# Iridium(III)-Catalyzed Regioselective Direct Arylation of $sp^2$ C-H Bonds with Diaryliodonium Salts

## (Supporting Information)

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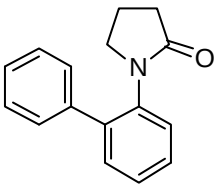
# Characterization of products

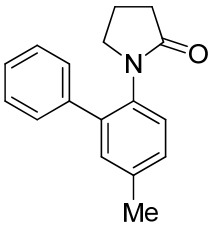
### 1-([1,1'-Biphenyl]-2-yl)pyrrolidin-2-one (3aa)



**3aa**

Viscous liquid (45.5 mg, 96%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.45 – 7.35 (m, 8H), 7.35 – 7.30 (m, 1H), 3.21 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 8.1 Hz, 2H), 1.92 – 1.80 (m, 2H).**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.65, 139.58, 139.05, 136.25, 130.79, 128.52, 128.38, 128.34, 128.30, 128.01, 127.54, 50.12, 31.15, 18.93.ATR-FTIR ($cm^{-1}$): 3132, 1672, 1499, 1403, 1305, 871, 825. HRMS m/z (ESI) calcd for $C_{16}H_{16}NO$ $(M + H)^+$ 238.1226, found 238.1226.

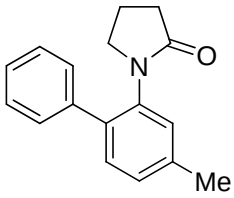
### 1-(5-Methylbiphenyl-2-yl)pyrrolidin-2-one (3ba)



**3ba**

Viscous liquid (47.2 mg, 94%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.44 – 7.30 (m, 5H), 7.25 – 7.16 (m, 3H), 3.18 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 8.1 Hz, 2H), 2.39 (s, 3H), 1.89 – 1.81 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.69, 139.31, 139.14, 137.88, 133.59, 131.40, 129.17, 128.29, 128.27, 128.08, 127.42, 50.17, 31.10, 21.04, 18.86.ATR-FTIR ($cm^{-1}$): 3133, 1699, 1495, 1400, 1305, 1238, 868, 825, 758. HRMS m/z (ESI) calcd for $C_{17}H_{18}NO$ $(M + H)^+$ 252.1383, found 252.1383.

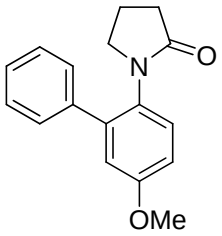
### 1-(4-Methylbiphenyl-2-yl)pyrrolidin-2-one (3ca)




**3ca**

Viscous liquid (37.7 mg, 75%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.42 – 7.31 (m, 5H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.21 – 7.17 (m, 1H), 7.16 – 7.11 (m, 1H), 3.19 (t, *J* = 7.0 Hz, 2H), 2.42 (t, J = 8 2H), 2.40 (s, 3H), 1.90 – 1.80 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.65, 139.05, 138.57, 136.67, 136.00, 130.61, 128.90, 128.83, 128.34, 128.3, 127.33, 50.18, 31.19, 20.95, 18.93. ATR-FTIR ($cm^{-1}$): 3133, 1698, 1495, 1401, 1305, 1239, 868, 825, 758. HRMS m/z (ESI) calcd for $C_{17}H_{18}NO$ $(M + H)^+$ 252.1383, found 252.1384.

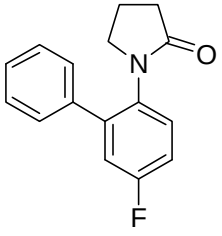
**1-(5-Methoxybiphenyl-2-yl)pyrrolidin-2-one (3da)**




**3da**

Viscous liquid (52.3 mg, 98%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.43 – 7.32 (m, 5H), 7.24 – 7.17 (m, 1H), 6.98 – 6.86 (m, 2H), 3.83 (s, 3H), 3.17 (t, *J* = 7.0 Hz, 2H), 2.44 – 2.36 (m, 2H), 1.88 – 1.79 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.92, 158.92, 140.88, 138.99, 138.11, 129.42, 129.01, 128.36, 128.25, 127.66, 113.95, 55.53, 50.38, 31.07, 18.81. ATR-FTIR ($cm^{-1}$): 3137, 1698, 1493, 1401, 1305, 1237, 866, 826, 758. HRMS m/z (ESI) calcd for $C_{17}H_{18}NO_2$ $(M + H)^+$ 268.1332, found 268.1334.

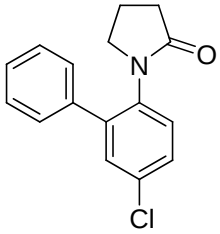
**1-(5-Fluorobiphenyl-2-yl)pyrrolidin-2-one (3ea)**




**3ea**

Viscous liquid (23.0 mg, 45%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.46 – 7.34 (m, 5H), 7.32 – 7.25 (m, 1H), 7.14 – 7.04 (m, 2H), 3.18 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 8.1 Hz, 2H), 1.86 (dt, *J* = 10.7, 7.5 Hz, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)**δ 175.81, 161.63 (d, *J* = 247.8 Hz), 141.65 (d, *J* = 8.4 Hz), 137.96 (d, *J* = 1.4 Hz), 132.21 (d, *J* = 3.0 Hz), 130.13 (d, *J* = 8.9 Hz), 128.51, 128.10, 128.04, 117.43 (d, *J* = 22.8 Hz), 115.30 (d, *J* = 22.4 Hz), 50.11, 30.99, 18.84. ATR-FTIR ($cm^{-1}$):3132, 1698, 1496, 1400. 1305, 1238, 863, 824, 758. HRMS m/z (ESI) calcd for $C_{16}H_{15}FNO$ $(M + H)^+$ 256.1132, found 256.1131.

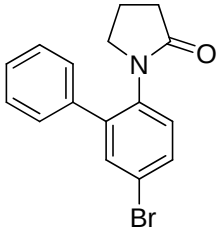
**1-(5-Chlorobiphenyl-2-yl)pyrrolidin-2-one (3fa)**



**3fa**

Viscous liquid (40.1 mg, 74%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.46 – 7.31 (m, 7H), 7.29 – 7.24 (m, 1H), 3.17 (t, *J* = 7.0 Hz, 2H), 2.41 (t, *J* = 8.1 Hz, 2H), 1.92 – 1.80 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)**δ 175.64, 141.09, 137.79, 134.84, 133.42, 130.69, 129.70, 128.53, 128.47, 128.09, 128.05, 49.92, 30.99, 18.88. ATR-FTIR ($cm^{-1}$): 3131, 1697, 1493, 1402. 1303, 1238, 865, 825, 758. HRMS m/z (ESI) calcd for $C_{16}H_{15}ClNO$ $(M + H)^+$ 272.0837, found 272.0838.

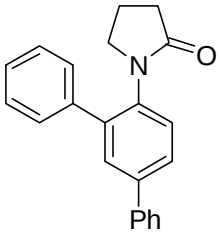
**1-(5-Bromobiphenyl-2-yl)pyrrolidin-2-one (3ga)**



**3ga**

Viscous liquid (36.7 mg, 58%), $^1$H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.49 (m, 2H), 7.45 – 7.30 (m, 5H), 7.20 (d, *J* = 8.3 Hz, 1H), 3.17 (t, *J* = 7.0 Hz, 2H), 2.40 (t, *J* = 8.1 Hz, 2H), 1.92 – 1.80 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 175.61, 141.41, 137.72, 135.39, 133.65, 131.48, 129.99, 128.55, 128.13, 128.09,121.46, 49.89, 31.02, 18.91. ATR-FTIR ($cm^{-1}$): 3131, 1697, 1496, 1401. 1308, 1237, 865, 825, 758. HRMS m/z (ESI) calcd for $C_{16}H_{15}BrNO$ $(M + H)^+$ 316.0332, found 316.0331.

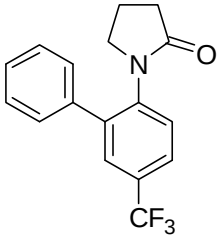
**1-(5-Phenylbiphenyl-2-yl)pyrrolidin-2-one (3ha)**



**3ha**

White solid (45.7 mg, 73%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.66 – 7.57 (m, 4H), 7.49 – 7.33 (m, 9H), 3.25 (t, *J* = 6.9 Hz, 2H), 2.45 (t, *J* = 8.0 Hz, 2H), 1.96 – 1.83 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.78, 141.05, 140.24, 139.81, 139.02, 135.40, 129.62, 128.77, 128.68, 128.45, 128.32, 127.67, 127.53, 127.21, 127.14, 50.13, 31.16, 18.96.ATR-FTIR ($cm^{-1}$): 3131, 1695, 1497, 1400. 1305, 1235, 860, 827, 756. HRMS m/z (ESI) calcd for $C_{22}H_{20}NO$ $(M + H)^+$ 314.1539, found 314.1539.

**1-(5-(Trifluoromethyl)biphenyl-2-yl)pyrrolidin-2-one (3ia)**

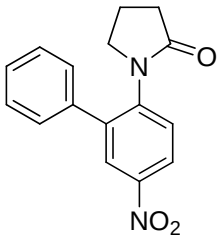


**3ia**

Viscous liquid (33.6 mg, 55%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.69 – 7.61 (m, 2H), 7.52 – 7.33 (m, 6H), 3.21 (t, *J* = 7.0 Hz, 2H),

2.44 (t, *J* = 8.0 Hz, 2H), 1.96 – 1.84 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.63, 140.04, 139.58, 137.83, 129.96 (q, *J* = 32.7 Hz), 128.96, 128.72, 128.27, 128.16, 127.93 (q, *J* = 3.7 Hz), 125.35 (q, 3.7 Hz), 123.76 (q, *J* = 272.3 Hz), 49.73, 31.06, 19.03. ATR-FTIR ($cm^{-1}$):3137, 1695, 1497, 1400. 1305, 1232, 858, 825, 754. HRMS m/z (ESI) calcd for $C_{17}H_{15}F_3NO$ $(M + H)^+$ 306.1100, found 306.1104.

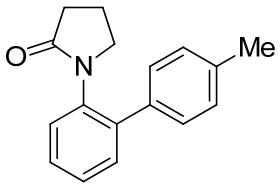
**1-(5-Nitrobiphenyl-2-yl)pyrrolidin-2-one (3ja)**



**3ja**

Viscous liquid (30.5 mg, 74%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.24 (dt, *J* = 8.4, 2.4 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.49 – 7.40 (m, 3H), 7.40 – 7.34 (m, 2H), 3.22 (t, *J* = 6.9 Hz, 2H), 2.45 (t, J = 8.0 Hz, 2H), 1.98 – 1.87 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)**δ 175.52), 146.47, 142.35, 140.23, 137.15, 129.24, 128.90, 128.64, 128.00, 126.09, 123.21, 49.54, 31.03, 19.06. ATR-FTIR ($cm^{-1}$): 3130, 1698, 1495, 1400. 1306, 1233, 865, 823, 755. HRMS m/z (ESI) calcd for $C_{16}H_{15}N_2O_3$ $(M + H)^+$ 283.1077, found 283.1079.

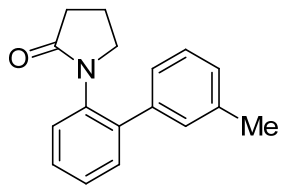
**1-(4'-Methyl-[1,1'-biphenyl]-2-yl)pyrrolidin-2-one (3ab)**



**3ab**

White solid (49.7 mg, 99%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.42 – 7.34 (m, 3H), 7.33 – 7.29 (m, 1H), 7.27 (s, 1H), 7.25 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 3.21 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 8.1 Hz, 2H), 2.39 (s, 3H), 1.93 – 1.82 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.75, 139.49, 137.30, 136.19, 136.10, 130.85, 129.13, 128.34, 128.30, 128.15, 50.08, 31.18, 21.18, 18.95; ATR-FTIR ($cm^{-1}$): 3129, 1697, 1493, 1403, 1307, 1238, 860, 828, 756; HRMS m/z (ESI) calcd for $C_{17}H_{18}NO$ $(M + H)^+$ 252.1383, found 252.1383.

**1-(3'-Methylbiphenyl-2-yl)pyrrolidin-2-one (3ac)**

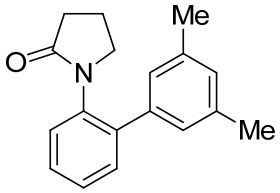


**3ac**

Viscous liquid (35 mg, 70%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.43 – 7.34 (m, 3H), 7.34 – 7.25 (m, 2H), 7.24 – 7.12 (m, 3H), 3.20 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 8.1 Hz, 2H), 2.38

(s, 3H), 1.94 – 1.80 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.53, 139.56, 138.99, 137.98, 136.20, 130.77, 128.96, 128.36, 128.33, 128.23 , 127.92, 125.34, 50.03, 31.17, 21.40, 18.97. ATR-FTIR ($cm^{-1}$): 3129, 1697, 1493, 1403, 1307, 1238, 860, 828, 761. HRMS m/z (ESI) calcd for $C_{17}H_{18}NO$ $(M + H)^+$ 252.1383, found 252.1384.

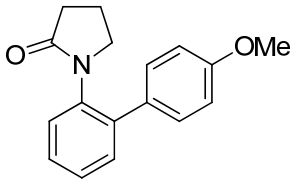
**1-(3',5'-Dimethylbiphenyl-2-yl)pyrrolidin-2-one (3ad)**




**3ad**

Viscous liquid (22.3 mg, 42%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.42 – 7.34 (m, 3H), 7.34 – 7.29 (m, 1H), 6.99 (s, 3H), 3.21 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 8.0 Hz, 2H), 2.34 (s, 6H), 1.98 – 1.80 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.53, 139.53, 138.94, 137.85, 136.12, 130.76, 129.11, 128.33, 128.24, 127.88, 126.03, 49.96, 31.21, 21.28, 19.03. ATR-FTIR ($cm^{-1}$): 3125, 1698, 1495, 1403, 1305, 1239, 866, 825, 758. HRMS m/z (ESI) calcd for $C_{18}H_{20}NO$ $(M + H)^+$ 266.1539, found 266.1539.

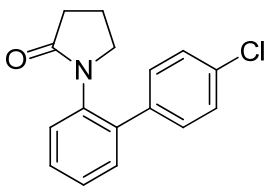
**1-(4'-Methoxybiphenyl-2-yl)pyrrolidin-2-one (3ae)**




**3ae**

White solid (51.3 mg, 96%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.41 – 7.34 (m, 3H), 7.34 – 7.27 (m, 3H), 6.96 – 6.90 (m, 2H), 3.84 (s, 3H), 3.22 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 8.1 Hz, 2H), 1.93 – 1.83 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)**δ 175.62, 159.07, 139.19, 136.23, 131.39, 130.77, 129.41, 128.32, 128.13, 127.96, 113.78, 55.19, 50.00, 31.17, 18.92. ATR-FTIR ($cm^{-1}$): 3132, 1695, 1499, 1400, 1307, 1237, 863, 828, 758. HRMS m/z (ESI) calcd for $C_{17}H_{18}NO_2$ $(M + H)^+$ 268.1332, found 268.1333.

**1-(4'-Chlorobiphenyl-2-yl)pyrrolidin-2-one (3af)**

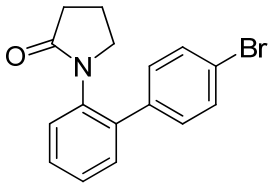



**3af**

Viscous liquid (40.1 mg, 74%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.45 – 7.28 (m, 8H), 3.25 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 8.1 Hz, 2H), 1.97 – 1.87 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)**δ 175.67, 138.49, 137.53, 136.23, 133.68, 130.67, 129.67,

128.93, 128.61, 128.39, 128.18, 50.26, 31.10, 18.94. ATR-FTIR ($cm^{-1}$): 1692, 1479, 1401, 1301, 1242, 1089, 834, 760. HRMS m/z (ESI) calcd for $C_{16}H_{15}ClNO$ $(M + H)^+$ 272.0837, found 272.0836.

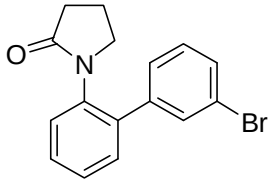
**1-(4'-Bromobiphenyl-2-yl)pyrrolidin-2-one (3ag)**



**3ag**

Viscous liquid (40.4 mg, 64%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.56 – 7.50 (m, 2H), 7.46 – 7.30 (m, 4H), 7.28 – 7.23 (m, 2H), 3.26 (t, *J* = 7.0 Hz, 2H), 2.44 (t, *J* = 8.1 Hz, 2H), 1.98 – 1.85 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.63, 138.51, 138.03, 136.21, 131.58, 130.63, 130.02, 128.97, 128.42, 128.20, 121.90, 50.28, 31.11, 18.96. ATR-FTIR ($cm^{-1}$):3132, 1690, 1401, 1322, 834, 758. HRMS m/z (ESI) calcd for $C_{16}H_{15}BrNO$ $(M + H)^+$ 316.0332, found 316.0333.

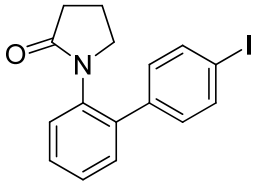
**1-(3'-Bromobiphenyl-2-yl)pyrrolidin-2-one (3ah)**



**3ah**

Viscous liquid (34.7 mg, 55%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.54 (t, *J* = 1.7 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.46 – 7.36 (m, 3H), 7.35 – 7.25 (m, 3H), 3.27 (t, *J* = 7.0 Hz, 2H), 2.44 (t, *J* = 8.1 Hz, 2H), 1.98 – 1.88 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)**δ 175.51, 141.08, 138.02, 136.22, 131.17, 130.59, 130.54, 129.93, 129.07, 128.36, 128.12, 127.03, 122.31, 50.23, 31.07, 18.96. ATR-FTIR ($cm^{-1}$): 3131, 1695, 1495, 1400, 1308, 1238, 865, 822, 758. HRMS m/z (ESI) calcd for $C_{16}H_{15}BrNO$ $(M + H)^+$ 316.0332, found 316.0332.

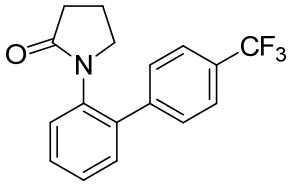
**1-(4'-Iodobiphenyl-2-yl)pyrrolidin-2-one (3ai)**



**3ai**

White solid (40.0 mg, 55%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.77 – 7.69 (m, 2H), 7.47 – 7.28 (m, 4H), 7.18 – 7.07 (m, 2H), 3.26 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 8.1 Hz, 2H), 1.97 – 1.87 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.64, 138.62, 138.53, 137.53, 136.13, 130.58, 130.22, 128.95, 128.40, 128.19, 93.53, 50.28, 31.09, 18.95. ATR-FTIR ($cm^{-1}$): 3139, 1693, 1497, 1400, 1305, 1237, 862, 827, 758. HRMS m/z (ESI) calcd for $C_{16}H_{15}INO$ $(M + H)^+$ 364.0193, found 364.0193.

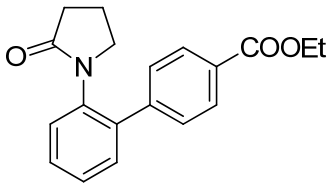
**1-(4'-(Trifluoromethyl)biphenyl-2-yl)pyrrolidin-2-one (3aj)**



**3aj**

Viscous liquid (30.0 mg, 49%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.67 (d, J = 8.1 Hz, 2H), 7.51 (d, J = 8.0 Hz, 2H), 7.48 – 7.32 (m, 4H), 3.28 (t, J = 7.0 Hz, 2H), 2.42 (t, J = 8.1 Hz, 2H), 1.98 – 1.87 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.51, 142.83, 138.35, 136.31, 130.66, 129.68 (q, *J* = 32.9 Hz), 129.33, 128.71, 128.34, 128.21, 125.30 (q, *J* = 3.54 Hz), 124.10 (q, *J* = 273.2 Hz), 50.39, 31.02, 18.91. ATR-FTIR ($cm^{-1}$): 3133, 1697, 1494, 1401, 1307, 1237, 866, 824, 758. HRMS m/z (ESI) calcd for $C_{17}H_{15}F_3NO$ $(M + H)^+$ 306.1100, found 306.1103.

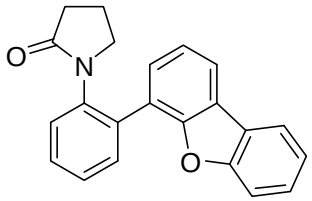
**Methyl 2'-(2-oxopyrrolidin-1-yl)biphenyl-4-carboxylate (3ak)**



**3ak**

Viscous liquid (26.6 mg, 43%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.11 – 8.04 (m, 2H), 7.48 – 7.37 (m, 5H), 7.35 – 7.31 (m, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 3.24 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 8.1 Hz, 2H), 1.94 – 1.85 (m, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.53, 166.39, 143.75, 138.63, 136.27, 130.63, 129.65, 129.61, 129.19, 128.34, 128.13, 61.06, 50.29, 31.07, 18.91, 14.31. ATR-FTIR ($cm^{-1}$): 3132, 1690, 1478, 1401, 1240, 835, 760. HRMS m/z (ESI) calcd for $C_{19}H_{20}NO_3$ $(M + H)^+$ 310.1438, found 310.1439.

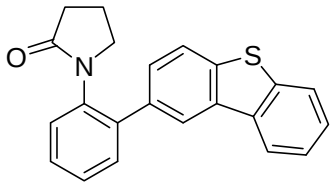
**1-(2-(Dibenzo[b,d]furan-4-yl)phenyl)pyrrolidin-2-one (3al)**



**3al**

White solid (57.0 mg, 87%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.12 – 8.04 (m, 2H), 7.67 – 7.60 (m, 1H), 7.58 – 7.32 (m, 8H), 3.29 (t, *J* = 6.9 Hz, 2H), 2.25 (t, *J* = 8.0 Hz, 2H), 1.73 – 1.58 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 174.91, 155.96, 153.09, 137.20, 133.78, 131.69, 129.09, 127.96, 127.87, 127.61, 127.32, 124.36, 124.04, 123.51, 122.98, 122.80, 120.65, 120.15, 111.69, 49.84, 31.09, 18.88. ATR-FTIR ($cm^{-1}$):3132, 1697, 1495, 1400, 1305, 1235, 866, 829, 758. HRMS m/z (ESI) calcd for $C_{22}H_{18}NO_2$ $(M + H)^+$ 328.1332, found 328.1333.

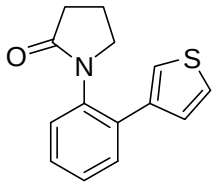
**1-(2-(Dibenzo[b,d]thiophen-2-yl)phenyl)pyrrolidin-2-one (3am)**



**3am**

White solid (55.6 mg, 81%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.23 – 8.11 (m, 2H), 7.93 – 7.84 (m, 2H), 7.56 – 7.42 (m, 6H), 7.42 – 7.35 (m, 1H), 3.22 (t, *J* = 7.0 Hz, 2H), 2.42 (t, *J* = 8.1 Hz, 2H), 1.89 – 1.74 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** 175.90, 139.76, 139.45, 138.79, 136.51, 135.79, 135.44, 135.37, 131.09, 128.72, 128.63, 128.23, 127.07, 126.95, 124.61, 122.88, 122.74, 121.60, 121.30, 50.19, 31.17, 18.96. ATR-FTIR ($cm^{-1}$): 3133, 1697, 1495, 1400, 1305, 1235, 863, 828, 761. HRMS m/z (ESI) calcd for $C_{22}H_{18}NOS$ $(M + H)^+$ 344.1104, found 344.1105.

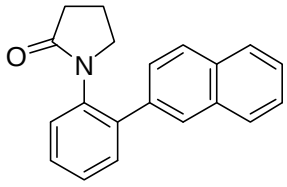
**1-(2-(Thiophen-3-yl)phenyl)pyrrolidin-2-one (3an)**



**3an**

Viscous liquid (39.4 mg, 81%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.47 – 7.42 (m, 1H), 7.41 – 7.34 (m, 3H), 7.33 – 7.28 (m, 2H), 7.16 (dd, *J* = 4.9, 1.2 Hz, 1H), 3.29 (t, *J* = 7.0 Hz, 2H), 2.48 (t, *J* = 8.1 Hz, 2H), 2.00 – 1.92 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.68, 139.35, 136.41, 134.56, 130.67, 128.61, 128.50, 128.11, 127.94, 125.77, 122.65, 50.23, 31.29, 19.03. ATR-FTIR ($cm^{-1}$): 3137, 1693, 1495, 1400, 1305, 1233, 868, 822, 761. HRMS m/z (ESI) calcd for $C_{14}H_{14}NOS$ $(M + H)^+$ 244.0791, found 244.0791.

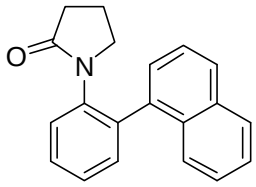
**1-(2-(Naphthalen-2-yl)phenyl)pyrrolidin-2-one (3ao)**



**3ao**

White solid (57.4 mg, 99%), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.88 (d, *J* = 8.0 Hz, 4H), 7.57 – 7.47 (m, 4H), 7.47 – 7.41 (m, 2H), 7.41 – 7.34 (m, 1H), 3.19 (t, *J* = 7.0 Hz, 2H), 2.43 (t, *J* = 8.0 Hz, 2H), 1.86 – 1.73 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.65, 139.32, 136.59, 136.42, 133.31, 132.51, 131.03, 128.60, 128.42, 128.03, 128.00, 127.88, 127.60, 127.08, 126.48, 126.23, 123.11, 50.03, 31.12, 18.85. ATR-FTIR ($cm^{-1}$): 3127, 1693, 1495, 1404, 1303, 1241, 860, 822, 758. HRMS m/z (ESI) calcd for $C_{20}H_{17}NO$ $(M + H)^+$ 288.1383, found 288.1383.

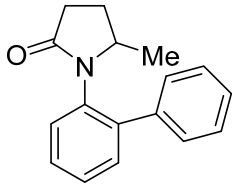
**1-(2-(Naphthalen-1-yl)phenyl)pyrrolidin-2-one (3ap)**



**3ap**

Viscous liquid (33.8 mg, 59%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.93 – 7.83 (m, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.56 – 7.37 (m, 8H), 2.98 – 2.84 (m, 2H), 2.25 – 2.08 (m, 2H), 1.58 – 1.43 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.12, 137.54, 137.38, 136.74, 133.46, 132.06, 131.43, 128.68, 128.28, 128.12, 127.45, 126.96, 126.15, 125.94, 125.86, 125.33, 49.81, 31.02, 18.90. ATR-FTIR ($cm^{-1}$): 3132, 1697, 1497, 1403, 1302, 1239, 862, 824, 758. HRMS m/z (ESI) calcd for $C_{20}H_{17}NO$ $(M + H)^+$ 288.1383, found 288.1384.

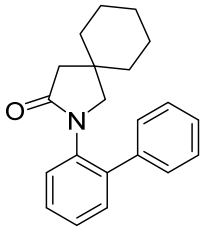
**1-(Biphenyl-2-yl)-5-methylpyrrolidin-2-one (3ka)**



**3ka**

Viscous liquid (32.6 mg, 65%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.44 – 7.31 (m, 8H), 7.26 – 7.21 (m, 1H), 2.55 – 2.45 (m, 1H), 2.43 – 2.31 (m, 1H), 2.02 – 1.91 (m, 1H), 1.58 – 1.47 (m, 1H), 1.35 – 1.25 (m, 1H), 0.86 (d, *J* = 6.3 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 175.69, 139.25, 134.81, 130.75, 130.15, 128.48, 128.35, 128.11, 127.51, 30.73, 27.57, 19.91. ATR-FTIR ($cm^{-1}$): 3130, 1696, 1498, 1401, 1301, 1239, 858, 823, 755. HRMS m/z (ESI) calcd for $C_{20}H_{17}NO$ $(M + H)^+$ 252.1383, found 252.1383.

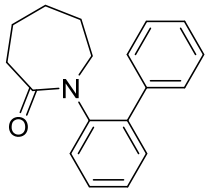
**2-(Biphenyl-2-yl)-2-azaspiro[4.5]decan-3-one (3la)**



**3la**

Viscous liquid (38.1 mg, 63%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.46 – 7.28 (m, 9H), 2.97 (s, 2H), 2.27 (s, 2H), 1.35 – 1.14 (m, 10H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 174.87, 140.06, 138.96, 136.43, 130.79, 128.59, 128.56, 128.29, 128.26, 127.91, 127.51, 61.21, 44.39, 36.56, 36.29, 25.39, 22.61. ATR-FTIR ($cm^{-1}$): 3132, 1698, 1494, 1401, 1303, 1238, 868, 825, 758. HRMS m/z (ESI) calcd for $C_{21}H_{24}NO$ $(M + H)^+$ 306.1852, found 306.1853.

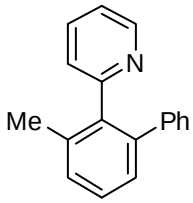
**1-(Biphenyl-2-yl)azepan-2-one (3ma)**



**3ma**

Viscous liquid (49.2 mg, 93%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 7.41 – 7.32 (m, 8H), 7.24 – 7.19 (m, 1H), 3.26 – 3.06 (m, 2H), 2.66 – 2.48 (m, 2H), 1.78 – 1.67 (m, 3H), 1.58 – 1.40 (m, 2H), 1.24 – 1.14 (m, 1H). **$^{13}$C NMR (101 MHz, CDCl$_3$)** δ 176.82, 142.59, 139.49, 139.21, 130.90, 128.73, 128.69, 128.39, 128.25, 127.57, 127.41, 52.79, 37.52, 29.87, 27.72, 23.10. ATR-FTIR (cm$^{-1}$): 3134, 1697, 1494, 1402, 1303, 1239, 869, 823, 758. HRMS m/z (ESI) calcd for $C_{18}H_{20}NO$ $(M + H)^+$ 266.1539, found 266.1538.

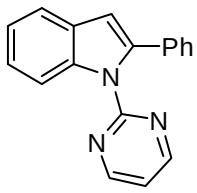
**2-(3-Methylbiphenyl-2-yl)pyridine (5aa)**



**5aa**

Viscous liquid (35.2 mg, 77%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 8.64 (ddd, *J* = 4.9, 1.7, 0.9 Hz, 1H), 7.45 (td, *J* = 7.7, 1.8 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.29 (t, *J* = 7.3 Hz, 2H), 7.17 – 7.05 (m, 6H), 6.89 (dt, *J* = 7.8, 1.0 Hz, 1H), 2.19 (s, 3H). **$^{13}$C NMR (101 MHz, CDCl$_3$)** δ 159.44, 148.67, 141.59, 141.24, 139.11, 136.68, 135.79, 129.60, 129.35, 128.03, 127.55, 126.19, 125.64, 121.31, 20.42 (s). ATR-FTIR (cm$^{-1}$): 3041, 1684, 1494, 1400, 1303, 1239, 869. HRMS m/z (ESI) calcd for $C_{18}H_{16}N$ $(M + H)^+$ 246.1277, found 246.1278.

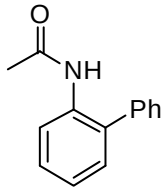
**2-Phenyl-1-(pyrimidin-2-yl)-1*H*-indole (5ba)**



**5ba**

White solid (43.0 mg, 78%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.11 (d, *J* = 8.3 Hz, 1H), 7.62 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.26 (s, 7H), 7.04 (t, *J* = 4.8 Hz, 1H), 6.78 (d, *J* = 0.4 Hz, 1H). **$^{13}$C NMR (101 MHz, CDCl$_3$)** δ 158.15, 158.02, 140.41, 138.03, 133.85, 129.27, 128.09, 128.07, 127.07, 123.50, 122.08, 120.63, 117.57, 112.72, 108.13. ATR-FTIR (cm$^{-1}$): 3135, 1682, 1517, 1505, 1452, 1404, 807. HRMS m/z (ESI) calcd for $C_{18}H_{14}N_3$ $(M + H)^+$ 272.1182, found 272.1182.

***N*-(Biphenyl-2-yl)acetamide (5ca)**

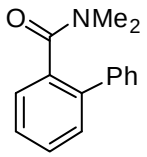


**5ca**

White solid (26.4 mg, 62%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 8.25 (d, *J* = 8.2 Hz, 1H), 7.55 – 7.41 (m, 3H), 7.39 – 7.34 (m, 3H), 7.26 – 7.07

(m, 3H), 2.01 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 168.23, 138.11, 134.61, 132.19, 130.01, 129.17, 129.03, 128.36, 127.91, 124.34, 121.68, 24.52. ATR-FTIR ($cm^{-1}$): 1631, 1586, 1521, 1440, 1405, 1108, 822. HRMS m/z (ESI) calcd for $C_{14}H_{14}NO$ $(M + H)^+$ 212.1070, found 212.1071.

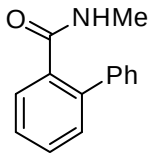
### *N*,*N*-Dimethylbiphenyl-2-carboxamide (5da)




**5da**

Viscous liquid (36.0 mg, 71%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.49 – 7.43 (m, 3H), 7.43 – 7.32 (m, 6H), 2.85 (s, 3H), 2.40 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 171.32, 139.94, 138.68, 135.76, 129.31, 129.29, 128.48, 128.36, 127.69, 127.58, 127.41, 37.93, 34.52. ATR-FTIR ($cm^{-1}$): 1633, 1506, 1402, 1270, 1209, 1110, 824. HRMS m/z (ESI) calcd for $C_{15}H_{16}NO$ $(M + H)^+$226.1226, found 226.1226.

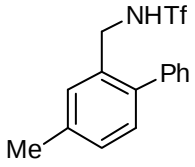
### *N*-Methylbiphenyl-2-carboxamide (5ea)




**5ea**

White solid (30.5 mg, 74%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.69 – 7.62 (m, 1H), 7.46 (td, *J* = 7.5, 1.5 Hz, 1H), 7.43 – 7.33 (m, 7H), 5.28 (s, 1H), 2.65 (d, *J* = 4.9 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 170.22, 140.09, 139.28, 135.67, 130.06, 130.02, 128.72, 128.55, 128.51, 127.68, 127.51, 26.56. ATR-FTIR ($cm^{-1}$): 1683, 1508, 1400, 825, 759 HRMS m/z (ESI) calcd for $C_{14}H_{14}NO$ $(M + H)^+$ 212.1070, found 212.1070.

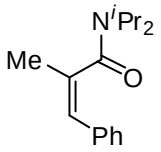
### 1,1,1-Trifluoro-N-((4-methylbiphenyl-2-yl)methyl)methanesulfonamide (5fa)




**5fa**

White solid (34.0 mg, 52%), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.46 – 7.37 (m, 3H), 7.27 – 7.24 (m, 3H), 7.22 – 7.16 (m, 2H), 4.69 (brs, 1H), 4.38 (d, *J* = 5.6 Hz, 2H), 2.41 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 139.79, 139.12, 138.07, 132.21, 130.46, 129.71, 129.39, 128.88, 128.73, 127.68, 119.50 (q, *J* = 323.2 Hz), 46.17, 21.08. ATR-FTIR ($cm^{-1}$): 3133, 1770, 1684, 1401, 1239, 1193, 1146. HRMS m/z (ESI) calcd for $C_{15}H_{15}F_3NO_2$ $(M + H)^+$ 330.0770, found 330.0772.

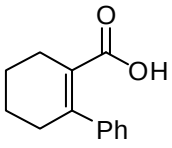
**(Z)-*N*,*N*-Diisopropyl-2-methyl-3-phenylacrylamide (5ga)**




**5ga**

Colorless liquid (40.6 mg, 83%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 7.39 – 7.33 (m, 2H), 7.27 – 7.22 (m, 2H), 7.21 – 7.15 (m, 1H), 6.27 (d, *J* = 1.3 Hz, 1H), 3.98 (dt, *J* = 13.4, 6.7 Hz, 1H), 3.27 (dt, *J* = 13.7, 6.8 Hz, 1H), 2.04 (d, *J* = 1.6 Hz, 3H), 1.46 (dd, *J* = 6.8, 3.7 Hz, 6H), 1.07 (d, *J* = 6.8 Hz, 3H), 0.49 (d, *J* = 6.6 Hz, 3H). **$^{13}$C NMR (101 MHz, CDCl$_3$)** δ 171.17, 136.37, 135.11, 128.09 , 127.96, 127.17, 125.73, 50.35, 45.41, 22.37, 21.40, 20.66, 19.85, 19.64. ATR-FTIR (cm$^{-1}$): 1770, 1684, 1672, 1400, 1303, 1245, 1043, 668 HRMS m/z (ESI) calcd for $C_{16}H_{24}NO$ $(M + H)^+$ 246.1852, found 246.1853.

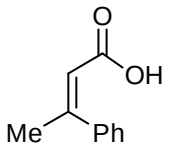
**2-Phenylcyclohex-1-enecarboxylic acid (5ha)**




**5ha**

White solid (33.0 mg, 83%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 7.31 – 7.21 (m, 3H), 7.15 – 7.06 (m, 2H), 2.42 – 2.33 (m, 4H), 1.74 – 1.65 (m, 4H). **$^{13}$C NMR (101 MHz, CDCl$_3$)** δ 174.30, 149.03, 143.08, 128.03, 127.10, 126.68, 126.47, 33.56, 26.48, 22.36, 21.89. ATR-FTIR (cm$^{-1}$): 1684, 1672, 1400, 558. HRMS m/z (ESI) calcd for $C_{13}H_{15}O_2$ $(M + H)^+$ 203.1067, found 203.1069.

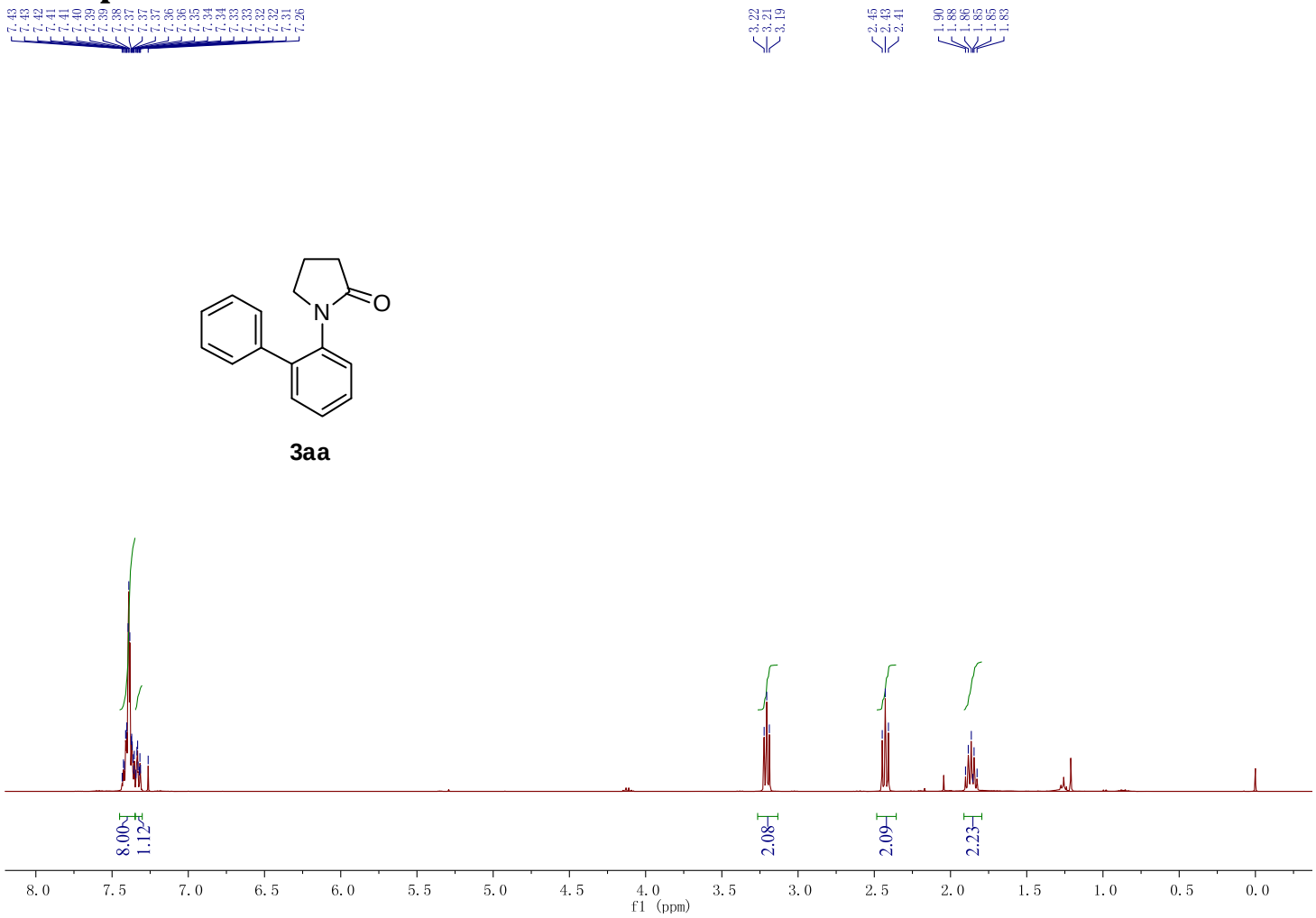
**(Z)-3-Phenylbut-2-enoic acid (5ia)**

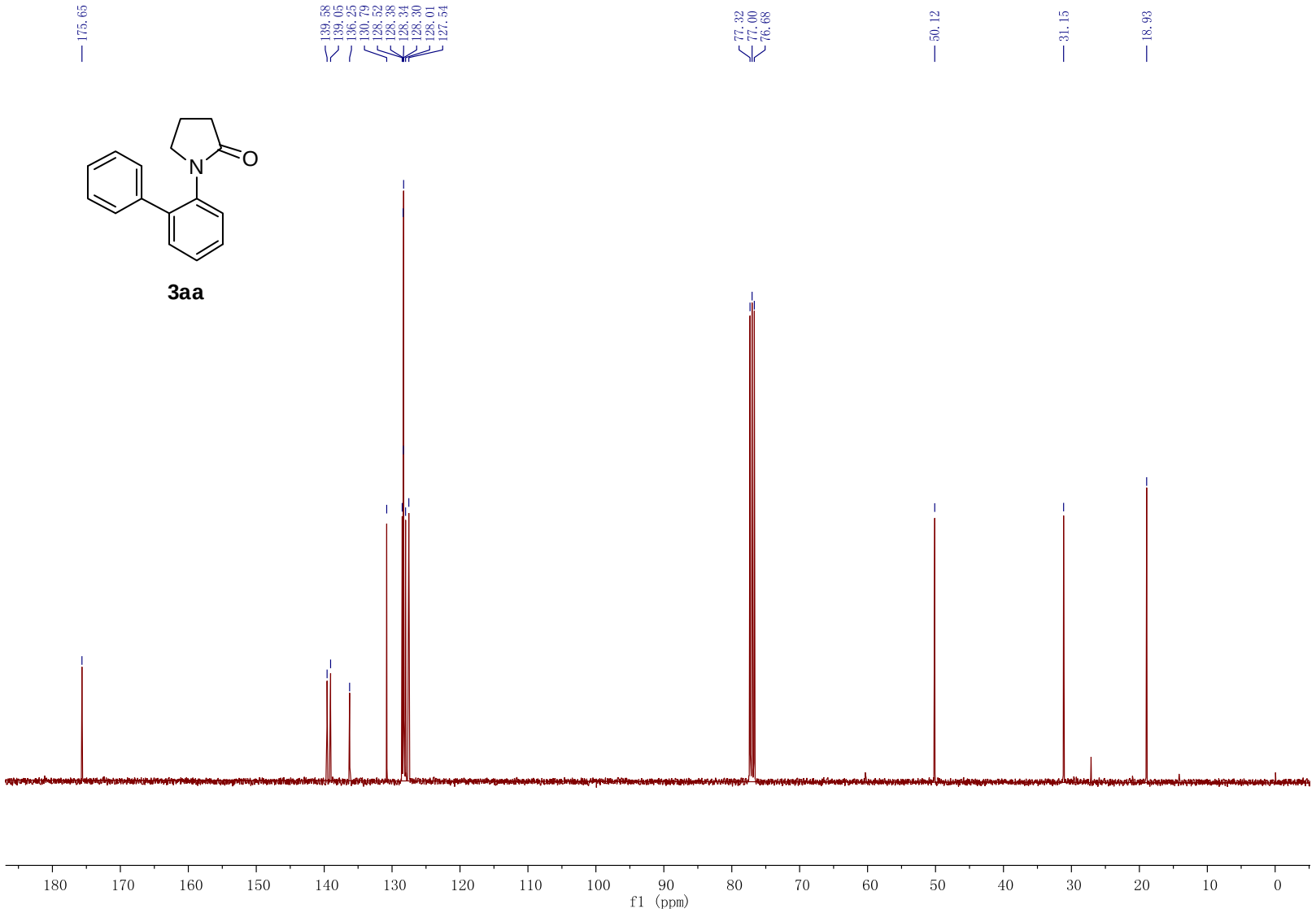



**5ia**

White solid (18.3 mg, 56%), **$^1$H NMR (400 MHz, CDCl$_3$)** δ 7.36 – 7.27 (m, 3H), 7.22 – 7.17 (m, 2H), 5.91 – 5.87 (m, 1H), 2.19 (d, *J* = 1.4 Hz, 3H). **$^{13}$C NMR (101 MHz, CDCl$_3$)** δ 170.40, 158.16, 140.18, 128.01, 127.96, 126.82, 116.84, 27.58. ATR-FTIR (cm$^{-1}$): 1765, 1684, 1616, 1405, 1323, 1244, 1112. HRMS m/z (ESI) calcd for $C_{10}H_{11}O_2$ $(M + H)^+$ 163.0754, found 163.0757.

# Copies of NMR Spectra

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31.15
18.93
N
O
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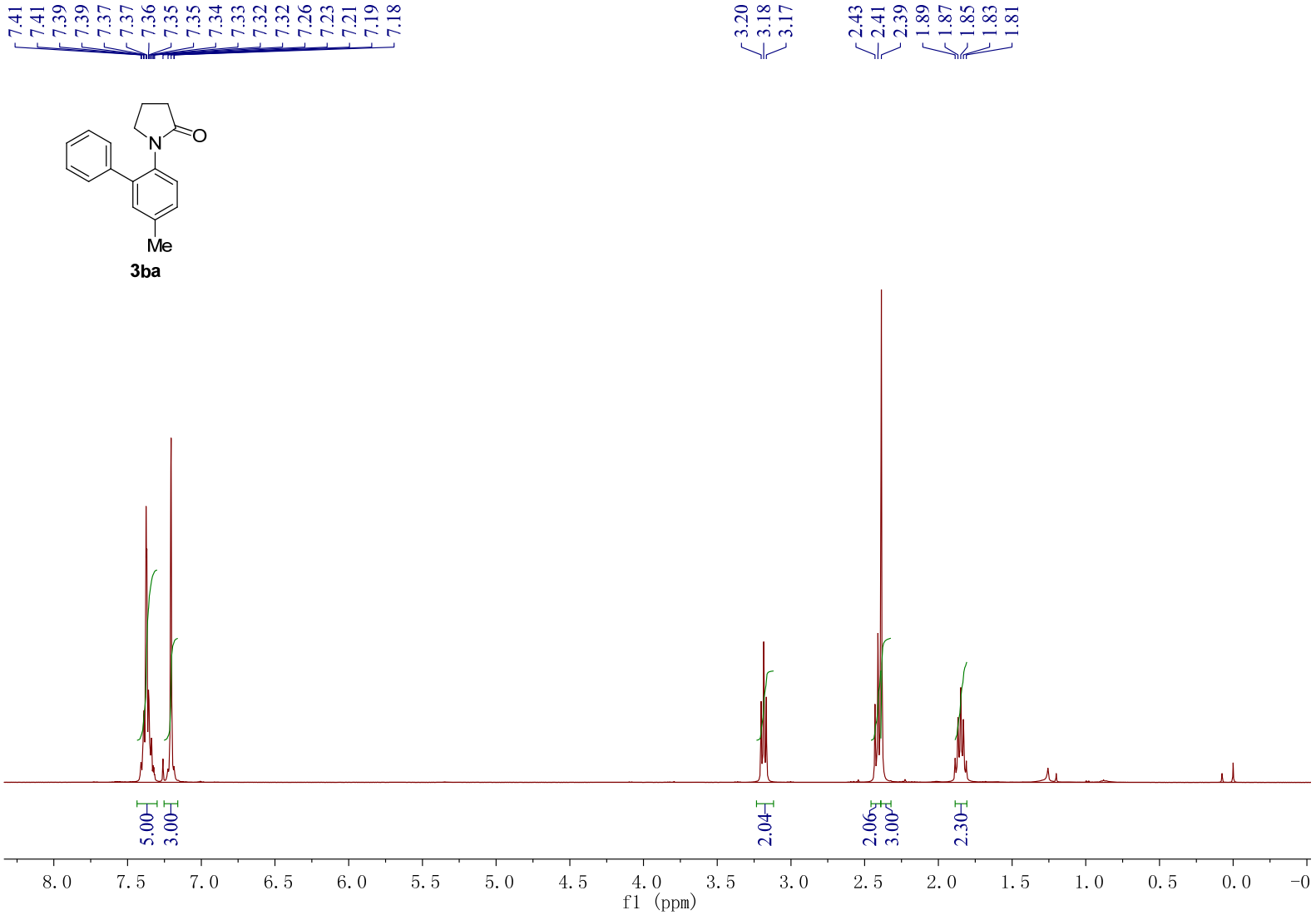
f1 (ppm)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7.23
7.21
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3.18
3.17
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2.41
2.39
1.89
1.87
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1.83
1.81
N
O
Me
3ba
5.00
3.00
2.04
2.06
3.00
2.30
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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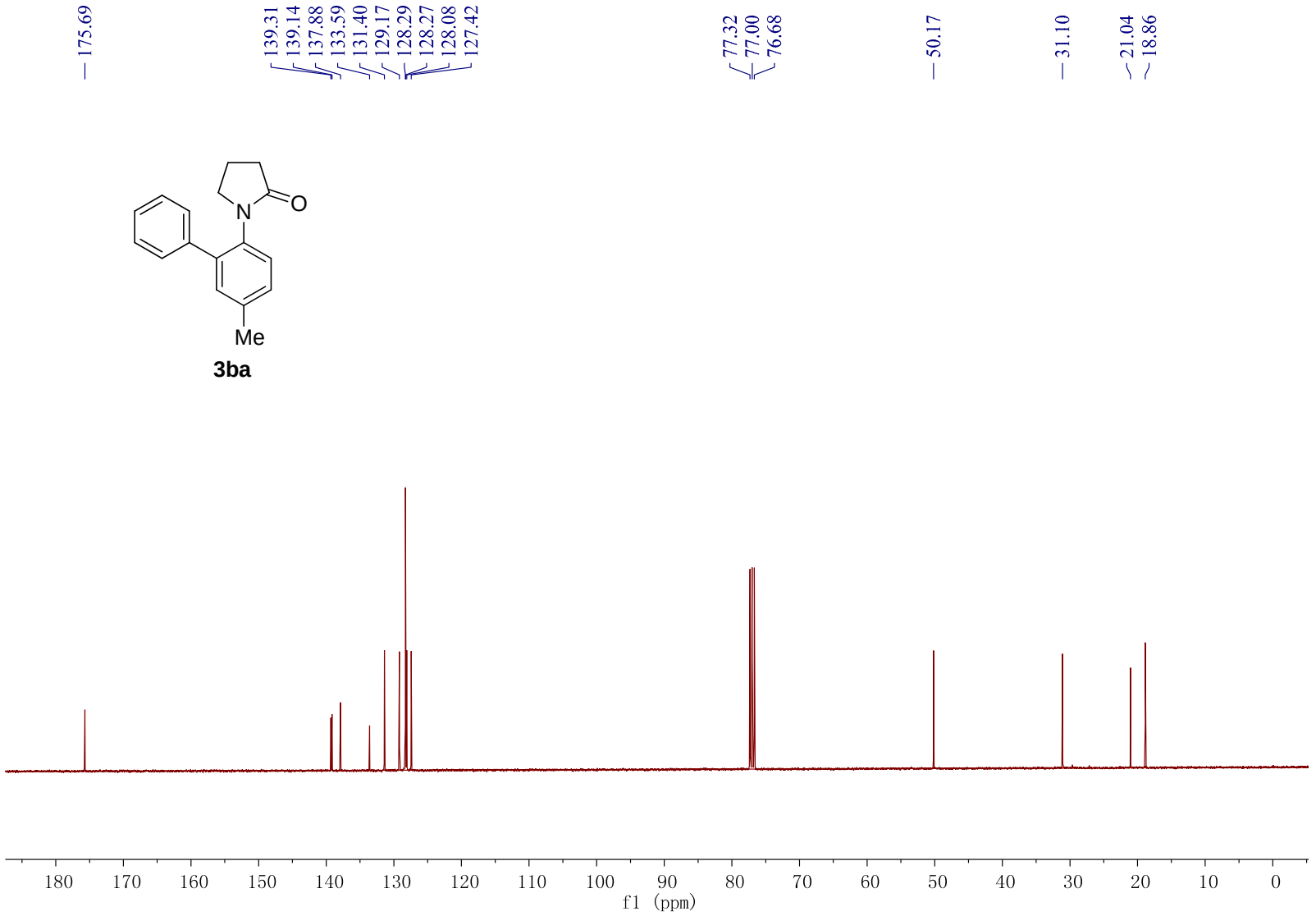
f1 (ppm)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77.00
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50.17
31.10
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Me
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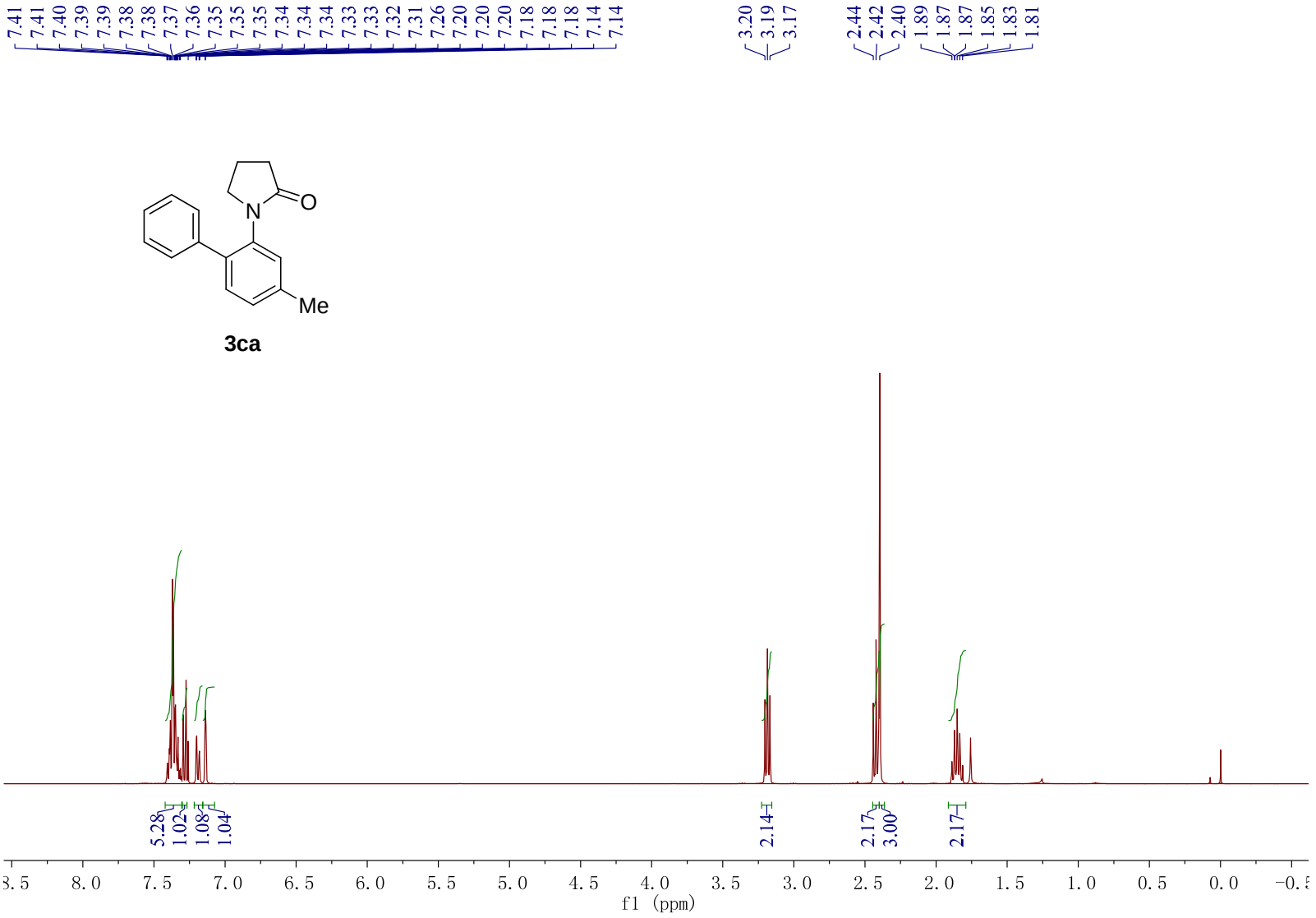
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7.14
3.20
3.19
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2.42
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1.89
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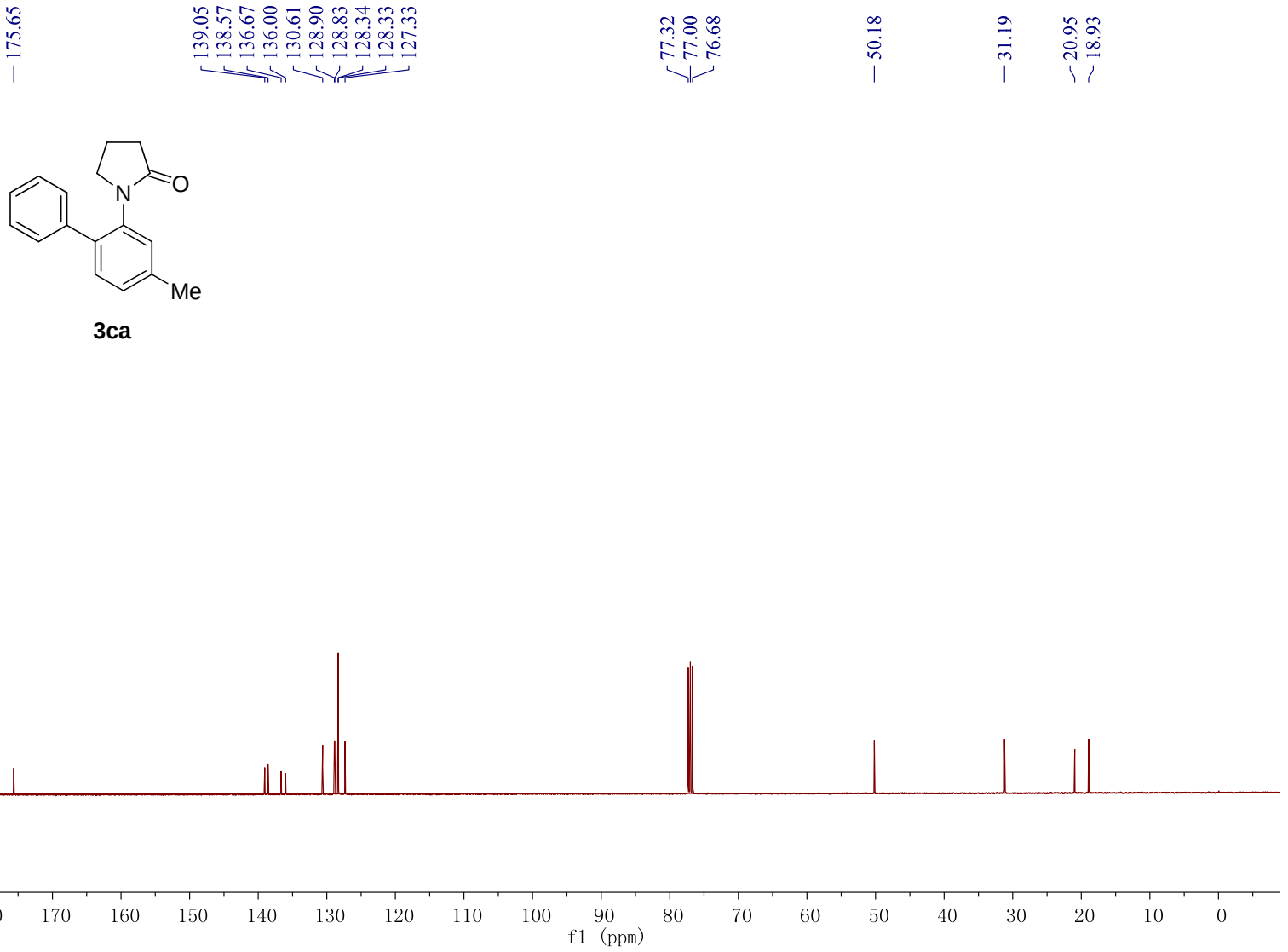
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31.19
20.95
18.93
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O
Me
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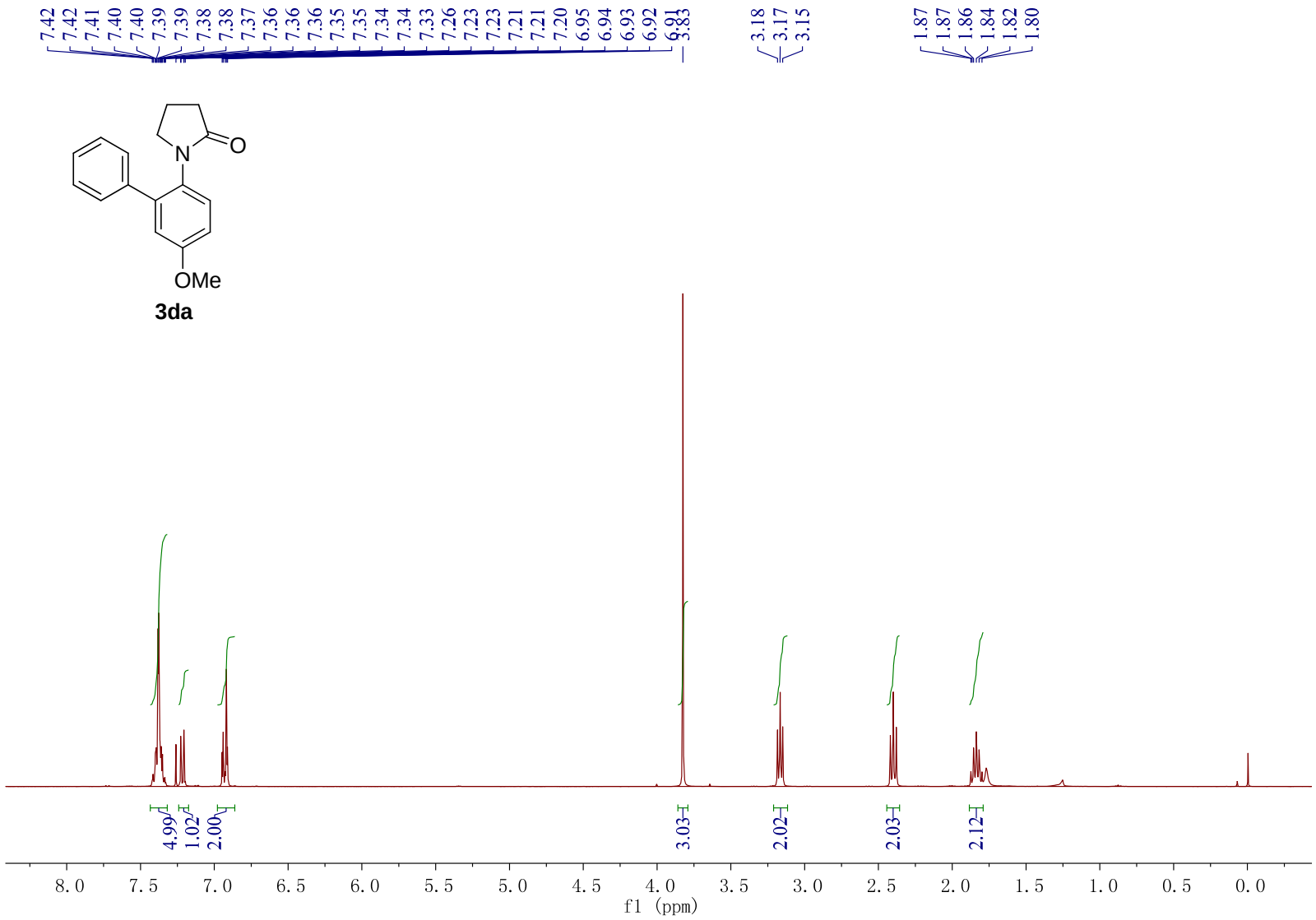
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7.21
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6.92
6.91
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3.18
3.17
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1.86
1.84
1.82
1.80
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O
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2.00
3.03
2.02
2.03
2.12
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6.0
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5.0
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f1 (ppm)

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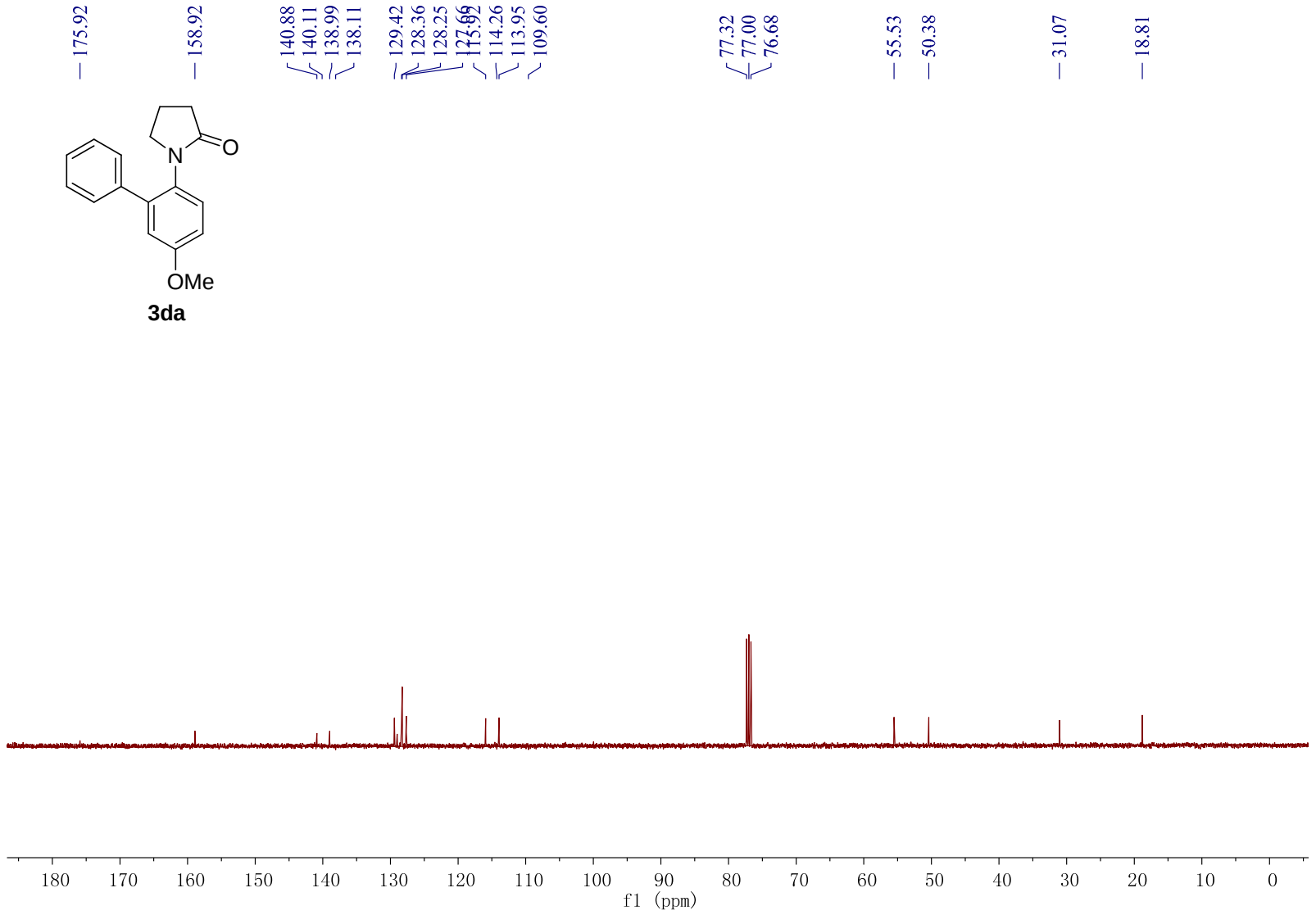
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128.25
114.26
113.95
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77.32
77.00
76.68
55.53
50.38
31.07
18.81
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O
OMe
3da
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160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


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7.43
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
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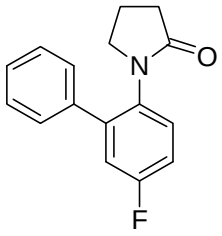
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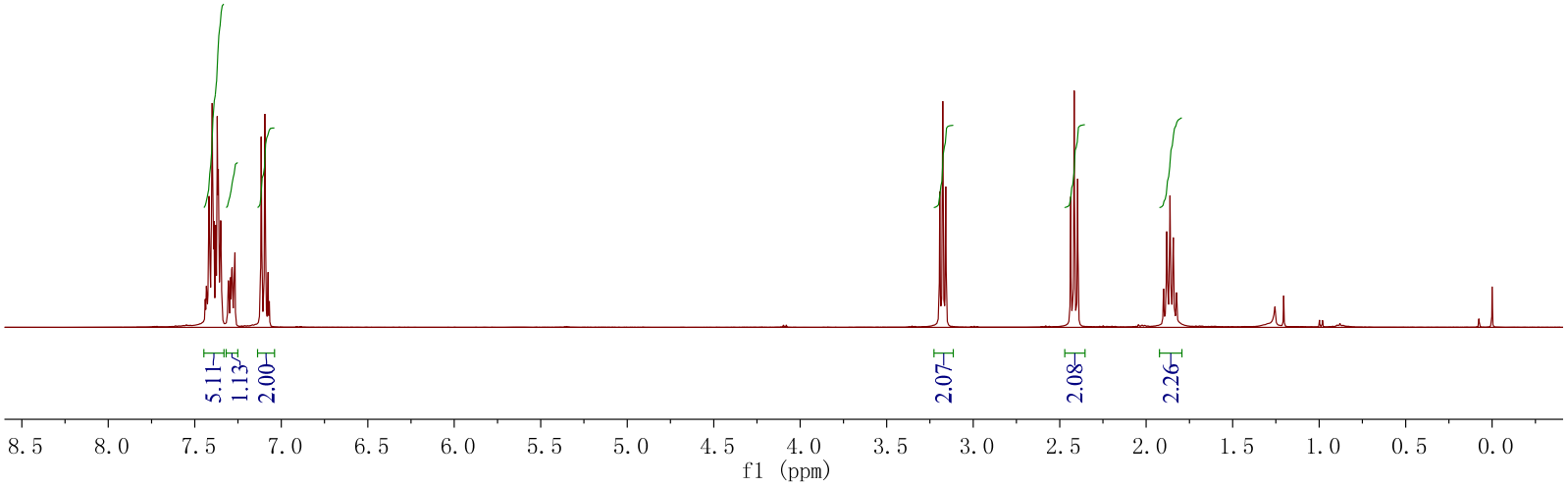
O
F

**3ea**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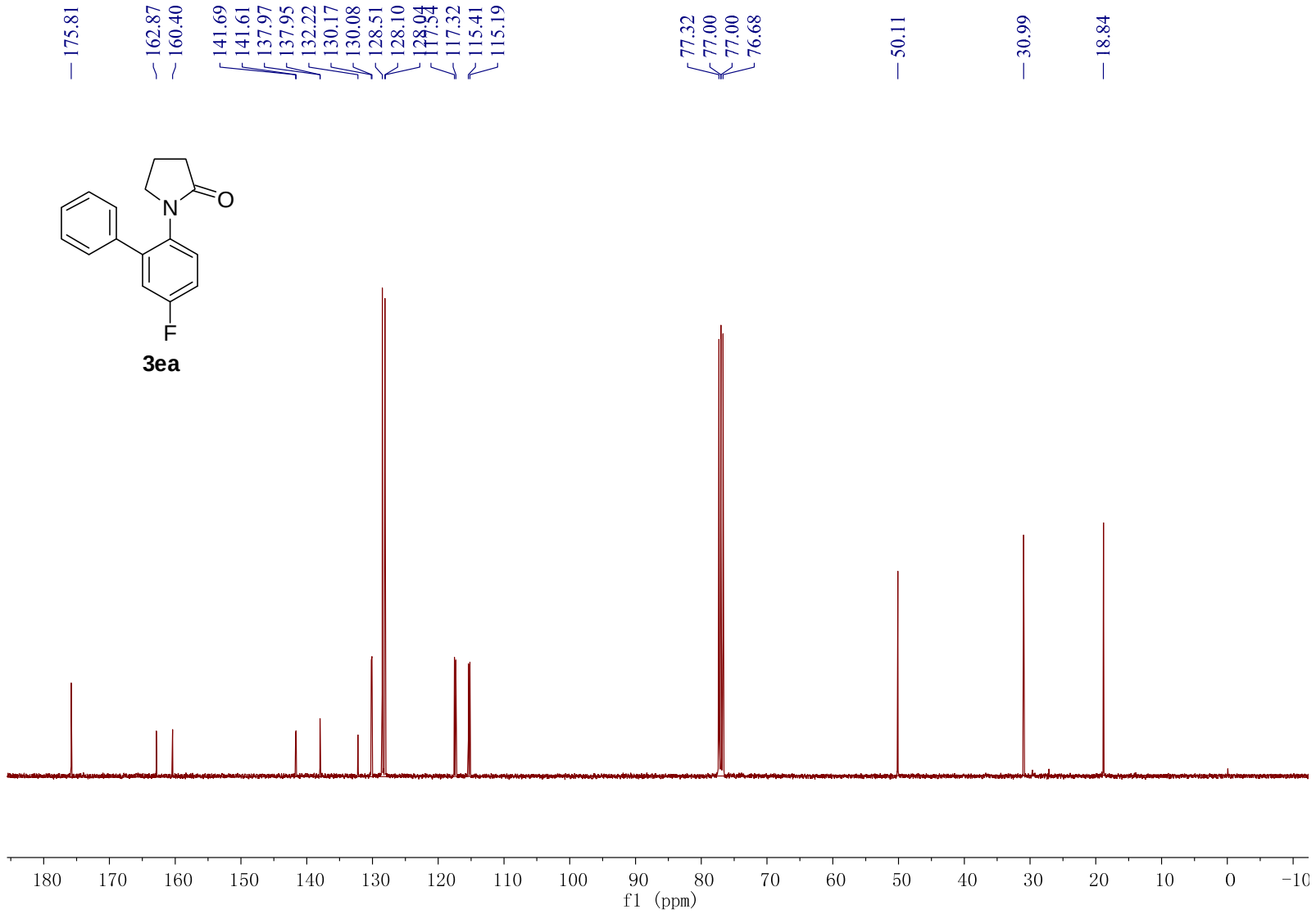
f1 (ppm)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F
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100
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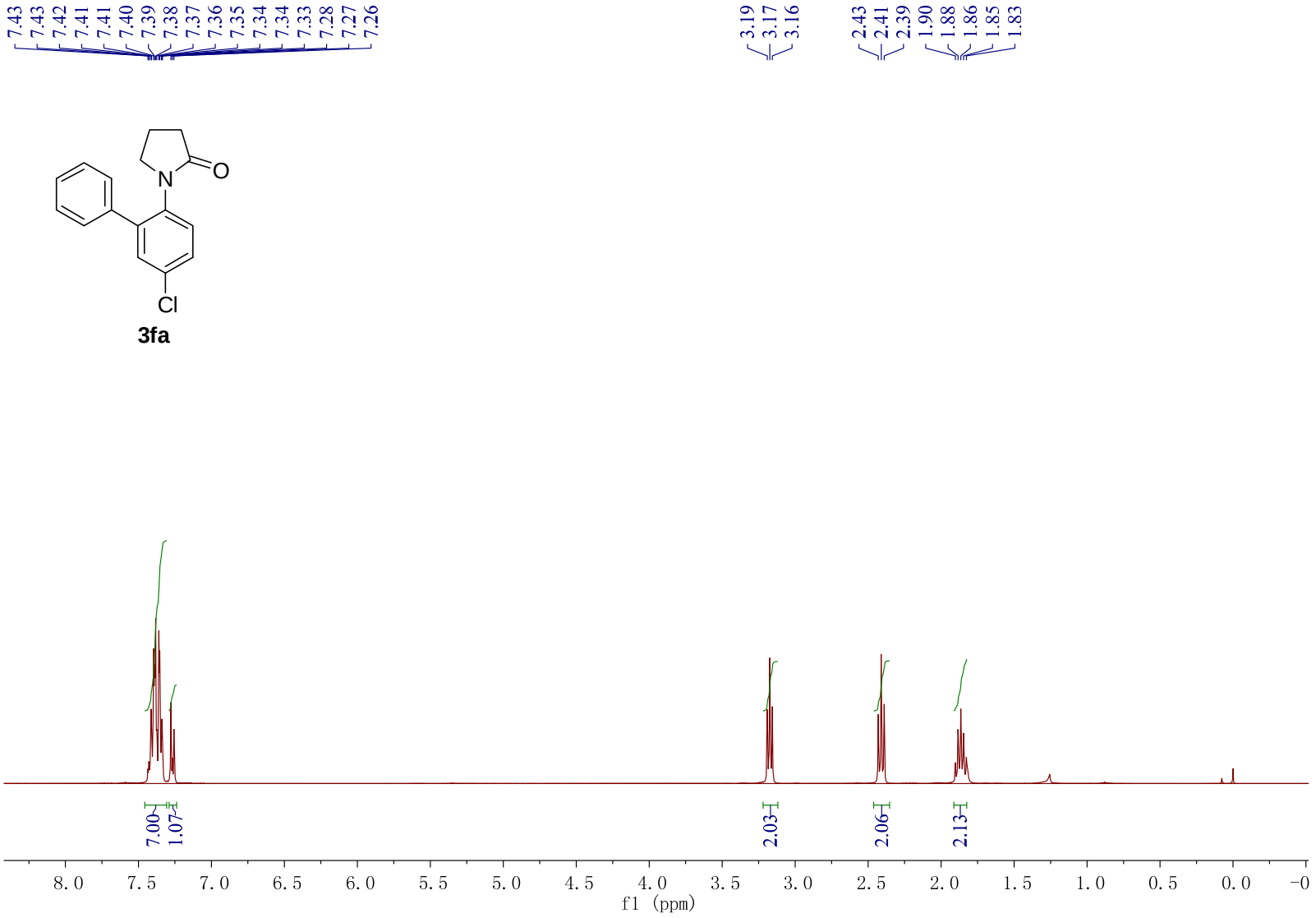
f1 (ppm)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1.85
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Cl
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f1 (ppm)

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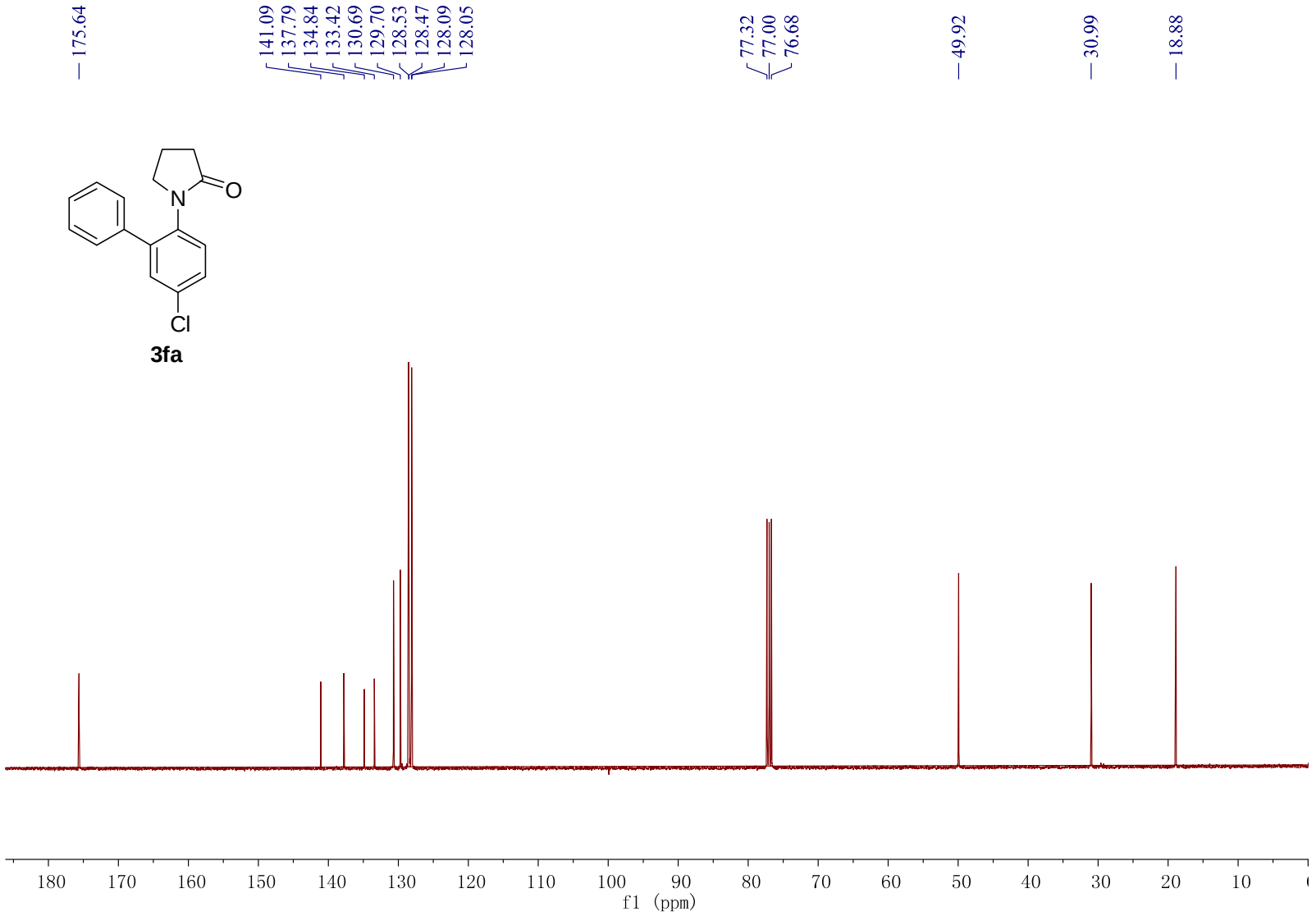
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77.32
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N
O
Cl
3fa
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60
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30
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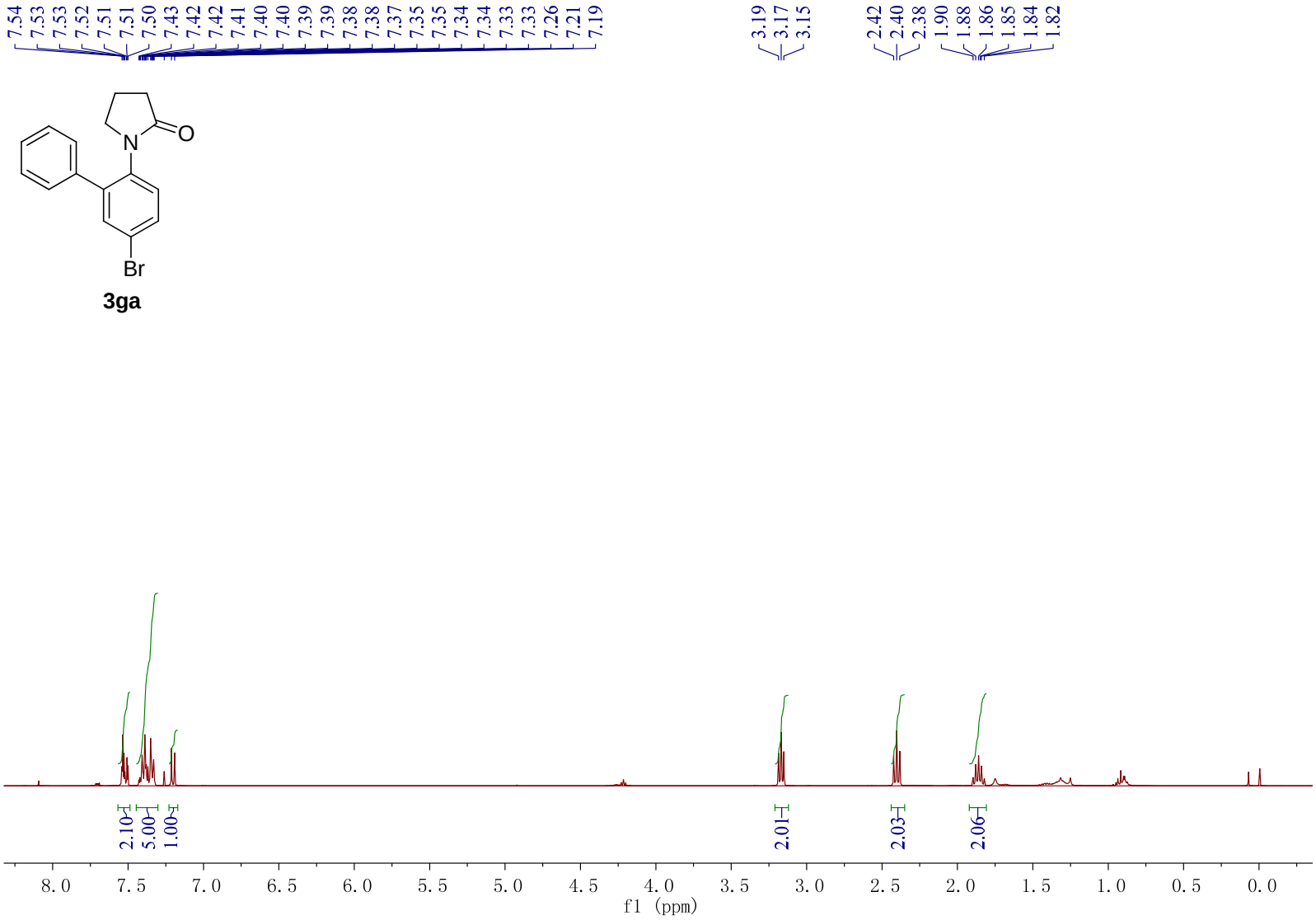
f1 (ppm)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2.40
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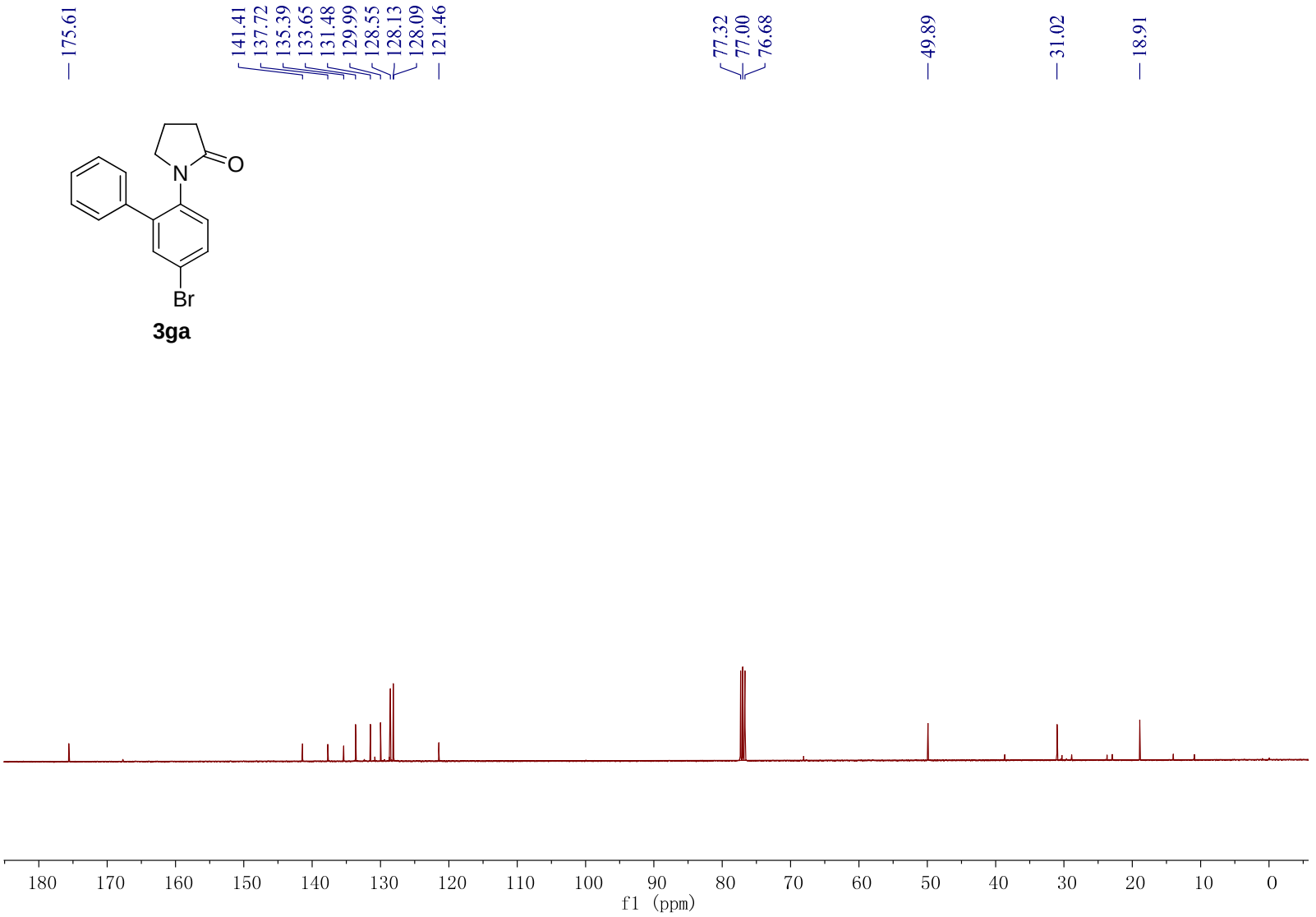
f1 (ppm)

**3ga**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76.68
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31.02
18.91
N
O
Br
3ga
180
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110
100
90
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70
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50
40
30
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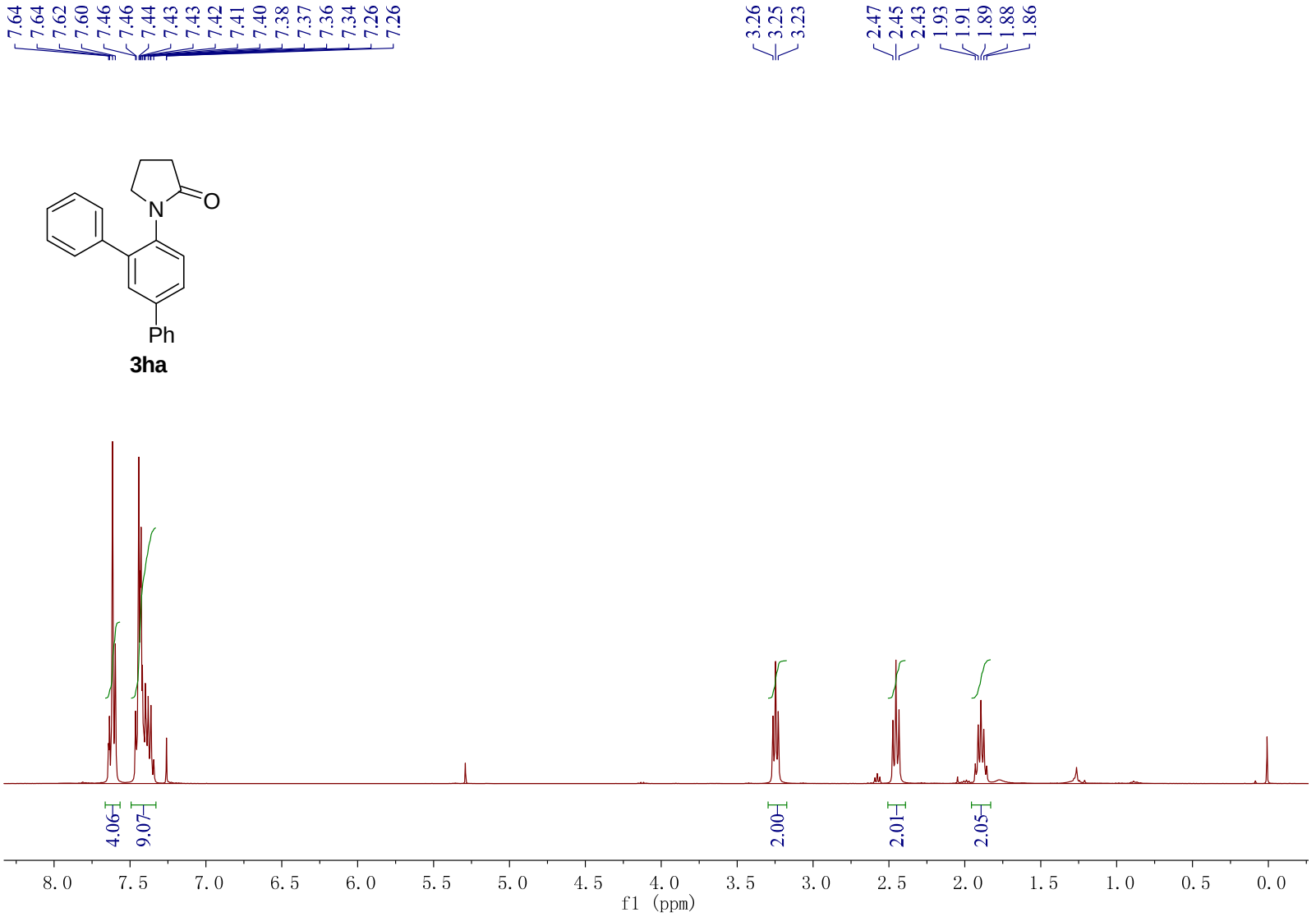
10
0
f1 (ppm)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7.26
7.26
3.26
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Ph
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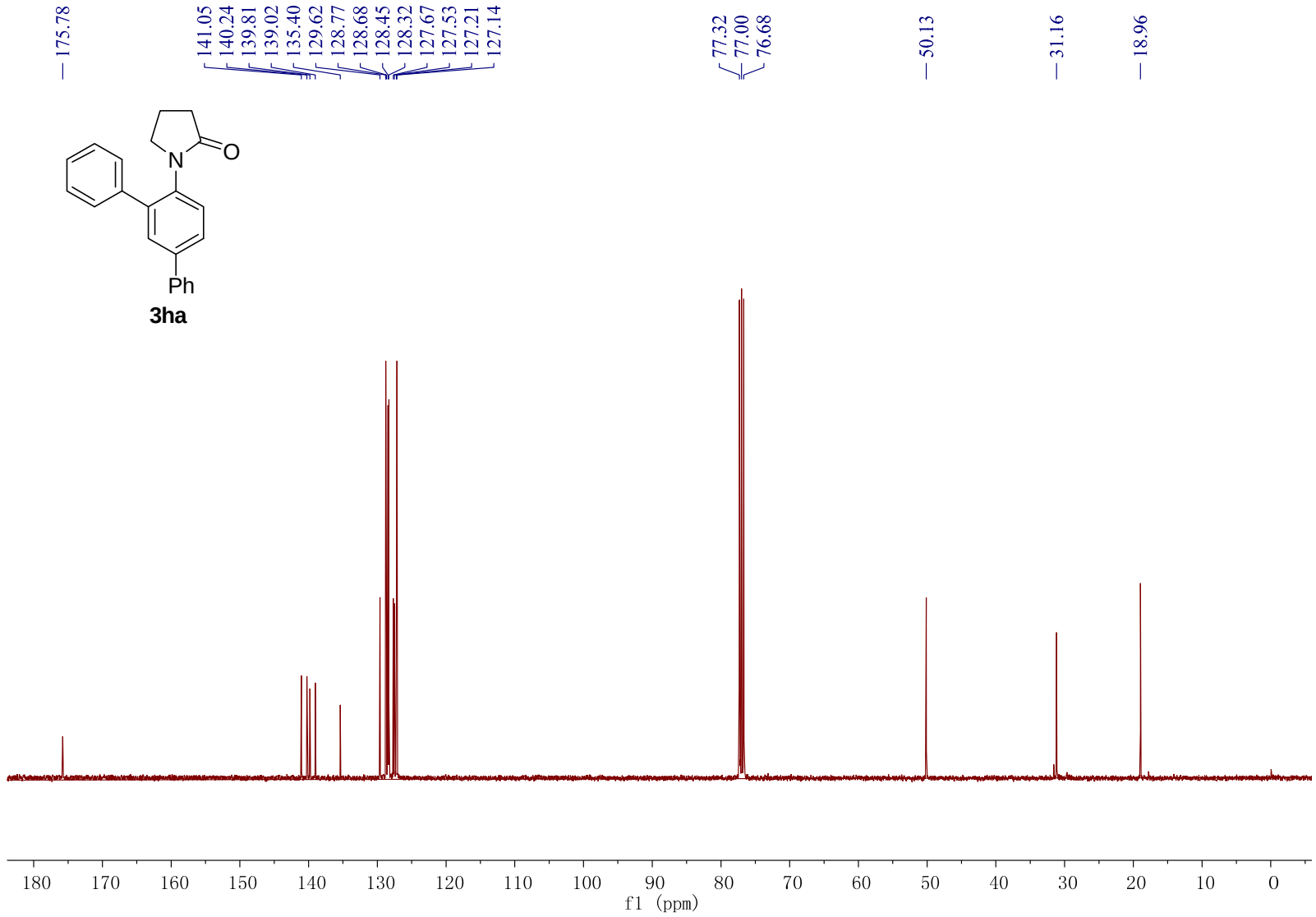
f1 (ppm)

**3ha**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127.14
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77.00
76.68
50.13
31.16
18.96
N
O
Ph
3ha
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100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.67
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7.36
7.36
7.26
7.26


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3.21
3.19


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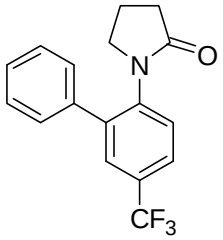
1.94
1.92
1.90
1.88
1.86


N
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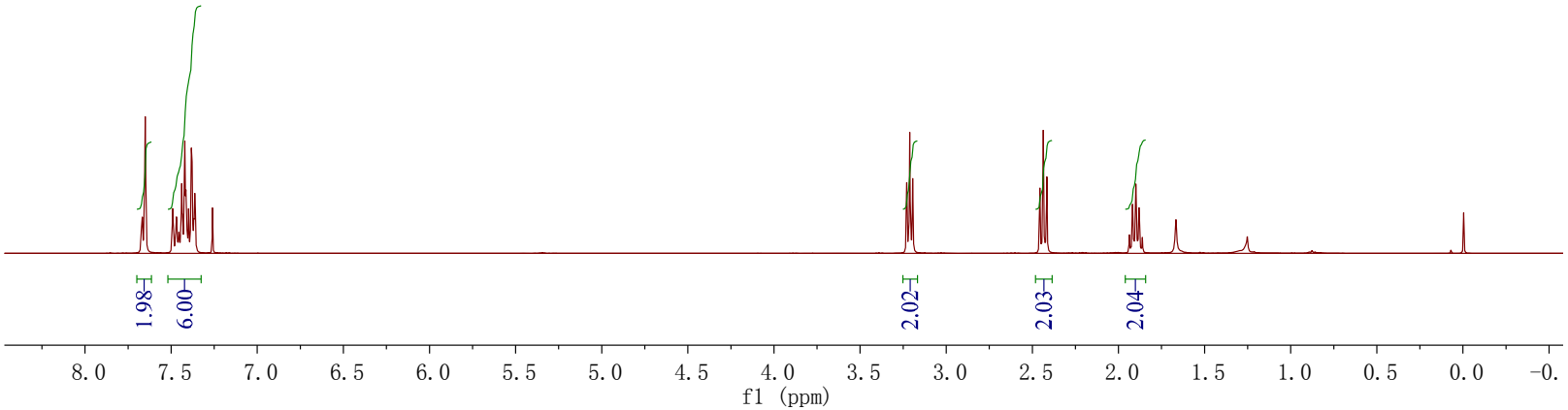
**3ia**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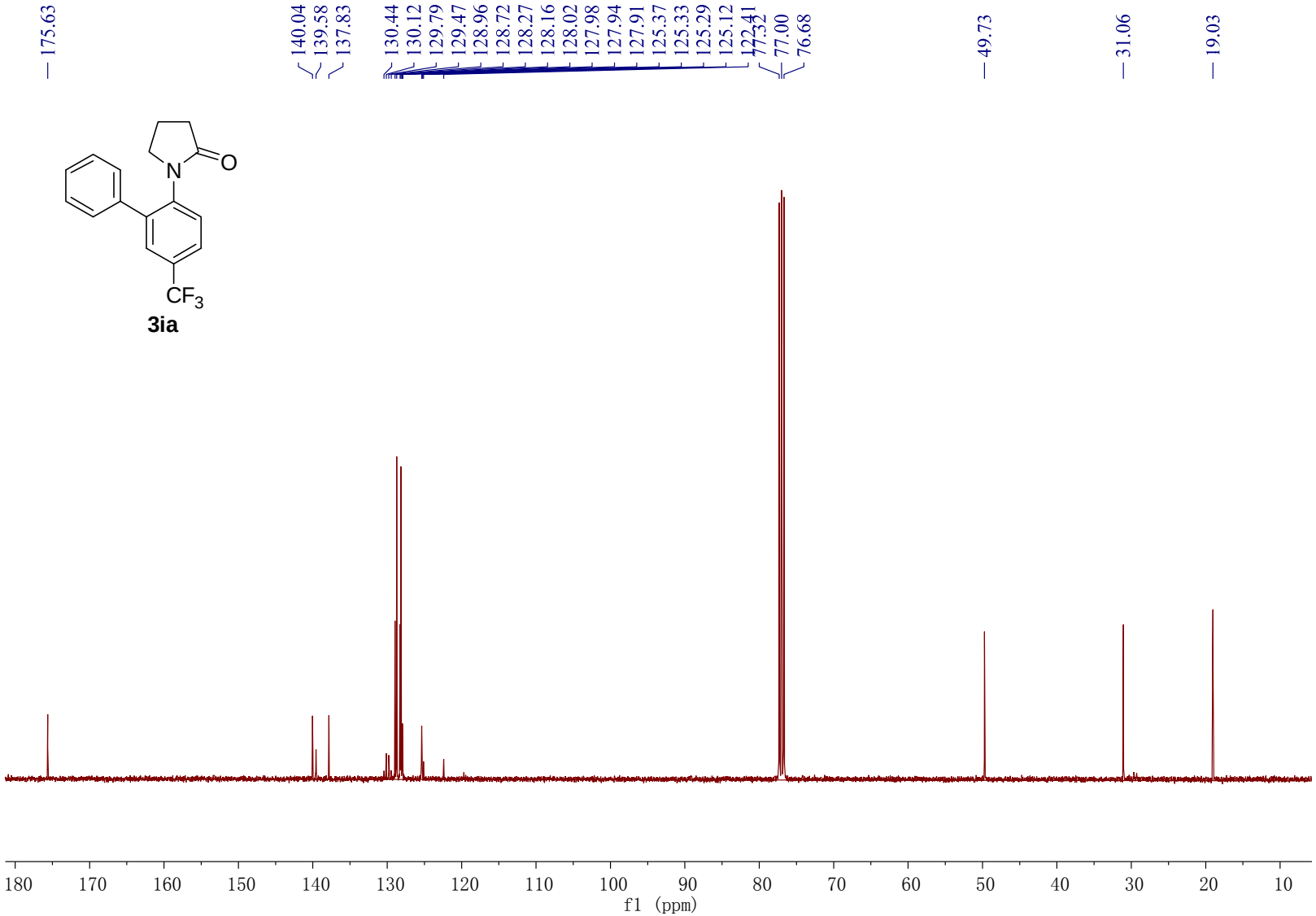
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127.91
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125.33
125.29
125.12
122.41
77.32
77.00
76.68
49.73
31.06
19.03
N
O
CF3
3ia
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60
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20
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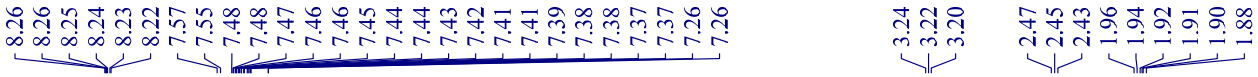
f1 (ppm)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7.26
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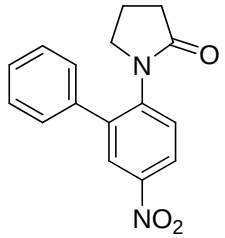
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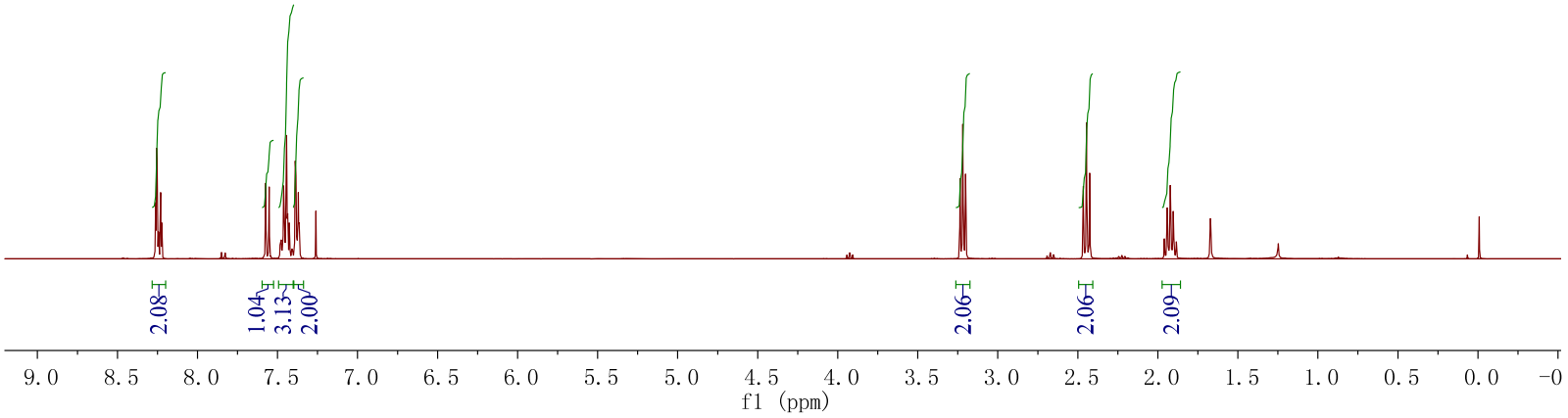
NO2

**3ja**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2.09
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8.0
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6.5
6.0
5.5
5.0
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2.5
2.0
1.5
1.0
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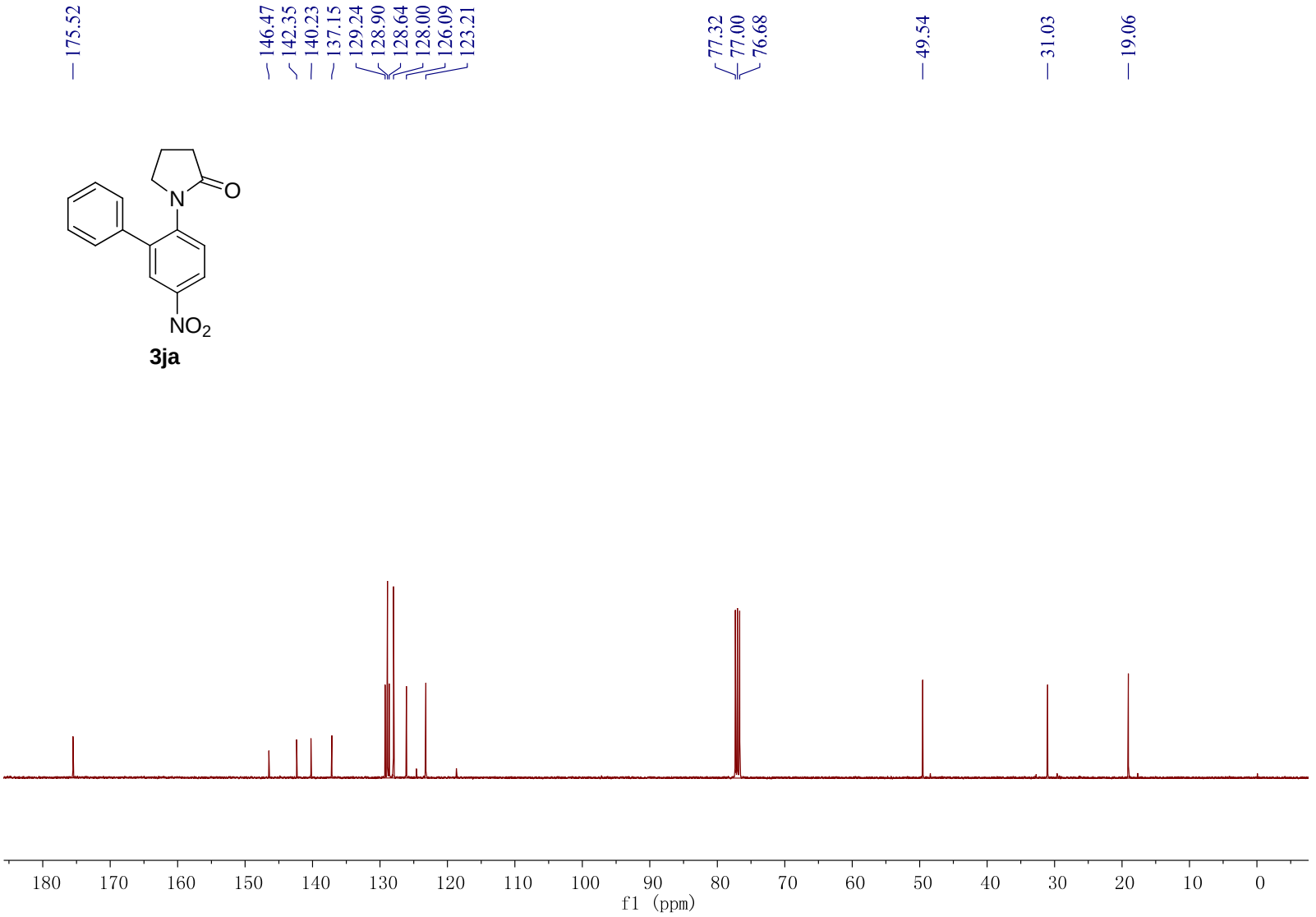
f1 (ppm)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128.90
128.64
128.00
126.09
123.21
77.32
77.00
76.68
49.54
31.03
19.06
O
N
NO2
3ja
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.41
7.40
7.40
7.39
7.38
7.37
7.36
7.35
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.27
7.26
7.25
7.21
7.19


3.23
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2.39
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1.90
1.89
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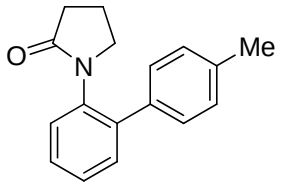
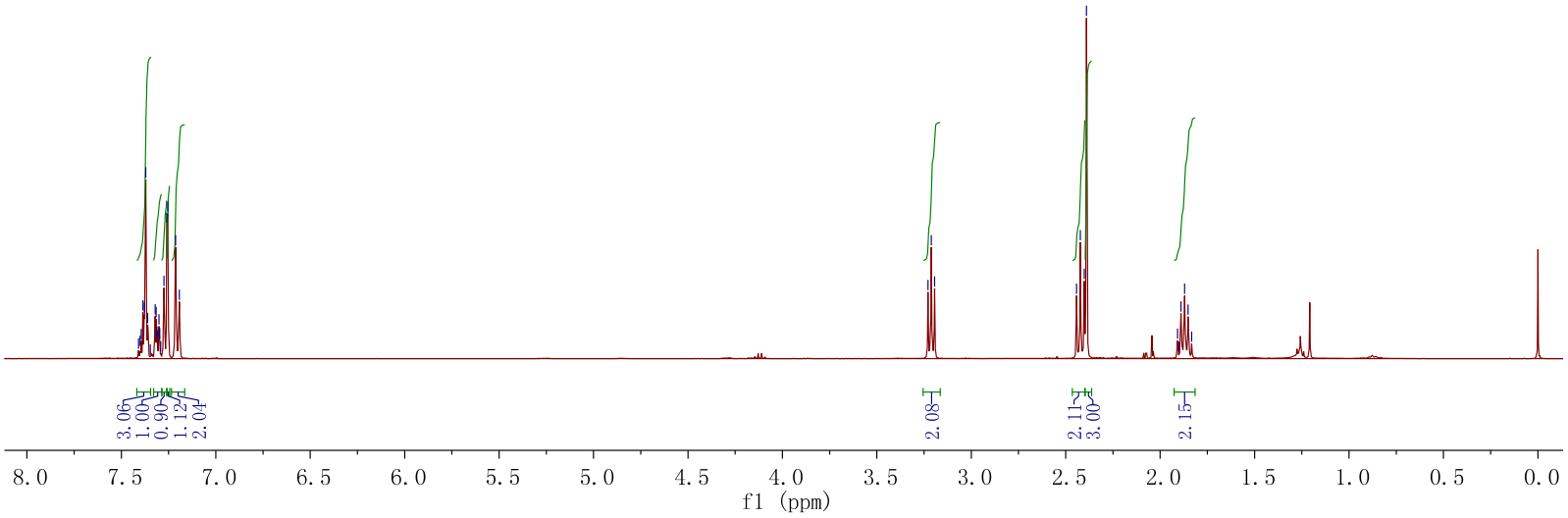
1.85
1.83


O
N
Me

**3ab**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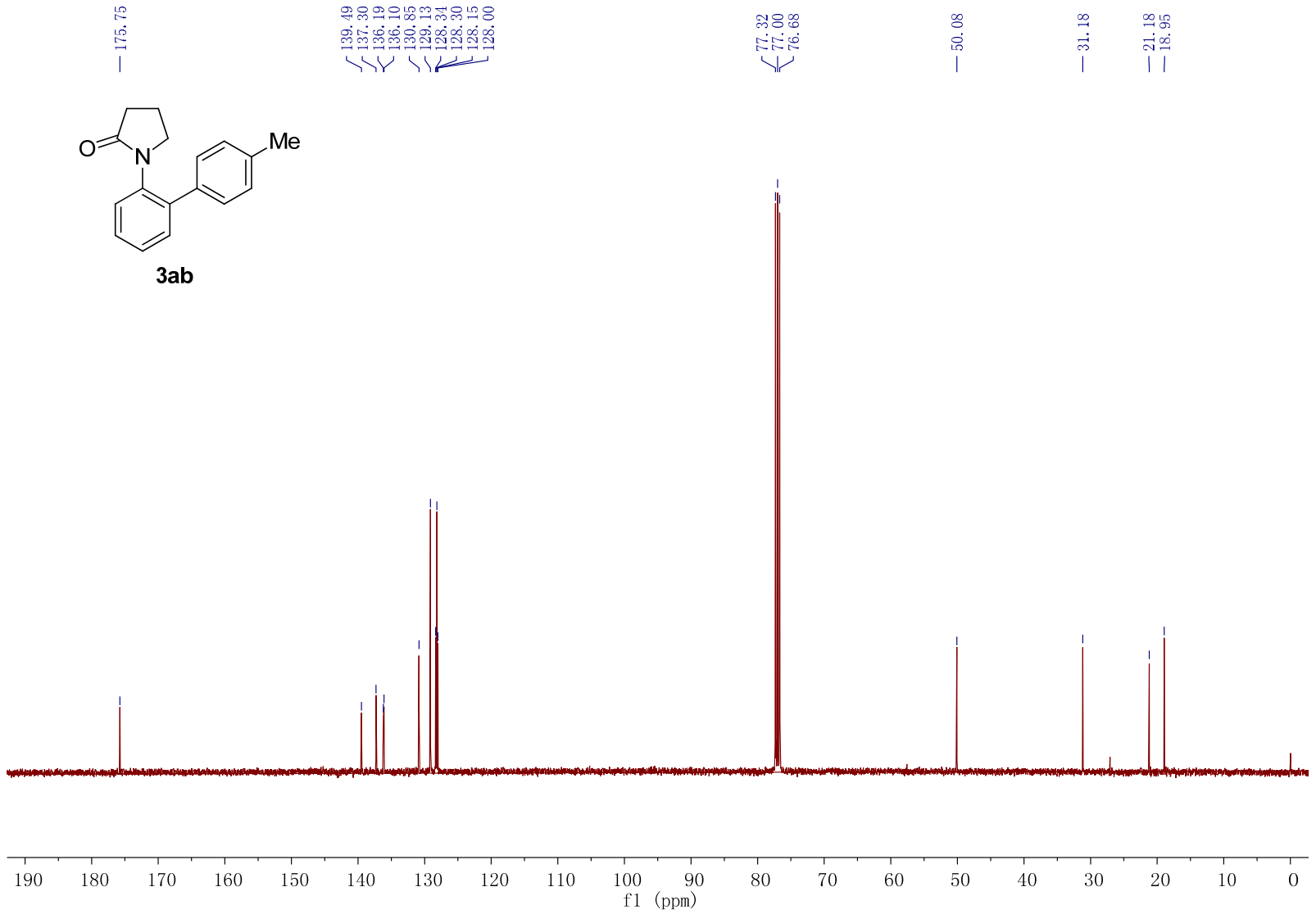
1.12
2.04
2.08
2.11
3.00
2.15
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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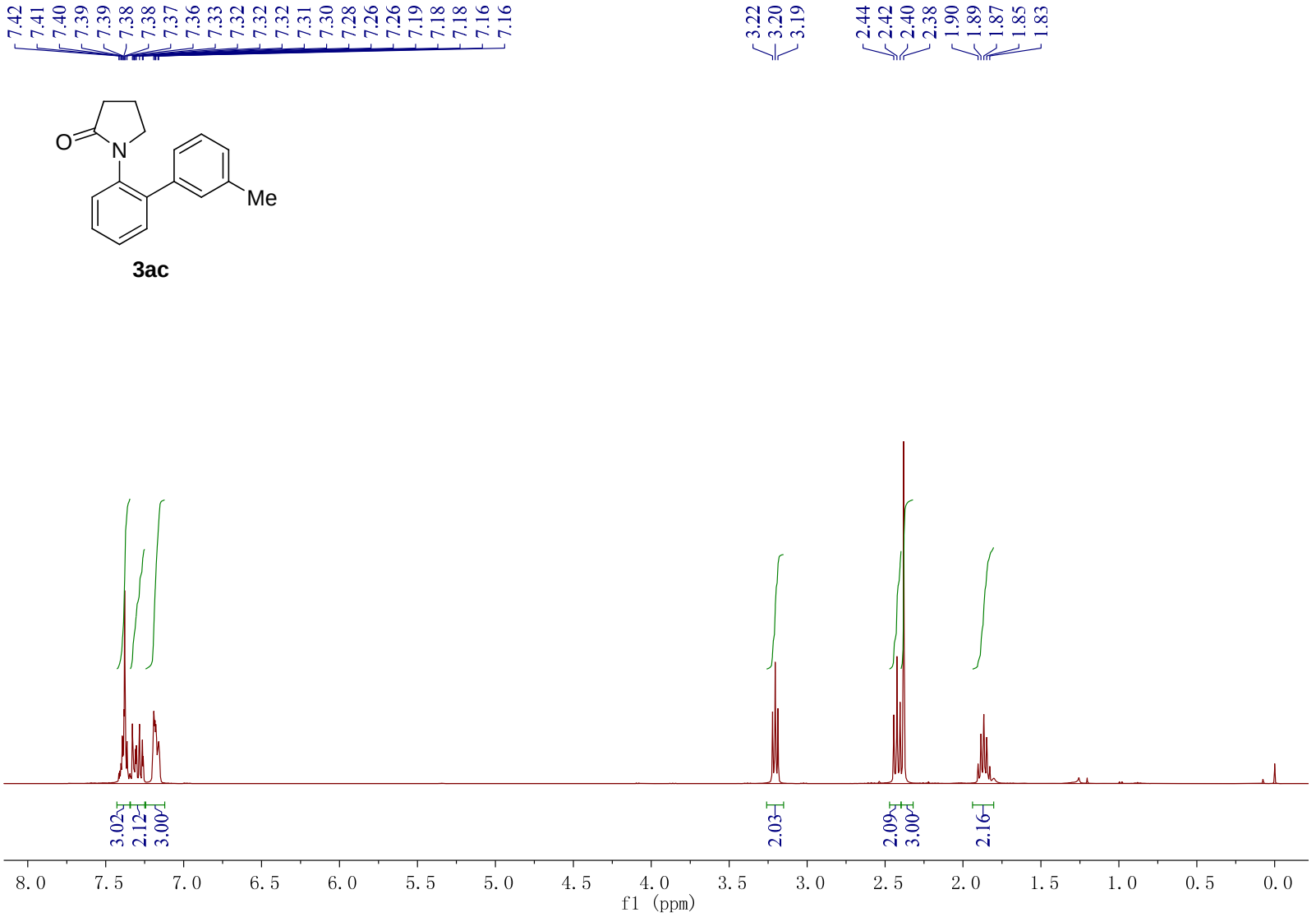
128.15
128.00
77.32
77.00
76.68
50.08
31.18
21.18
18.95
O
N
Me
3ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.32
7.32
7.32
7.31
7.30
7.28
7.26
7.26
7.19
7.18
7.18
7.16
7.16
3.22
3.20
3.19
2.44
2.42
2.40
2.38
1.90
1.89
1.87
1.85
1.83
O
N
Me
3ac
3.02
2.12
3.00
2.03
2.09
3.00
2.16
8.0
7.5
7.0
6.5
6.0
5.5
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1.0
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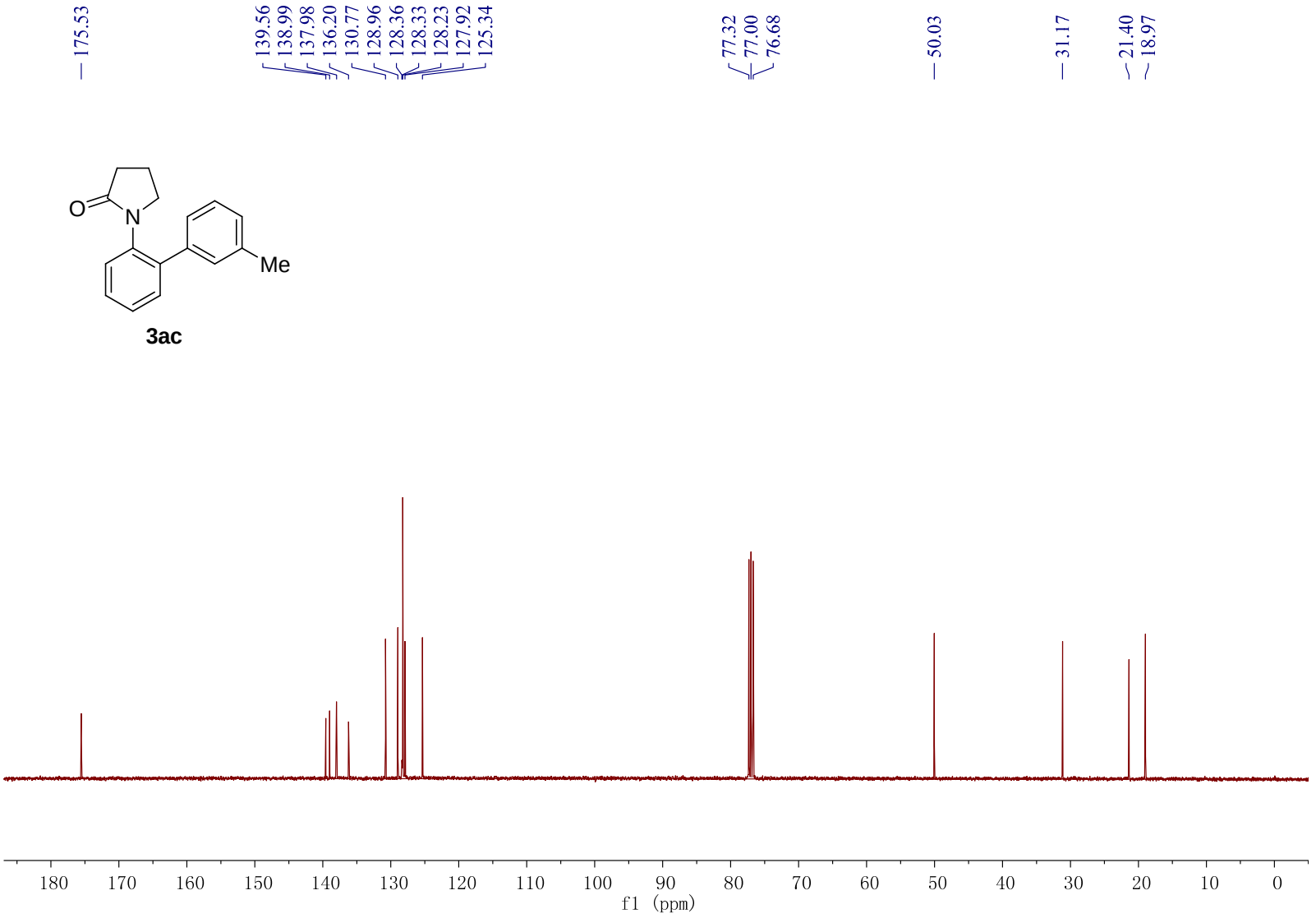
0.0
f1 (ppm)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128.23
127.92
125.34
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77.00
76.68
50.03
31.17
21.40
18.97
O
N
Me
3ac
180
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160
150
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130
120
110
100
90
80
70
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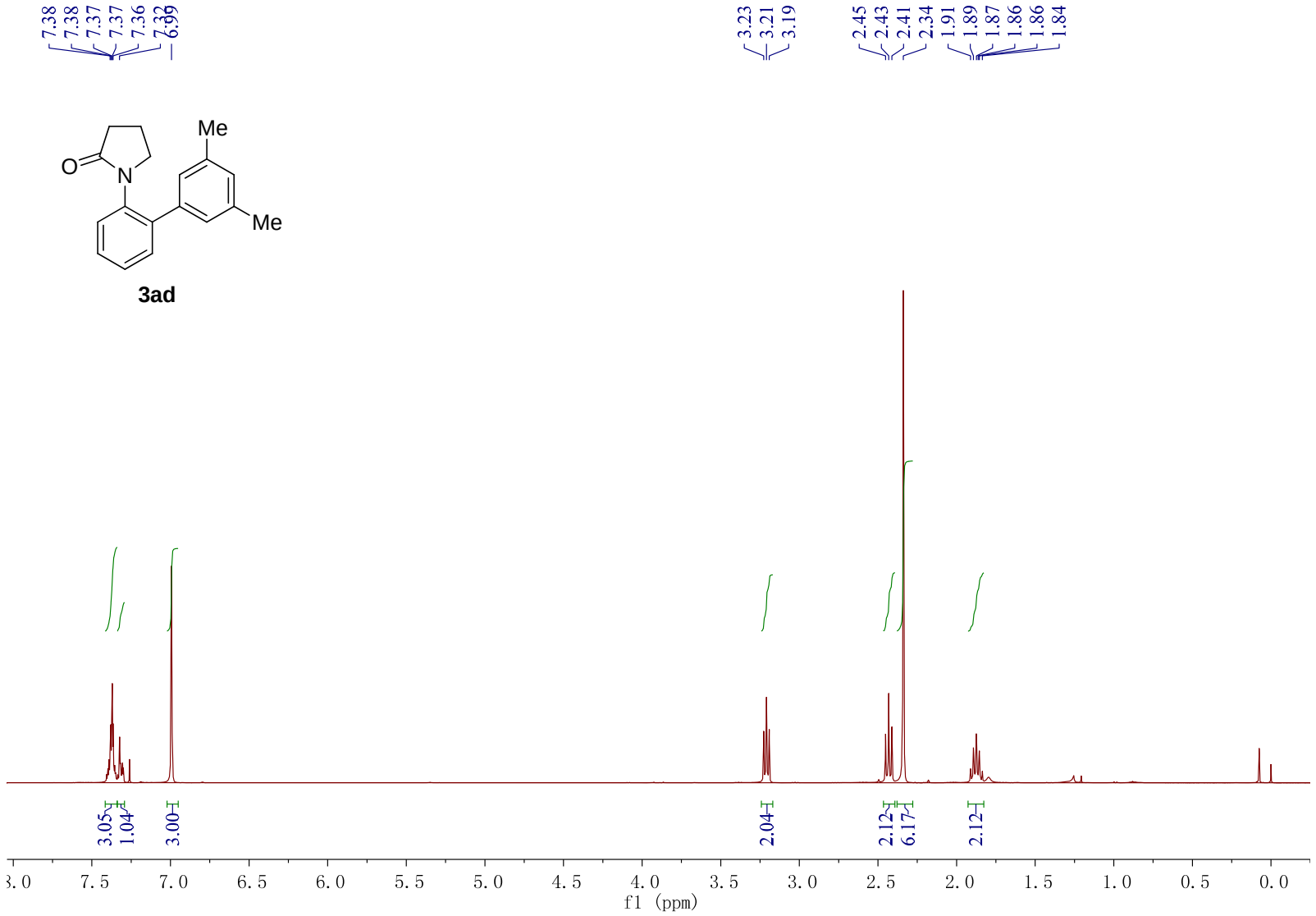
50
40
30
20
10
0
f1 (ppm)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7.36
7.32
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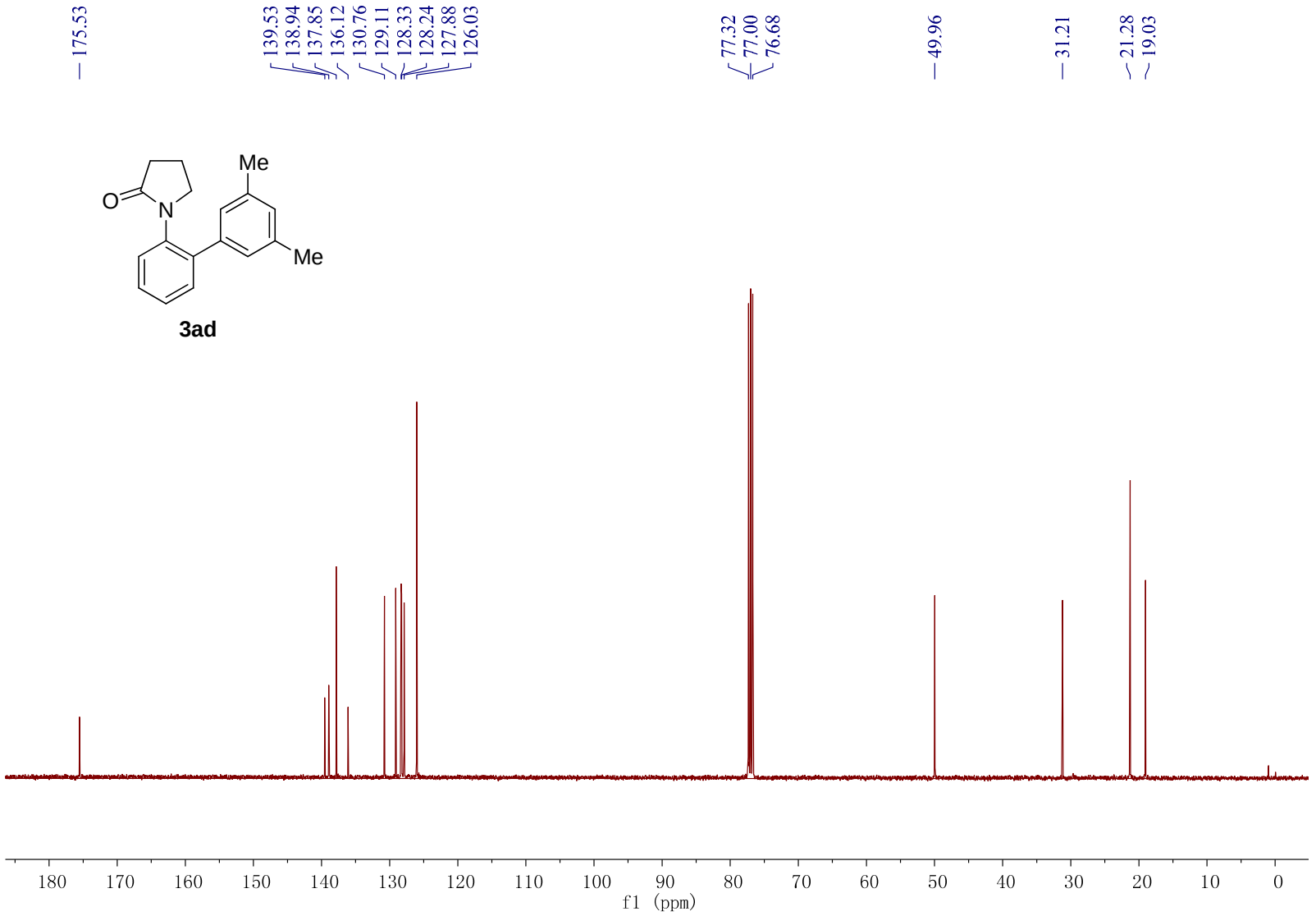
3.23
3.21
3.19
2.45
2.43
2.41
2.34
1.91
1.89
1.87
1.86
1.86
1.84
Me
Me
O
N
3ad
3.05
1.04
3.00
2.04
2.12
6.17
2.12
f1 (ppm)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127.88
126.03
77.32
77.00
76.68
49.96
31.21
21.28
19.03
O
N
Me
Me
3ad
180
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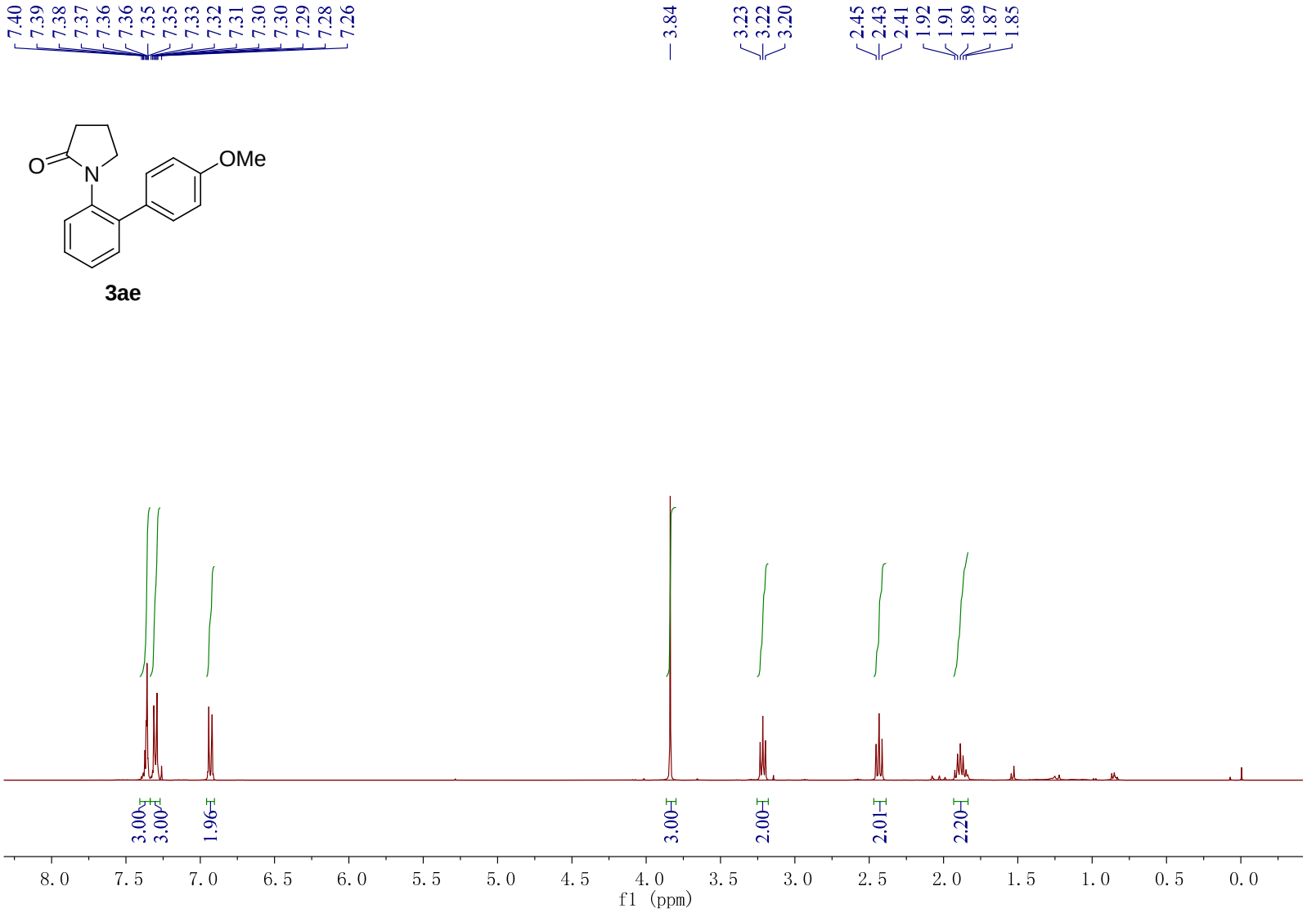
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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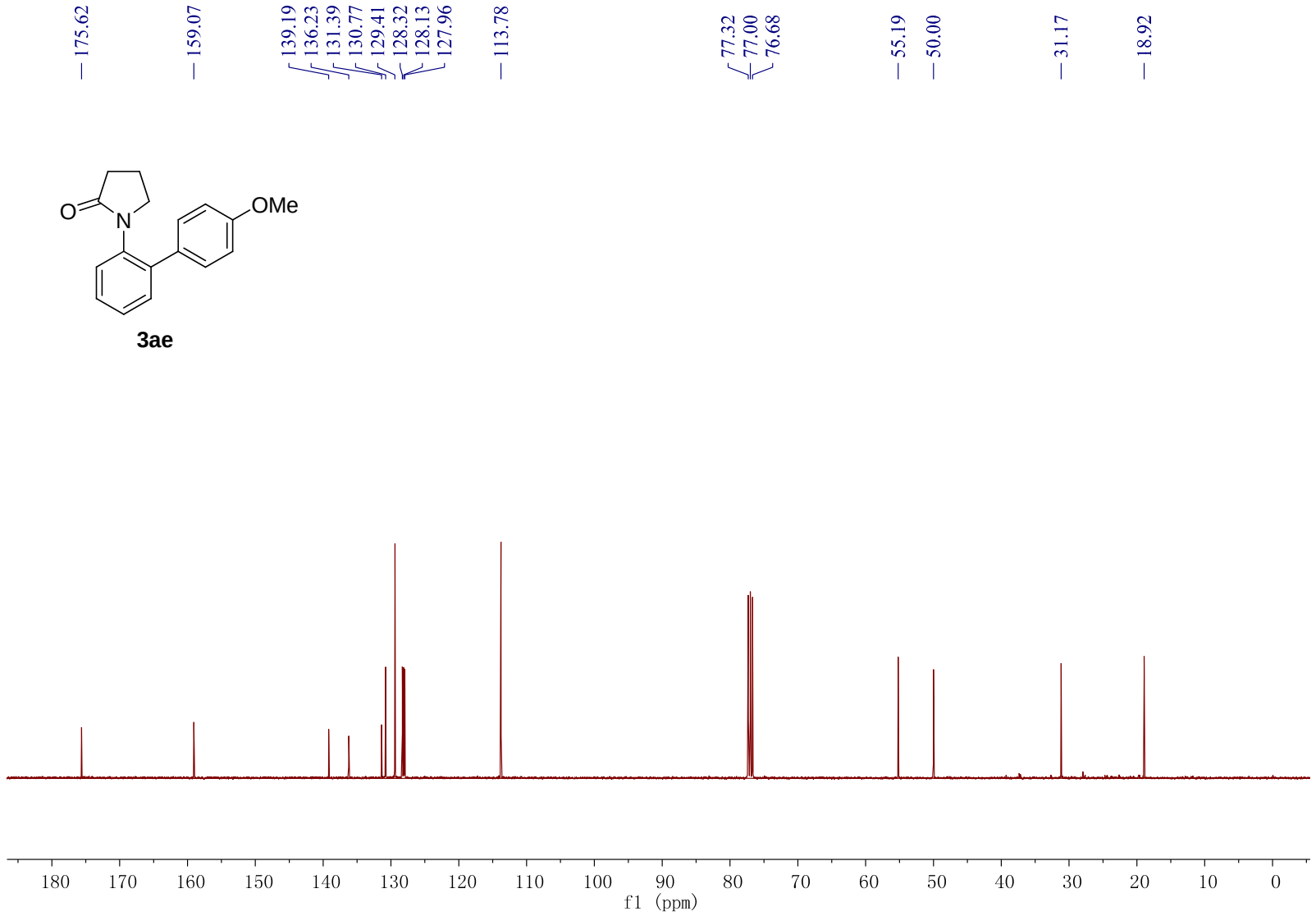
7.30
7.29
7.28
7.26
3.84
3.23
3.22
3.20
2.45
2.43
2.41
1.92
1.91
1.89
1.87
1.85
O
N
OMe
3ae
3.00
3.00
1.96
3.00
2.00
2.01
2.20
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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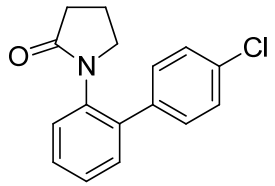
127.96
113.78
77.32
77.00
76.68
55.19
50.00
31.17
18.92
O
N
OMe
3ae
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

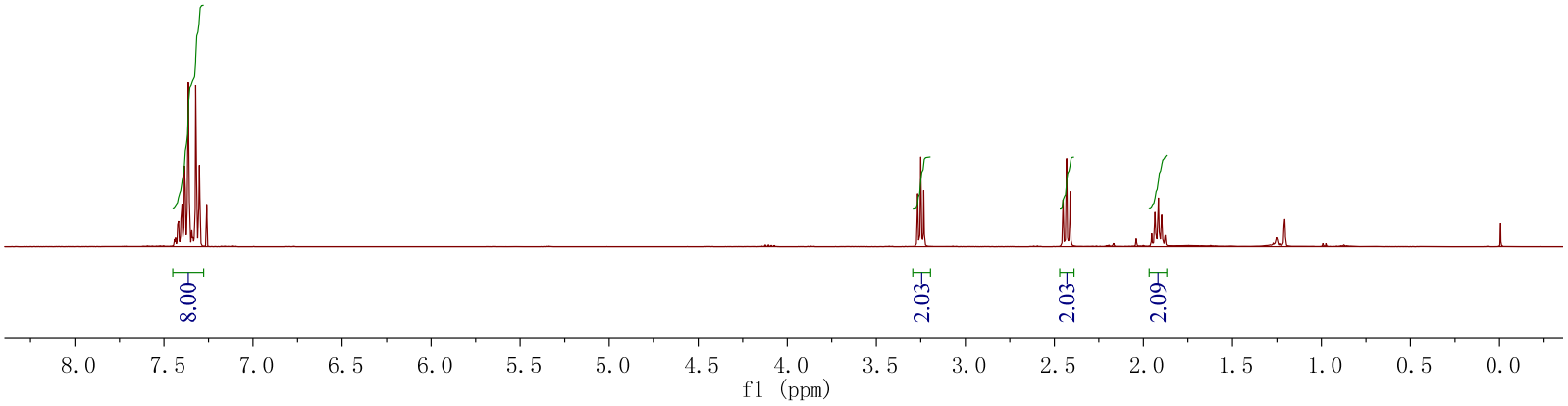

7.44
7.44
7.42
7.42
7.41
7.40
7.39
7.38
7.36
7.36
7.34
7.34
7.33
7.32
7.32
7.30
7.26


3.27
3.25
3.23


1.95
1.93
1.92
1.90
1.88


O
N
Cl

**3af**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2.03
2.09
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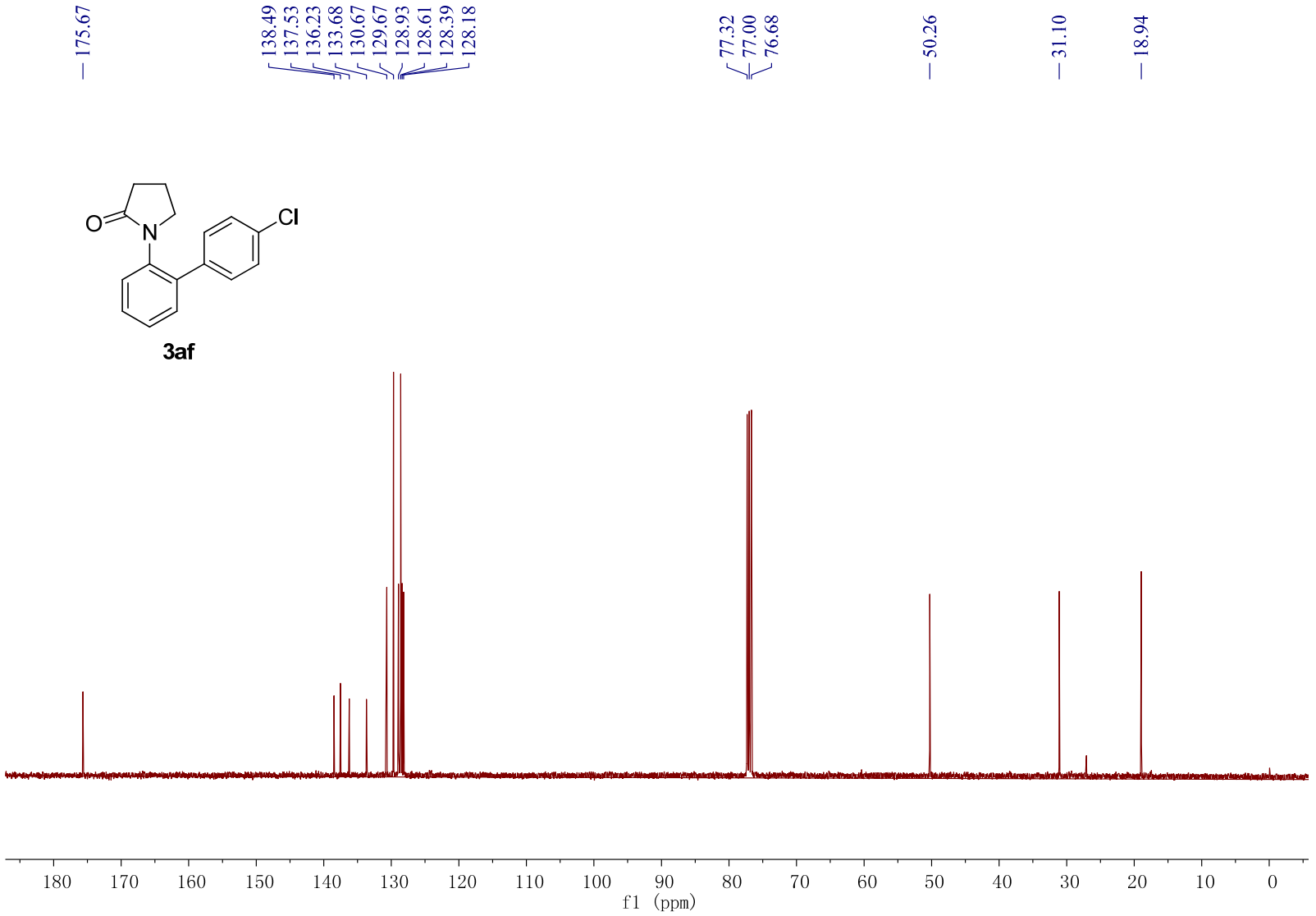
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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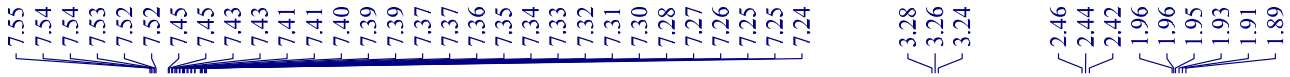
128.61
128.39
128.18
77.32
77.00
76.68
50.26
31.10
18.94
O
N
Cl
3af
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.43
7.41
7.41
7.40
7.39
7.39
7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.30
7.28
7.27
7.26
7.25
7.25
7.24
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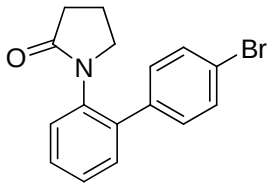
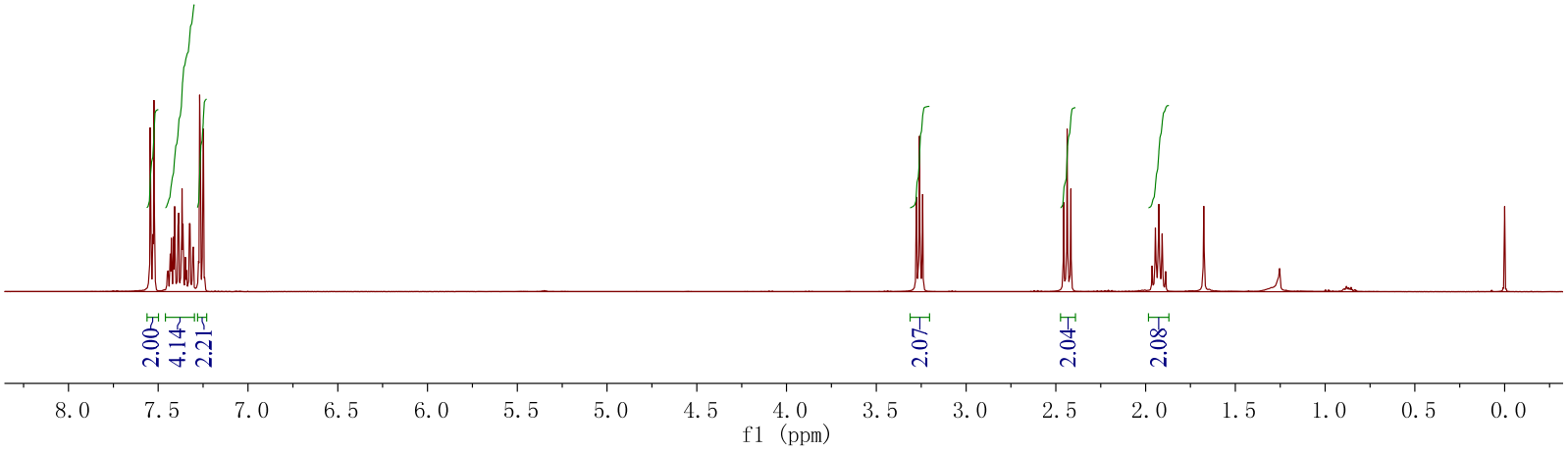
1.96
1.96
1.95
1.93
1.91
1.89


O
N
Br

**3ag**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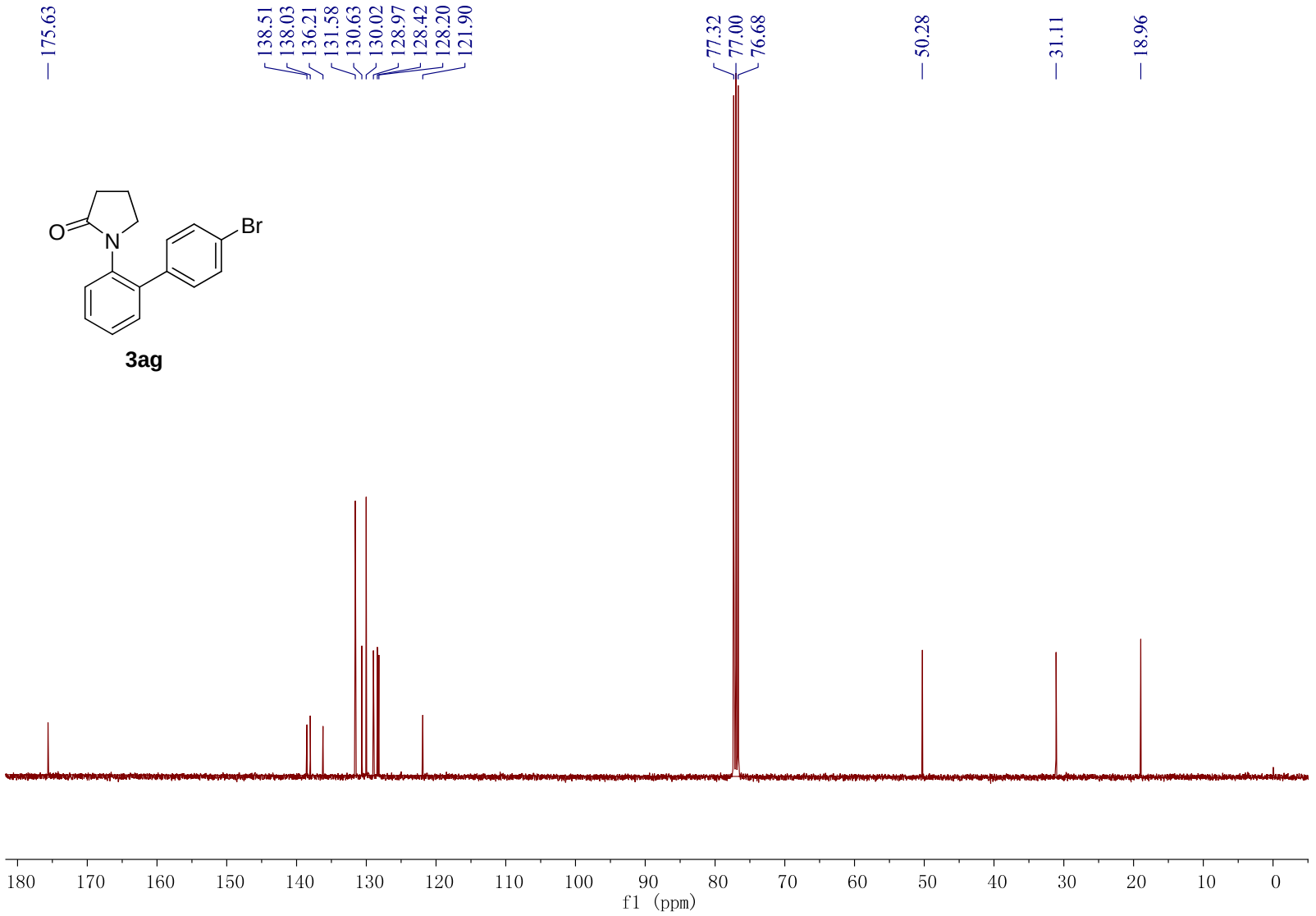
2.04
2.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.58
130.63
130.02
128.97
128.42
128.20
121.90
77.32
77.00
76.68
50.28
31.11
18.96
O
N
Br
3ag
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.54
7.54
7.53
7.50
7.50
7.50
7.48
7.48
7.48
7.44
7.43
7.43
7.42
7.41
7.41
7.39
7.39
7.38
7.38
7.37
7.34
7.34
7.33
7.32
7.32
7.32
7.31
7.29
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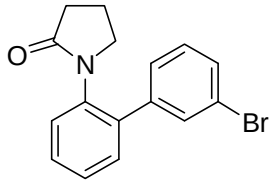
2.42
1.97
1.95
1.93
1.91
1.89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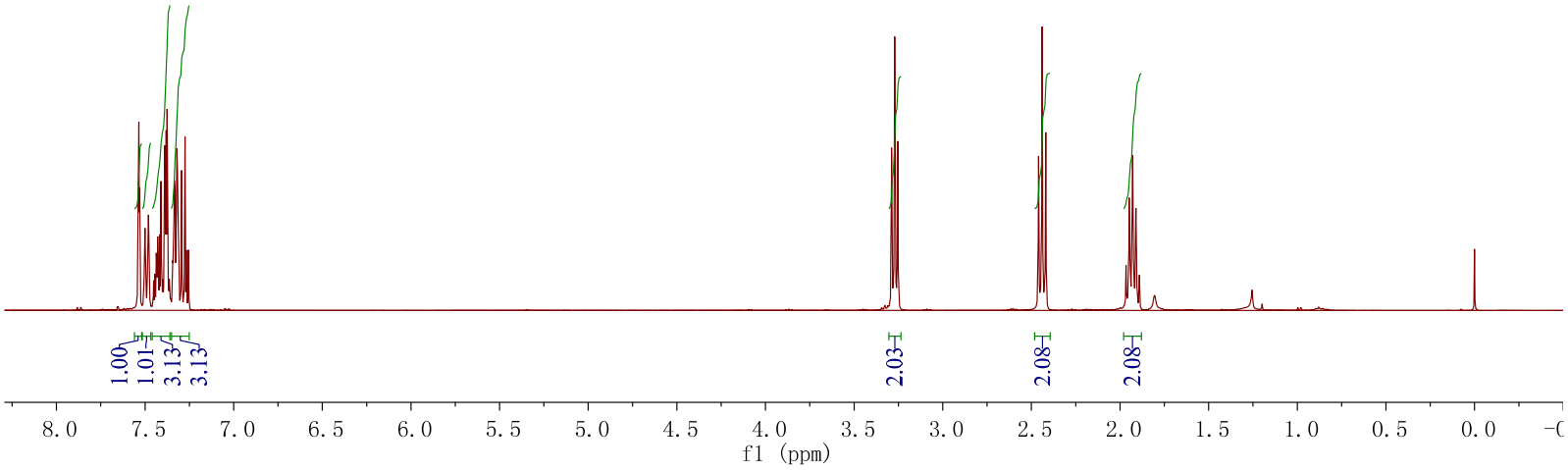
N
Br

**3ah**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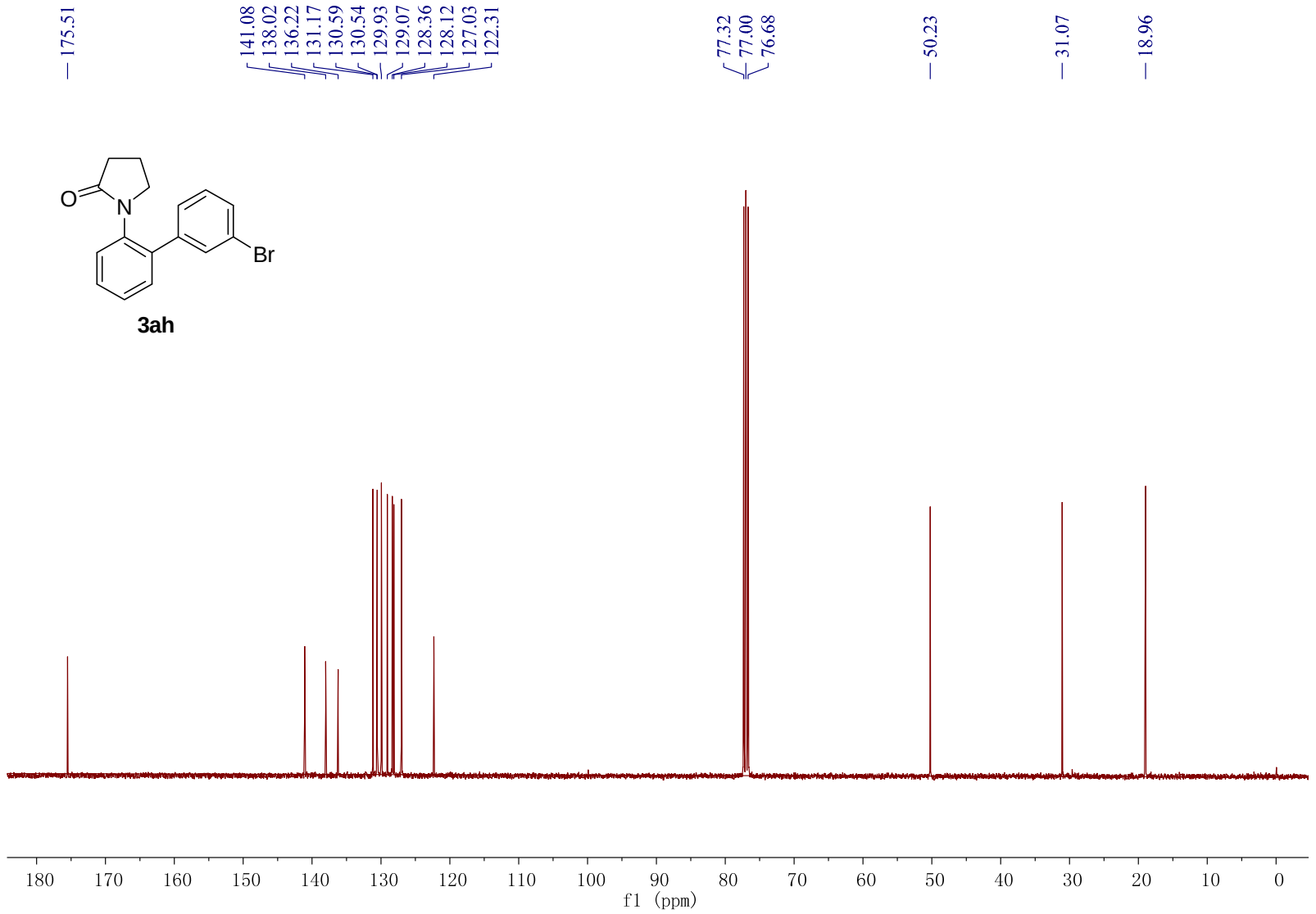
2.03
2.08
2.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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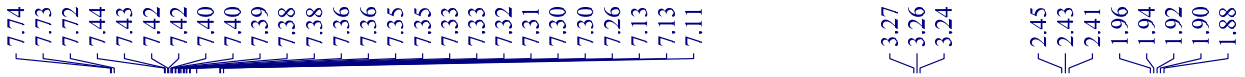
136.22
131.17
130.59
130.54
129.93
129.07
128.36
128.12
127.03
122.31
77.32
77.00
76.68
50.23
31.07
18.96
O
N
Br
3ah
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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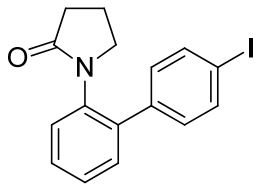
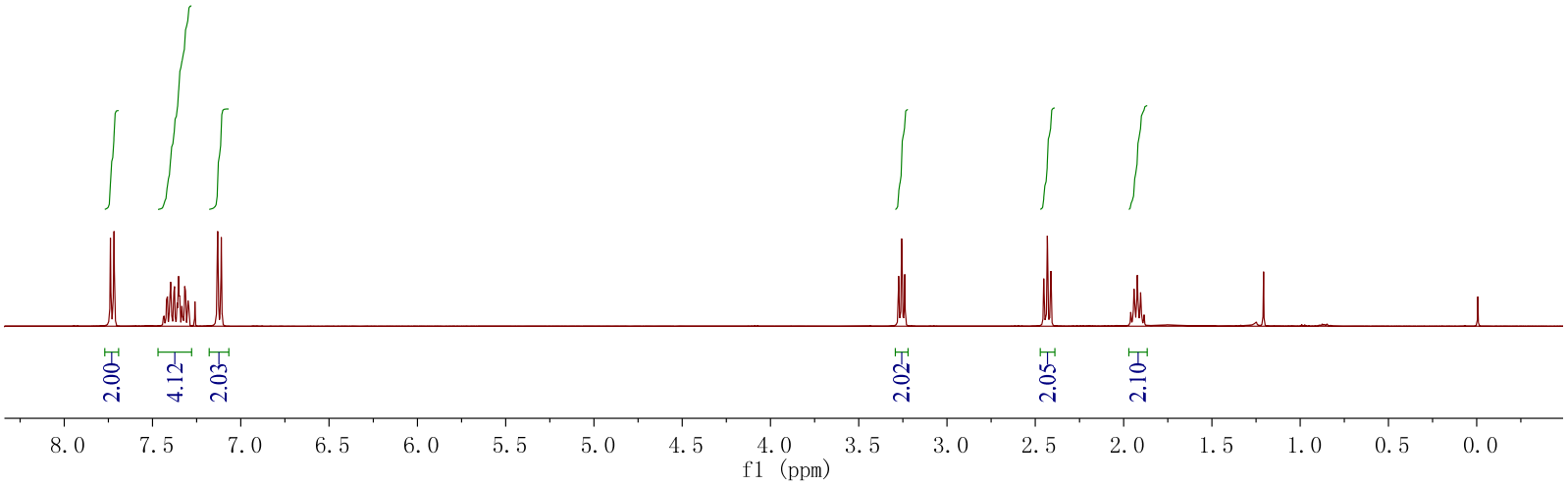
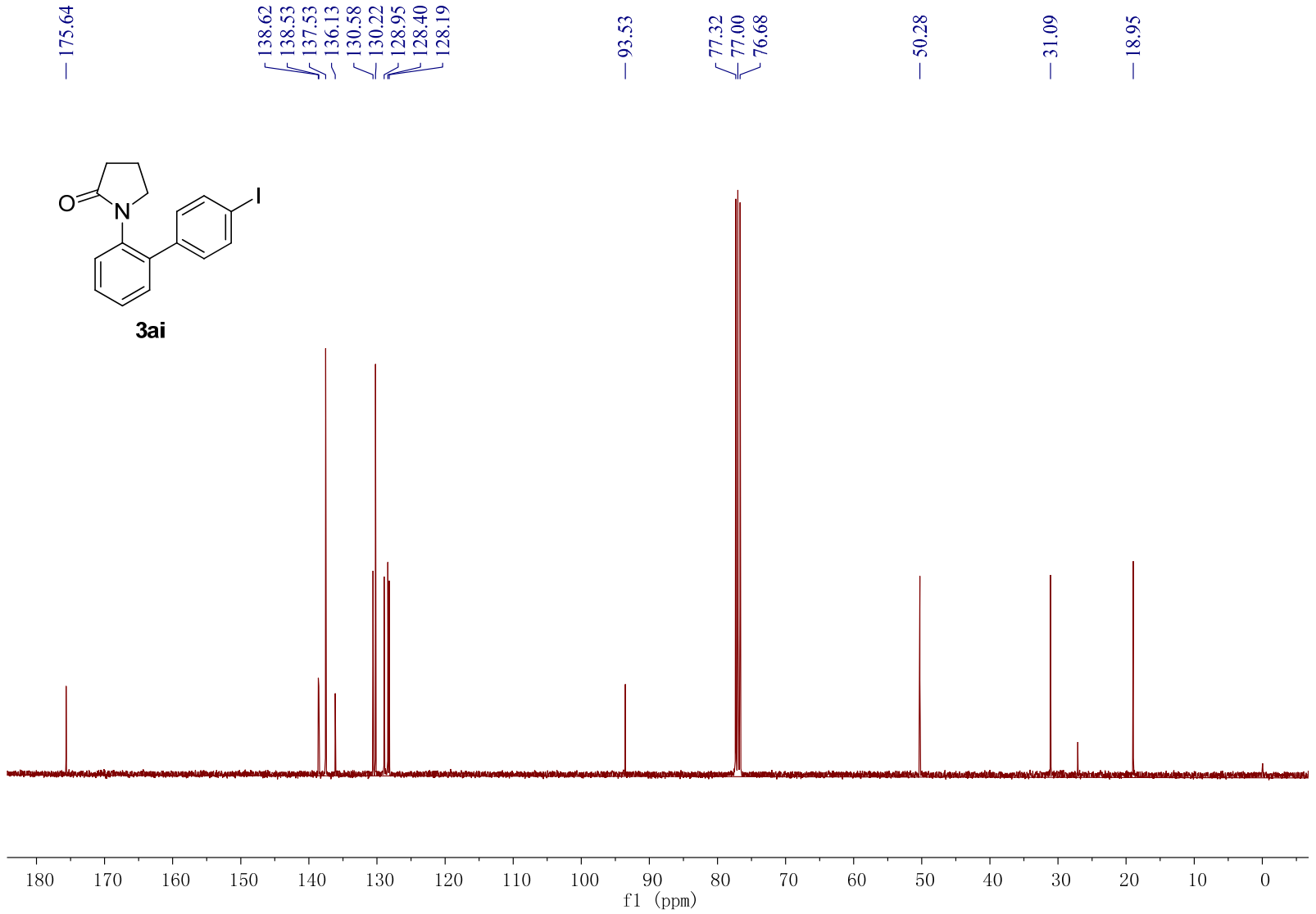
7.38
7.38
7.36
7.36
7.35
7.35
7.33
7.33
7.32
7.31
7.30
7.30
7.26
7.13
7.13
7.11
3.27
3.26
3.24
2.45
2.43
2.41
1.96
1.94
1.92
1.90
1.88


O
N
I

**3ai**


2.00
4.12
2.03
2.02
2.05
2.10
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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136.13
130.58
130.22
128.95
128.40
128.19
93.53
77.32
77.00
76.68
50.28
31.09
18.95
O
N
I
3ai
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.68
7.66
7.52
7.50
7.48
7.48
7.46
7.46
7.44
7.44
7.43
7.43
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.35
7.35
7.33
7.33
7.33
7.27
3.30
3.28
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2.40
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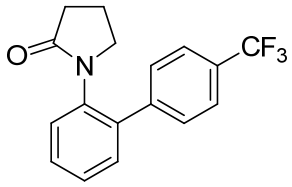
1.95
1.94
1.93
1.92
1.91
1.90
1.88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CF3

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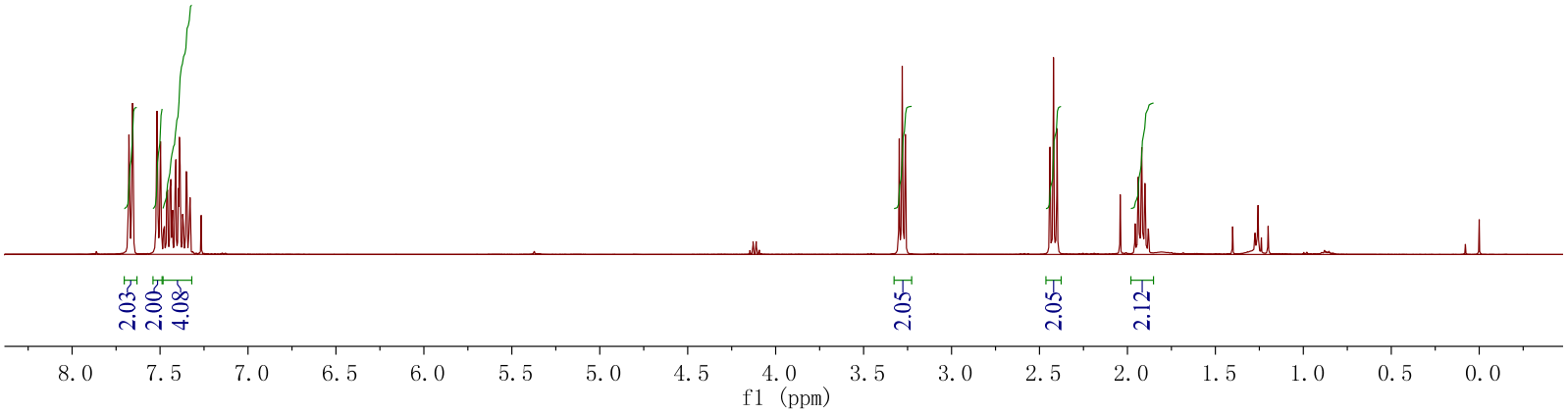
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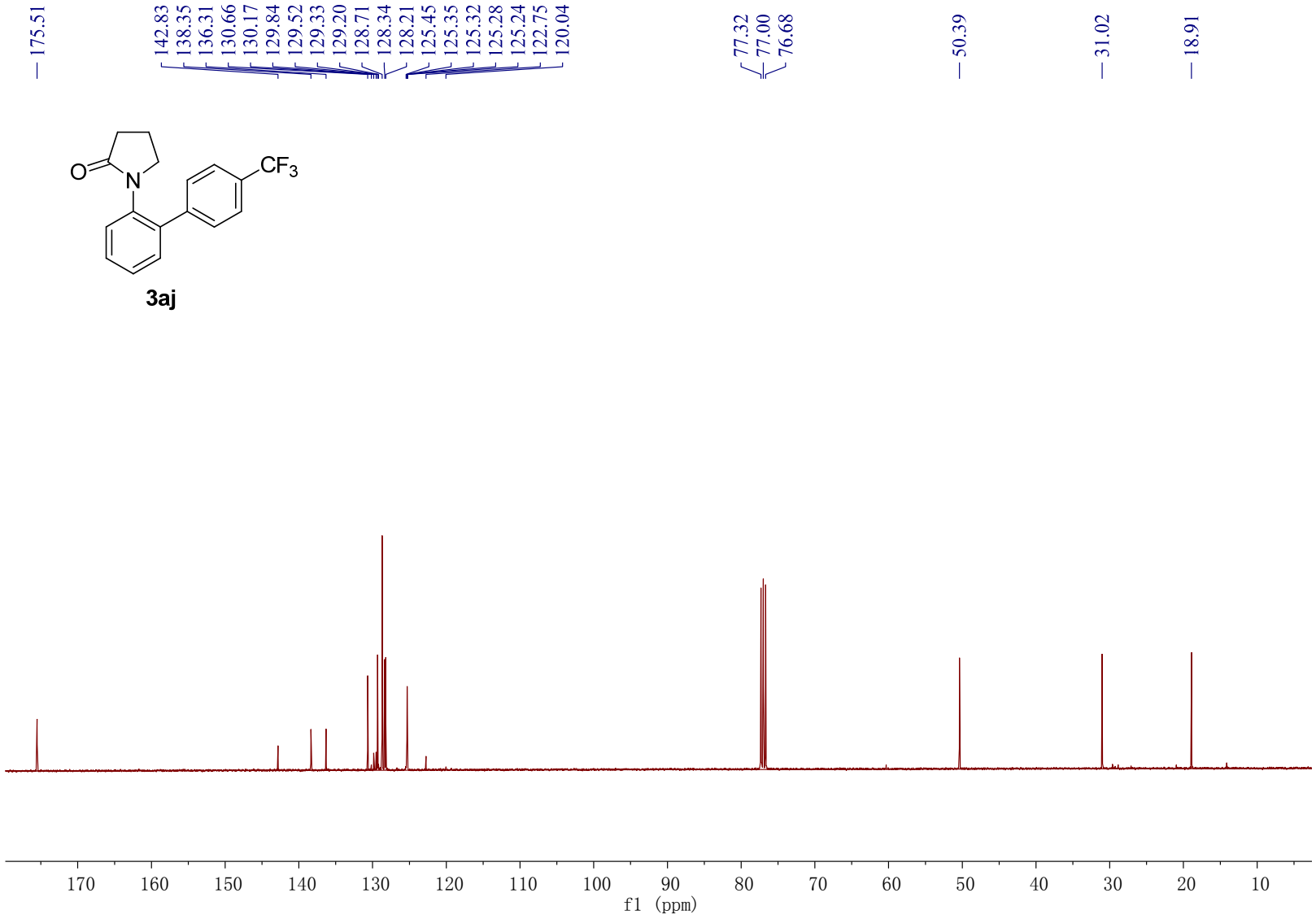
4.08
2.05
2.05
2.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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142.83
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136.31
130.66
130.17
129.84
129.52
129.33
129.20
128.71
128.34
128.21
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125.35
125.32
125.28
125.24
122.75
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77.32
77.00
76.68
50.39
31.02
18.91
O
N
CF3
3aj
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.09
8.08
8.07
8.07
8.06
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.40
7.40
7.39
7.39
7.34
7.32
7.32
7.26
4.42
4.41
4.39
4.37
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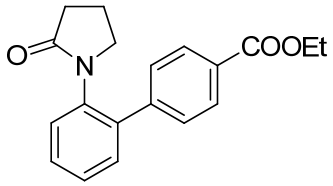
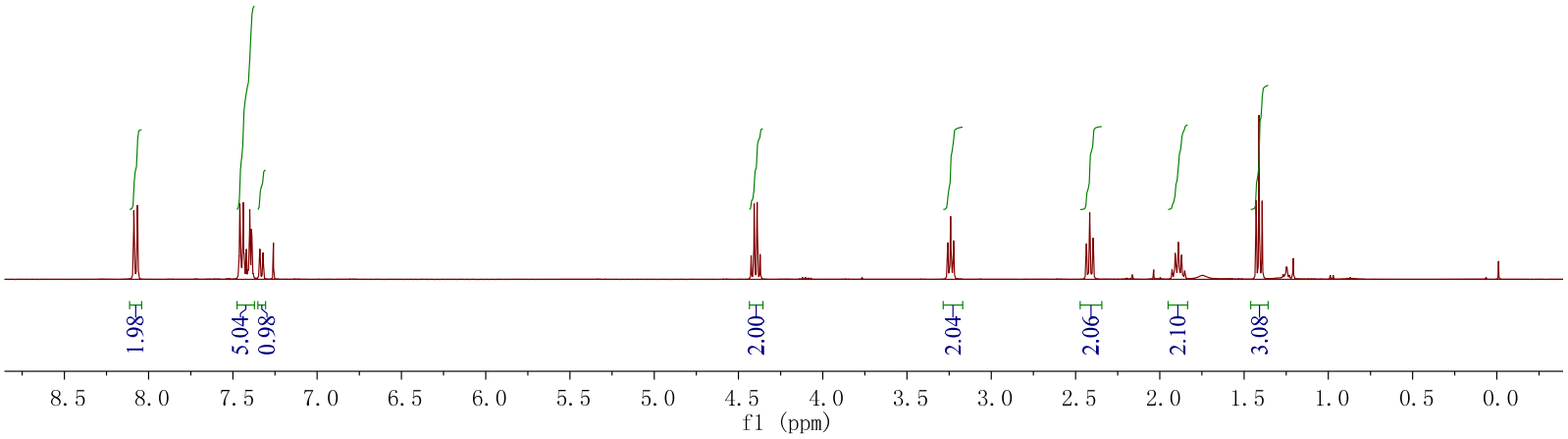
1.41
1.39


O
N
COOEt

**3ak**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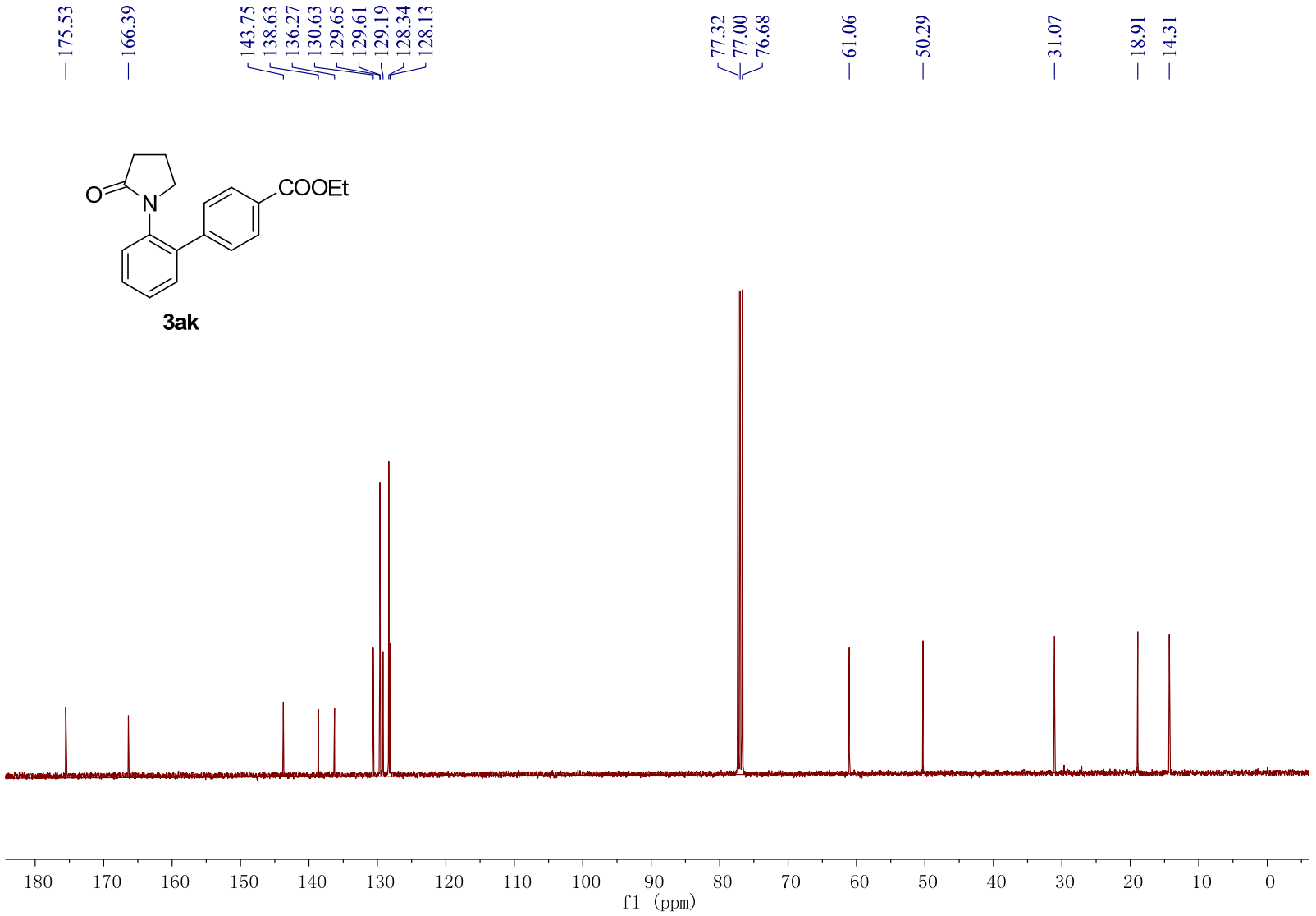
0.98
2.00
2.04
2.06
2.10
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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143.75
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136.27
130.63
129.65
129.61
129.19
128.34
128.13
77.32
77.00
76.68
61.06
50.29
31.07
18.91
14.31
O
N
COOEt
3ak
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.00
7.98
7.96
7.96
7.64
7.64
7.62
7.62
7.56
7.54
7.52
7.50
7.50
7.49
7.48
7.48
7.47
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.43
7.41
7.39
7.38
7.38
7.36
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3.27
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2.25
2.23
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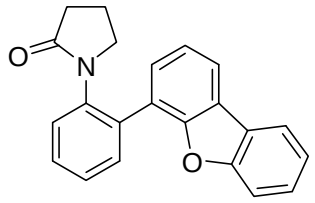
1.65
1.63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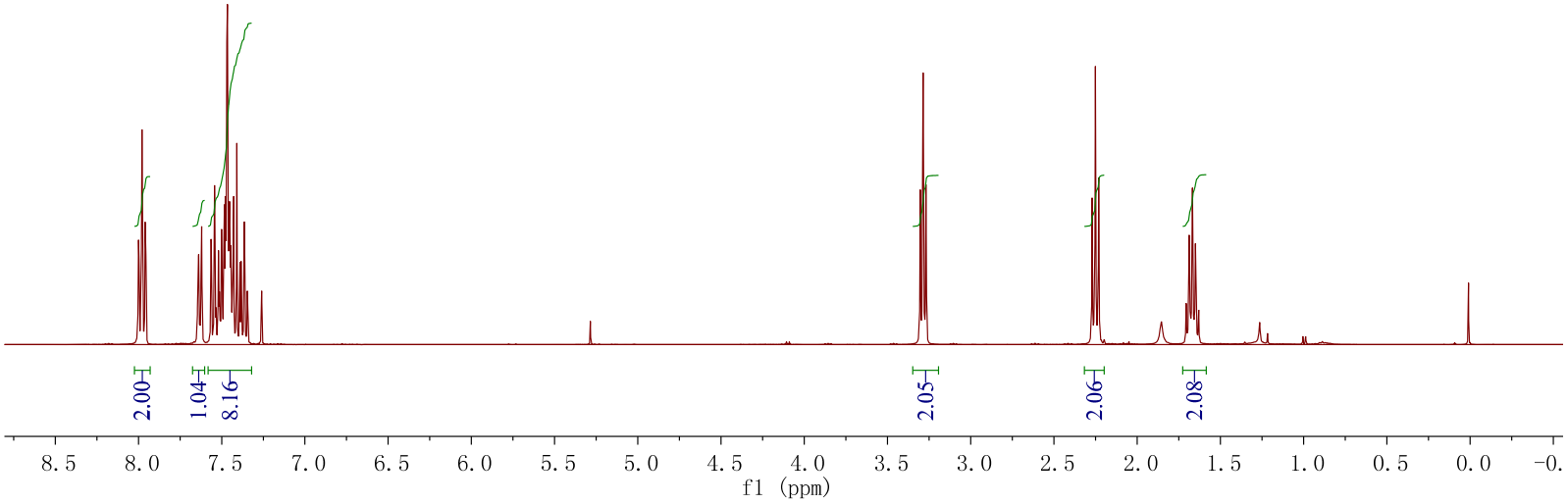
N
O

**3al**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1.04
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2.06
2.08
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
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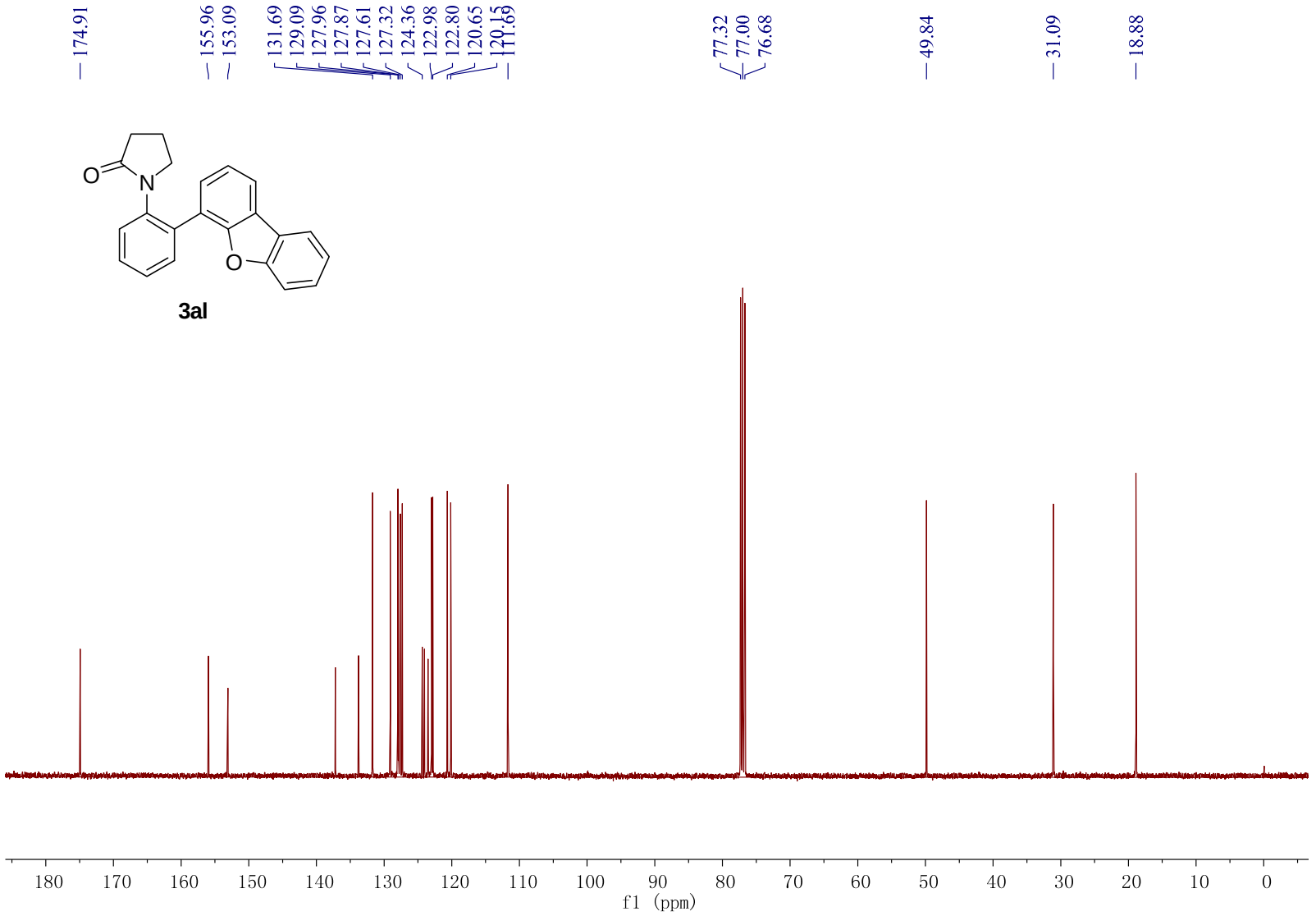
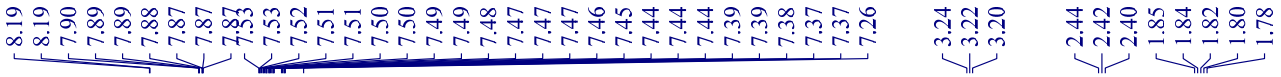
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


174.91
155.96
153.09
131.69
129.09
127.96
127.87
127.61
127.32
124.36
122.98
122.80
120.65
120.15
111.68
77.32
77.00
76.68
49.84
31.09
18.88
O
N
O
3al
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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8.19
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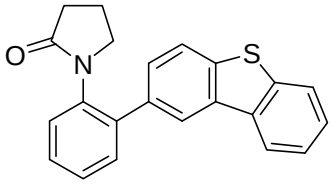
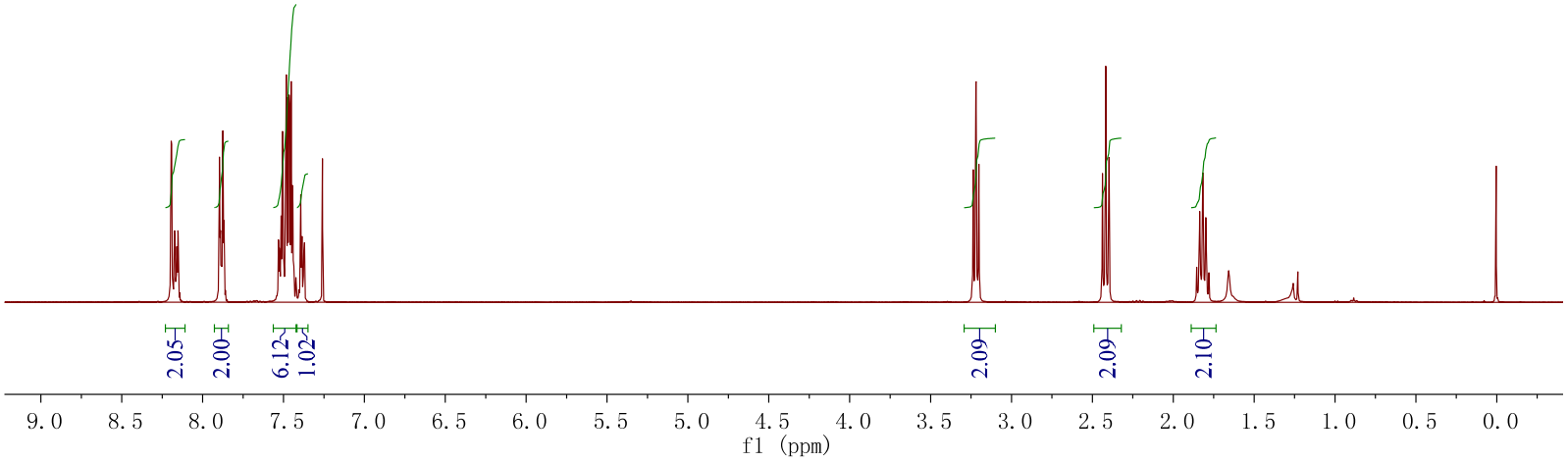
7.89
7.88
7.87
7.87
7.87
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.47
7.47
7.47
7.46
7.45
7.44
7.44
7.44
7.39
7.39
7.38
7.37
7.37
7.26
3.24
3.22
3.20
2.44
2.42
2.40
1.85
1.84
1.82
1.80
1.78


O
N
S

**3am**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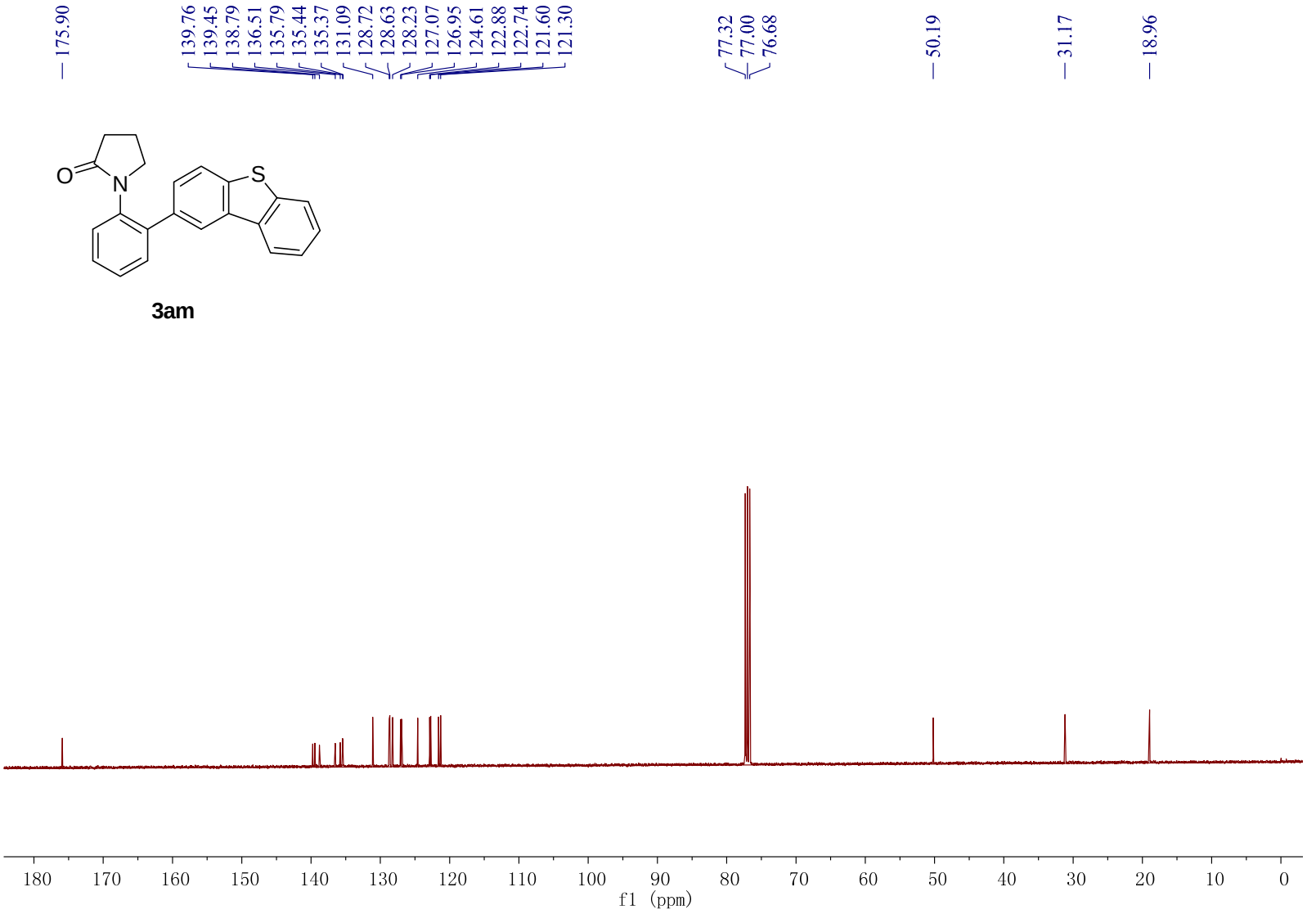
2.00
6.12
1.02
2.09
2.09
2.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


175.90
139.76
139.45
138.79
136.51
135.79
135.44
135.37
131.09
128.72
128.63
128.23
127.07
126.95
124.61
122.88
122.74
121.60
121.30
77.32
77.00
76.68
50.19
31.17
18.96
O
N
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**3am**


7.46
7.45
7.45
7.44
7.43
7.41
7.40
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.32
7.31
7.31
7.30
7.30
7.29
7.26
7.17
7.16
7.15
7.15
3.31
3.29
3.27
2.50
2.48
2.46
2.00
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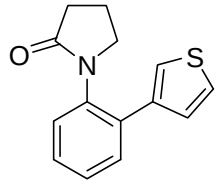
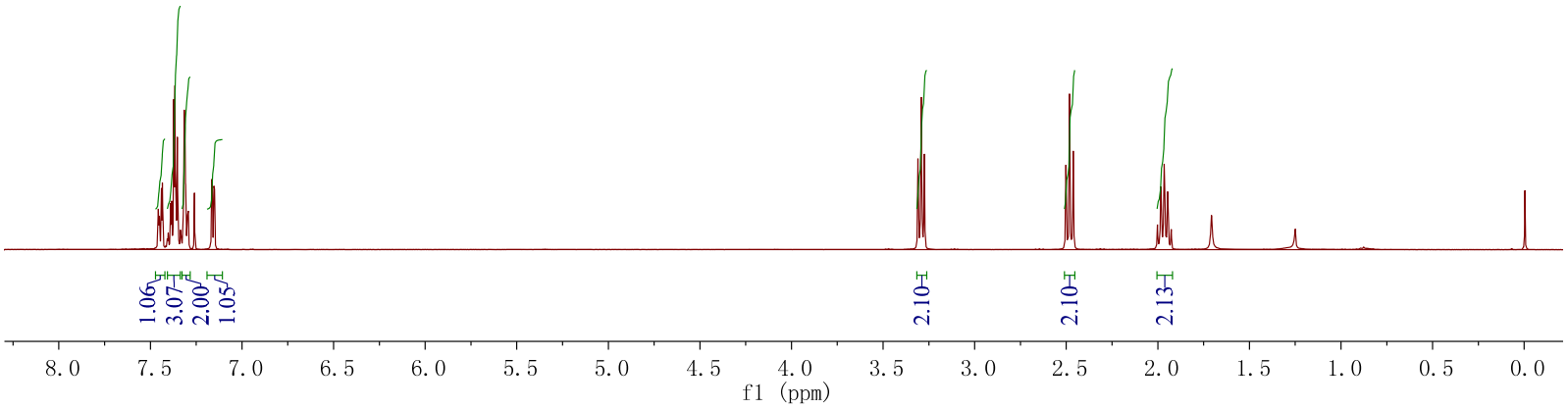
1.97
1.95
1.93


O
N
S

**3an**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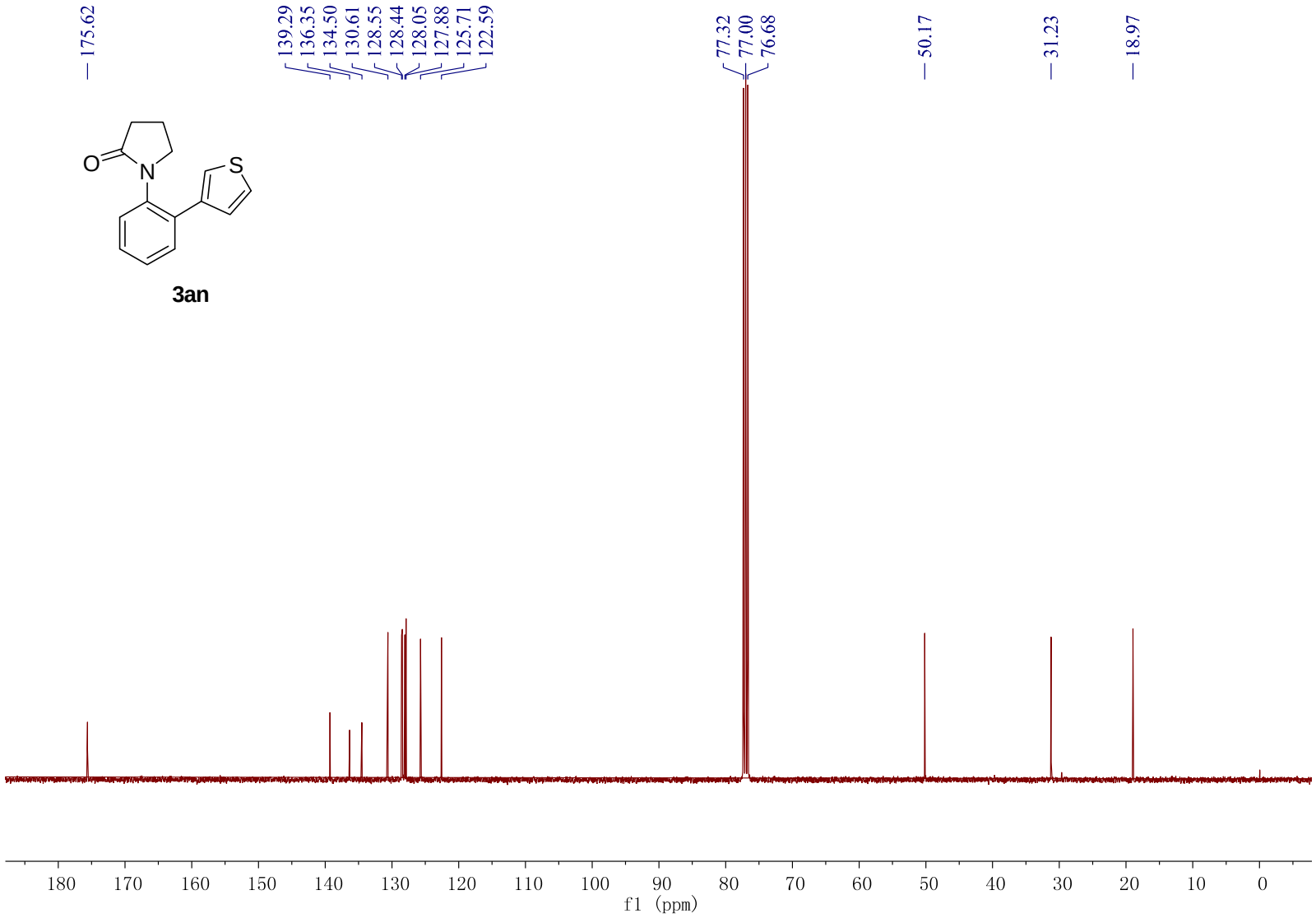
3.07
2.00
1.05
2.10
2.10
2.13
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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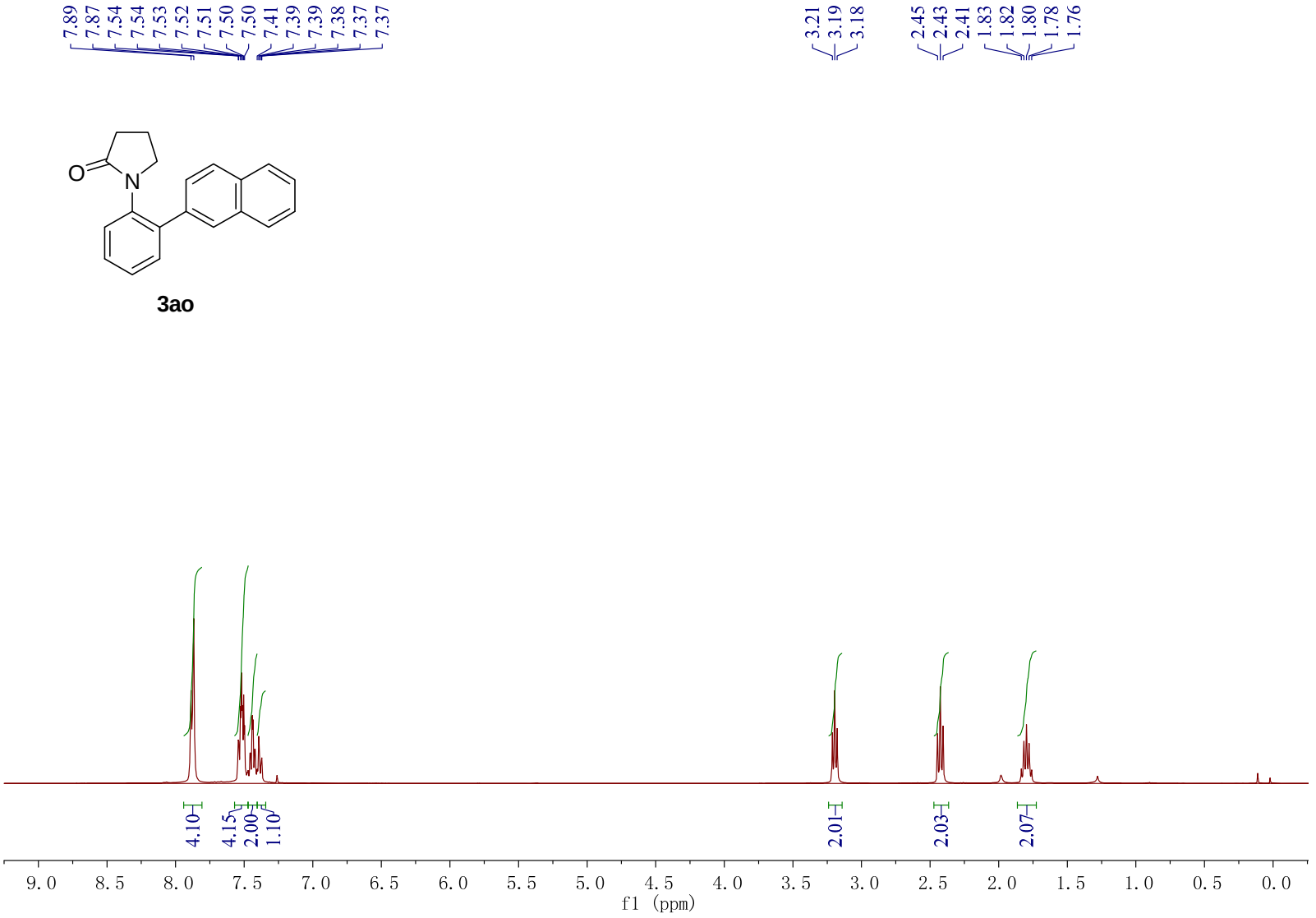
128.44
128.05
127.88
125.71
122.59
77.32
77.00
76.68
50.17
31.23
18.97
O
N
S
3an
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**3ao**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7.50
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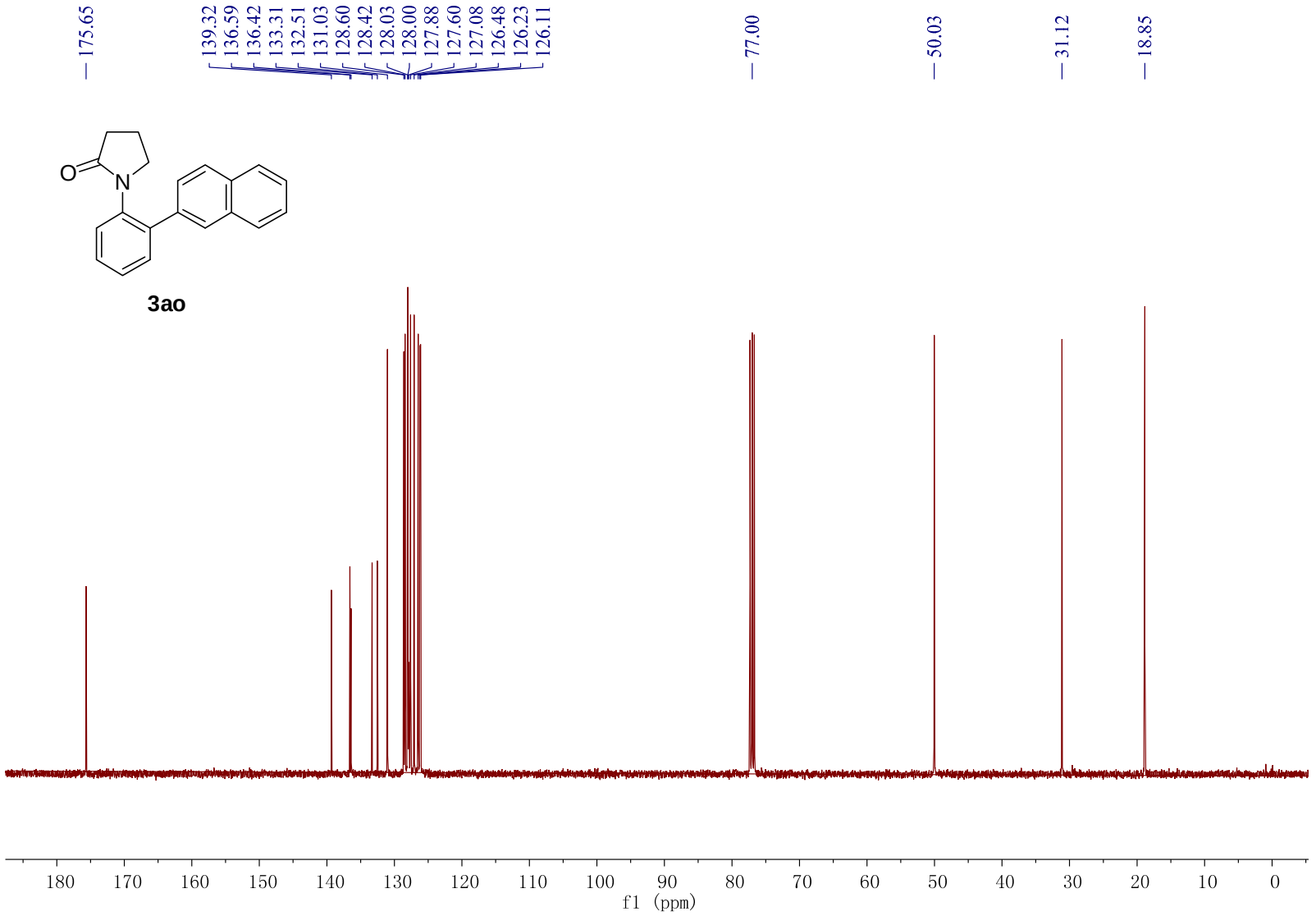
7.41
7.39
7.39
7.38
7.37
7.37
3.21
3.19
3.18
2.45
2.43
2.41
1.83
1.82
1.80
1.78
1.76
4.10
4.15
2.00
1.10
2.01
2.03
2.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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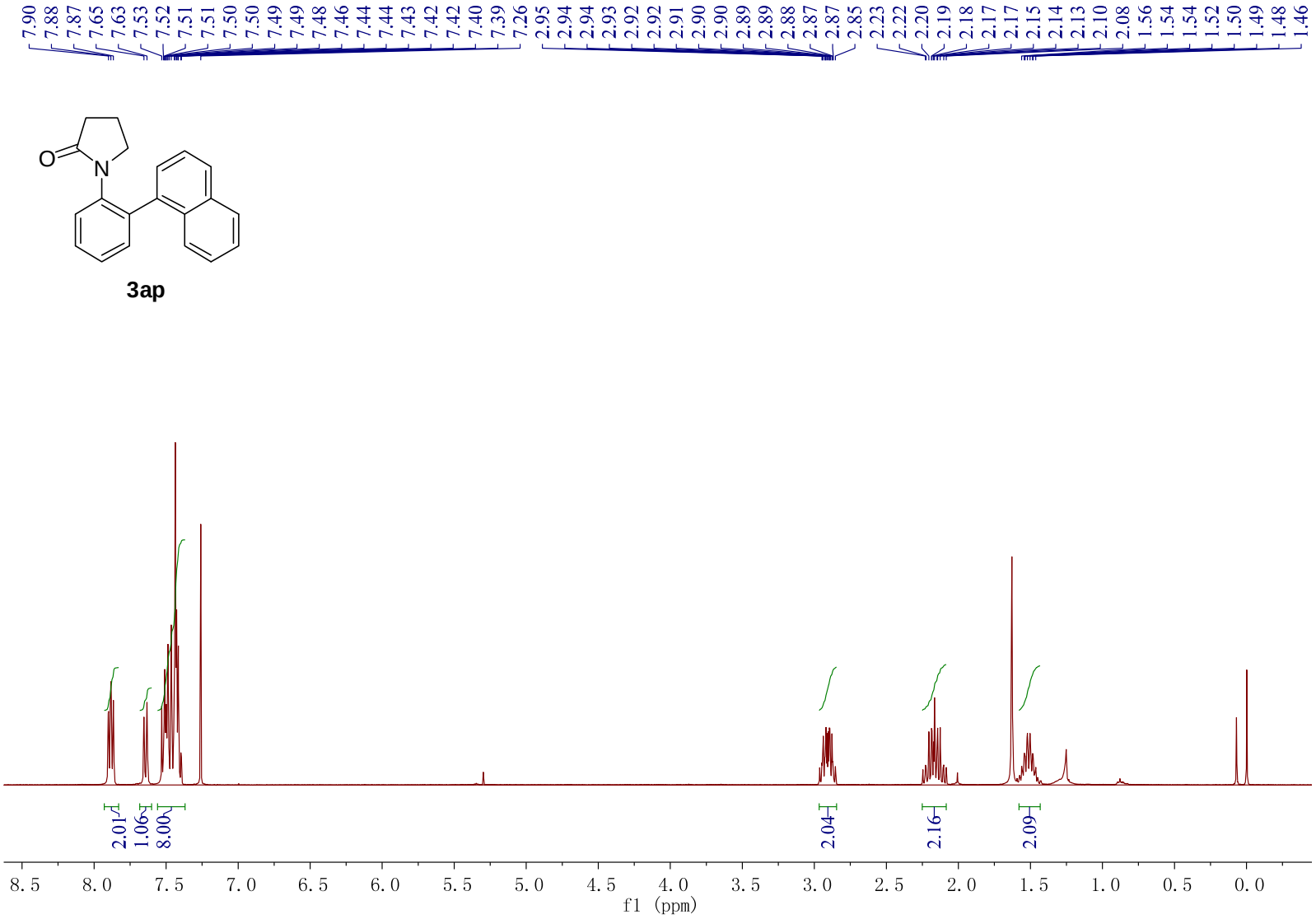
128.03
128.00
127.88
127.60
127.08
126.48
126.23
126.11
77.00
50.03
31.12
18.85
O
N
3ao
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.87
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7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.46
7.44
7.44
7.43
7.42
7.42
7.40
7.39
7.26
2.95
2.94
2.94
2.93
2.92
2.92
2.91
2.90
2.90
2.89
2.89
2.88
2.87
2.87
2.85
2.23
2.22
2.20
2.19
2.18
2.17
2.17
2.15
2.14
2.13
2.10
2.08
1.56
1.54
1.54
1.52
1.50
1.49
1.48
1.46
O
N
2.01
1.06
8.00
2.04
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2.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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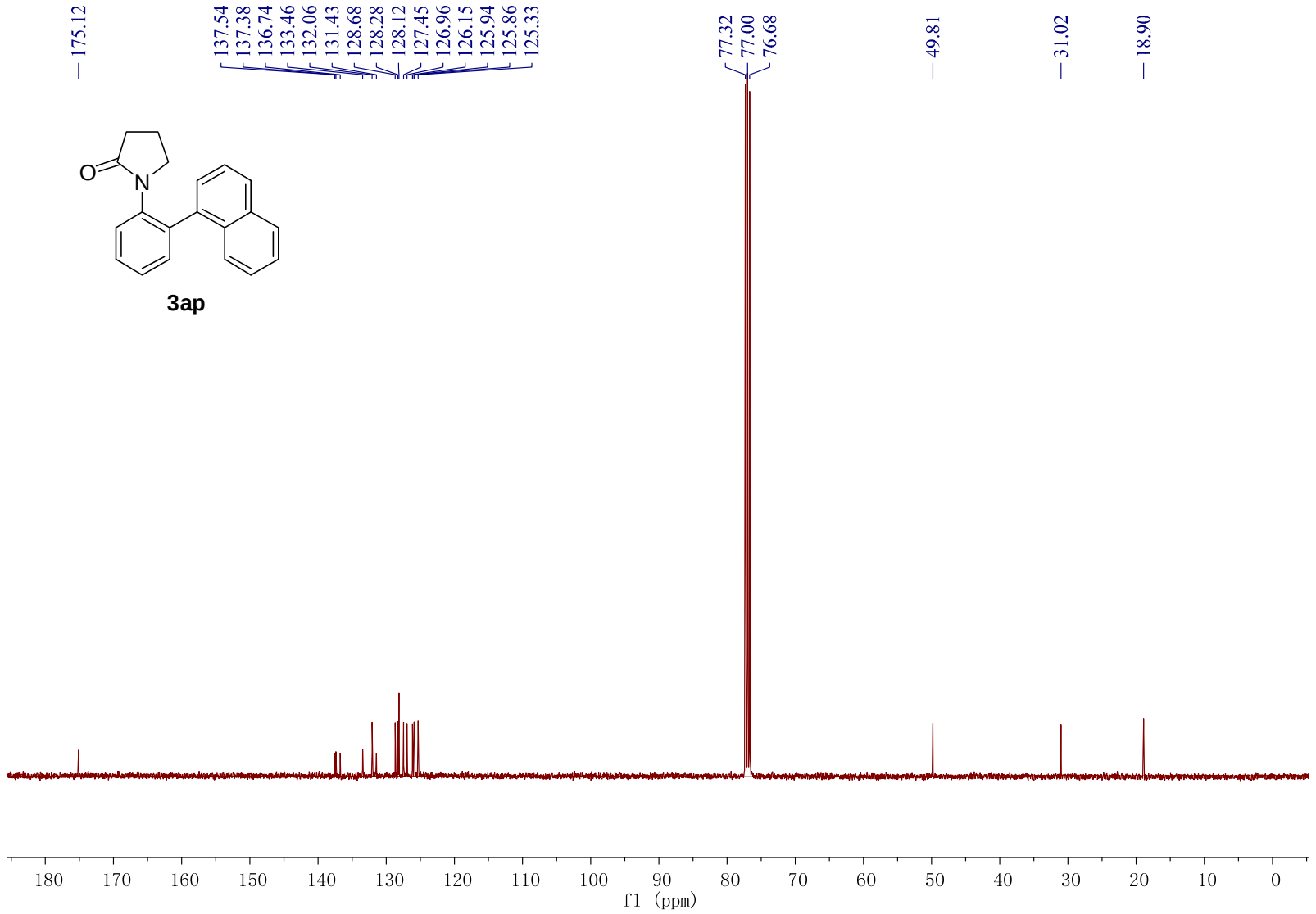
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

**3ap**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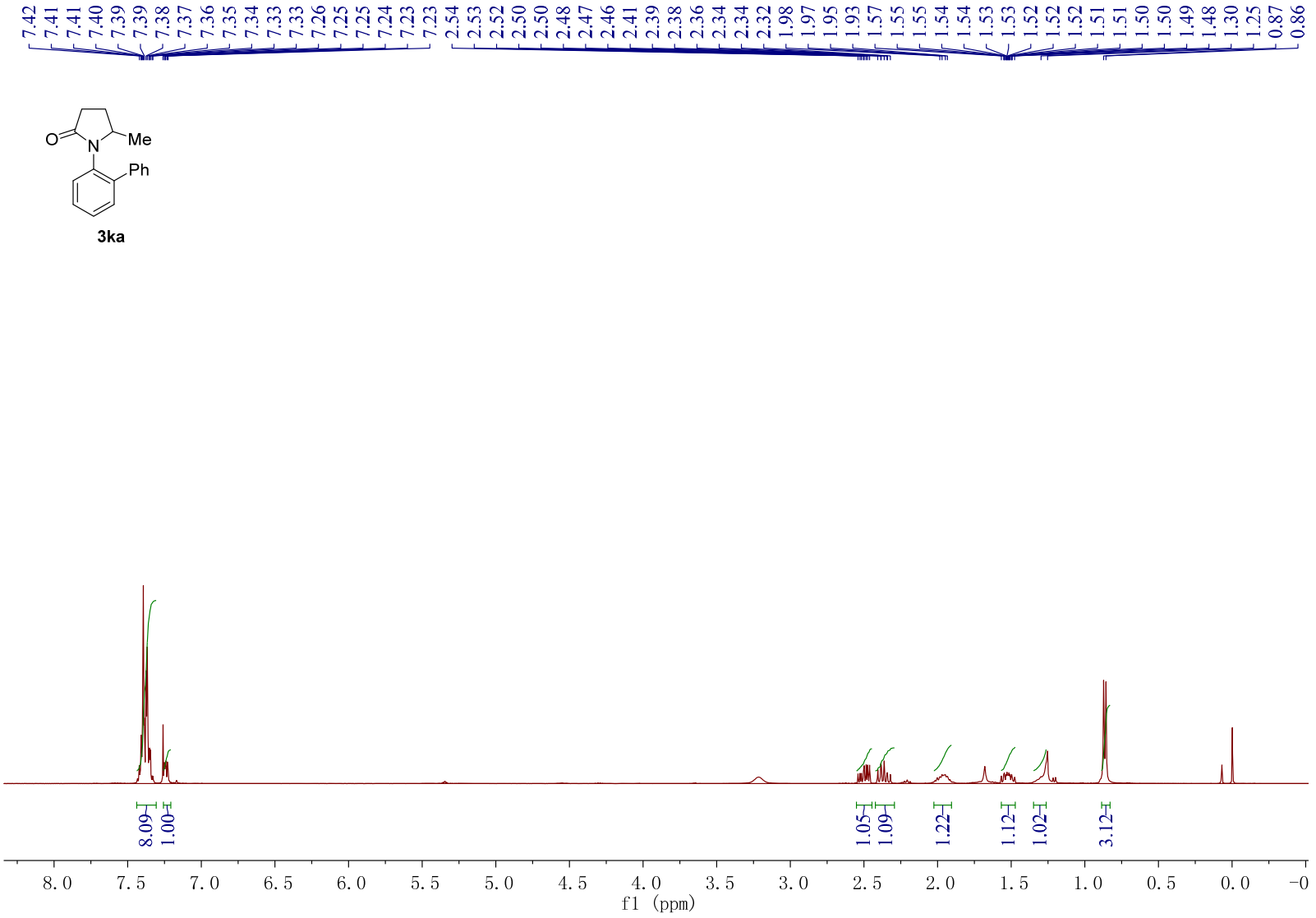
128.68
128.28
128.12
127.45
126.96
126.15
125.94
125.86
125.33
77.32
77.00
76.68
49.81
31.02
18.90
O
N
3ap
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.33
7.26
7.25
7.25
7.24
7.23
7.23
2.54
2.53
2.52
2.50
2.50
2.48
2.47
2.46
2.41
2.39
2.38
2.36
2.34
2.34
2.32
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1.97
1.95
1.93
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1.52
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1.52
1.51
1.51
1.50
1.50
1.49
1.48
1.30
1.25
0.87
0.86
O
N
Me
Ph
3ka
8.09
1.00
1.05
1.09
1.22
1.12
1.02
3.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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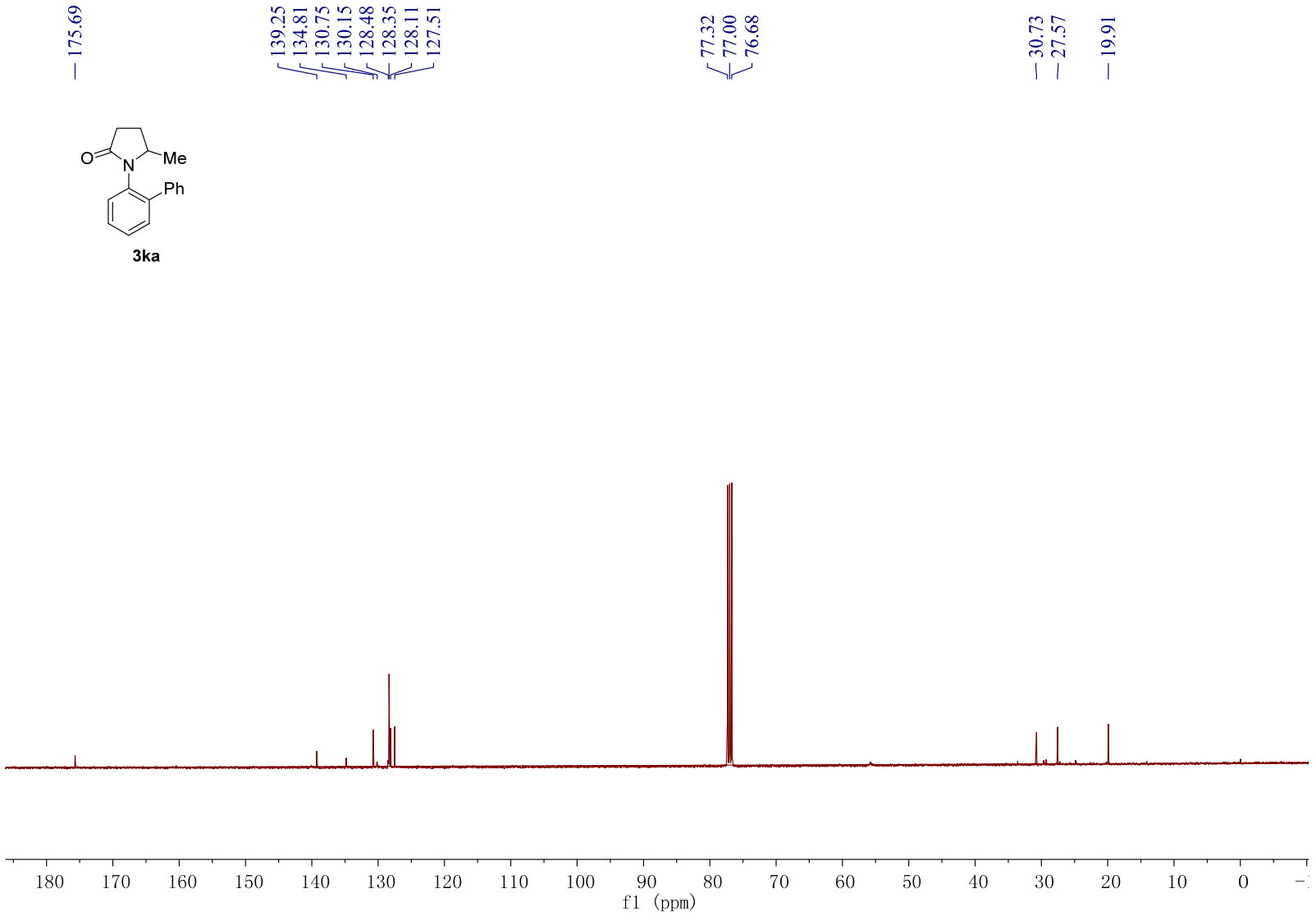
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0
f1 (ppm)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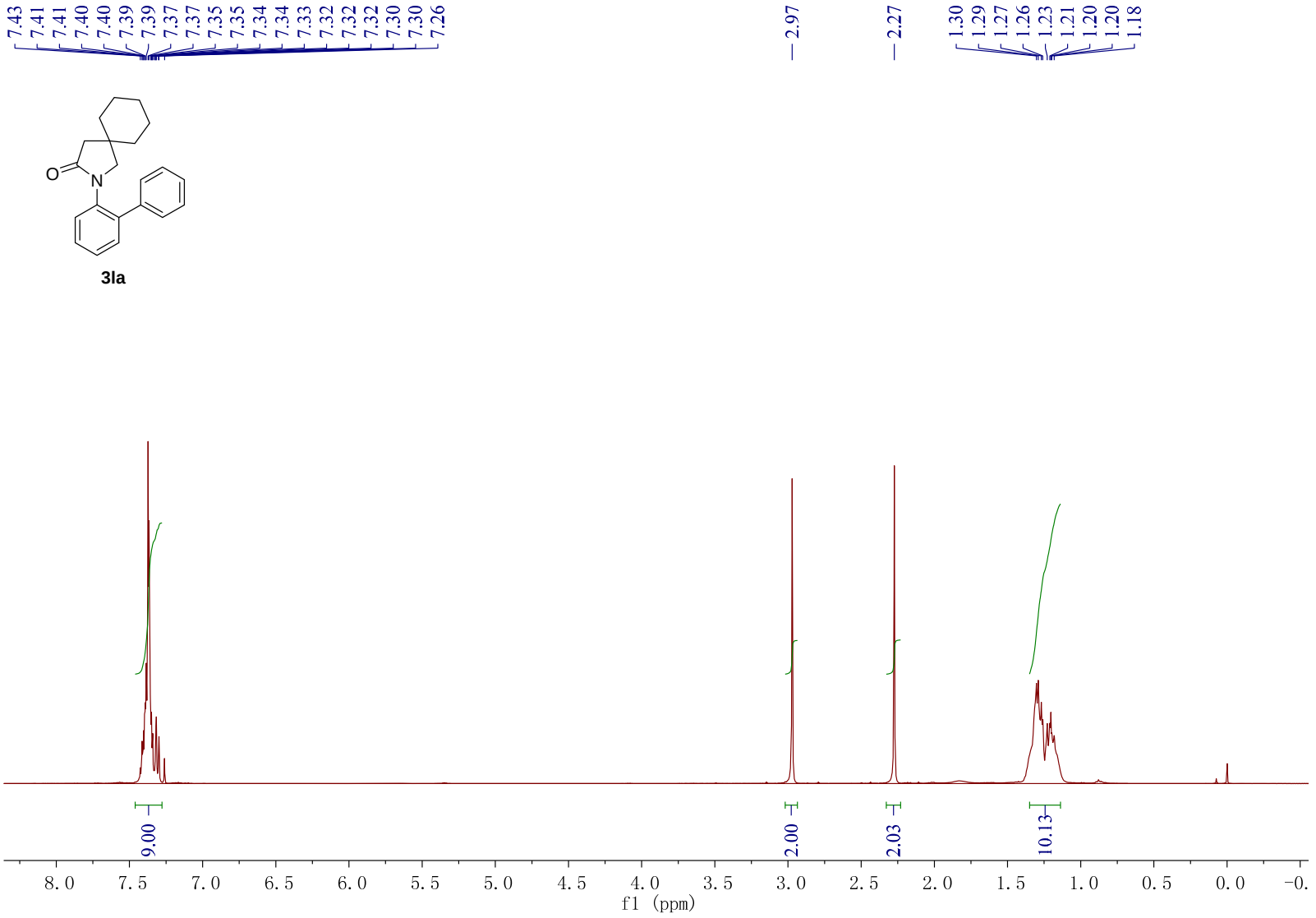
128.48
128.35
128.11
127.51
77.32
77.00
76.68
30.73
27.57
19.91
O
N
Me
Ph
3ka
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.34
7.33
7.32
7.32
7.32
7.30
7.30
7.26
2.97
2.27
1.30
1.29
1.27
1.26
1.23
1.21
1.20
1.20
1.18
O
N
9.00
2.00
2.03
10.13
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.0
1.5
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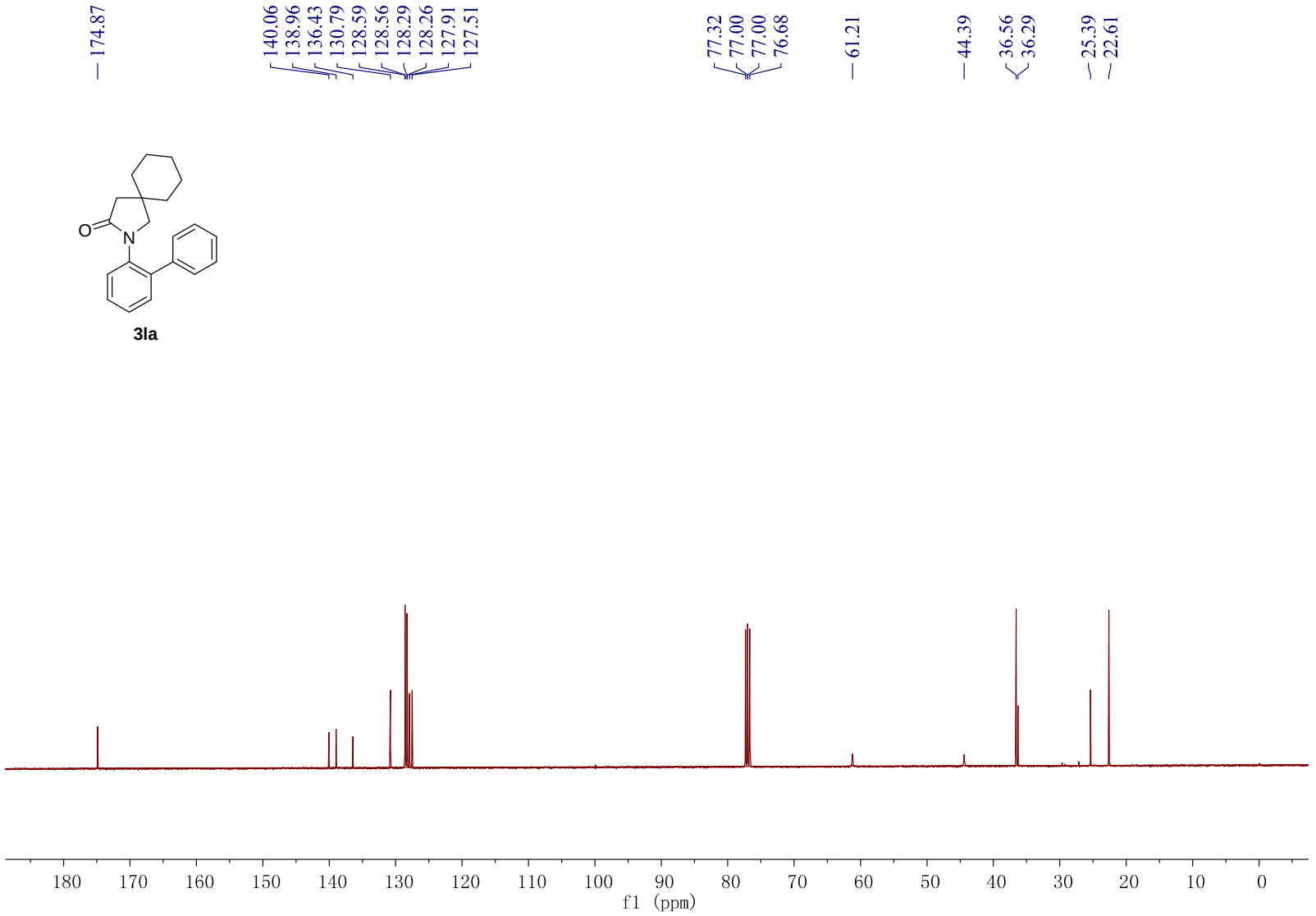
0.5
0.0
-0.
f1 (ppm)

**3la**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127.91
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77.32
77.00
77.00
76.68
61.21
44.39
36.56
36.29
25.39
22.61
O
N
3la
180
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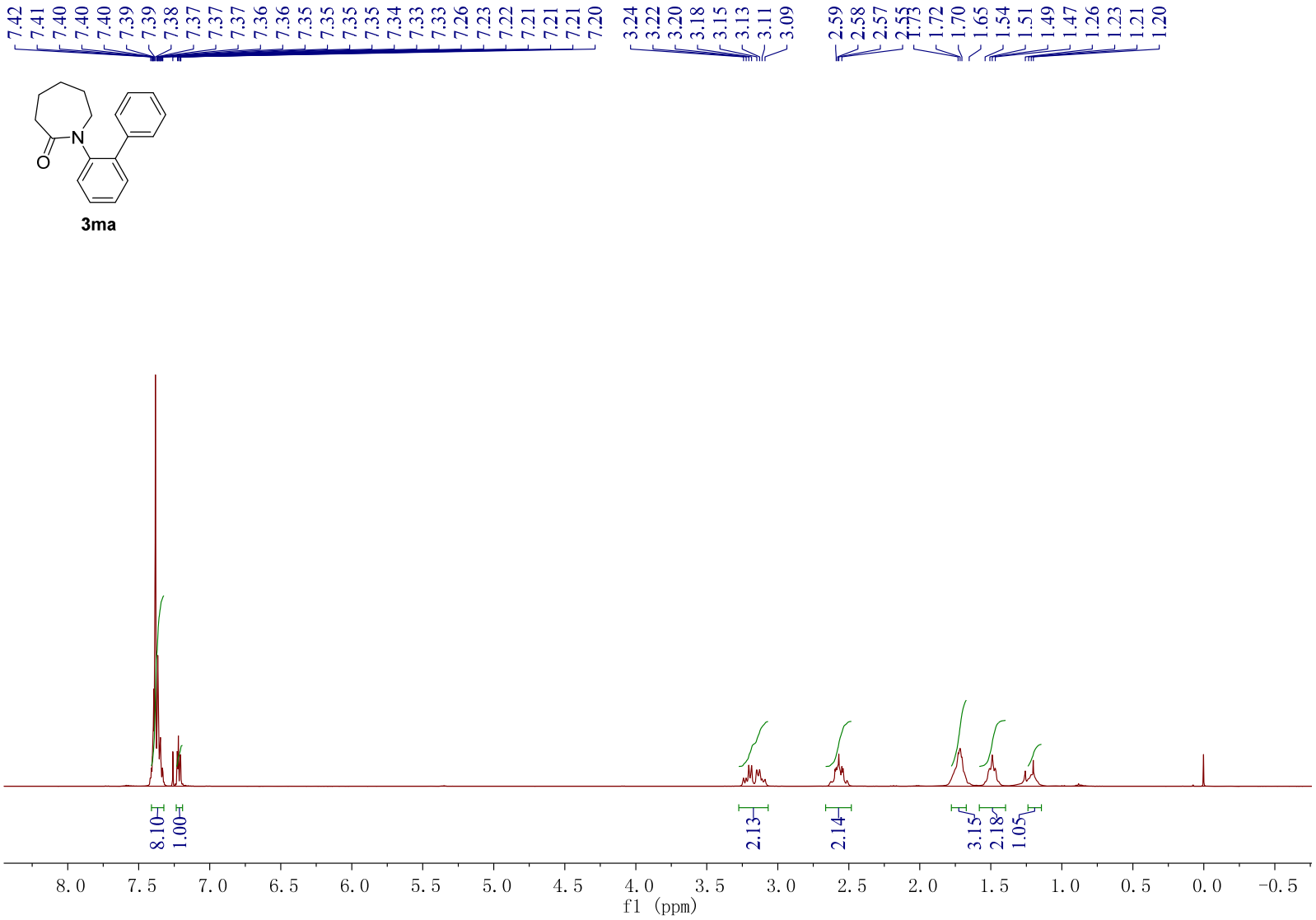
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.35
7.35
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7.35
7.34
7.33
7.33
7.26
7.23
7.22
7.21
7.21
7.21
7.20
3.24
3.22
3.20
3.18
3.15
3.13
3.11
3.09
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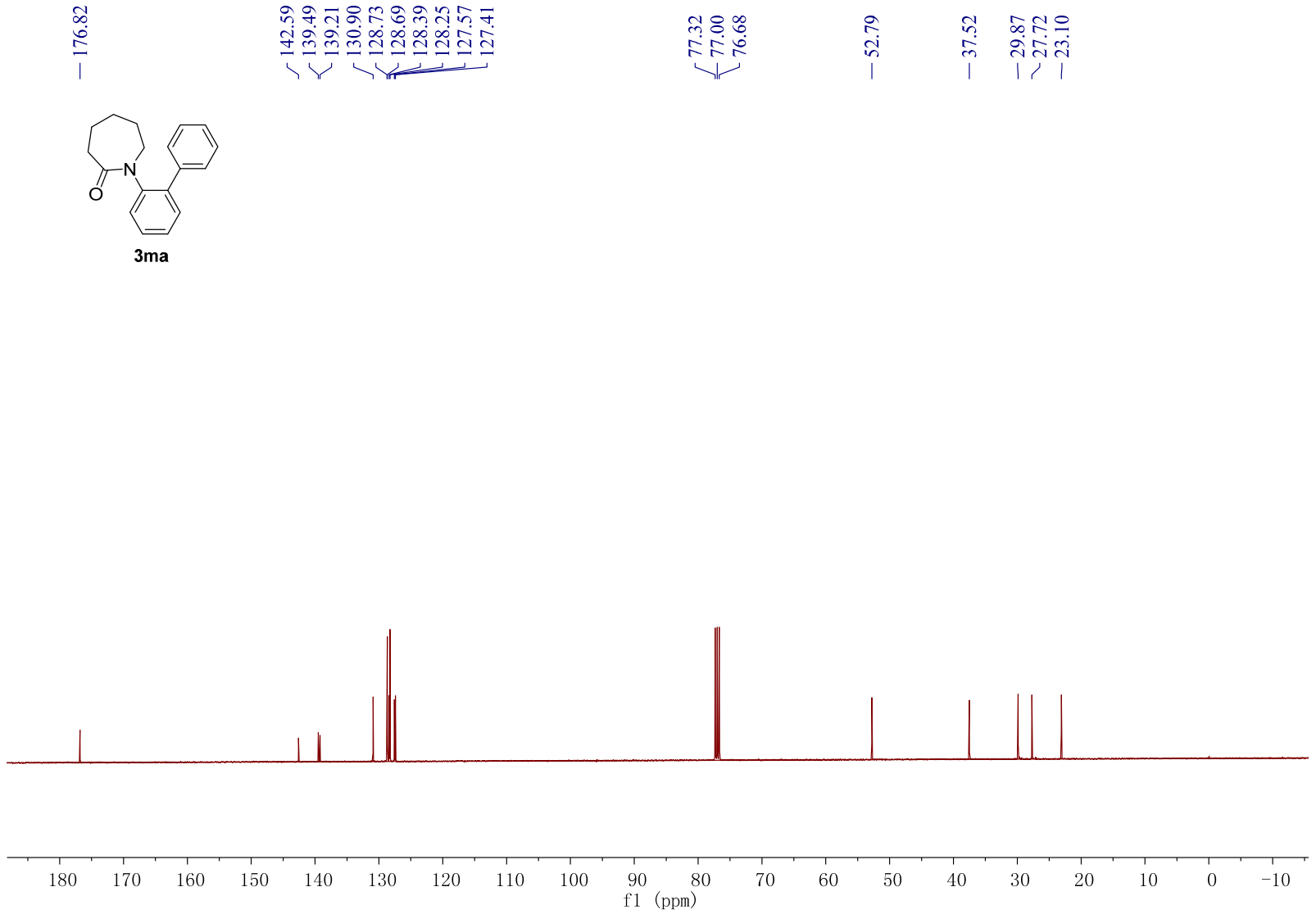
2.58
2.57
2.55
1.73
1.72
1.70
1.65
1.54
1.51
1.49
1.47
1.26
1.23
1.21
1.20
N
O
3ma
8.10
1.00
2.13
2.14
3.15
2.18
1.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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128.39
128.25
127.57
127.41
77.32
77.00
76.68
52.79
37.52
29.87
27.72
23.10
O
N
3ma
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.65
8.65
8.65
8.64
8.64
8.64
7.45
7.45
7.43
7.43
7.39
7.37
7.35
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7.29
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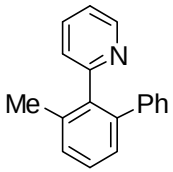
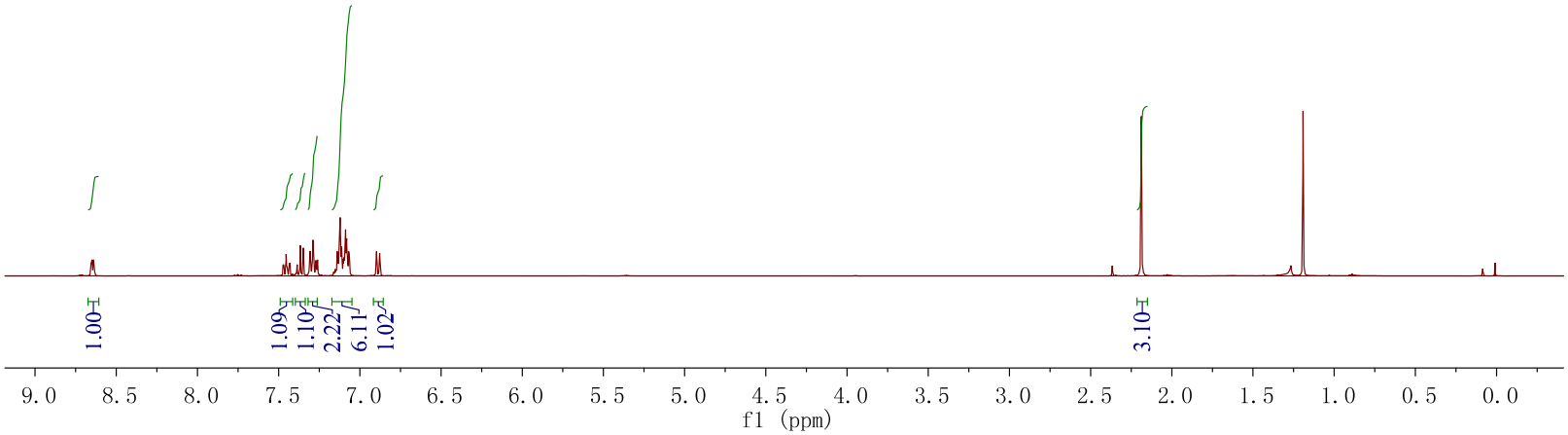
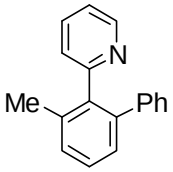
6.88
6.88
2.19


N
Me
Ph

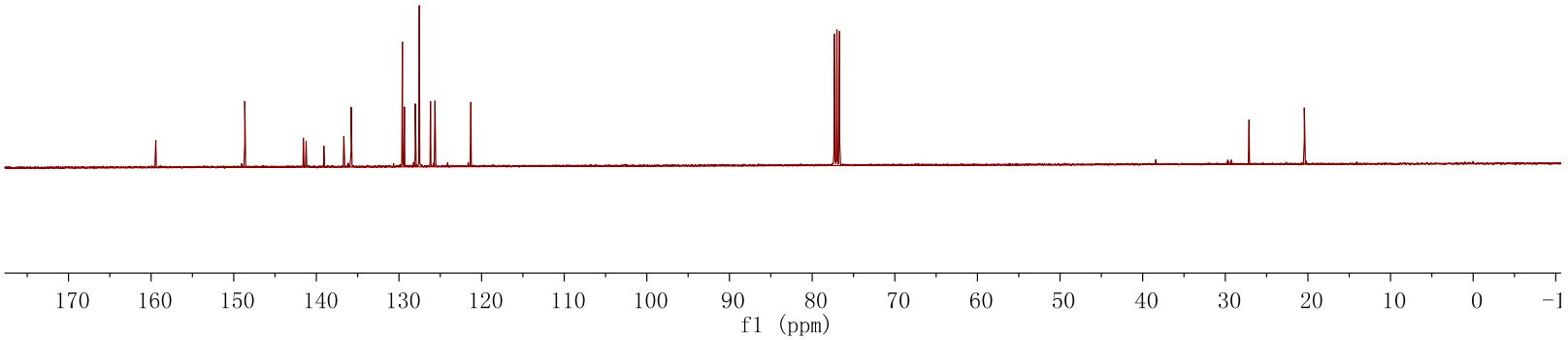
**5aa**


1.00
1.09
1.10
2.22
6.11
1.02
3.10
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)

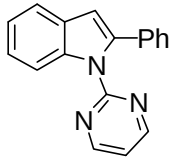
159.44
148.67
141.59
141.24
139.11
136.68
135.79
129.60
129.35
128.03
127.55
126.19
125.64
121.31
77.32
77.00
76.68
20.42



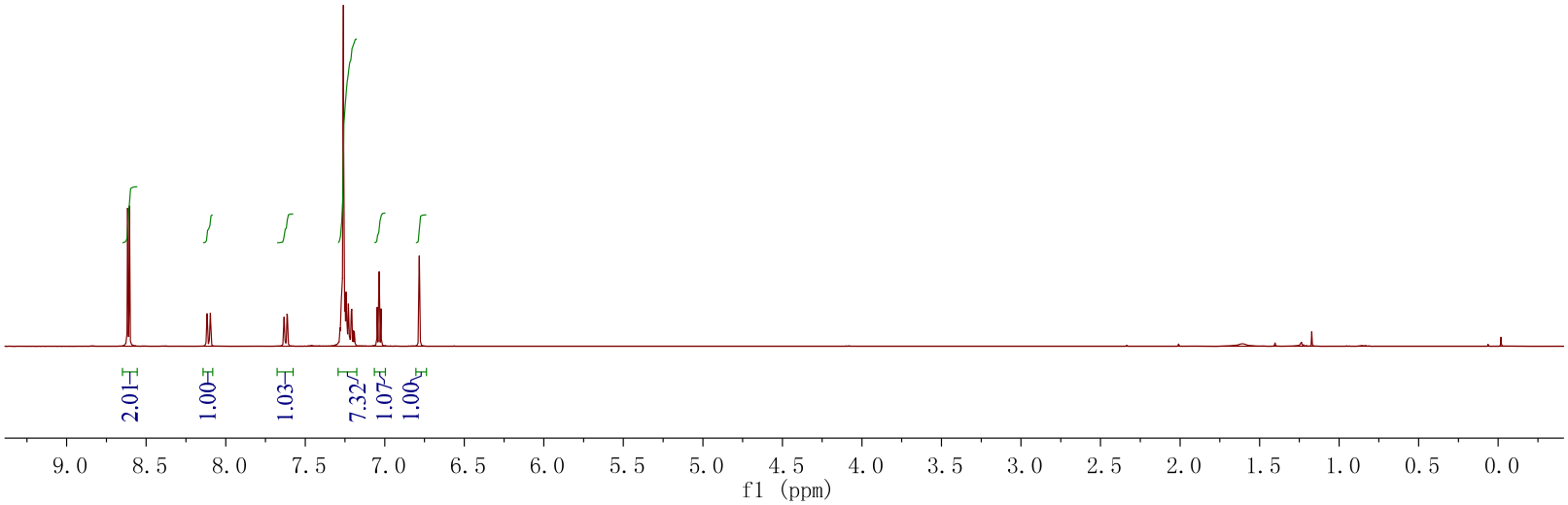

**5aa**

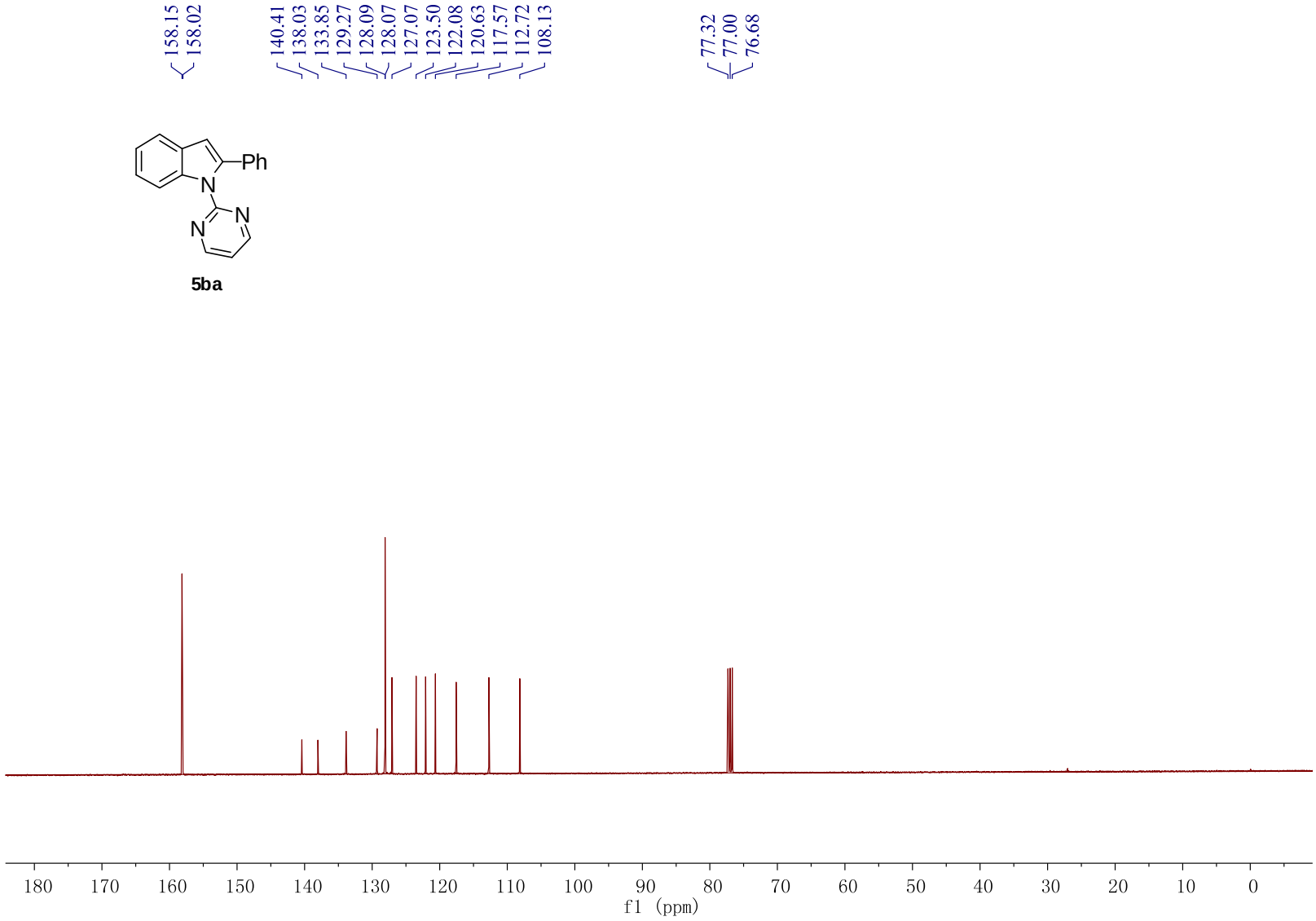



8.62
8.61
8.12
8.10
7.63
7.63
7.61
7.61
7.28
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.21
7.20
7.19
7.19
7.05
7.04
7.02
6.78
6.78

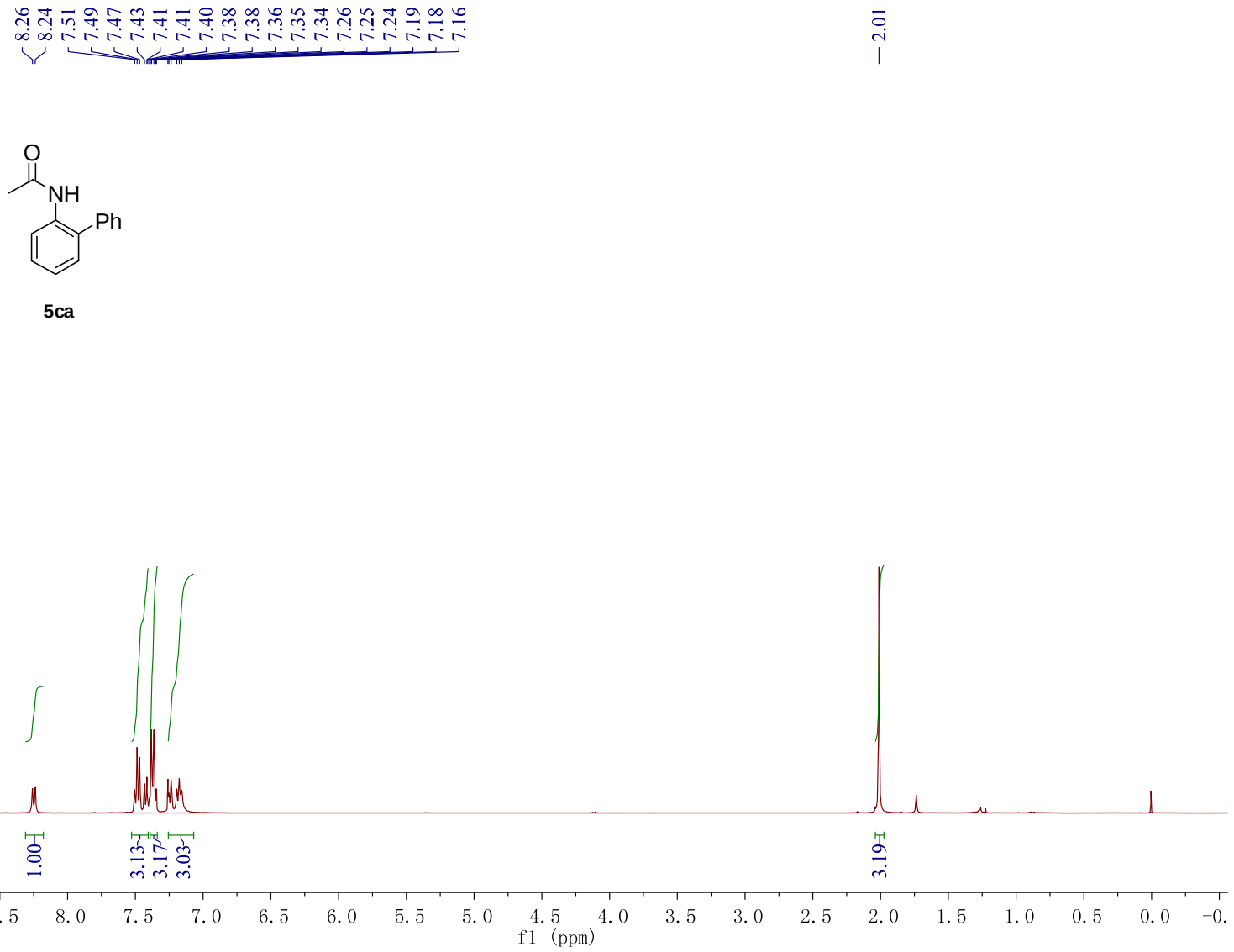

Ph
N
N
N

**5ba**

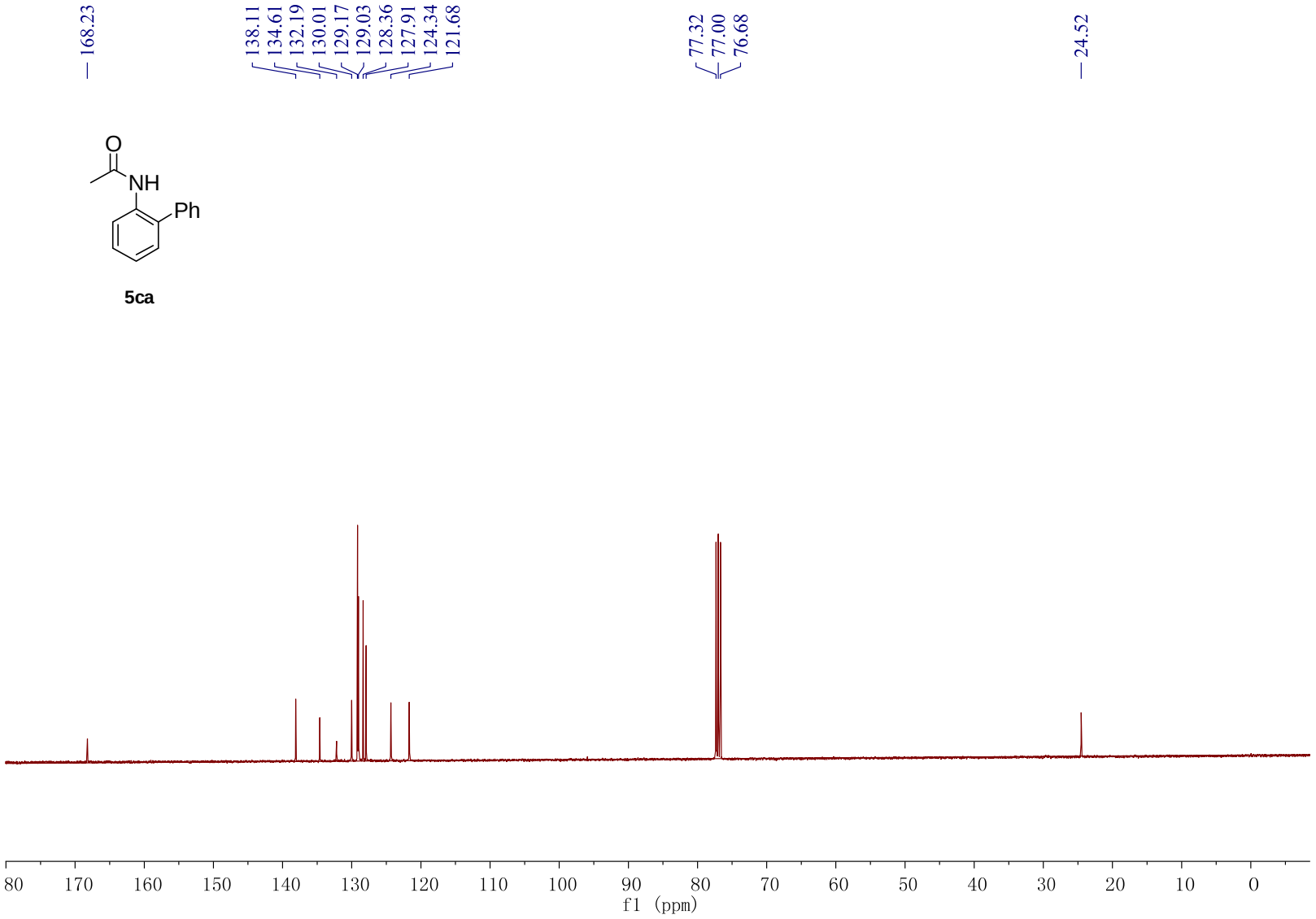

2.01
1.00
1.03
7.32
1.07
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.15
158.02
140.41
138.03
133.85
129.27
128.09
128.07
127.07
123.50
122.08
120.63
117.57
112.72
108.13
77.32
77.00
76.68
Ph
N
N
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

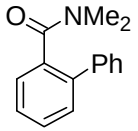
**5ba**


8.26
8.24
7.51
7.49
7.47
7.43
7.41
7.41
7.40
7.38
7.38
7.36
7.35
7.34
7.26
7.25
7.24
7.19
7.18
7.16
2.01
O
NH
Ph
1.00
3.13
3.17
3.03
3.19
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.
f1 (ppm)

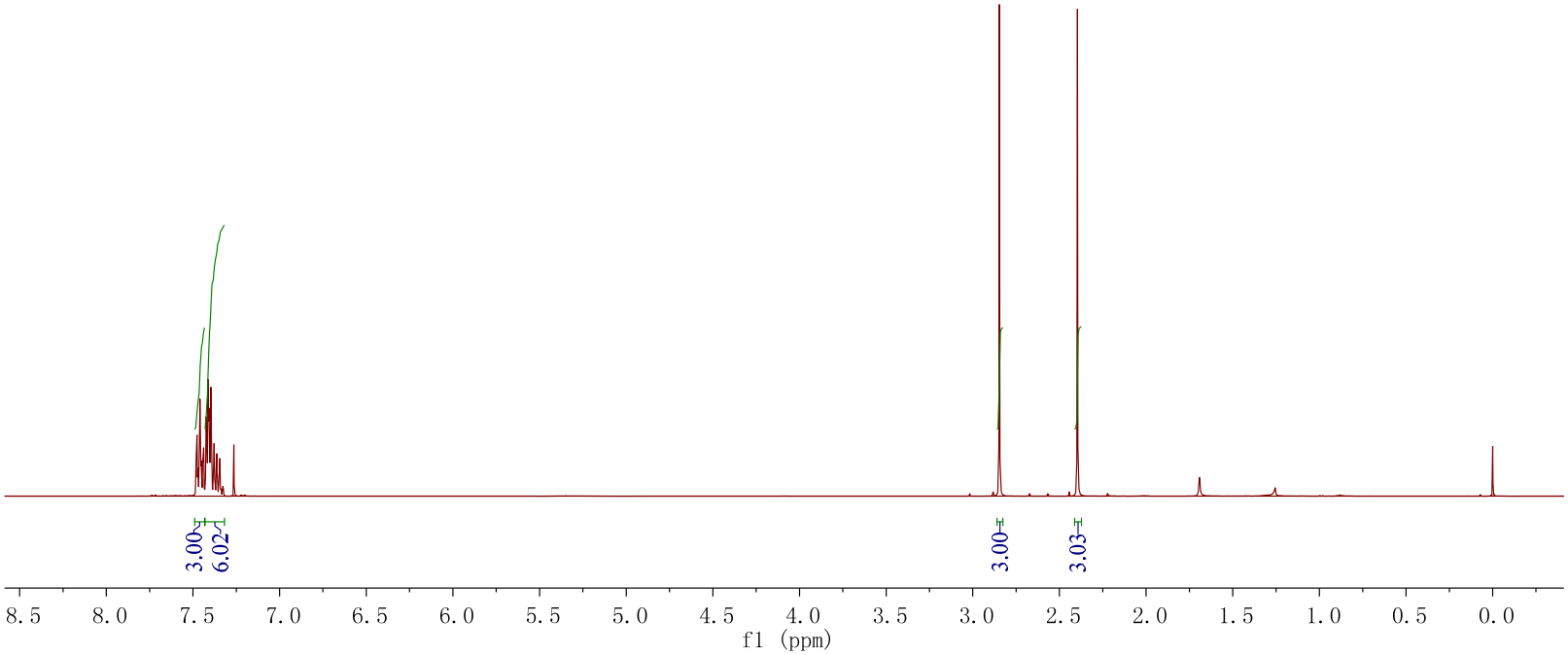
**5ca**

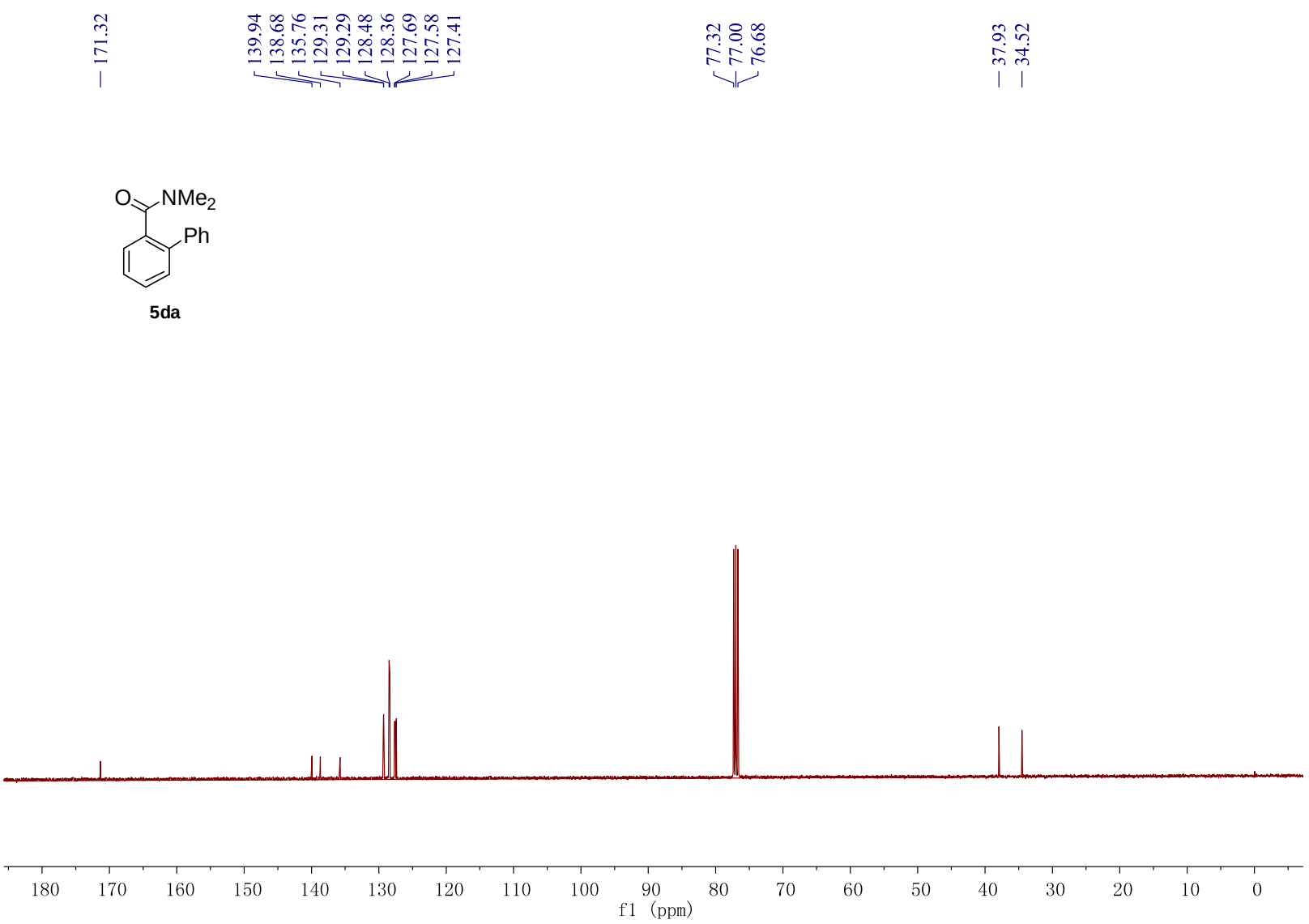

168.23
138.11
134.61
132.19
130.01
129.17
129.03
128.36
127.91
124.34
121.68
77.32
77.00
76.68
24.52
O
NH
Ph
5ca
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

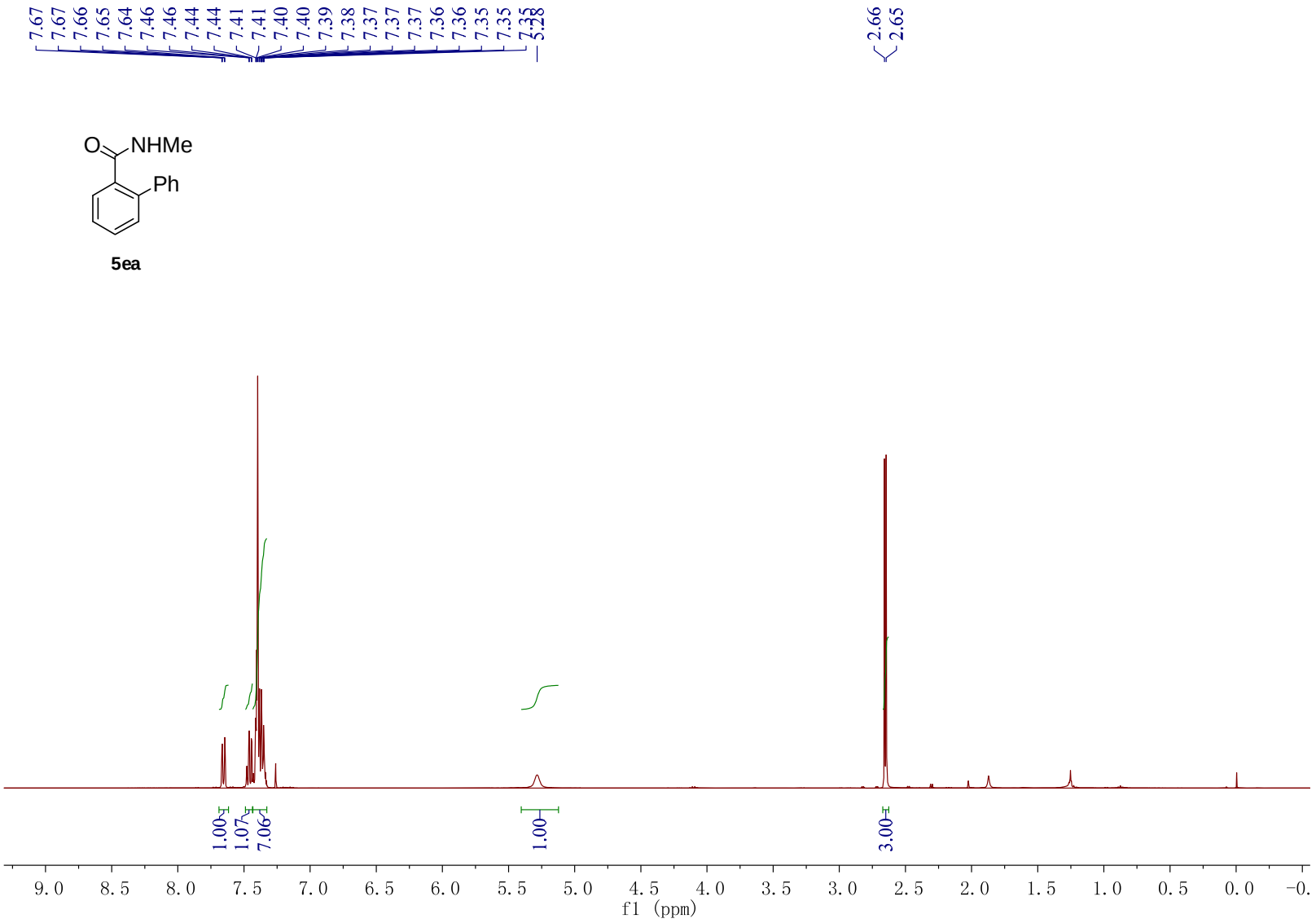

7.48
7.48
7.47
7.46
7.46
7.46
7.45
7.44
7.44
7.42
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.26
2.85
2.40


O
NMe2
Ph

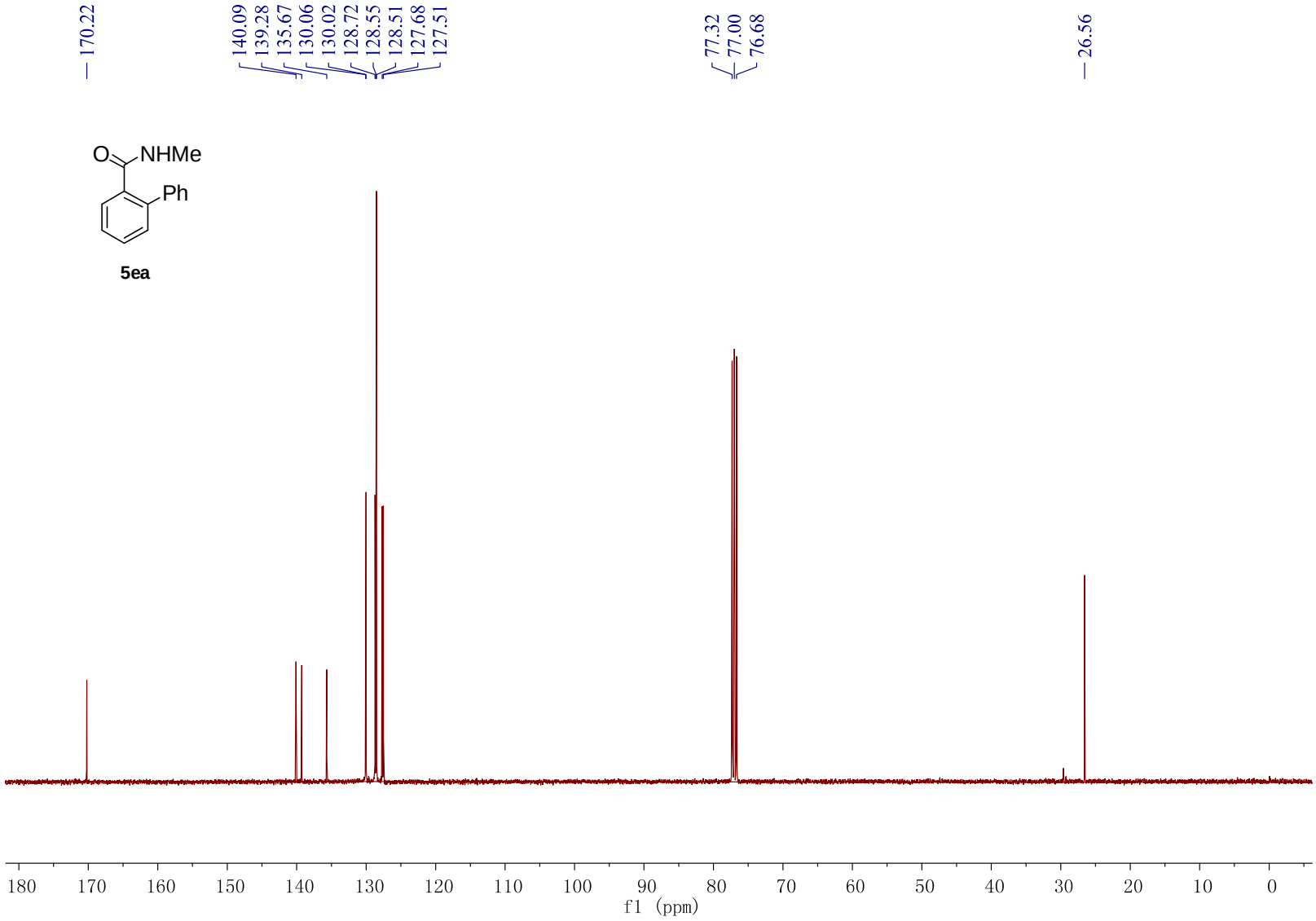
**5da**

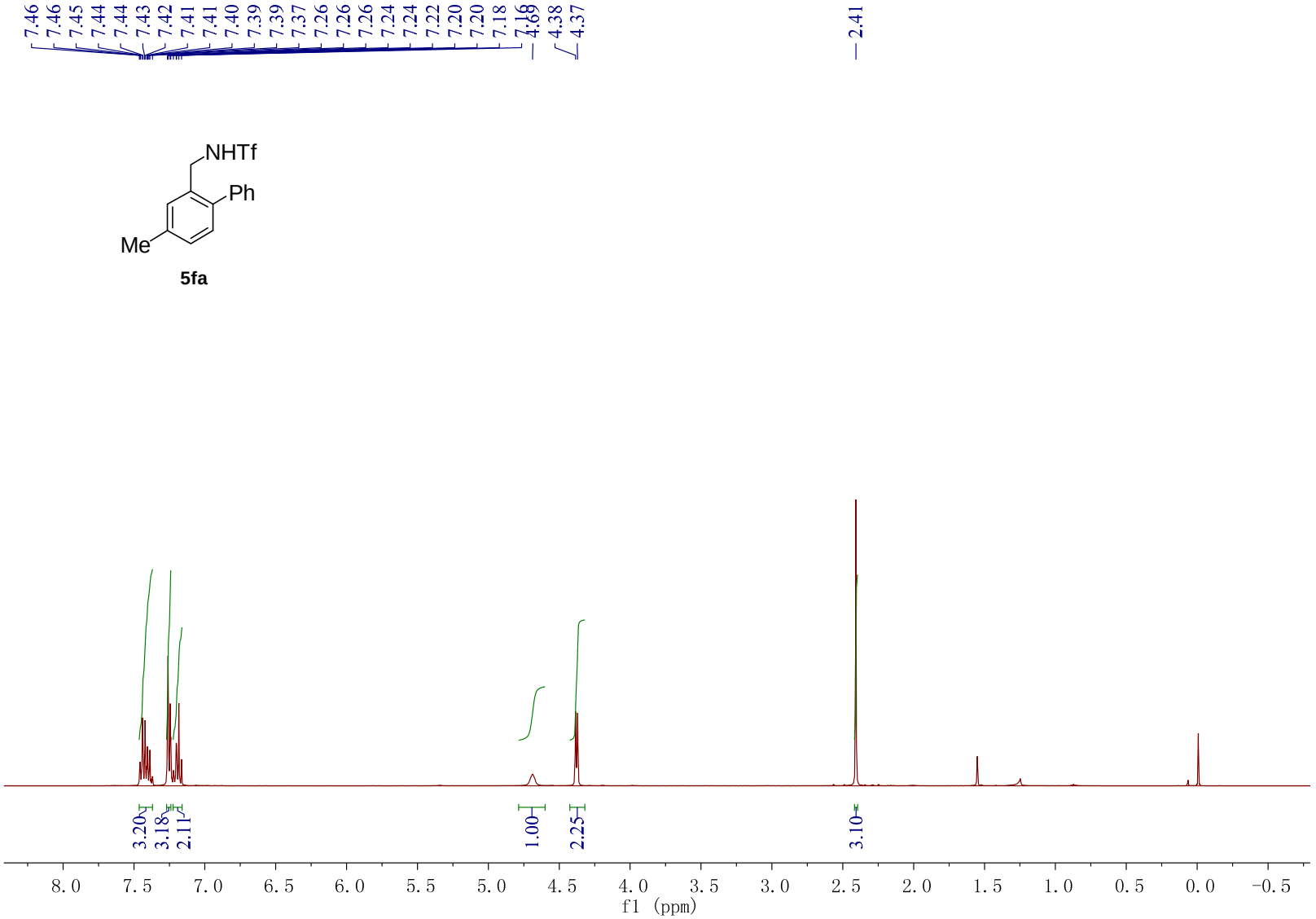

3.00
6.02
3.00
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


171.32
139.94
138.68
135.76
129.31
129.29
128.48
128.36
127.69
127.58
127.41
77.32
77.00
76.68
37.93
34.52
O
NMe2
Ph
5da
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

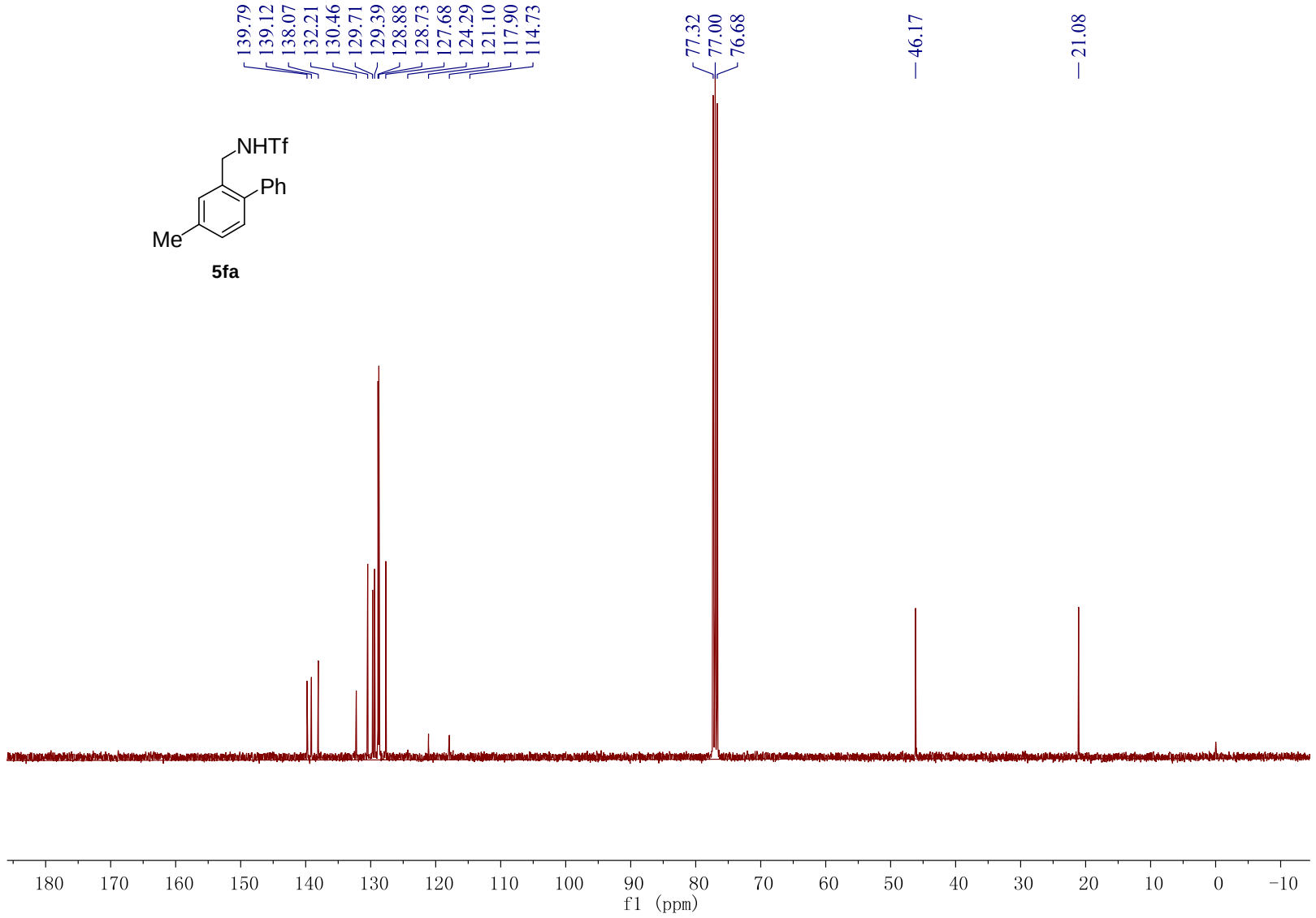

7.67
7.67
7.66
7.65
7.64
7.46
7.46
7.44
7.44
7.41
7.41
7.40
7.40
7.39
7.38
7.37
7.37
7.37
7.36
7.36
7.35
7.35
2.66
2.65
O
NHMe
Ph
1.00
1.07
7.06
1.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

**5ea**

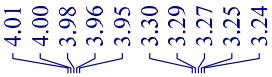

170.22
140.09
139.28
135.67
130.06
130.02
128.72
128.55
128.51
127.68
127.51
77.32
77.00
76.68
26.56
O
NHMe
Ph
5ea
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

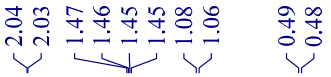

7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.37
7.26
7.26
7.26
7.24
7.24
7.22
7.20
7.20
7.18
7.16
4.69
4.38
4.37
2.41
NHTf
Ph
Me
3.20
3.18
2.11
1.00
2.25
3.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

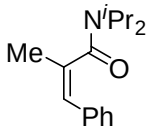
**5fa**


139.79
139.12
138.07
132.21
130.46
129.71
129.39
128.88
128.73
127.68
124.29
121.10
117.90
114.73
77.32
77.00
76.68
46.17
21.08
NHTf
Ph
Me
5fa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

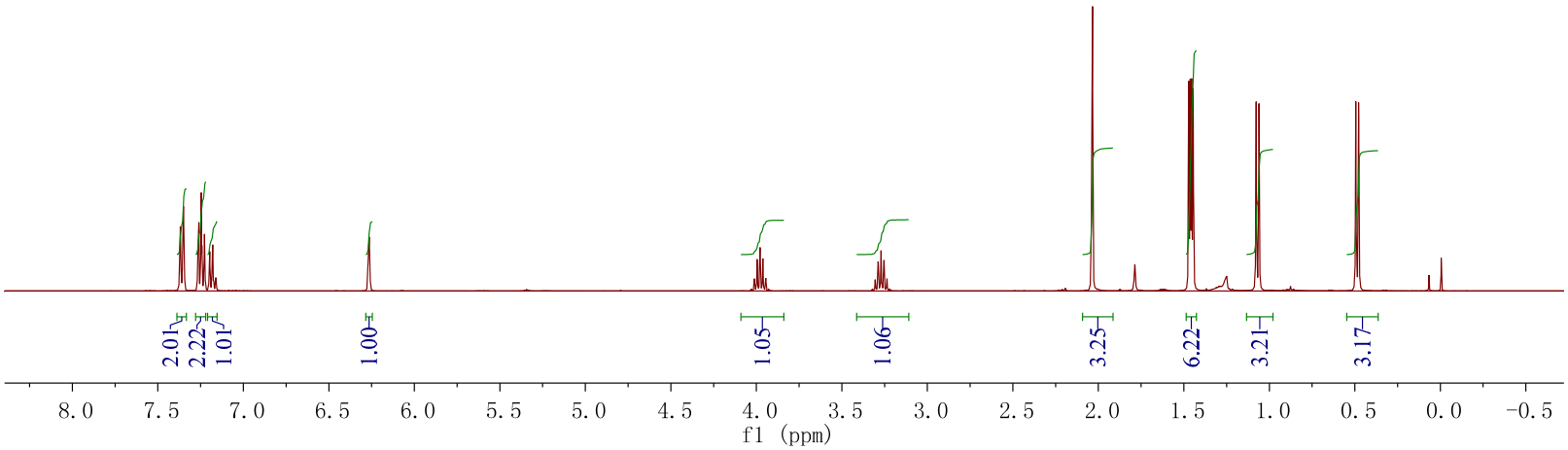

7.37
7.37
7.35
7.27
7.26
7.26
7.26
7.25
7.24
7.23
7.20
7.18
6.27
6.26

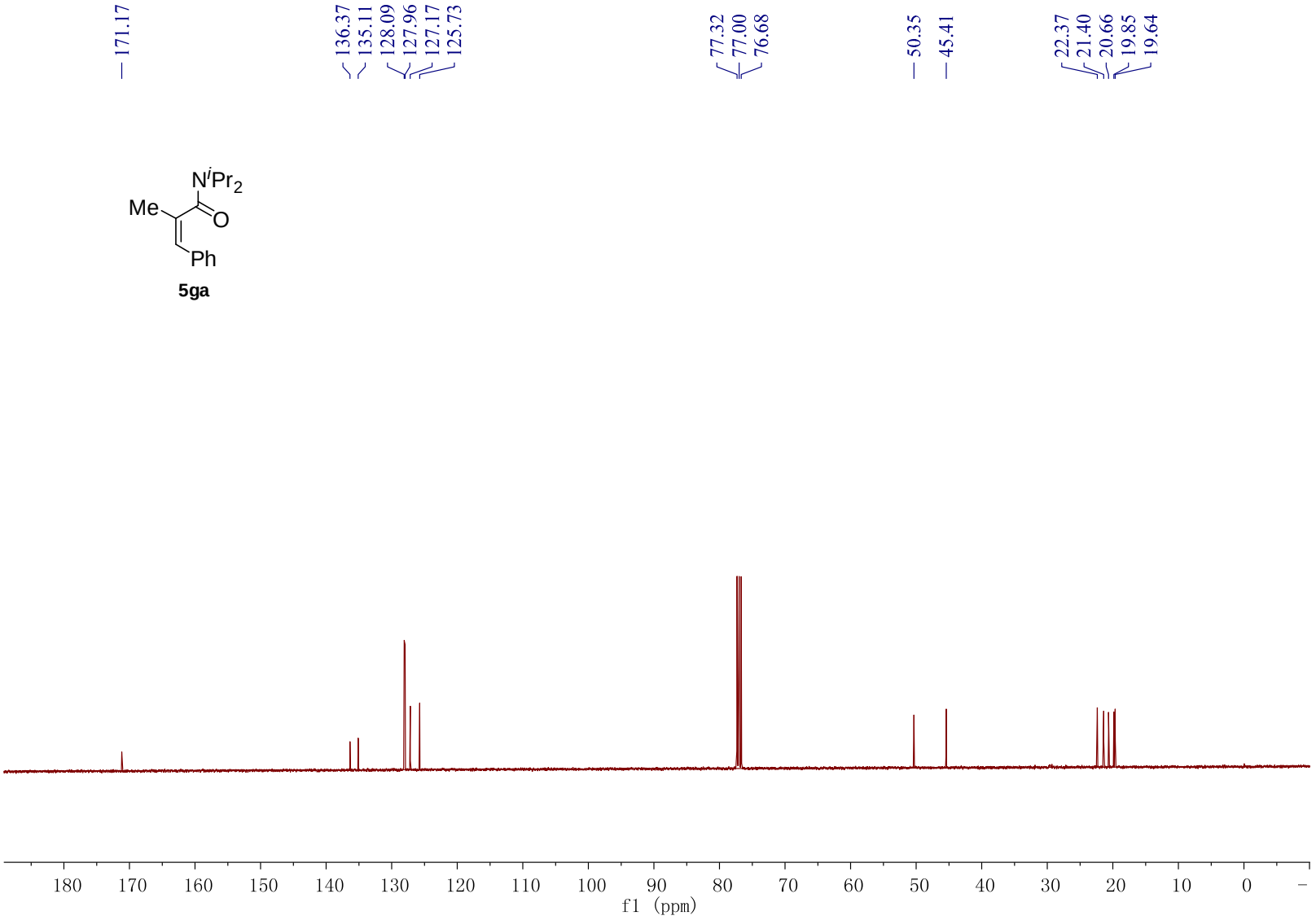

4.01
4.00
3.98
3.96
3.95
3.30
3.29
3.27
3.25
3.24


2.04
2.03
1.47
1.46
1.45
1.45
1.08
1.06
0.49
0.48

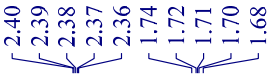

N$^i$Pr$_2$
Me
O
Ph

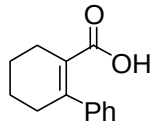
**5ga**


2.01
2.22
1.01
1.00
1.05
1.06
3.25
6.22
3.21
3.17
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)

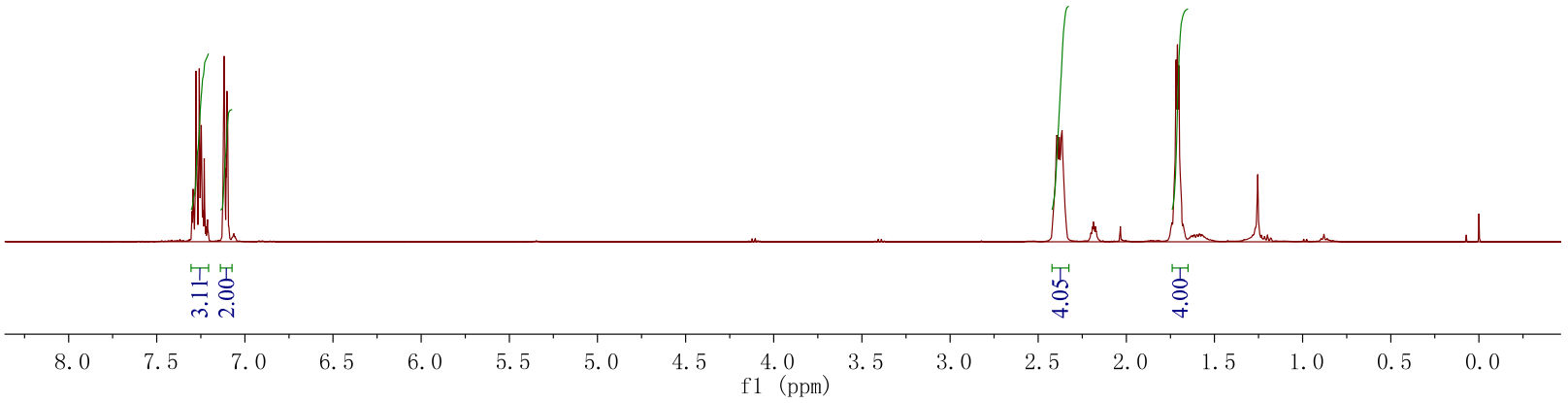

171.17
136.37
135.11
128.09
127.96
127.17
125.73
77.32
77.00
76.68
50.35
45.41
22.37
21.40
20.66
19.85
19.64
N$^{i}$Pr$_2$
Me
O
Ph
5ga
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

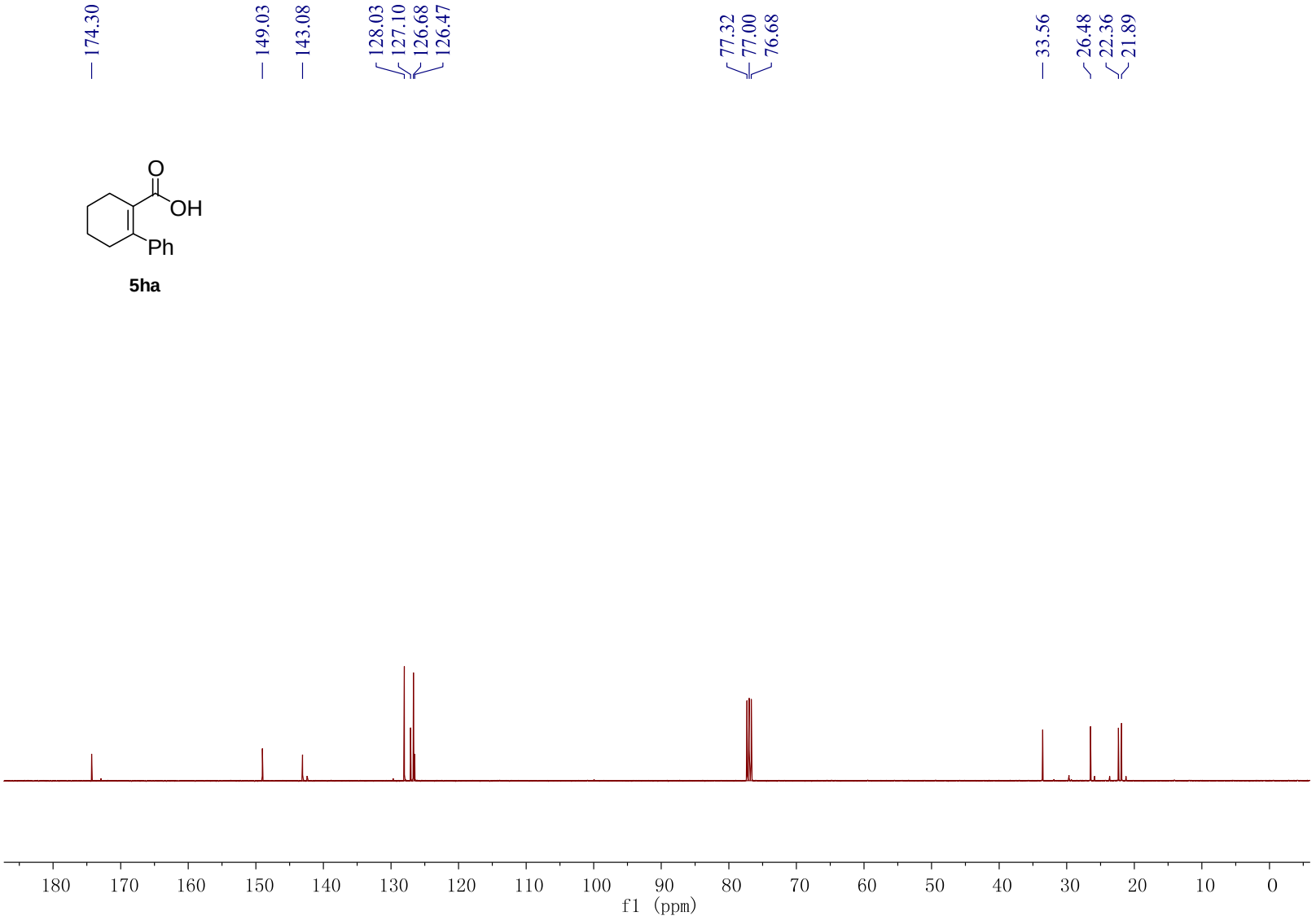

7.30
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.21
7.12
7.12
7.11
7.11
7.10
7.10

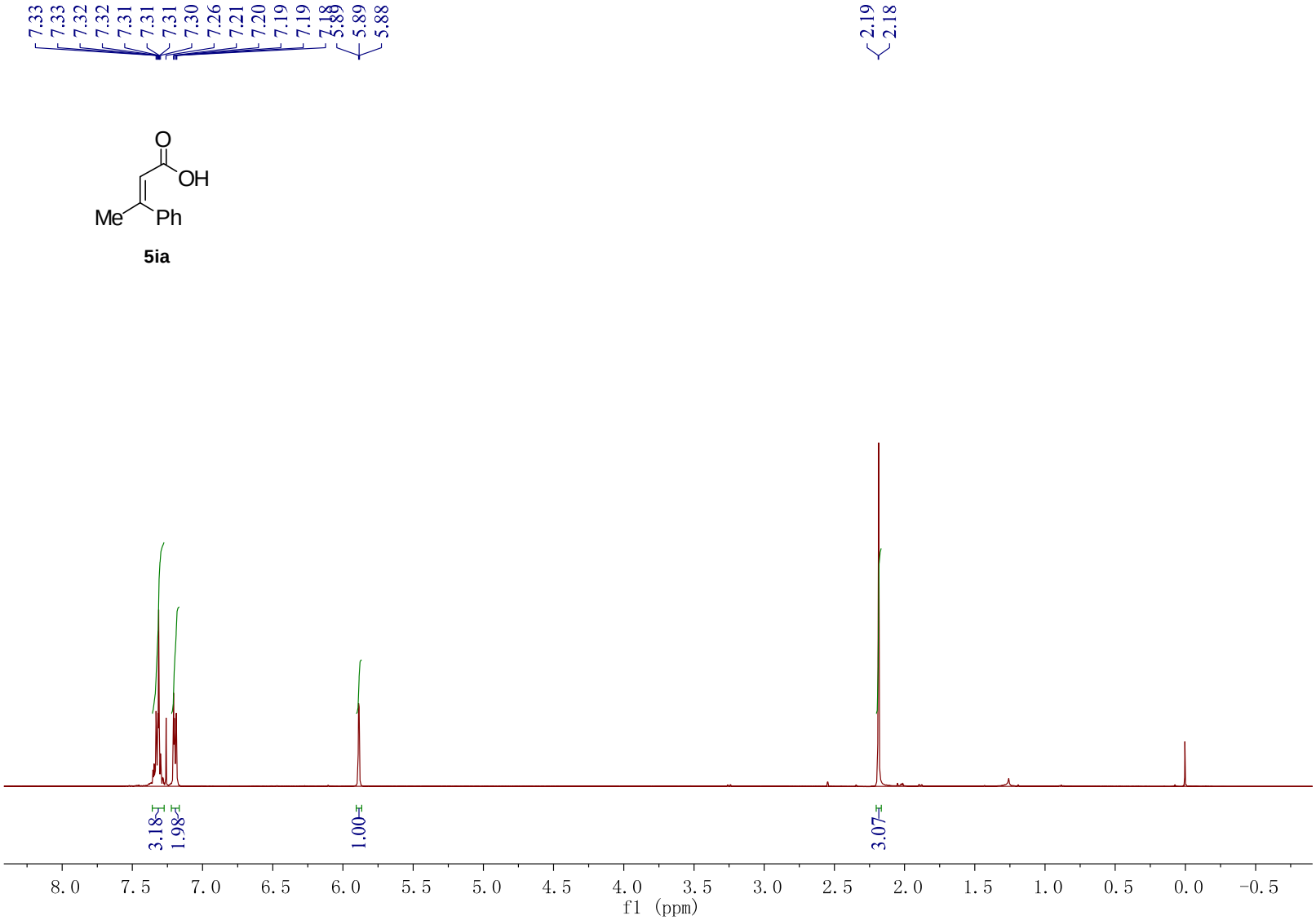

2.40
2.39
2.38
2.37
2.36
1.74
1.72
1.71
1.70
1.68

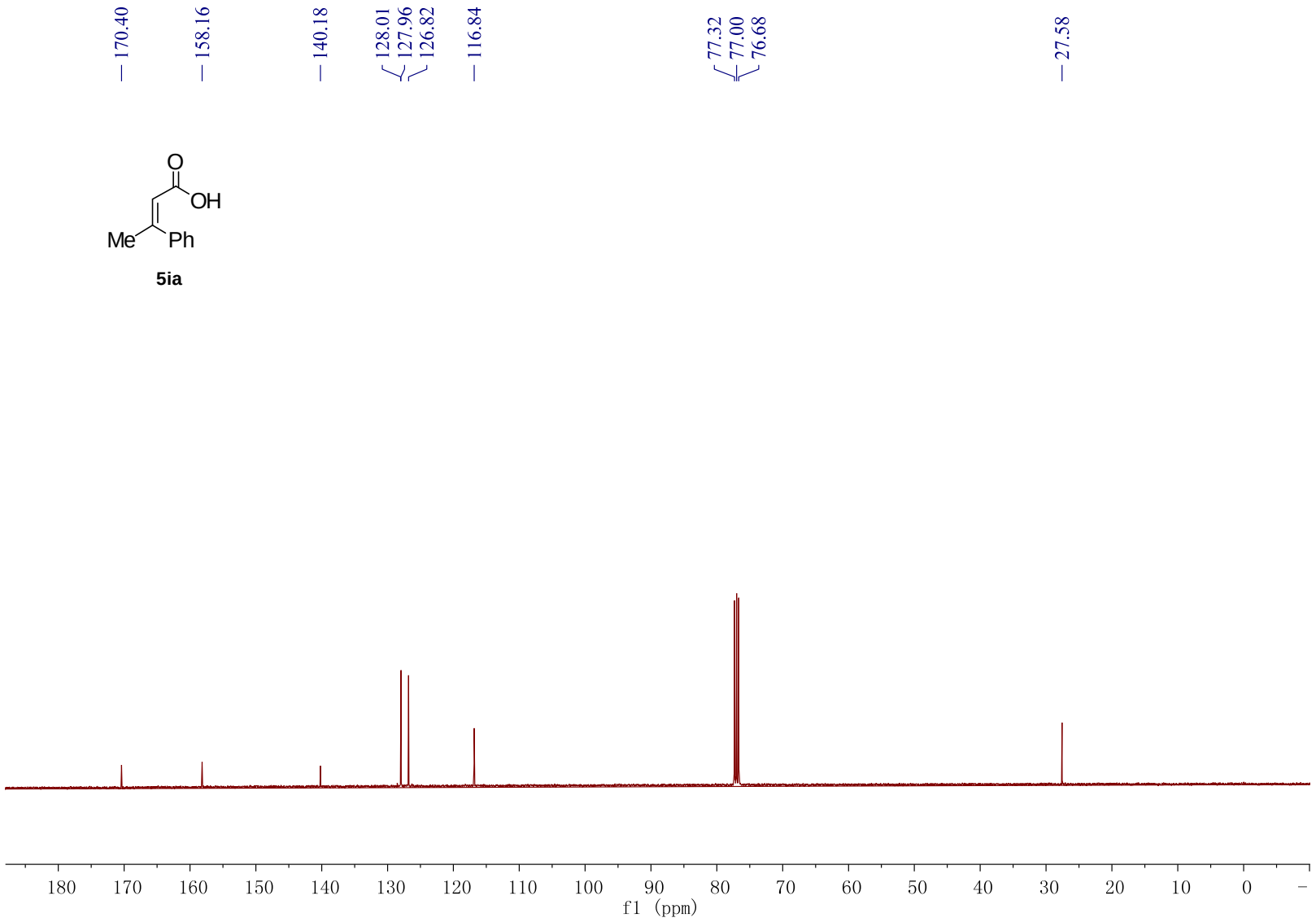

O
OH
Ph

**5ha**


3.11
2.00
4.05
4.00
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)


174.30
149.03
143.08
128.03
127.10
126.68
126.47
77.32
77.00
76.68
33.56
26.48
22.36
21.89
O
OH
Ph
5ha
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.33
7.33
7.32
7.32
7.31
7.31
7.31
7.30
7.26
7.21
7.20
7.19
7.19
7.18
5.89
5.89
5.88
2.19
2.18
O
OH
Me
Ph
5ia
3.18
1.98
1.00
3.07
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)


170.40
158.16
140.18
128.01
127.96
126.82
116.84
77.32
77.00
76.68
27.58
O
OH
Me
Ph
5ia
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)