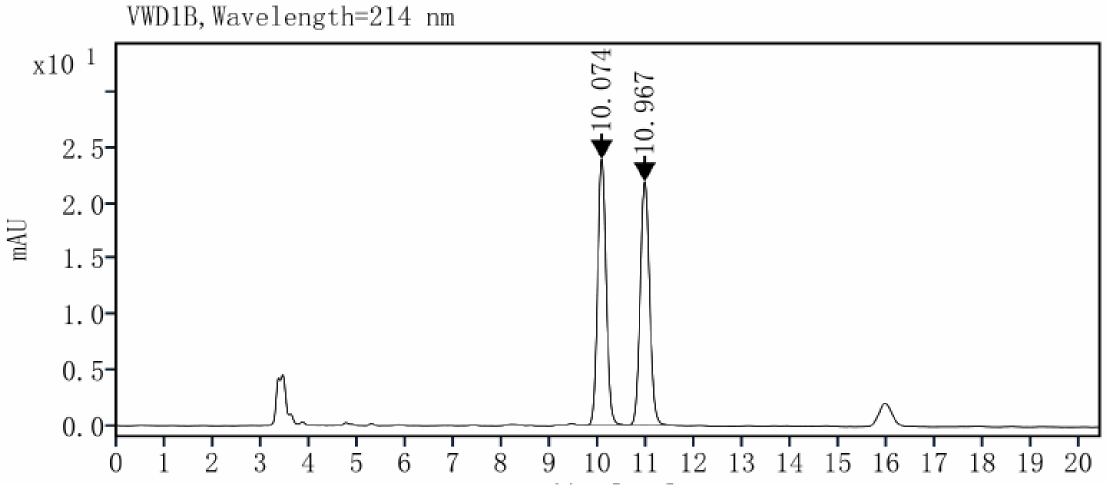
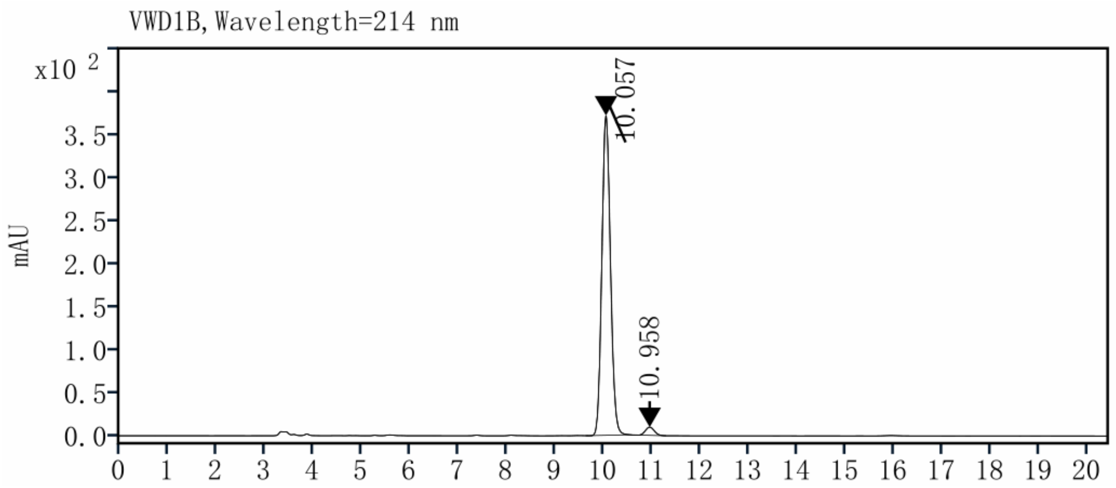


Fig. 2a, entry 2
(*S*)-**L1**: 95% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.074	MM m	294.20	50.05
	10.967	MM m	293.58	49.95



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.057	MM m	4586.42	97.47
	10.958	MM m	119.25	2.53

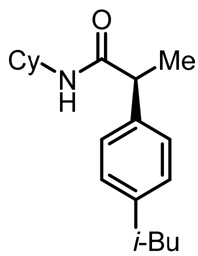
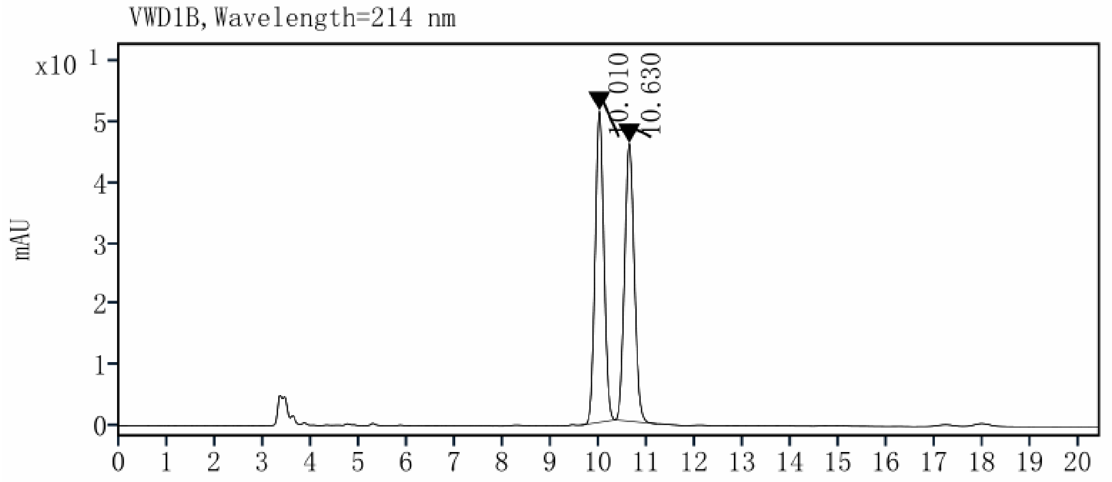
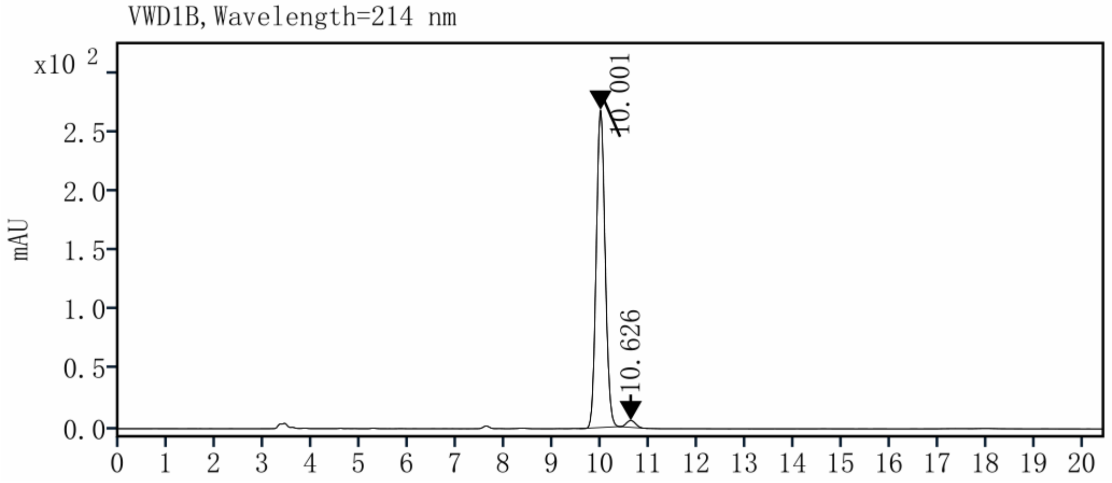


Fig. 2a, entry 3
(*S*)-**L1**: 96% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.010	MM m	650.34	50.10
	10.630	MM m	647.72	49.90



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.001	MM m	3409.43	97.83
	10.626	MM m	75.48	2.17

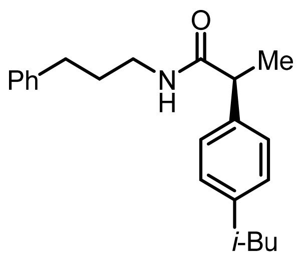
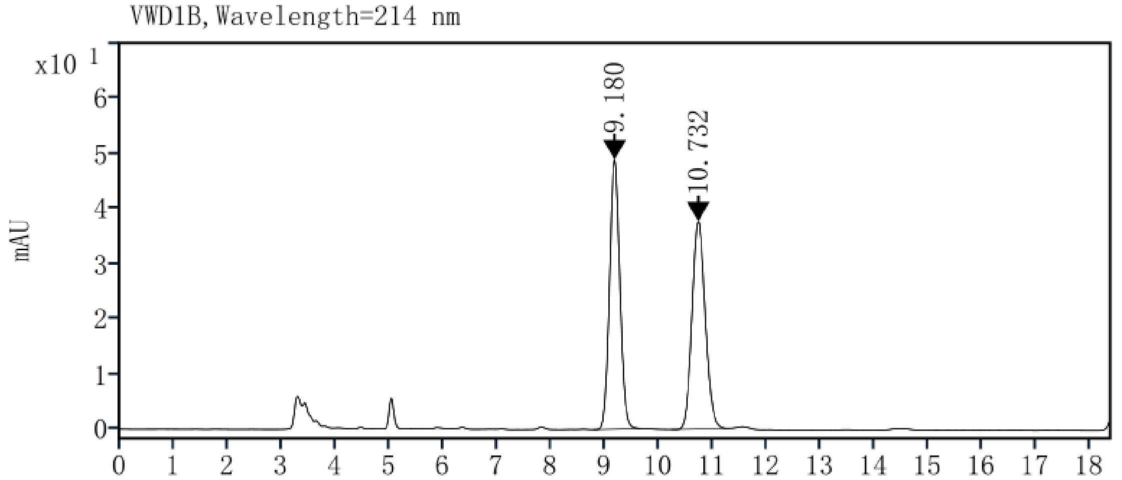
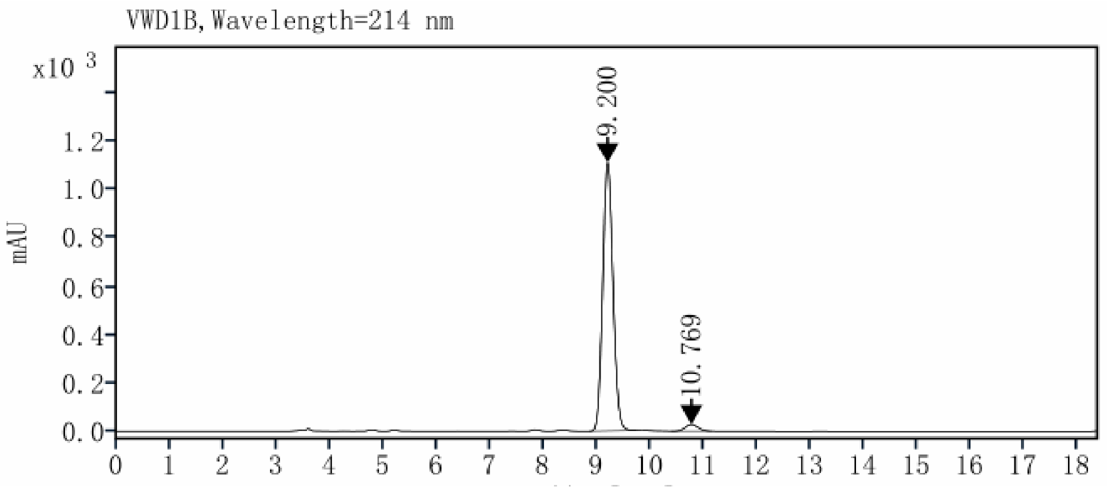


Fig. 2a, entry 4
(S)-**L1**: 94% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.180	MM m	651.54	50.30
	10.732	MM m	643.71	49.70



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.200	MM m	14932.88	96.91
	10.769	MM m	476.91	3.09

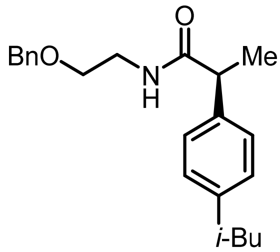
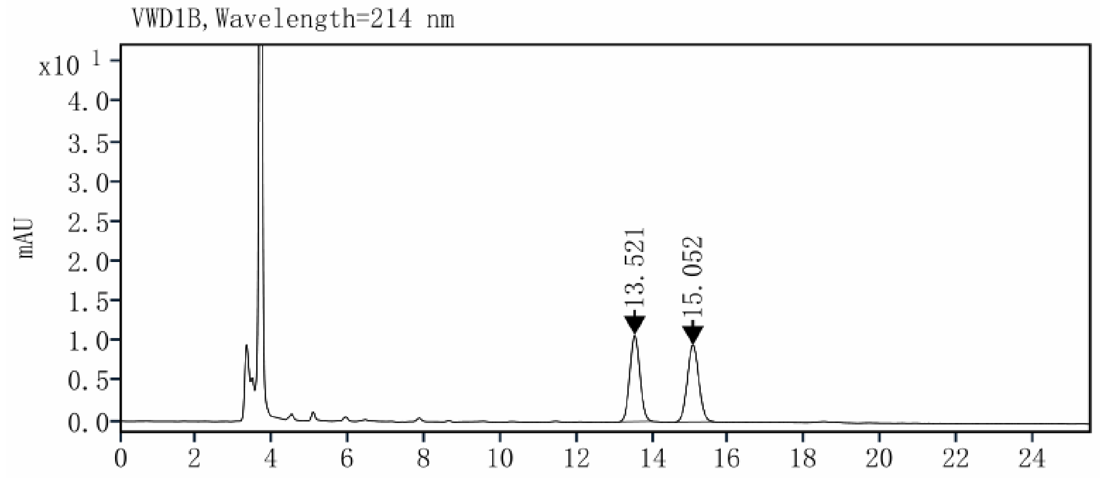
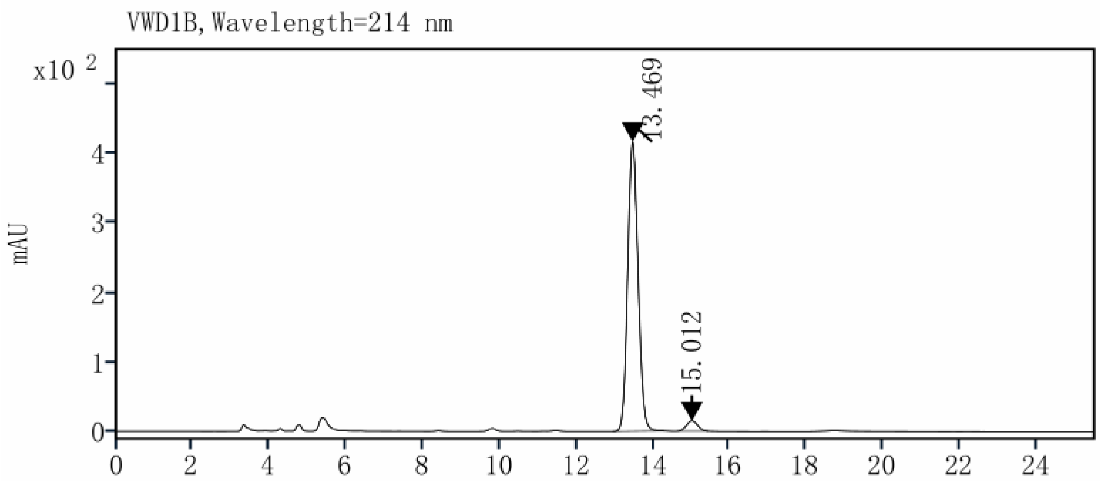


Fig. 2a, entry 5
(*S*)-**L1**: 93% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	13.521	MM m	200.41	49.79
	15.052	MM m	202.06	50.21



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	13.469	MM m	7887.93	96.33
	15.012	MM m	300.33	3.67

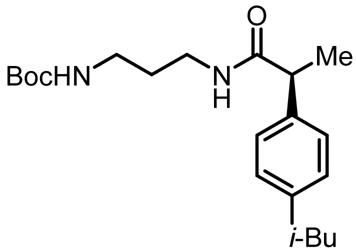
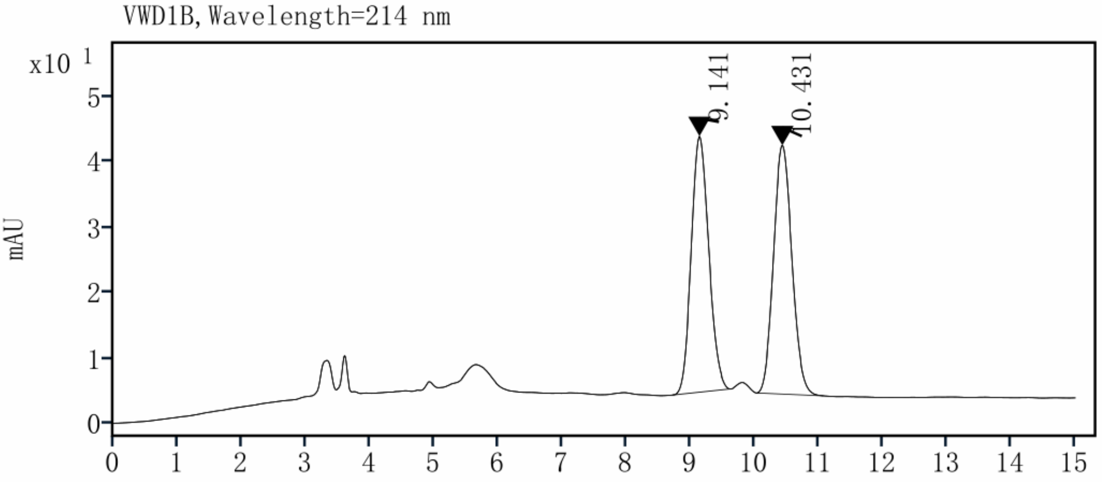
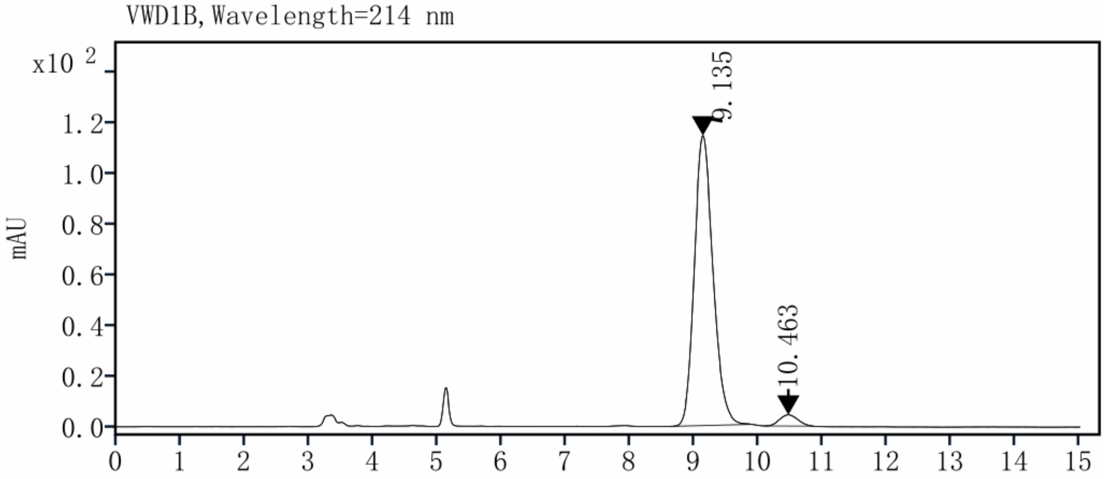


Fig. 2a, entry 6
(*S*)-**L1**: 93% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.141	MM m	743.37	49.52
	10.431	MM m	757.72	50.48



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.135	MM m	2308.52	96.34
	10.463	MM m	87.63	3.66

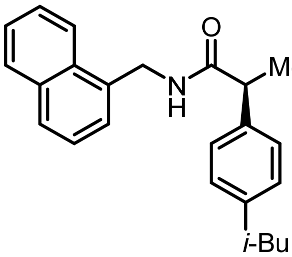
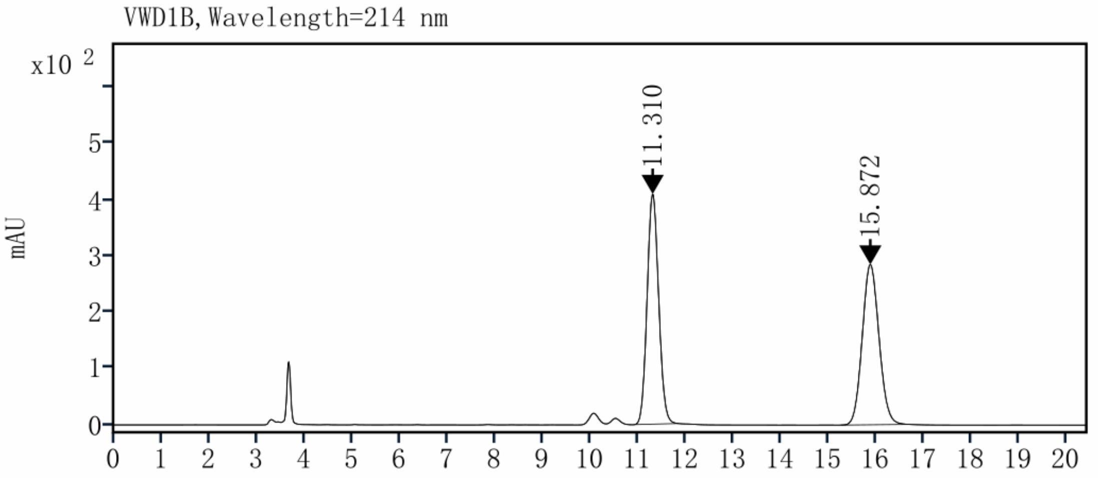
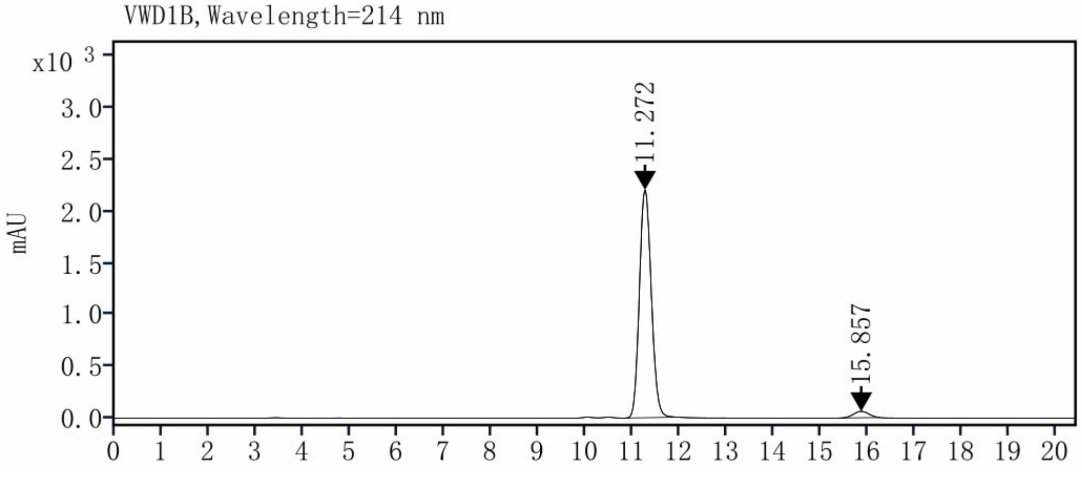


Fig. 2a, entry 7
(*S*)-**L1**: 93% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.310	MM m	6880.34	49.71
	15.872	MM m	6960.56	50.29



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.272	MM m	38719.90	96.51
	15.857	MM m	1401.69	3.49

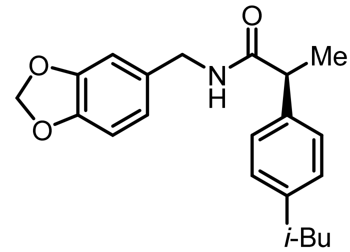
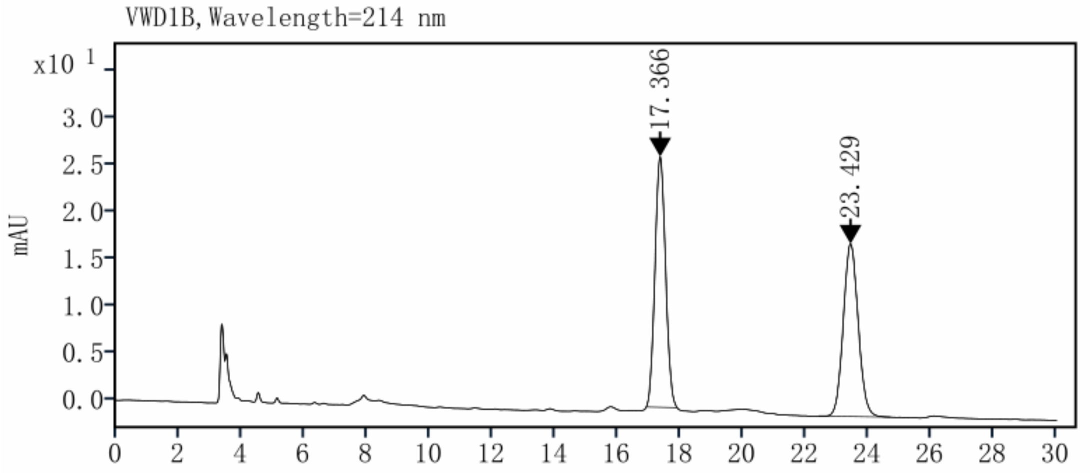
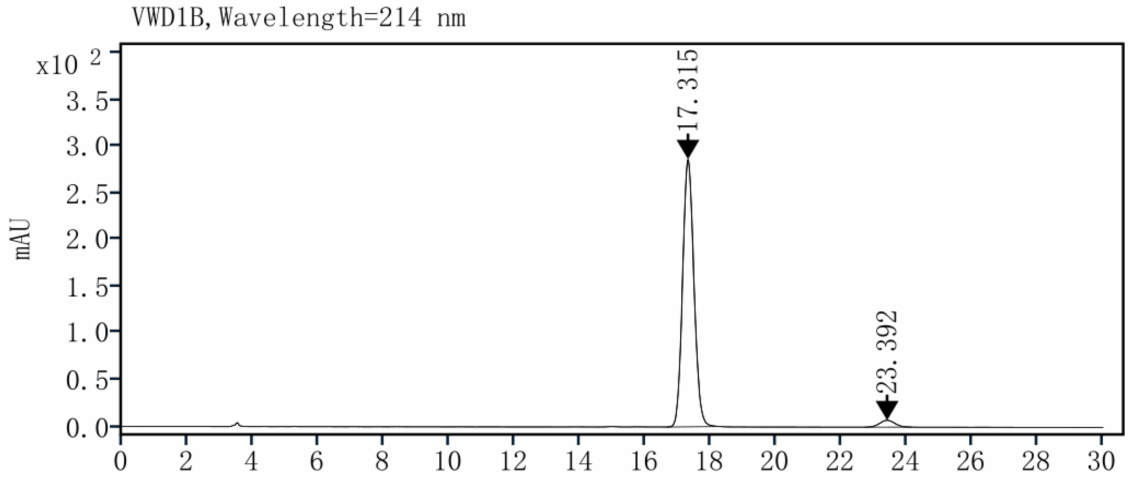


Fig. 2a, entry 8
(*S*)-**L1**: 93% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	17.366	MM m	626. 64	50. 72
	23.429	MM m	608. 91	49. 28



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	17.315	MM m	6921. 03	96. 68
	23.392	MM m	237. 39	3. 32

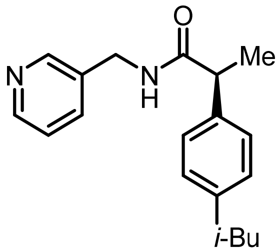
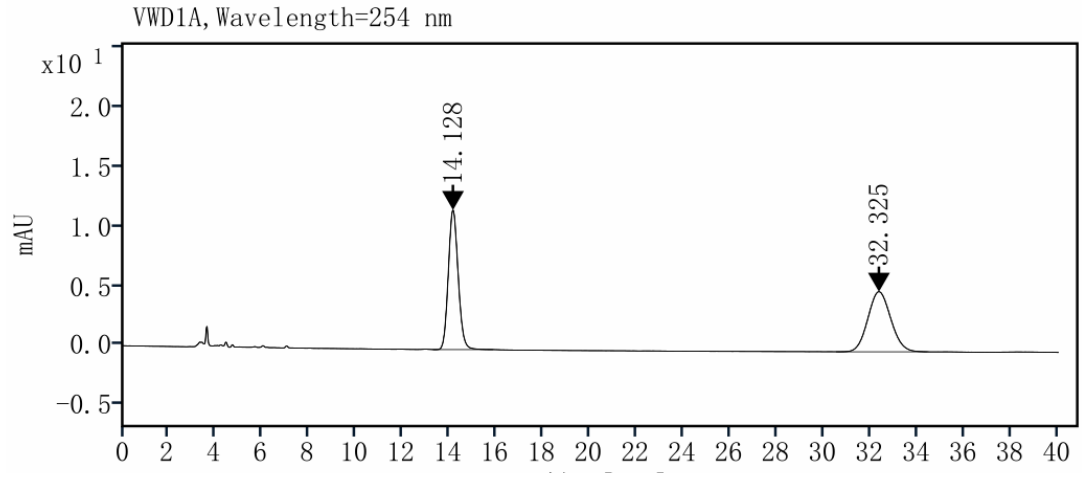
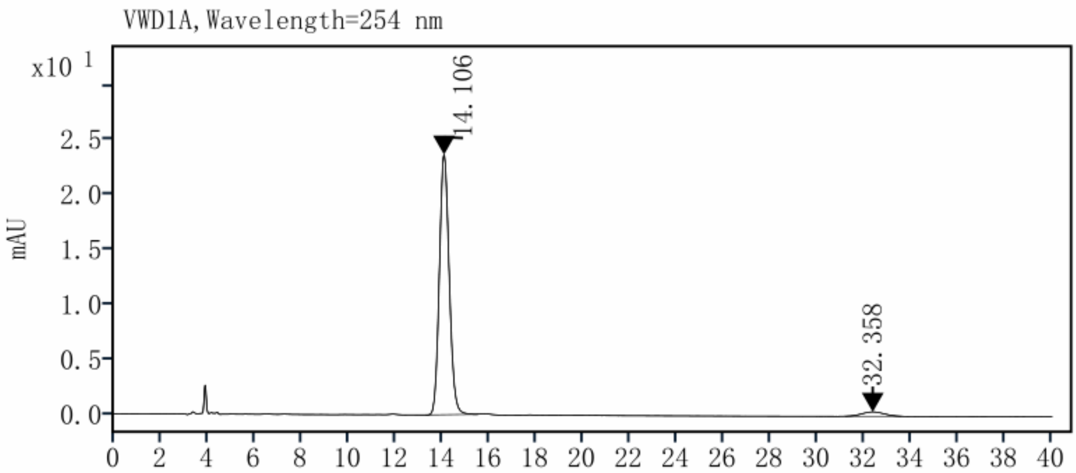


Fig. 2a, entry 9
(*S*)-**L1**: 93% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.128	MM m	343. 89	49. 92
	32.325	MM m	345. 04	50. 08



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.106	MM m	691. 92	96. 33
	32.358	MM m	26. 36	3. 67

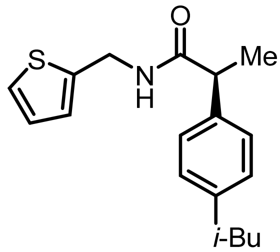
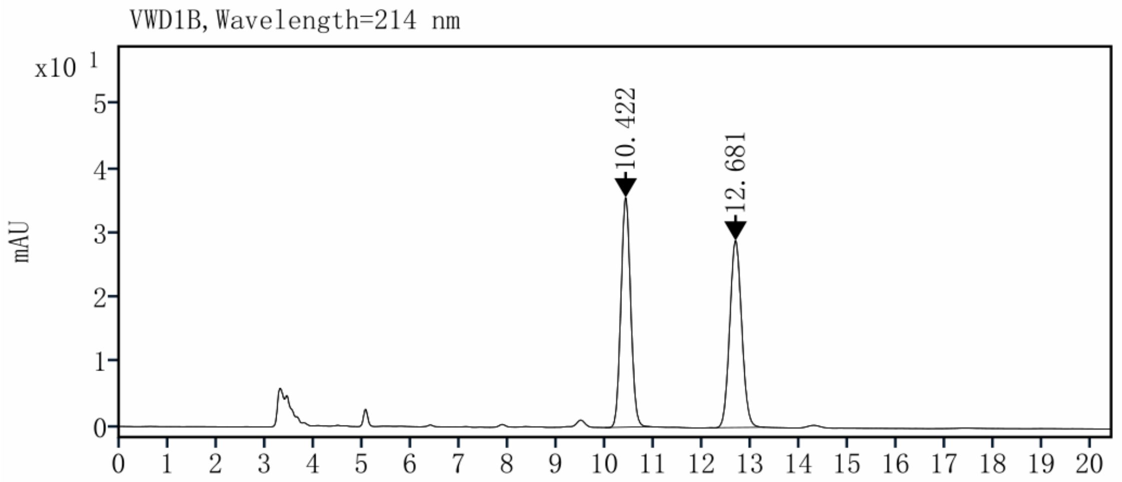
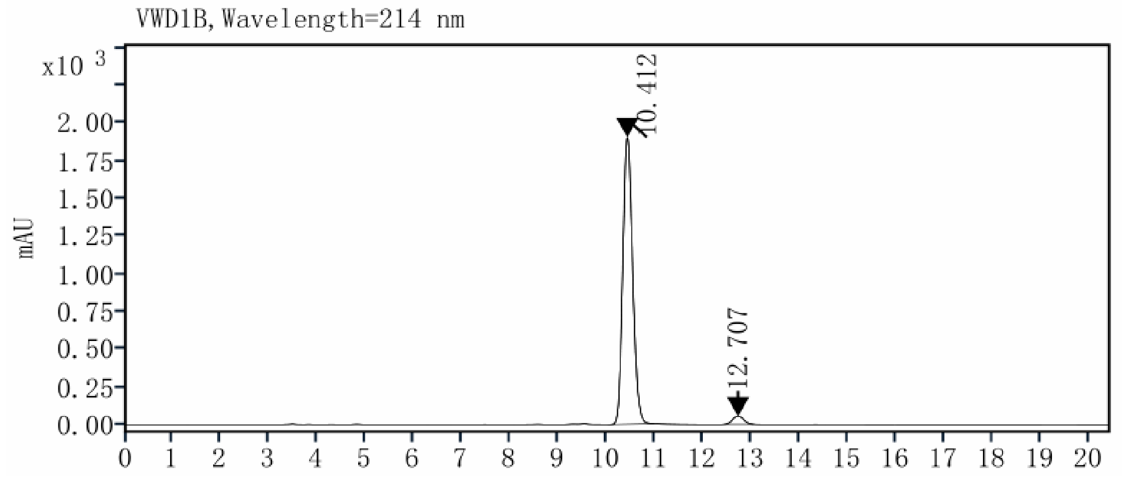


Fig. 2a, entry 10
(*S*)-**L1**: 94% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.422	MM m	495.41	49.89
	12.681	MM m	497.61	50.11



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.412	MM m	26861.36	96.83
	12.707	MM m	878.57	3.17

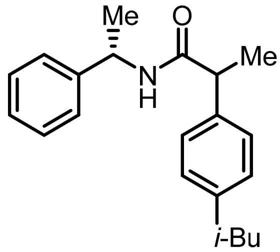
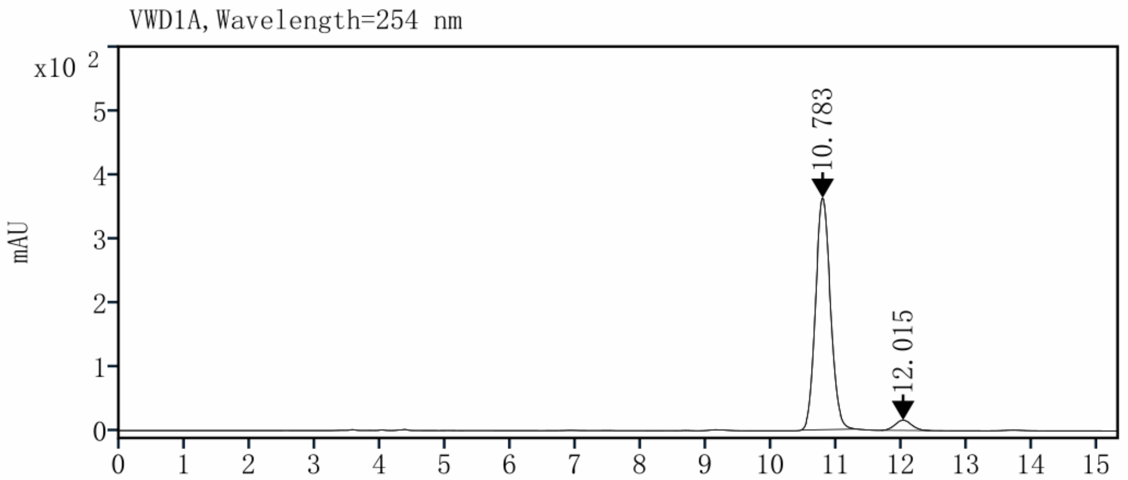
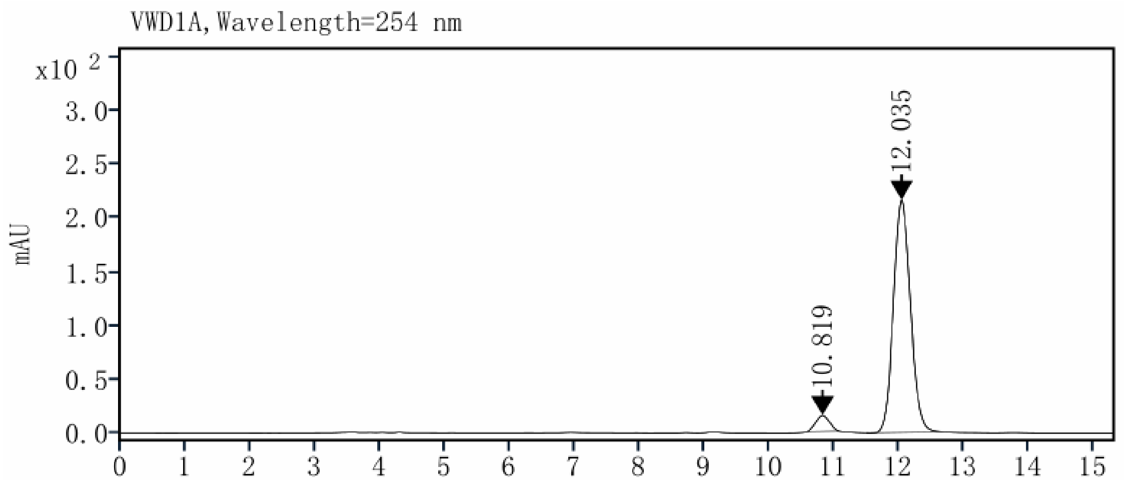


Fig. 2a, entries 11 and 12
(*S*)-**L1**: 95:5 dr, (*R*)-**L1**: 5:95 dr



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.783	MM m	5781.79	95.32
	12.015	MM m	283.94	4.68



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.819	MM m	216.15	5.18
	12.035	MM m	3958.26	94.82

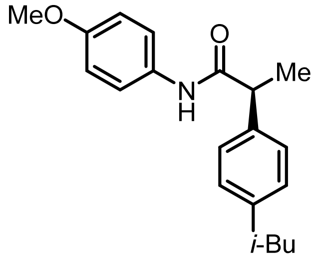
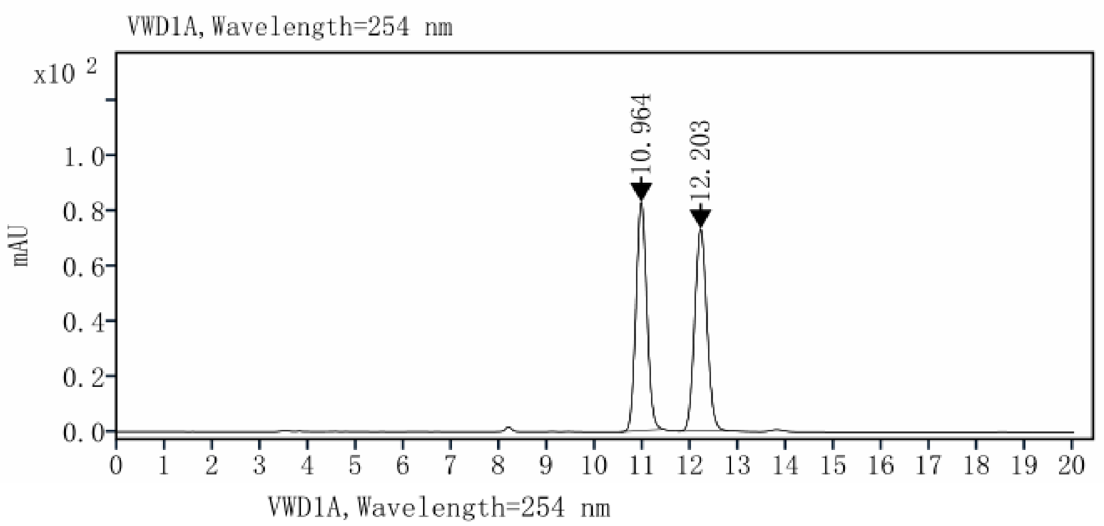
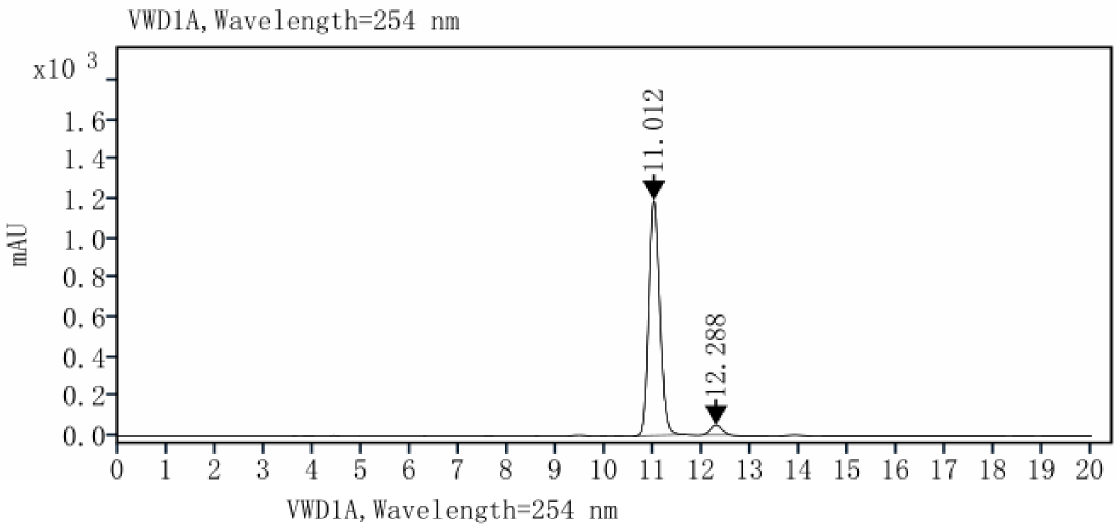


Fig. 2a, entry 13
(*S*)-**L1**: 92% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.964	MM m	1295.15	49.96
	12.203	MM m	1297.30	50.04



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.012	MM m	18901.83	95.87
	12.288	MM m	815.05	4.13

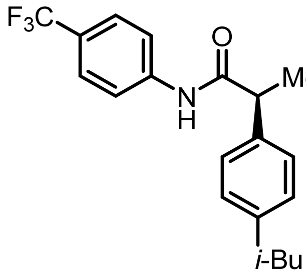
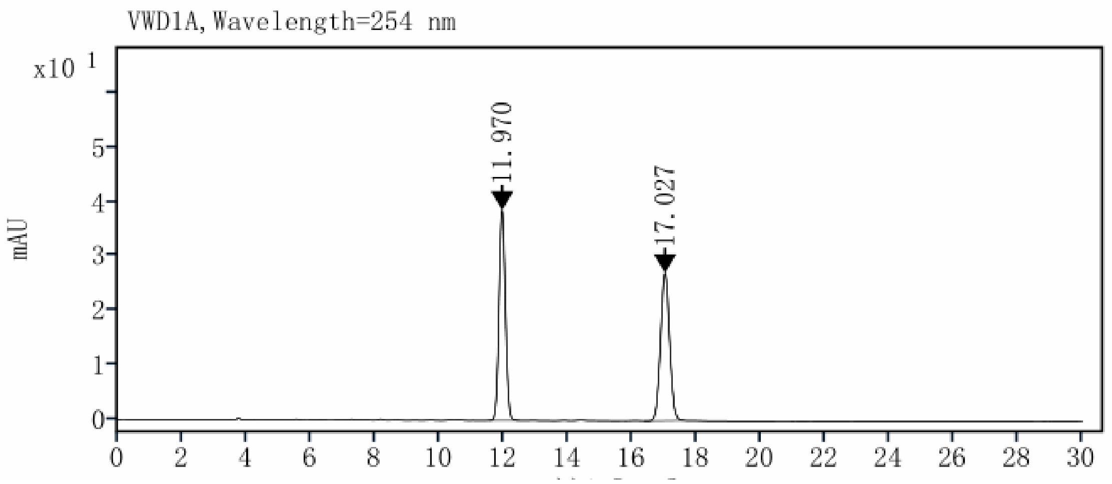
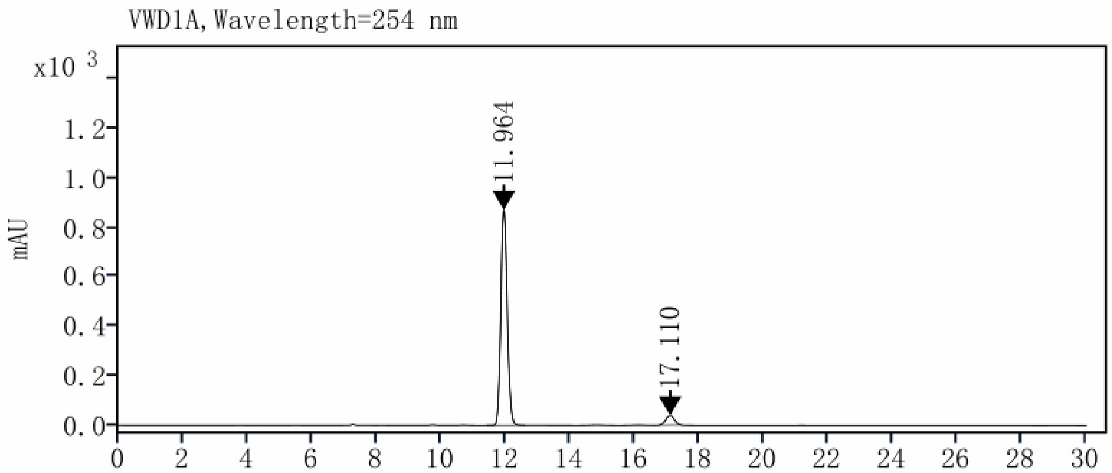


Fig. 2a, entry 14
(*S*)-**L1**: 89% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.970	MM m	531.54	50.12
	17.027	MM m	529.09	49.88



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.964	MM m	12076.93	94.38
	17.110	MM m	719.27	5.62

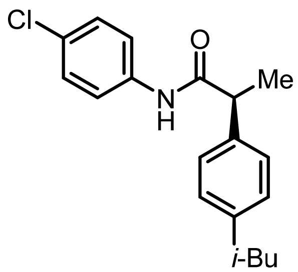
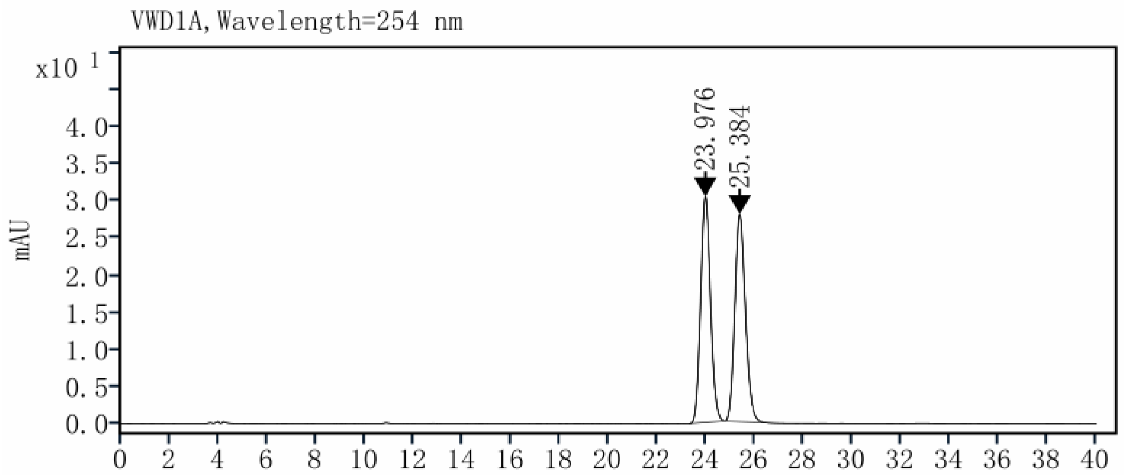
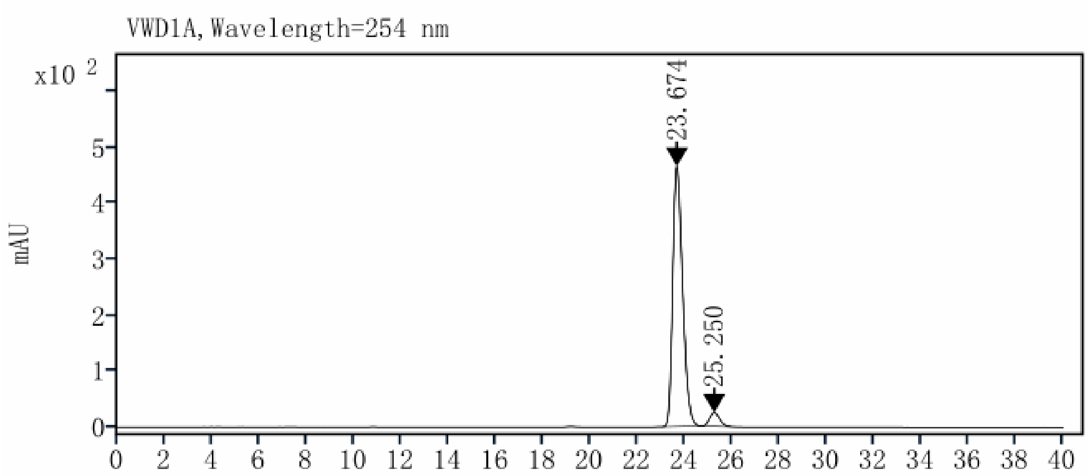


Fig. 2a, entry 15
(*S*)-**L1**: 90% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	23.976	MM m	854.79	50.09
	25.384	MM m	851.58	49.91



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	23.674	MM m	13451.37	95.03
	25.250	MM m	703.92	4.97

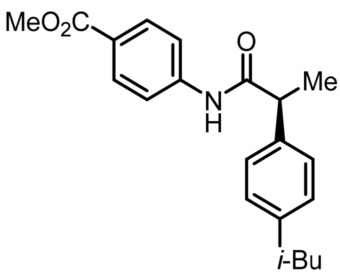
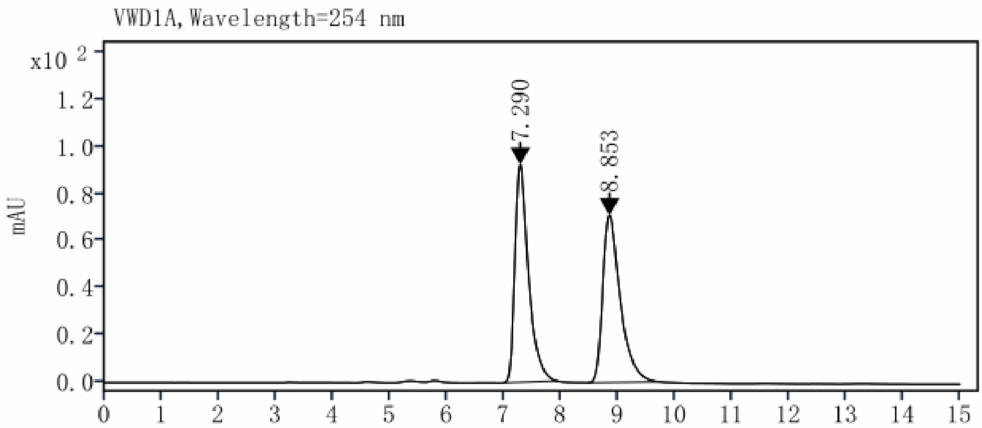
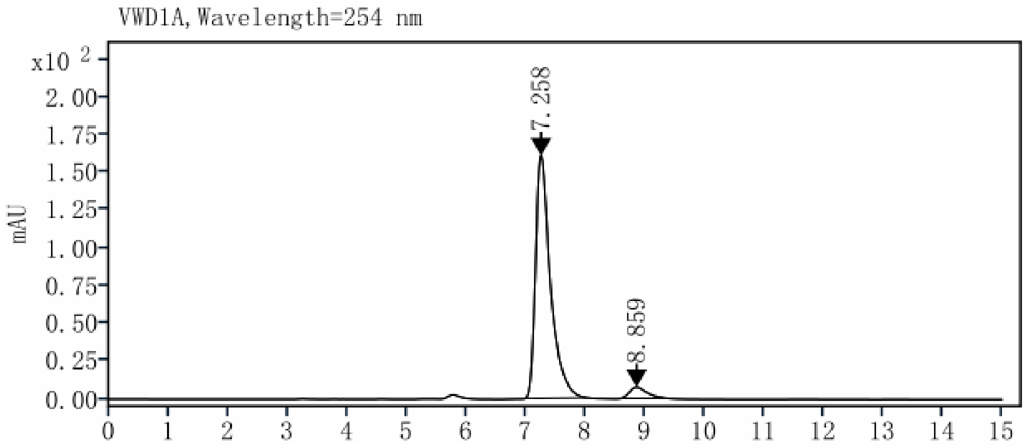


Fig. 2a, entry 16
(*S*)-**L1**: 90% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.290	MM m	1522.94	50.08
	8.853	MM m	1517.95	49.92
		总和	3040.89	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.258	MM m	2788.05	94.89
	8.859	MM m	150.02	5.11
		总和	2938.08	

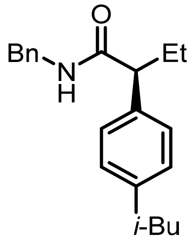
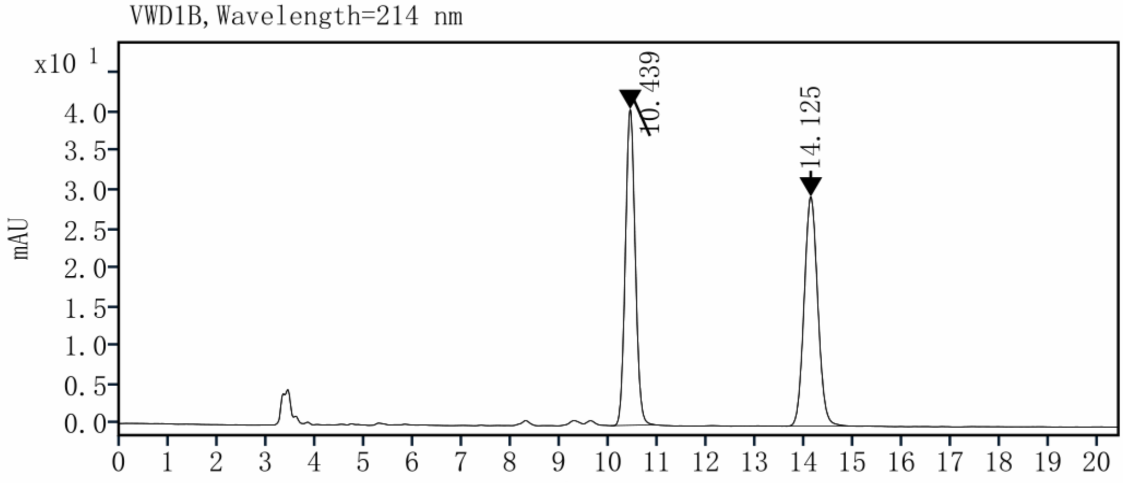
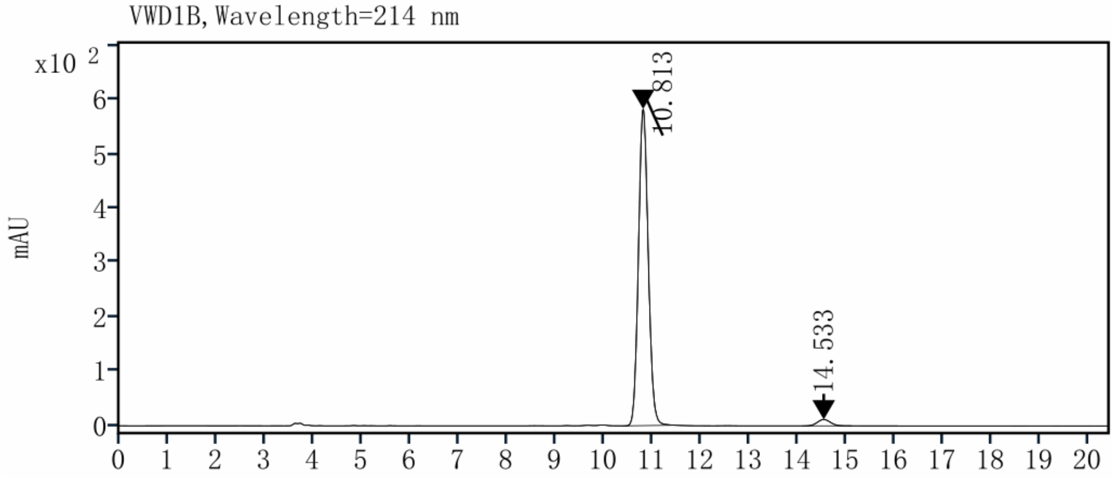


Fig. 2b, entry 17
(S)-**L1**: 95% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.439	MM m	565.47	49.85
	14.125	MM m	568.90	50.15



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.813	MM m	8163.73	97.32
	14.533	MM m	224.93	2.68

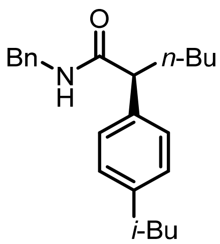
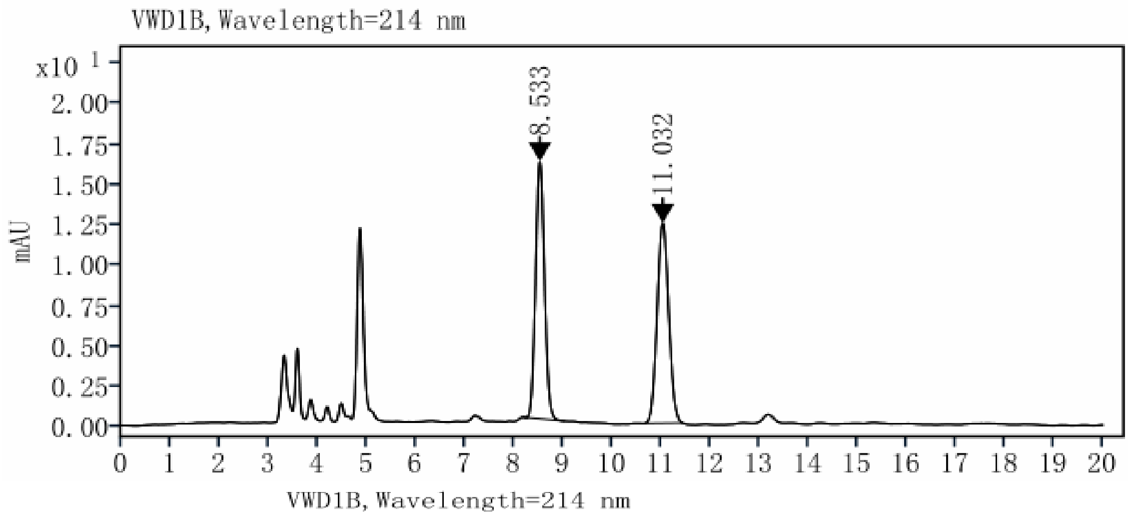
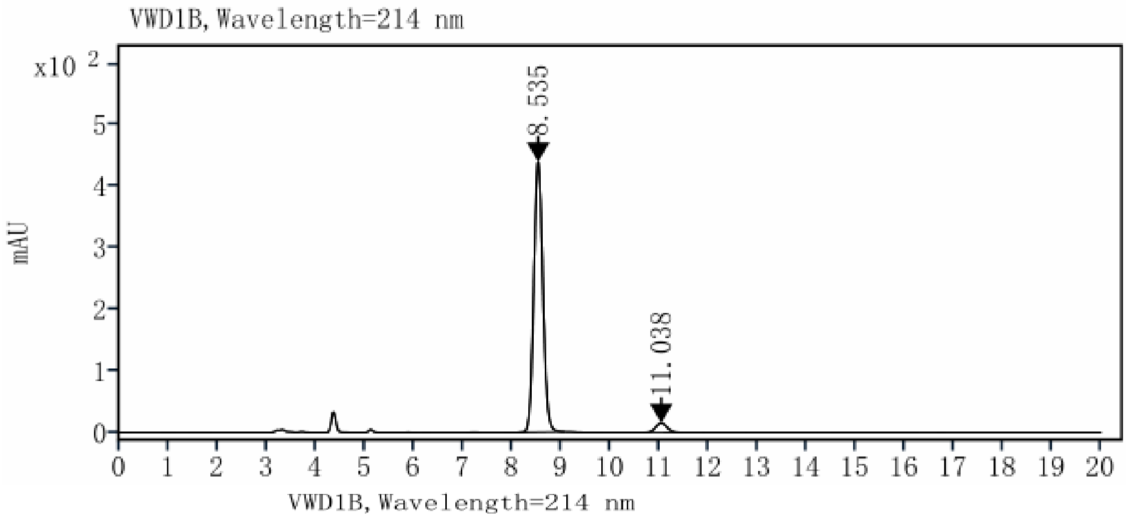


Fig. 2b, entry 18
(*S*)-**L1**: 92% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	8.533	MM m	199.47	49.54
	11.032	MM m	203.16	50.46
		总和	**402.63**	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	8.535	MM m	5608.99	95.97
	11.038	MM m	235.74	4.03
		总和	**5844.73**	

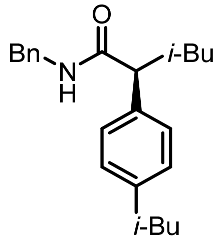
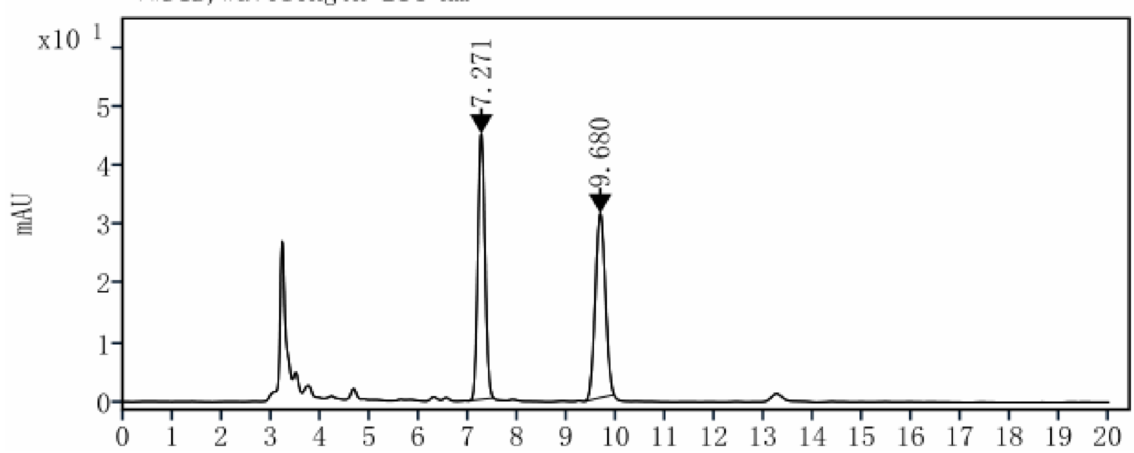


Fig. 2b, entry 19
(*S*)-**L1**: 87% ee

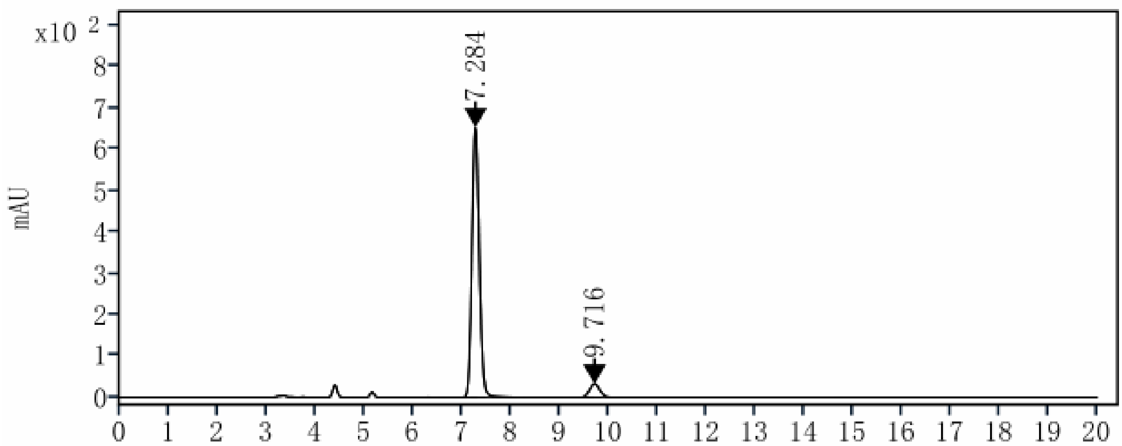
VWD1B, Wavelength=214 nm



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.271	MM m	453.33	50.61
	9.680	MM m	442.41	49.39
		总和	895.74	

VWD1B, Wavelength=214 nm



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.284	MM m	6765.38	93.67
	9.716	MM m	457.38	6.33
		总和	7222.76	

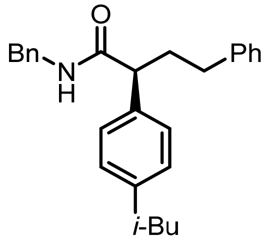
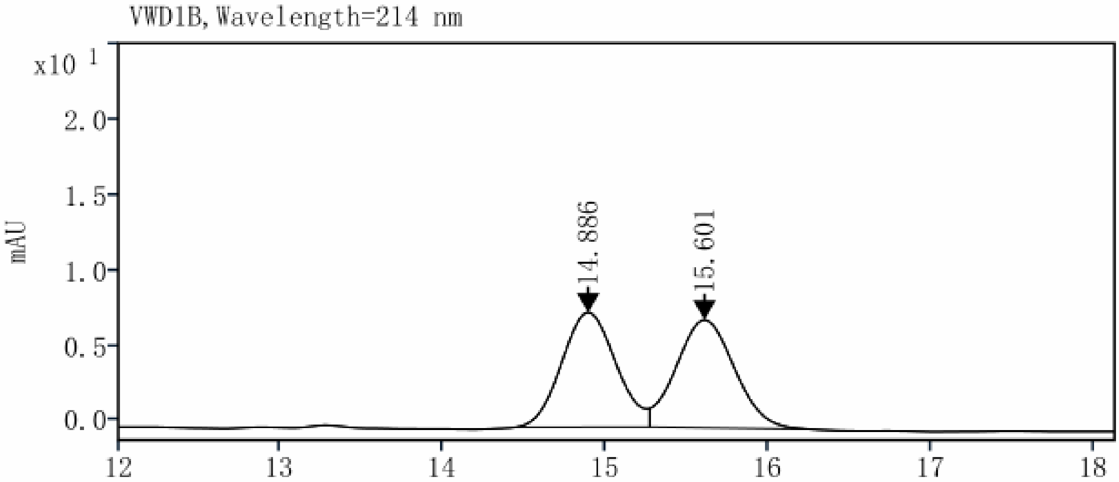
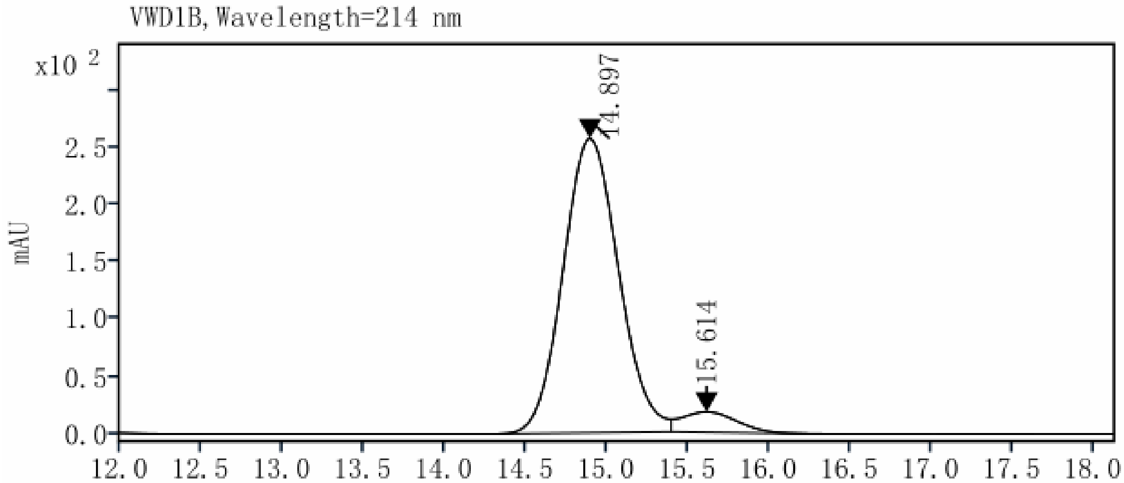


Fig. 2b, entry 20
(*S*)-**L1**: 87% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.886	MM m	177.24	49.79
	15.601	MM m	178.76	50.21
		总和	356.00	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.897	MM m	6149.04	93.55
	15.614	MM m	423.91	6.45
		总和	6572.95	

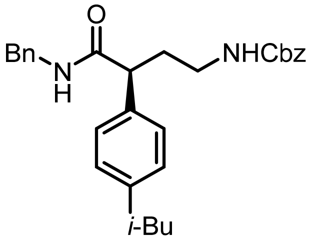
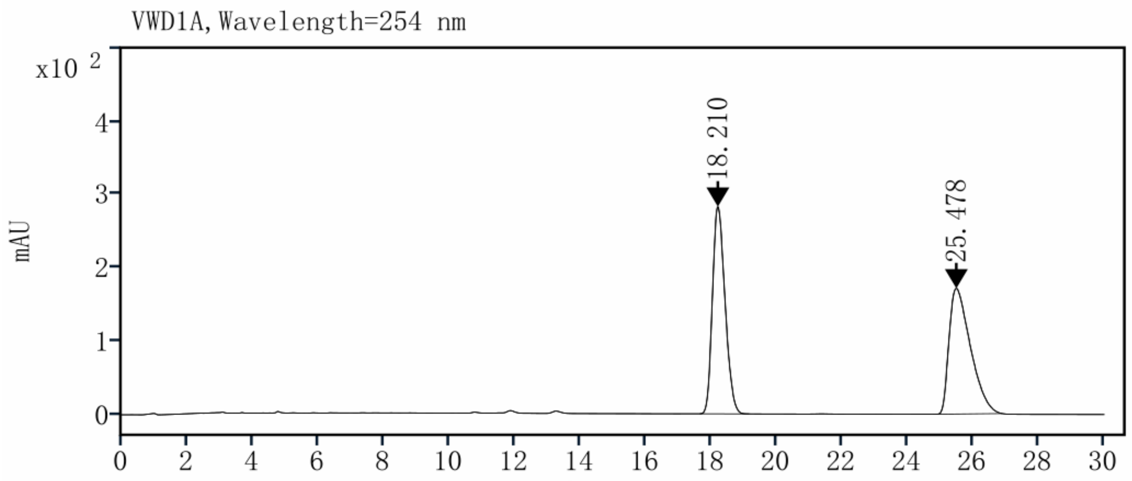
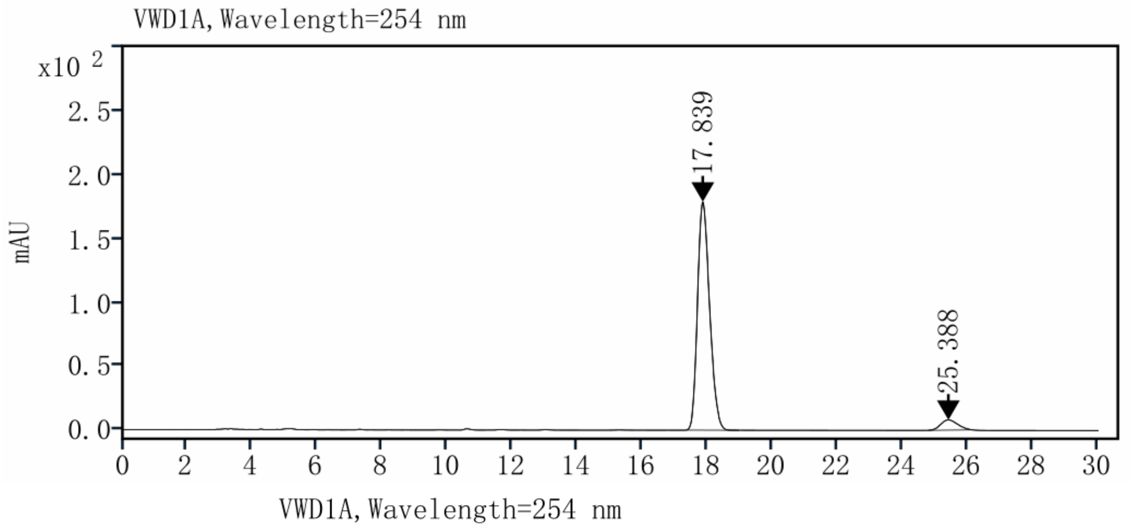


Fig. 2b, entry 21
(*S*)-**L1**: 88% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	18.210	MM m	7566.52	49.31
	25.478	MM m	7779.36	50.69



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	17.839	MM m	4651.64	94.11
	25.388	MM m	290.88	5.89

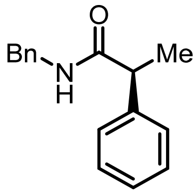
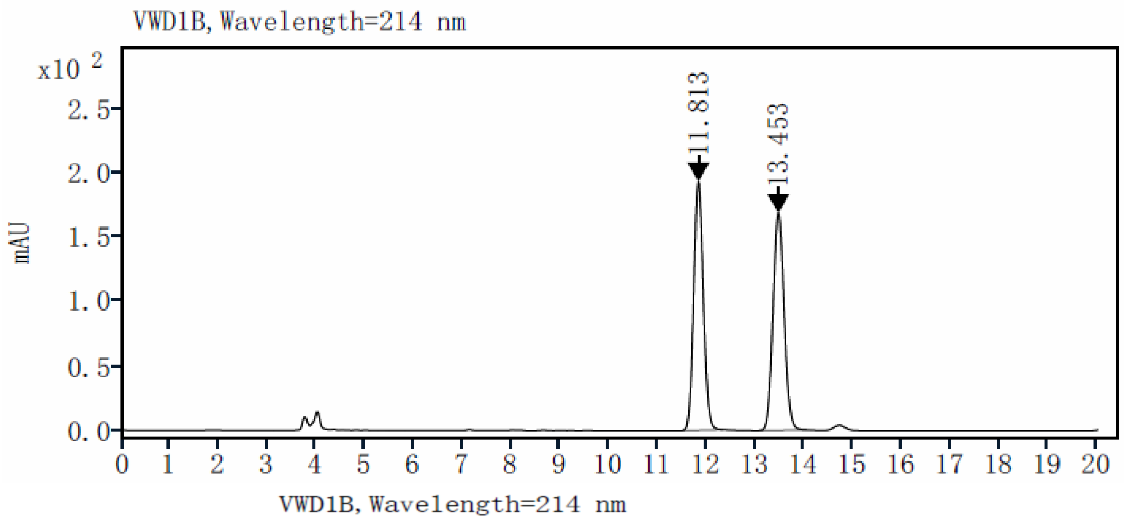
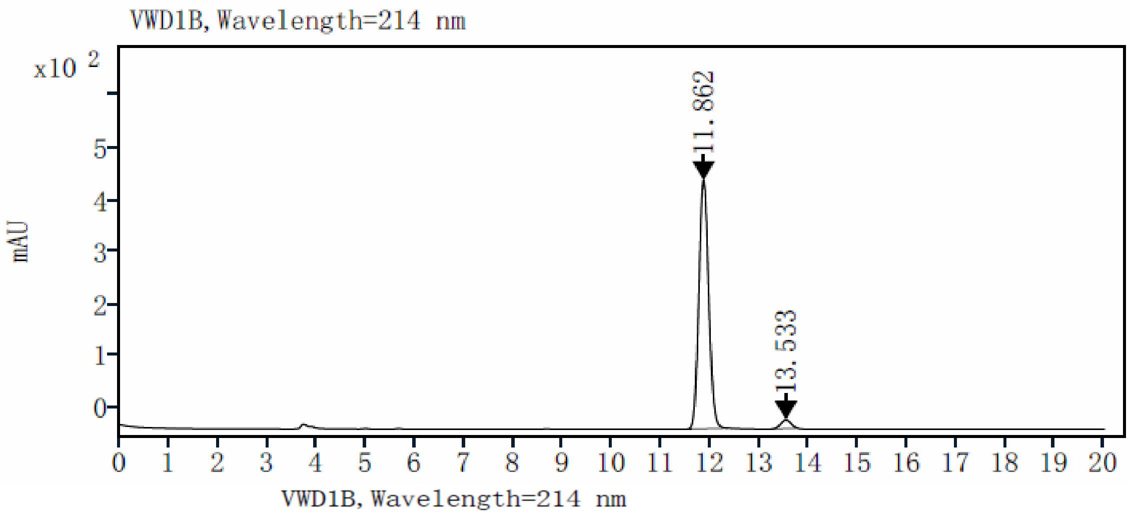


Fig. 2c, entry 22
(*S*)-**L1**: 93% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.813	MM m	2668.54	49.87
	13.453	MM m	2682.14	50.13
		总和	5350.68	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.862	MM m	6607.18	96.43
	13.533	MM m	244.43	3.57
		总和	6851.61	

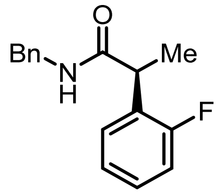
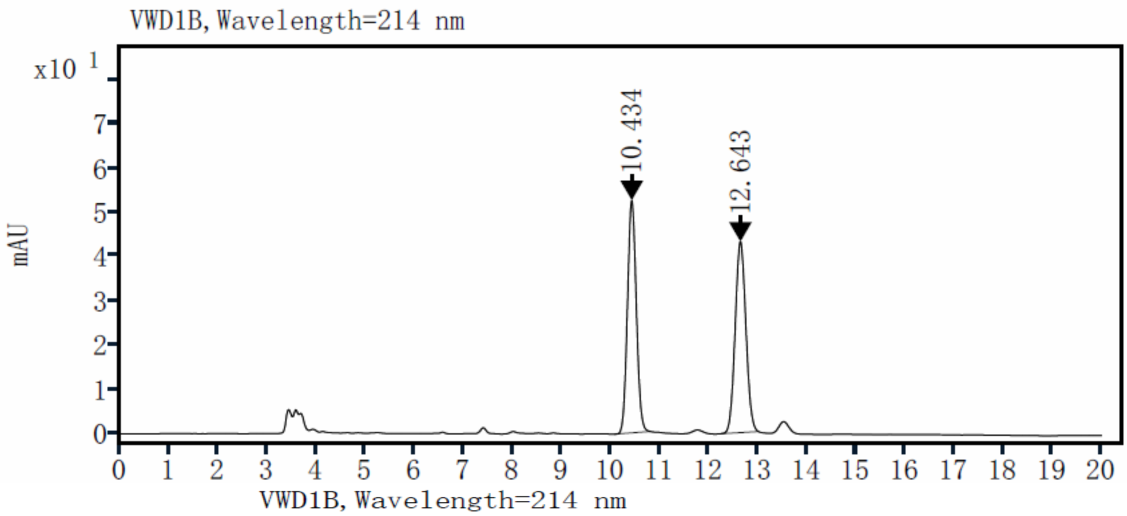
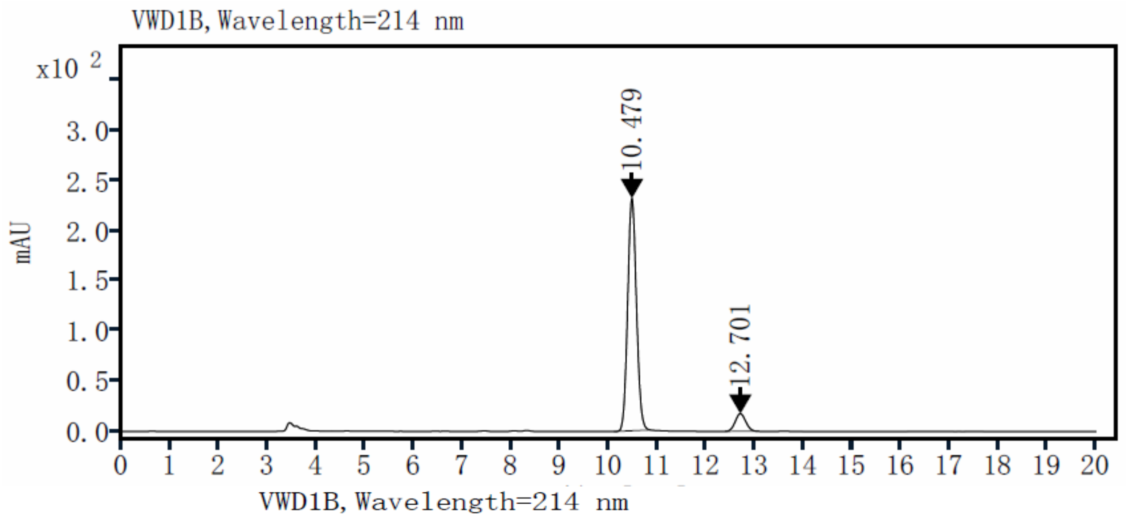


Fig. 2c, entry 23
(*S*)-**L1**: 83% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.434	MM m	656. 80	50. 12
	12.643	MM m	653. 61	49. 88
		总和	**1310. 41**	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.479	MM m	2899. 63	91. 63
	12.701	MM m	264. 98	8. 37
		总和	**3164. 61**	

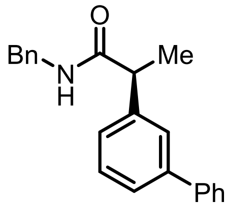
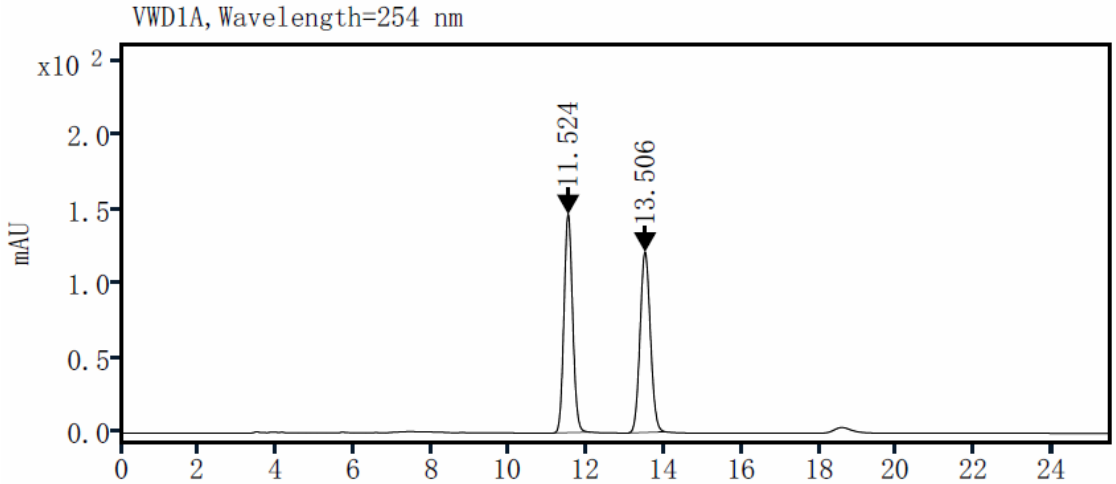
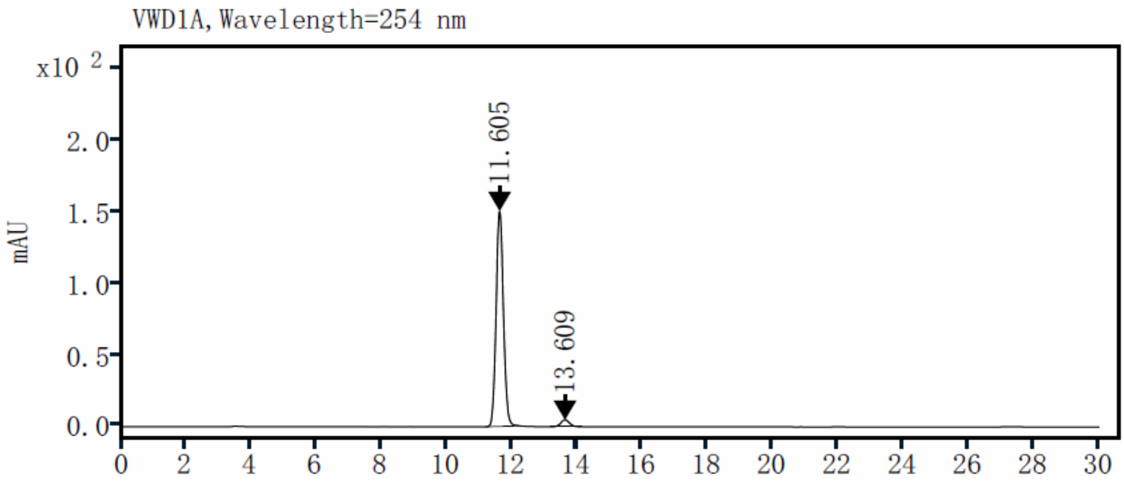


Fig. 2c, entry 24
(*S*)-**L1**: 93% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.524	MM m	2278.22	50.21
	13.506	MM m	2258.82	49.79
		总和	4537.04	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.605	MM m	2341.96	96.31
	13.609	MM m	89.72	3.69
		总和	2431.69	

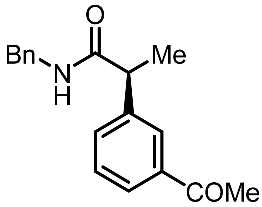
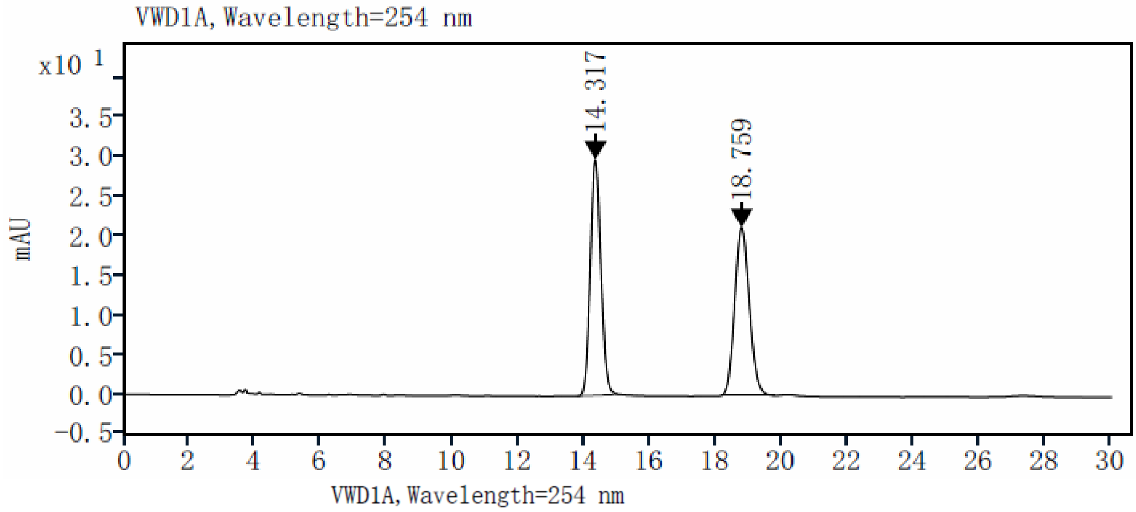
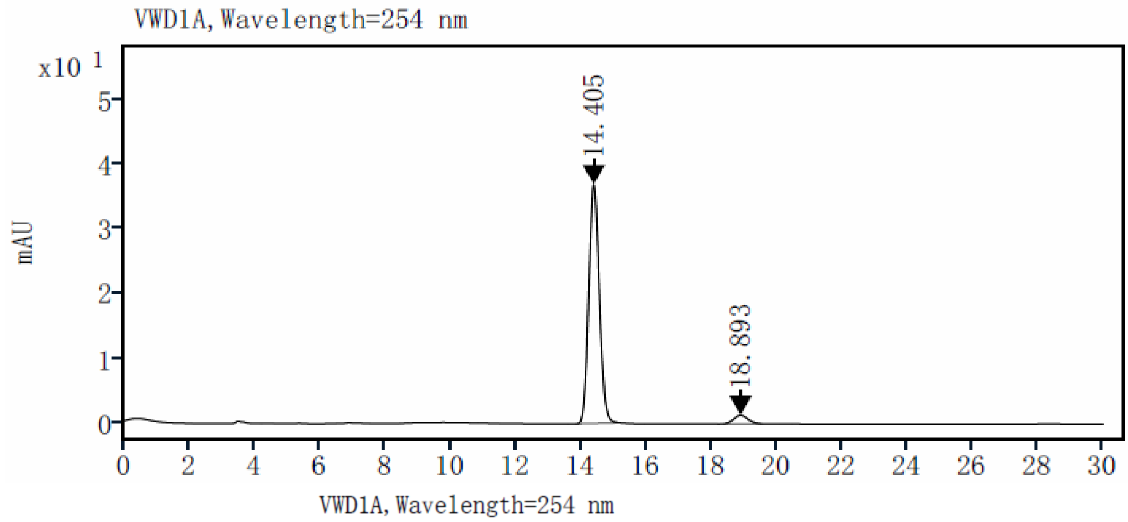


Fig. 2c, entry 25
(*S*)-**L1**: 91% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.317	MM m	663. 07	50. 14
	18.759	MM m	659. 38	49. 86
		总和	1322. 44	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.405	MM m	825. 74	95. 27
	18.893	MM m	41. 01	4. 73
		总和	866. 75	

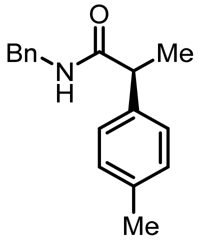
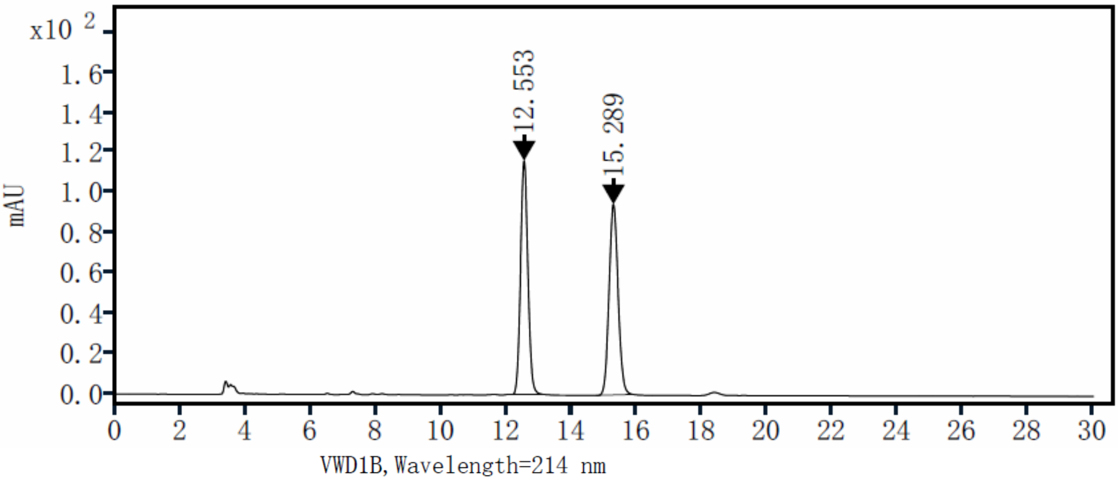


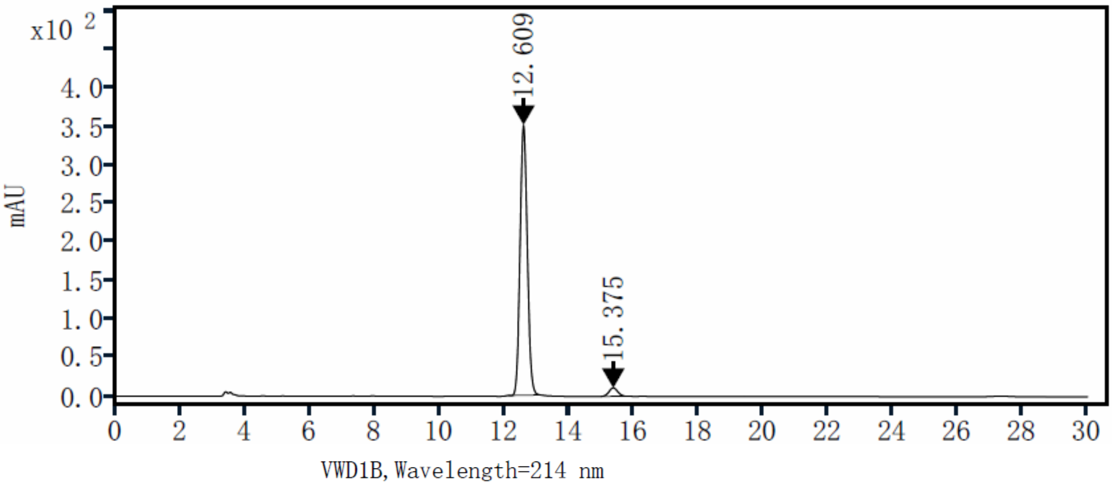
Fig. 2c, entry 26
(*S*)-**L1**: 93% ee

VWD1B, Wavelength=214 nm



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	12.553	MM m	1814.46	49.95
	15.289	MM m	1818.11	50.05
		总和	3632.57	

VWD1B, Wavelength=214 nm



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	12.609	MM m	5453.93	96.36
	15.375	MM m	206.28	3.64
		总和	5660.21	

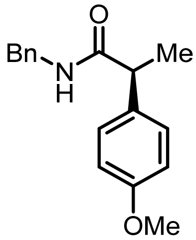
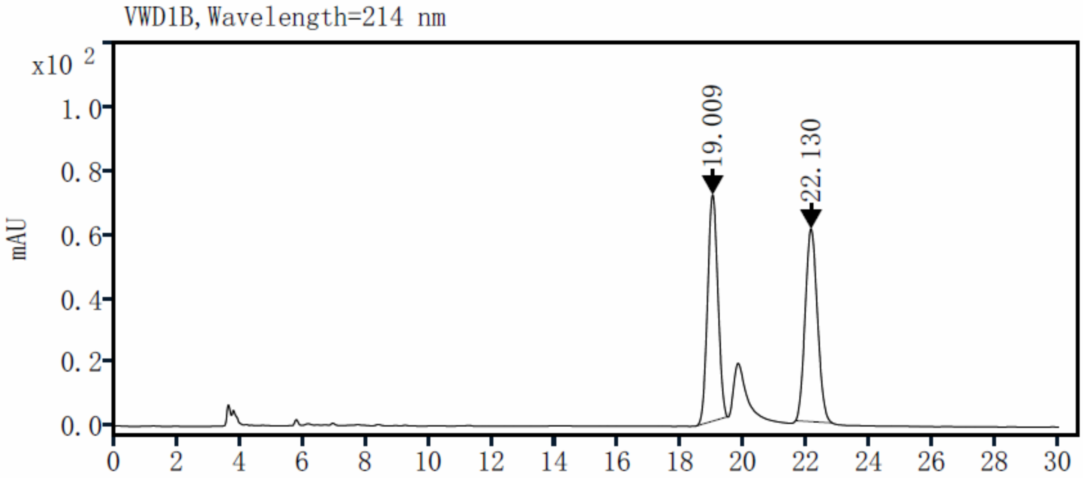


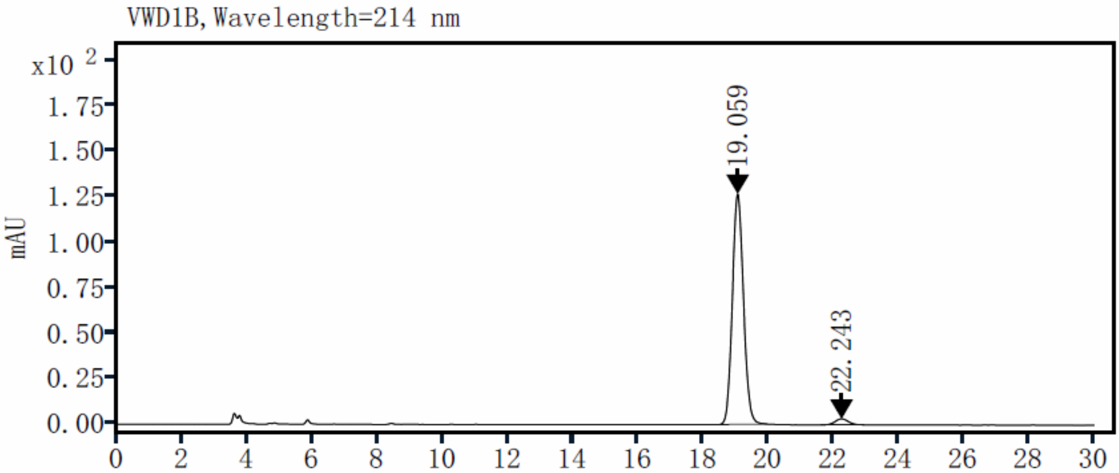
Fig. 2c, entry 27

(*S*)-**L1**: 94% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	19.009	MM m	1606.08	49.51
	22.130	MM m	1638.11	50.49
		总和	3244.19	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	19.059	MM m	2998.66	97.05
	22.243	MM m	91.05	2.95
		总和	3089.71	

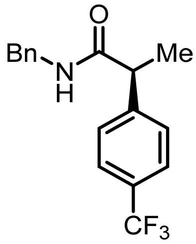
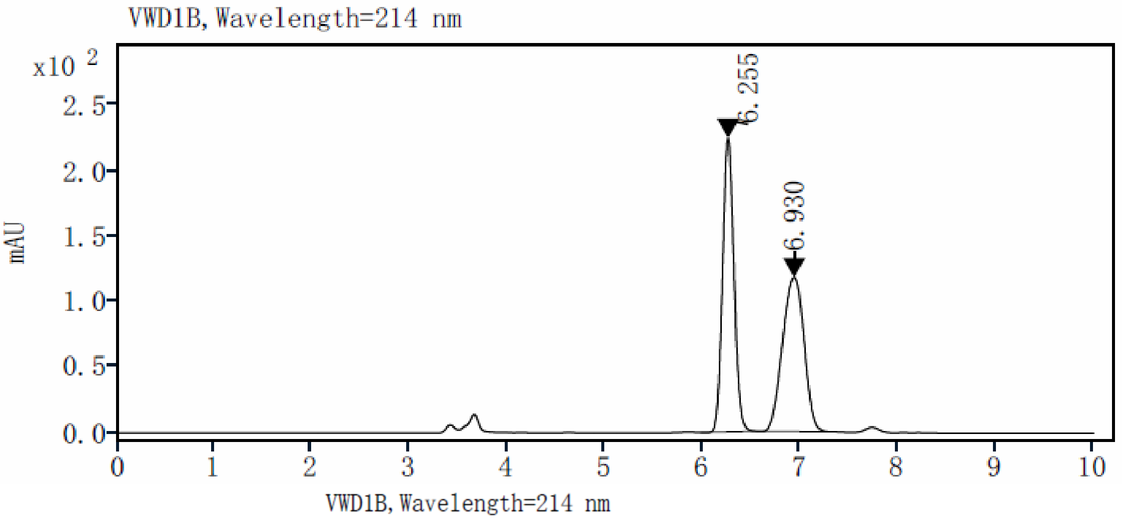
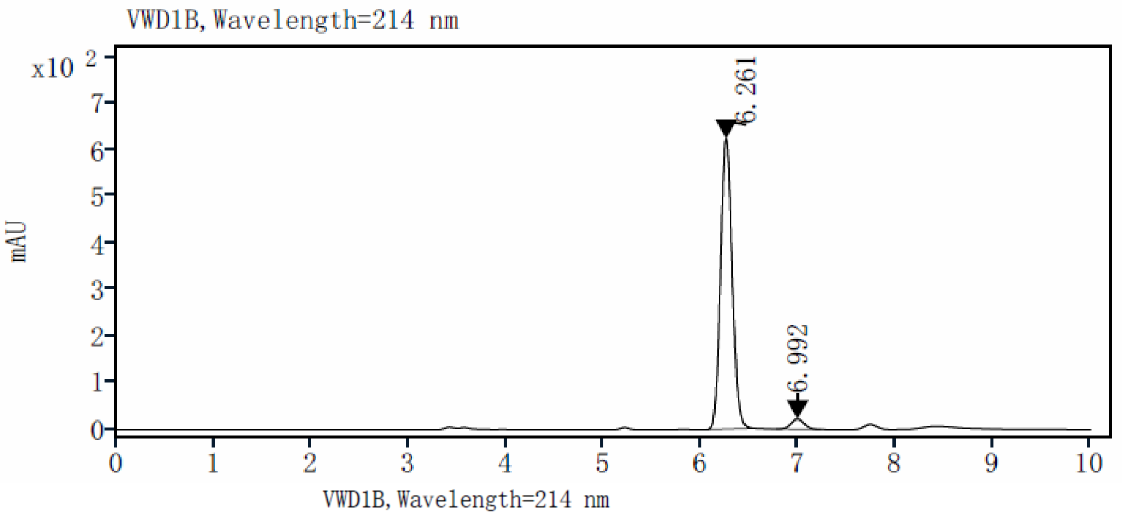


Fig. 2c, entry 28
(*S*)-**L1**: 92% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	6.255	MM m	1809.08	50.11
	6.930	MM m	1800.78	49.89
		总和	**3609.86**	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	6.261	MM m	5160.01	96.12
	6.992	MM m	208.44	3.88
		总和	**5368.44**	

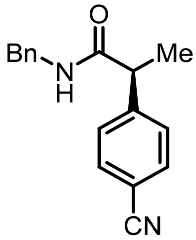
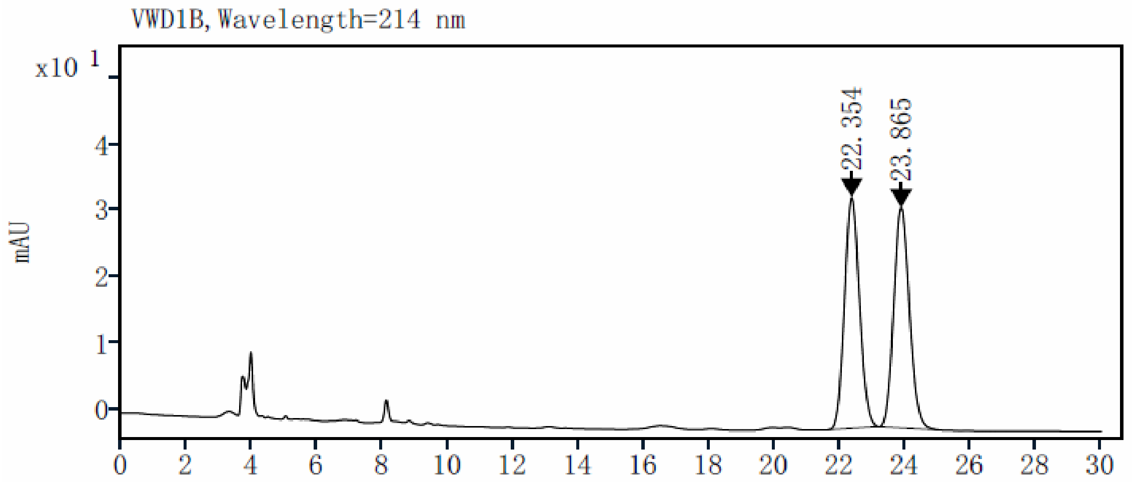
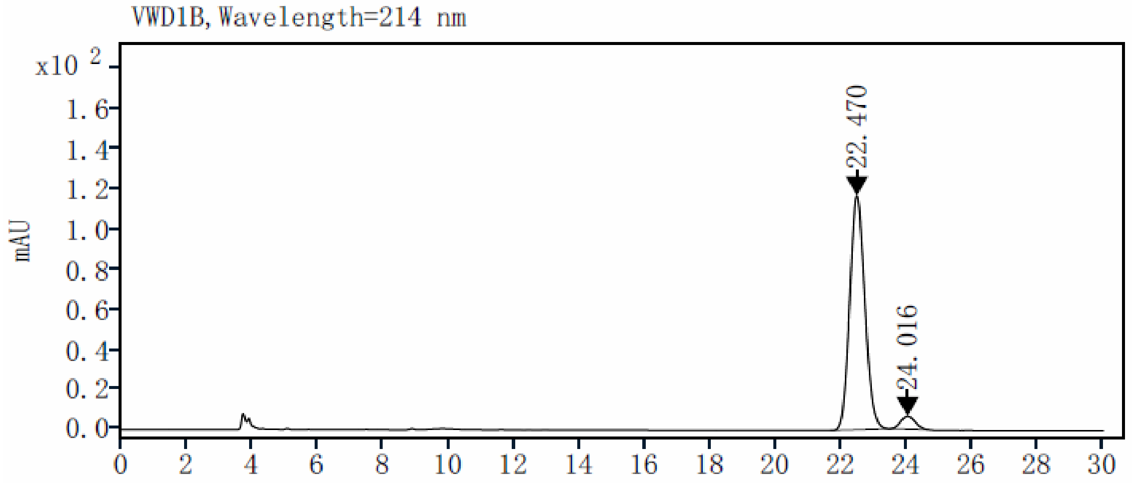


Fig. 2c, entry 29
(*S*)-**L1**: 90% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	22.354	MM m	1103. 43	49. 98
	23.865	MM m	1104. 17	50. 02
		总和	2207. 60	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	22.470	MM m	3739. 94	94. 96
	24.016	MM m	198. 41	5. 04
		总和	3938. 35	

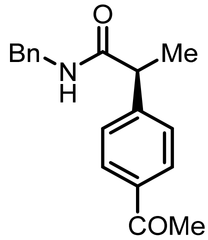
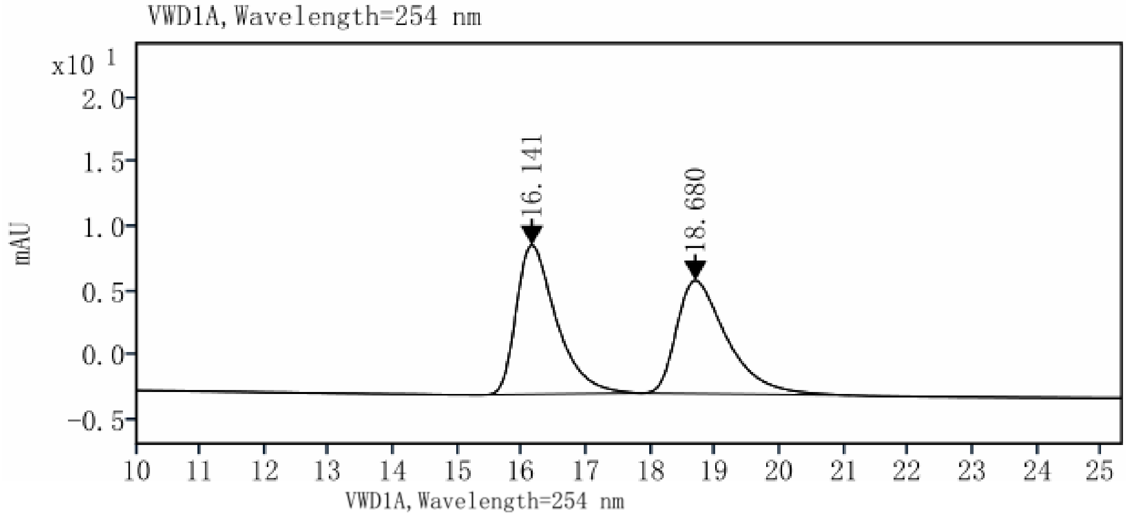
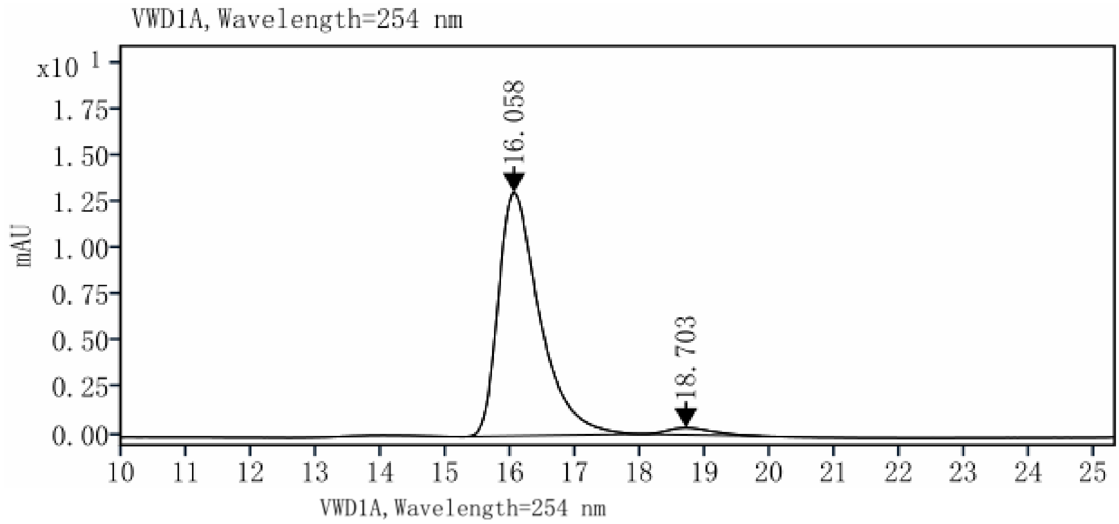


Fig. 2c, entry 30
(*S*)-**L1**: 94% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	16.141	MM m	503.51	50.24
	18.680	MM m	479.07	49.76
		总和	**982.58**	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	16.058	MM m	579.28	97.01
	18.703	MM m	17.83	2.99
		总和	**597.11**	

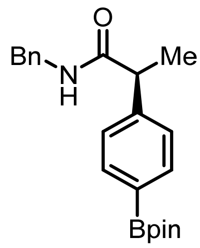
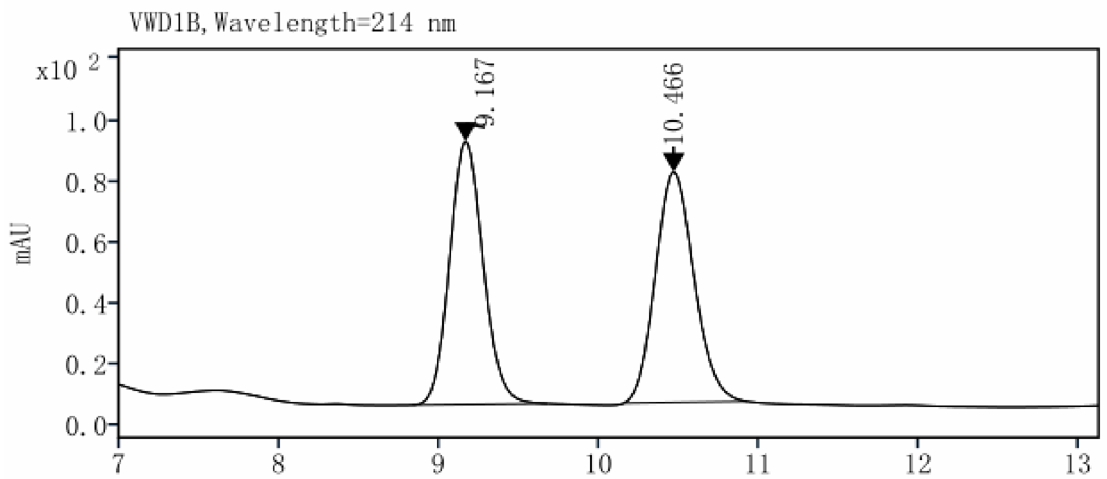
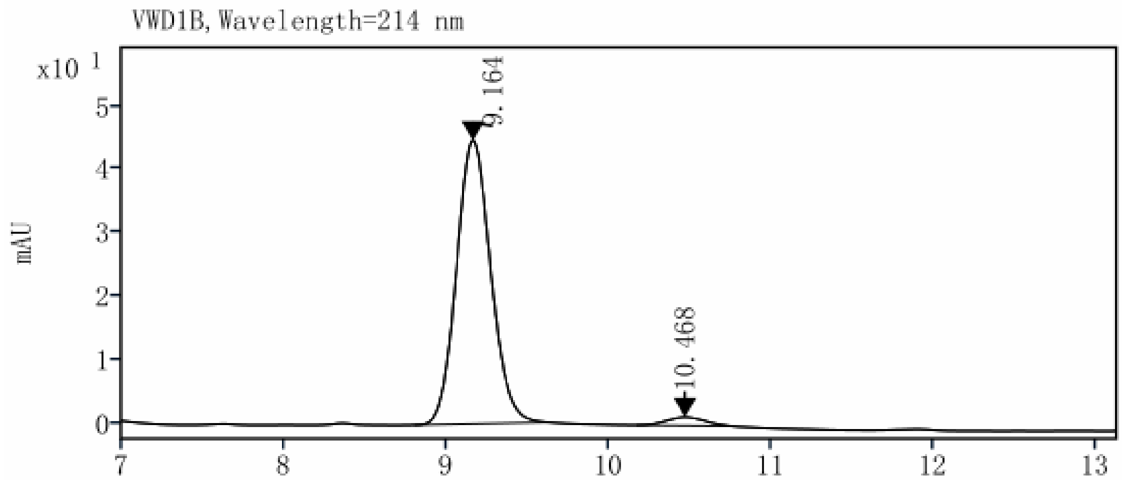


Fig. 2c, entry 31
(*S*)-**L1**: 94% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.167	MM m	1255.91	49.74
	10.466	MM m	1269.08	50.26
		总和	2524.99	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.164	MM m	655.34	96.79
	10.468	MM m	21.70	3.21
		总和	677.04	

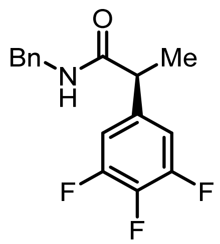
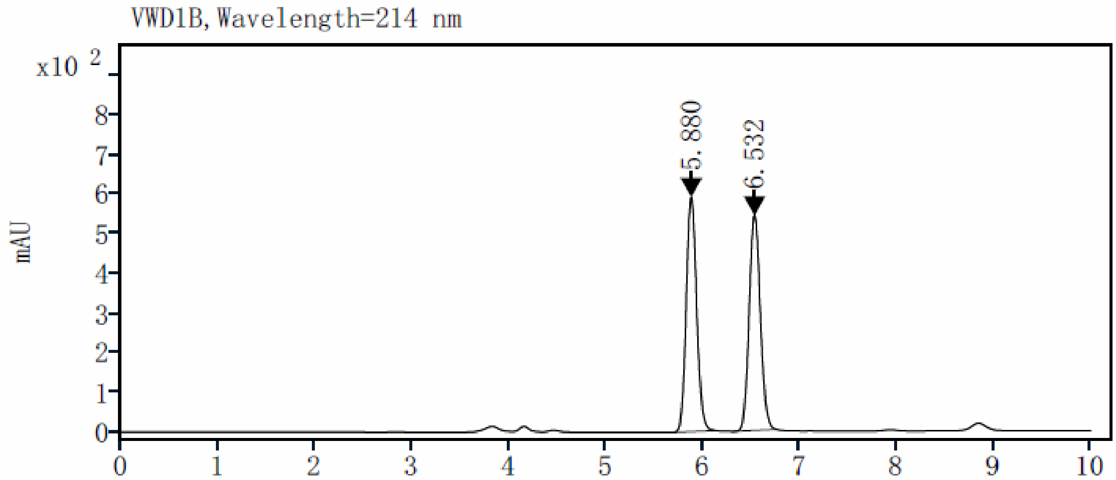
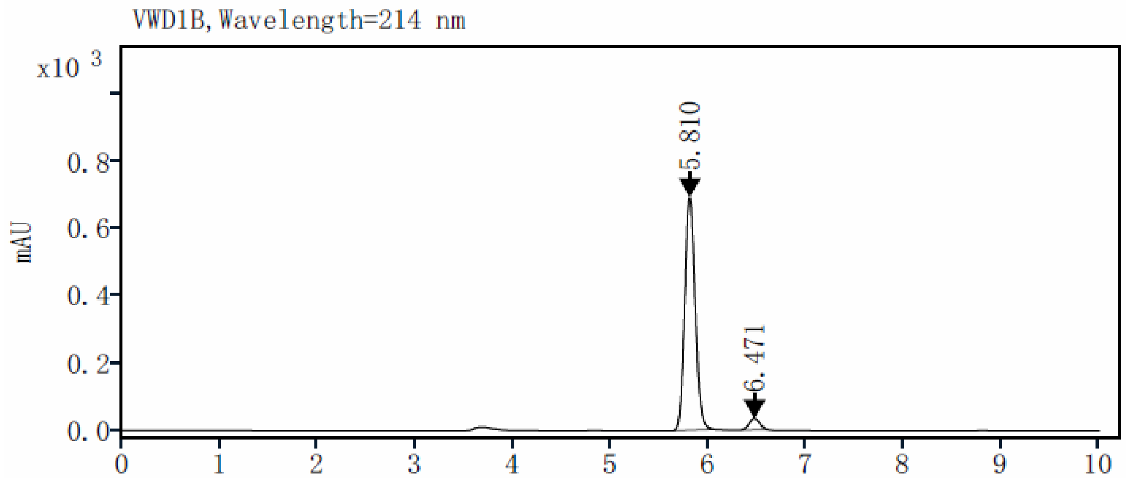


Fig. 2c, entry 32
(*S*)-**L1**: 91% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.880	MM m	4398.01	50.19
	6.532	MM m	4365.02	49.81
		总和	8763.03	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.810	MM m	5149.37	95.45
	6.471	MM m	245.47	4.55
		总和	5394.83	

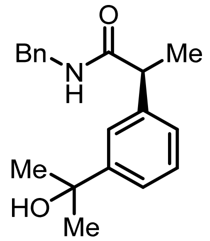
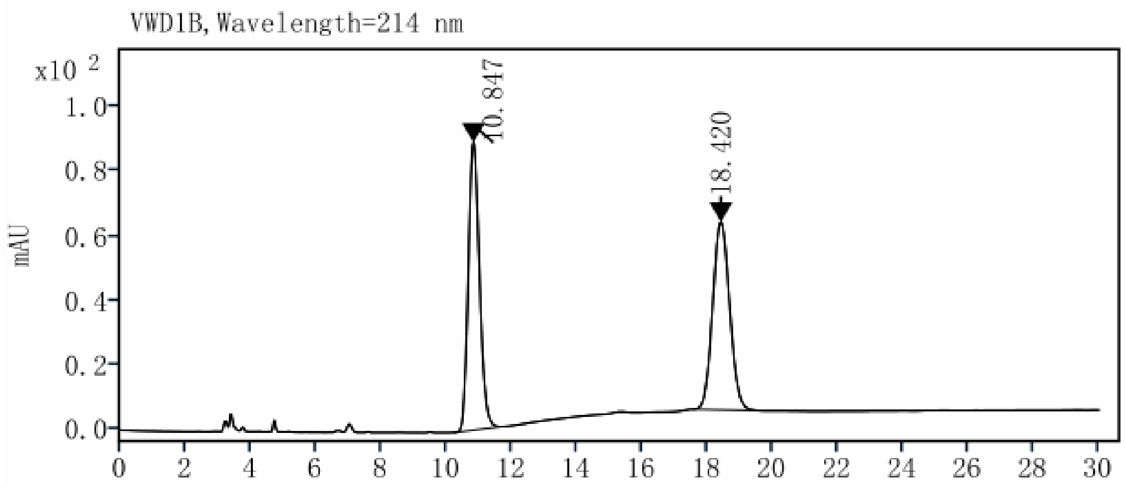
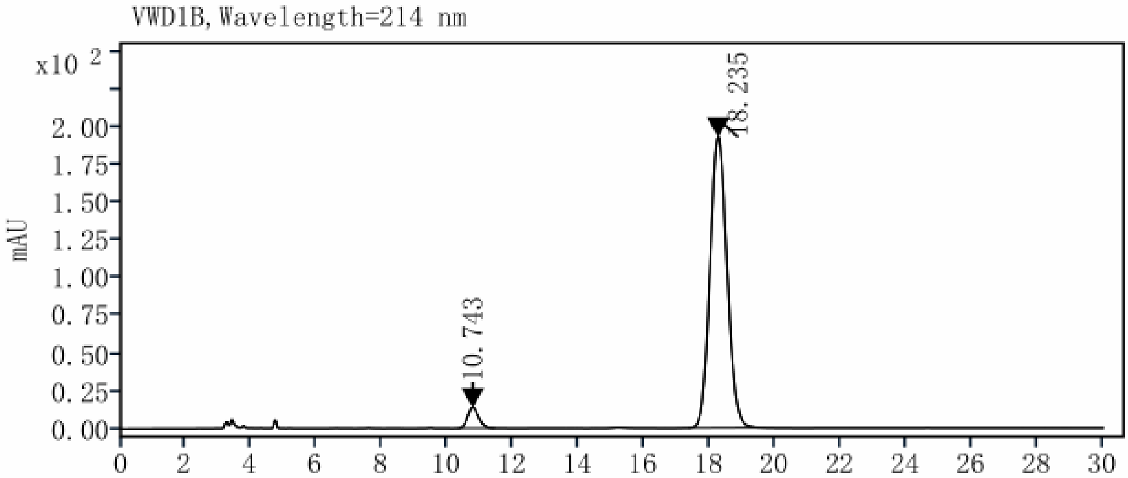


Fig. 2c, entry 33
(*S*)-**L1**: 91% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.847	MM m	2111.79	50.13
	18.420	MM m	2100.67	49.87
		总和	4212.46	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.743	MM m	323.10	4.42
	18.235	MM m	6992.05	95.58
		总和	7315.16	

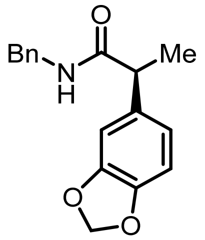
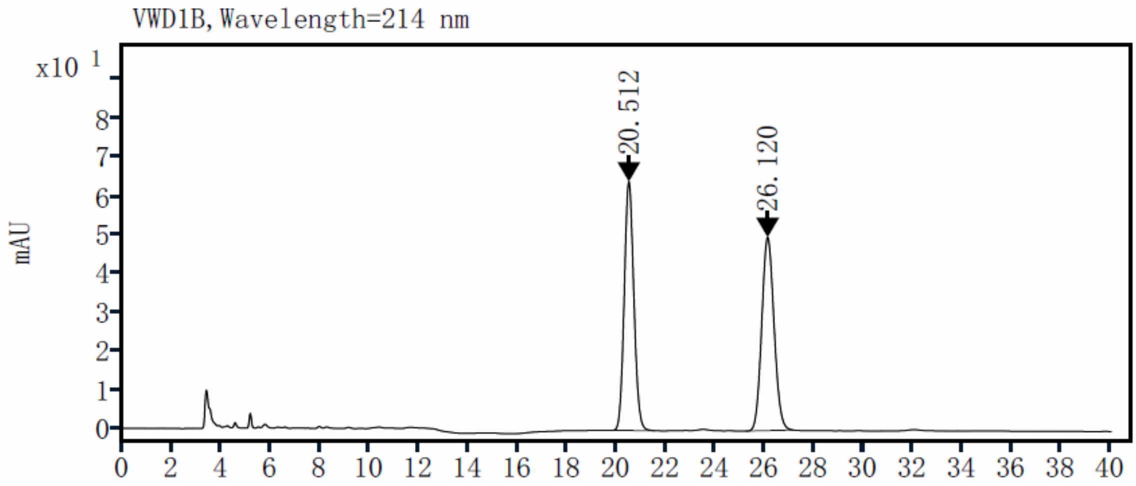
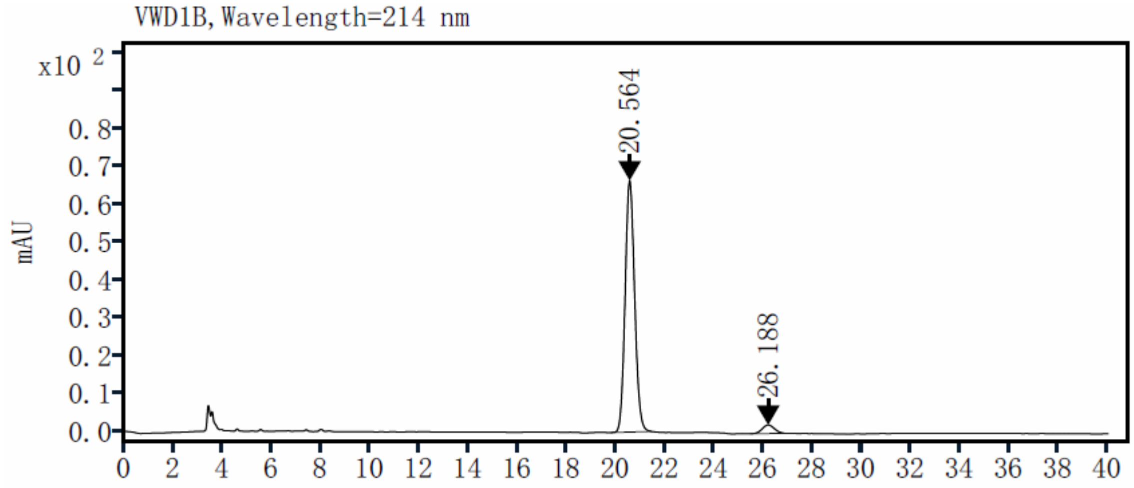


Fig. 2c, entry 34
(*S*)-**L1**: 92% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	20.512	MM m	1727.77	50.02
	26.120	MM m	1726.29	49.98
		总和	3454.05	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	20.564	MM m	1788.81	95.81
	26.188	MM m	78.14	4.19
		总和	1866.95	

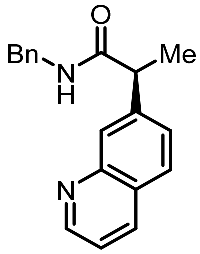
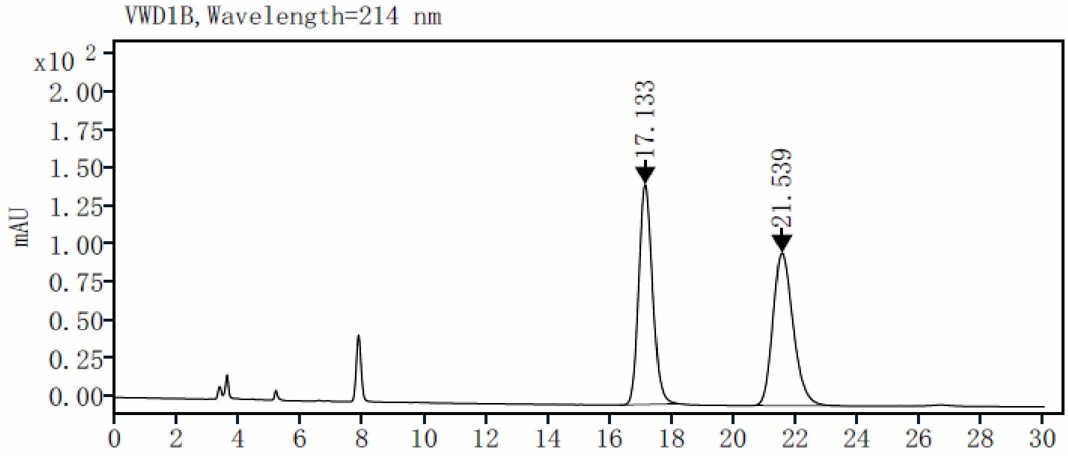
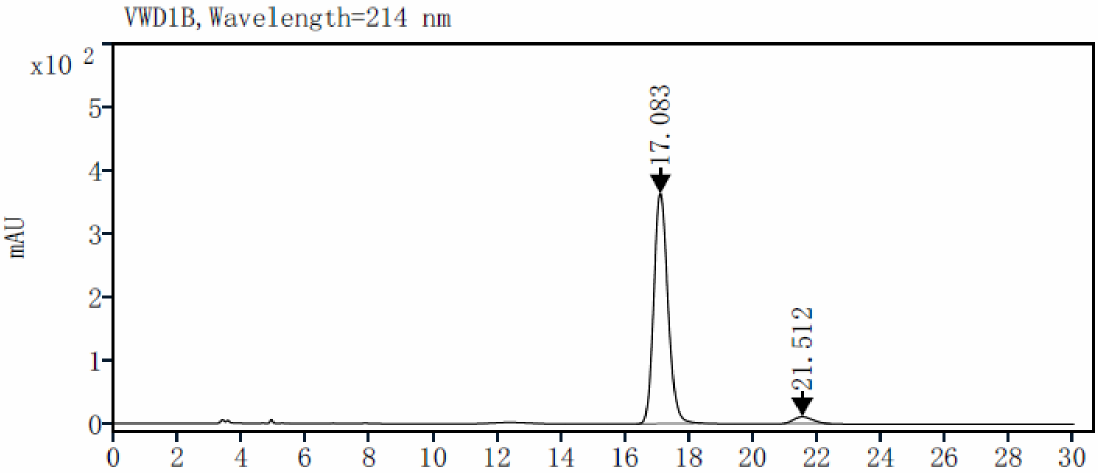


Fig. 2c, entry 35
(*S*)-**L1**: 92% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	17.133	MM m	4463.88	49.78
	21.539	MM m	4503.74	50.22
		总和	8967.62	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	17.083	MM m	11190.27	96.12
	21.512	MM m	451.83	3.88
		总和	11642.10	

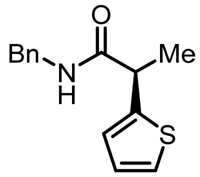
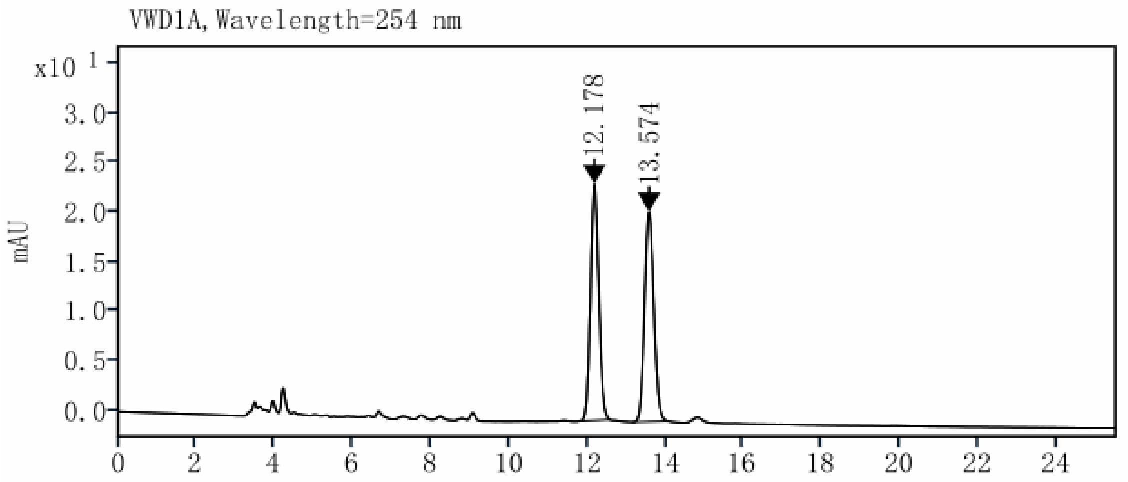
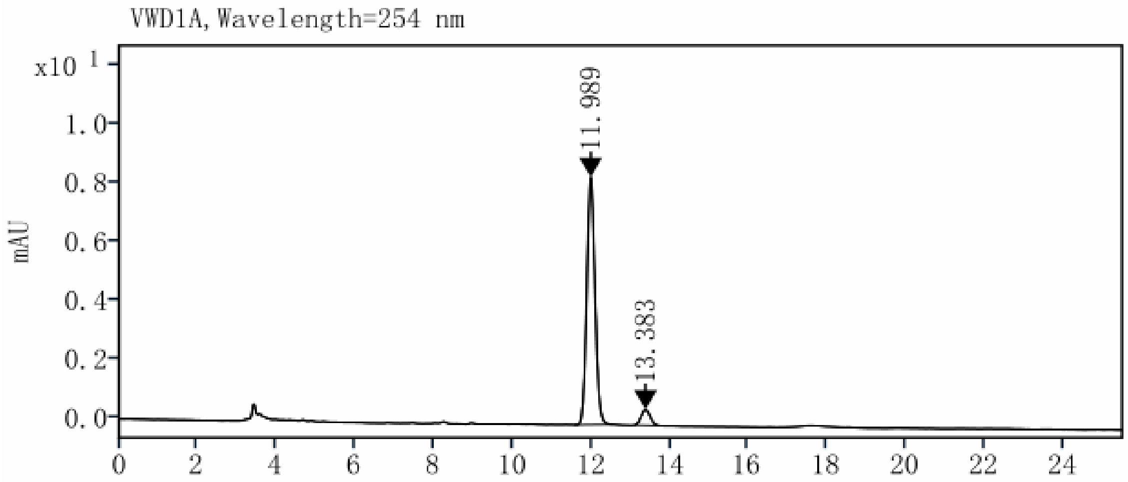


Fig. 2c, entry 36
(*S*)-**L1**: 87% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	12.178	MM m	353.18	50.13
	13.574	MM m	351.29	49.87
		总和	704.47	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	11.989	MM m	123.88	93.50
	13.383	MM m	8.61	6.50
		总和	132.49	

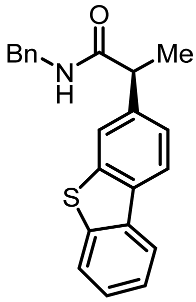
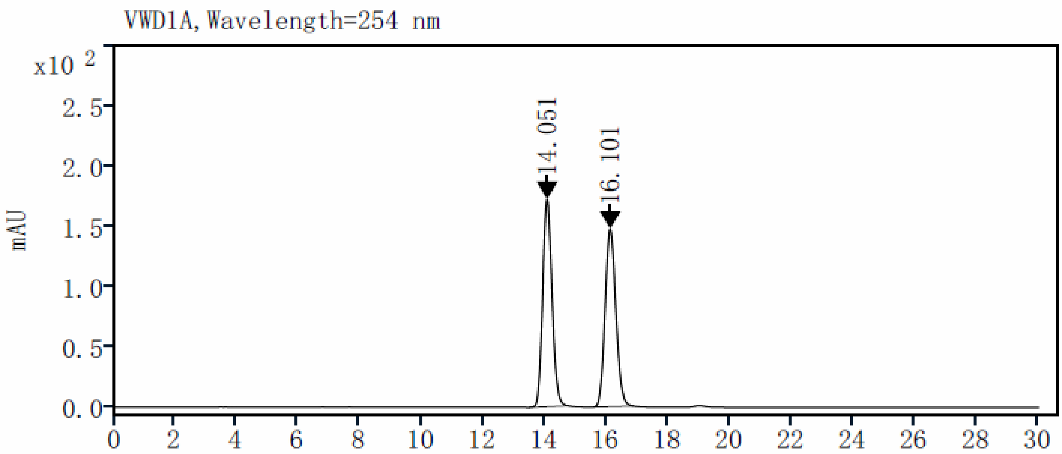
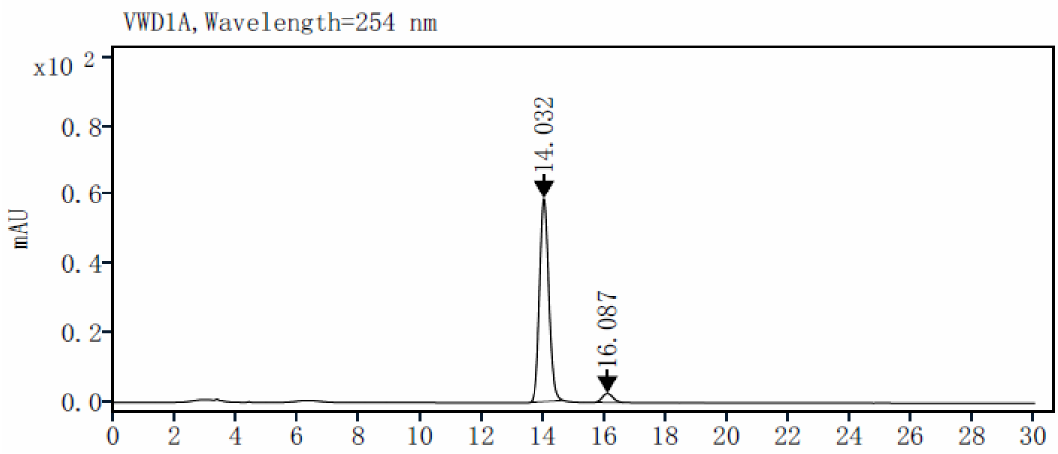


Fig. 2c, entry 37
(*S*)-**L1**: 91% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.051	MM m	3638.36	50.32
	16.101	MM m	3592.52	49.68
		总和	7230.88	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.032	MM m	1241.12	95.43
	16.087	MM m	59.44	4.57
		总和	1300.56	

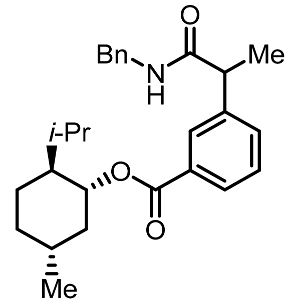
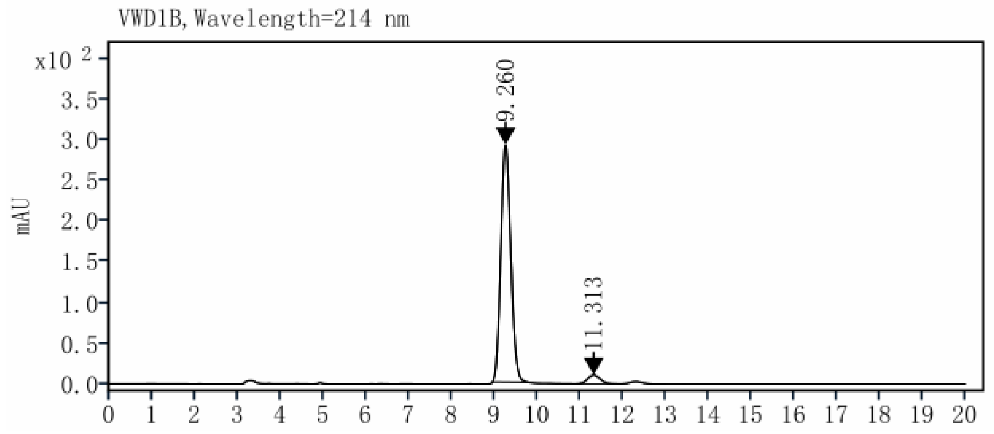
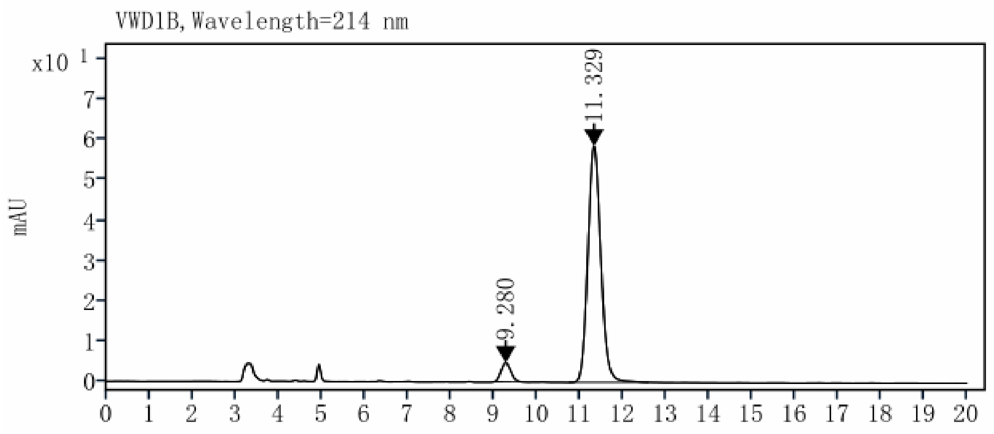


Fig. 2c, entries 38 and 39
(*S*)-**L1**: 95:5 dr, (*R*)-**L1**: 5:95 dr



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.260	MM m	4708.47	95.47
	11.313	MM m	223.16	4.53
		总和	4931.63	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.280	MM m	71.47	5.47
	11.329	MM m	1234.41	94.53
		总和	1305.88	

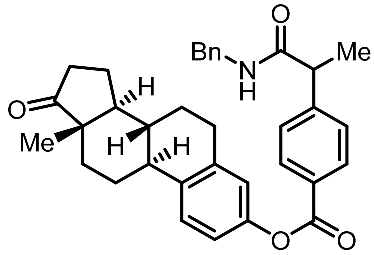
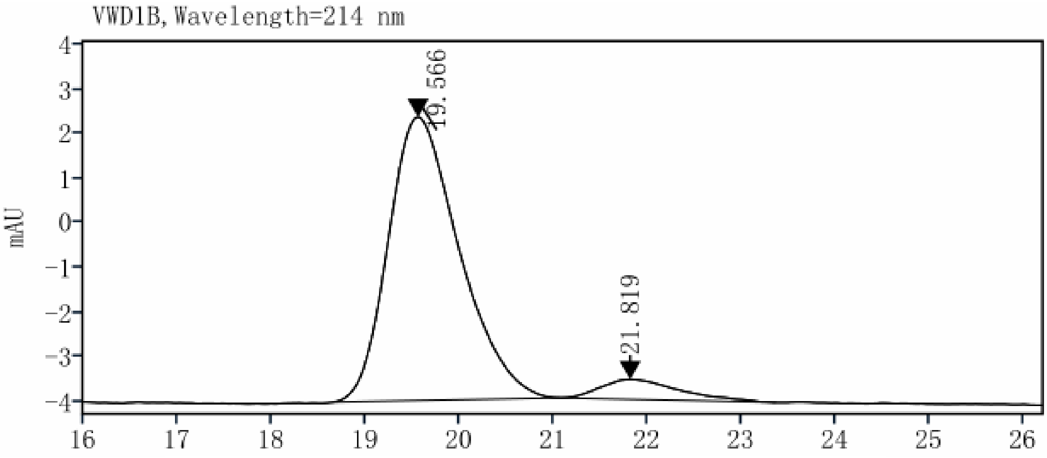
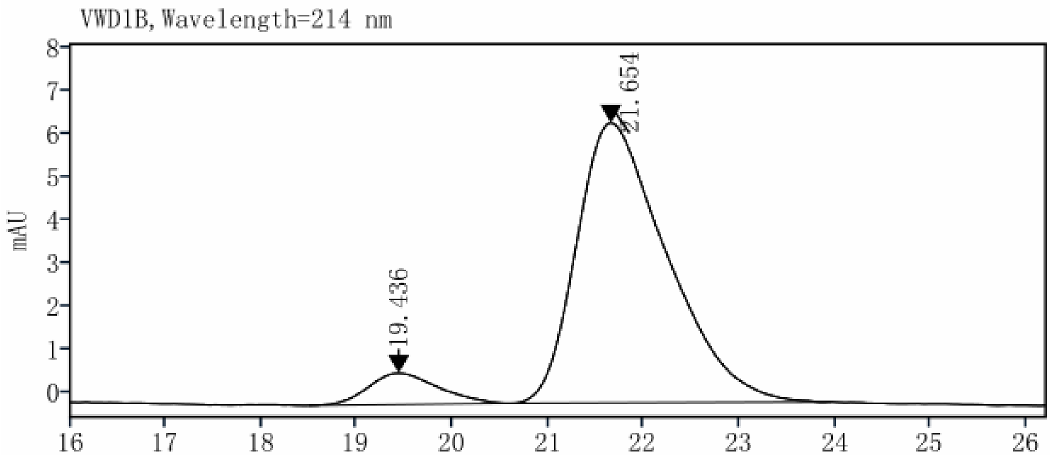


Fig. 2c, entries 40 and 41
(*S*)-**L1**: 93:7 dr, (*R*)-**L1**: 8:92 dr



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	19.566	MM m	334.36	92.80
	21.819	MM m	25.94	7.20
		总和	**360.30**	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	19.436	MM m	36.60	7.92
	21.654	MM m	425.76	92.08
		总和	**462.36**	

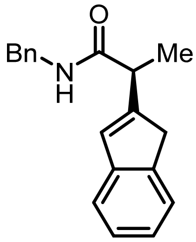
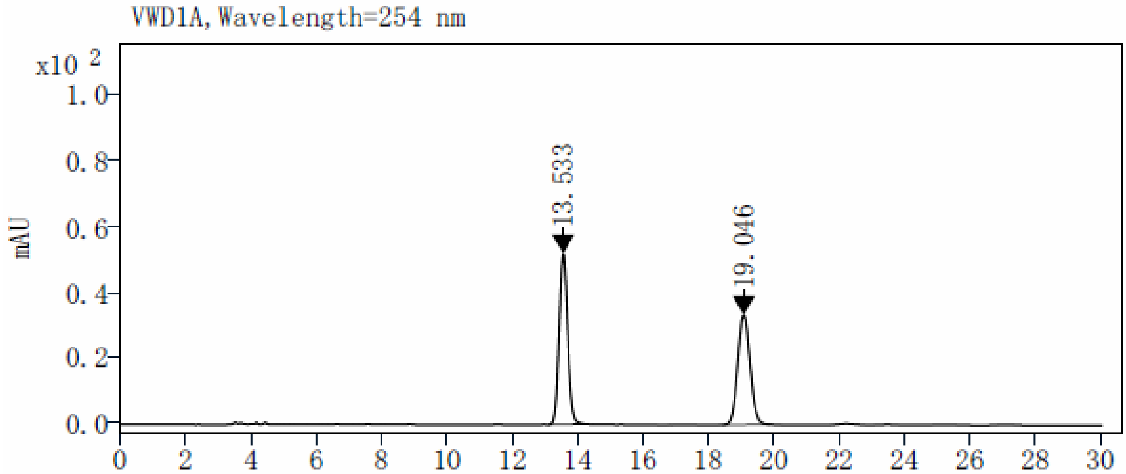
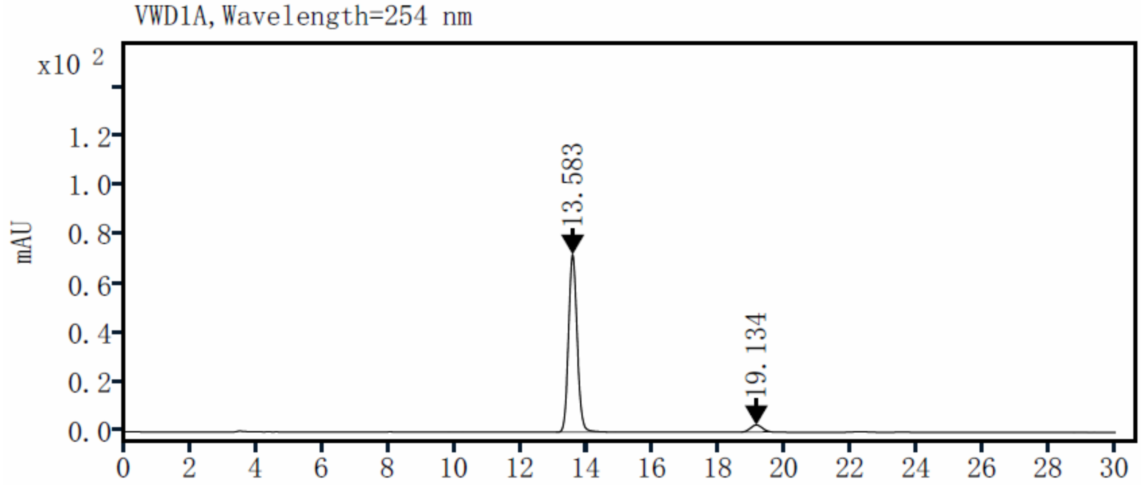


Fig. 2d, entry 42
(*S*)-**L1**: 90% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	13.533	MM m	939.59	50.67
	19.046	MM m	864.96	49.33
		总和	1804.55	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	13.583	MM m	1310.02	94.95
	19.134	MM m	69.69	5.05
		总和	1379.71	

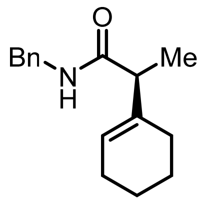
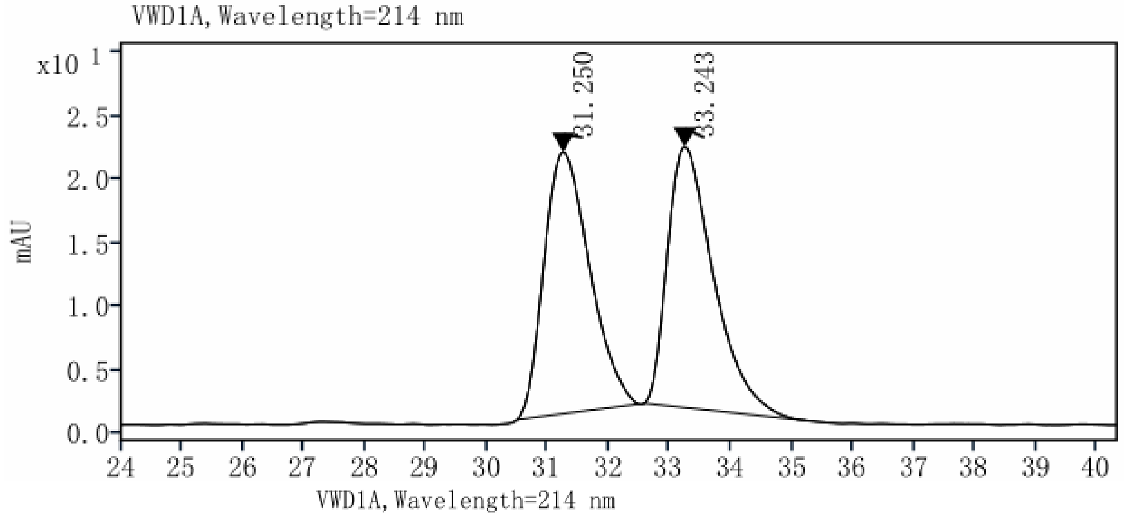
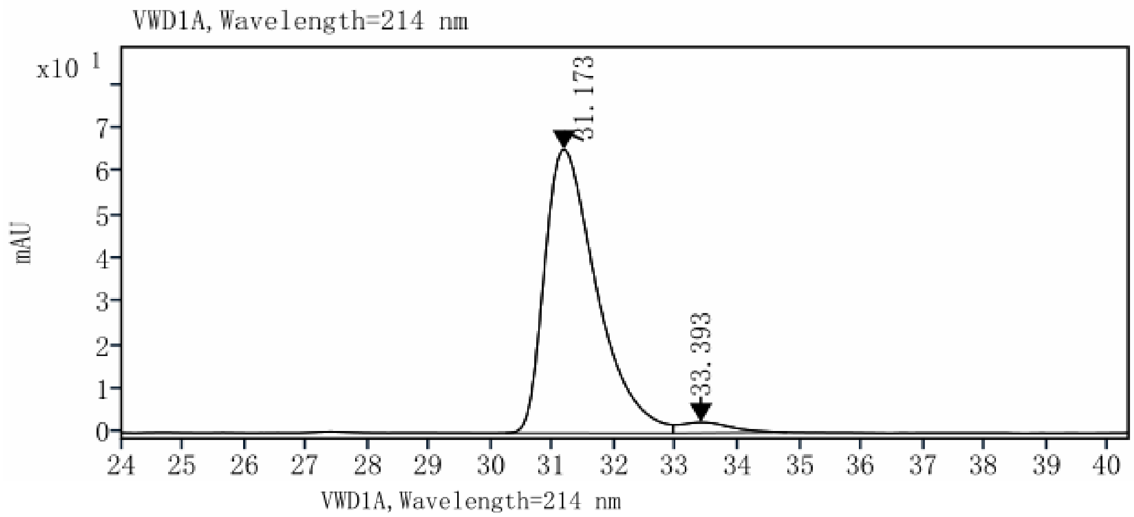


Fig. 2d, entry 43
(*S*)-**L1**: 93% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	31.250	MM m	1074.02	49.75
	33.243	MM m	1084.65	50.25
		总和	2158.66	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	31.173	MM m	3844.38	96.36
	33.393	MM m	145.34	3.64
		总和	3989.72	

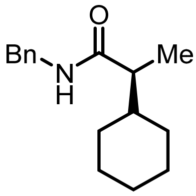
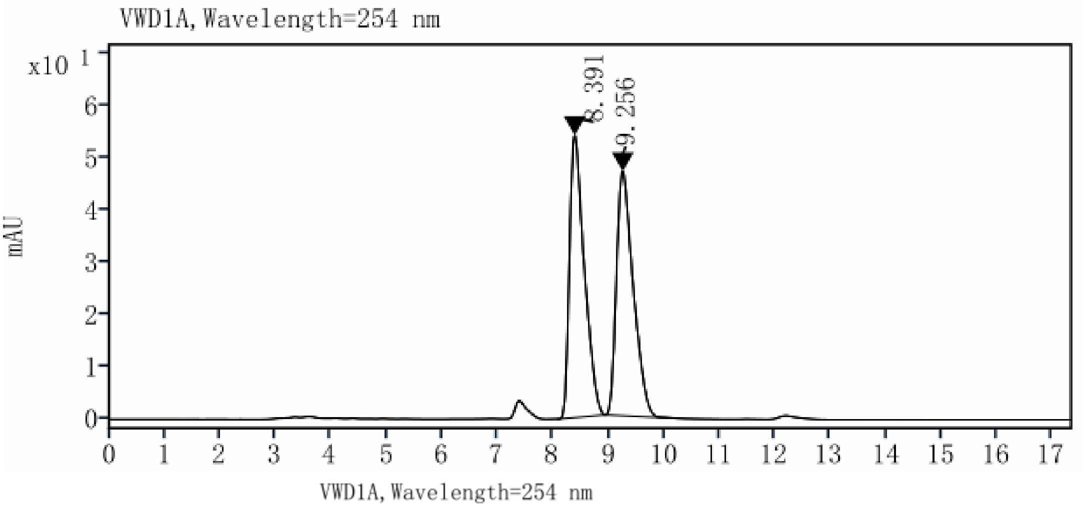
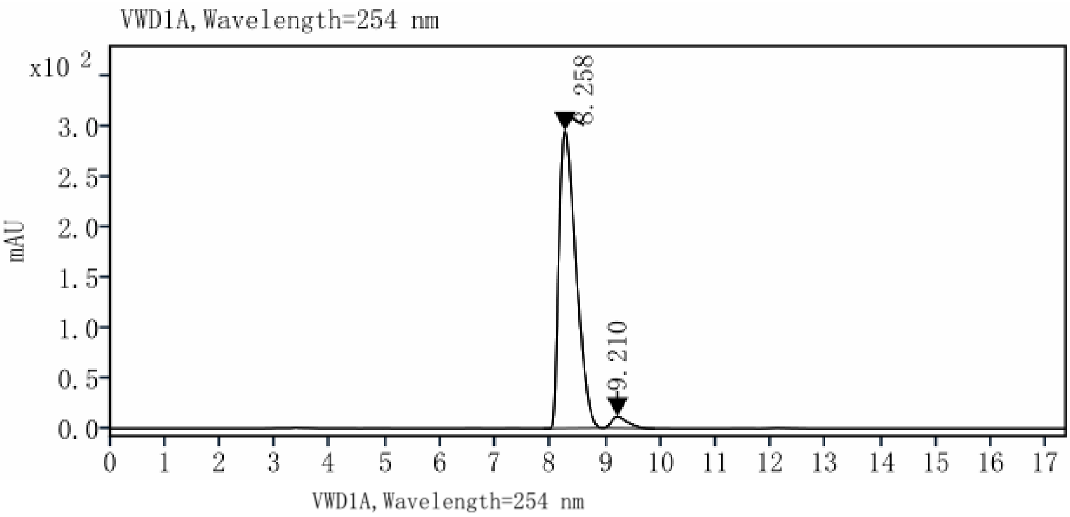


Fig. 2d, entry 44
(*S*)-**L1**: 93% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	8.391	MM m	997.45	50.42
	9.256	MM m	980.80	49.58
		总和	1978.25	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	8.258	MM m	6411.84	96.40
	9.210	MM m	239.19	3.60
		总和	6651.03	

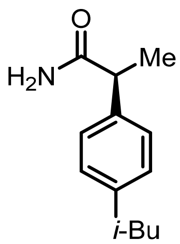
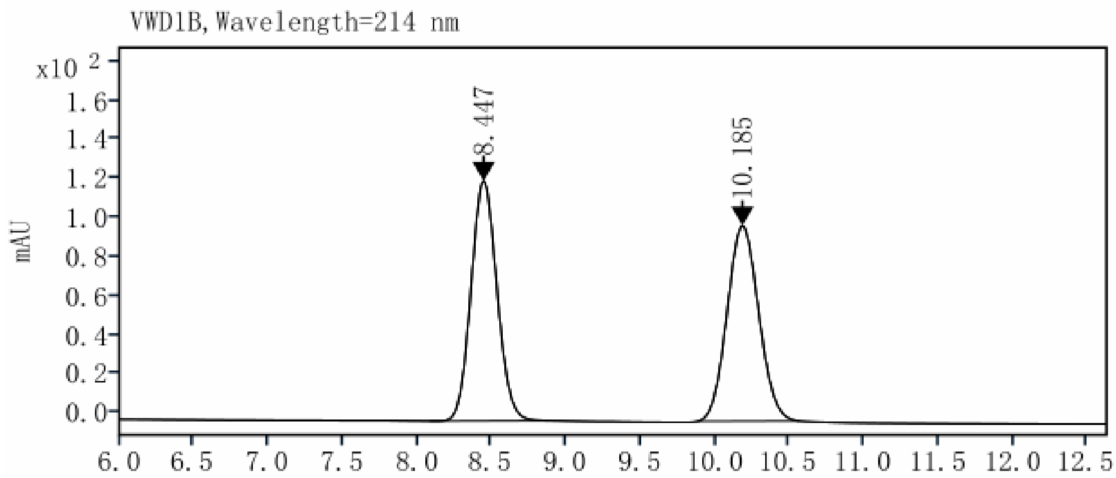
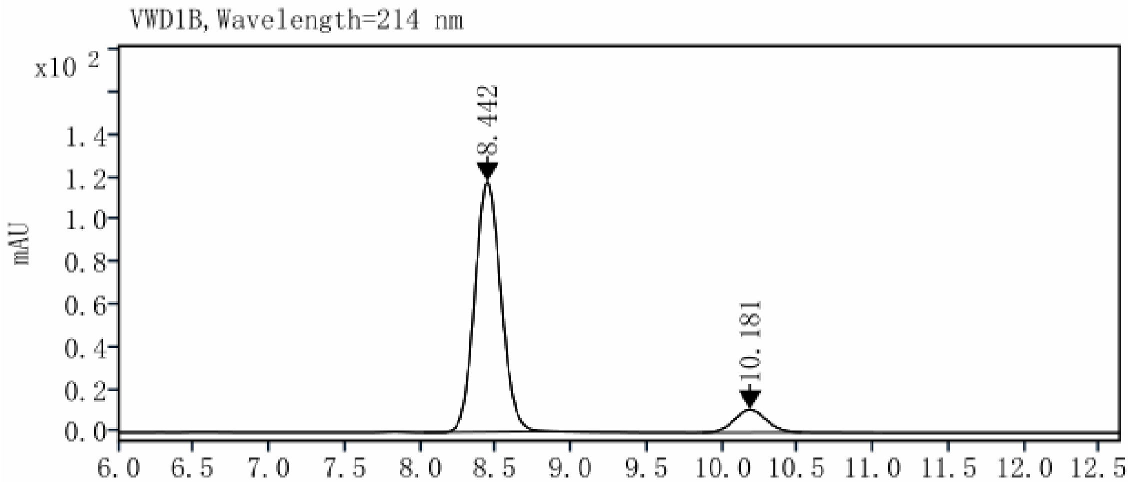


Fig. 2e, entry 45
(*S*)-**L1**: 80% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	8.447	MM m	1492.06	50.12
	10.185	MM m	1484.86	49.88
		总和	2976.92	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	8.442	MM m	1432.00	90.04
	10.181	MM m	158.46	9.96
		总和	1590.47	

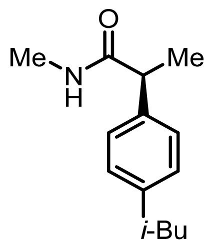
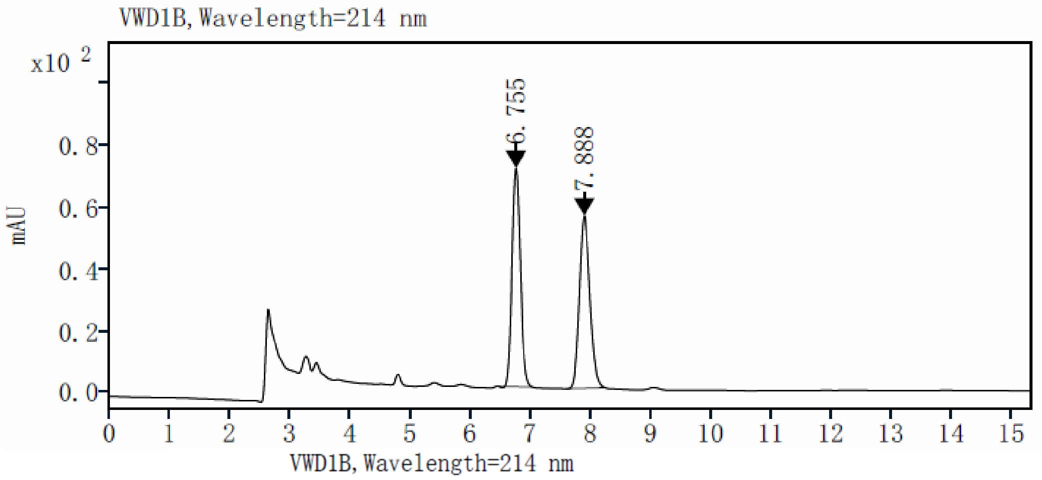
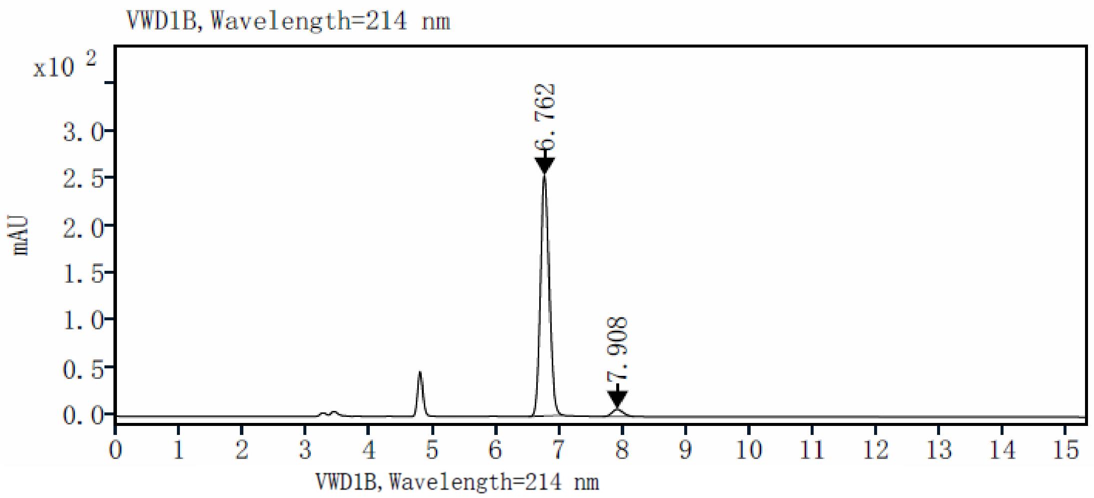


Fig. 2e, entry 46
(*S*)-**L1**: 93% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	6.755	MM m	667.57	49.86
	7.888	MM m	671.45	50.14
		总和	1339.02	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	6.762	MM m	2441.93	96.47
	7.908	MM m	89.48	3.53
		总和	2531.41	

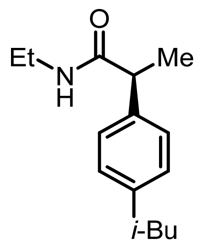
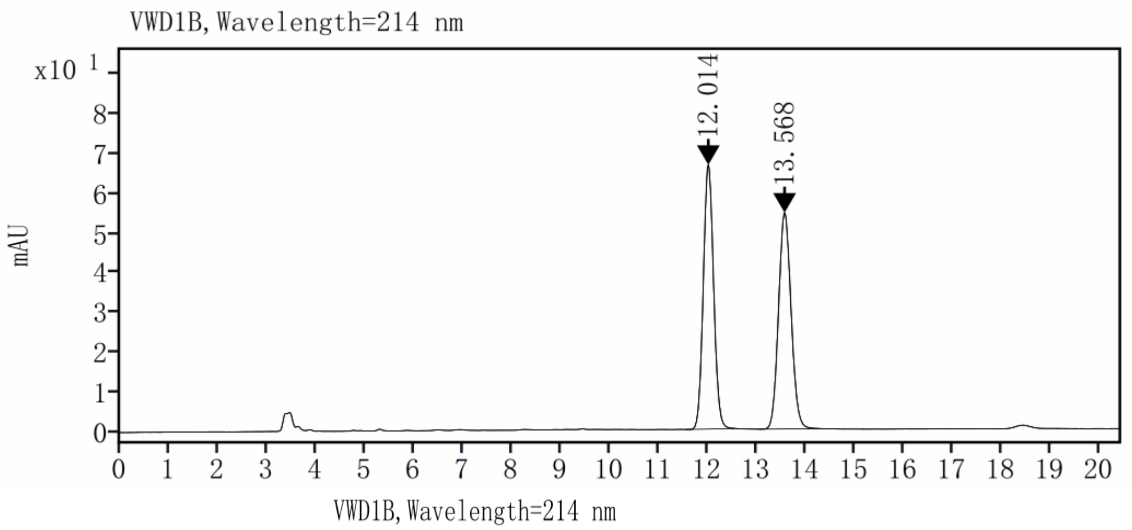
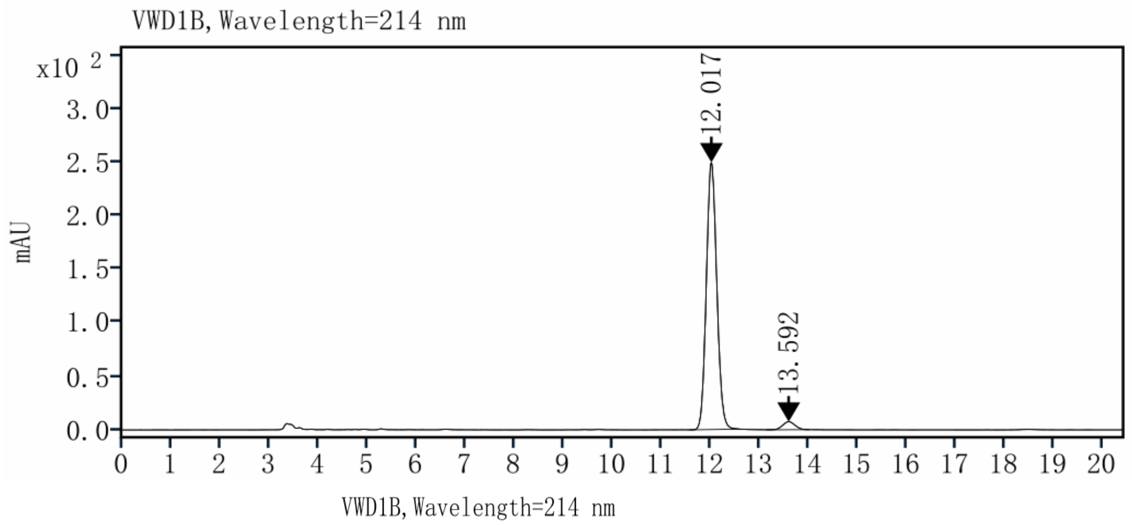


Fig. 2e, entry 47
(*S*)-**L1**: 93% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	12.014	MM m	966.81	50.00
	13.568	MM m	966.98	50.00



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	12.017	MM m	3688.24	96.57
	13.592	MM m	131.10	3.43

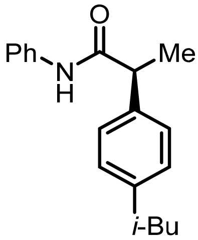
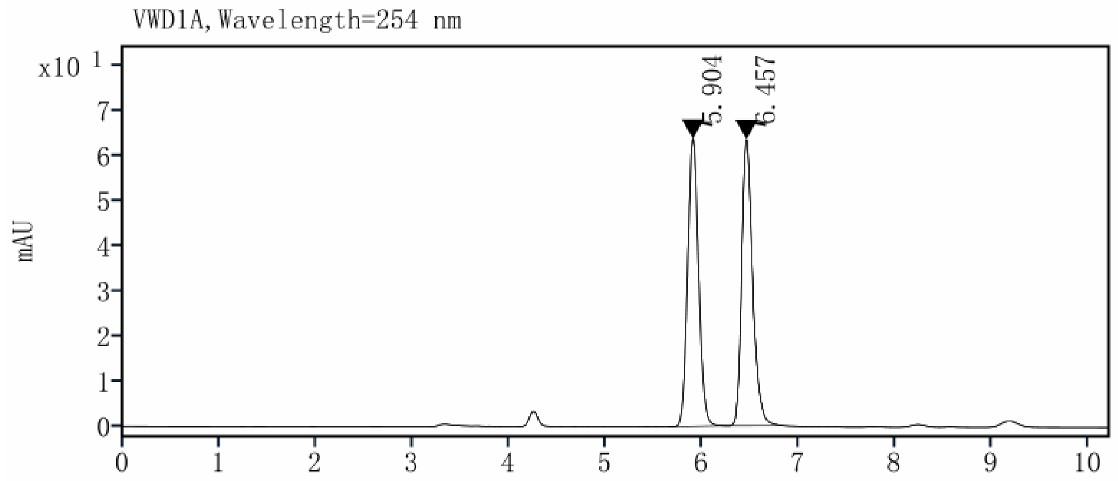
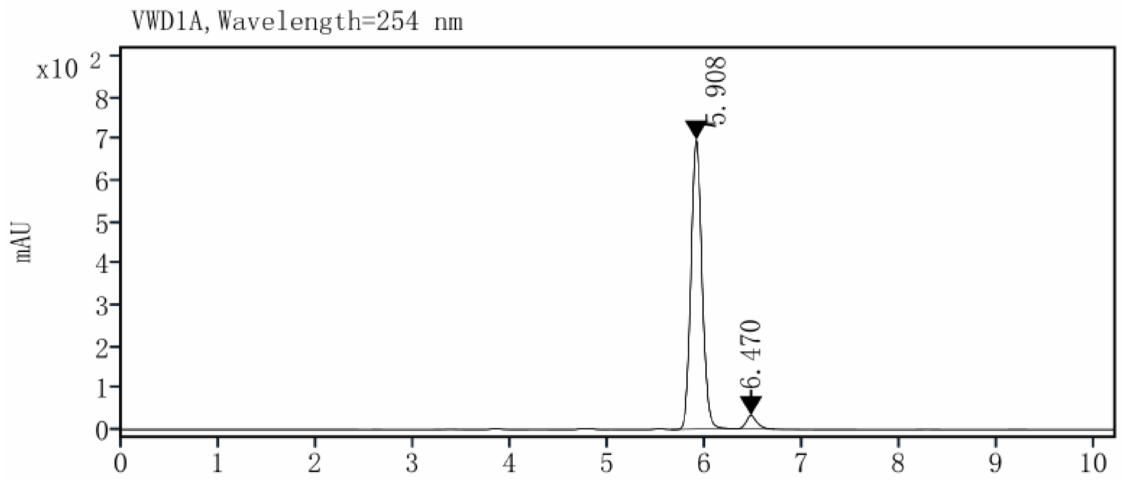


Fig. 2e, entry 48
(*S*)-**L1**: 92% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.904	MM m	502.03	50.00
	6.457	MM m	501.98	50.00



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.908	MM m	5544.70	95.83
	6.470	MM m	241.48	4.17

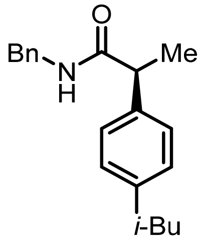
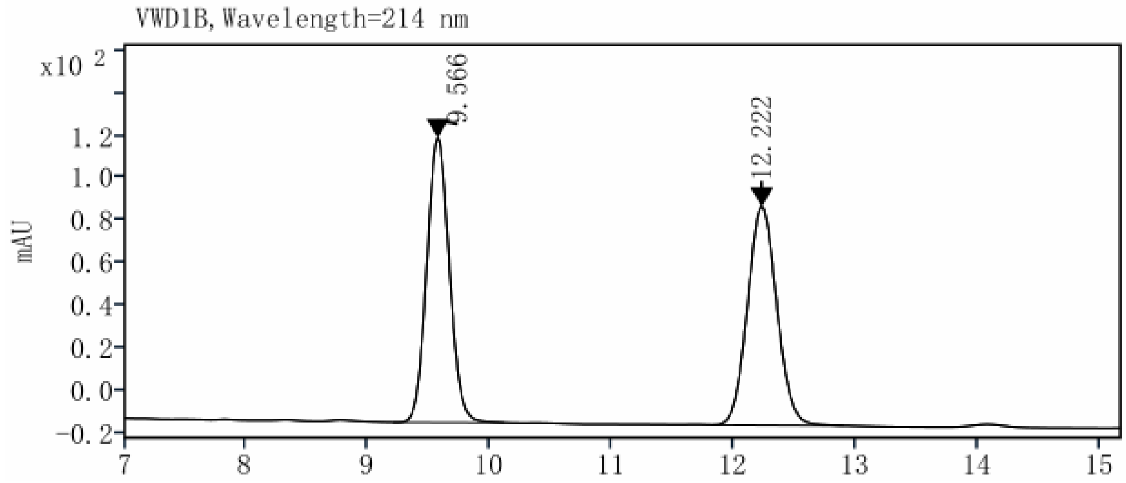
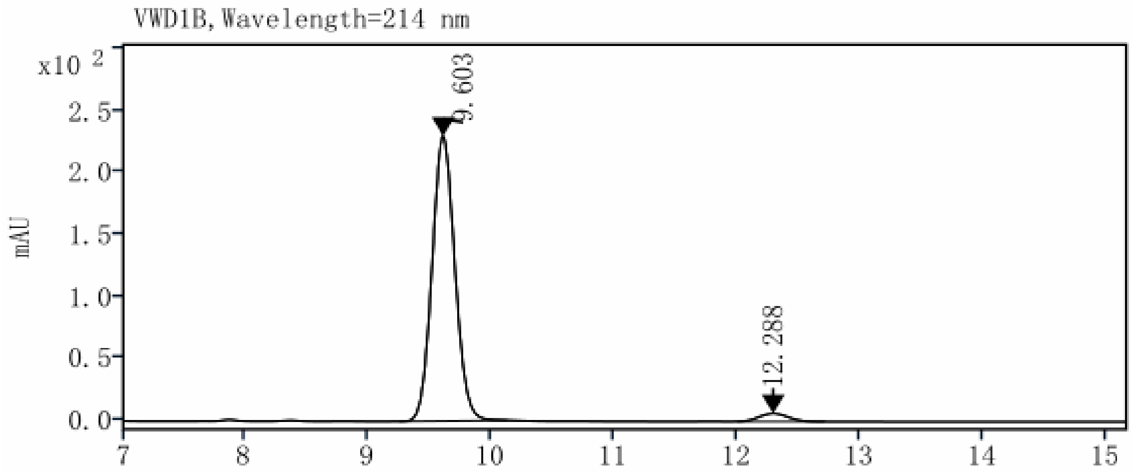


Fig. 2e, entry 49
(*S*)-**L1**: 93% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.566	MM m	1725.54	49.98
	12.222	MM m	1727.04	50.02
		总和	3452.58	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	9.603	MM m	2993.43	96.57
	12.288	MM m	106.28	3.43
		总和	3099.71	

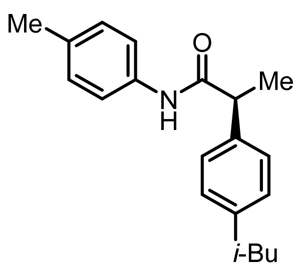
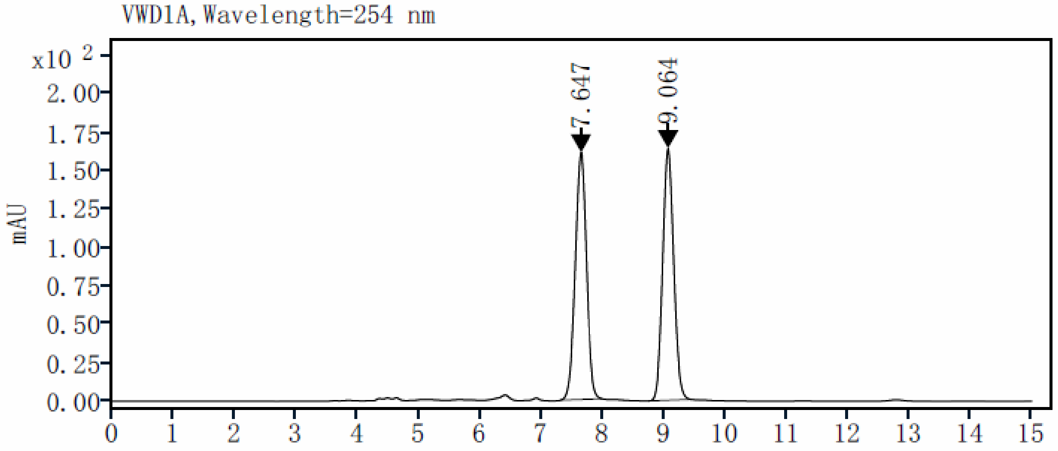
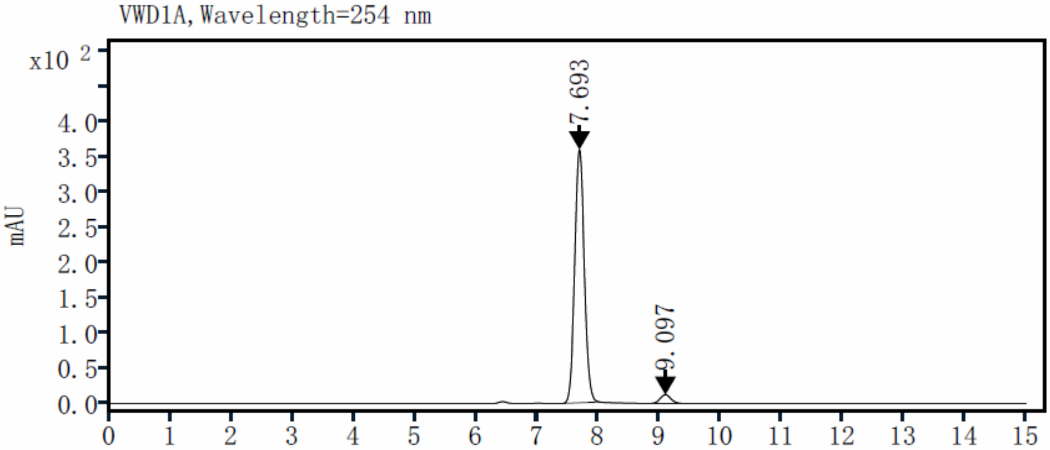


Fig. 2e, entry 50
(*S*)-**L1**: 93% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.647	MM m	2065.86	50.29
	9.064	MM m	2042.11	49.71
		总和	4107.97	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.693	MM m	3903.28	96.44
	9.097	MM m	144.11	3.56
		总和	4047.39	

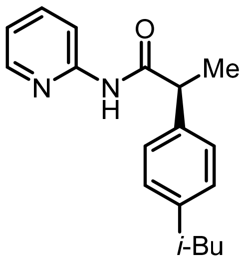
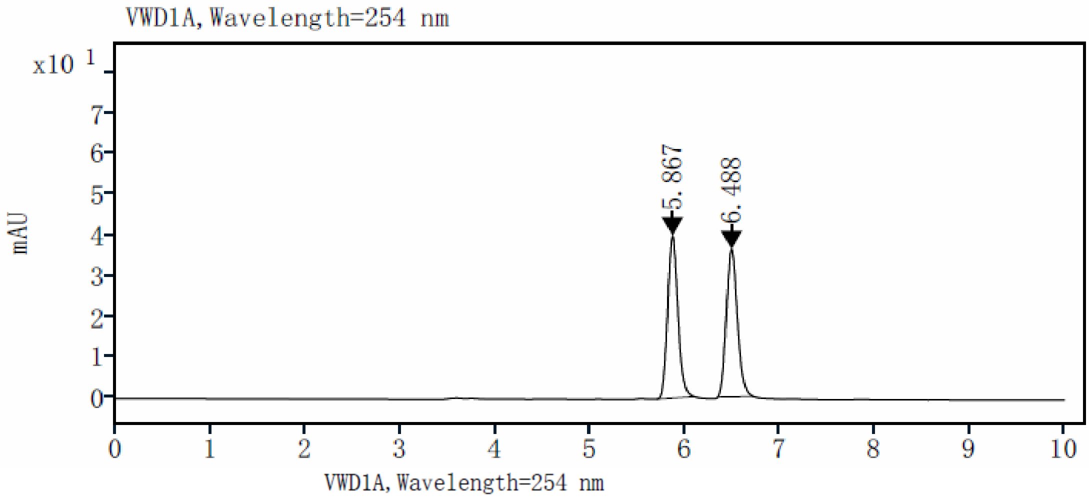
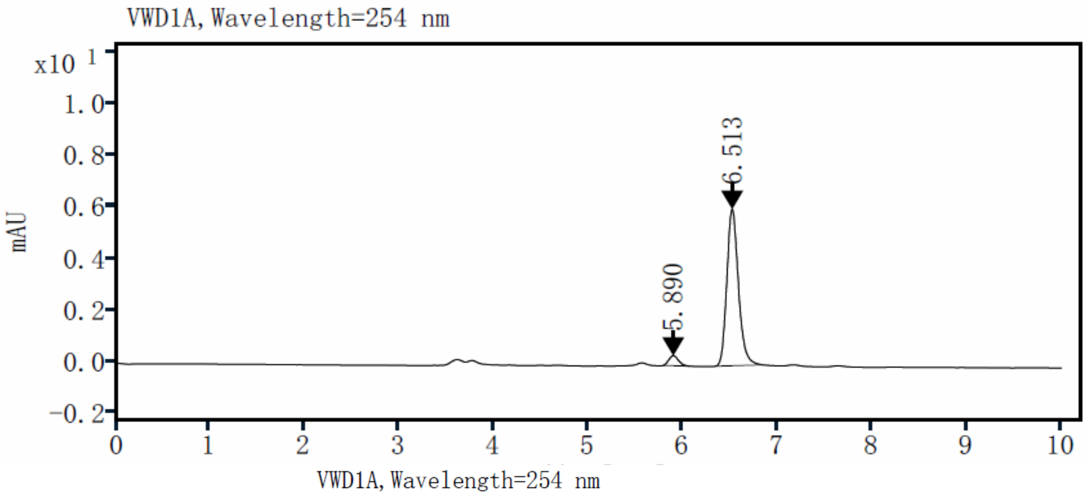


Fig. 2e, entry 51

(*S*)-**L1**: 90% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.867	MM m	298.03	50.45
	6.488	MM m	292.68	49.55
		总和	590.70	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.890	MM m	2.74	5.04
	6.513	MM m	51.51	94.96
		总和	54.25	

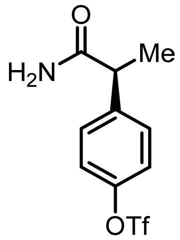
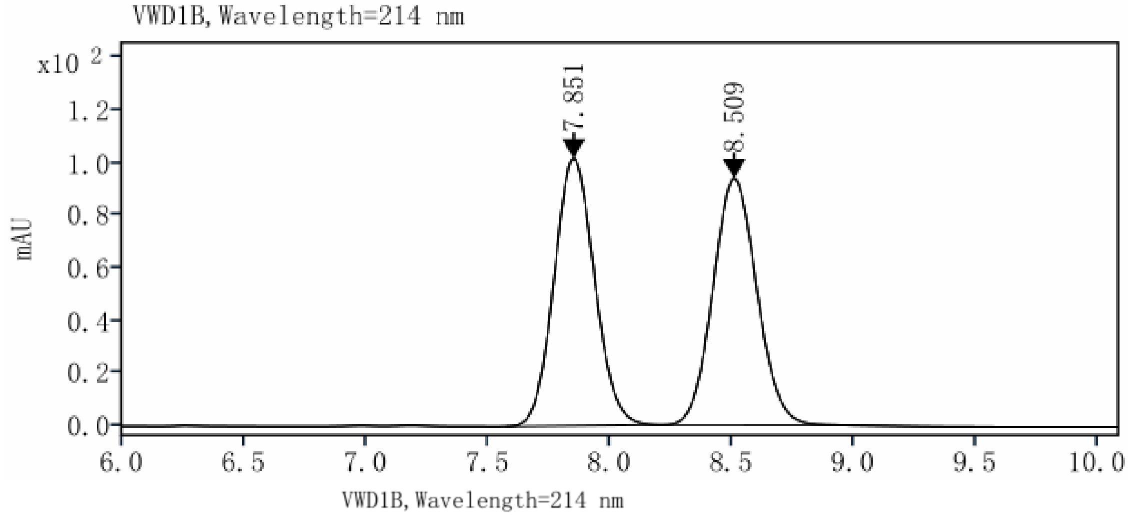
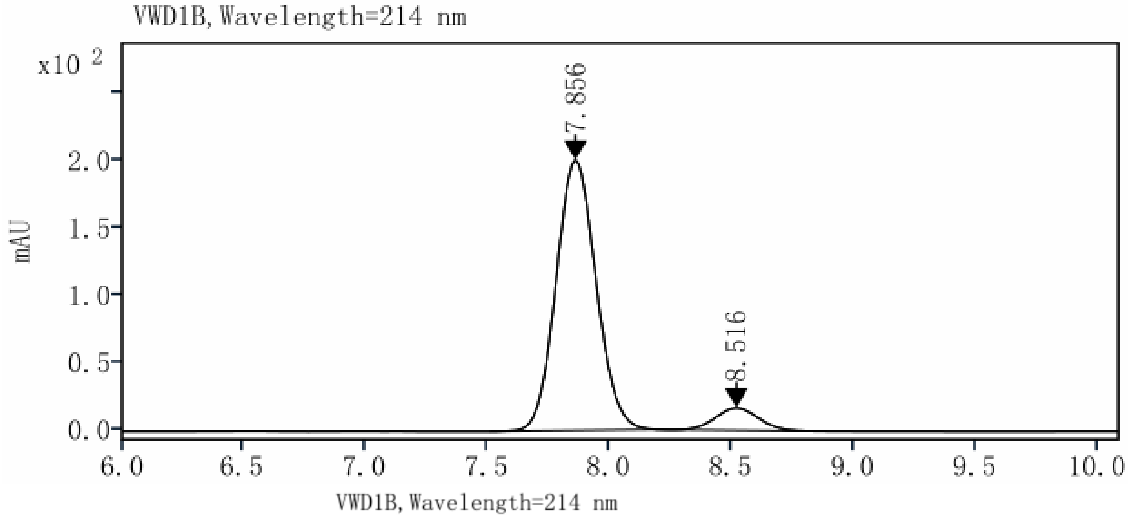


Fig. 2e, entry 53
(*S*)-**L1**: 84% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.851	MM m	1168.09	50.02
	8.509	MM m	1166.94	49.98
		总和	2335.03	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	7.856	MM m	2283.73	91.92
	8.516	MM m	200.76	8.08
		总和	2484.49	

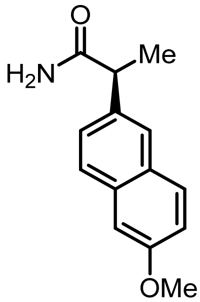
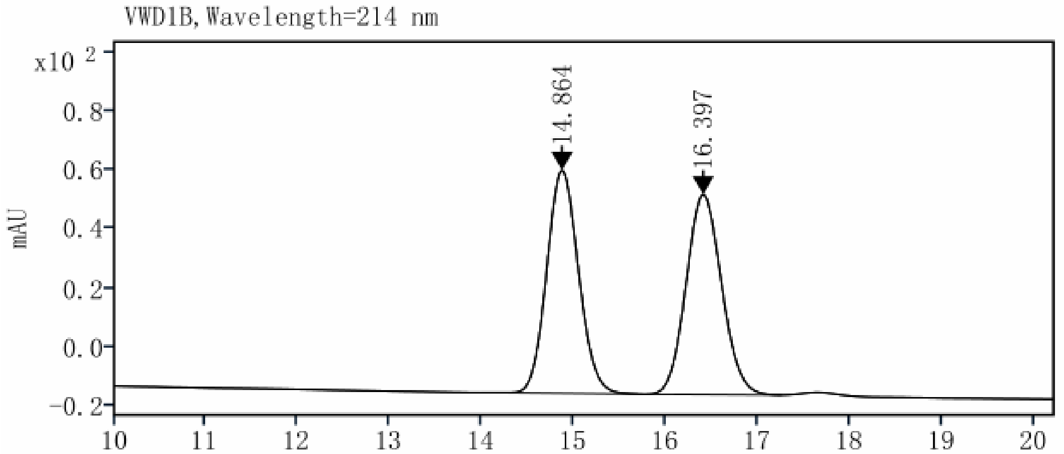


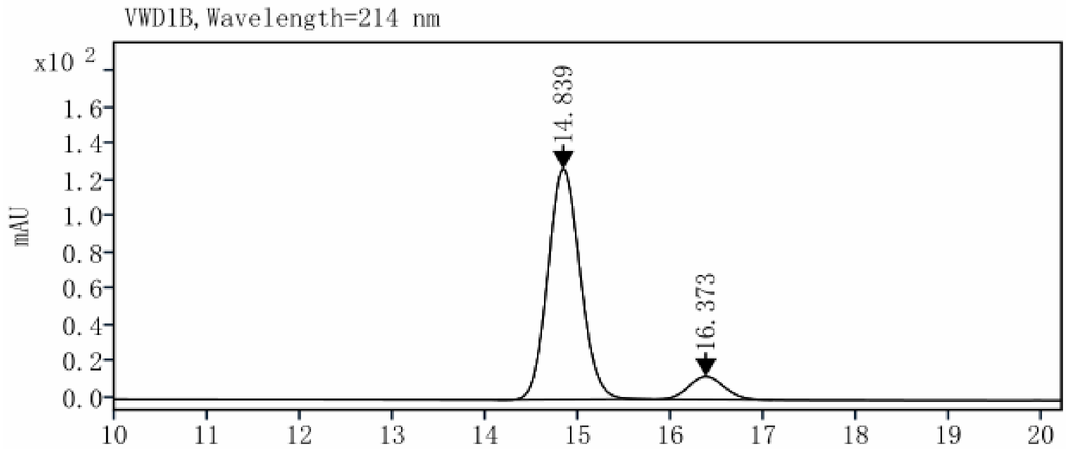
Fig. 2e, entry 54

(*S*)-**L1**: 80% ee



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.864	MM m	1828.88	49.95
	16.397	MM m	1832.69	50.05
		总和	3661.58	



VWD1B, Wavelength=214 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	14.839	MM m	3082.05	90.12
	16.373	MM m	337.81	9.88
		总和	3419.86	

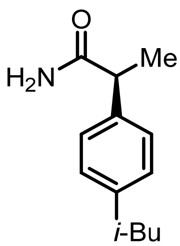
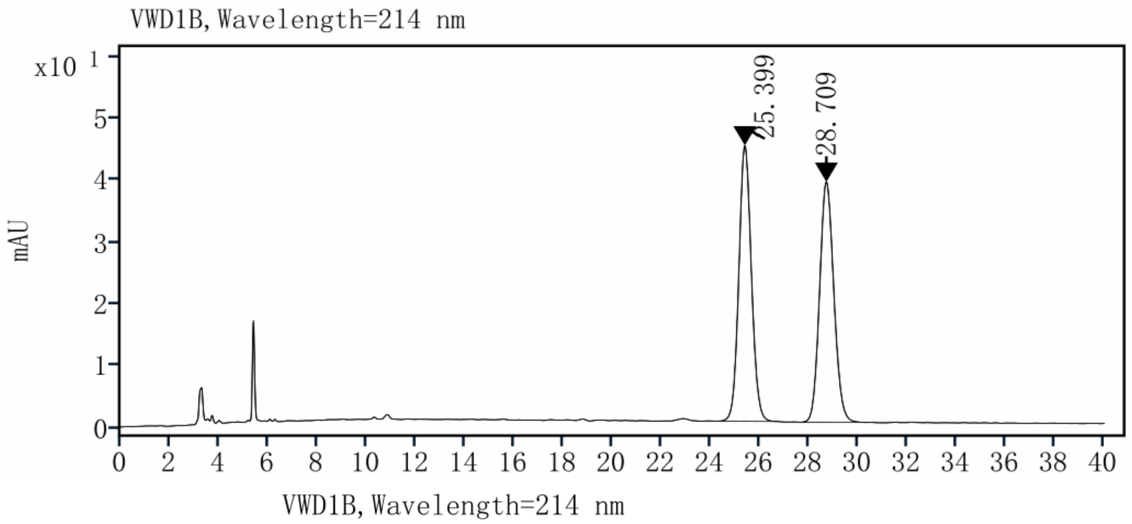
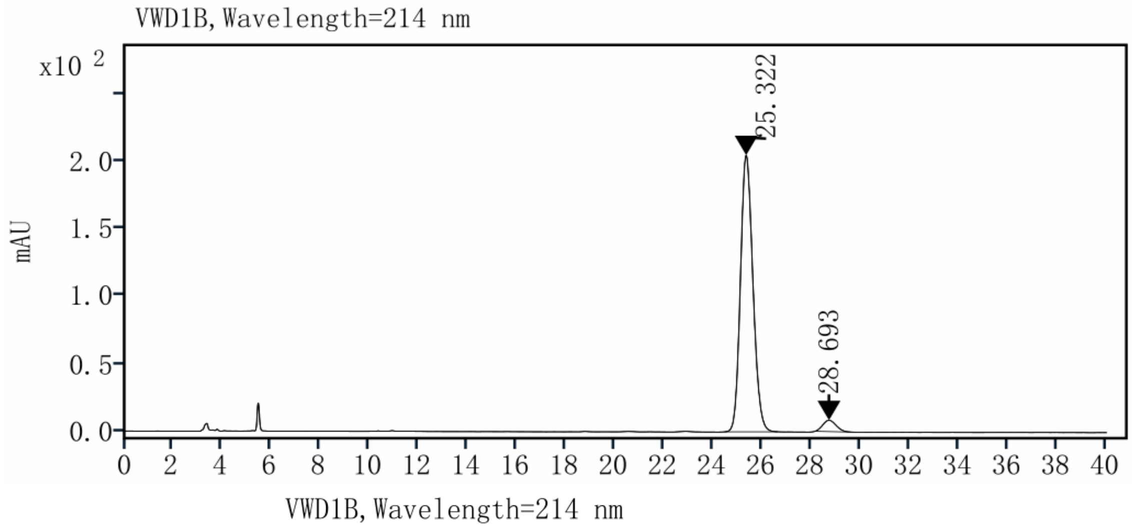


Fig. 3, entry 45
(*S*)-**L1**: 92% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	25.399	MM m	1580.83	50.28
	28.709	MM m	1563.47	49.72



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	25.322	MM m	7244.65	95.82
	28.693	MM m	315.80	4.18

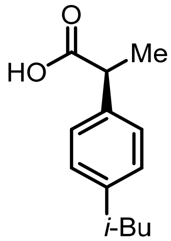
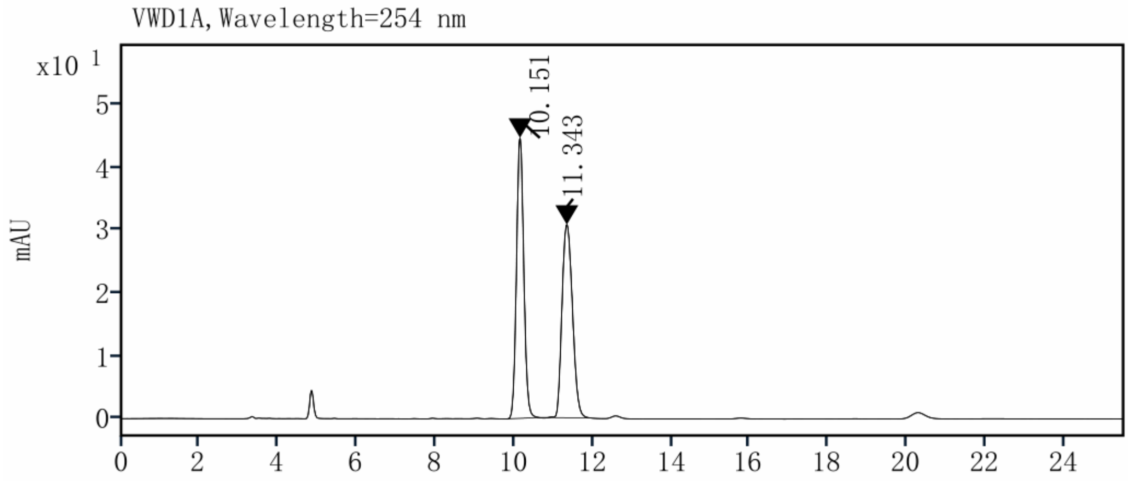
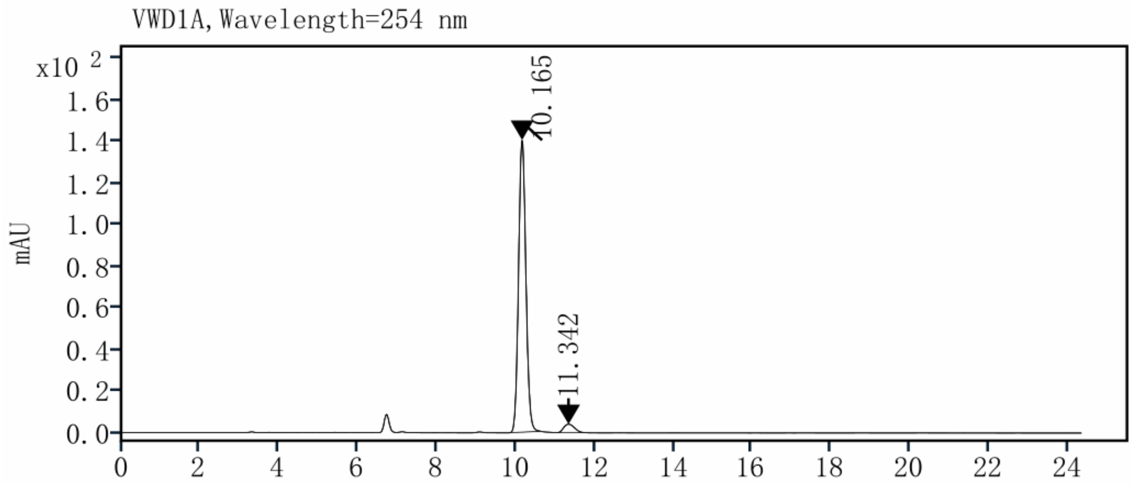


Fig. 3, entry 55
(*S*)-**L1**: 92% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.151	MM m	575.62	50.25
	11.343	MM m	569.89	49.75



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	10.165	MM m	1814.87	95.87
	11.342	MM m	78.25	4.13

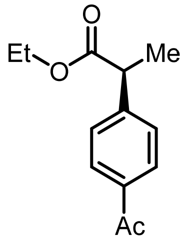
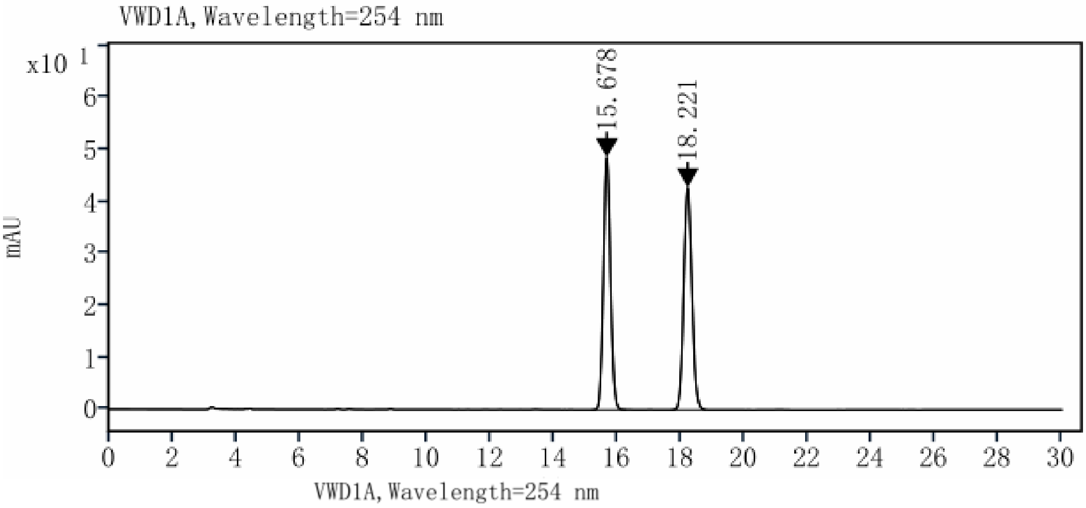
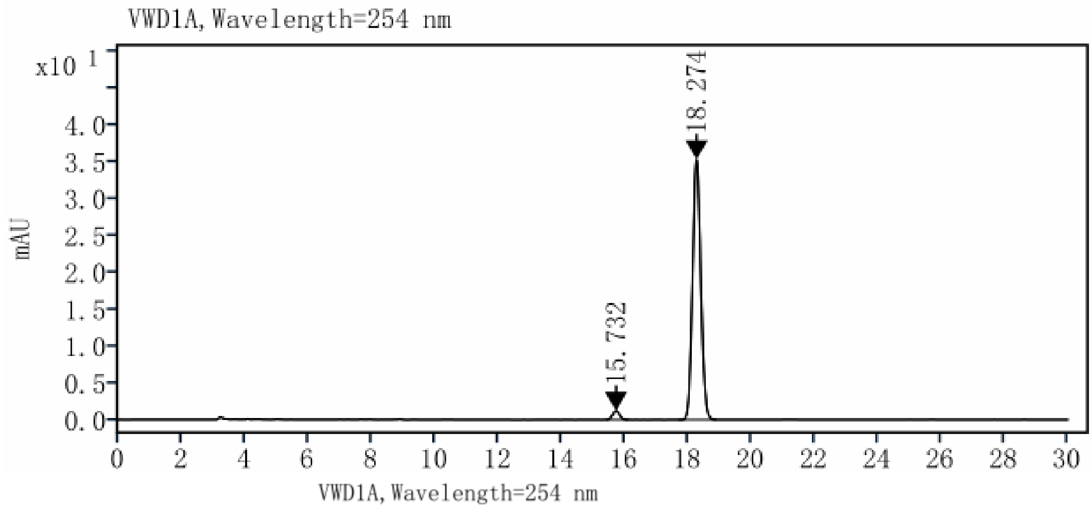


Fig. 3, entry 56
(*S*)-**L1**: 94% ee



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	15.678	MM m	760.83	49.45
	18.221	MM m	777.76	50.55
		总和	1538.59	



No.	RetTime[min]	Type	Area [mAu*s]	Area%
	15.732	MM m	18.33	2.78
	18.274	MM m	640.94	97.22
		总和	659.27	

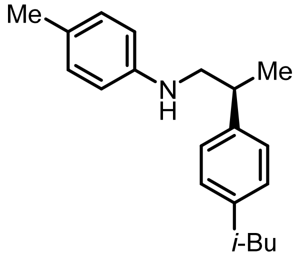
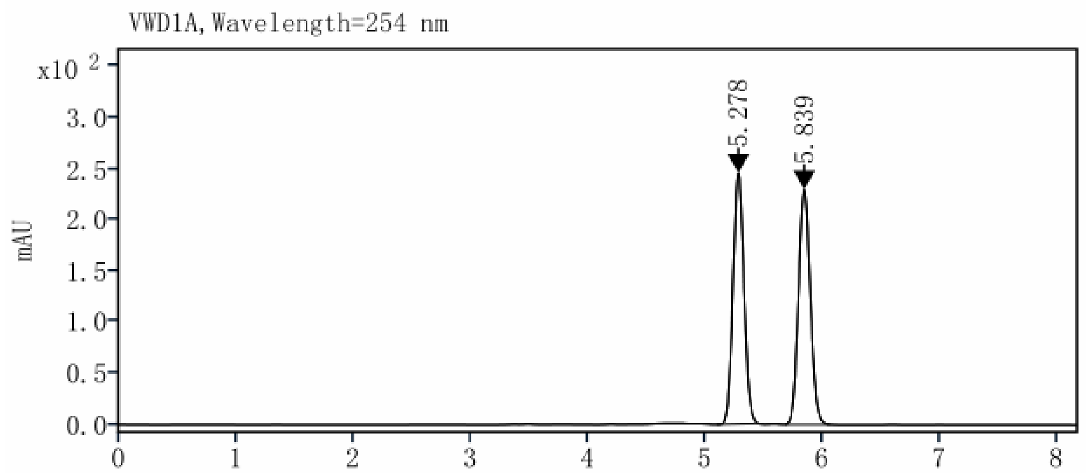
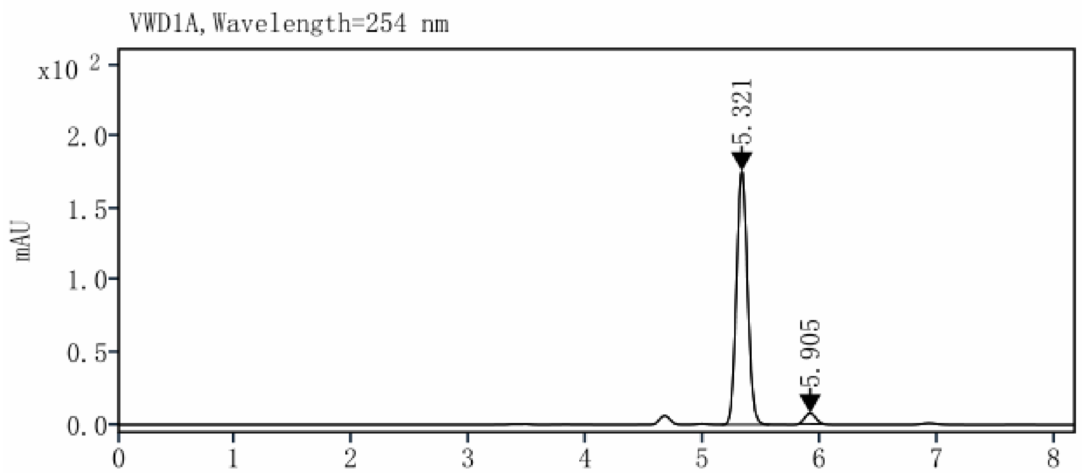


Fig. 3, entry 57
(*S*)-**L1**: 92% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.278	MM m	1596.74	49.85
	5.839	MM m	1606.34	50.15
		总和	3203.08	



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	5.321	MM m	1157.66	96.01
	5.905	MM m	48.10	3.99
		总和	1205.77	

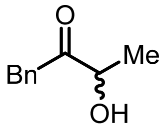
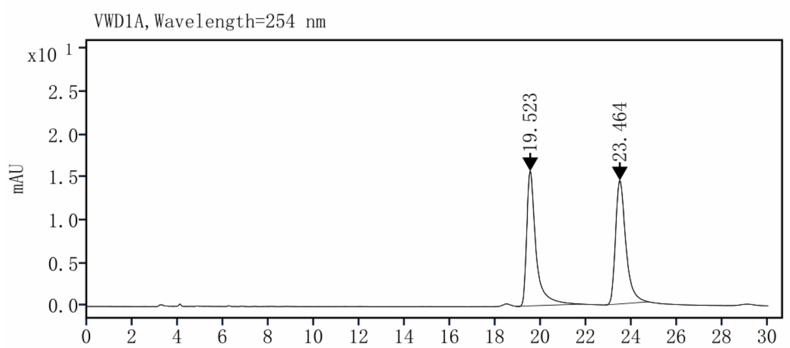
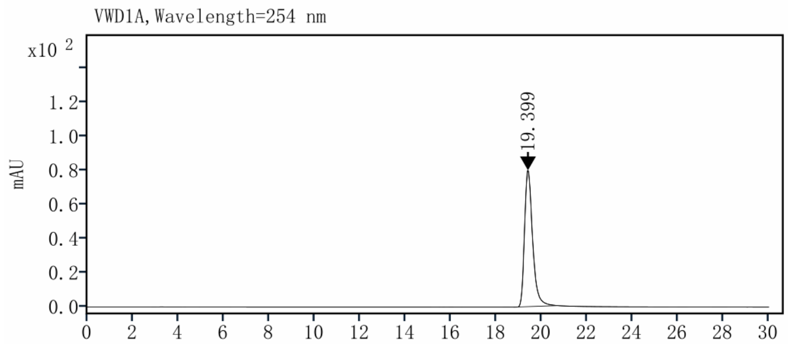


Fig. 4d
recovery of alcohol



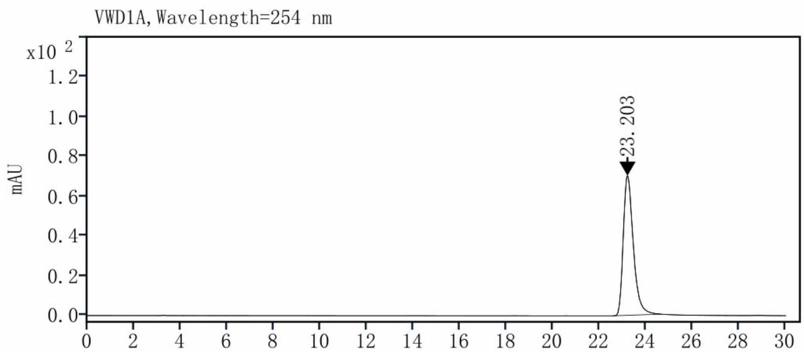
VWD1A,Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	19.523	MM m	449.49	49.75
	23.464	MM m	453.96	50.25



VWD1A,Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	19.399	MM m	1967.15	100.00



VWD1A,Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	23.203	MM m	2108.69	100.00

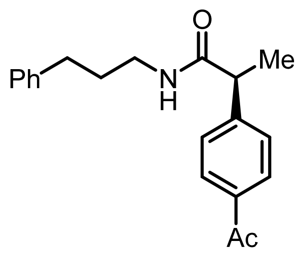
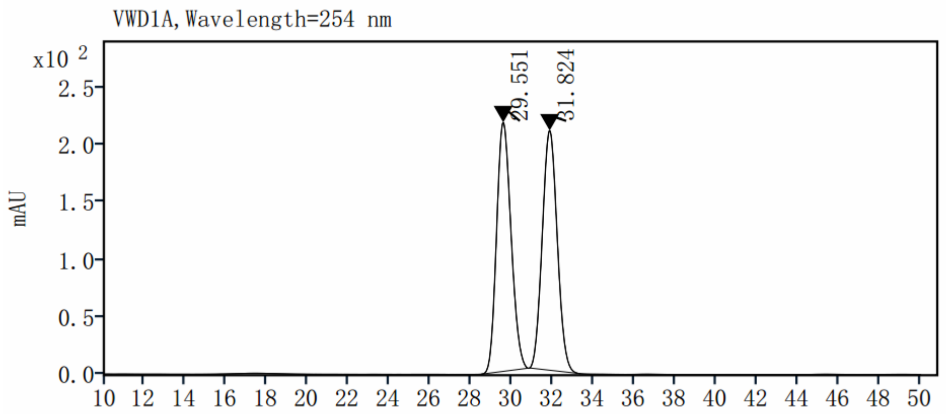


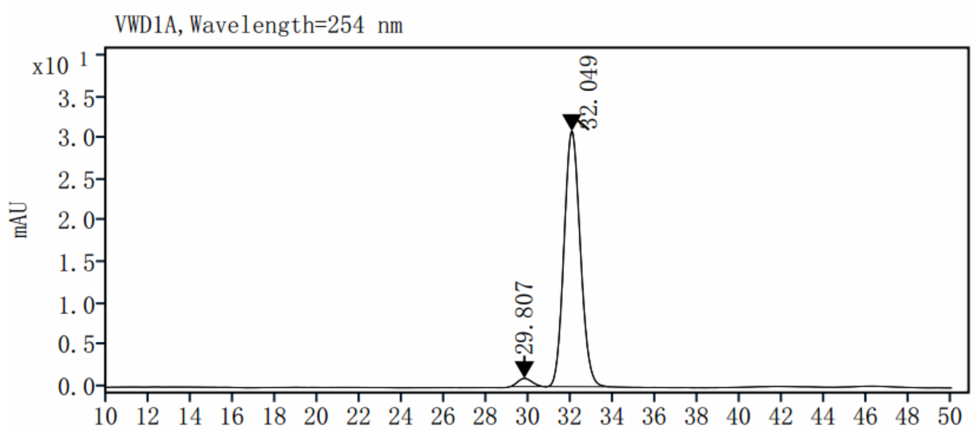
Fig. 5, entry 58

using Ni^2 as the catalyst: 95% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	29.551	MM m	10748.01	50.07
	31.824	MM m	10717.56	49.93



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	29.807	MM m	45.80	2.69
	32.049	MM m	1659.33	97.31

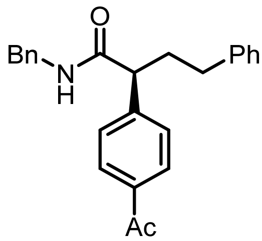
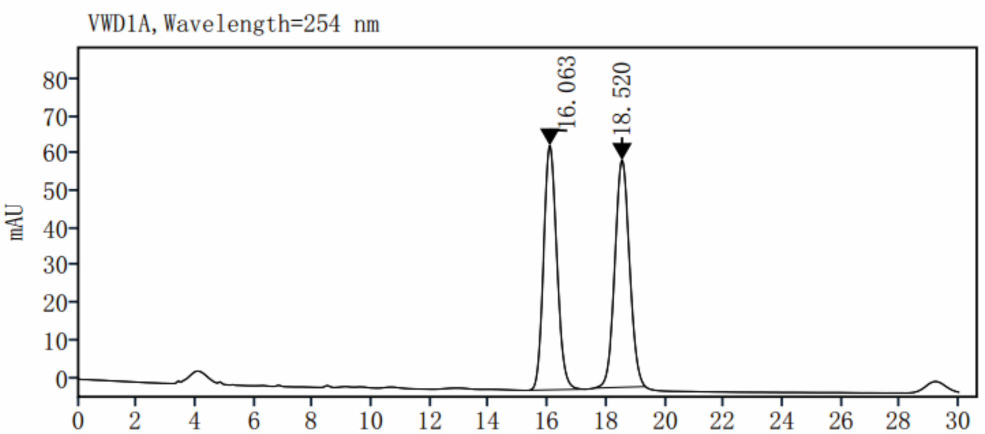


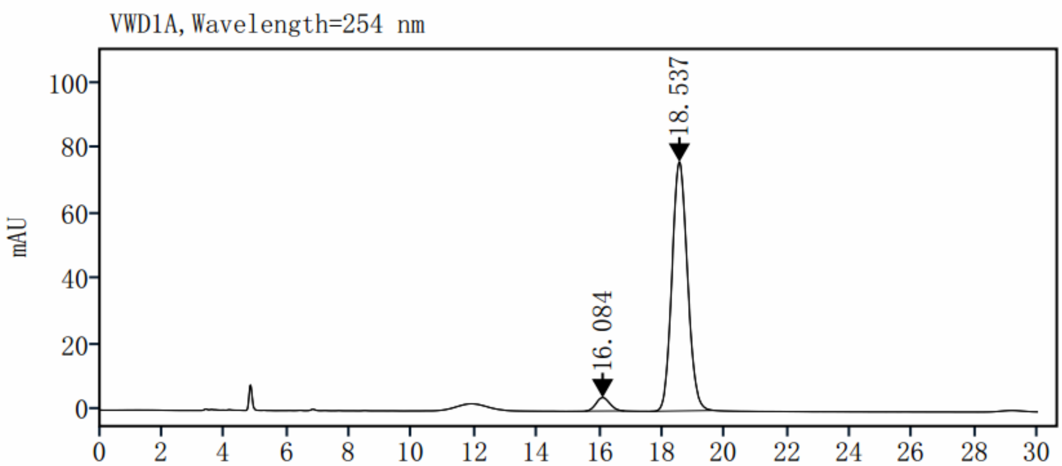
Fig. 5, entry 59

using Ni^2 as the catalyst: 91% ee



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	16.063	MM m	2053.78	49.19
	18.520	MM m	2121.32	50.81



VWD1A, Wavelength=254 nm

No.	RetTime[min]	Type	Area [mAu*s]	Area%
	16.084	MM m	126.83	4.60
	18.537	MM m	2632.80	95.40