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Supporting Information

TBHP Promoted Demethylation of *α*-Amino Carbonyl Compounds: a Concise Approach to Substituted *γ*-Lactams

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Electronic Supplementary Information Table of Contents

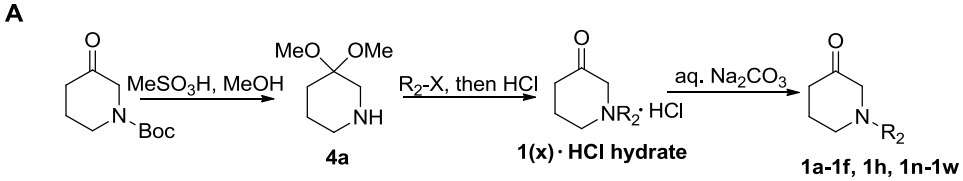
1. General Information:

All reactions were carried out in a dry solvent under dry oxygen or dry air atmosphere unless otherwise noted. NMR spectra were recorded on Bruker 400 MHz (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) spectrometers. Proton chemical shifts are reported relative to a residual solvent peak ($CDCl_3$ at 7.260 ppm). Carbon chemical shifts are reported relative to a residual solvent peak ($CDCl_3$ at 77.300 ppm). The following abbreviations were used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, br = broad. Fourier transform infrared spectra (FT-IR) were recorded on an Agilent Technologies Cary 630 instrument. High-resolution mass spectra (HRMS) were measured on a Brucker Daltonics Apex II 47e Specification. Gas chromatography-mass spectra (GC-MS) were detected on a Agilent 7890B system equipped with a Agilent 19091S-433UI column. Substrates were purchased from commercial sources and used as received. Substrates **2a, 2b** and **2l** are commercially available. Substrates **1a-1f**[1], **1g**[2], **1h**[1], **1i**[6], **1j-v**[1], **2c**[3], **2d**[2], **2e**[4], **2f**[5], **2g**[7], **2h**[6], **2i**[6], **2j**[7], **2k**[8] are prepared according to literature procedures.

2. Preparation of Substrates：

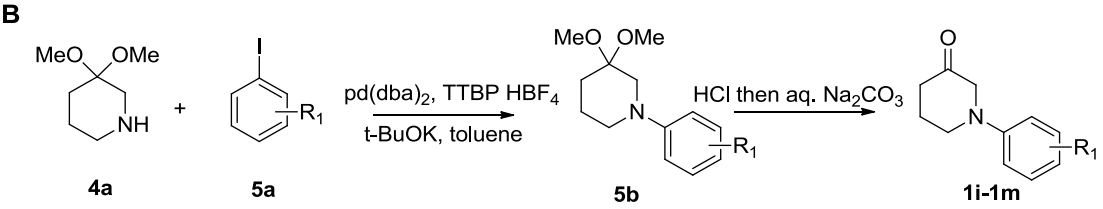
1a-1f, **1h, 1j-v** and **1w** were prepared according to literature procedure[1].

N-substituted piperidinones were prepared from commercially available N-Boc-piperidin-3-one through N-substitution of the common intermediate **4a** and subsequent hydrolysis of the ketal moiety yielding either the ketone **1(x)**. The piperidinones **2(x)** themselves were liberated from their salt prior to use.



Common intermediate **4a** react with various aryl halide via Buchwald-Hartwig amination to afford **5b**. Then through the same procedures in route A, **1i-1m** were synthesized.

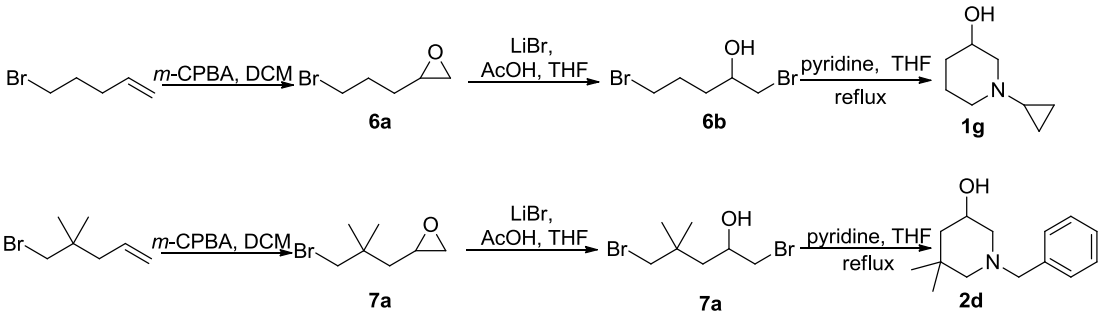
B



1g and **2d** were prepared according to literature procedure[2].

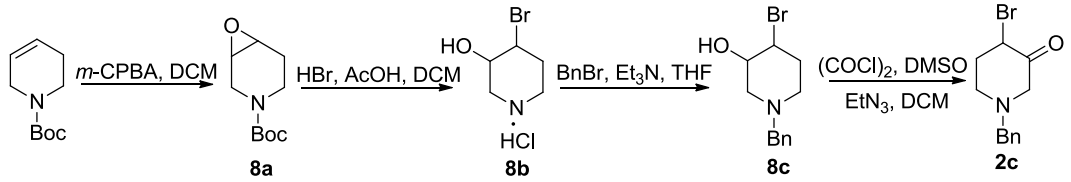
5-bromo-1-pentene was oxidized by 3-chloroperbenzoic acid (*m*-CPBA) to provide compound **6a**. Opening of the epoxide 6a with BrLi gave **6b** and subsequent reaction with cyclopropanamine in THF provided **1g**.

2d was synthesized by the same procedures with commercial available compound 5-bromo-4, 4-dimethyl-1-pentene and benzylamine.



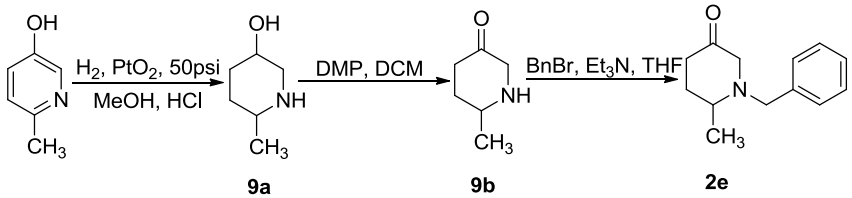
2c was prepared according to literature procedure[3].

Boc-protected tetrahydropyridine was oxidized to its epoxide **8a** with *m*-CPBA. Then treatment of **8a** with HBr selectively gave bromide **8b,** which was converted to its benzyl derivative **8c** followed by the Swern oxidation to produce **2c**



2e was prepared according to literature procedure[4].

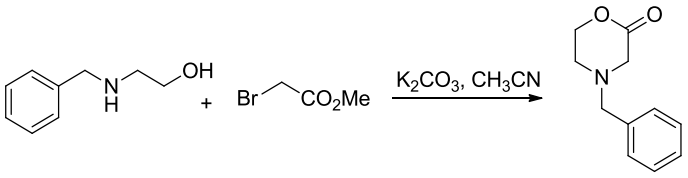
PtO_2 catalyzed hydrogenation of 3-hydroxy-6-methylpyridine to give piperidine **9a**. **9a** was then oxidized by DMP to produce **9b** followed by the conversion to its benzyl derivative **2e**.



9a **9b** **2e**

2f was prepared according to literature procedure[5]

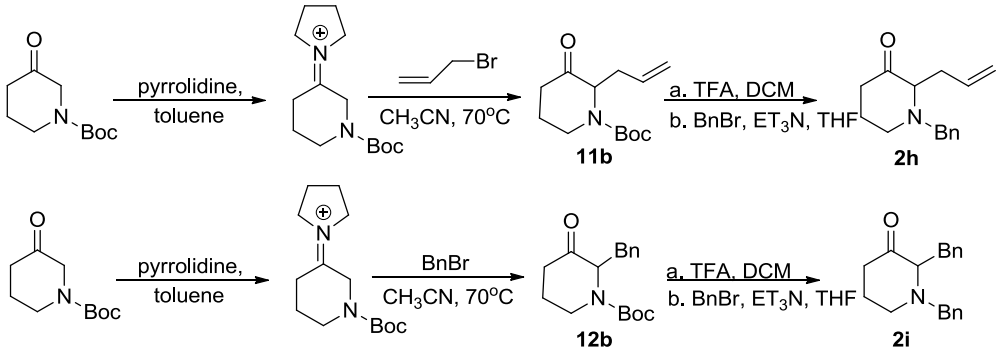
The alkylation of N-benzylethanolamine with methyl bromoacetate in the presence of K_2CO_3 as a base and in CH_3CN at room temperature provided exclusively the lactonization product 4-benzylmorpholin-2-one (**2f**).



2f

2h and **2i** were prepared according to literature procedure[6].

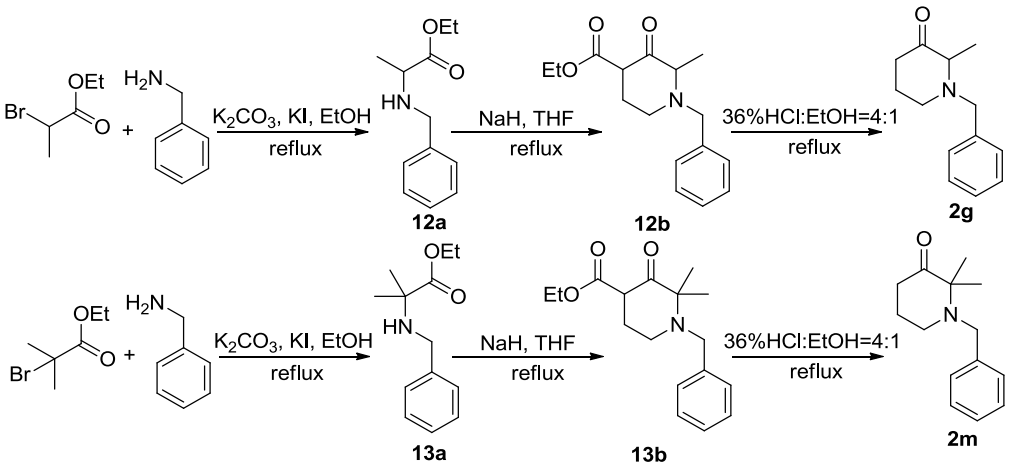
Commercial available N-Boc-piperidin-3-one was subjected to an enamine alkylation with allyl bromide or BnBr to provide **11b** or 1**2b** respectively which was transformed to its benzyl derivant in the presence of EtN_3.



11b **2h** **12b** **2i**

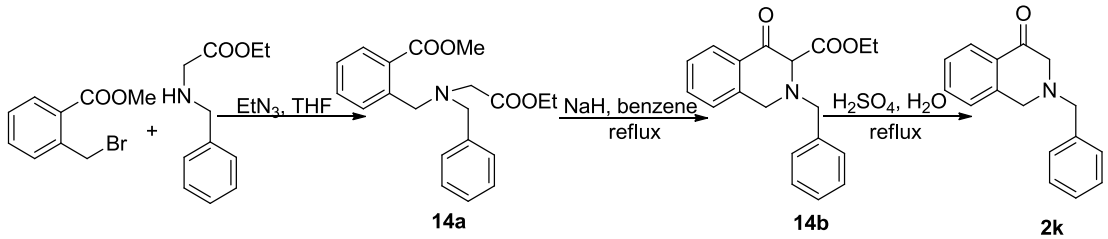
2g and **2j** were prepared according to literature procedure[7].

Heating benzylamine with Ethyl 2-bromopropionate or ethyl 2-bromoisobutyrate in ethanol in the presence of a catalytic amount of KI gave **12a** and **13a**. Dieckmann condensation of diester 12 with sodium hydride in THF gave keto ester **12b** and **13b** respectively followed by hydrolytic decarboxylation afforded **2g** and **2j**.



2k was prepared according to literature procedure[8]

Methyl 2-bromomethylbenzoate react with either *N*-benzylglycine ethyl ester to afford **14a**. Then Dieckmann cyclization of **14a** was accomplished in refluxing benzene in the presence of sodium hydride. Hydrolysis and decarboxylation of **14b** was carried out in sulfuric acid solution to yield the expected **2k**.



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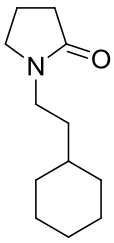
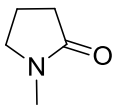
3. General Procedure for the Synthesis of Substituted *γ*-Lactams：

A sealed tube charged with *α*-amino carbonyl compound (0.1 mmol) was added 2.0 mL of toluene as solvent. Then the mixture was degassed for three times, added TBHP (0.3 mmol, *tert*-Butyl hydroperoxide) and kept stirring under nitrogen at 90 ℃ for 3h. The mixture was then cooled to room temperature, diluted with water, extracted with ethyl acetate, dried over sodium sulfate and concentrated. The crude products were purified by column chromatography on silica gel to give the corresponding products.

4. Characterization Data of all Products：

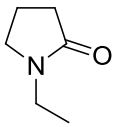


1-(2-cyclohexylethyl)pyrrolidin-2-one (1aa) Colorless oil (16.39 mg, 84% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.34 (t, *J* = 7.1 Hz, 2H), 3.30 – 3.23 (m, 2H), 2.36 (t, *J* = 8.1 Hz, 2H), 1.98 (p, *J* = 7.5 Hz, 2H), 1.67 (q, *J* = 16.6, 15.6 Hz, 5H), 1.41 – 1.33 (m, 2H), 1.24 – 1.08 (m, 4H), 0.88 (q, *J* = 10.8, 9.7 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.95, 47.24, 40.65, 35.67, 34.89, 33.39, 31.41, 26.74, 26.45, 18.14; IR (KBr ν/cm^{-1}) 2926, 2855, 1425, 1463, 1496, 1287, 1267, 806; HRMS (ESI^{+}) Calcd for $C_{12}H_{22}NO$ [M + H]$^{+}$ 196.1696, found 196.1692.

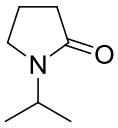


1-cyclopropylpyrrolidin-2-one (1ab): Colorless oil (8.42 mg, 85% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.35 (t, *J* = 7.1 Hz, 2H), 2.81 (s, 3H), 2.33 (t, *J* = 8.1 Hz, 2H), 2.04 – 1.93 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.27, 49.63, 30.89, 29.78, 17.87; IR (KBr ν/cm^{-1}) 1836, 1855, 1322, 1243, 1176, 1077, 926; HRMS (ESI^{+}) Calcd for $C_5H_{10}NO$ [M + H]$^{+}$ 100.0757, found 100.0754.

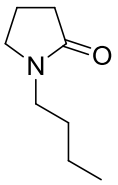
1-ethylpyrrolidin-2-one (1ac): Colorless oil (9.49 mg, 84% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ3.39 – 3.27 (m, 4H), 2.35 (t, *J* = 8.1 Hz, 2H), 2.06 – 1.86 (m, 2H), 1.09 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ174.80, 46.72, 37.32, 31.39, 18.03, 12.73.; IR (KBr ν/cm^{-1}) 2937, 2972, 1881, 1498, 1459, 1127, 839; HRMS (ESI^{+}) Calcd for $C_6H_{12}NO$ $[M + H]^{+}$ 114.0913, found 114.0917.



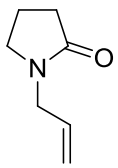
1-isopropylpyrrolidin-2-one (1ad): Colorless oil (10.42 mg, 82% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.36 (m, *J* = 6.8 Hz, 1H), 3.32 (t, *J* = 7.0 Hz, 2H), 2.37 (t, *J* = 8.1 Hz, 2H), 1.98 (p, *J* = 7.5 Hz, 2H), 1.12 (d, *J* = 6.8 Hz, 6H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.45, 42.63, 41.96, 31.92, 20.09, 18.28.; IR (KBr ν/cm^{-1}) 2972, 1677, 1241, 1366, 1459, 1164, 1066, 962; HRMS (ESI^{+}) Calcd for $C_7H_{14}NO$ $[M + H]^{+}$ 128.1070, found 128.1073.



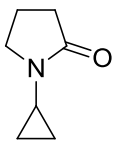
1-butylpyrrolidin-2-one (1ae): Colorless oil (12.70 mg, 90% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.36 (t, *J* = 7.0 Hz, 2H), 3.26 (t, *J* = 7.4 Hz, 2H), 2.37 (t, *J* = 8.1 Hz, 2H), 2.05 – 1.93 (m, 2H), 1.48 (dt, *J* = 15.0, 7.6 Hz, 2H), 1.37 – 1.23 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.10, 47.36, 42.54, 31.40, 29.66, 20.34, 18.20, 14.05; IR (KBr ν/cm^{-1}) 1688, 1261, 1322, 1422, 1276, 1126, 751; HRMS (ESI^{+}) Calcd for $C_8H_{16}NO$ $[M + H]^{+}$ 142.1226, found 142.1222.



1-allylpyrrolidin-2-one (1af): Colorless oil (10.76 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ5.73 – 5.60 (m, 1H), 5.17 – 5.07 (m, 2H), 3.82 (d, *J* = 6.0 Hz, 2H), 3.29 (t, *J* = 7.1 Hz, 2H), 2.34 (t, *J* = 8.1 Hz, 2H), 2.03 – 1.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ174.87, 132.62, 117.87, 46.87, 45.32, 31.11, 17.92; IR (KBr ν/cm^{-1}) 1688, 1440, 1488, 1464, 1306, 1284, 926; HRMS (ESI^{+}) Calcd for $C_7H_{12}NO$ $[M + H]^{+}$ 126.0913, found 126.0916.

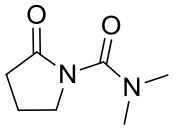


1-cyclopropylpyrrolidin-2-one (1ag): Colorless oil (10.88 mg, 87% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ3.31 (t, *J* = 7.1 Hz, 2H), 2.69 – 2.61 (m, 1H), 2.39 (t, *J* = 8.1 Hz, 2H), 2.02 – 1.92 (m, 2H), 0.80 – 0.73 (m, 2H), 0.68 (td, *J* = 7.6, 4.3 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ176.37, 47.58,

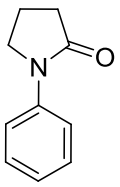


31.91, 25.24, 18.10, 4.93.; IR (KBr ν/cm^{-1}) 2368, 1686, 1459, 1276, 834, 766,; HRMS (ESI$^+$) Calcd for $C_7H_{12}NO$ $[M + H]^+$ 126.0913, found 126.0917.

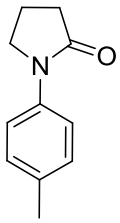
N,N-dimethyl-2-oxopyrrolidine-1-carboxamide (1ah): Colorless oil (8.27 mg, 53% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.69 (t, *J* = 7.0 Hz, 2H), 2.94 (s, 6H), 2.41 (t, *J* = 8.0 Hz, 2H), 2.10 – 1.97 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.50, 154.88, 47.05, 38.72, 36.83, 32.28, 18.63; IR (KBr ν/cm^{-1}) 2372, 2342, 1720, 1671, 1489, 1019, 939, 773; HRMS (ESI$^+$) Calcd for $C_7H_{13}N_2O_2$ $[M + H]^+$157.0972, found 157.0968.



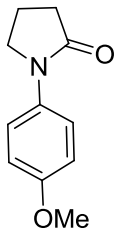
1-phenylpyrrolidin-2-one (1ai): Colorless oil (10.79 mg, 67% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.7 Hz, 2H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.15 (t, *J* = 7.4 Hz, 1H), 3.87 (t, *J* = 7.0 Hz, 2H), 2.62 (t, *J* = 8.1 Hz, 2H), 2.17 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.51, 139.68, 129.11, 124.80, 120.26, 49.08, 33.04, 18.33.; IR (KBr ν/cm^{-1}) 1686, 1489, 1339, 1226, 1123, 942, 693; HRMS (ESI$^+$) Calcd for $C_{10}H_{12}NO$ $[M + H]^+$ 162.0913, found 162.0910.



1-(p-tolyl)pyrrolidin-2-one (1ak): White solid (13.31 mg, 76% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.5 Hz, 2H), 7.16 (d, *J* = 8.2 Hz, 2H), 3.83 (t, *J* = 7.0 Hz, 2H), 2.59 (t, *J* = 8.1 Hz, 2H), 2.32 (s, 3H), 2.14 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.34, 137.15, 134.46, 129.61, 120.35, 49.19, 32.93, 21.12, 18.30.; IR (KBr ν/cm^{-1}) 2361, 2344, 1686, 1517, 1395, 821, 719; HRMS (ESI$^+$) Calcd for $C_{11}H_{14}NO$ $[M + H]^+$ 176.1070, found 176.1074.

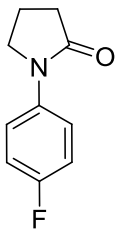


1-(4-methoxyphenyl)pyrrolidin-2-one (1al): White solid (15.29 mg, 80% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ7.49 (d, *J* = 9.1 Hz, 2H), 6.90 (d, *J* = 9.1 Hz, 2H), 3.84 (d, *J* = 7.0 Hz, 2H), 3.80 (s, 3H), 2.59 (t, *J* = 8.1 Hz, 2H), 2.15 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.22, 156.87, 132.92, 122.15, 114.34, 55.77, 49.50, 32.76, 18.34.; IR (KBr ν/cm^{-1}) 2372, 2687, 1682, 1517, 1256, 1181, 829; HRMS (ESI$^+$) Calcd for $C_{11}H_{14}NO_2$ $[M + H]^+$

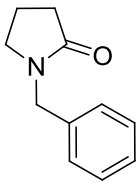


192.1019, found 192.1016.

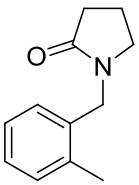
1-(4-fluorophenyl)pyrrolidin-2-one (1am): White solid (9.67 mg, 54% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ7.62 – 7.50 (m, 2H), 7.11 – 7.00 (m, 2H), 3.84 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.1 Hz, 2H), 2.17 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.40, 159.77 (d, *J* = 244.0 Hz), 135.78 (d, *J* = 2.8 Hz), 121.98 (d, *J* = 7.9 Hz), 115.77 (d, *J* = 22.4 Hz), 49.29, 32.79, 18.25.; IR (KBr ν/cm^{-1}) 1686, 1511, 1394, 1297, 1228, 1121, 818, 681; HRMS (ESI^{+}) Calcd for $C_{10}H_{11}FNO$ $[M + H]^{+}$180.0819, found 180.0823.



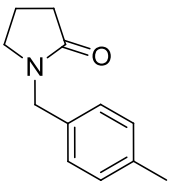
1-benzylpyrrolidin-2-one (1an): Yellow solid (13.13 mg, 75% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ7.35 – 7.22 (m, 5H), 4.45 (s, 2H), 3.26 (t, *J* = 7.1 Hz, 2H), 2.45 (t, *J* = 8.1 Hz, 2H), 1.99 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.24, 136.85, 128.94, 128.40, 127.82, 77.50, 46.88, 31.22, 18.01.; IR (KBr ν/cm^{-1}) 1686, 1656, 1474, 11276, 1080, 766; HRMS (ESI^{+}) Calcd for $C_{11}H_{14}NO$ $[M + H]^{+}$ 176.1070, found 176.1074.



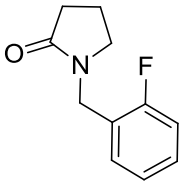
1-(2-methylbenzyl)pyrrolidin-2-one (1ao): Yellow solid (13.62 mg, 72% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ7.17 (m, *J* = 15.6, 7.8 Hz, 4H), 4.47 (s, 2H), 3.20 (t, *J* = 7.1 Hz, 2H), 2.45 (t, *J* = 8.1 Hz, 2H), 2.30 (s, 3H), 1.98 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.69, 136.73, 134.21, 130.57, 128.82, 127.72, 126.07, 46.61, 44.67, 30.97, 19.15, 17.77.; IR (KBr ν/cm^{-1}) 1688, 1556, 1478, 1336, 1261, 1048, 983, 816; HRMS (ESI^{+}) Calcd for $C_{12}H_{16}NO$ $[M + H]^{+}$190.1226, found 190.1223.



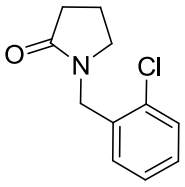
1-(4-methylbenzyl)pyrrolidin-2-one (1ap): Yellow solid (15.13 mg, 80% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (s, 4H), 4.41 (s, 2H), 3.24 (t, *J* = 7.1 Hz, 2H), 2.43 (t, *J* = 8.1 Hz, 2H), 2.33 (s, 3H), 2.04 – 1.91 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.14, 137.50, 133.81, 129.60, 128.43, 46.81, 46.58, 31.28, 21.38, 17.99.; IR (KBr ν/cm^{-1}) 1684, 1486, 1459, 1423, 1261, 1023, 883, 736; HRMS (ESI^{+}) Calcd for $C_{12}H_{16}NO$ $[M + H]^{+}$ 190.1226, found 190.1230.



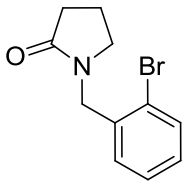
1-(2-fluorobenzyl)pyrrolidin-2-one (1aq): Yellow solid (14.10 mg, 73% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.22 (m, 2H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.08 – 7.02 (m, 1H), 4.53 (s, 2H), 3.32 (t, *J* = 7.1 Hz, 2H), 2.43 (t, *J* = 8.1 Hz, 2H), 2.09 – 1.94 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.32, 161.31 (d, *J* = 246.3 Hz), 130.84 (d, *J* = 4.1 Hz), 129.66 (d, *J* = 8.1 Hz), 124.71 (d, *J* = 3.6 Hz), 123.75 (d, *J* = 15.1 Hz), 115.65 (d, *J* = 21.7 Hz), 47.07, 40.10, 31.06, 18.03.; IR (KBr ν/cm^{-1}) 1686, 1490, 1457, 1422, 1280, 1228, 1030, 758; HRMS (ESI^{+}) Calcd for $C_{11}H_{13}FNO$ $[M + H]^{+}$ 194.0976, found 194.0979.



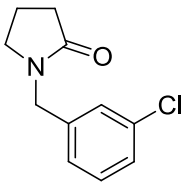
1-(2-chlorobenzyl)pyrrolidin-2-one (1ar): Yellow solid (15.89 mg, 76% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ7.37 (dd, *J* = 6.7, 2.3 Hz, 1H), 7.29 – 7.20 (m, 3H), 4.61 (s, 2H), 3.32 (t, *J* = 7.1 Hz, 2H), 2.45 (t, *J* = 8.1 Hz, 2H), 2.03 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.44, 134.33, 134.02, 130.07, 129.88, 129.17, 127.45, 47.23, 44.18, 31.02, 18.15.; IR (KBr ν/cm^{-1}) 2365, 2338, 1686, 1422, 1287, 1056, 1126, 751; HRMS (ESI^{+}) Calcd for $C_{11}H_{13}ClNO$ $[M + H]^{+}$ 210.0680, found 210.0677.



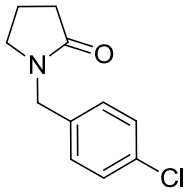
1-(2-bromobenzyl)pyrrolidin-2-one (1as): Yellow solid (18.22 mg, 72% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 1.3 Hz, 1H), 7.26 (d, *J* = 1.0 Hz, 1H), 7.23 (s, 1H), 7.15 – 7.11 (m, 1H), 4.43 (s, 2H), 3.27 (t, *J* = 7.1 Hz, 2H), 2.46 (t, *J* = 8.1 Hz, 2H), 2.07 – 1.92 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.34, 138.97, 134.85, 130.27, 128.38, 128.08, 126.50, 46.94, 46.39, 31.07, 18.02.; IR (KBr ν/cm^{-1}) 1686, 1599, 1541, 1507, 1474, 1284, 1079, 948; HRMS (ESI^{+}) Calcd for $C_1H_{13}BrNO$ $[M + H]^{+}$ 254.0175, found 254.0171.



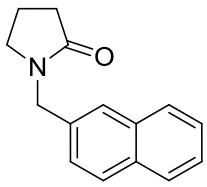
1-(3-chlorobenzyl)pyrrolidin-2-one (1at): Yellow solid (14.43 mg, 69% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 1.4 Hz, 1H), 7.26 (d, *J* = 1.1 Hz, 1H), 7.23 (s, 1H), 7.15 – 7.10 (m, 1H), 4.43 (s, 2H), 3.27 (t, *J* = 7.1 Hz, 2H), 2.46 (t, *J* = 8.1 Hz, 2H), 2.11 – 1.84 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.33, 138.98, 134.86, 130.27, 128.39, 128.08, 126.50, 46.93, 46.39, 31.07, 18.03.; IR (KBr ν/cm^{-1}) 1686, 1588, 1459, 1362, 1189, 904, 768; HRMS (ESI^{+}) Calcd for $C_{11}H_{13}ClNO$ $[M + H]^{+}$ 210.0680, found 210.0676.



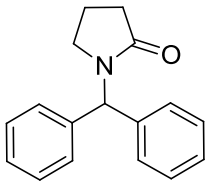
1-(4-chlorobenzyl)pyrrolidin-2-one (1au): Yellow solid (15.47 mg, 74% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ7.30 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 8.3 Hz, 2H), 4.42 (s, 2H), 3.25 (t, *J* = 7.1 Hz, 2H), 2.44 (t, *J* = 8.1 Hz, 2H), 2.00 (p, *J* = 7.5 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.29, 135.41, 133.70, 129.77, 129.12, 46.85, 46.23, 31.11, 18.02.; IR (KBr ν/cm^{-1}) 1686, 1492, 1408, 1261, 1094, 853, 751; HRMS (ESI^{+}) Calcd for $C_{11}H_{13}ClNO$ $[M + H]^{+}$ 210.0680, found 210.0683.



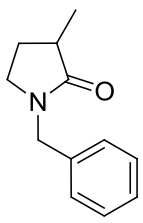
1-(naphthalen-2-ylmethyl)pyrrolidin-2-one (1av): White solid (17.56 mg, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.76 (m, 3H), 7.69 (s, 1H), 7.51 – 7.42 (m, 2H), 7.37 (dd, *J* = 8.4, 1.4 Hz, 1H), 4.61 (s, 2H), 3.28 (t, *J* = 7.1 Hz, 2H), 2.48 (t, *J* = 8.1 Hz, 2H), 2.06 – 1.90 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) 175.30, 134.40, 133.59, 133.10, 128.86, 127.98, 127.22, 126.56, 126.41, 126.25, 47.07, 46.90, 31.27, 18.03.; IR (KBr ν/cm^{-1}) 2361, 2342, 1684, 1602, 1541, 1492, 1265, 784; HRMS (ESI^{+}) Calcd for $C_{15}H_{16}NO$ $[M + H]^{+}$ 226.1226, found 226.1229.



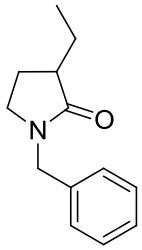
1-benzhydrylpyrrolidin-2-one (1aw): White solid (17.08 mg, 68% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.27 (m, 6H), 7.18 (d, *J* = 6.8 Hz, 4H), 6.62 (s, 1H), 3.20 (t, *J* = 7.0 Hz, 2H), 2.49 (t, *J* = 8.0 Hz, 2H), 2.09 – 1.94 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.06, 138.72, 128.53, 128.51, 127.52, 58.51, 44.30, 31.20, 18.20. IR (KBr ν/cm^{-1}) 21686, 1600, 1494, 1276, 1077, 1030, 893, 751; HRMS (ESI^{+}) Calcd for $C_{17}H_{18}NO$ $[M + H]^{+}$ 252.1383, found 252.1379.



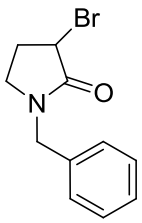
cyclopropylpyrrolidin-2-one (2aa): Yellow solid (16.26 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.16 (m, 5H), 4.54 – 4.36 (m, 2H), 3.24 – 3.09 (m, 2H), 2.51 (h, *J* = 7.5 Hz, 1H), 2.26 – 2.13 (m, 1H), 1.59 (dq, *J* = 12.5, 8.5 Hz, 1H), 1.23 (d, *J* = 7.1 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ177.59, 136.96, 128.89, 128.32, 127.72, 47.01, 44.88, 36.99, 27.32, 16.67.; IR (KBr ν/cm^{-1}) 1686, 1455, 1297, 1203, 1082, 989; HRMS (ESI^{+}) Calcd for $C_{12}H_{16}NO$ $[M + H]^{+}$ 190.1226, found 190.1222.



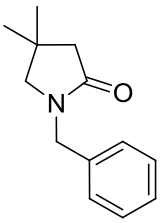
1-benzyl-3-ethylpyrrolidin-2-one (2ab): Yellow solid (17.06 mg, 84% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.19 (m, 5H), 4.45 (q, *J* = 14.7 Hz, 2H), 3.21 – 3.13 (m, 2H), 2.40 (m, *J* = 8.7, 4.4 Hz, 1H), 2.22 – 2.06 (m, 1H), 2.01 – 1.85 (m, 1H), 1.65 (m, *J* = 12.7, 8.3 Hz, 1H), 1.53 – 1.33 (m, 1H), 0.97 (t, *J* = 7.4 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ176.90, 137.00, 128.89, 128.35, 127.72, 46.92, 45.12, 43.55, 24.55, 24.38, 11.68.; IR (KBr ν/cm^{-1}) 1686, 1565, 1438, 1288, 1162, 1102, 1050, 972, 864,; HRMS (ESI^{+}) Calcd for $C_{13}H_{18}NO$ $[M + H]^{+}$ 204.1383, found 204.1386.



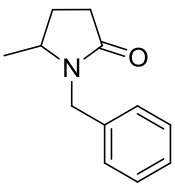
1-benzyl-3-bromopyrrolidin-2-one (2ac): Yellow oil (15.69 mg, 62% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.25 (m, 5H), 4.59 – 4.40 (m, 3H), 3.42 (dt, *J* = 9.9, 7.5 Hz, 1H), 3.20 (m, *J* = 10.1, 8.0, 2.3 Hz, 1H), 2.56 (m, *J* = 15.1, 7.7 Hz, 1H), 2.34 – 2.25 (m, 1H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ170.93, 135.84, 129.04, 128.29, 128.08, 47.34, 44.80, 44.52, 30.38.; IR (KBr ν/cm^{-1}) 2383, 2344, 1701, 1494, 1425, 1282, 1161, 950; HRMS (ESI^{+}) Calcd for $C_{11}H_{13}BrNO$ $[M + H]^{+}$ 254.0175, found 254.0173.



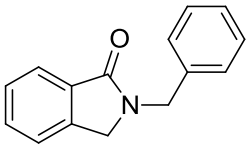
1-benzyl-4,4-dimethylpyrrolidin-2-one (2ad): Yellow solid (16.45 mg, 81% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 5H), 4.44 (s, 2H), 2.96 (s, 2H), 2.27 (s, 2H), 1.09 (s, 6H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ174.40, 136.78, 128.87, 128.38, 127.75, 59.95, 46.70, 46.52, 32.82, 28.02.; IR (KBr ν/cm^{-1}) 1686, 1560, 1469, 1257, 1197, 1072, 903, 802; HRMS (ESI^{+}) Calcd for $C_{13}H_{18}NO$ $[M + H]^{+}$ 204.1383, found 204.1379.



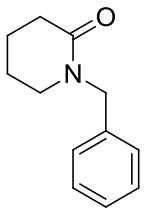
1-benzyl-5-methylpyrrolidin-2-one (2ae): Yellow solid (14.75 mg, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.21 (m, 5H), 4.97 (d, *J* = 15.0 Hz, 1H), 3.98 (d, *J* = 15.0 Hz, 1H), 3.58 – 3.33 (m, 1H), 2.56 – 2.34 (m, 2H), 2.21 – 2.10 (m, 1H), 1.66 – 1.54 (m, 1H), 1.16 (d, *J* = 6.3 Hz, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ175.25, 137.07, 128.88, 128.24, 127.67, 53.04, 44.12, 30.59, 26.91, 19.87.; IR (KBr ν/cm^{-1}) 1686, 1490, 1313, 1127, 803, 745; HRMS (ESI^{+}) Calcd for $C_{12}H_{16}NO$ $[M + H]^{+}$ 190.1226, found 190.1221.



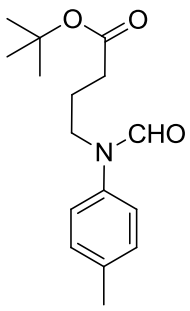
2-benzylisoindolin-1-one (2ak): White solid (9.82 mg, 44% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.2 Hz, 1H), 7.55 – 7.44 (m, 2H), 7.41 – 7.28 (m, 6H), 4.81 (s, 2H), 4.27 (s, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ168.75, 141.50, 137.32, 132.92, 131.62, 129.07, 128.44, 128.32, 127.95, 124.18, 123.02, 49.70, 46.67.; IR (KBr ν/cm^{-1}) 1638, 1545, 1490, 1469, 1265, 914, 839; HRMS (ESI^{+}) Calcd for $C_{15}H_{14}NO$ $[M + H]^{+}$ 224.1070, found 224.1073.



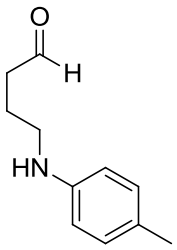
1-benzylpiperidin-2-one (2al): Colorless oil (16.45 mg, 87% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.21 (m, 5H), 4.60 (s, 2H), 3.19 (t, *J* = 5.6 Hz, 2H), 2.47 (t, *J* = 6.3 Hz, 2H), 1.84 – 1.74 (m, 4H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ170.10, 137.58, 128.81, 128.31, 127.54, 50.34, 47.50, 32.68, 23.45, 21.66.; IR (KBr ν/cm^{-1}) 1638, 1449, 1418, 1282, 1261, 1071, 993, 764, 711; HRMS (ESI^{+}) Calcd for $C_{12}H_{16}NO$ $[M + H]^{+}$ 190.1226, found 190.1222.

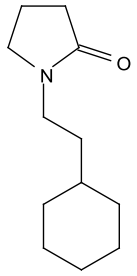


tert-butyl 4-(N-p-tolylformamido)butanoate (1bk): Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 3.86 – 3.75 (m, 2H), 2.36 (s, 3H), 2.23 (t, *J* = 7.4 Hz, 2H), 1.86 – 1.78 (m, 2H), 1.41 (s, 9H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ172.41, 162.70, 138.52, 137.19, 130.54, 124.52, 80.70, 44.63, 32.90, 28.33, 23.36, 21.18.; IR (KBr ν/cm^{-1}) 1756, 1738, 1378, 1346,1253, 893, 764; HRMS (ESI^{+}) Calcd for $C_{16}H_{23}NNaO_3$ $[M + Na]^{+}$ 300.1570, found 300.1564.



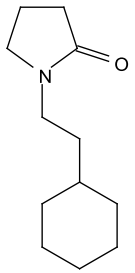
4-(p-tolylamino)butanal (1ck): Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 3.78 – 3.71 (m, 2H), 2.36 (s, 3H), 1.54 (h, *J* = 7.4 Hz, 2H), 0.88 (t, *J* = 7.4 Hz, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.72, 138.72, 137.09, 130.44, 124.70, 46.90, 21.19, 21.11, 11.48; IR (KBr ν/cm^{-1}) 1724, 1658, 1267, 1076, 853, 806; HRMS (ESI^{+}) Calcd for $C_{11}H_{15}NNaO$ $[M + Na]^{+}$ 200.1046, found 200.1056.




N
O

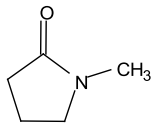
1aa

3.36
3.34
3.32
3.29
3.27
3.25
2.38
2.36
2.34
2.02
2.00
1.98
1.97
1.95
1.72
1.69
1.65
1.60
1.40
1.38
1.36
1.34
1.23
1.22
1.21
1.20
1.18
1.15
1.12
1.09
0.93
0.90
0.87
0.84
2.08
2.03
2.00
2.21
5.32
2.11
4.36
2.22
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


O
N

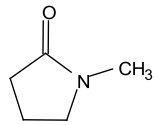
1aa

174.95
47.24
40.65
35.67
34.89
33.39
31.41
26.74
26.45
18.14
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


O
N
CH3

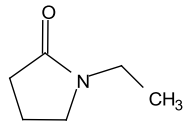
1ab

3.36
3.35
3.33
2.81
2.35
2.33
2.31
2.02
2.00
1.99
1.97
1.95
2.09
3.00
2.05
2.21
f1 (ppm)


O
N
CH3

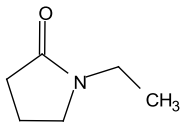
1ab

175.27
49.63
30.89
29.78
17.87
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
CH3

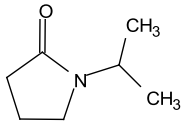
1ac

3.38
3.36
3.34
3.33
3.32
3.30
3.28
2.37
2.35
2.33
2.03
2.01
1.99
1.97
1.95
1.11
1.09
1.07
4.18
2.00
2.37
3.05
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)


O
N
CH3

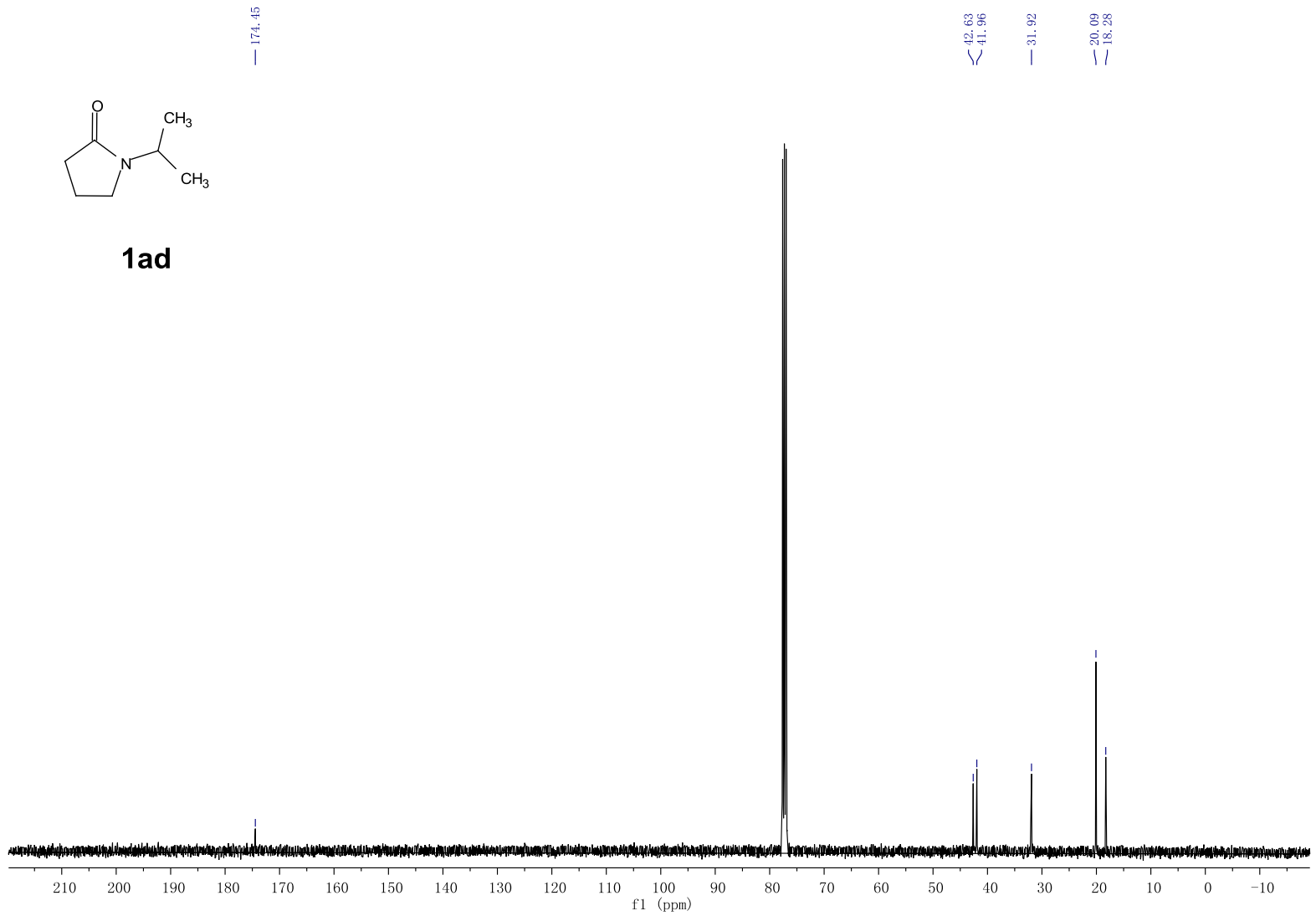
1ac

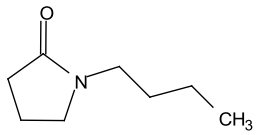
174.80
46.72
37.32
31.39
18.03
12.73
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
CH3
N
CH3

1ad

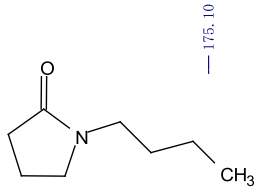
4.41
4.40
4.38
4.36
4.35
4.33
4.31
3.34
3.32
3.30
2.39
2.37
2.35
2.02
2.00
1.98
1.97
1.95
1.13
1.12
1.00
2.11
2.04
2.09
6.00
f1 (ppm)


174.45
42.63
41.96
31.92
20.09
18.28
O
N
CH3
CH3
1ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N
CH3

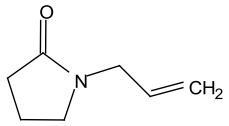
1ae

3.38
3.36
3.34
3.28
3.26
3.24
2.39
2.37
2.35
2.01
2.00
1.98
1.50
1.48
1.47
1.31
1.29
0.93
0.91
0.90
2.00
2.02
2.02
2.19
2.22
2.40
3.11
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)


O
N
CH3

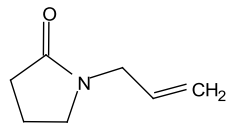
1ae

175.10
47.36
42.54
31.40
29.66
20.34
18.20
14.05
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
CH2

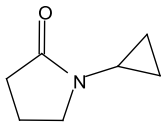
1af

5.71
5.70
5.69
5.68
5.67
5.66
5.66
5.65
5.64
5.64
5.63
5.61
5.13
5.13
5.10
5.10
5.10
5.09
5.09
3.83
3.81
3.31
3.29
3.27
2.36
2.34
2.32
2.00
1.98
1.96
1.94
1.92
1.02
1.97
2.00
2.09
2.34
2.17
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


O
N
CH2

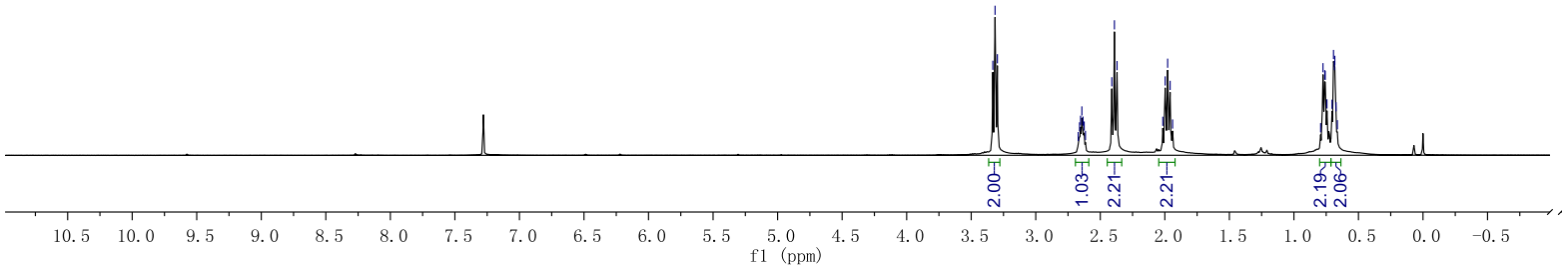
1af

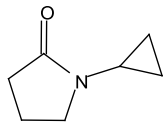
174.87
132.62
117.87
46.87
45.32
31.11
17.92
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N

1ag

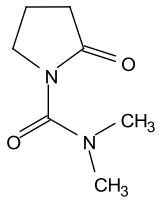

3.33
3.32
3.30
2.65
2.64
2.63
2.63
2.41
2.39
2.37
2.02
2.00
1.98
1.96
1.94
0.79
0.77
0.76
0.76
0.74
0.70
0.69
0.69
0.68
0.67
0.66


2.00
1.03
2.21
2.21
2.19
2.06
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)


O
N

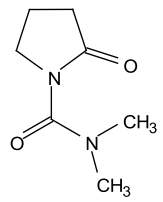
1ag

176.62
47.83
32.16
25.49
18.35
5.19
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


O
N
O
N
CH3
CH3

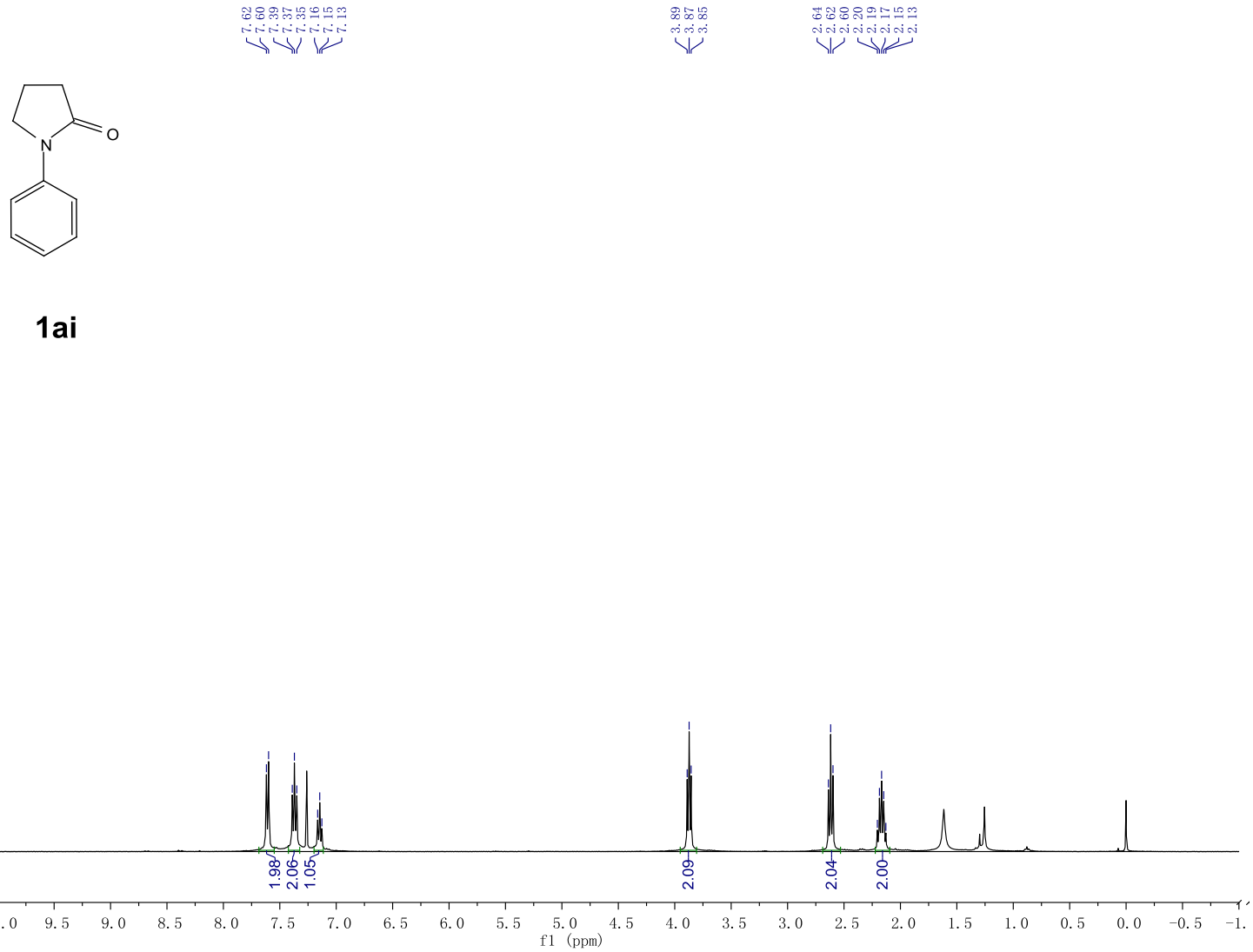
1ah

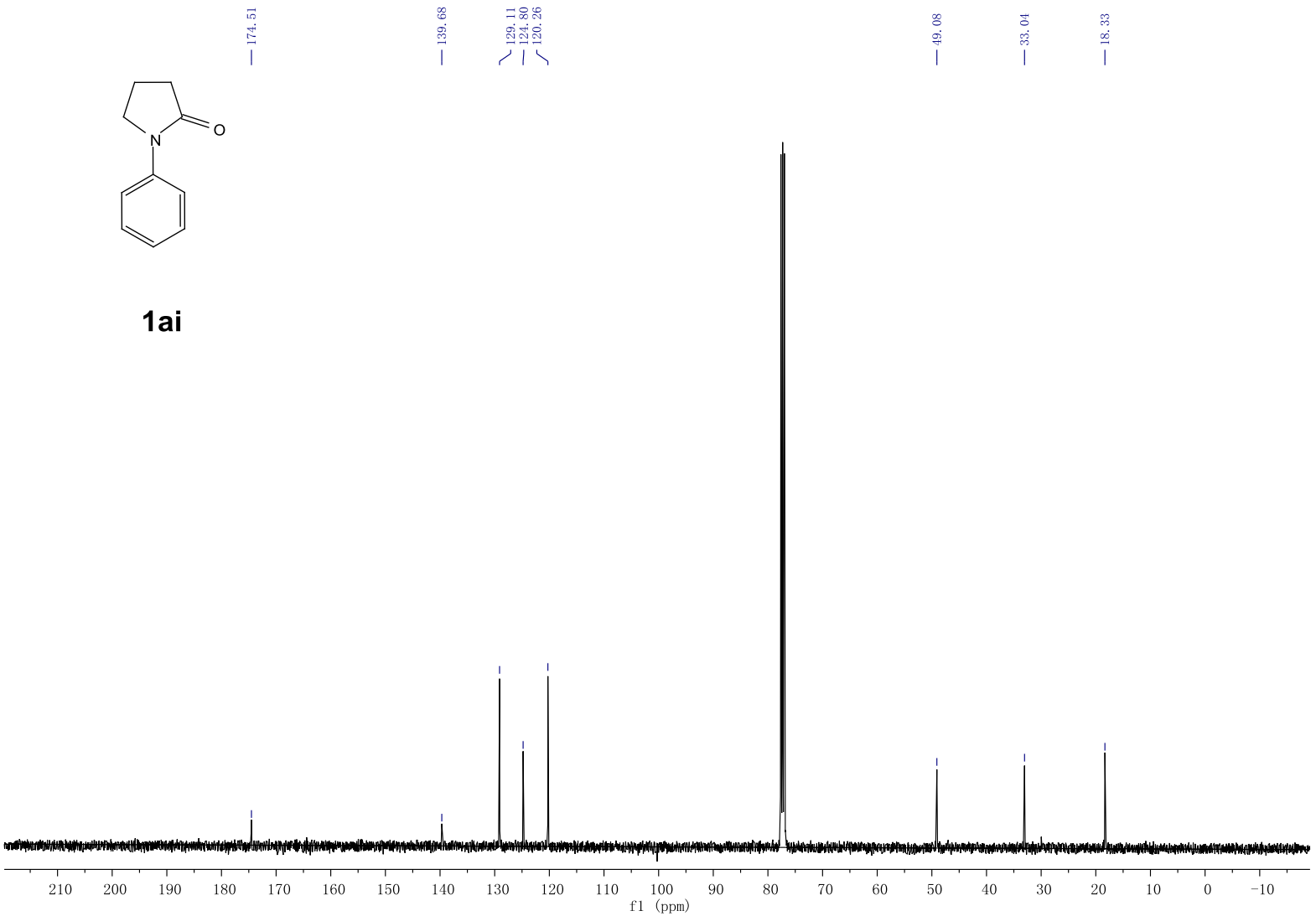
3.70
3.69
3.67
2.94
2.43
2.41
2.39
2.07
2.05
2.03
2.01
1.99
2.00
6.00
2.01
2.18
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

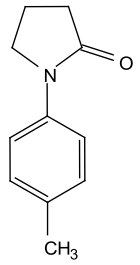

O
N
CH3
O
N
CH3

1ah

174.50
154.88
47.05
38.72
36.83
32.28
18.63
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

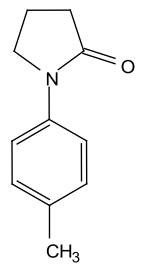

7.62
7.60
7.39
7.37
7.35
7.16
7.15
7.13
3.89
3.87
3.85
2.64
2.62
2.60
2.20
2.19
2.17
2.15
2.13
O
N
1ai
1.98
2.06
1.05
2.09
2.04
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


174.51
139.68
129.11
124.80
120.26
49.08
33.04
18.33
O
N
1ai
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
CH3

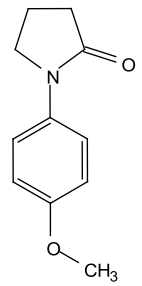
1ak

7.48
7.46
7.17
7.15
3.85
3.83
3.82
2.61
2.59
2.57
2.32
2.18
2.16
2.14
2.13
2.11
2.00
2.02
2.10
2.10
3.05
2.19
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)


O
N
CH3

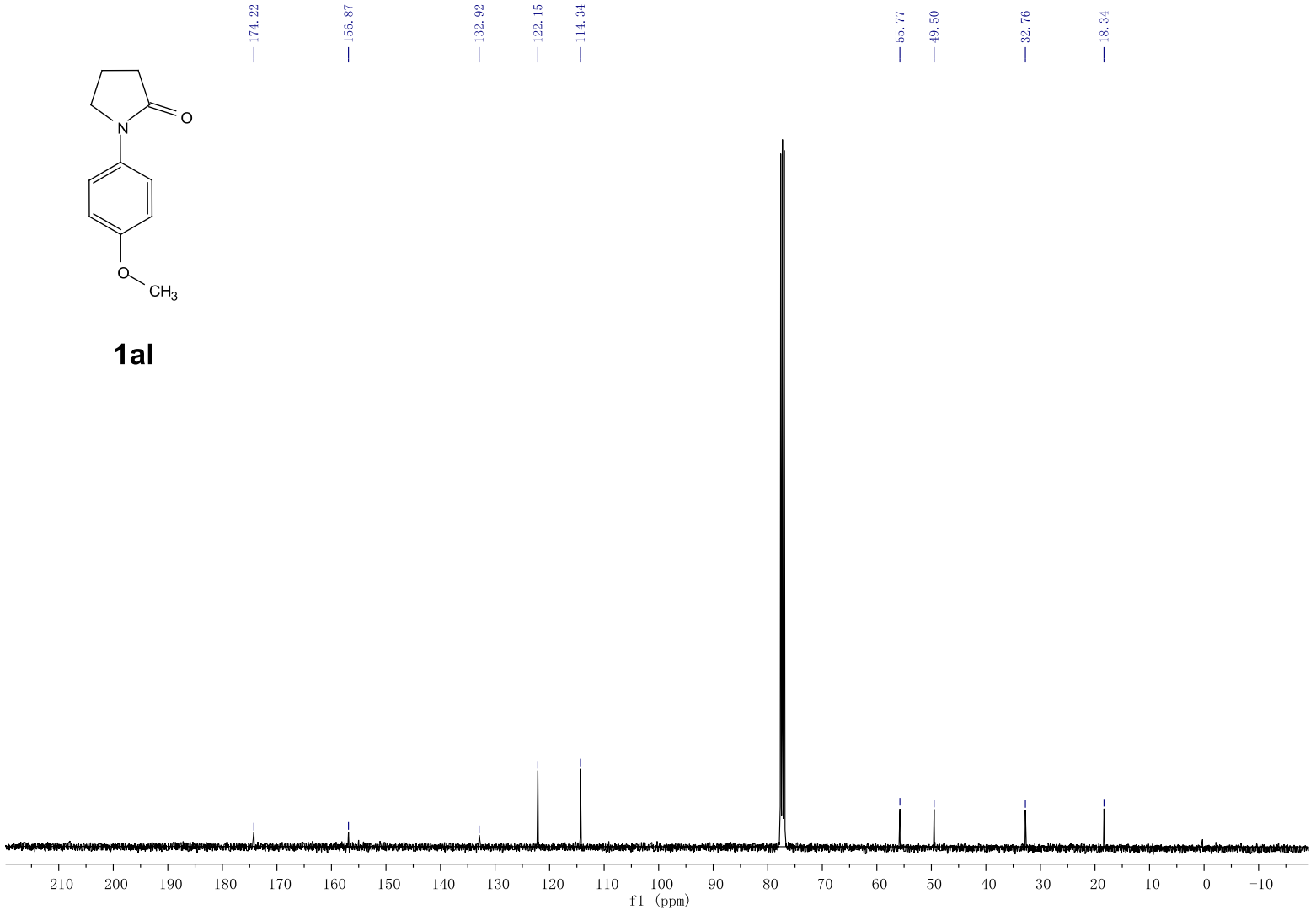
1ak

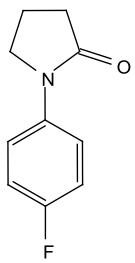
174.34
137.15
134.46
129.61
120.35
49.19
32.93
21.12
18.30
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N
O
CH3

1al

7.51
7.48
6.91
6.89
3.85
3.83
3.81
3.80
2.61
2.59
2.57
2.19
2.17
2.15
2.14
2.12
2.00
2.14
2.23
3.09
2.02
2.18
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)


174.22
156.87
132.92
122.15
114.34
55.77
49.50
32.76
18.34
O
N
O
CH3
1al
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

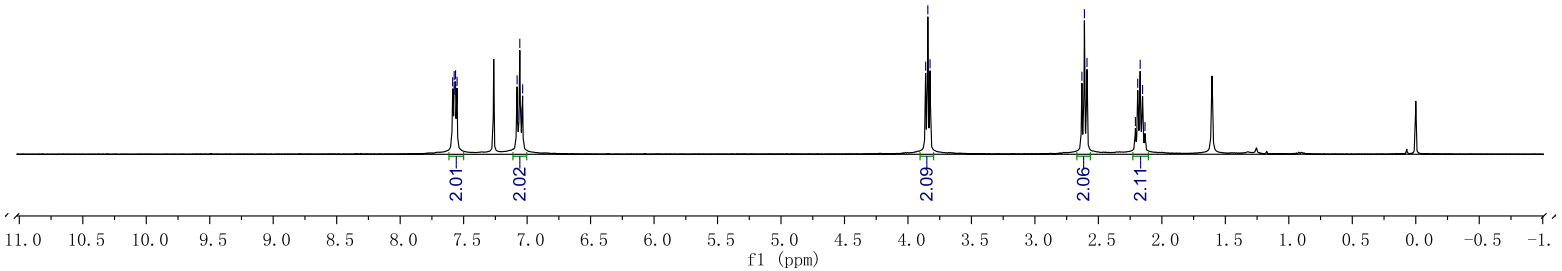

O
N
F

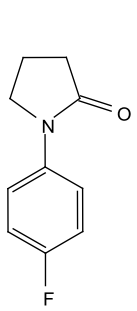
1am


7.59
7.58
7.57
7.57
7.57
7.56
7.55
7.08
7.07
7.06
7.04
7.04


3.86
3.84
3.83

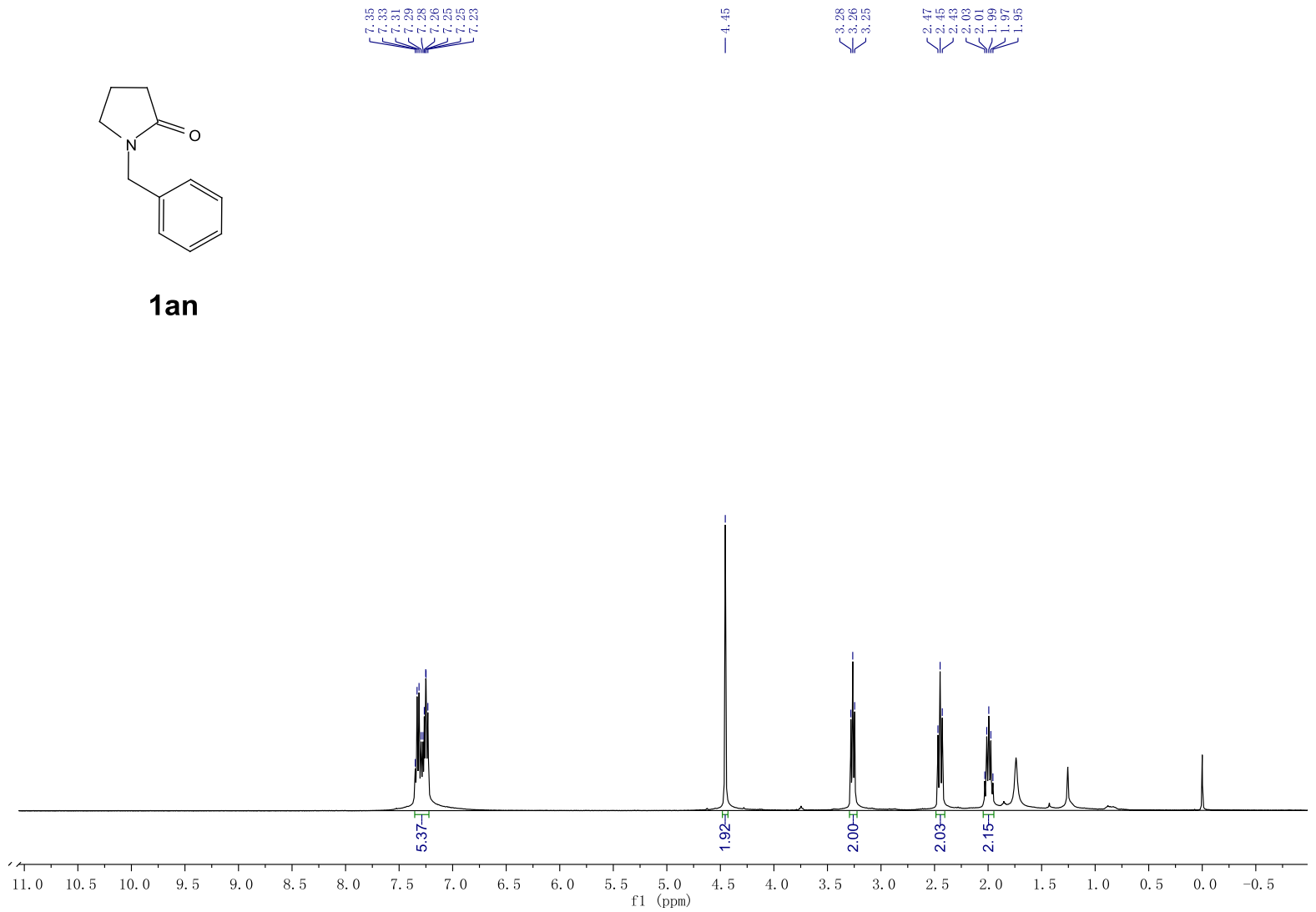

2.63
2.61
2.59
2.21
2.19
2.17
2.15
2.13


2.01
2.02
2.09
2.06
2.11
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

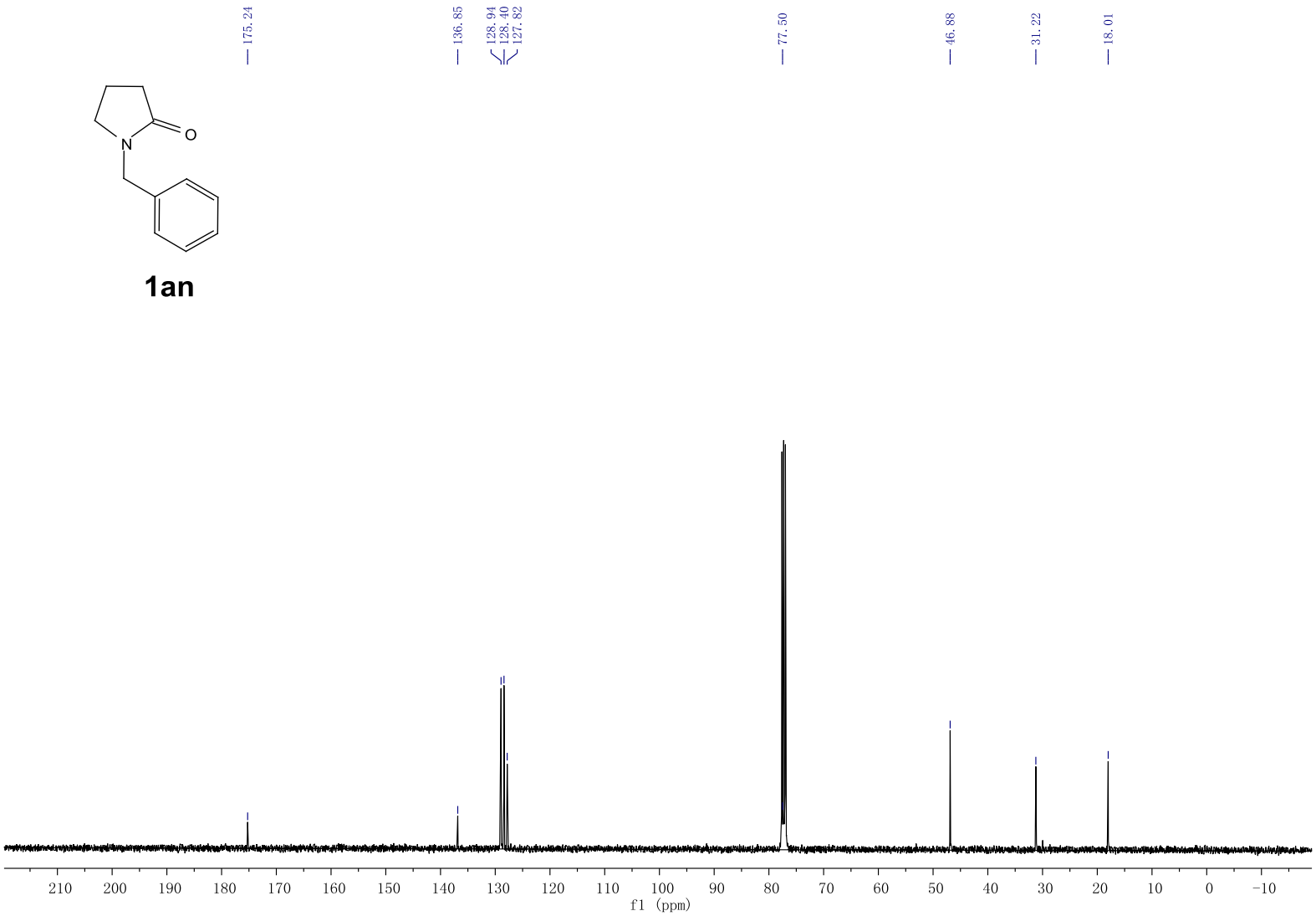

O
N
F

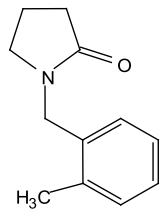
1am

174.40
160.98
158.55
135.80
135.77
122.02
121.94
115.88
115.66
49.29
32.79
18.25
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.35
7.33
7.31
7.29
7.28
7.26
7.25
7.25
7.23
4.45
3.28
3.26
3.25
2.47
2.45
2.43
2.03
2.01
1.99
1.97
1.95
O
N
5.37
1.92
2.00
2.03
2.15
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

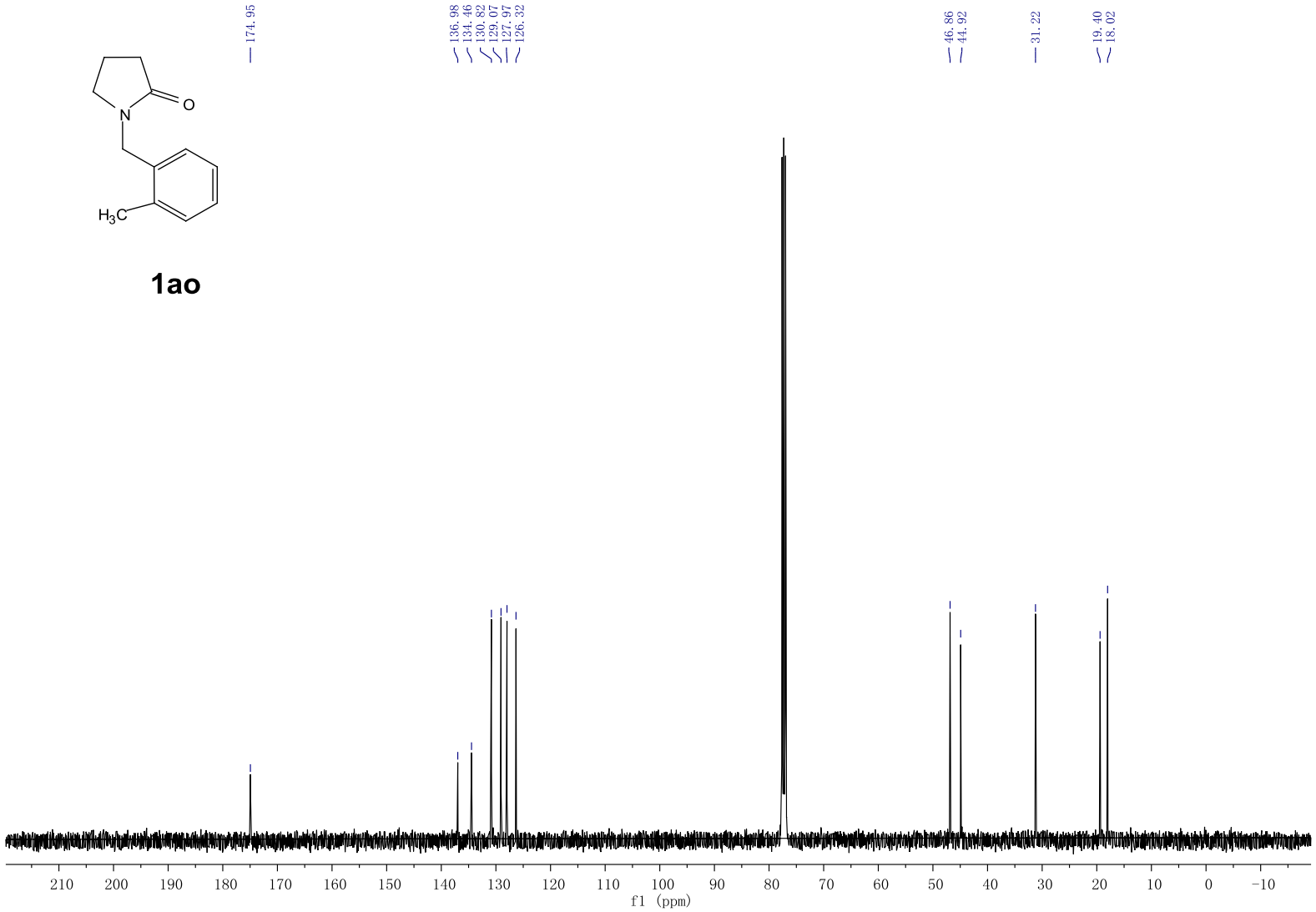
1an

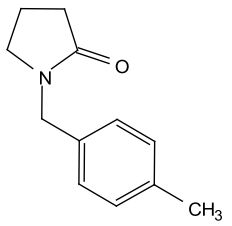

175.24
136.85
128.94
128.40
127.82
77.50
46.88
31.22
18.01
O
N
1an
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N
H3C

1ao

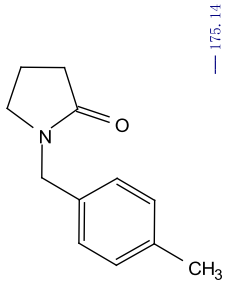
7.21
7.19
7.18
7.16
7.14
7.12
4.47
3.22
3.20
3.18
2.47
2.45
2.43
2.30
2.02
2.00
1.99
1.97
1.95
4.13
2.01
2.00
2.14
3.07
2.18
f1 (ppm)


174.95
136.98
134.46
130.82
129.07
127.97
126.32
46.86
44.92
31.22
19.40
18.02
O
N
H3C
1ao
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N
CH3

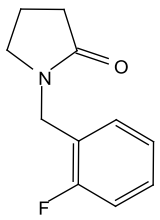
1ap

7.13
4.41
3.26
3.24
3.23
2.45
2.43
2.41
2.33
2.01
1.99
1.97
1.95
1.93
3.93
2.00
2.22
2.25
3.26
2.32
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


O
N
CH3

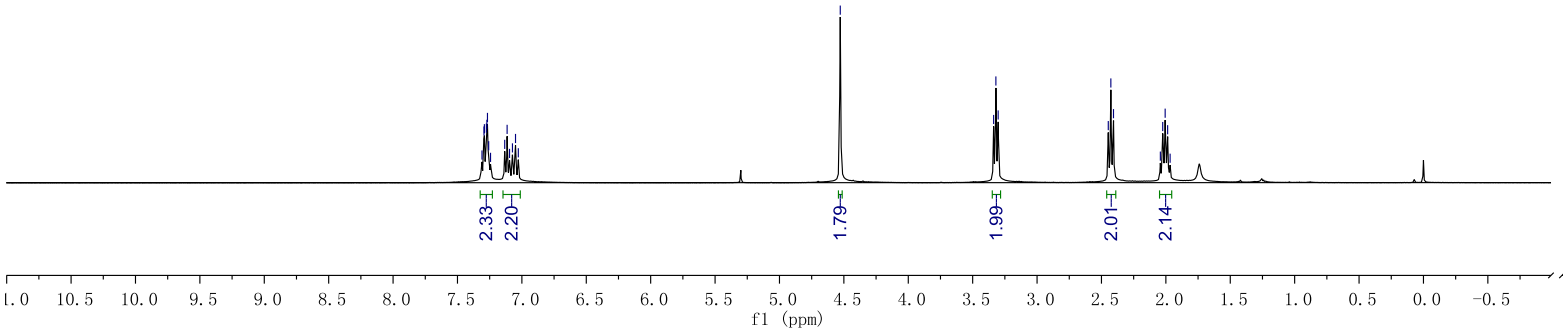
1ap

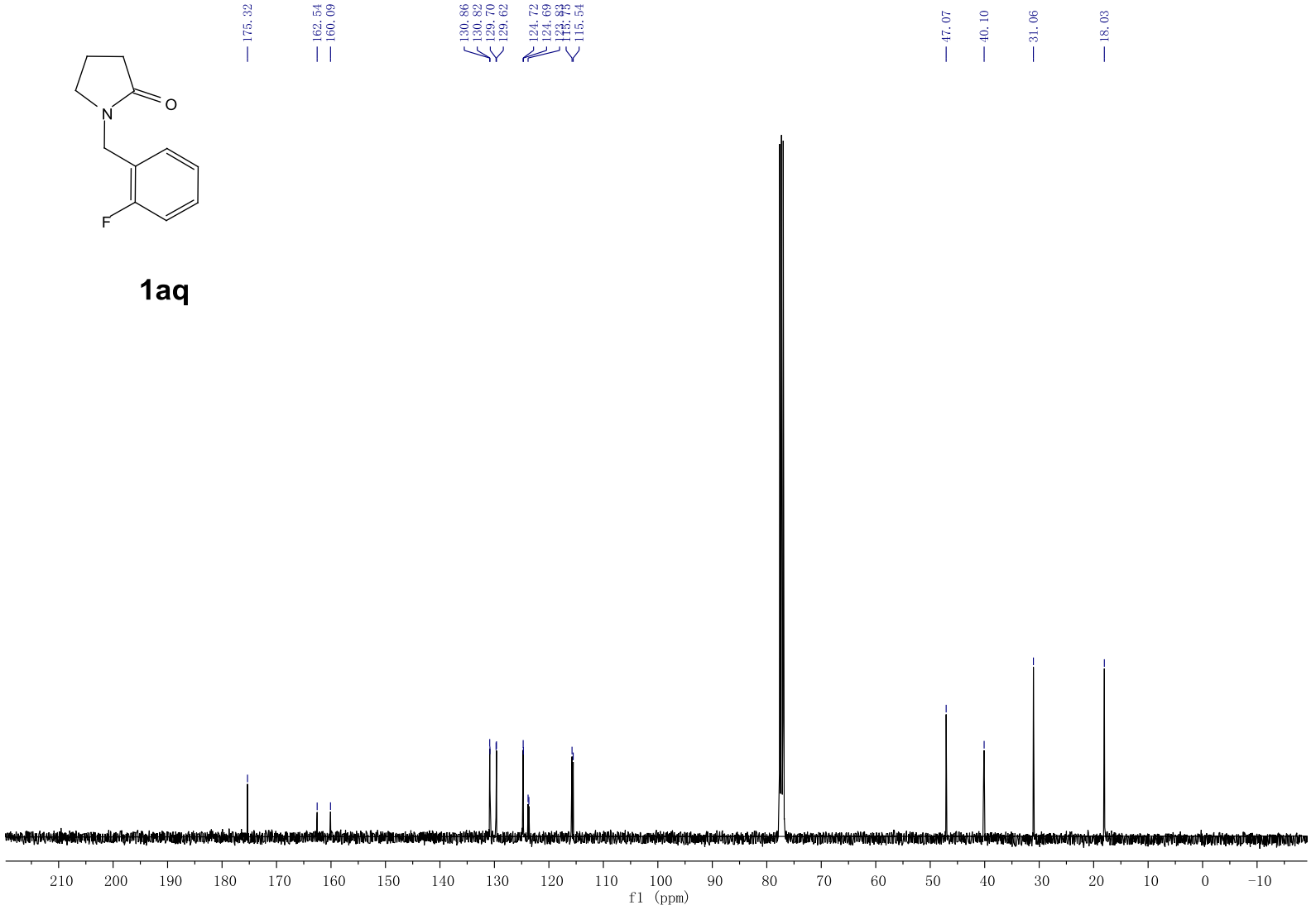
175.14
137.50
133.81
129.60
128.43
46.81
46.58
31.28
21.38
17.99
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

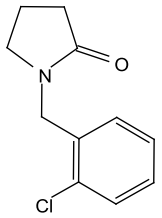

O
N
F

1aq


7.31
7.29
7.29
7.28
7.27
7.27
7.26
7.24
7.13
7.11
7.10
7.07
7.05
7.03
4.53
3.34
3.32
3.30
2.45
2.43
2.41
2.04
2.02
2.01
1.99
1.97

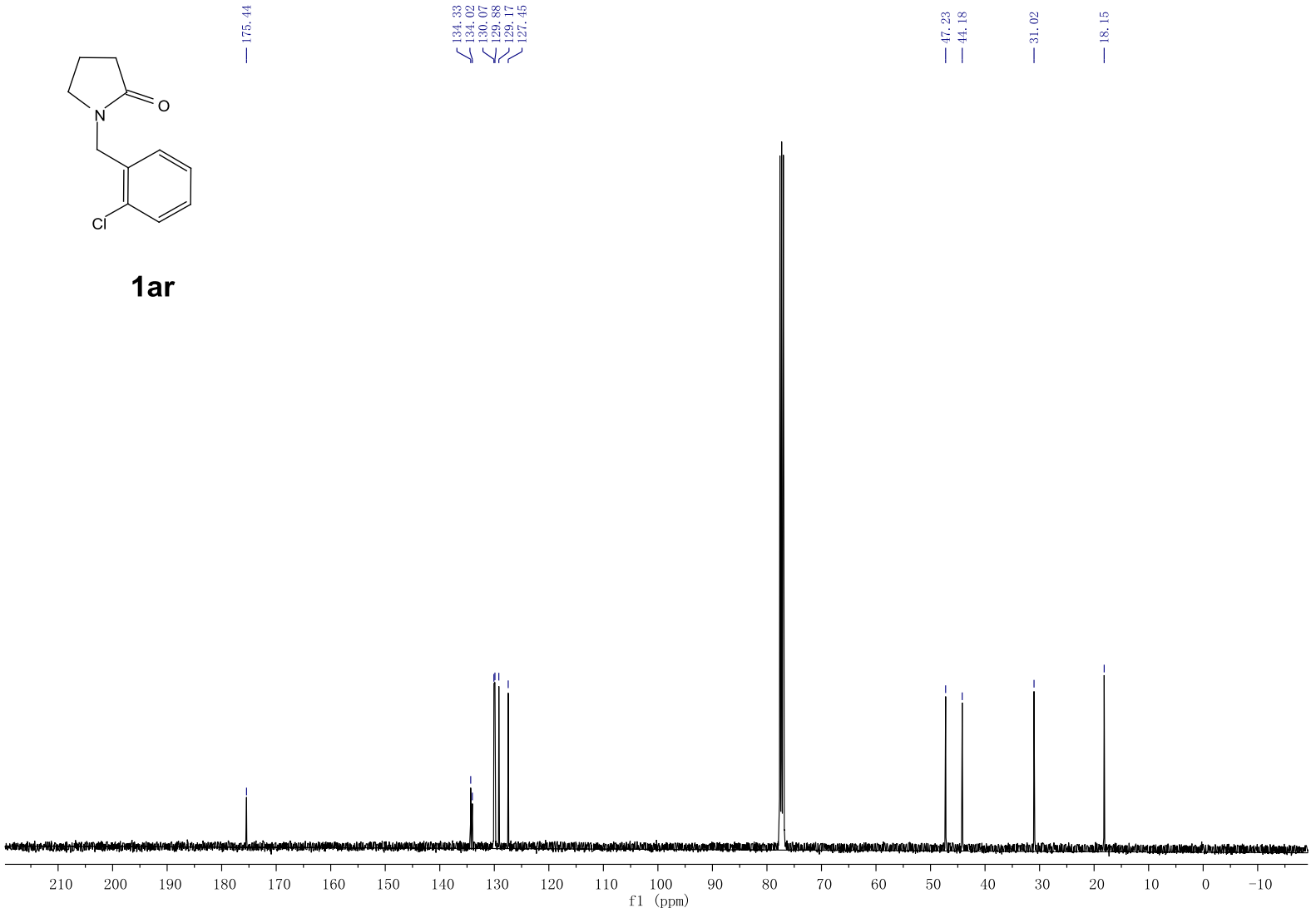

2.33
2.20
1.79
1.99
2.01
2.14
f1 (ppm)

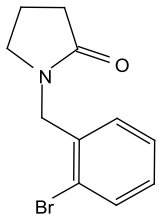

175.32
162.54
160.09
130.86
130.82
129.70
129.62
124.72
124.69
123.83
115.75
115.54
47.07
40.10
31.06
18.03
O
N
F
1aq
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


O
N
Cl

1ar

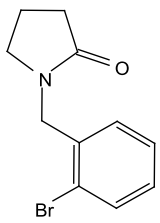
7.38
7.38
7.36
7.36
7.29
7.28
7.27
7.25
7.24
7.23
7.22
7.21
4.61
3.34
3.32
3.30
2.47
2.45
2.43
2.06
2.05
2.03
2.01
1.99
0.93
3.32
1.87
2.00
2.07
2.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


175.44
134.33
134.02
130.07
129.88
129.17
127.45
47.23
44.18
31.02
18.15
O
N
Cl
1ar
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
Br

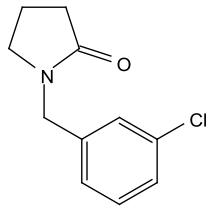
1as

7.27
7.26
7.26
7.26
7.23
7.14
7.14
7.13
7.12
4.43
3.29
3.27
3.26
2.48
2.46
2.44
2.06
2.04
2.02
2.00
1.98
1.09
0.94
0.93
1.05
1.86
2.00
2.03
2.28
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)


O
N
Br

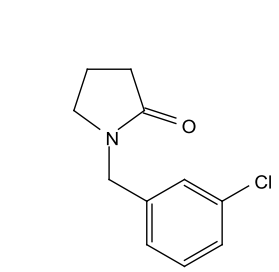
1as

175.34
138.97
134.85
130.27
128.38
128.08
126.50
46.94
46.39
31.07
18.02
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N
Cl

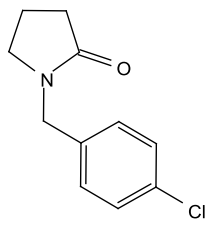
1at

7.27
7.26
7.26
7.25
7.23
7.14
7.14
7.13
7.12
4.43
3.29
3.27
3.26
2.48
2.46
2.44
2.06
2.04
2.02
2.00
1.98
2.21
0.88
0.91
1.72
2.03
1.98
2.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


O
N
Cl

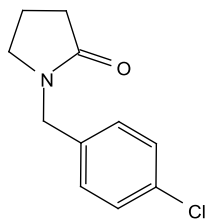
1at

175.33
138.98
134.86
130.27
128.39
128.08
126.50
46.93
46.39
31.07
18.03
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
Cl

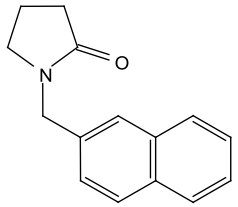
1au

7.31
7.29
7.19
7.17
4.42
3.27
3.25
3.24
2.46
2.44
2.42
2.04
2.02
2.00
1.98
1.96
2.02
2.00
1.88
2.14
2.15
2.35
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)


O
N
Cl

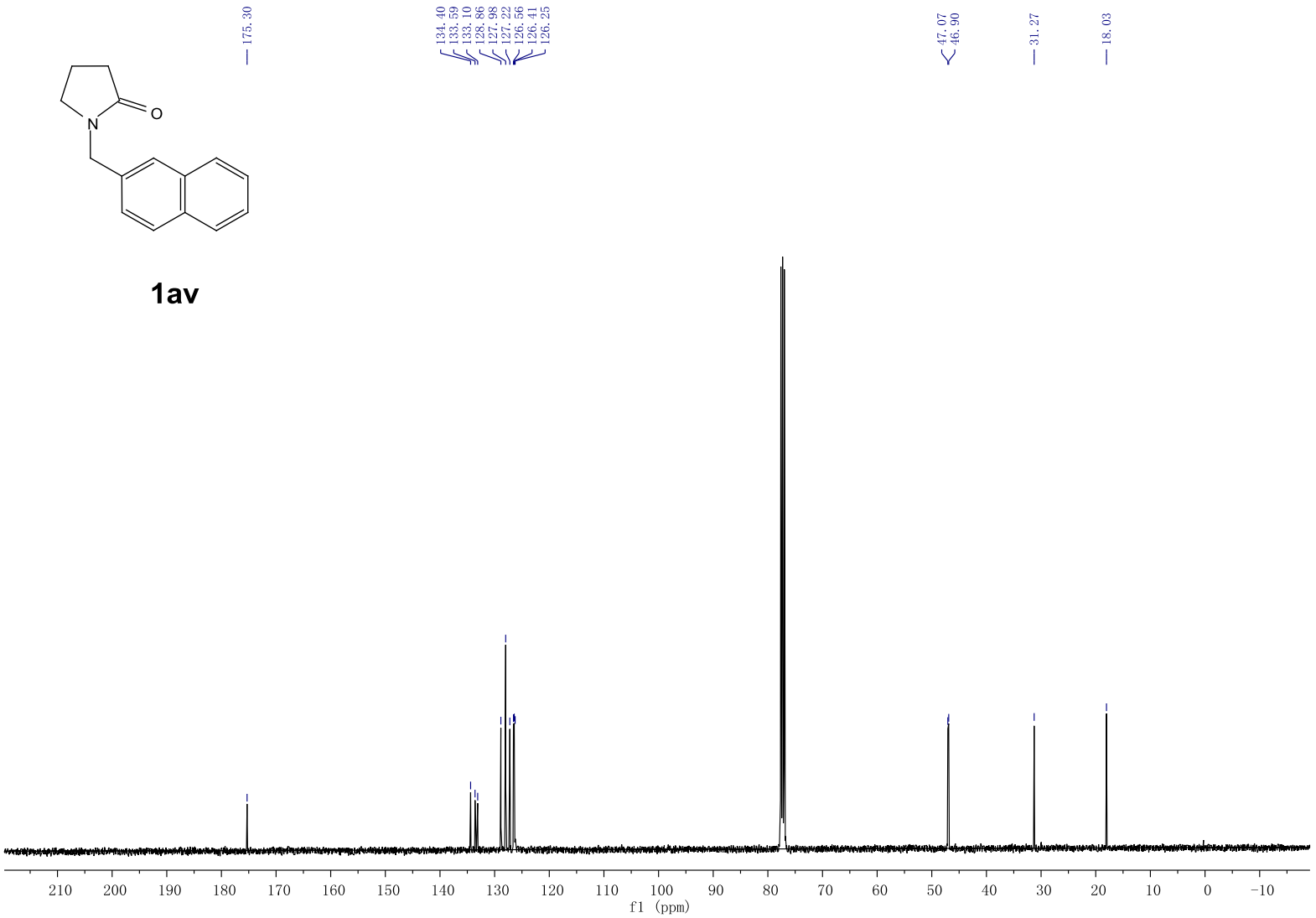
1au

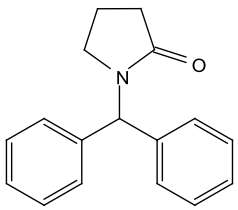
175.29
135.41
133.70
129.77
129.12
46.85
46.23
31.11
18.02
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N

1av

7.84
7.82
7.81
7.80
7.69
7.50
7.49
7.49
7.48
7.47
7.46
7.45
7.38
7.38
7.36
7.36
4.61
3.30
3.28
3.26
2.50
2.48
2.46
2.03
2.01
1.99
1.97
1.96
3.15
1.07
2.12
1.05
2.00
2.06
2.09
2.17
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)

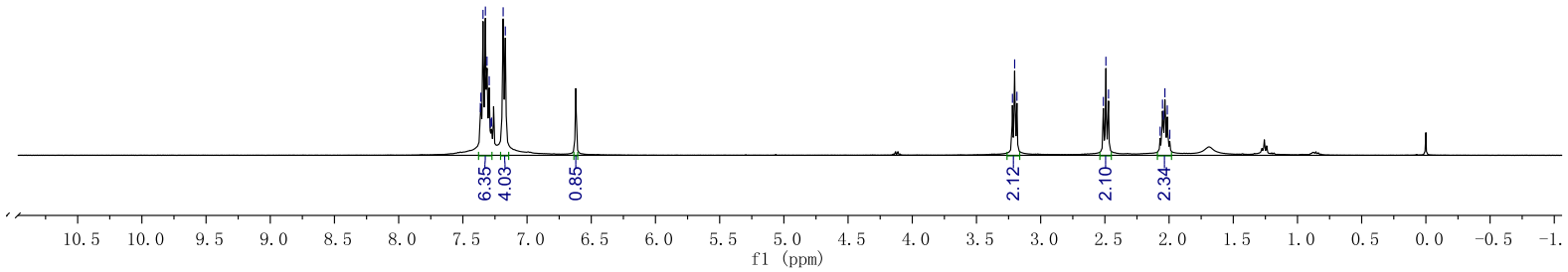

175.30
134.40
133.59
133.10
128.86
127.98
127.22
126.56
126.41
126.25
47.07
46.90
31.27
18.03
O
N
1av
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

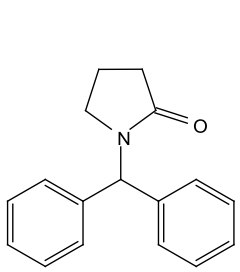

O
N

1aw


7.36
7.36
7.34
7.32
7.31
7.29
7.29
7.28
7.19
7.17

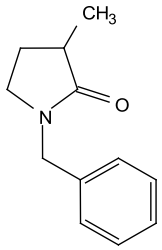

3.22
3.20
3.19
2.51
2.49
2.47
2.07
2.05
2.04
2.03
2.01
1.99


6.35
4.03
0.85
2.12
2.10
2.34
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 -1.
f1 (ppm)


O
N

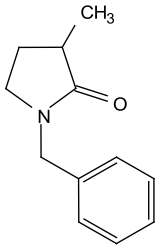
1aw

175.06
138.72
128.53
128.51
127.52
58.51
44.30
31.20
18.20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CH3
O
N

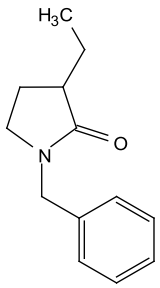
2aa

7.33
7.32
7.30
7.28
7.26
7.23
7.21
4.49
4.45
4.44
4.40
3.18
3.17
3.16
3.16
3.15
2.52
2.50
2.48
2.21
2.20
2.19
2.19
1.61
1.59
1.58
1.56
1.24
1.22
5.04
2.04
2.01
0.98
1.03
1.11
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


CH3
O
N

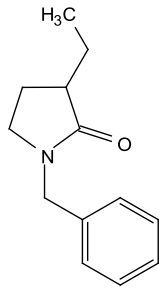
2aa

177.59
136.96
128.89
128.32
127.72
47.01
44.88
36.99
27.32
16.67
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


H3C
O
N

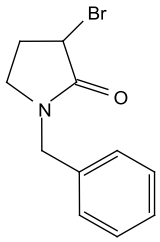
2ab

7.33
7.31
7.30
7.28
7.26
7.23
7.21
4.51
4.47
4.42
4.39
3.18
3.16
3.15
2.42
2.41
2.40
2.39
2.16
2.14
1.92
1.91
1.67
1.65
1.64
1.62
1.47
0.97
0.95
5.06
2.09
2.13
0.99
1.09
1.13
1.15
1.10
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 -1.0
f1 (ppm)


H3C
O
N

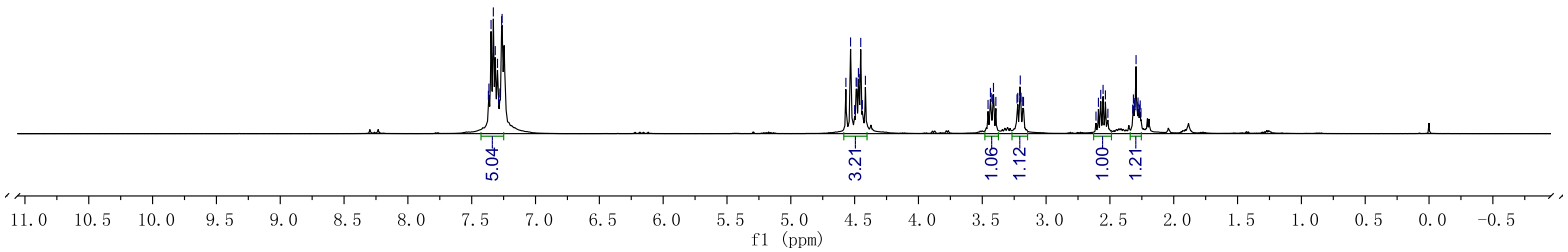
2ab

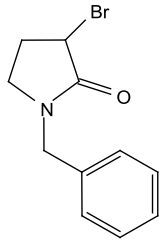
176.90
137.00
128.89
128.35
127.72
46.92
45.12
43.55
24.55
24.38
11.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


Br
O
N

2ac

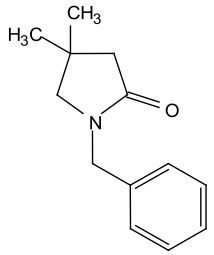

7.37
7.37
7.35
7.33
7.32
7.30
7.29
7.28
7.27
7.26
4.57
4.53
4.50
4.49
4.48
4.47
4.46
4.45
4.44
4.42
3.44
3.43
3.41
3.23
3.22
3.21
3.20
2.61
2.59
2.57
2.55
2.54
2.52
2.32
2.32
2.31
2.30
2.30
2.29
2.28
2.27
2.27
2.26
2.26


5.04
3.21
1.06
1.12
1.00
1.21
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Br
O
N

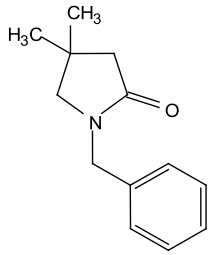
2ac

170.93
135.84
129.04
128.29
128.08
47.34
44.80
44.52
30.38
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


CH3
H3C
O
N

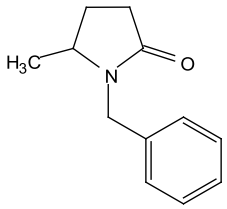
2ad

7.35
7.33
7.31
7.29
7.27
7.27
7.24
7.23
4.44
2.96
2.27
1.09
5.30
2.00
2.02
2.00
6.34
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


CH3
H3C
O
N

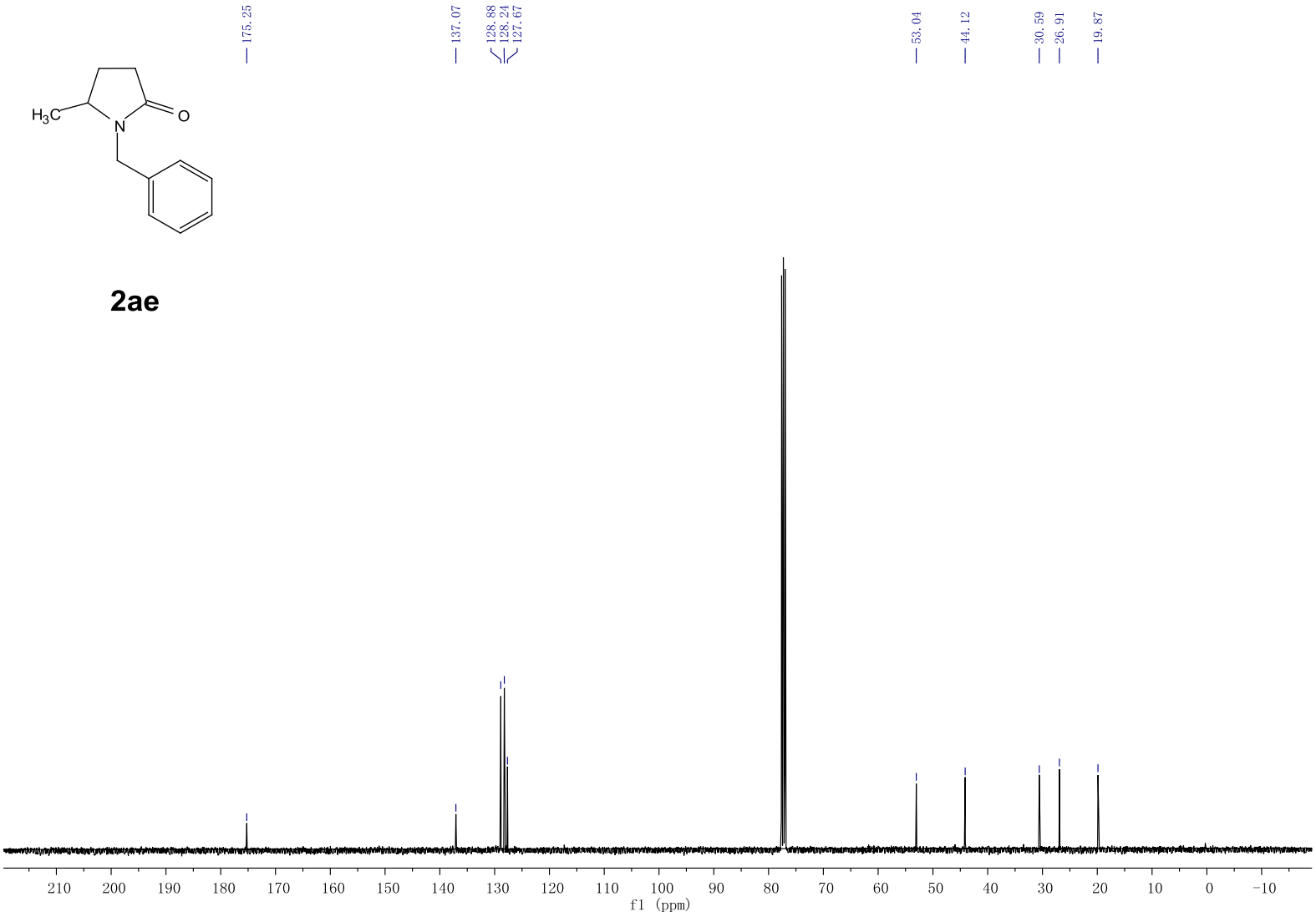
2ad

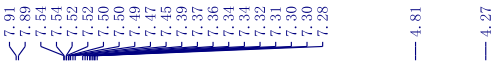
174.40
136.78
128.87
128.38
127.75
59.95
46.70
46.52
32.82
28.02
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

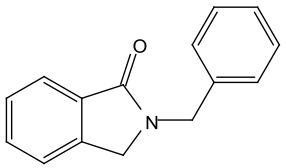

H3C
N
O

2ae

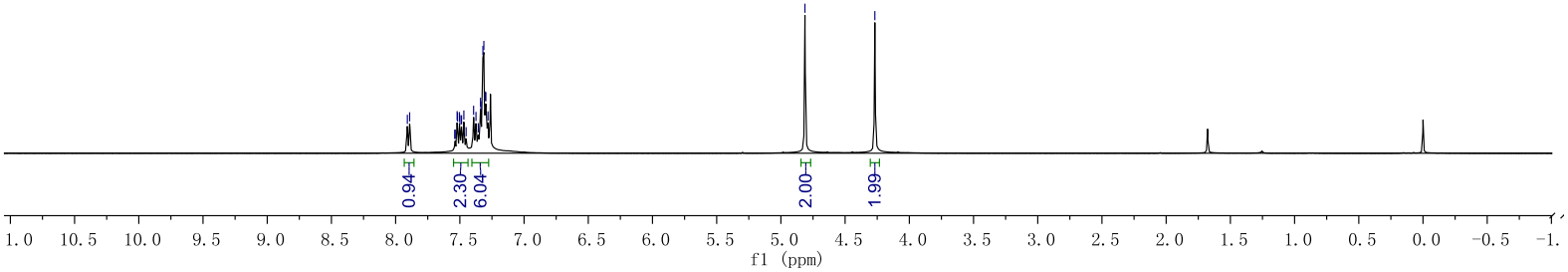
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.28
7.27
7.24
7.24
7.22
4.99
4.96
3.99
3.96
3.54
3.53
3.53
3.51
3.49
3.48
2.50
2.49
2.48
2.46
2.46
2.45
2.43
2.42
2.40
1.61
1.60
1.59
1.58
1.17
1.15
2.72
2.05
1.00
1.02
0.98
2.04
1.05
1.14
3.07
f1 (ppm)

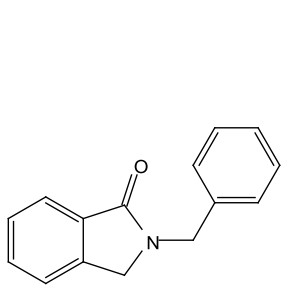

175.25
137.07
128.88
128.24
127.67
53.04
44.12
30.59
26.91
19.87
H3C
N
O
2ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.91
7.89
7.54
7.54
7.52
7.52
7.50
7.50
7.49
7.47
7.45
7.39
7.37
7.36
7.34
7.34
7.32
7.31
7.30
7.30
7.28
4.81
4.27


O
N

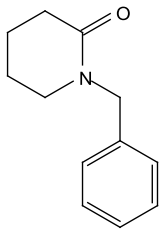
2ak


0.94
2.30
6.04
2.00
1.99
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)


O
N

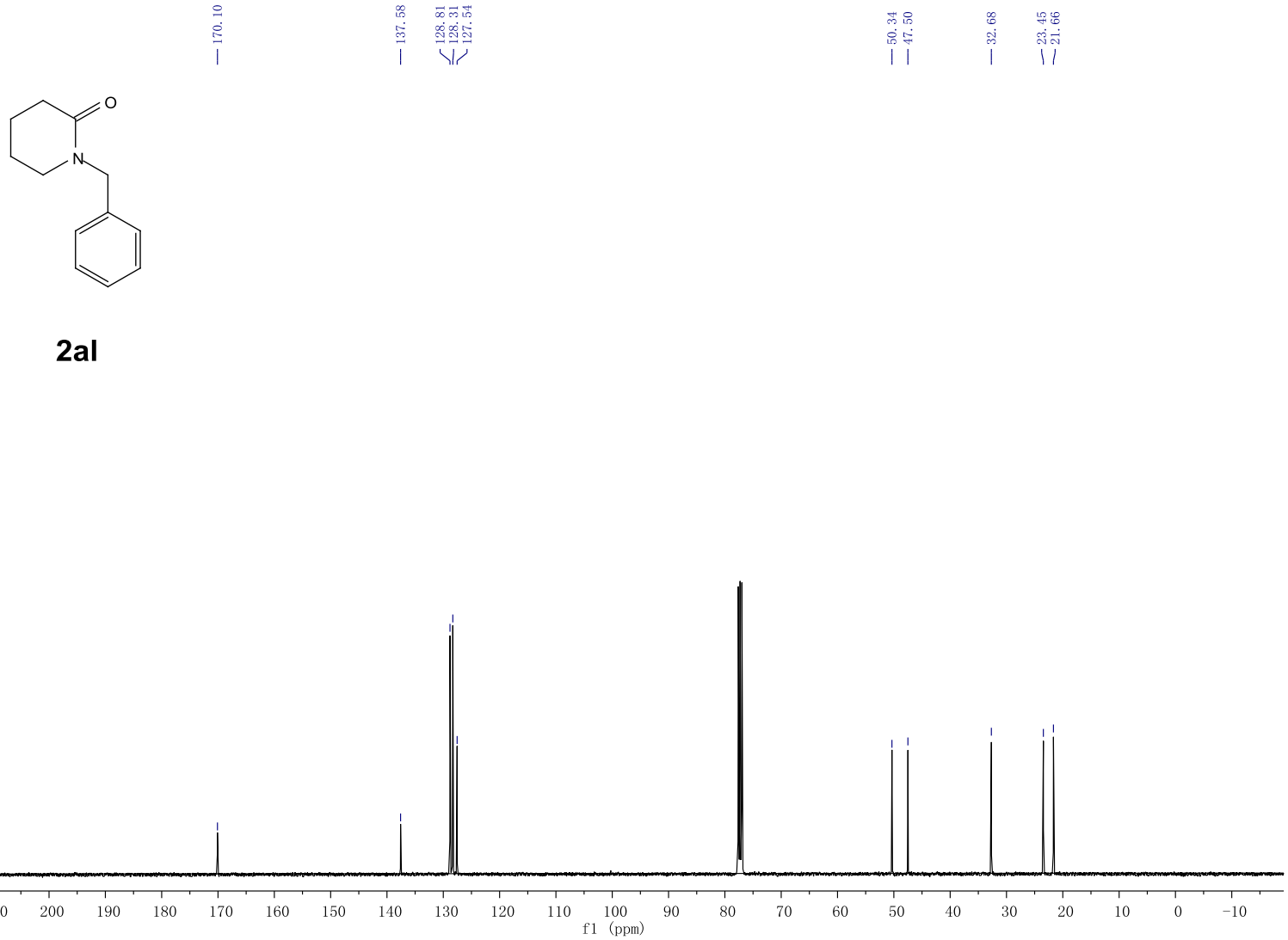
2ak

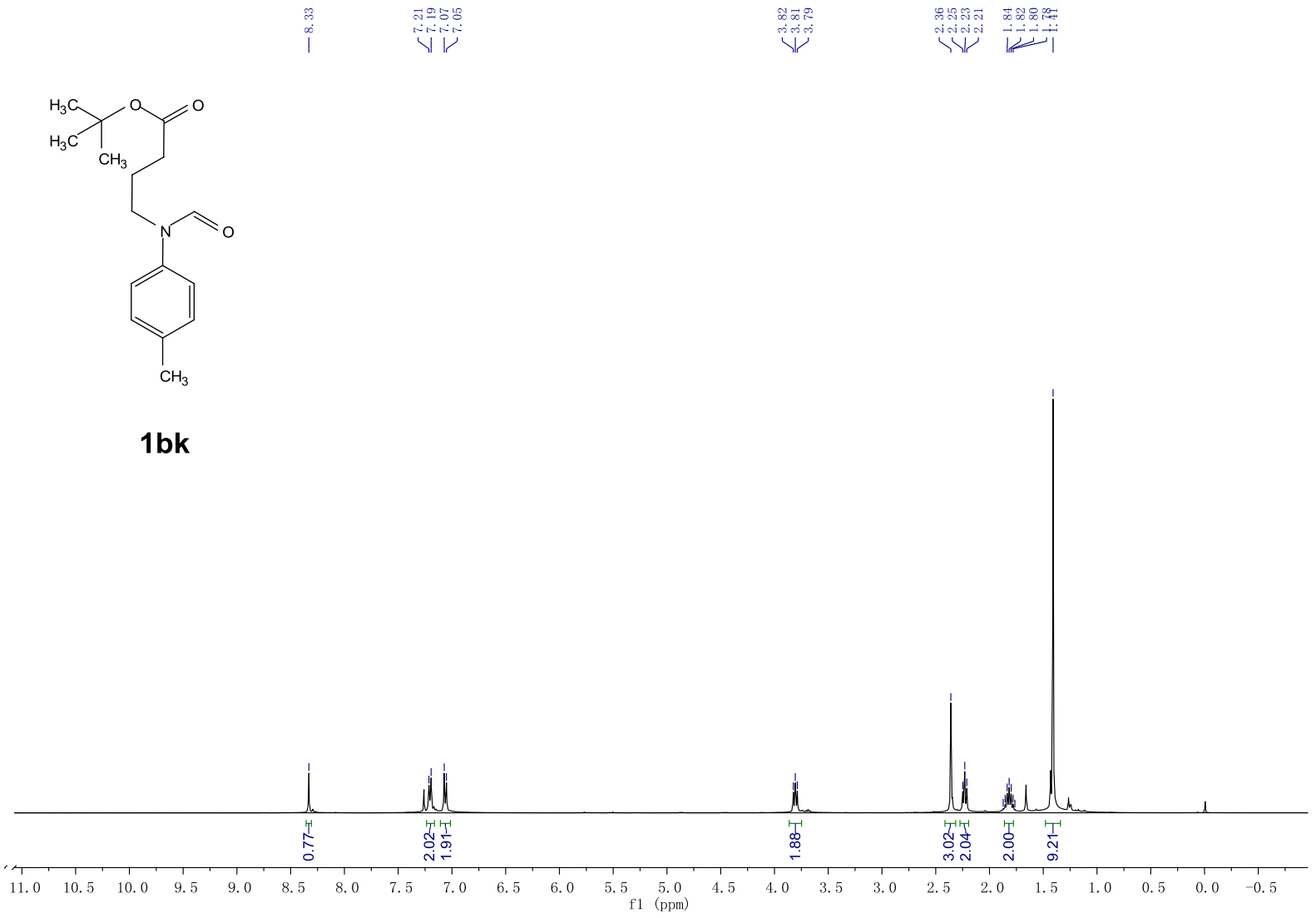
168.75
141.50
137.32
132.92
131.62
129.07
128.44
128.32
127.95
124.18
123.02
49.70
46.67
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
N

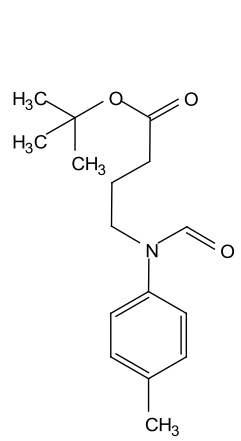
2al

7.34
7.32
7.30
7.27
7.27
7.26
7.24
4.60
3.21
3.19
3.18
2.48
2.47
2.45
1.79
1.78
1.78
1.77
1.76
5.08
2.03
2.01
2.00
4.17
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


170.10
137.58
128.81
128.31
127.54
50.34
47.50
32.68
23.45
21.66
O
N
2al
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

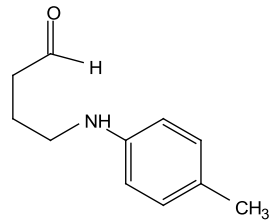

8.33
7.21
7.19
7.07
7.05
3.82
3.81
3.79
2.36
2.25
2.23
2.21
1.84
1.82
1.80
1.78
1.41
0.77
2.02
1.91
1.88
3.02
2.04
2.00
9.21
f1 (ppm)

1bk


H3C
O
O
H3C
CH3
N
O
CH3

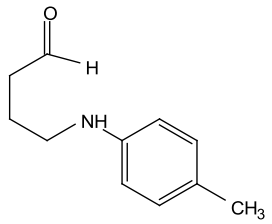
1bk

172.41
162.70
138.52
137.19
130.54
124.52
80.70
44.63
32.90
28.33
23.36
21.18
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
H
NH
CH3

1ck

8.33
7.21
7.19
7.06
7.04
3.76
3.74
3.72
2.36
1.59
1.57
1.55
1.53
1.51
1.50
0.90
0.88
0.86
0.89
2.03
1.85
1.77
3.00
2.16
2.47
f1 (ppm)


O
H
NH
CH3

1ck

162.72
138.72
137.09
130.44
124.70
46.90
21.19
21.11
11.48
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)