Electronic Supplementary Material (ESI) for ChemComm.

Supporting information

Ruthenium-Catalyzed Synthesis of *N*-substituted Lactams by Acceptorless Dehydrogenative Coupling of Diols with Primary Amines

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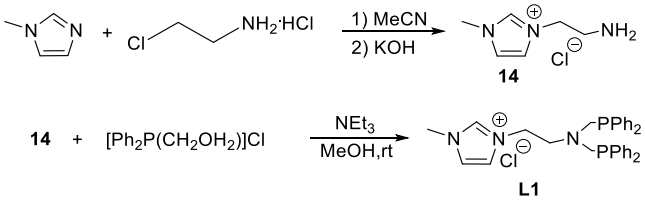
I. General remarks

Unless otherwise noted, all operations were performed in the nitrogen. All solvents were purified with standard methods. Reagents were purchased from commercial suppliers and used as received, and moisture sensitive compounds were stored in glovebox. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on the Bruker AVENCE III HD-400 MHz in $CDCl_3$, DMSO-d_6. GC analysis was performed with Agilent 7890B (KB-1, 30 m × 0.32 mm × 0.25 μm) and AT (C-2000, 3 m × 3 mm). GC-MS analysis was performed with SHIMADZU GCMS-QP2020 (SH-Rtx-35MS, 30 m × 0.25 mm × 0.25 μm). HRMS was measured on SHIMADZU LCMS-IT-TOF mass spectrometer.

II. General procedures

1. Synthesis of Ligand L1

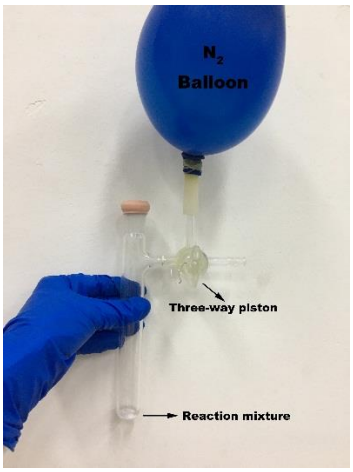


Ligand **L1** was synthesized according to the reported method.[1] 2-Chloroethylamine hydrochloride (0.05 mol, 5.8 g), dried acetonitrile (60 mL) and 1-methylimidazole (0.1 mol, 8.2 g) were added successively into a dried two-neck flask, and then the mixture was stirred overnight at reflex condition to form colourless oil layer. At the end of reaction, solvent was removed and oil layer was washed with dried acetonitrile (10 mL× 2). The washed oil layer was recrystallized in EtOH/EtOAc to give a white solid. The solid was solved in minimal water and pH of the aqueous solution was adjusted to 8-9 with solid KOH. All water in the resulting aqueous solution was removed by rotary evaporation, and then THF/EtOH (1:4, 50 mL) was added to remove KCl. The mixture solution was filtered and filtrate was evaporated to dryness under vacuum to give pale yellow liquid (**14**), and then **14** (5 mmol, 0.81 g), $[Ph_2P(CH_2OH)_2]Cl$ (10 mmol, 2.82 g), MeOH (30 mL), and Et_3N (3 mL) were added into a two-neck flask at N_2 atmosphere successively. This mixture solution was stirred at room temperature for 5 h, and then the solution was evaporated to dryness under vacuum. H_2O (10 mL) was added into the residue and the resulting aqueous solution was extract with CH_2Cl_2 (30

mL). The isolated CH_2Cl_2 solution was dried over $MgSO_4$, filtered, and evaporated to about 10 mL, and then Et_2O (30 mL) was added into it to give colourless crystal (1.98 g, 71% yield).

2. Details of the optimization of reaction conditions.

Reaction procedure: Unless other conditions are specified, catalyst, ligand, base and amines were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then diols and solvent were sequentially injected into it. The mixture was stirred at corresponding temperature for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the residue was purified by flash column chromatography on silica gel to afford the product **3**.



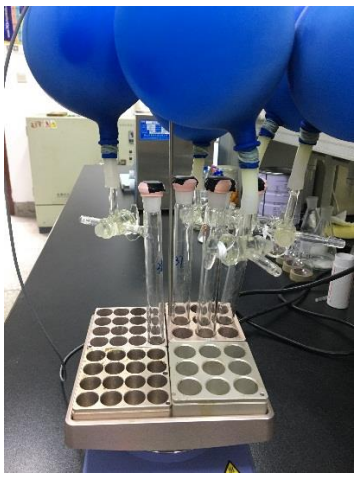
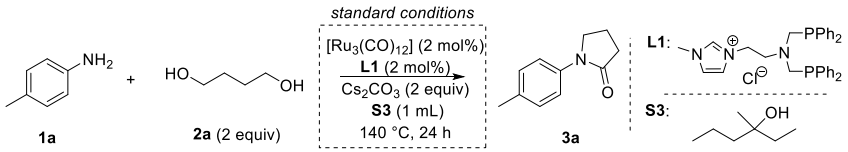


Table S1 Complementary Experiments on optimization of the reaction conditions.[a]



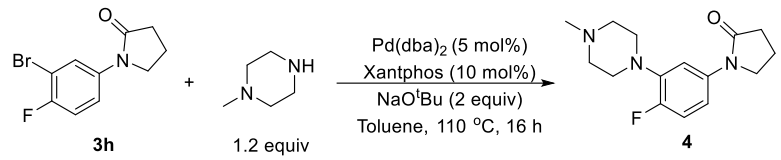
Entry	Changes	Yield[b]	Entry	Changes	Yield[b]
1	None	81%	16	Cs_2CO_3 (3 equiv)	80%
2	Replace **S3** with Toluene	31%	17	Cs_2CO_3 (4 equiv)	77%
3	Replace **S3** with Toluene, 110 °C	18%	18	Replace Cs_2CO_3 with NaH	44%
4	Replace **S3** with Toluene, 120 °C	20%	19	Replace Cs_2CO_3 with KO^{t}Bu	trace
5	Replace **S3** with Toluene, 130 °C	25%	20	Replace Cs_2CO_3 with K_2CO_3	0
6	Replace **S3** with Toluene, 150 °C	30%	21	Replace Cs_2CO_3 with Na_2CO_3	0
7	Replace **S3** with Toluene (closed vessel)[c]	trace	22	Replace Cs_2CO_3 with KOH	trace
8	Replace **S3** with xylene	16%	23	Replace Cs_2CO_3 with K_3PO_4	0
9	Replace **S3** with mesitylene	trace	24	n(**2a**) = 0.25 mmol (1 equiv)	55%
10	Replace **S3** with anisole	trace	25	n(**2a**) = 0.375 mmol (1.5 equiv)	61%
11	Replace **S3** with DMF	trace	26	n(**2a**) = 0.625 mmol (2.5 equiv)	82%
12	Replace **S3** with DMSO	trace	27	n(**2a**) = 0.75 mmol (3 equiv)	76%
13	Cs_2CO_3 (10 mol%)	12%	28	n(**2a**) = 1 mmol (4 equiv)	71%
14	Cs_2CO_3 (50 mol%)	22%	29	n(**2a**) = 1.25 mmol (5 equiv)	63%
15	Cs_2CO_3 (1 equiv)	40%			

[a]Unless otherwise noted, the reaction was carried out under open condition to nitrogen on a 0.25 mmol scale. [b]Isolated yields. [c]the reaction was carried out under nitrogen protection in a sealed 25 mL Schlenk tube without the balloon.

3. Typical procedures for the preparation of *N*-substituted lactams from diols and amines.

Unless other conditions are specified, $Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and amines (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then diols (0.5 mmol) and **S3** (1 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the residue was purified by flash column chromatography on silica gel to afford the product **3**.

4. Procedures for the preparation of *N*-[4-fluoro-3-(4-methylpiperazin-1-yl)phenyl]pyrrolidin-2-one (4)



To a solution of 1-methylpiperazine (0.24 mmol, 24 mg), $Pd(dba)_2$ (0.01 mmol, 5.8 mg), xantphos (0.02 mmol, 11.6 mg) and NaO^tBu (0.4 mmol, 38.4 mg) in toluene (1 mL) was added *N*-(3-bromo-4-fluorophenyl)pyrrolidin-2-one (**3h**) (0.2 mmol, 51.2 mg) dropwise. The mixture was stirred at 110 °C for 16 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the desired product was separated by flash column chromatography to give a white solid **4** (49.8 mg, 90%).

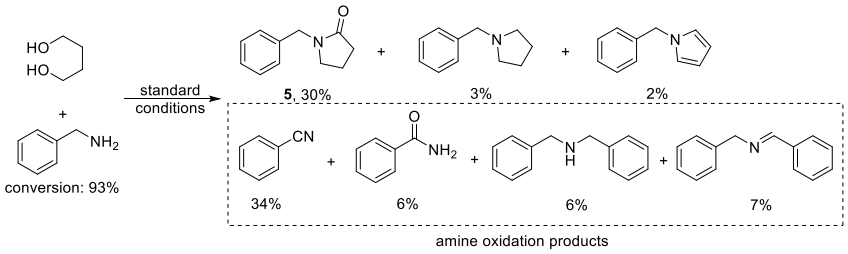
5. Gram scale reaction

$Ru_3(CO)_{12}$ (2 mol%, 128 mg), ligand **L1** (2 mol%, 112 mg) and Cs_2CO_3 (20 mmol) and amines (10 mmol) were added into a dried Schlenk tube with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then diols (20 mmol) and **S3** (50 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 5 d. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 30 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the residue was purified by flash column chromatography on silica gel to afford the product **3aa** (1.14 g, 65%).

6. Detailed results of the reaction using benzylamine as substrate

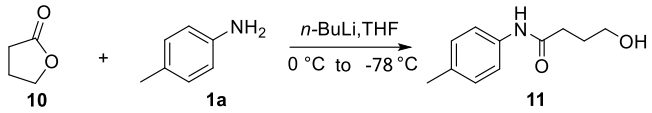
$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (1.0 mmol, 325 mg) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then benzylamine (0.25 mmol, 26.8 mg), diols (0.5 mmol, 45 mg) and **S3** (1 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL

of dichloromethane and filtered with *Celite*, and the filtrate was analyzed by GC-MS. Detailed results were shown below. The lower yield of desired product **5** might due to the generation of amine oxidation byproducts.[2]

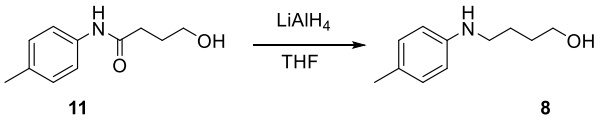


III. Mechanistic studies

1. Synthesis of the intermediates

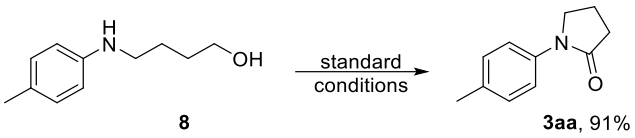


To a solution of *p*-toluidine (214 mg, 2 mmol) in THF (20 mL) was added *n*-BuLi (2.5 M in hexanes, 10 mL, 4 mmol) at 0 °C. The resulting reaction mixture was stirred at 0 °C and then cooled down to −78 °C. γ-Butyrolactone **10** (156 mg, 1.8 mmol) was added drop-wise. The reaction mixture was stirred for 1 h at the same temperature. The reaction was quenched with saturated NH_4Cl and extracted with ethyl acetate. The combined organic extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography through silica gel (CH_2Cl_2/MeOH) to give **11** as a white solid (4.9 g, 90% yield).[3]



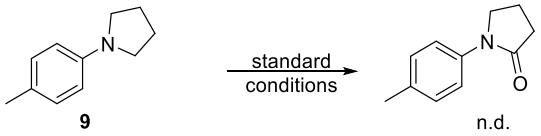
Hydroxyamide **11** (193 mg, 1 mmol) and $LiAlH_4$ (113 mg, 3 mmol) was added in a Schlenk tube and it was subject to three cycles of vacuum and refilled with nitrogen. After that, under the protection of nitrogen, THF (15 mL) was added at 0 ºC, and the reaction mixture was slowly warmed to room temperature and stirred for 10 h. The reaction mixture was evaporated and purified by flash column chromatography to afford the compound **8** as a yellow oil (163 mg, 91%).[4]

2. Control experiments



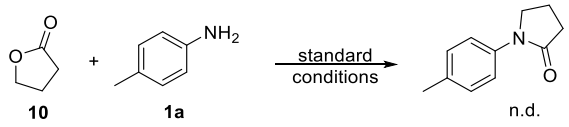
8 **3aa**, 91%

$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and amino alcohol **8** (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then **S3** (1 mL) was sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the desired product was separated by flash column chromatography to give a white solid **3aa** (39.8 mg, 91%).



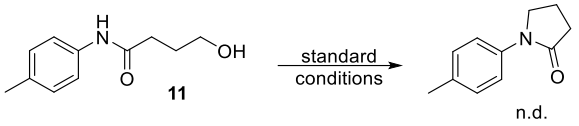
9 n.d.

$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and pyrrolidine **9** (26.8 mg, 0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then **S3** (1 mL) was sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. The component of the completed reaction was analyzed by GC-MS, and no desired product was observed.

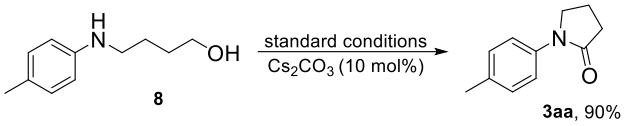


10 **1a** n.d.

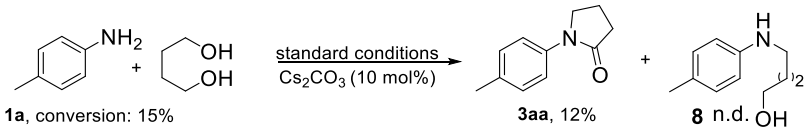
$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and *p*-toluidine (26.8 mg, 0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then **10** (0.5 mmol, 43 mg), **S3** (1 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. The component of the completed reaction was analyzed by GC-MS, and no desired product was observed. Nevertheless, a trace amount of **10** was detected of model reaction under standard conditions.



$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and hydroxylamide **11** (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then **S3** (1 mL) was sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. The component of the completed reaction was analyzed by GC-MS, and no desired product was observed.

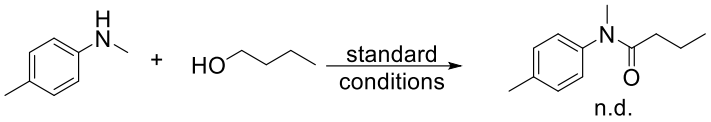


$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (10 mol%, 16.2 mg) and amino alcohol **8** (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then **S3** (1 mL) was sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the desired product was separated by flash column chromatography to give a white solid **3aa** (39.8 mg, 90%).



$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (10 mol%, 16.2 mg) and amines (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then diols (0.5 mmol) and **S3** (1 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature and diluted with 3 mL of dichloromethane and filtered with *Celite*. The filtrate was evaporated to dry, and the residue was purified by flash column chromatography on silica gel to afford the product **3aa** (12%), without

amino alcohol **8** being detected.



$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and amines (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then *n*-butyl alcohol (0.5 mmol) and **S3** (1 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was analyzed by GC-MS, and no *N*-methyl-*N*-(*p*-tolyl)butyramide was observed.

3. Profile of monitoring on reaction process

$Ru_3(CO)_{12}$ (2 mol%, 12.8 mg), ligand **L1** (2 mol%, 11.2 mg) and Cs_2CO_3 (2.0 mmol, 650 mg) and amines (1.0 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then diols (2.0 mmol) and **S3** (5 mL) were sequentially injected into it. The mixture's ingredient was determined by GC-MS, based on amine consumption and lactam production, and the profile of the *in situ* relative composition of *p*-toluidine (**1a**), imine **7**, amino alcohol **8** and the desired product **3aa** was shown in **Fig. S1**.

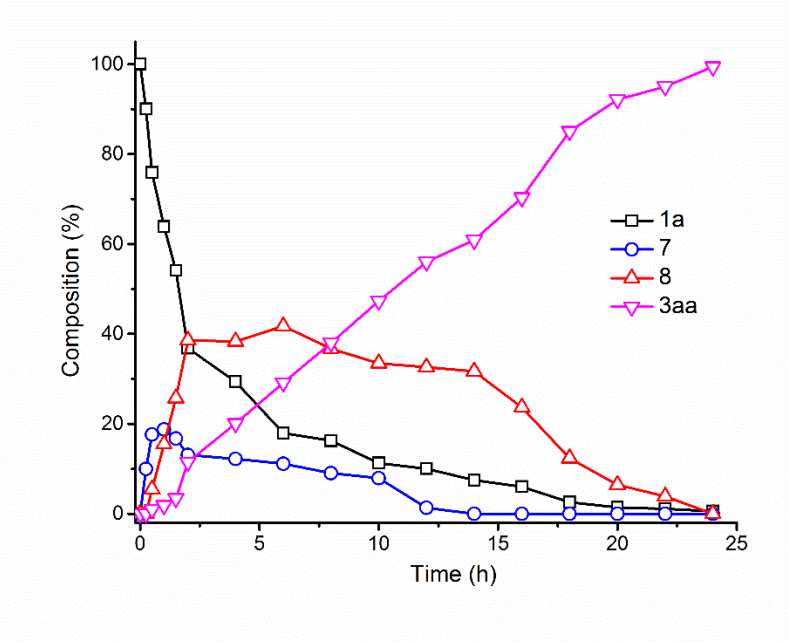


Fig. S1 Reaction profile of the preparation of *N*-substituted γ-lactam.

4. Detection of H_2

$Ru_3(CO)_{12}$ (2 mol%, 3.2 mg), ligand **L1** (2 mol%, 2.8 mg) and Cs_2CO_3 (0.5 mmol, 162 mg) and amines (0.25 mmol) were added into a dried Schlenk tube equipped with a balloon, and it was subject to three cycles of vacuum and refilled with nitrogen. Then diols (0.5 mmol) and **S3** (1 mL) were sequentially injected into it. The mixture was stirred at 140 ºC for 24 h. At the end of the reaction, the mixture was slowly cooled to room temperature. Then the gas was vented off carefully and an aliquot of the gas was collected and analyzed by GC, showing formation of H_2 (**Fig. S2**)

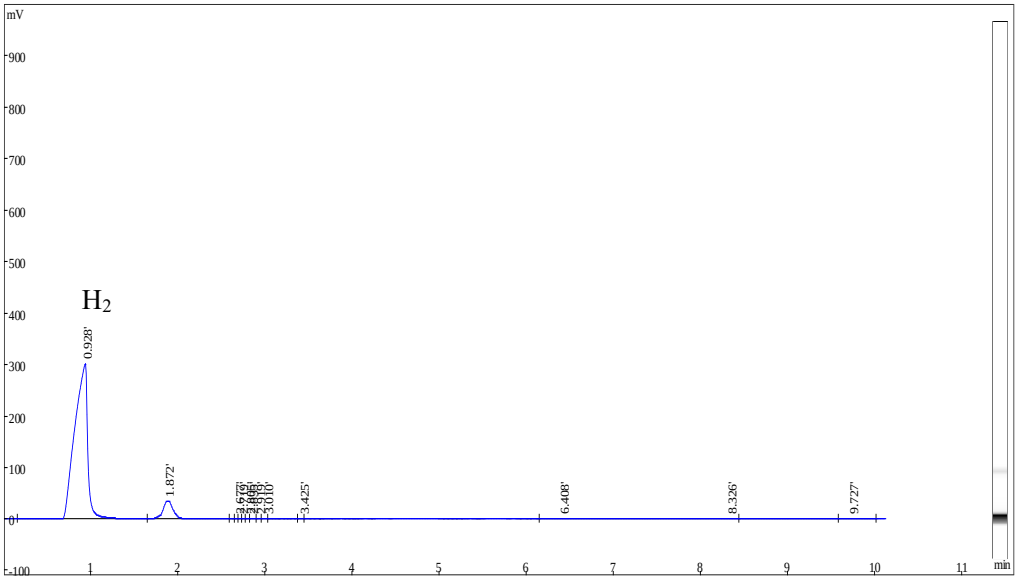
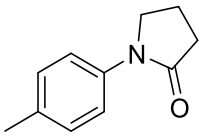


Fig. S2 GC chromatograph of the gas collected from the reaction.

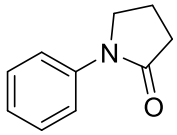
IV. Characterization data of compounds



***N*-(4-methylphenyl)-2-pyrrolidinone (3aa)**

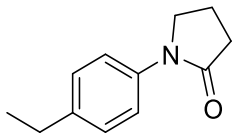
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.5 Hz, 2H), 7.16 (d, J = 8.6 Hz, 2H), 3.83 (t, J = 7.0 Hz, 2H), 2.59 (t, J = 8.1 Hz, 2H), 2.32 (s, 3H), 2.14 (p, J = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ

174.02, 136.86, 134.15, 129.31, 120.04, 48.89, 32.64, 20.83, 18.01. HRMS (ESI^+): calcd for $C_{11}H_{14}NO$ $[M+H]^+$ 176.1075, found: 176.1069.



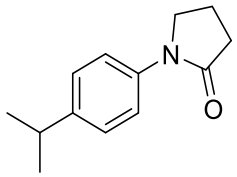
***N*-Phenylbutyrolactam (3ab)**

^1H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.8 Hz, 2H), 7.36 (t, J = 8.0 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 3.85 (t, J = 7.0 Hz, 2H), 2.61 (t, J = 8.1 Hz, 2H), 2.15 (p, J = 7.6 Hz, 2H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 174.26, 139.39, 128.82, 124.51, 119.97, 48.82, 32.79, 18.05. HRMS (ESI^+): calcd for $C_{10}H_{12}NO$ $[M+H]^+$ 162.0919, found: 162.0924.



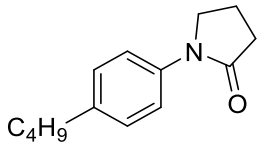
***N*-(4-Ethylphenyl)-2-pyrrolidinone (3ac)**

^1H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.6 Hz, 2H), 7.19 (d, J = 8.6 Hz, 2H), 3.84 (t, J = 7.0 Hz, 2H), 2.61 (dt, J = 16.4, 7.9 Hz, 4H), 2.14 (p, J = 7.5 Hz, 2H), 1.25 – 1.16 (m, 3H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 174.11, 140.65, 137.04, 128.19, 120.20, 48.96, 32.69, 28.33, 18.08, 15.69. HRMS (ESI^+): calcd for $C_{12}H_{16}NO$ $[M+H]^+$ 190.1232, found: 190.1240.



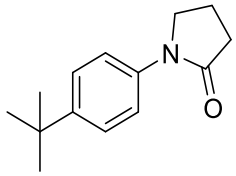
***N*-(4-propan-2-ylphenyl)pyrrolidin-2-one (3ad)**

^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.6 Hz, 2H), 7.22 (d, J = 8.6 Hz, 2H), 3.84 (t, J = 7.0 Hz, 2H), 2.94 – 2.84 (m, 1H), 2.59 (dd, J = 8.5, 7.7 Hz, 2H), 2.14 (td, J = 7.7, 1.2 Hz, 2H), 1.23 (d, J = 7.0 Hz, 6H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 174.11, 145.28, 137.08, 126.76, 120.22, 48.97, 33.62, 32.68, 24.02, 18.11. HRMS (ESI^+): calcd for $C_{13}H_{18}NO$ $[M+H]^+$ 204.1388, found: 204.1391



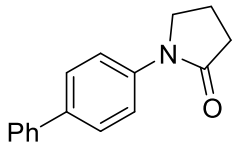
***N*-(4-butyphenyl)pyrrolidin-2-one (3ae)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.6 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 3.84 (t, *J* = 7.0 Hz, 2H), 2.63 – 2.54 (m, 4H), 2.14 (p, *J* = 7.5 Hz, 2H), 1.57 (q, *J* = 7.5 Hz, 2H), 1.34 (dq, *J* = 14.6, 7.3 Hz, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.10, 139.29, 137.01, 128.74, 120.07, 48.95, 35.06, 33.66, 32.70, 22.29, 18.09, 13.96. HRMS (ESI$^+$): calcd for $C_{14}H_{20}NO$ $[M+H]^+$ 218.1545, found: 218.1547.



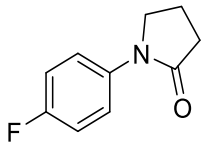
***N*-[4-(*tert*-buty)phenyl]pyrrolidin-2-one (3af)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.7 Hz, 2H), 7.39 (d, *J* = 8.7 Hz, 2H), 3.85 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.1 Hz, 2H), 2.15 (p, *J* = 7.6 Hz, 2H), 1.31 (s, 9H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.14, 147.50, 136.76, 125.69, 119.86, 48.90, 34.39, 32.68, 31.35, 18.12.HRMS (ESI$^+$): calcd for $C_{14}H_{20}NO$ $[M+H]^+$ 218.1545, found: 218.1543.



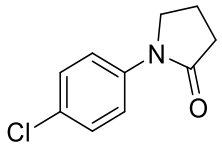
***N*-Biphenyl-4-yl-2-pyrrolidinone (3ag)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.7 Hz, 2H), 7.65 – 7.55 (m, 4H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.38 – 7.30 (m, 1H), 3.90 (t, *J* = 7.0 Hz, 2H), 2.64 (t, *J* = 8.1 Hz, 2H), 2.24 – 2.13 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.32, 140.48, 138.66, 137.25, 128.81, 127.44, 127.17, 126.90, 120.17, 48.80, 32.79, 18.05. HRMS (ESI$^+$): calcd for $C_{16}H_{16}NO$ $[M+H]^+$ 238.1232, found: 238.1232



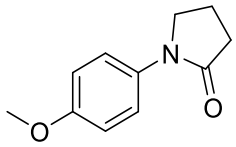
***N*-(4-Fluorophenyl)-2-pyrrolidinone (3ah)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.49 (m, 2H), 7.03 (t, *J* = 8.7 Hz, 2H), 3.81 (t, *J* = 7.0 Hz, 2H), 2.58 (t, *J* = 8.1 Hz, 2H), 2.14 (m, *J* = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.15, 159.44(d, *J* = 245.43 Hz), 135.50 (d, *J* = 3.03 Hz), 121.68 (d, *J* = 7.07 Hz), 115.45(d, *J* = 22.22 Hz), 49.00, 32.51, 17.95. HRMS (ESI^{+}): calcd for $C_{10}H_{11}FNO$ $[M+H]^{+}$ 180.0825, found: 180.0830.



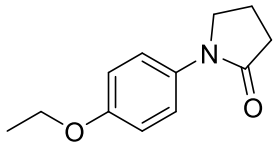
***N*-(4-Chlorophenyl)-2-pyrrolidinone (3ai)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 9.0 Hz, 2H), 7.32 (d, *J* = 9.0 Hz, 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{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.28, 137.97, 129.52, 128.82, 120.95, 48.67, 32.66, 17.90. HRMS (ESI^{+}): calcd for $C_{10}H_{11}ClNO$ $[M+H]^{+}$ 196.0529, found:196.0536.



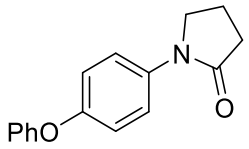
***N*-(4-(Methoxyphenyl)pyrrolidin-2-one (3aj)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 9.1 Hz, 2H), 6.88 (d, *J* = 9.1 Hz, 2H), 3.78 (d, *J* = 9.4 Hz, 5H), 2.56 (t, *J* = 8.1 Hz, 2H), 2.12 (p, *J* = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 173.97, 156.55, 132.60, 121.85, 114.02, 55.47, 49.21, 32.48, 18.02. HRMS (ESI^{+}): calcd for $C_{11}H_{14}NO_2$ $[M+H]^{+}$ 192.1025, found: 192.1032.



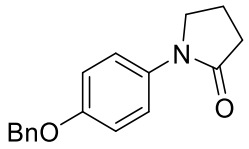
***N*-(4-Ethoxyphenyl)-2-pyrrolidinone (3ak)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 9.1 Hz, 2H), 6.87 (d, *J* = 9.1 Hz, 2H), 3.99 (q, *J* = 7.0 Hz, 2H), 3.79 (t, *J* = 7.0 Hz, 2H), 2.56 (t, *J* = 8.1 Hz, 2H), 2.11 (p, *J* = 7.5 Hz, 2H), 1.38 (t, *J* = 7.0 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 173.91, 155.90, 132.49, 121.78, 114.62, 63.65, 49.19, 32.49, 18.02, 14.84. HRMS (ESI^+): calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$ 206.1181, found: 206.1186.



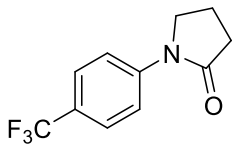
***N*-(4-phenoxyphenyl)-2-pyrrolidinone (3al)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 9.0 Hz, 2H), 7.31 (dd, *J* = 8.6, 7.4 Hz, 2H), 7.15 – 6.92 (m, 5H), 3.83 (t, *J* = 7.0 Hz, 2H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.15 (p, *J* = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.10, 157.46, 153.64, 134.97, 129.75, 123.15, 121.66, 119.39, 118.51, 49.05, 32.57, 18.02. HRMS (ESI^+): calcd for $C_{16}H_{16}NO_2$ $[M+H]^+$ 254.1181, found: 254.1178.



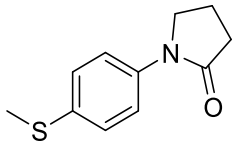
***N*-(3-Benzyloxyphenyl)pyrrolidin-2-one (3am)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.28 (m, 7H), 7.05 – 6.88 (m, 2H), 5.04 (s, 2H), 3.79 (t, *J* = 7.0 Hz, 2H), 2.57 (t, *J* = 8.1 Hz, 2H), 2.16 – 2.07 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.01, 155.72, 136.97, 132.84, 128.62, 128.00, 127.48, 121.78, 115.08, 70.24, 49.17, 32.53, 18.02. HRMS (ESI^+): calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$ 268.1338, found: 268.1347.



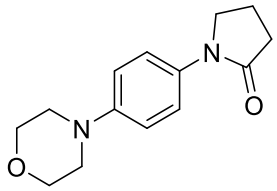
***N*-[4-(Trifluoromethyl)phenyl]-2-pyrrolidinone (3an)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.6 Hz, 2H), 7.61 (d, *J* = 8.9 Hz, 2H), 3.89 (t, *J* = 7.0 Hz, 2H), 2.64 (t, *J* = 8.1 Hz, 2H), 2.29 – 2.09 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.65, 142.34, 125.99 (q, *J* = 3.7 Hz), 122.78, 119.18, 48.47, 32.78, 17.89. HRMS (ESI^+): calcd for $C_{11}H_{11}F_3NO$ $[M+H]^+$ 230.0793, found: 230.0783.



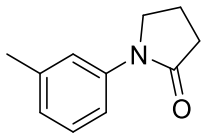
***N*-[4-(Methylthio)phenyl]pyrrolidin-2-one (3ao)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.9 Hz, 2H), 7.27 (d, *J* = 8.9 Hz, 2H), 3.96 – 3.71 (m, 2H), 2.60 (t, *J* = 6.6 Hz, 2H), 2.46 (s, 3H), 2.23 – 2.05 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.19, 137.00, 133.88, 127.65, 120.44, 48.75, 32.69, 17.96, 16.57. HRMS (ESI$^+$): calcd for $C_{11}H_{14}NOS$ $[M+H]^+$ 208.0796, found: 208.0801.



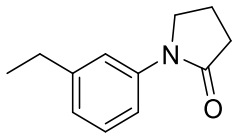
***N*-[4-(4-morpholinyl)phenyl]-2-pyrrolidinone (3ap)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.8 Hz, 2H), 7.61 (d, *J* = 8.9 Hz, 2H), 3.91 – 3.72 (m, 6H), 3.15 – 3.03 (m, 4H), 2.57 (t, *J* = 8.1 Hz, 2H), 2.18 – 2.06 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 173.97, 148.34, 132.17, 121.43, 116.07, 66.87, 49.63, 49.09, 32.53, 18.03. HRMS (ESI$^+$): calcd for $C_{14}H_{19}N_2O_2$ $[M+H]^+$ 247.1447, found: 247.1458.



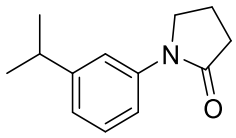
***N*-(m-Tolyl)pyrrolidin-2-one (3ba)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.00 (d, *J* = 7.5 Hz, 1H), 3.88 (t, *J* = 7.0 Hz, 2H), 2.63 (t, *J* = 8.1 Hz, 2H), 2.40 (s, 3H), 2.17 (p, *J* = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.20, 139.34, 138.66, 128.63, 125.38, 120.83, 117.17, 48.97, 32.80, 21.64, 18.08. HRMS (ESI$^+$): calcd for $C_{11}H_{14}NO$ $[M+H]^+$ 176.1075, found: 176.1074.



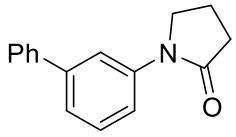
***N*-(3-Ethylphenyl)-2-pyrrolidinone (3bb)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.41 (d, *J* = 9.4 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 3.88 (t, *J* = 7.0 Hz, 2H), 2.78 – 2.48 (m, 4H), 2.17 (p, *J* = 7.5 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.21, 145.06, 139.39, 128.72, 124.18, 119.73, 117.46, 49.00, 32.81, 29.01, 18.11, 15.62. HRMS (ESI^+): calcd for $C_{12}H_{16}NO$ $[M+H]^+$ 190.1232, found: 190.1251.



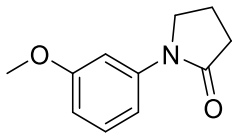
***N*-[3-(1-methylethyl)phenyl]-2-pyrrolidinone (3bc)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.31 – 7.25 (m, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 3.86 (t, *J* = 7.0 Hz, 2H), 2.91 (p, *J* = 6.9 Hz, 1H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.14 (p, *J* = 7.6 Hz, 2H), 1.25 (d, *J* = 6.9 Hz, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.21, 149.70, 139.37, 128.71, 122.64, 118.43, 117.66, 49.01, 34.28, 32.80, 23.99, 18.10. HRMS (ESI^+): calcd for $C_{13}H_{18}NO$ $[M+H]^+$ 204.1388, found: 204.1403.



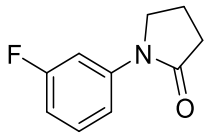
***N*-Biphenyl -3-yl-2-pyrrolidinon (3bd)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (t, *J* = 1.8 Hz, 1H), 7.69 – 7.56 (m, 3H), 7.49 – 7.40 (m, 3H), 7.41 – 7.31 (m, 2H), 3.86 (t, *J* = 7.0 Hz, 2H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.24 – 2.06 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.41, 141.92, 140.90, 139.93, 129.23, 128.83, 127.55, 127.29, 123.32, 118.90, 118.79, 48.91, 32.83, 18.04. HRMS (ESI^+): calcd for $C_{16}H_{16}NO$ $[M+H]^+$ 238.1232, found: 238.1227.



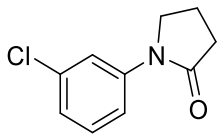
***N*-(3-Methoxyphenyl)pyrrolidin-2-one (3be)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (t, *J* = 2.3 Hz, 1H), 7.29 – 7.21 (m, 1H), 7.11 (ddd, *J* = 8.2, 2.1, 0.9 Hz, 1H), 6.78 – 6.61 (m, 1H), 3.82 (d, *J* = 9.8 Hz, 5H), 2.60 (t, J = 8.1 Hz, 2H), 2.14 (p, *J* = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.33, 159.91, 140.62, 129.46, 112.00, 110.05, 106.03, 55.33, 48.92, 32.91, 17.96. HRMS (ESI$^+$): calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$ 192.1025, found: 192.1032.



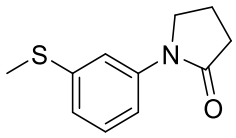
***N*-(3-Fluorophenyl)pyrrolidin-2-one (3bf)**

^{1}H NMR (400 MHz,$CDCl_3$) δ 7.52 (d, *J* = 11.4 Hz, 1H), 7.40 – 7.27 (m, 2H), 6.96 – 6.76 (m, 1H), 3.84 (t, *J* = 7.1 Hz, 2H), 2.62 (t, J = 8.1 Hz, 2H), 2.16 (p, *J* = 7.9 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.39, 162.85 (d, *J* = 244.5 Hz), 140.84 (s), 129.89 (d, *J* = 9.3 Hz), 114.75 (d, *J* = 3.0 Hz), 111.06 (d, *J* = 21.3 Hz), 107.13 (d, *J* = 26.2 Hz). 48.66, 32.83, 17.86. HRMS (ESI$^+$): calcd for $C_{10}H_{11}FNO$ $[M+H]^+$ 180.0825, found: 180.0830.



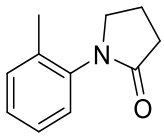
***N*-(3-Chlorophenyl)pyrrolidin-2-one (3bg)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (t, *J* = 2.0 Hz, 1H), 7.52 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.28 (t, *J* = 8.1 Hz, 1H), 7.11 (dd, *J* = 7.7, 1.5 Hz, 1H), 3.83 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.1 Hz, 2H), 2.16 (p, *J* = 7.6 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.39, 140.54, 134.45, 129.79, 124.32, 119.71, 117.62, 48.60, 32.74, 17.87. HRMS (ESI+): calcd for $C_{10}H_{11}ClNO$ $[M+H]^+$ 196.0529, found: 196.0538.



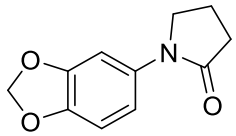
***N*-[3-(methylthio)phenyl]pyrrolidi-2-none (3bh)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.34 – 7.26 (m, 2H), 7.03 (d, *J* = 7.3 Hz, 1H), 3.84 (dd, *J* = 6.7, 3.6 Hz, 2H), 2.60 – 2.58 (m, 2H), 2.49 (s, 3H), 2.27 – 2.11 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.37, 139.92, 139.30, 129.08, 122.48, 117.85, 116.49, 48.79, 32.81, 18.00, 15.80. HRMS (ESI$^+$): calcd for $C_{11}H_{14}NOS$ $[M+H]^+$ 208.0796, found: 208.0801.



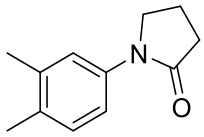
***N*-(o-tolyl)pyrrolidin-2-one (3c)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.12 (m, 4H), 3.72 – 3.69 (m, 2H), 2.58 – 2.54 (m, 2H), 2.24 – 2.17 (m, 5H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.54, 137.45, 135.57, 131.17, 127.93, 126.87, 126.65, 50.78, 31.26, 19.10, 17.93. HRMS (ESI$^+$): calcd for $C_{11}H_{14}NO$ $[M+H]^+$ 176.1075, found: 176.1079.



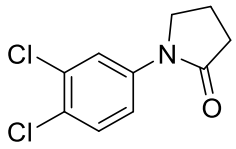
***N*-(1,3-Benzodioxol-5-yl)pyrrolidin-2-one (3d)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 2.1 Hz, 1H), 6.84 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 1H), 5.93 (s, 2H), 3.78 (t, *J* = 7.0 Hz, 2H), 2.56 (t, *J* = 8.1 Hz, 2H), 2.12 (p, *J* = 7.5 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.01, 147.77, 144.50, 133.78, 113.28, 107.88, 103.00, 101.29, 49.53, 32.54, 17.99. HRMS (ESI$^+$): calcd for $C_{11}H_{12}NO_3$ $[M+H]^+$ 206.0817, found: 206.0822.



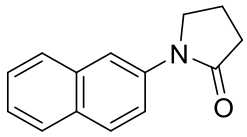
***N*-(3,4-dimethylphenyl)pyrrolidin-2-one (3e)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (br, 2H), 6.80 (s, 1H), 3.83 (t, *J* = 7.0 Hz, 2H), 2.59 (t, *J* = 8.1 Hz, 2H), 2.32 (br, 6H), 2.23 – 2.05 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.27, 139.22, 138.48, 126.49, 118.16, 49.21, 32.78, 21.51, 18.13. HRMS (ESI^+): calcd for $C_{12}H_{16}NO$ $[M+H]^+$ 190.1232, found: 190.1237.



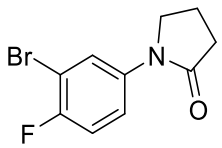
***N*-(3,4-Dichlorophenyl)pyrrolidin-2-one (3f)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 2.6 Hz, 1H), 7.51 (dd, *J* = 8.9, 2.6 Hz, 1H), 7.38 (d, *J* = 8.9 Hz, 1H), 3.80 (t, *J* = 7.1 Hz, 2H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.24 – 2.08 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.42, 138.88, 132.58, 130.28, 127.51, 121.14 , 118.74, 48.50, 32.65, 17.75. HRMS (ESI^+): calcd for $C_{10}H_9Cl_2NaNO$ $[M+Na]^+$ 251.9959, found: 251.9950.



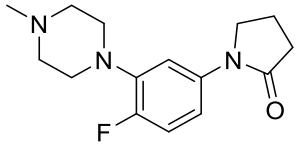
***N*-(2-Naphthyl)pyrrolidin-2-one (3g)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.88 – 7.73 (m, 4H), 7.51 – 7.36 (m, 2H), 3.92 (t, *J* = 7.0 Hz, 2H), 2.63 (t, *J* = 8.1 Hz, 2H), 2.15 (p, *J* = 7.6 Hz, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.48, 137.19, 133.51, 130.67, 128.55, 127.71, 127.55, 126.40, 125.24, 119.87, 116.76, 49.04, 32.87, 18.03. HRMS (ESI^+): calcd for $C_{14}H_{13}KNO$ $[M+K]^+$ 250.0634, found: 250.0637.



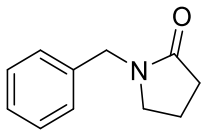
***N*-(3-bromo-4-fluorophenyl)pyrrolidin-2-one (3h)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 6.0, 2.7 Hz, 1H), 7.62 – 7.50 (m, 1H), 7.10 (t, *J* = 8.5 Hz, 1H), 3.82 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.1 Hz, 2H), 2.24 – 2.08 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.23, 157.03, 154.59, 136.36, 124.64, 120.29 (d, *J* = 6.9 Hz), 116.25 (d, *J* = 23.2 Hz), 48.82, 32.39, 17.98. HRMS (ESI^+): calcd for $C_{10}H_{10}BrFNO$ $[M+H]^+$ 257.9930, found: 257.9937.



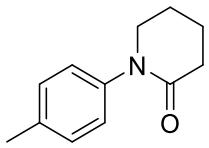
***N*-[4-fluoro-3-(4-methylpiperazin-1-yl)phenyl]pyrrolidin-2-one (4)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.6 Hz, 1H), 6.96 – 6.92 (m, 2H), 3.79 (t, *J* = 7.0 Hz, 2H), 3.11 (br, 4H), 2.57 – 2.53 (m, 6H), 2.32 (s, 3H), 2.21 – 1.97 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.14 , 152.41 (d, *J* = 244.2 Hz), 140.03 (d, *J* = 9.3 Hz), 135.89 (d, *J* = 2.8 Hz), 115.88 (d, *J* = 22.1 Hz), 113.51 (d, *J* = 7.8 Hz), 111.70 (d, *J* = 3.0 Hz), 55.05, 50.23 (d, *J* = 3.6 Hz), 49.16, 46.06 , 32.61, 17.93. HRMS (ESI^{+}): calcd for $C_{15}H_{21}FN_3O$ $[M+H]^{+}$ 278.1669, found: 278.1659.



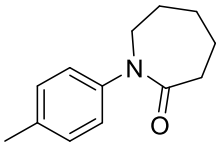
***N*-benzylpyrrolidin-2-one (5)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.23 (m, 5H), 4.45 (s, 2H), 3.27 – 3.24 (m, 2H), 2.44 (t, *J* = 8.1 Hz, 2H), 2.02 – 1.94 (m, 2H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 174.97, 136.57, 128.67, 128.11, 127.54, 46.61, 46.58, 30.95, 17.73. HRMS (ESI^{+}): calcd for $C_{11}H_{14}NO$ $[M+H]^{+}$ 176.1075, found: 176.1078.



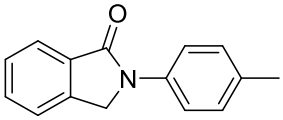
***N*-(*p*-tolyl)piperidin-2-one (6a)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.1 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 3.61 (dd, *J* = 7.8, 3.9 Hz, 2H), 2.54 (t, *J* = 5.7 Hz, 2H), 2.34 (s, 3H), 1.94 – 1.92 (m, 4H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 170.15, 140.84, 136.55, 129.85, 126.09, 51.83, 32.86, 23.59, 21.51, 21.07. HRMS (ESI+): calcd for $C_{12}H_{16}NO$ $[M+H]^{+}$ 190.1232, found: 190.1238.



***N*-(*p*-tolyl)azepan-2-one (6b)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 3.73 – 3.72 (m, 2H), 2.70 – 2.69 (m, 2H), 2.33 (s, 3H), 1.81 (br, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 175.74, 142.05, 136.26, 129.77, 126.07, 53.16, 37.65, 29.92, 28.87, 23.58, 21.03. HRMS (ESI^+): calcd for $C_{13}H_{18}NO$ $[M+H]^+$ 204.1388, found: 204.1398.



***N*-(*p*-tolyl)isoindolin-2-one (6c)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.2 Hz, 1H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.53 – 7.45 (m, 1H), 7.42 (t, *J* = 7.2 Hz, 2H), 7.13 (d, *J* = 8.3 Hz, 2H), 4.64 (s, 2H), 2.28 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 167.33, 140.20, 136.95, 134.00, 133.27, 131.88, 129.60, 128.22, 123.87, 122.61, 119.35, 50.72, 20.84. HRMS (ESI^+): calcd for $C_{15}H_{14}NO$ $[M+H]^+$ 224.1075, found: 224.1077.

V. References

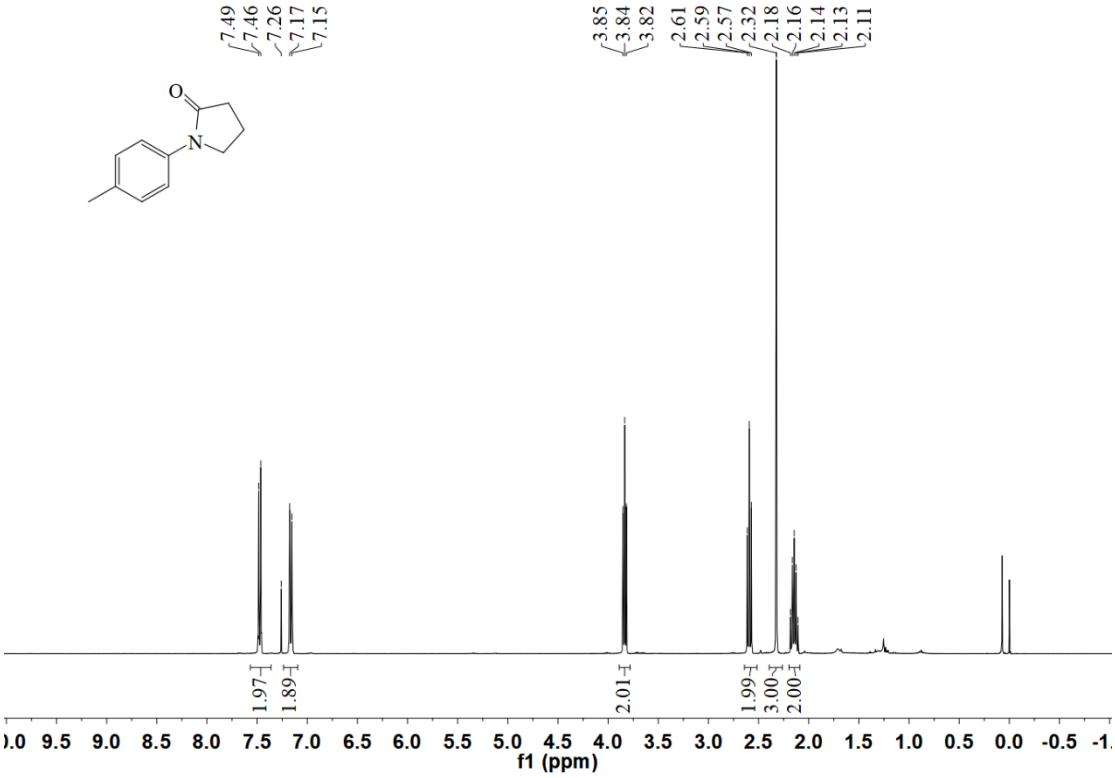
1 X.-J. Yu, H.-Y. He, L. Yang, H.-Y. Fu, X.-L. Zheng, H. Chen, R.-X. Li, *Catal. Commun.*, 2017, **95**, 54.

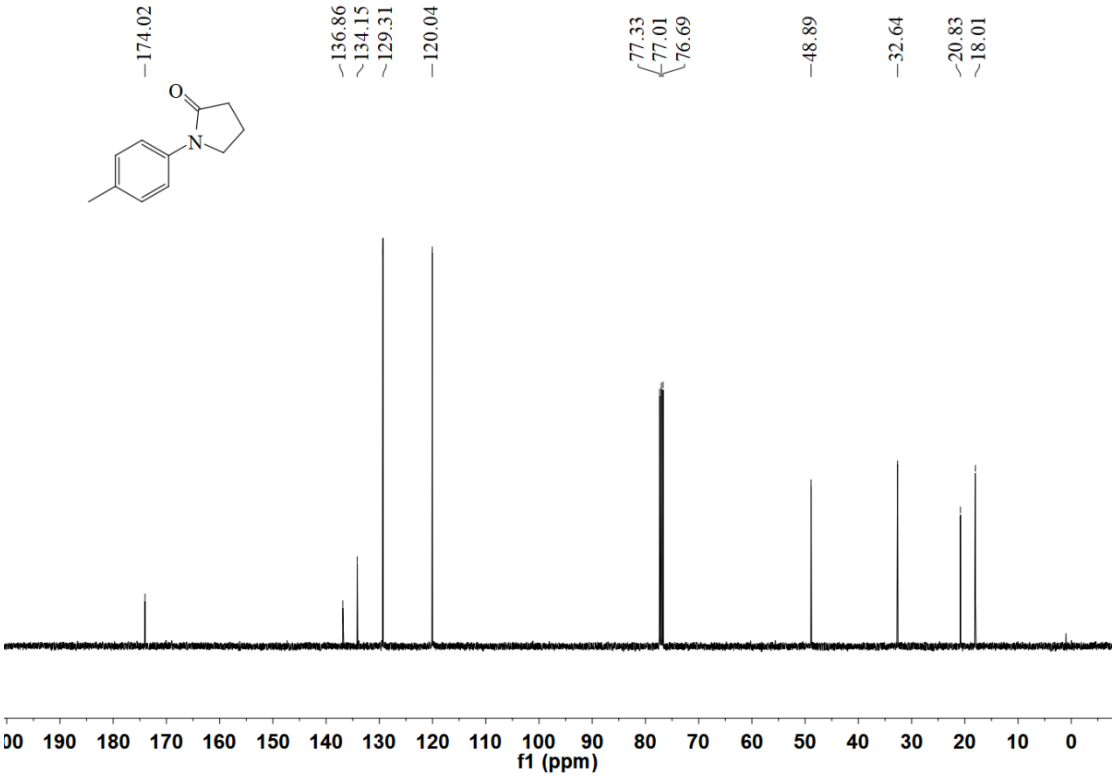
2 a) J. W. Kim, K. Yamaguchi, and N. Mizuno, Angew. Chem. Int. Ed., 2008, 47, 9249; b) R. Ray, S. Chandra, V. Yadav, P. Mondal, D. Maiti, and G. K. Lahiri, Chem. Commun., 2017, 53, 4006.

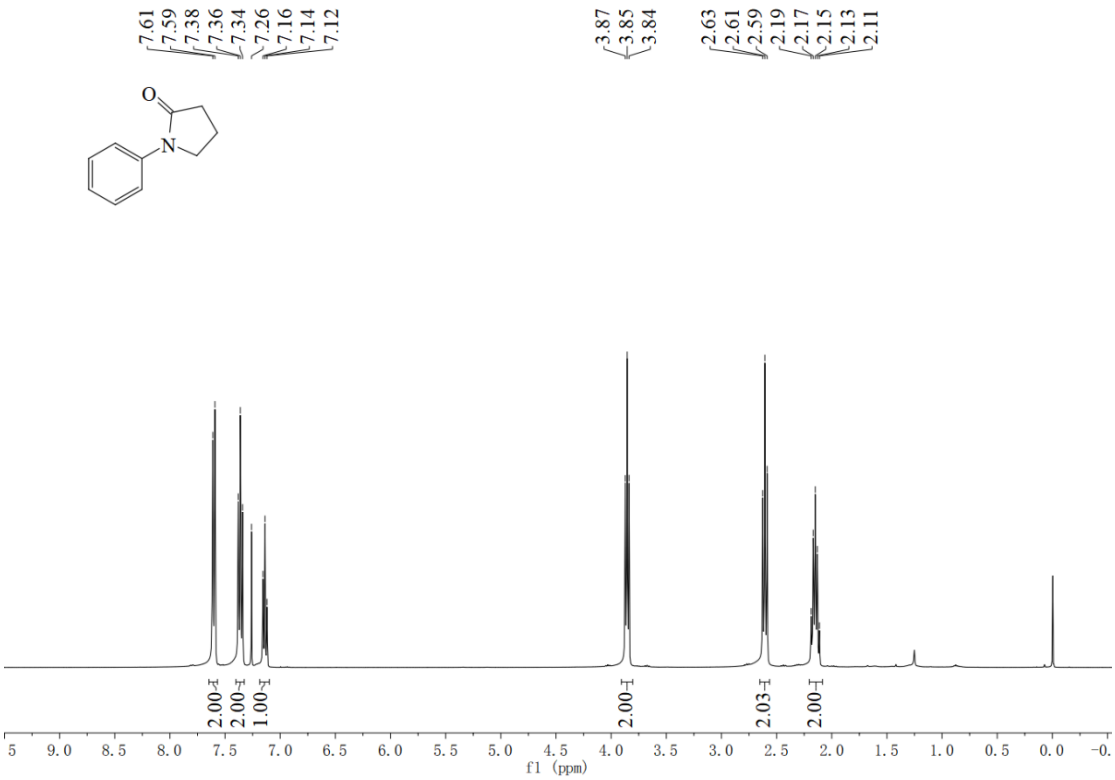
3 A. A. F.-Amador, X.-Y. Qian, H.-C. Xu, and T. Wirth, *Chem. Eur. J.*, 2018, **24**, 487.

4 W. Guo, J. E. Gómez, L. M.-Rodríguez, N. A. G. Bandeira, C. Bo, and A. W. Kleij, *ChemSusChem*., 2017, **9**, 1969.

VI. Copies of ^{1}H and $^{13}C\{^{1}H\}$ spectra



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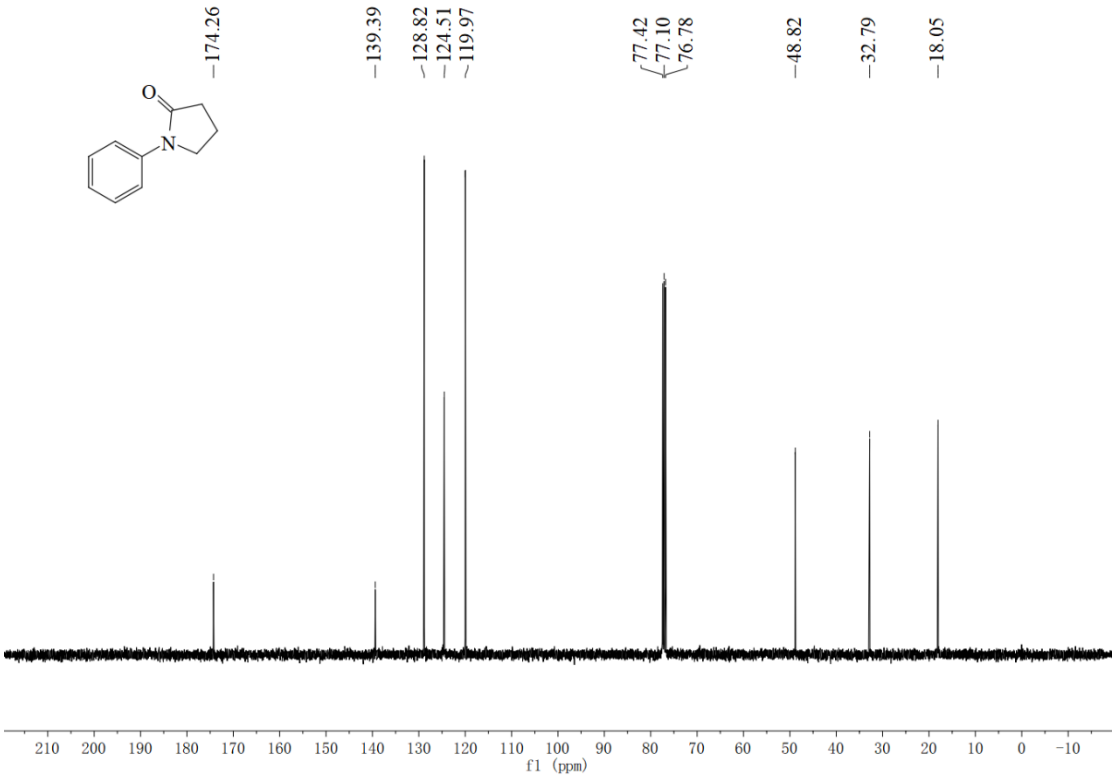
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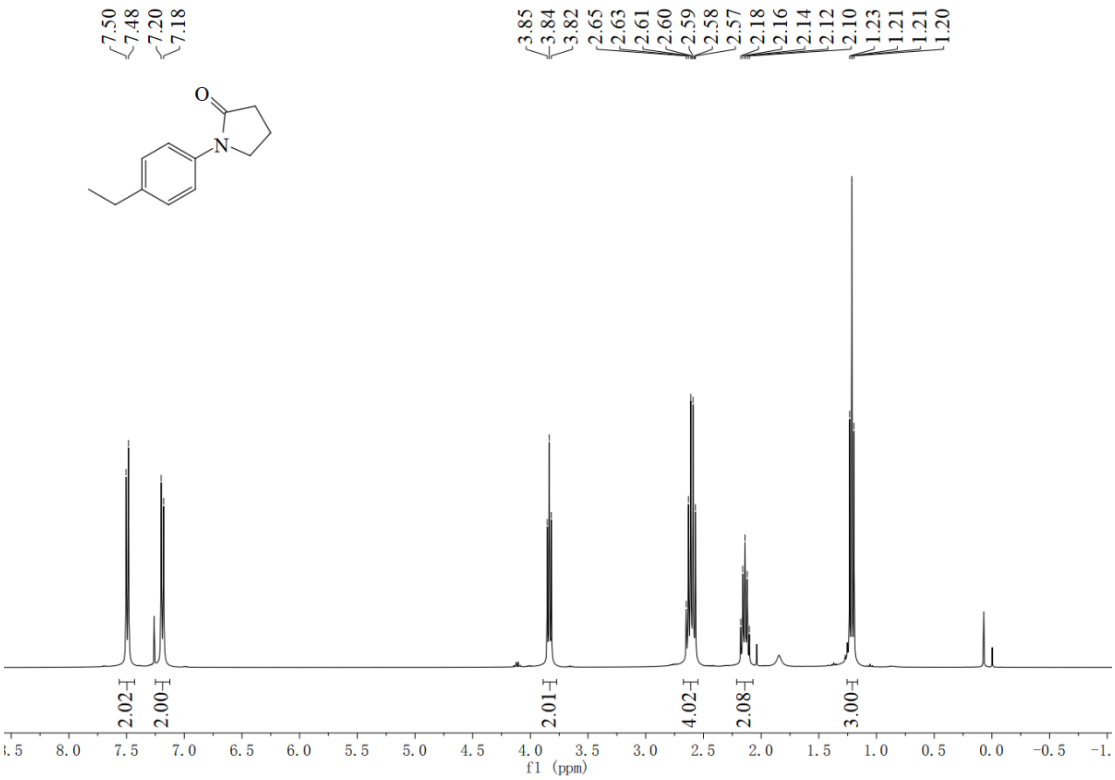
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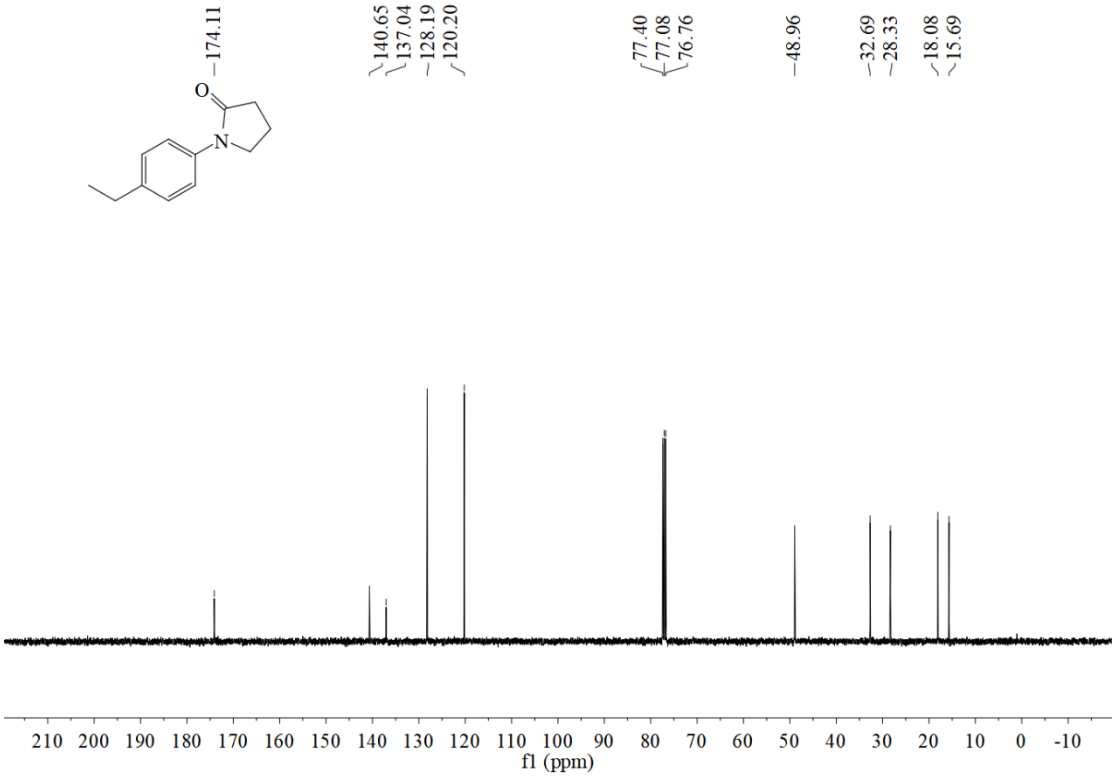
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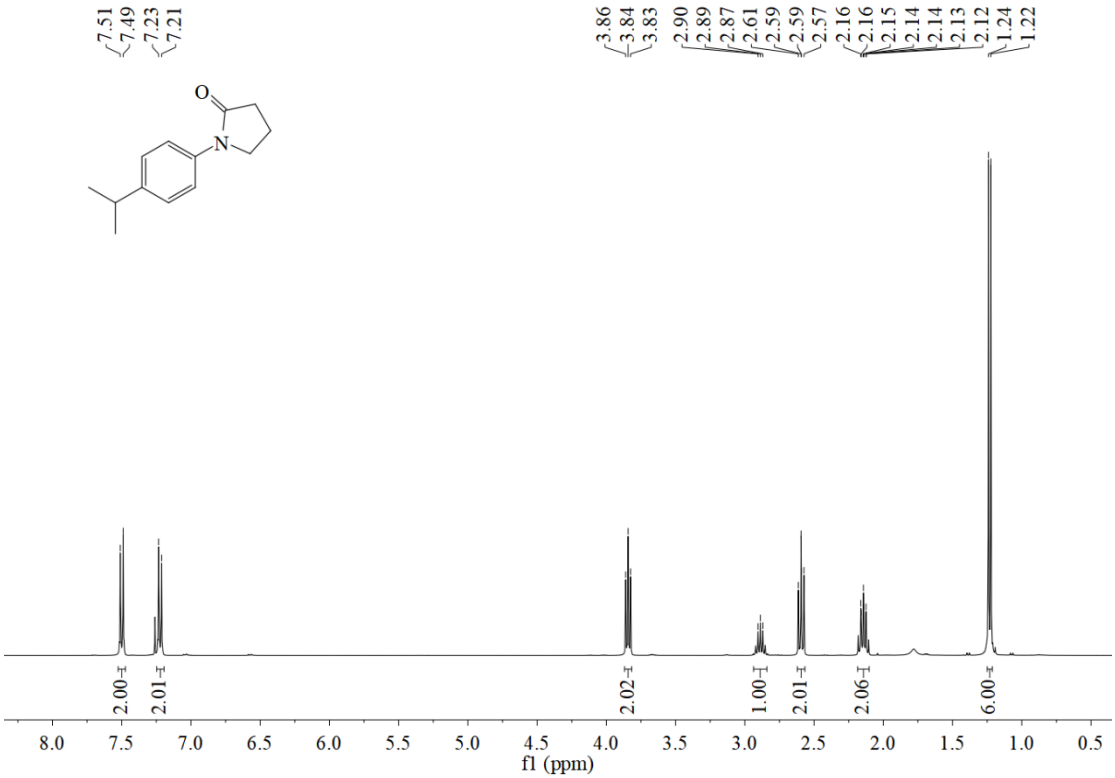
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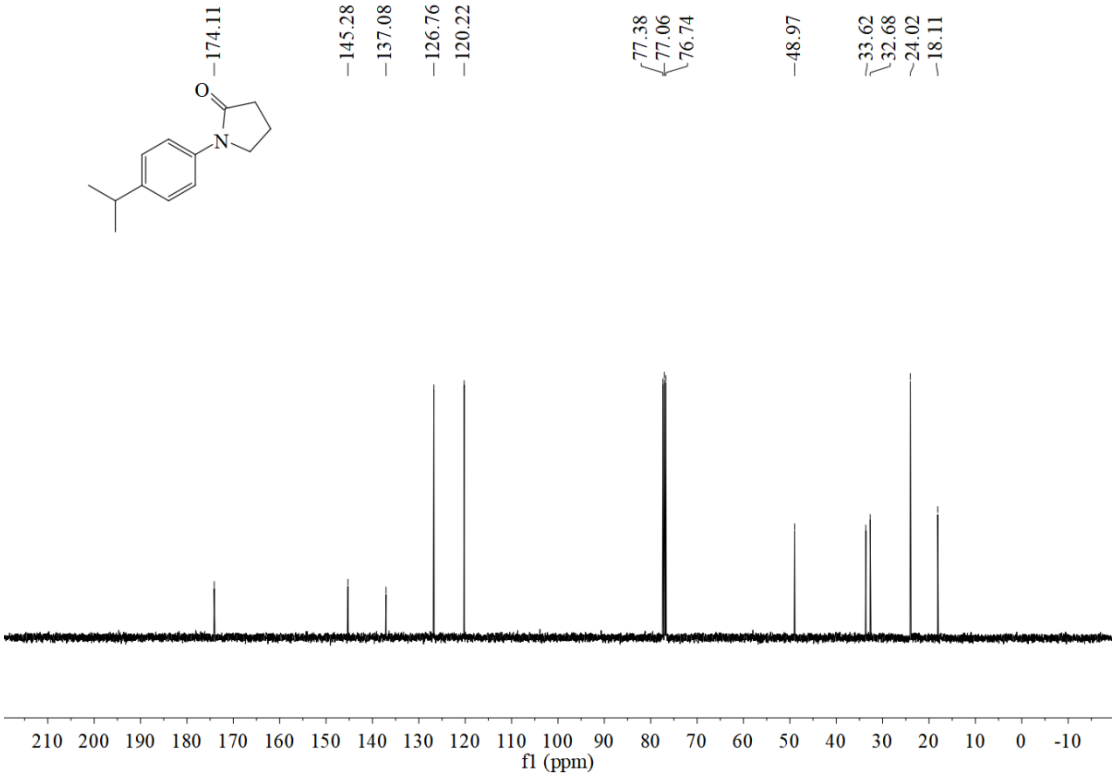
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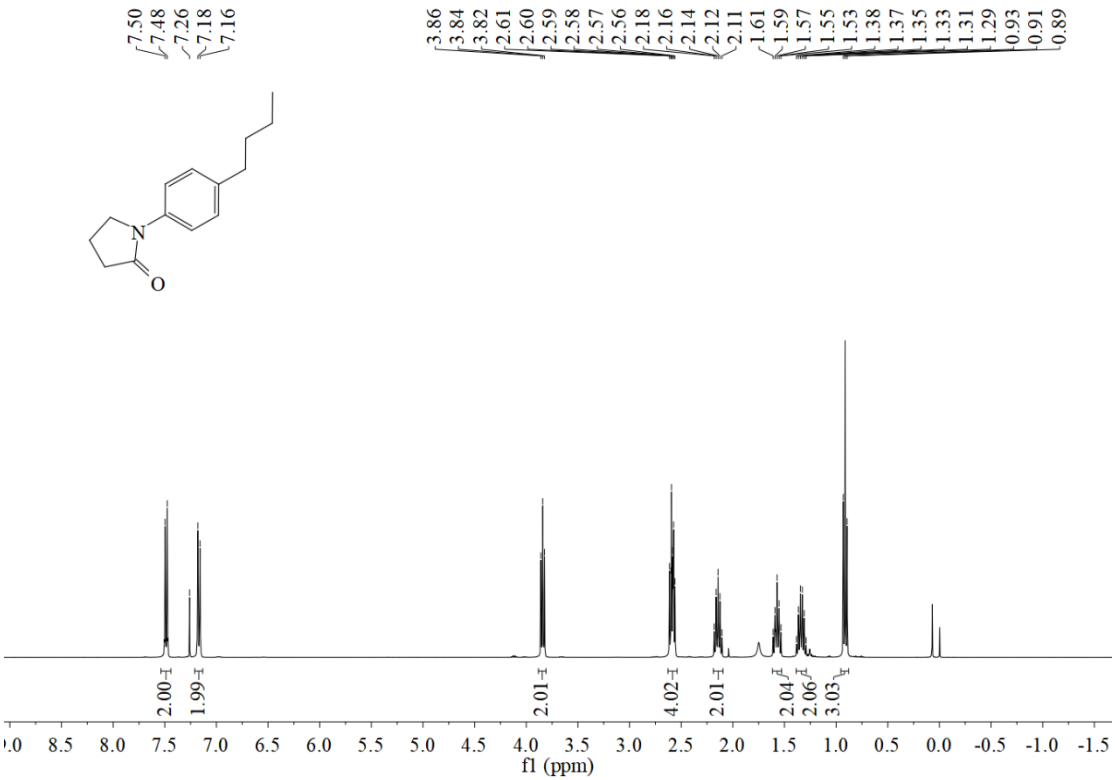
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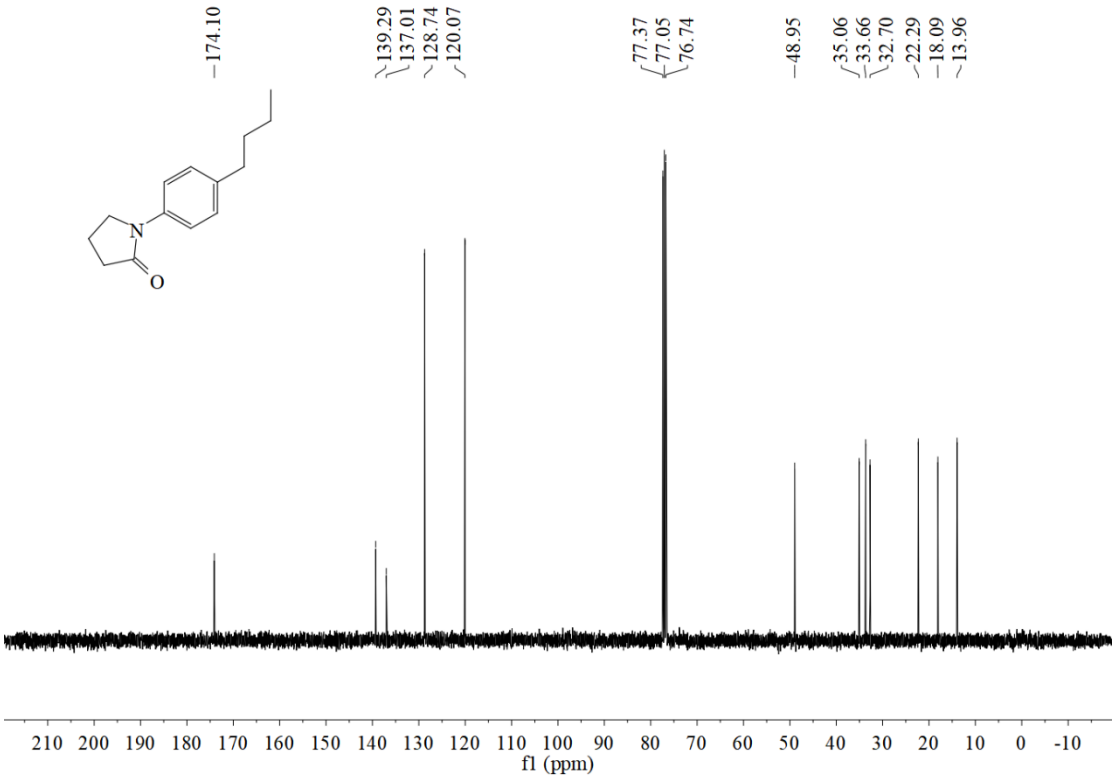
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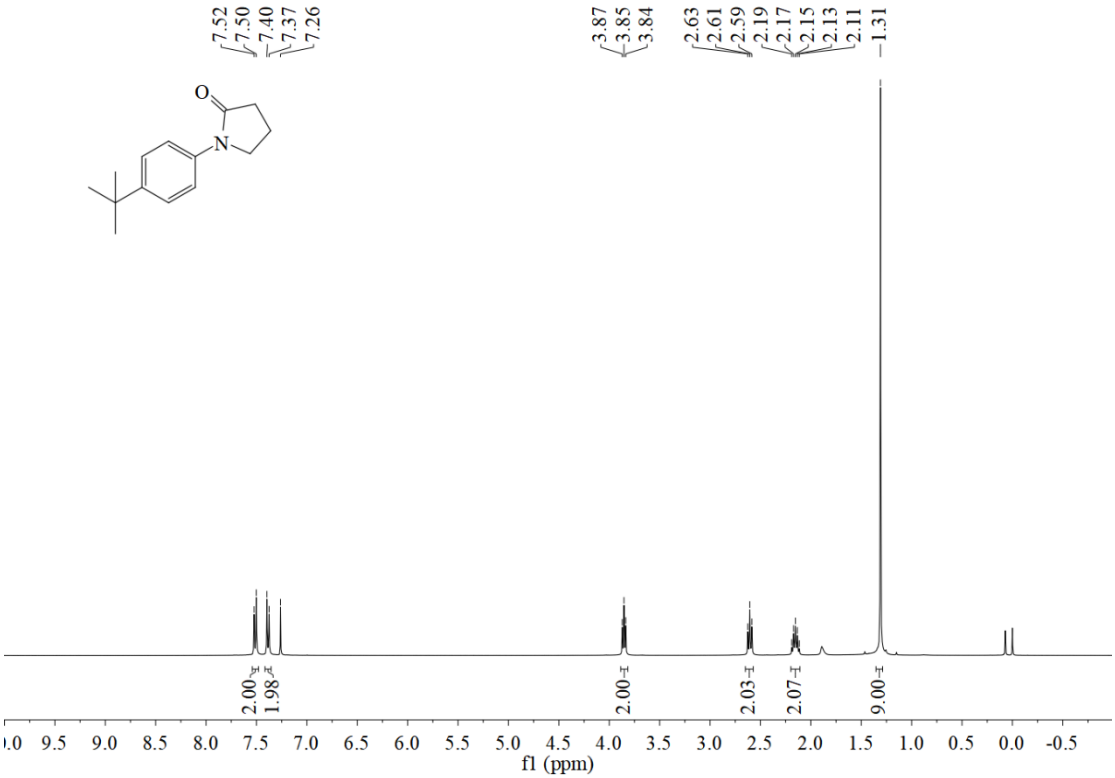
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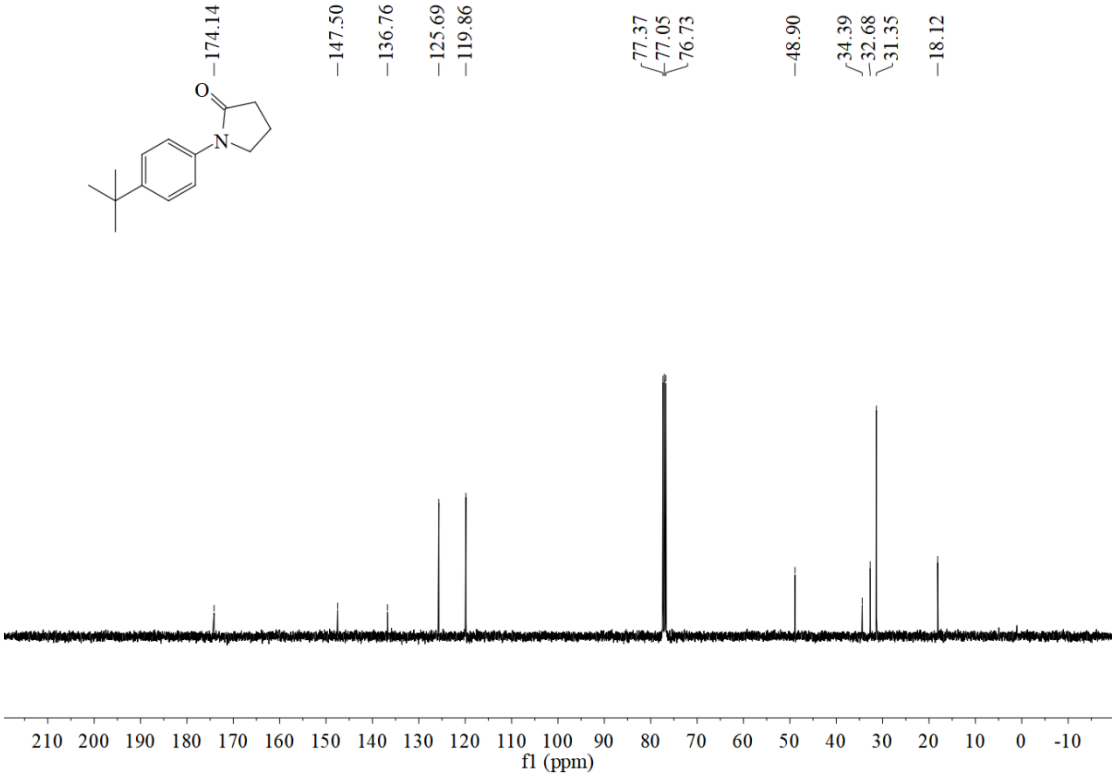
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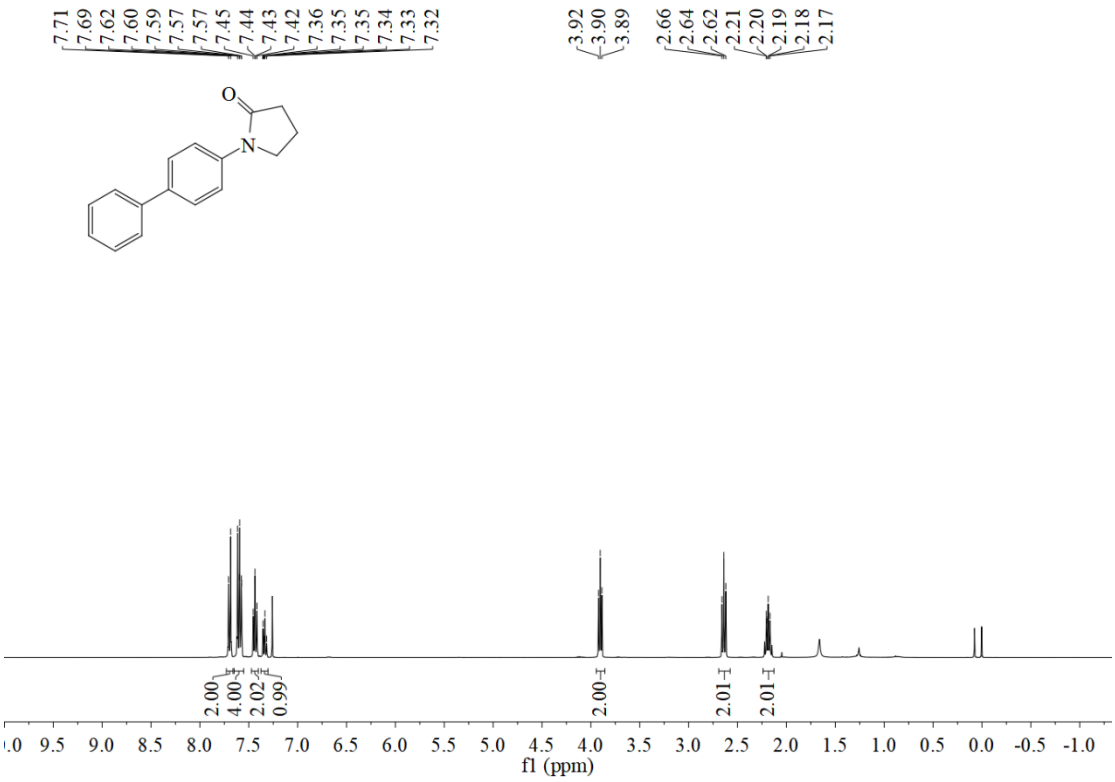
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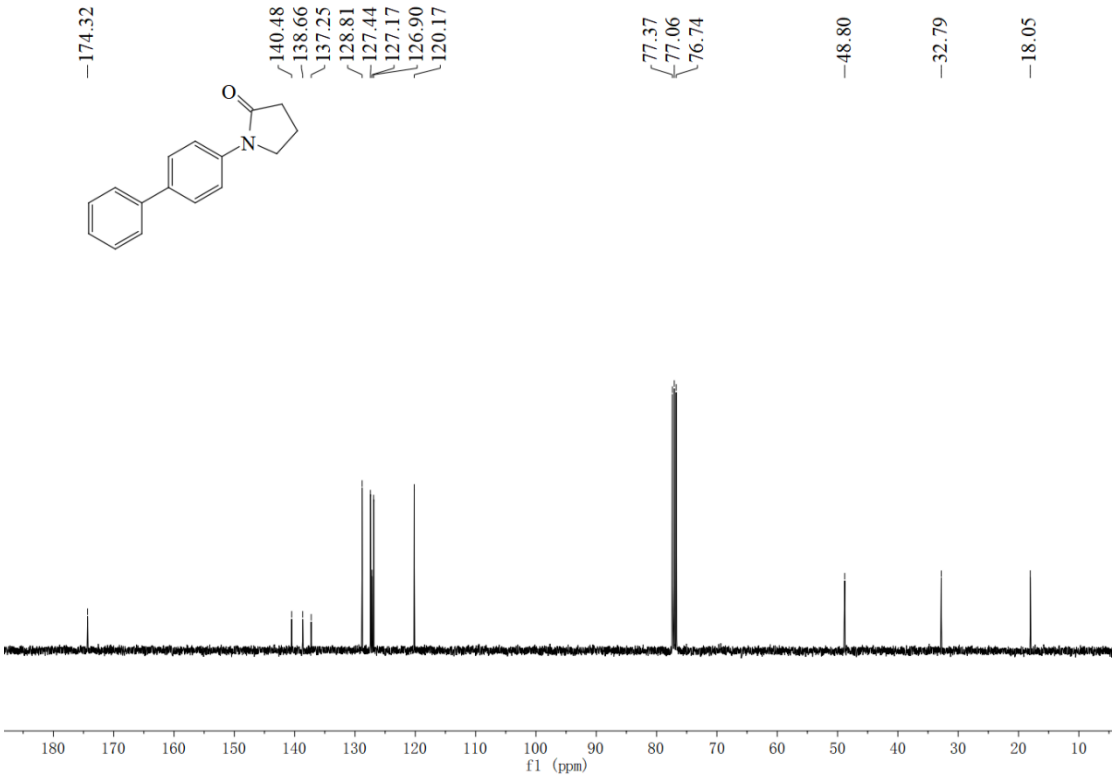
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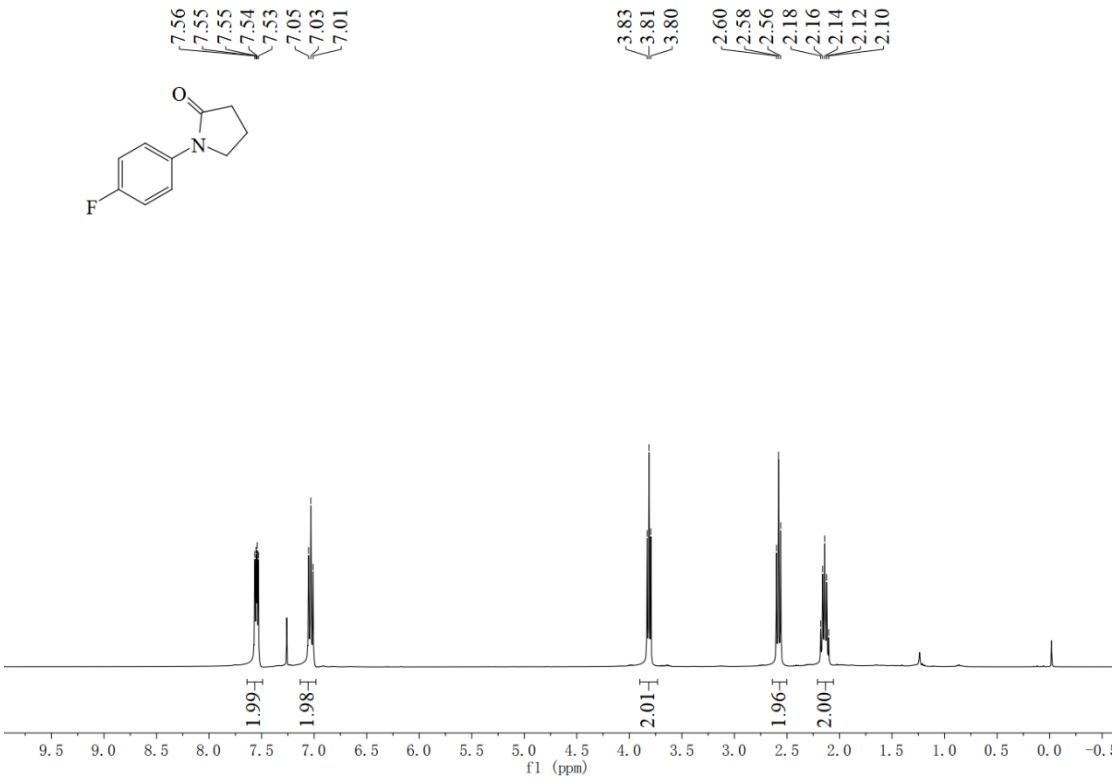
N
f1 (ppm)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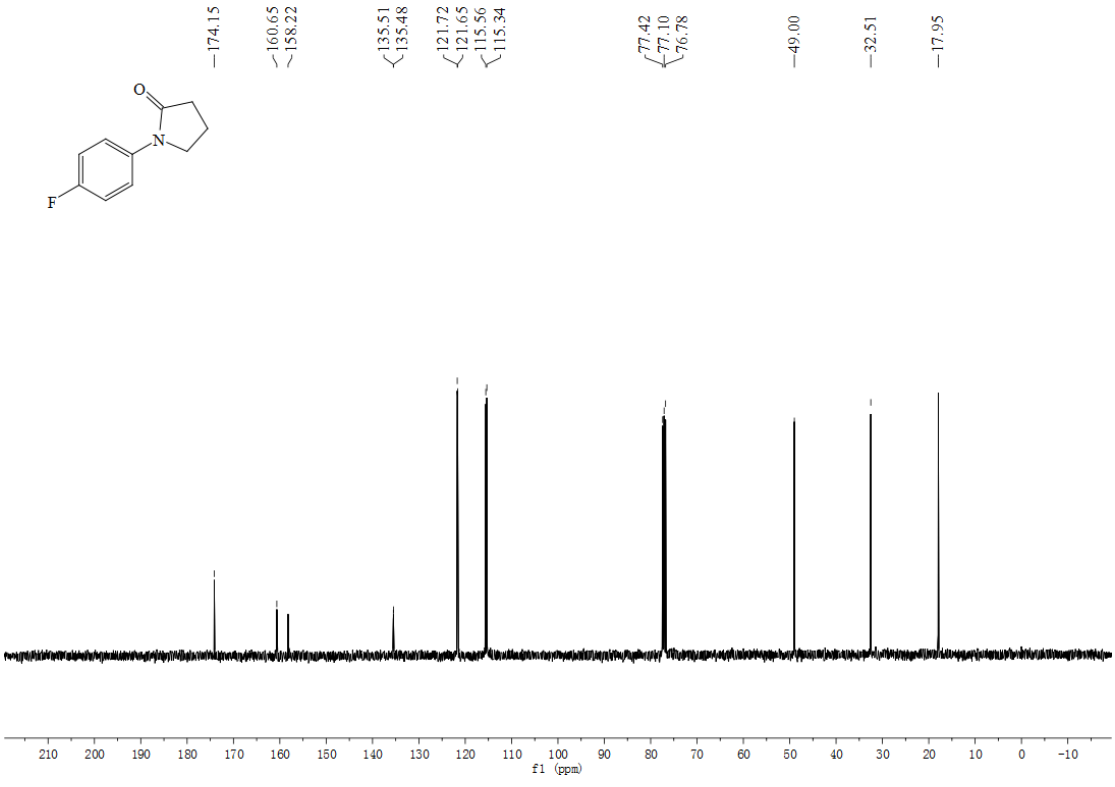
7.55
7.55
7.54
7.53
7.05
7.03
7.01
3.83
3.81
3.80
2.60
2.58
2.56
2.18
2.16
2.14
2.12
2.10
O
N
F
1.99
1.98
2.01
1.96
2.00
f1 (ppm)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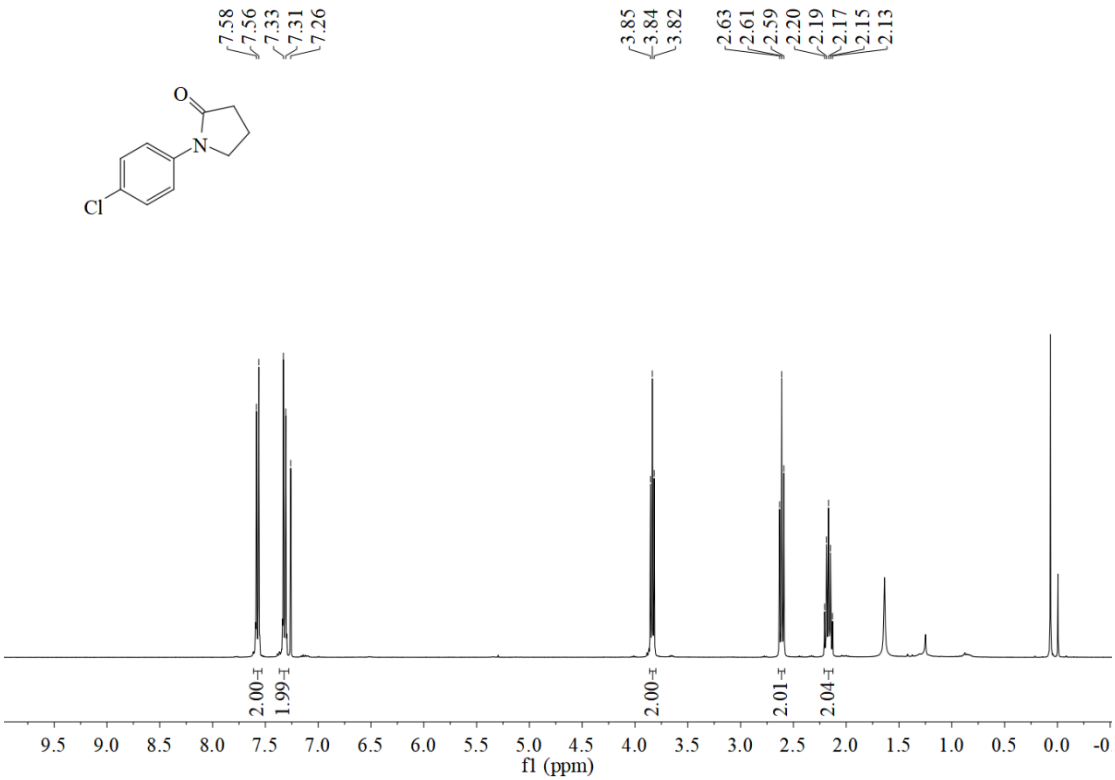
158.22
135.51
135.48
121.72
121.65
115.56
115.34
77.42
77.10
76.78
49.00
32.51
17.95
O
N
F
f1 (ppm)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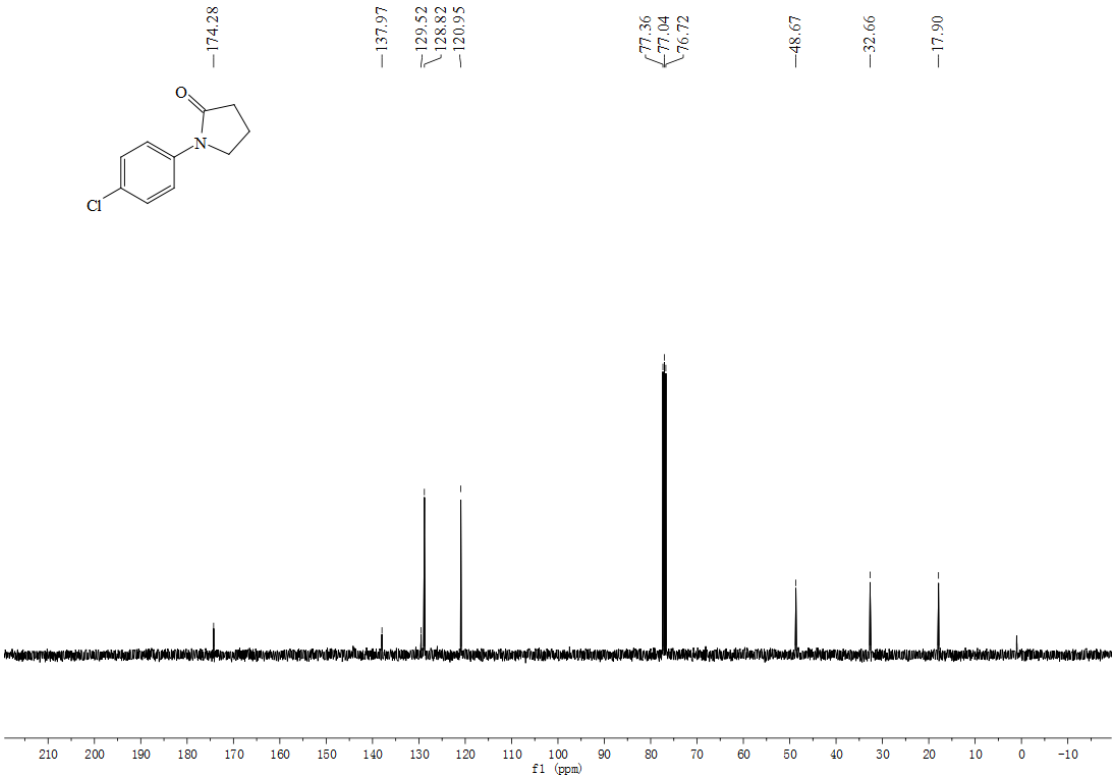
7.33
7.31
7.26
3.85
3.84
3.82
2.63
2.61
2.59
2.20
2.19
2.17
2.15
2.13
O
N
Cl
2.00
1.99
2.00
2.01
2.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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120.95
77.36
77.04
76.72
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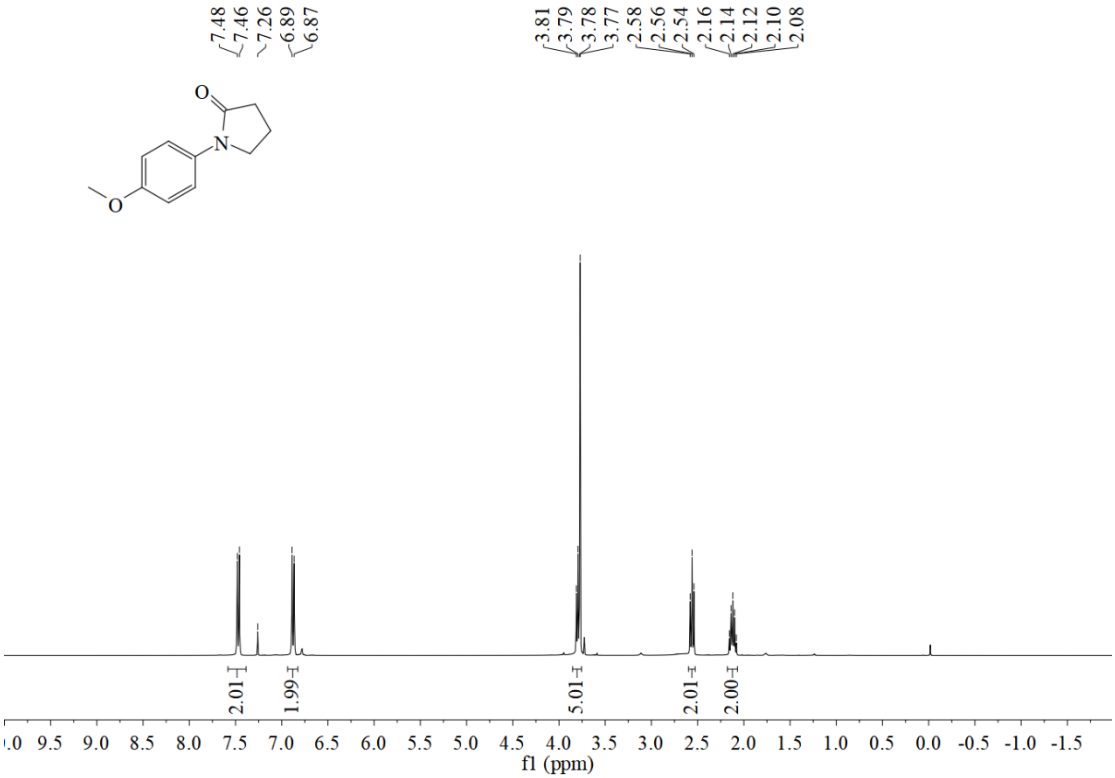
17.90
O
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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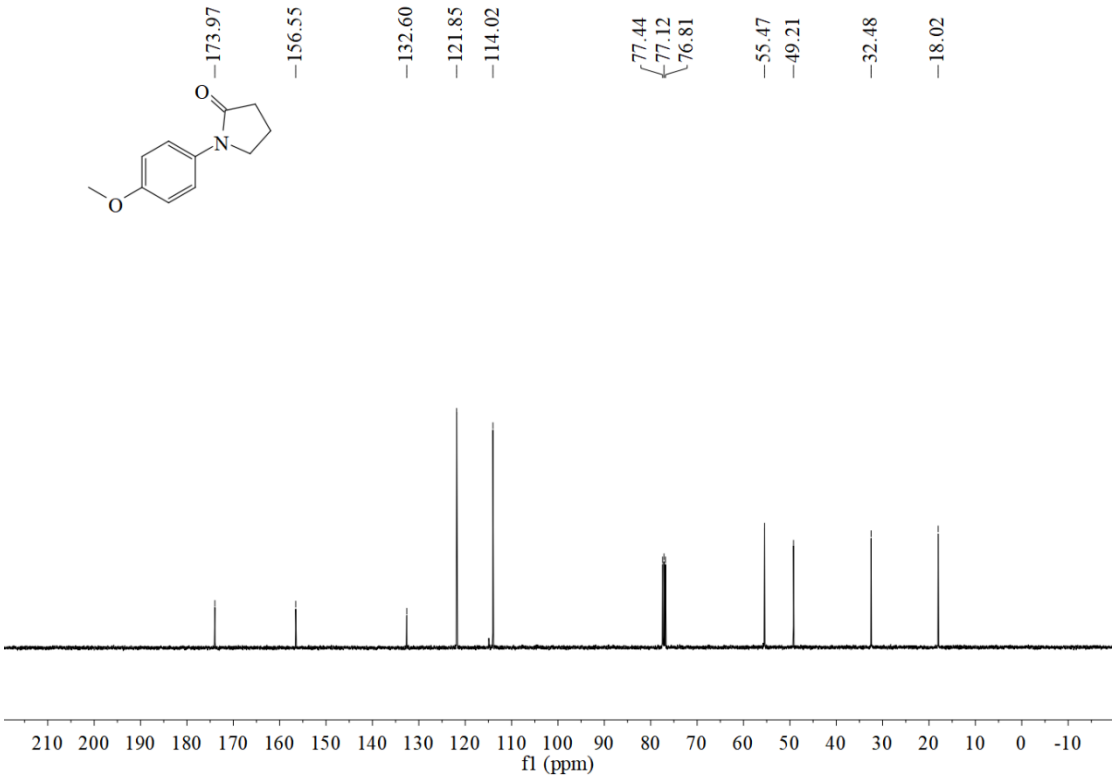
3.81
3.79
3.78
3.77
2.58
2.56
2.54
2.16
2.14
2.12
2.10
2.08
O
N
O
2.01
1.99
5.01
2.01
2.00
f1 (ppm)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114.02
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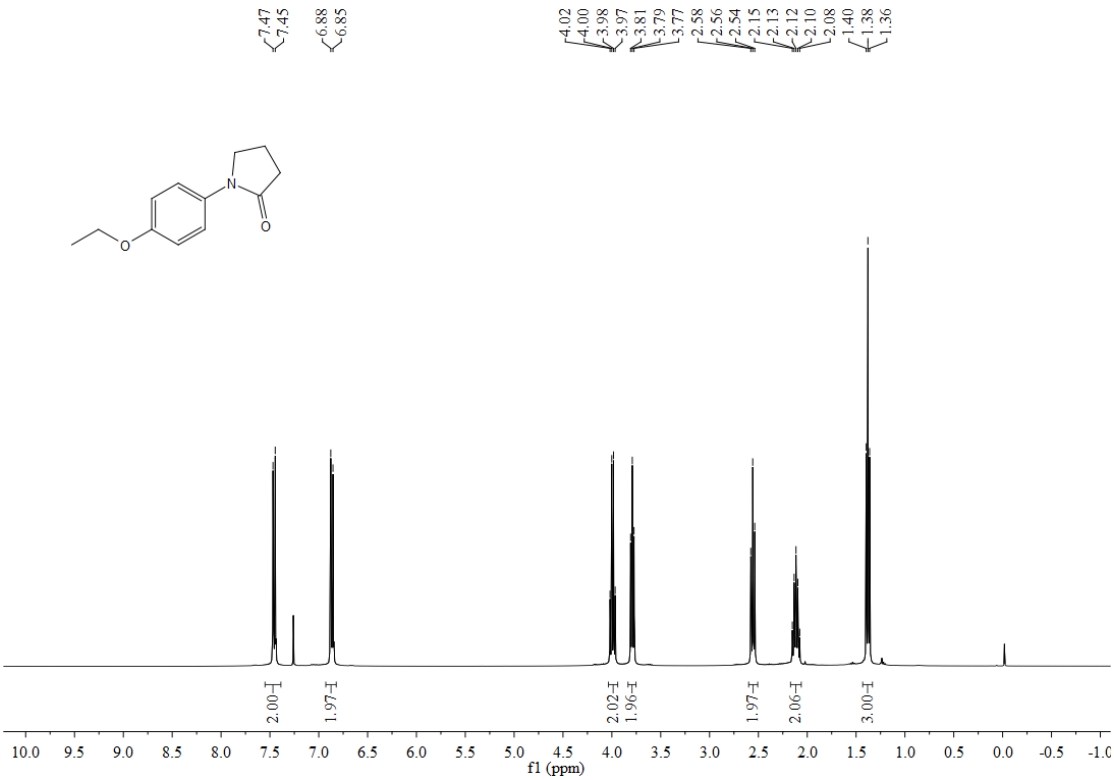
49.21
32.48
18.02
O
N
O
f1 (ppm)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6.85
4.02
4.00
3.98
3.97
3.81
3.79
3.77
2.58
2.56
2.54
2.15
2.13
2.12
2.10
2.08
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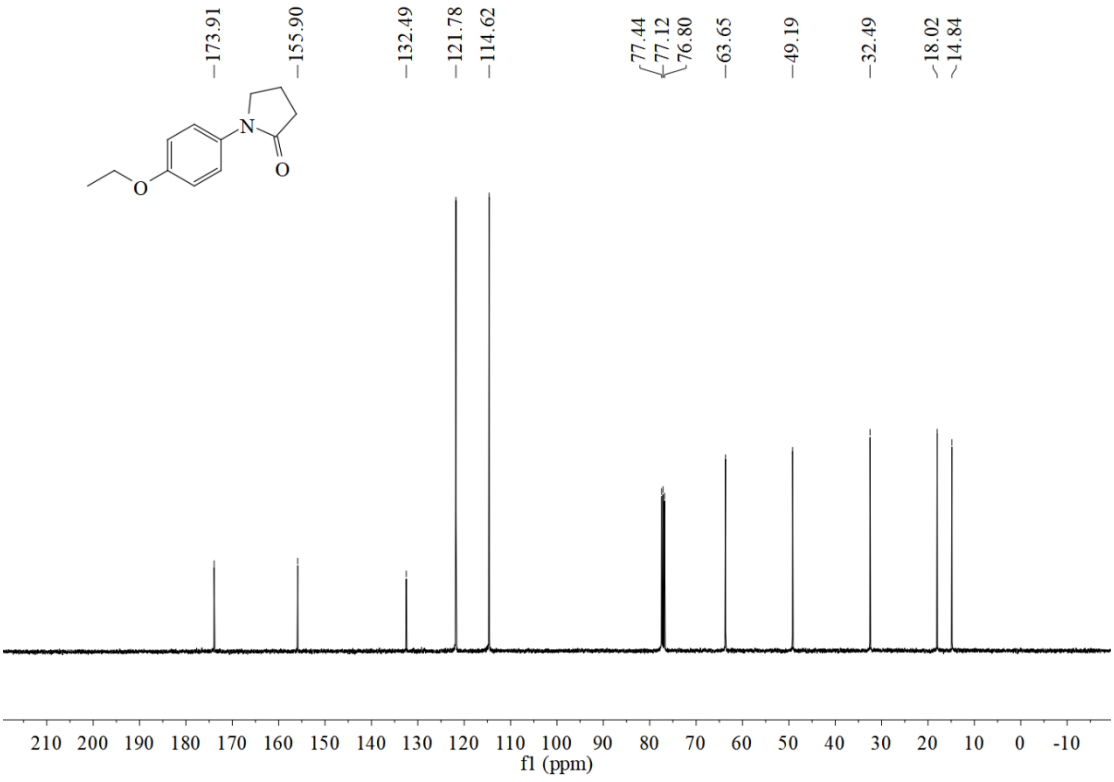
1.97
2.02
1.96
1.97
2.06
3.00
f1 (ppm)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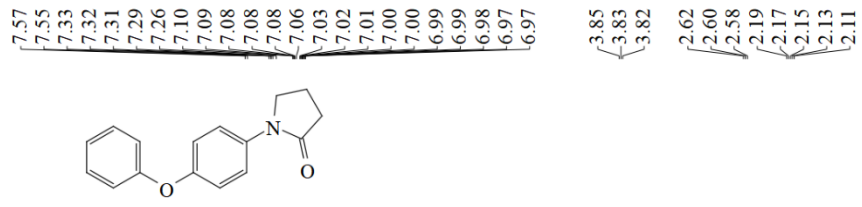
121.78
114.62
77.44
77.12
76.80
63.65
49.19
32.49
18.02
14.84
f1 (ppm)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7.26
7.10
7.09
7.08
7.08
7.08
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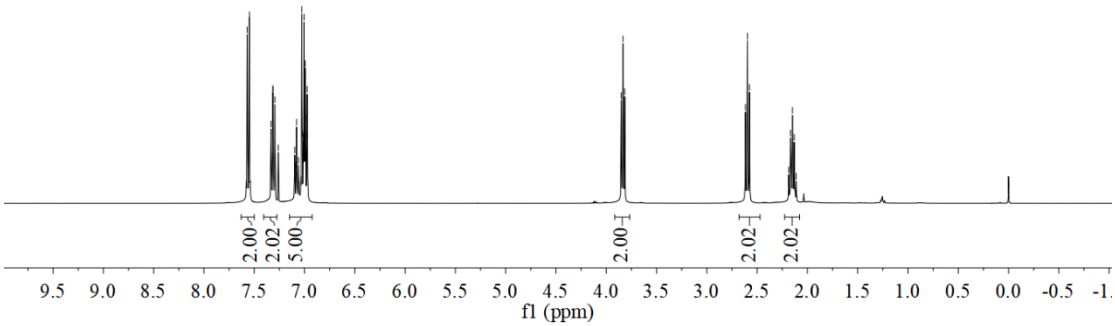
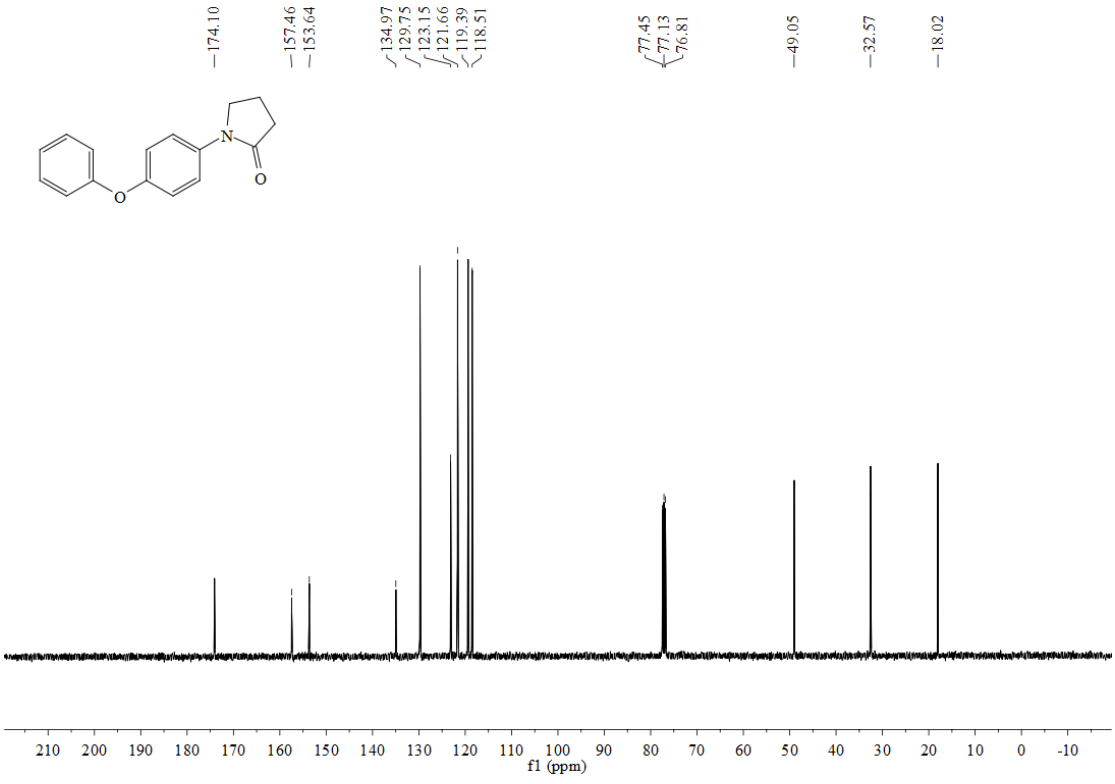
7.03
7.02
7.01
7.00
7.00
6.99
6.99
6.98
6.97
6.97
3.85
3.83
3.82
2.62
2.60
2.58
2.19
2.17
2.15
2.13
2.11
N
O
O


2.00
2.02
5.00
2.00
2.02
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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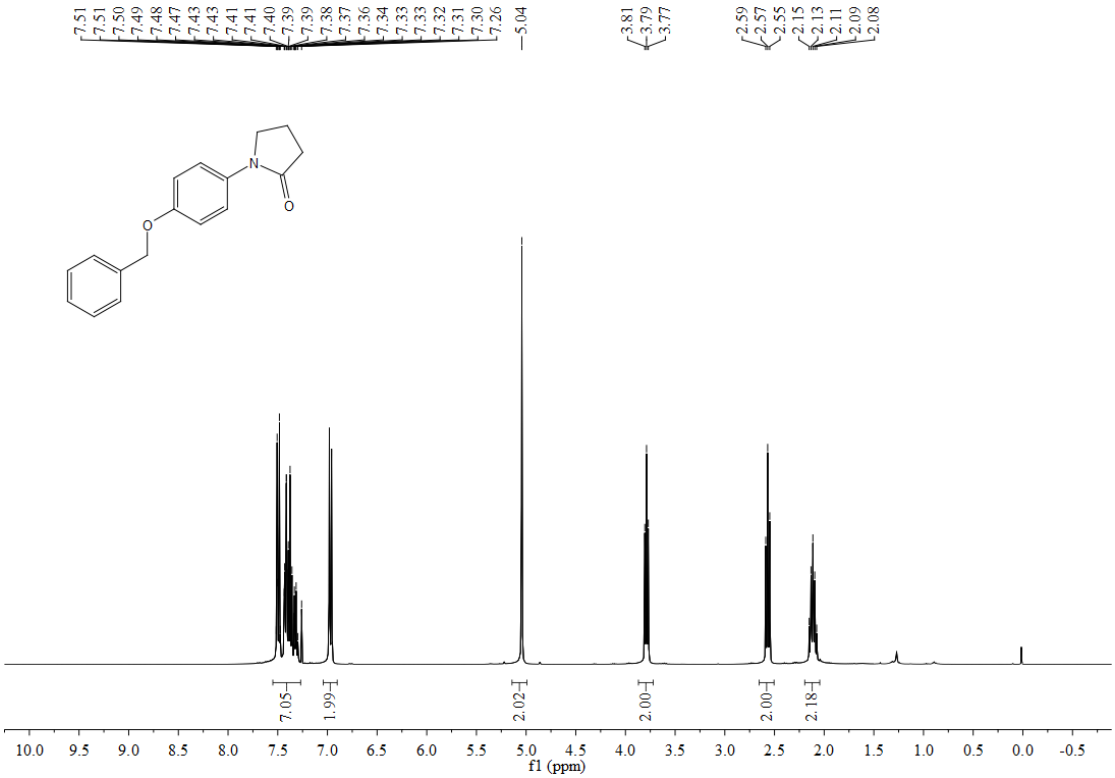
157.46
153.64
134.97
129.75
123.15
121.66
119.39
118.51
77.45
77.13
76.81
49.05
32.57
18.02
N
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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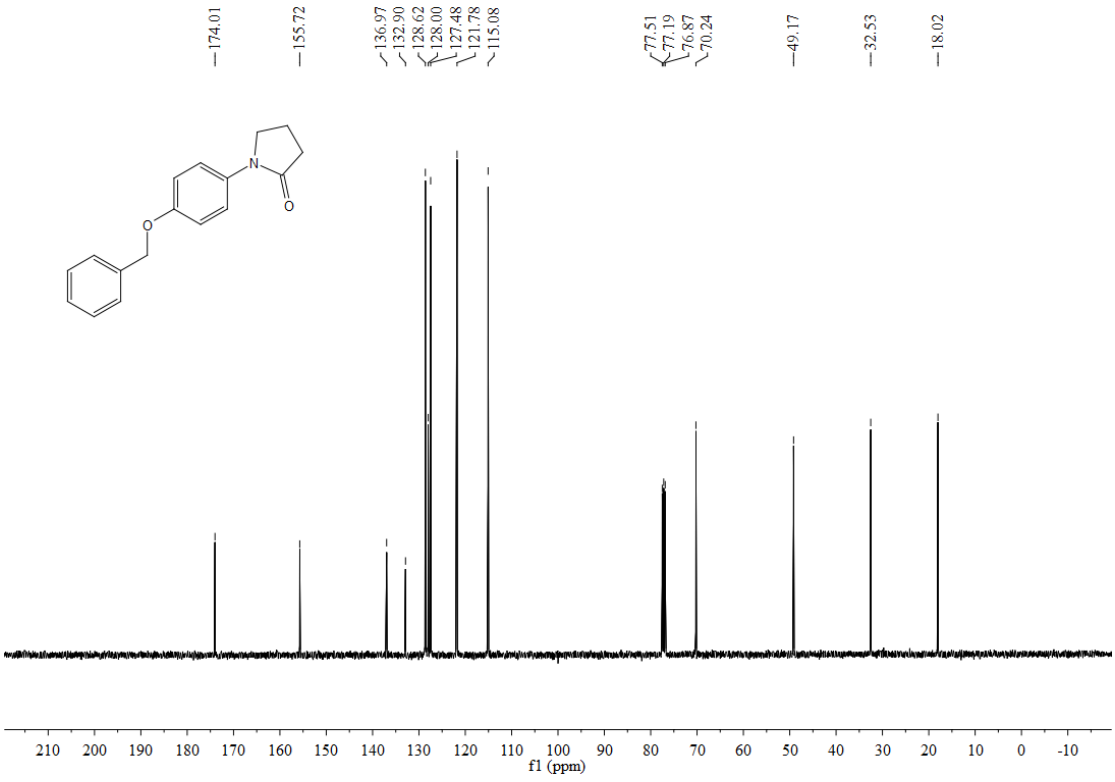
7.36
7.34
7.33
7.33
7.32
7.31
7.30
7.26
5.04
3.81
3.79
3.77
2.59
2.57
2.55
2.15
2.13
2.11
2.09
2.08
O
N
O
7.05
1.99
2.02
2.00
2.00
2.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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132.90
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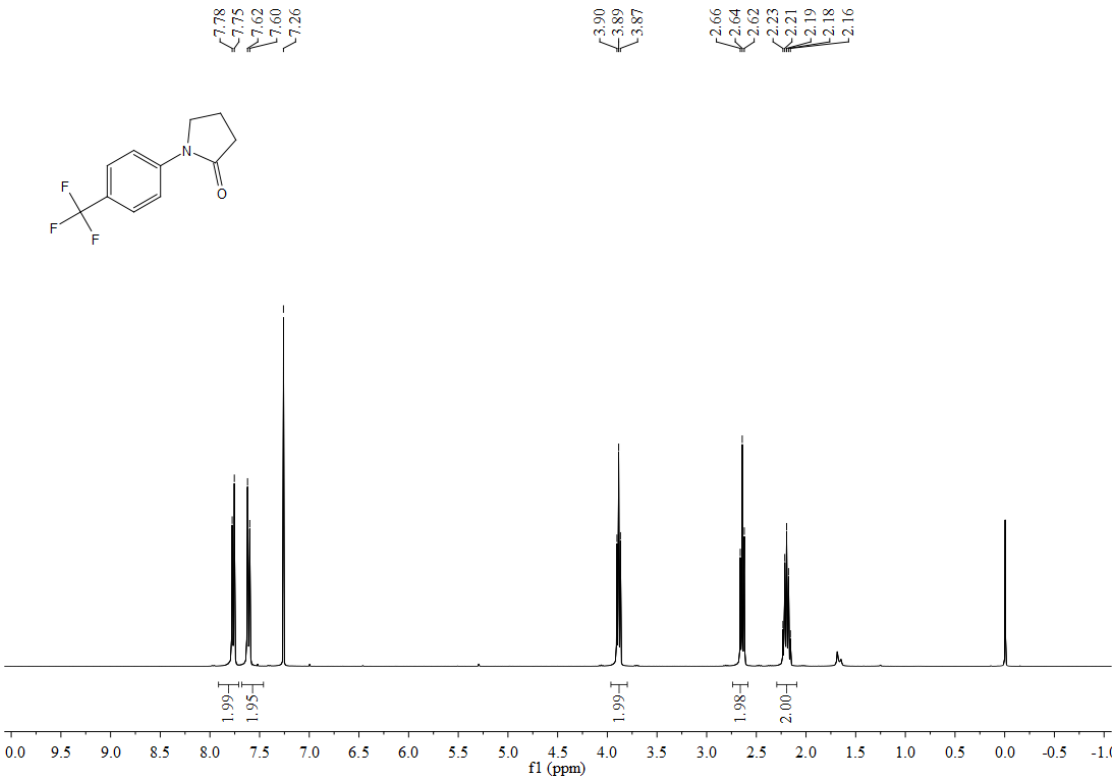
128.00
127.48
121.78
115.08
77.51
77.19
76.87
70.24
49.17
32.53
18.02
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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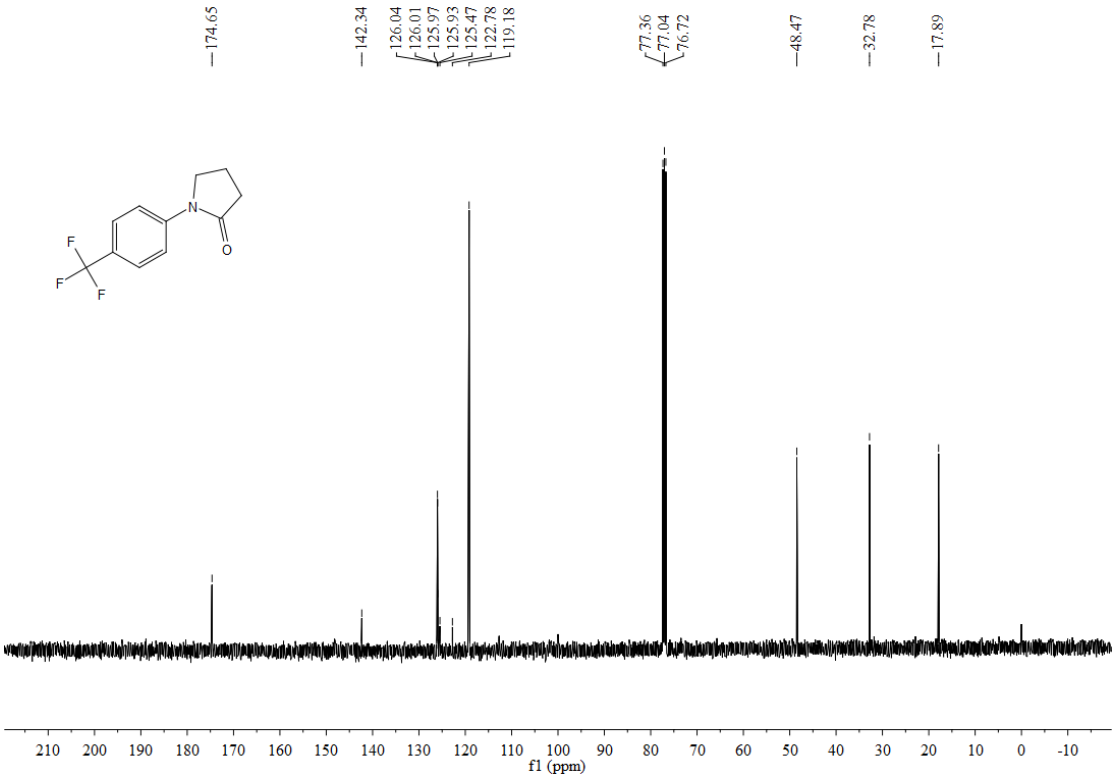
7.26
3.90
3.89
3.87
2.66
2.64
2.62
2.23
2.21
2.19
2.18
2.16
F
F
F
N
O
1.99
1.95
1.99
1.98
2.00
f1 (ppm)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142.34
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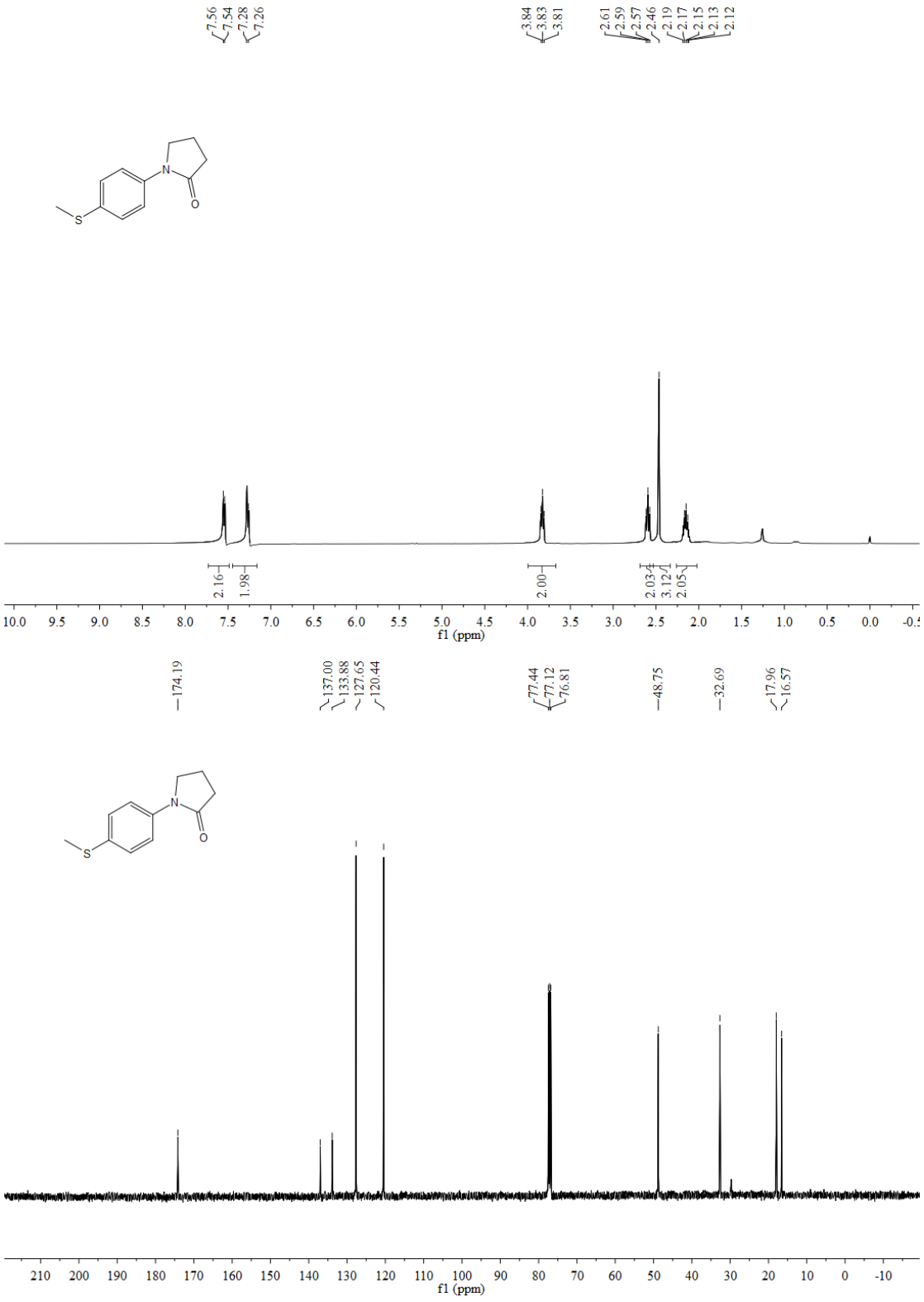
126.01
125.97
125.93
125.47
122.78
119.18
77.36
77.04
76.72
48.47
32.78
17.89
F
F
F
N
O
f1 (ppm)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3.83
3.81
2.61
2.59
2.57
2.46
2.19
2.17
2.15
2.13
2.12
N
O
S
2.16
1.98
2.00
2.03
3.12
2.05
f1 (ppm)
174.19
137.00
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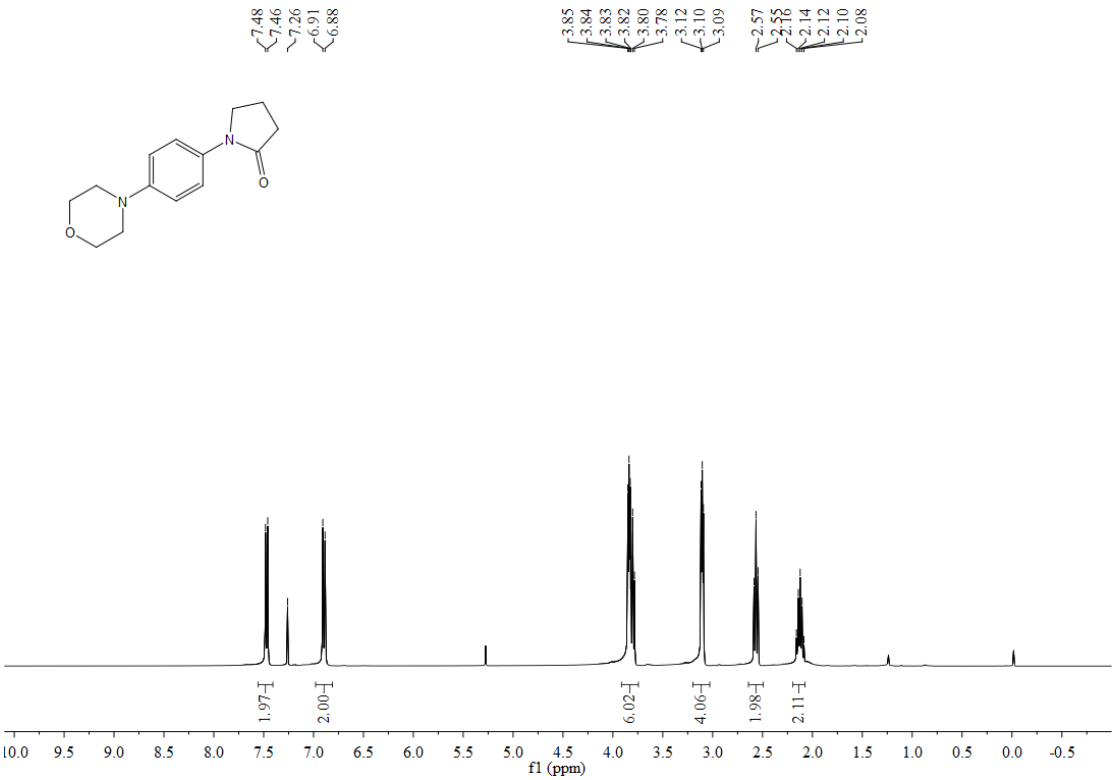
120.44
77.44
77.12
76.81
48.75
32.69
17.96
16.57
f1 (ppm)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3.82
3.80
3.78
3.12
3.10
3.09
2.57
2.55
2.16
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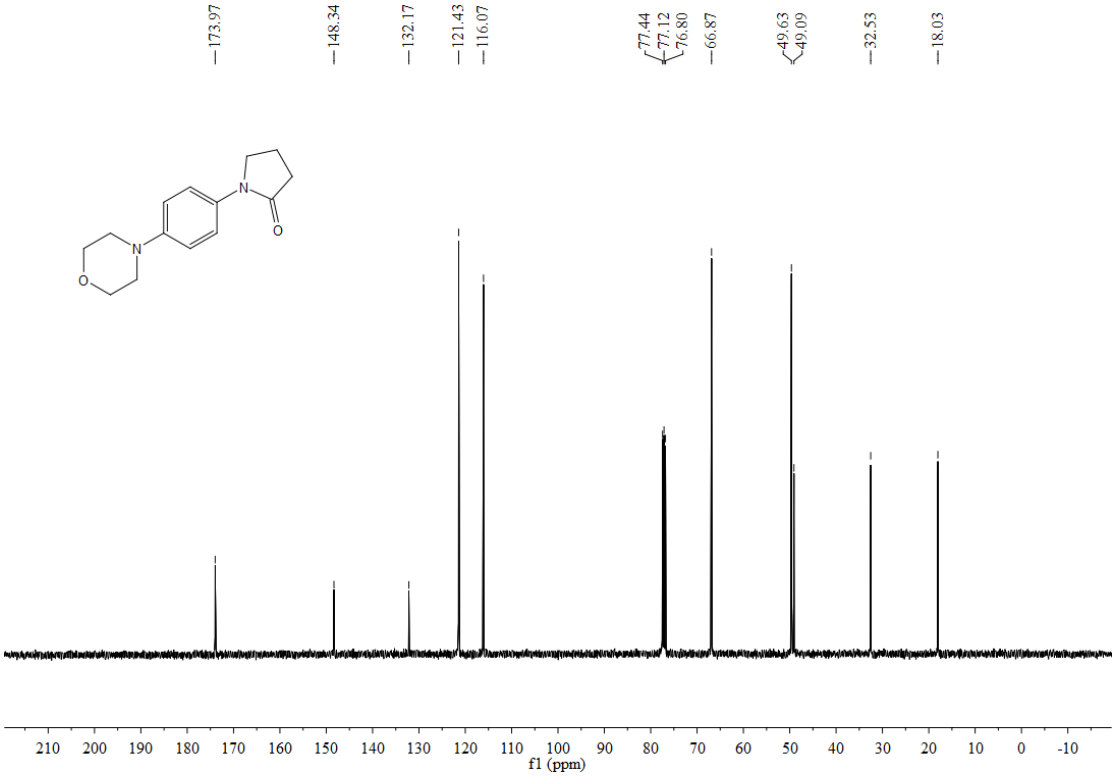
2.10
2.08
1.97
2.00
6.02
4.06
1.98
2.11
f1 (ppm)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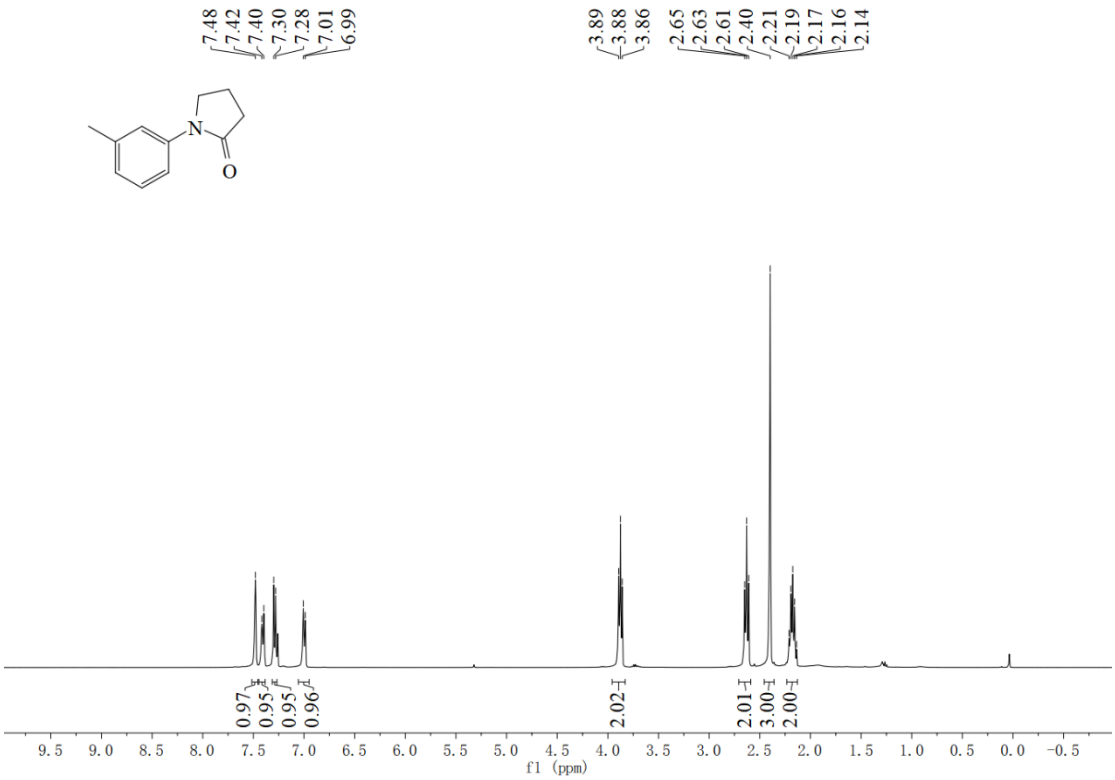
66.87
49.63
49.09
32.53
18.03
f1 (ppm)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3.88
3.86
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2.63
2.61
2.40
2.21
2.19
2.17
2.16
2.14
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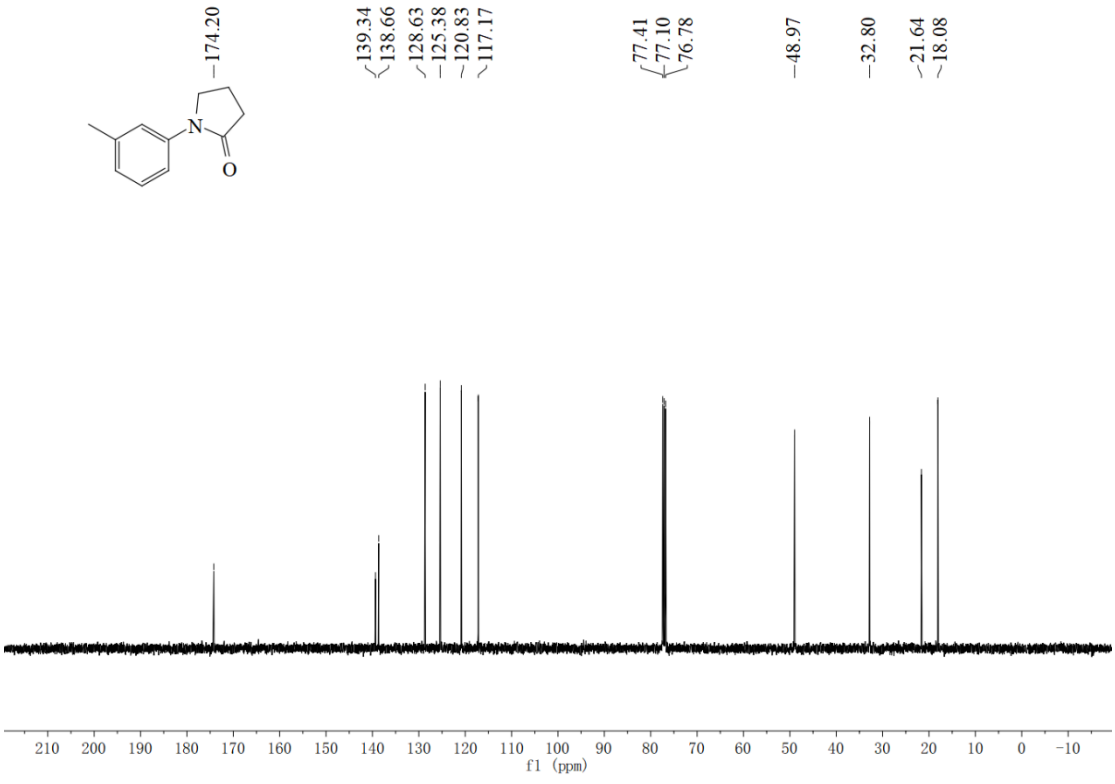
O
0.97
0.95
0.95
0.96
2.02
2.01
3.00
2.00
f1 (ppm)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128.63
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120.83
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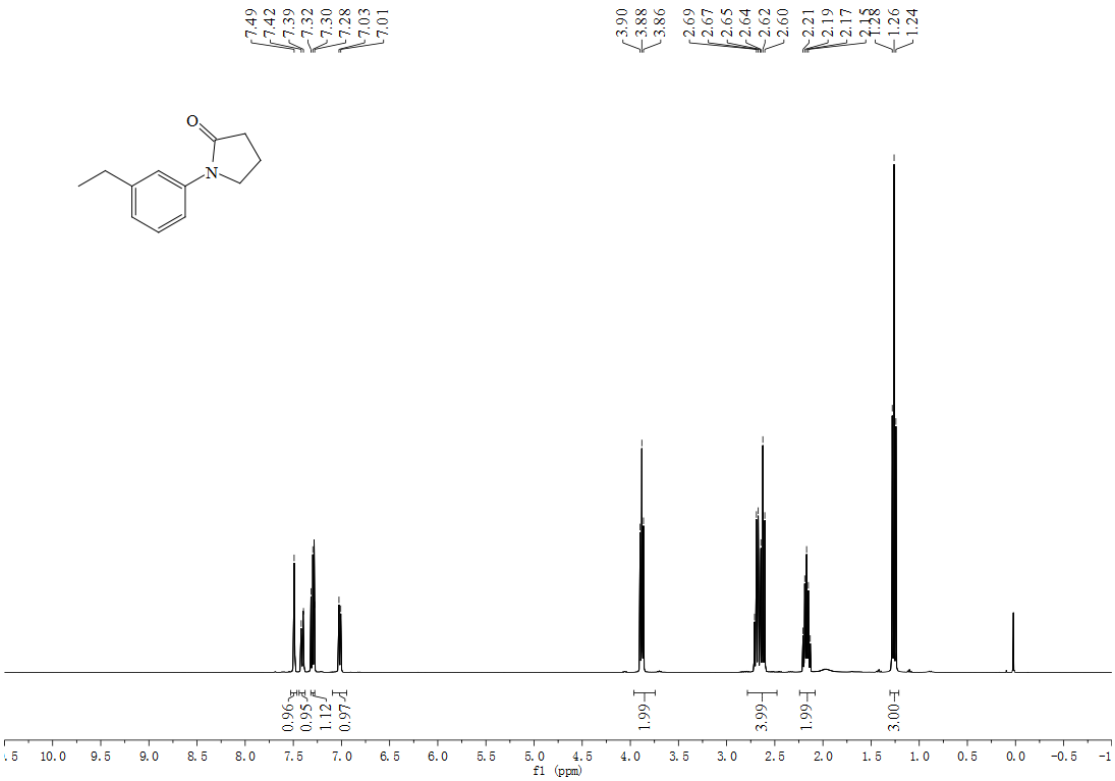
77.41
77.10
76.78
48.97
32.80
21.64
18.08
N
O
f1 (ppm)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2.69
2.67
2.65
2.64
2.62
2.60
2.21
2.19
2.17
2.15
2.13
1.26
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O
N
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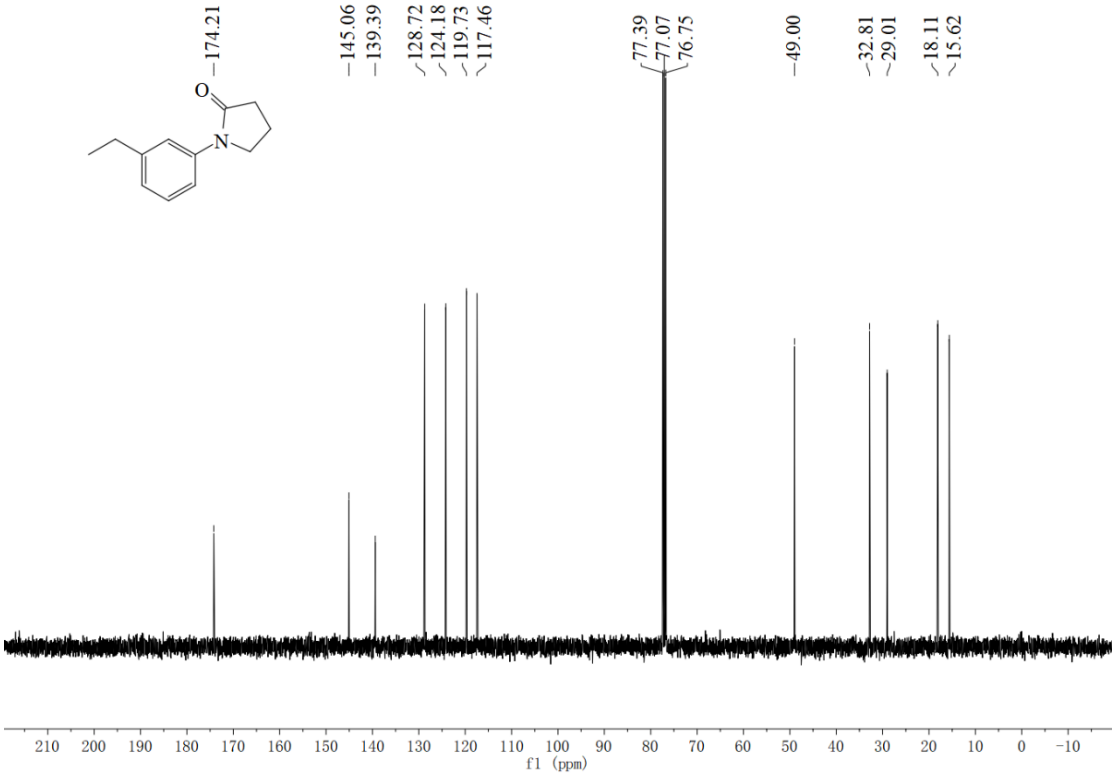
0.95
1.12
0.97
1.99
3.99
1.99
3.00
f1 (ppm)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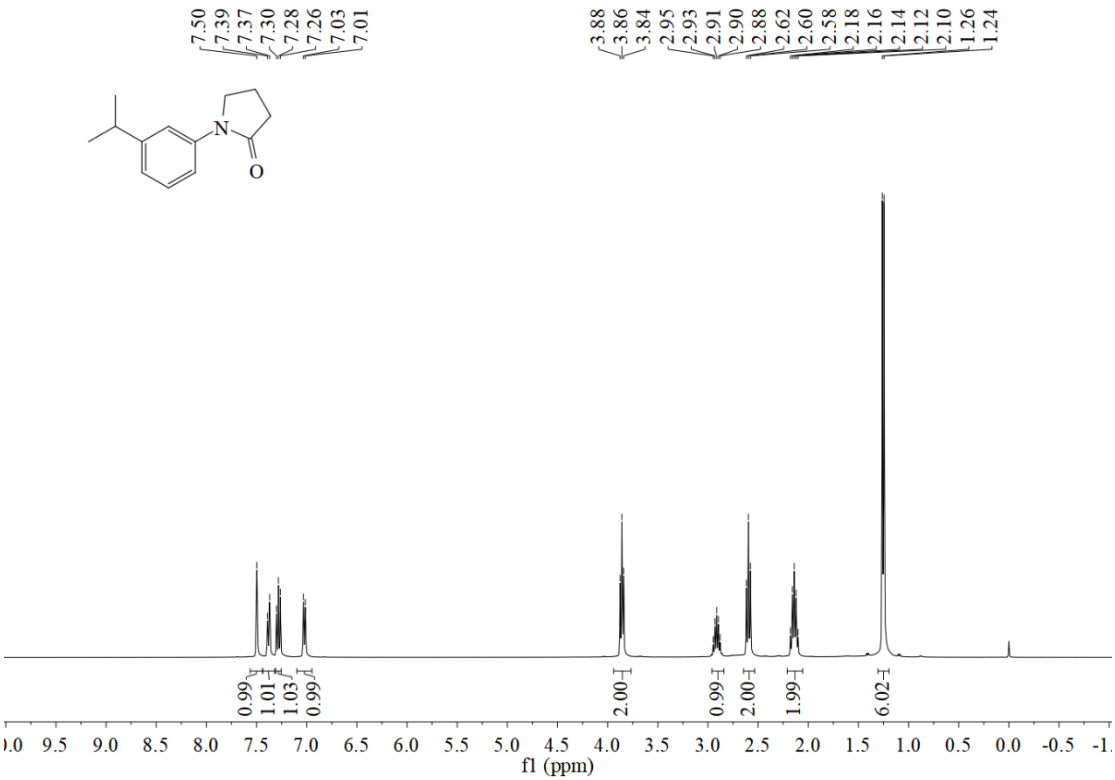
77.07
76.75
49.00
32.81
29.01
18.11
15.62
O
N
f1 (ppm)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7.01
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3.86
3.84
2.95
2.93
2.91
2.90
2.88
2.62
2.60
2.58
2.18
2.16
2.14
2.12
2.10
1.26
1.24
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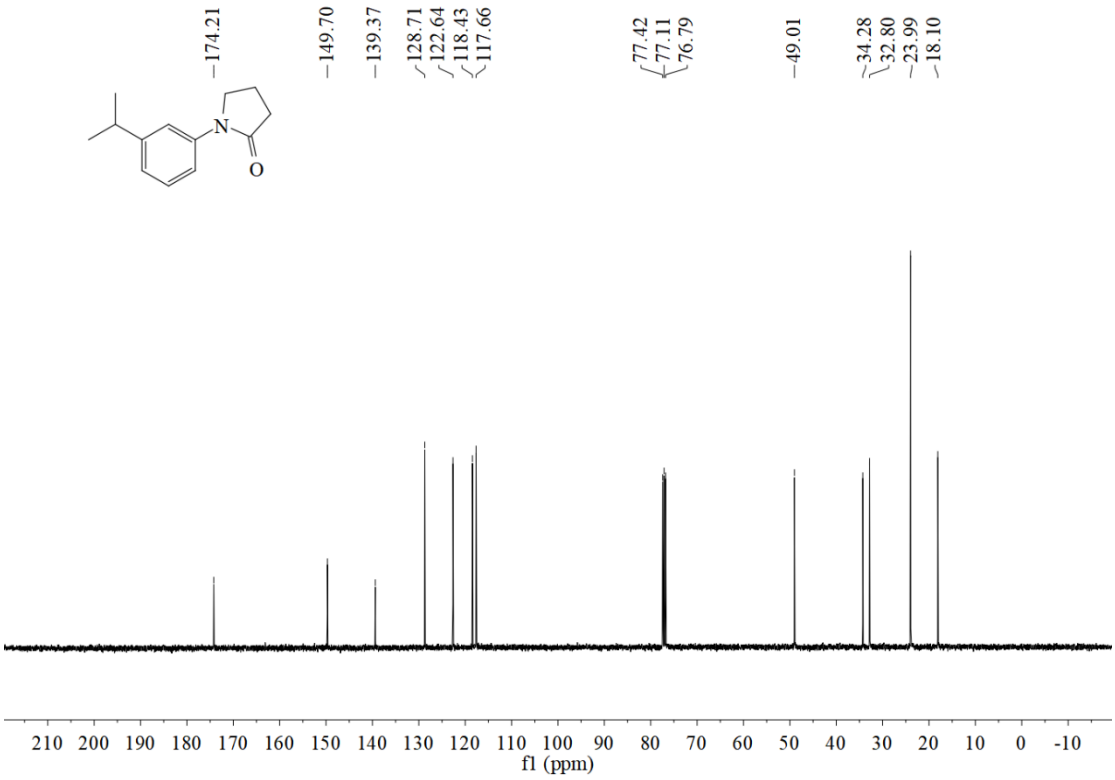
1.01
1.03
0.99
2.00
0.99
2.00
1.99
6.02
fl (ppm)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77.11
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49.01
34.28
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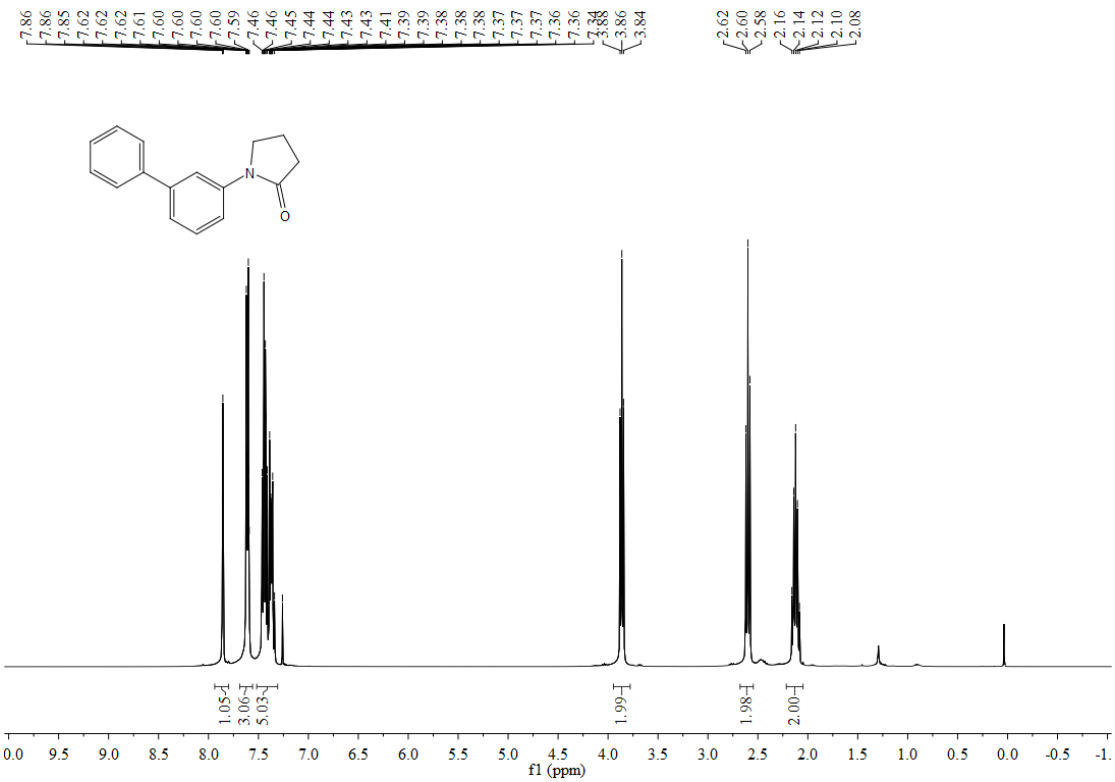
23.99
18.10
N
O
fl (ppm)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3.86
3.84
2.62
2.60
2.58
2.16
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3.06
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1.99
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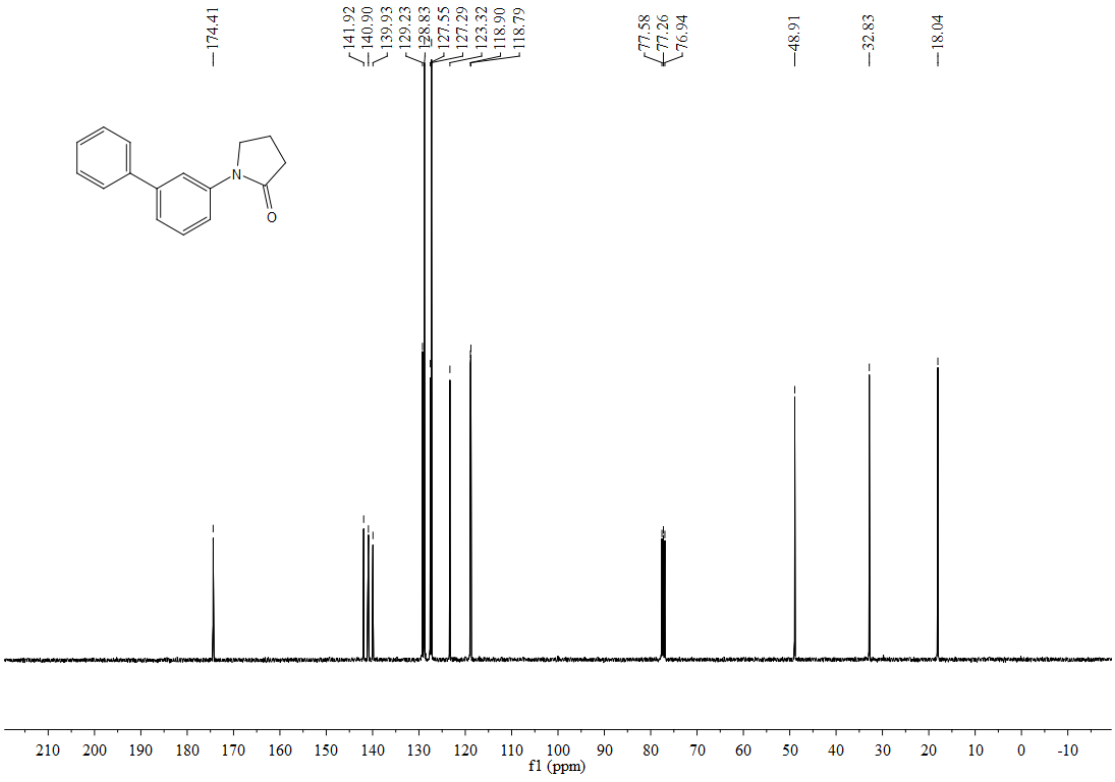
2.00
f1 (ppm)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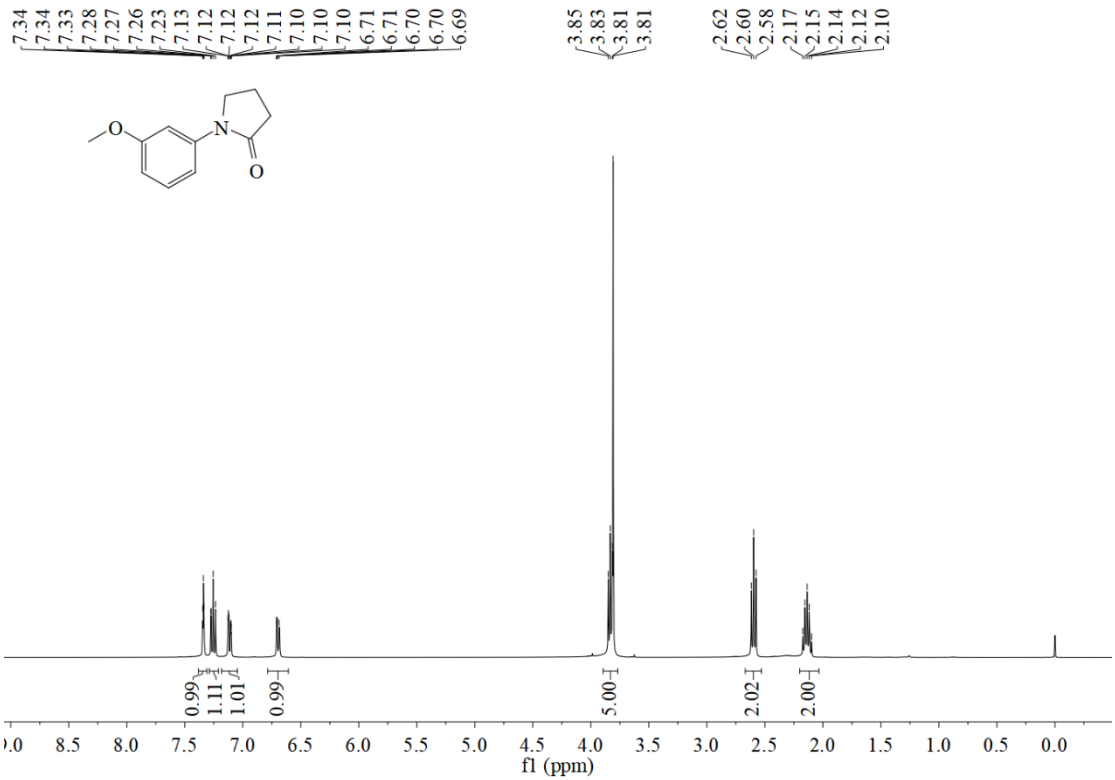
77.26
76.94
48.91
32.83
18.04
N
O
f1 (ppm)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7.10
7.10
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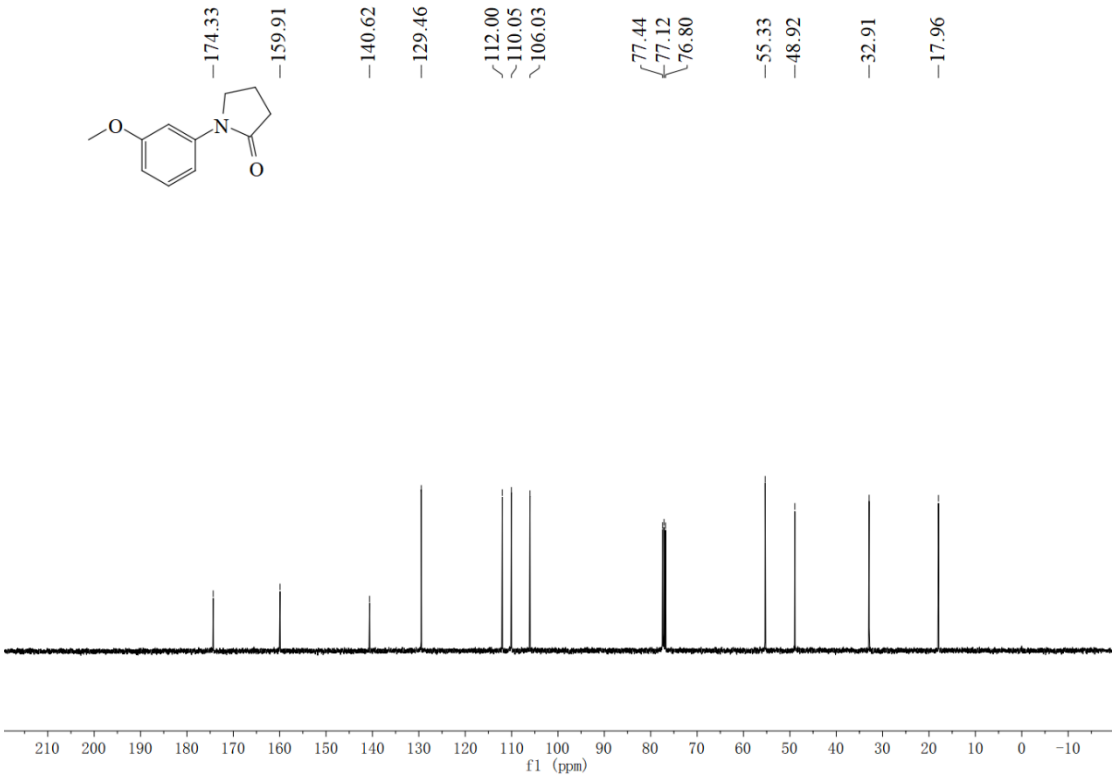
3.83
3.81
3.81
2.62
2.60
2.58
2.17
2.15
2.14
2.12
2.10
O
N
O
0.99
1.11
1.01
0.99
5.00
2.02
2.00
f1 (ppm)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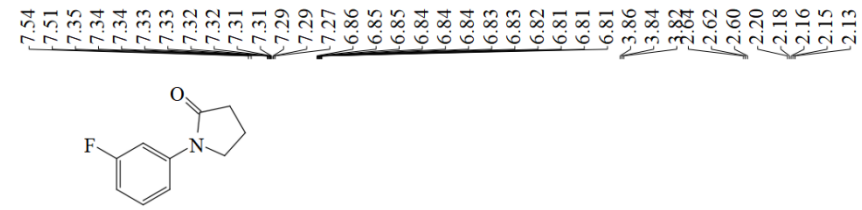
77.12
76.80
55.33
48.92
32.91
17.96
O
N
O
f1 (ppm)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7.29
7.27
6.86
6.85
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6.84
6.84
6.84
6.83
6.83
6.82
6.81
6.81
6.81
3.86
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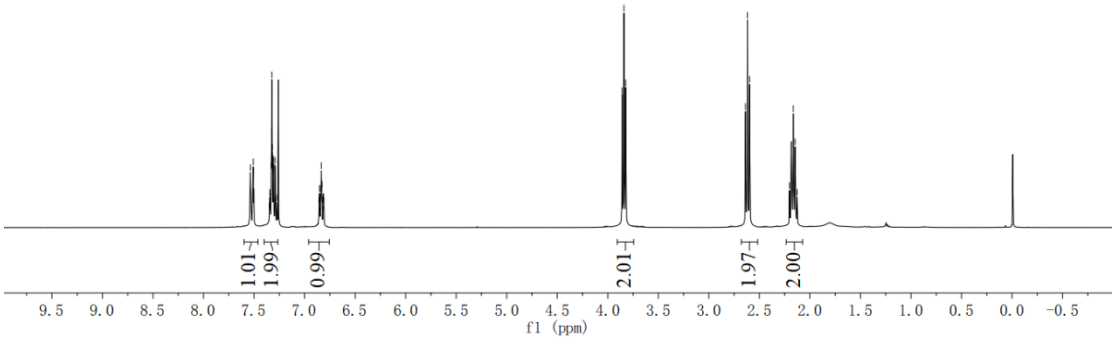
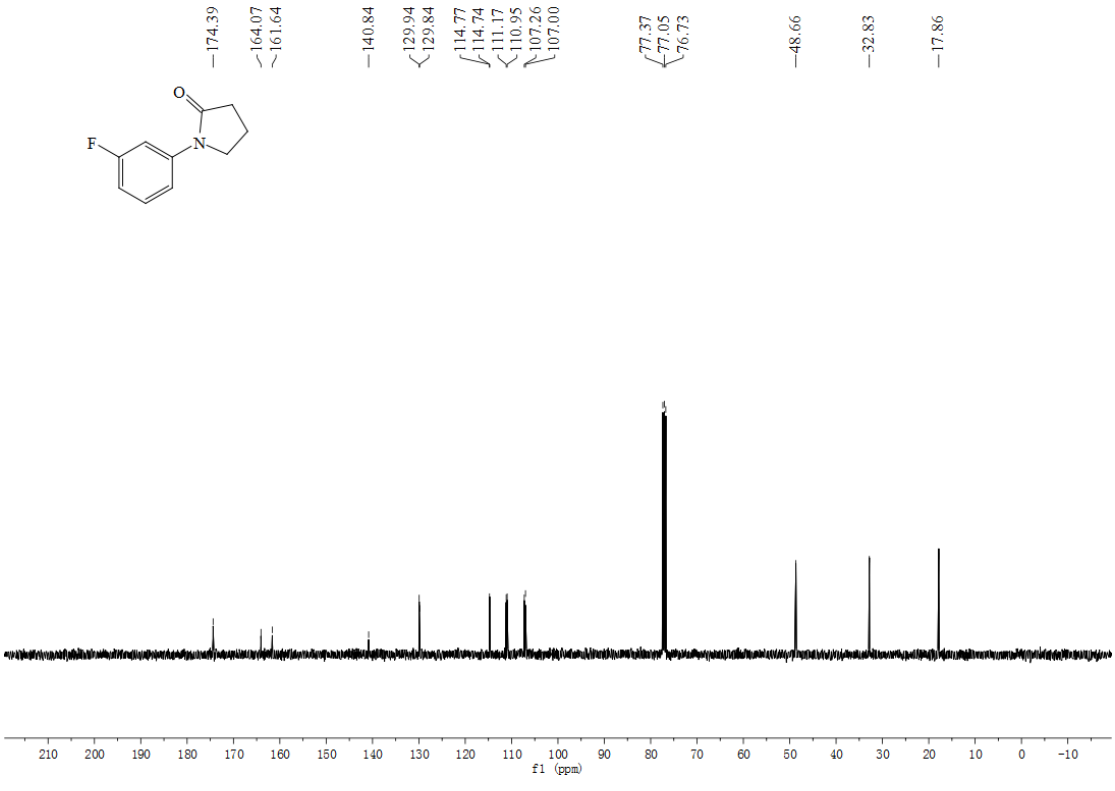
2.16
2.15
2.13
O
N
F


1.01
1.99
0.99
2.01
1.97
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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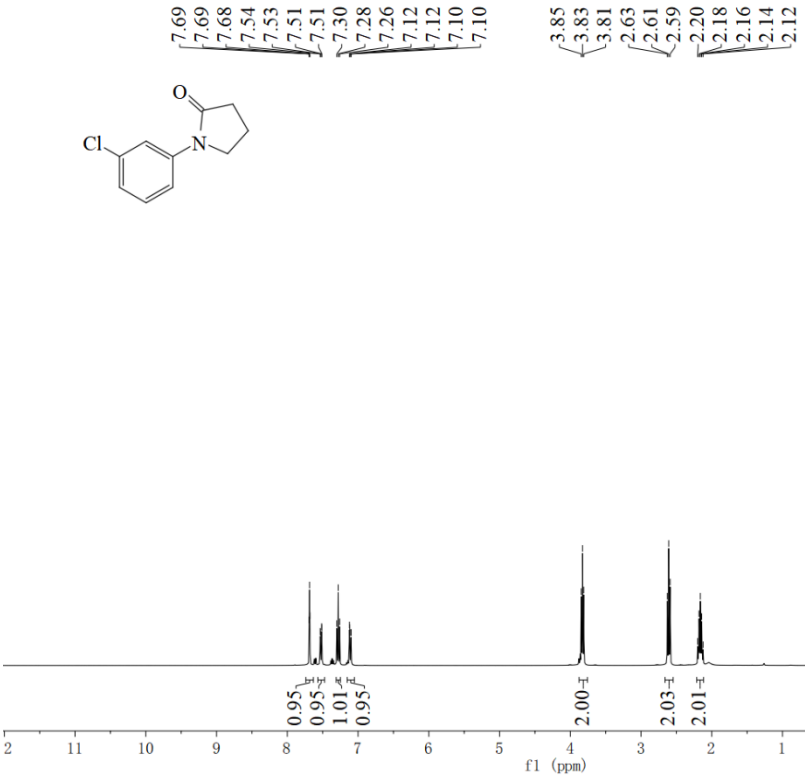
164.07
161.64
140.84
129.94
129.84
114.77
114.74
111.17
110.95
107.26
107.00
77.37
77.05
76.73
48.66
32.83
17.86
O
N
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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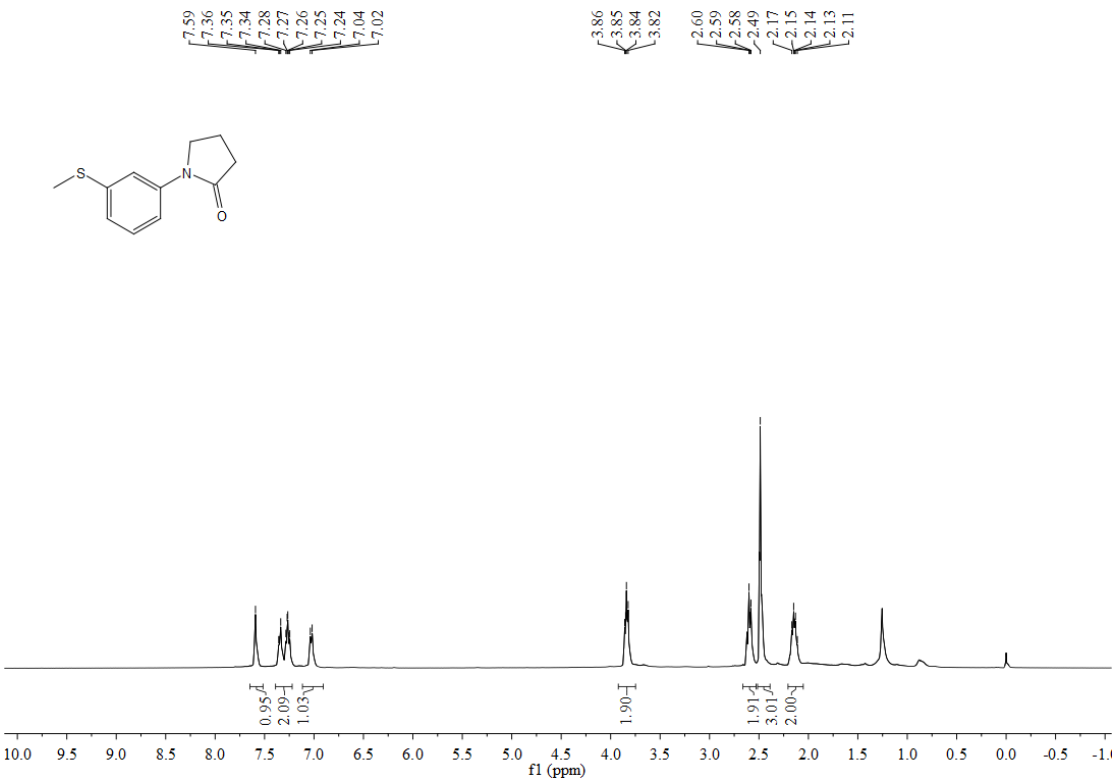
7.69
7.68
7.54
7.53
7.51
7.51
7.30
7.28
7.26
7.12
7.12
7.10
7.10
3.85
3.83
3.81
2.63
2.61
2.59
2.20
2.18
2.16
2.14
2.12
O
N
Cl
0.95
0.95
1.01
0.95
2.00
2.03
2.01
f1 (ppm)
174.39
140.54
134.45
129.79
124.32
119.71
117.62
77.43
77.12
76.80
48.60
32.74
17.87
f1 (ppm)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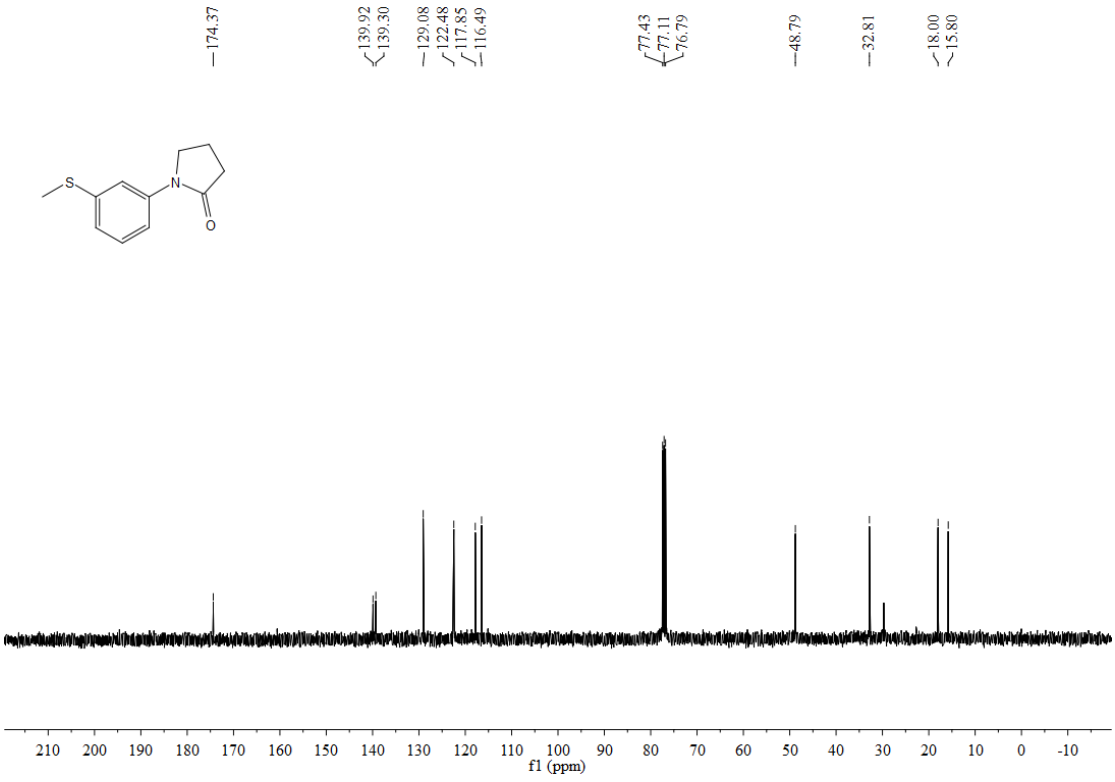
7.27
7.26
7.25
7.24
7.04
7.02
3.86
3.85
3.84
3.82
2.60
2.59
2.58
2.49
2.17
2.15
2.14
2.13
2.11
S
N
O
0.95
2.09
1.03
1.90
1.91
3.01
2.00
f1 (ppm)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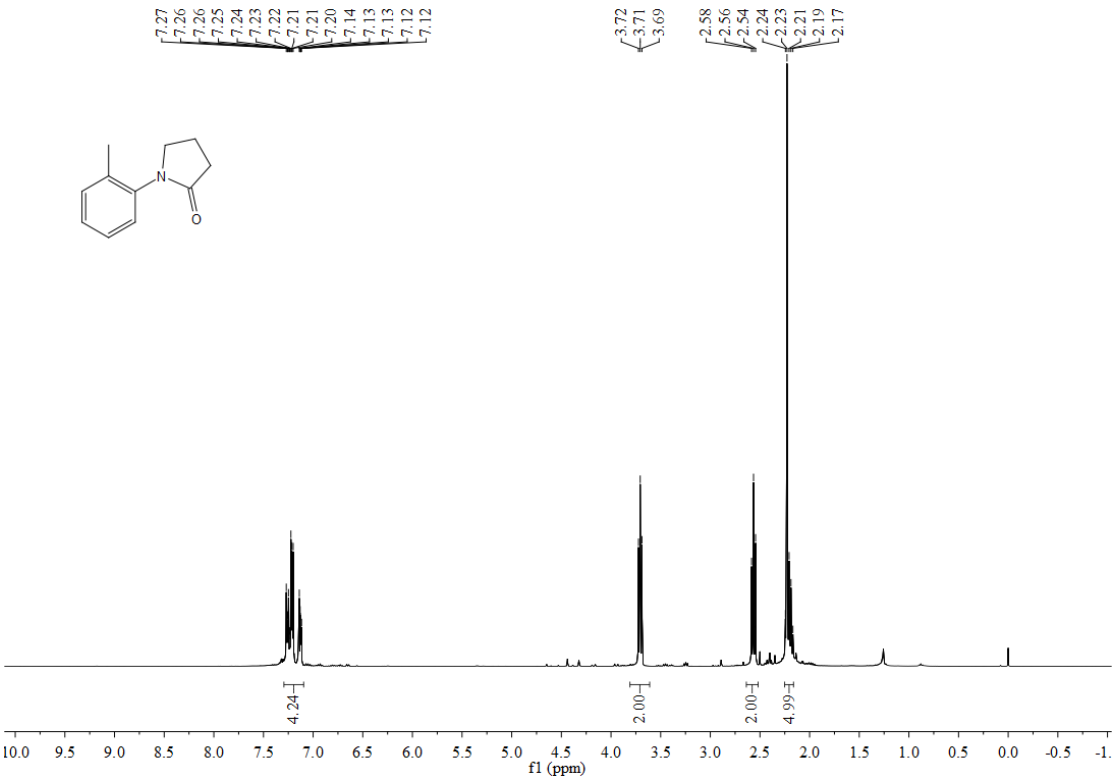
139.30
129.08
122.48
117.85
116.49
77.43
77.11
76.79
48.79
32.81
18.00
15.80
S
N
O
f1 (ppm)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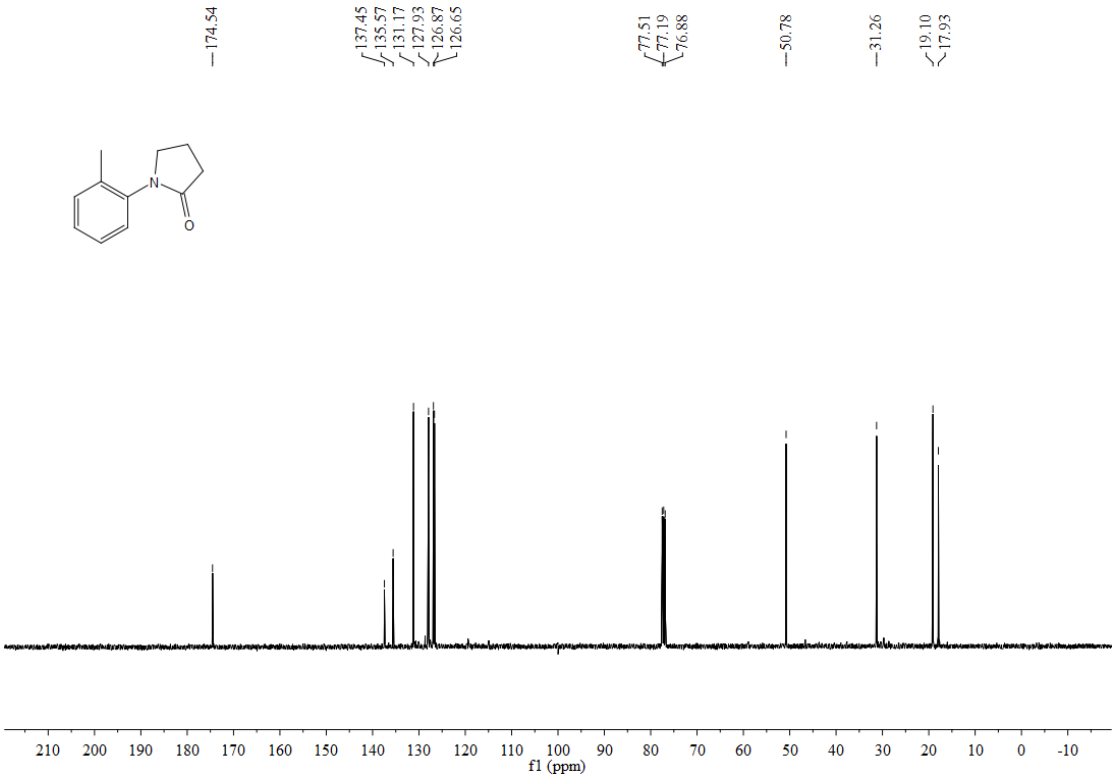
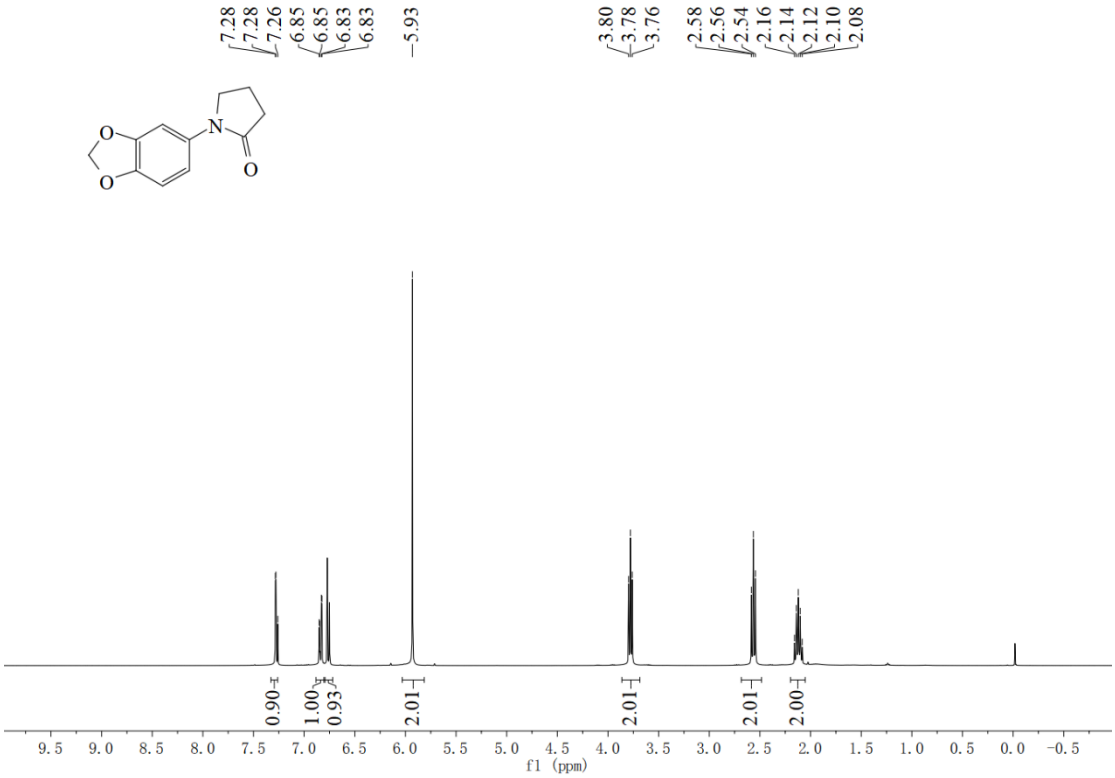
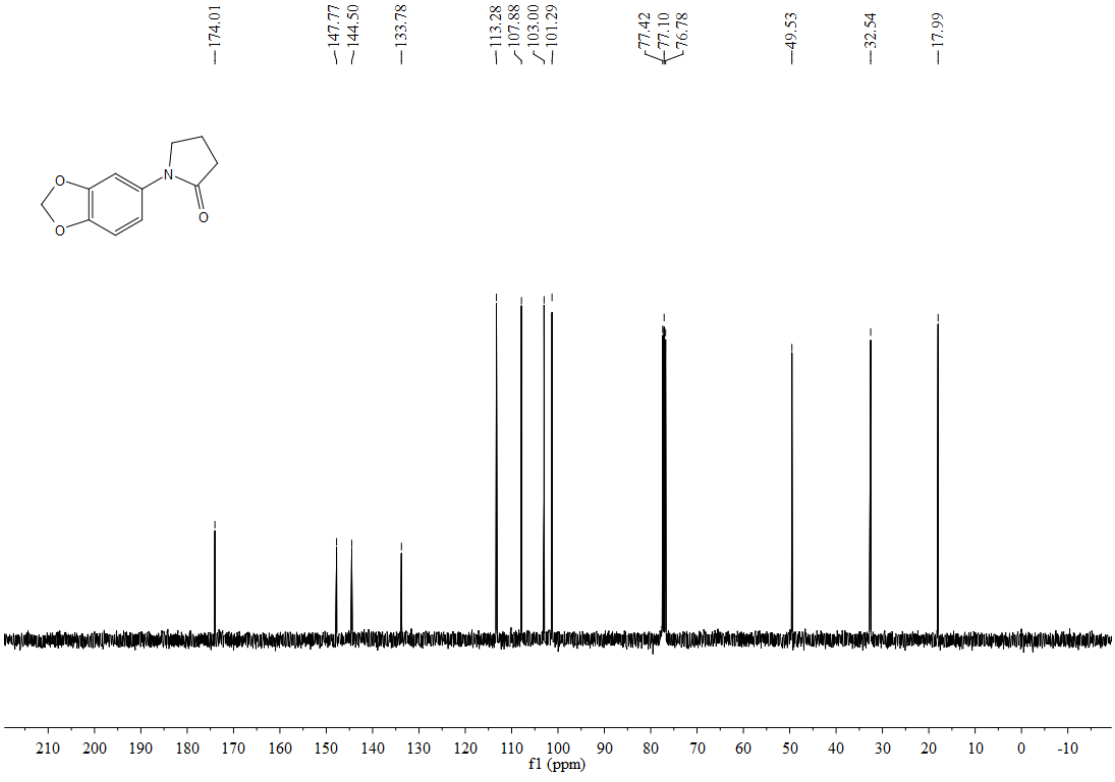
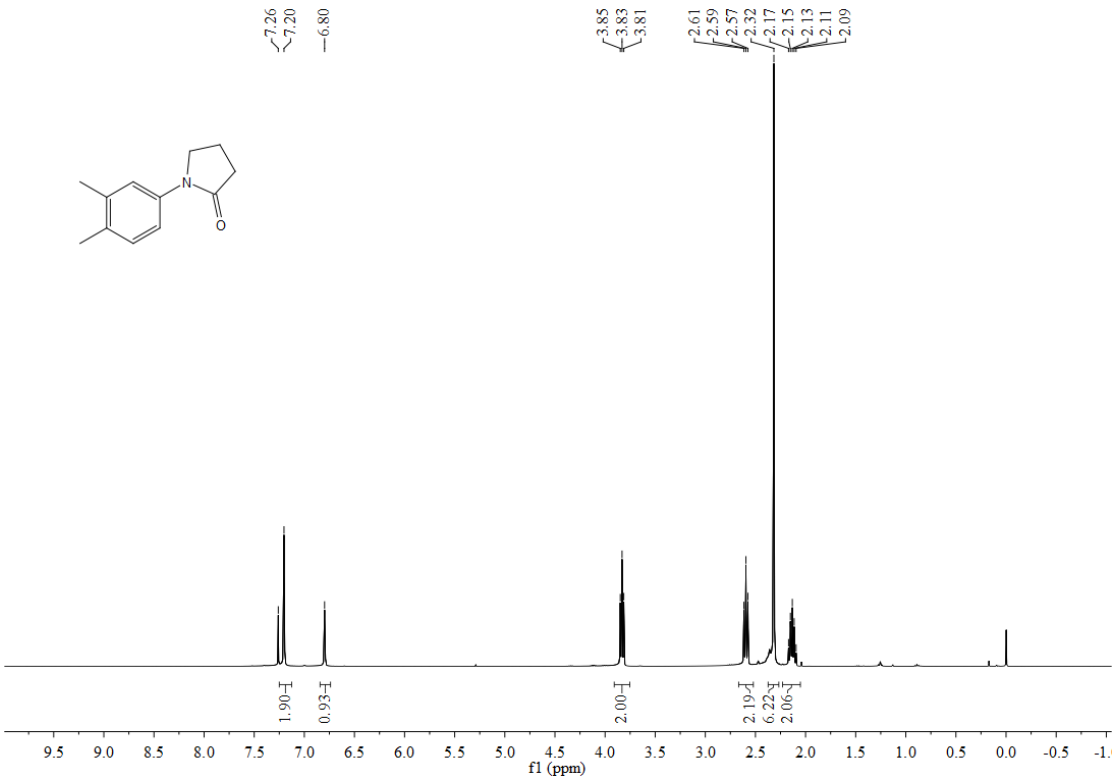
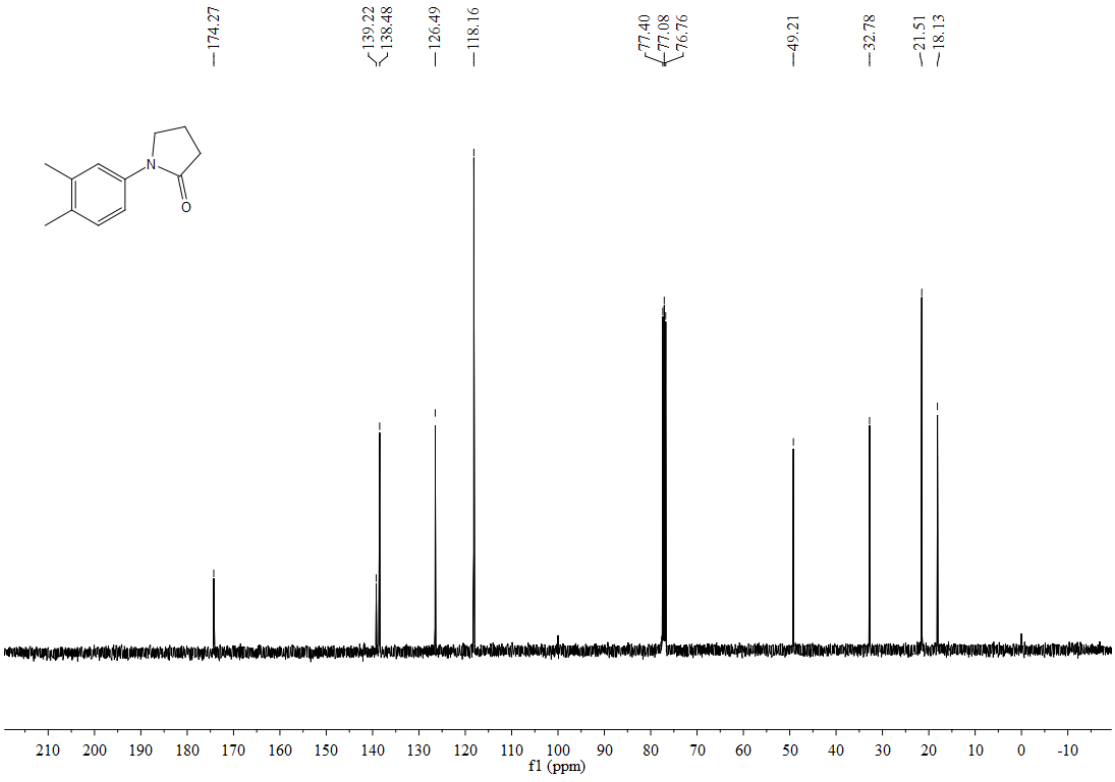
7.26
7.26
7.25
7.24
7.23
7.22
7.21
7.21
7.20
7.14
7.13
7.13
7.12
7.12
3.72
3.71
3.69
2.58
2.56
2.54
2.24
2.23
2.21
2.19
2.17
N
O
4.24
2.00
2.00
4.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

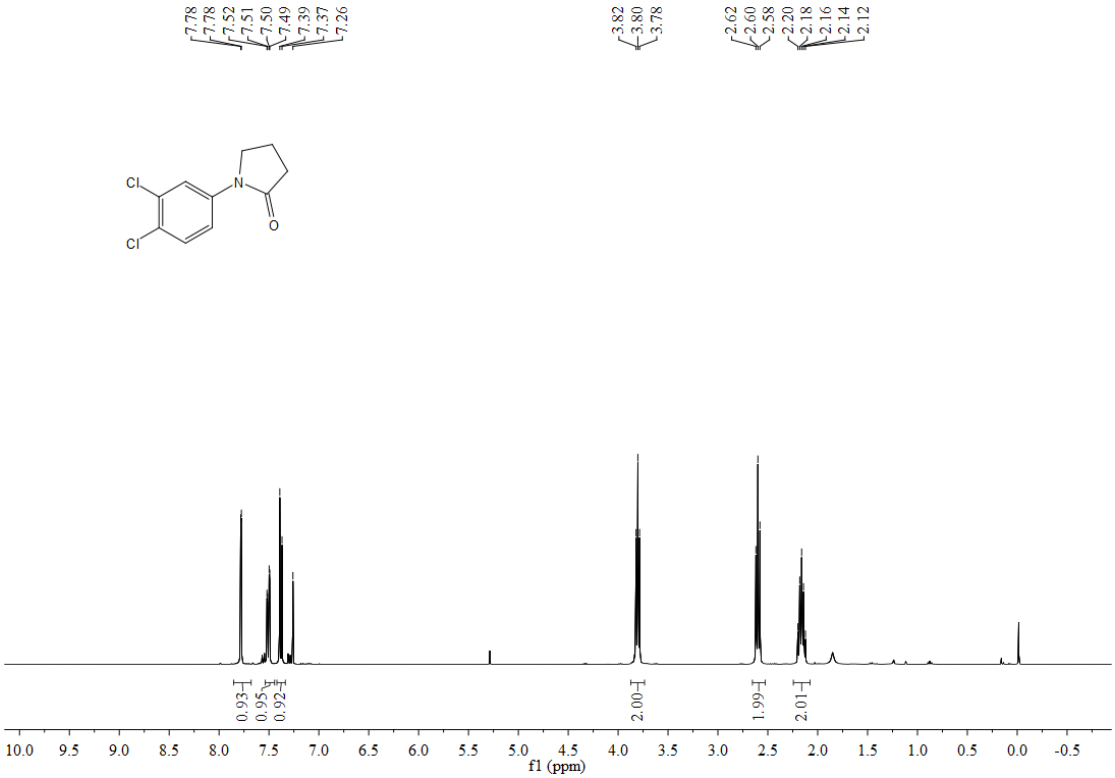

174.54
137.45
135.57
131.17
127.93
126.87
126.65
77.51
77.19
76.88
50.78
31.26
19.10
17.93
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

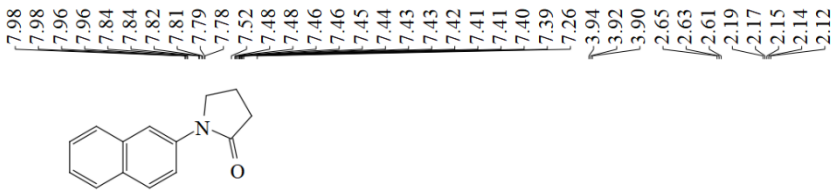

7.28
7.28
7.26
6.85
6.85
6.83
6.83
5.93
3.80
3.78
3.76
2.58
2.56
2.54
2.16
2.14
2.12
2.10
2.08
0.90
1.00
0.93
2.01
2.01
2.01
2.00
f1 (ppm)


174.01
147.77
144.50
133.78
113.28
107.88
103.00
101.29
77.42
77.10
76.78
49.53
32.54
17.99
f1 (ppm)


7.26
7.20
6.80
3.85
3.83
3.81
2.61
2.59
2.57
2.32
2.17
2.15
2.13
2.11
2.09
1.90
0.93
2.00
2.19
6.22
2.06
f1 (ppm)


174.27
139.22
138.48
126.49
118.16
77.40
77.08
76.76
49.21
32.78
21.51
18.13
f1 (ppm)


7.78
7.78
7.52
7.51
7.50
7.49
7.39
7.37
7.26
3.82
3.80
3.78
2.62
2.60
2.58
2.20
2.18
2.16
2.14
2.12
Cl
Cl
N
O
0.93
0.95
0.92
2.00
1.99
2.01
f1 (ppm)
174.42
138.88
132.58
130.28
127.51
121.14
118.74
77.40
77.08
76.76
48.50
32.65
17.75
f1 (ppm)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7.98
7.96
7.96
7.84
7.84
7.82
7.81
7.79
7.78
7.52
7.48
7.48
7.46
7.46
7.45
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.39
7.26
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3.92
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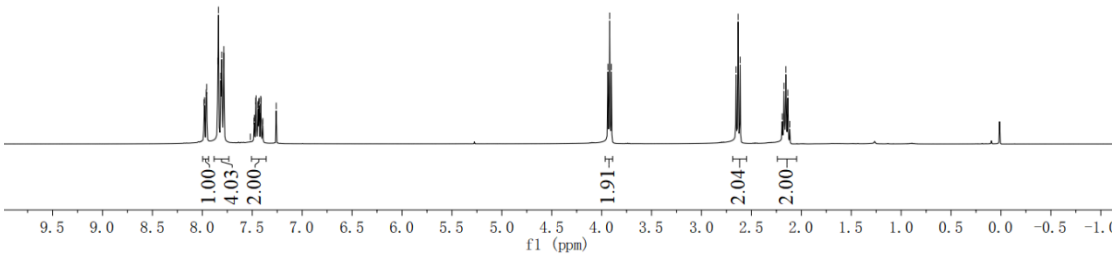
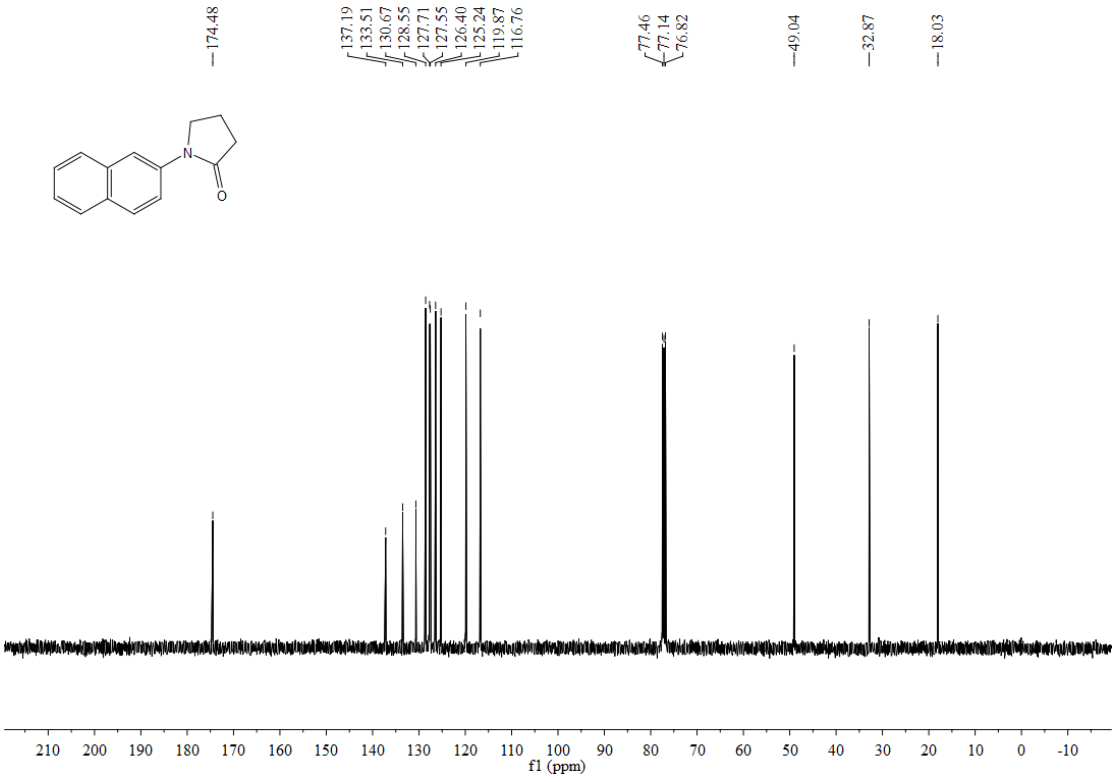
2.65
2.63
2.61
2.19
2.17
2.15
2.14
2.12
N
O


1.00
4.03
2.00
1.91
2.04
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)


174.48
137.19
133.51
130.67
128.55
127.71
127.55
126.40
125.24
119.87
116.76
77.46
77.14
76.82
49.04
32.87
18.03
N
O
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)


7.85
7.84
7.83
7.83
7.59
7.58
7.57
7.57
7.56
7.56
7.55
7.26
7.13
7.10
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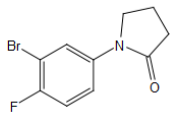
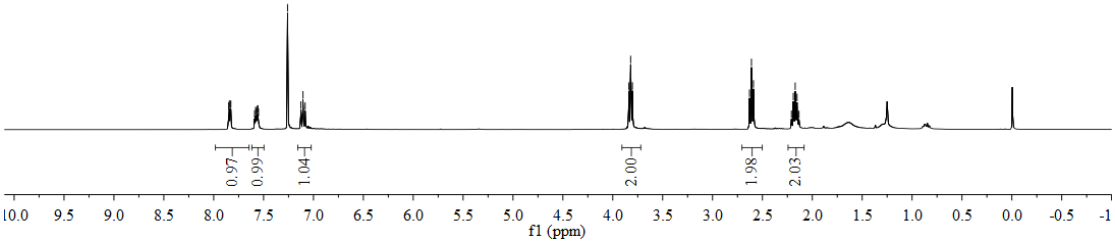
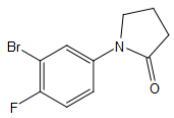
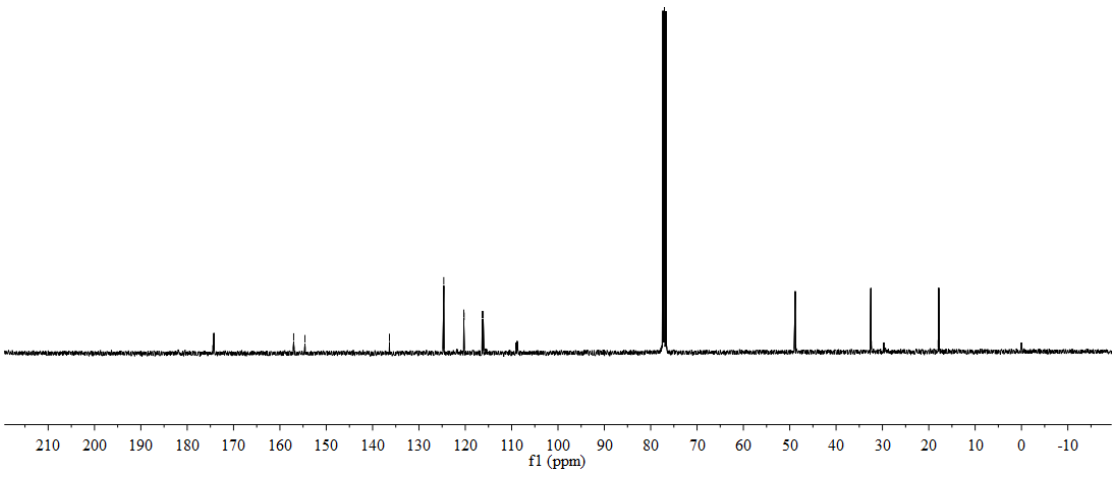
2.59
2.21
2.19
2.17
2.15
2.13

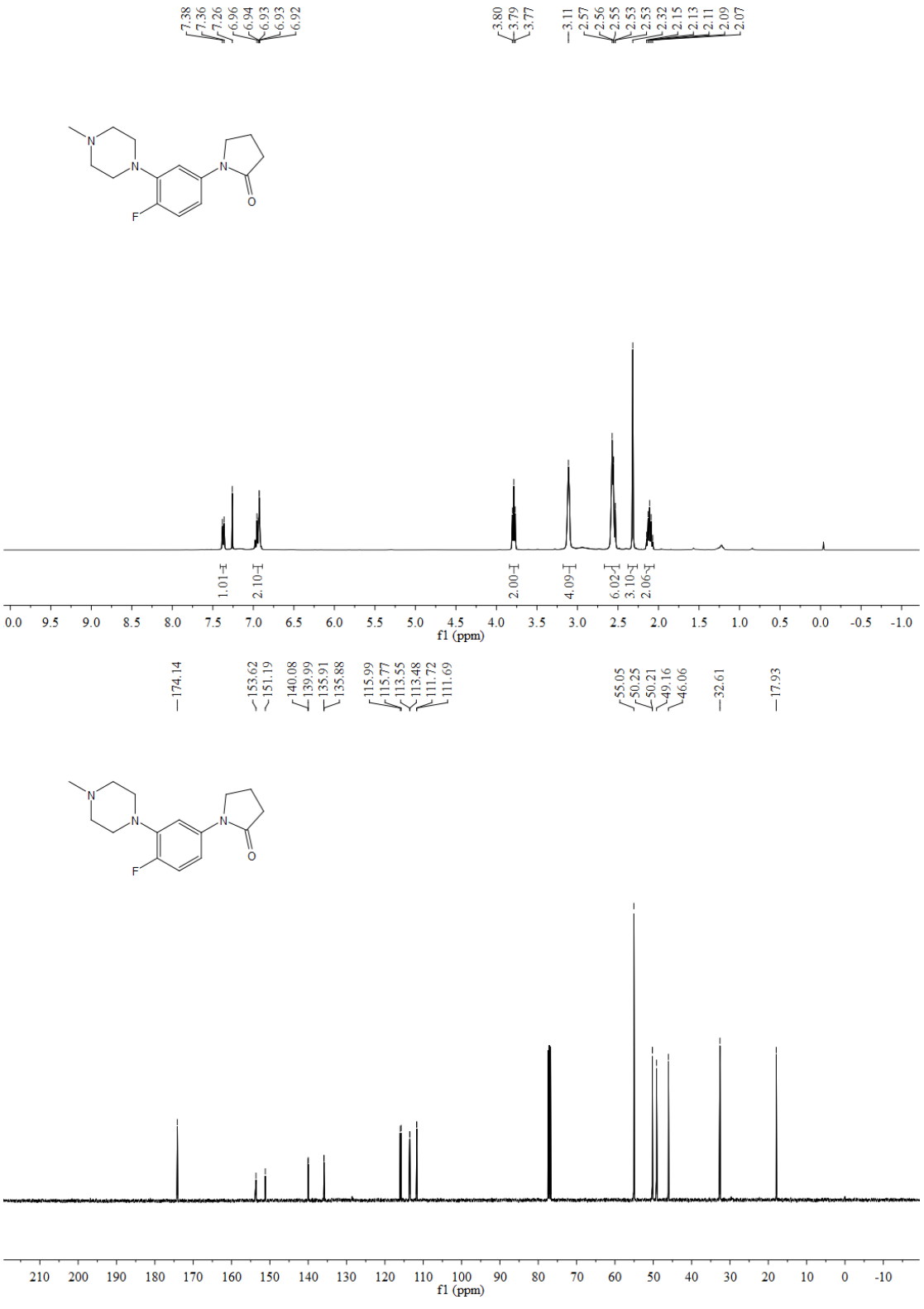

Br
F
N
O


0.97
0.99
1.04
2.00
1.98
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


174.48
157.03
154.59
136.36
124.64
120.33
120.26
116.37
116.14
48.69
32.39
17.98


Br
F
N
O


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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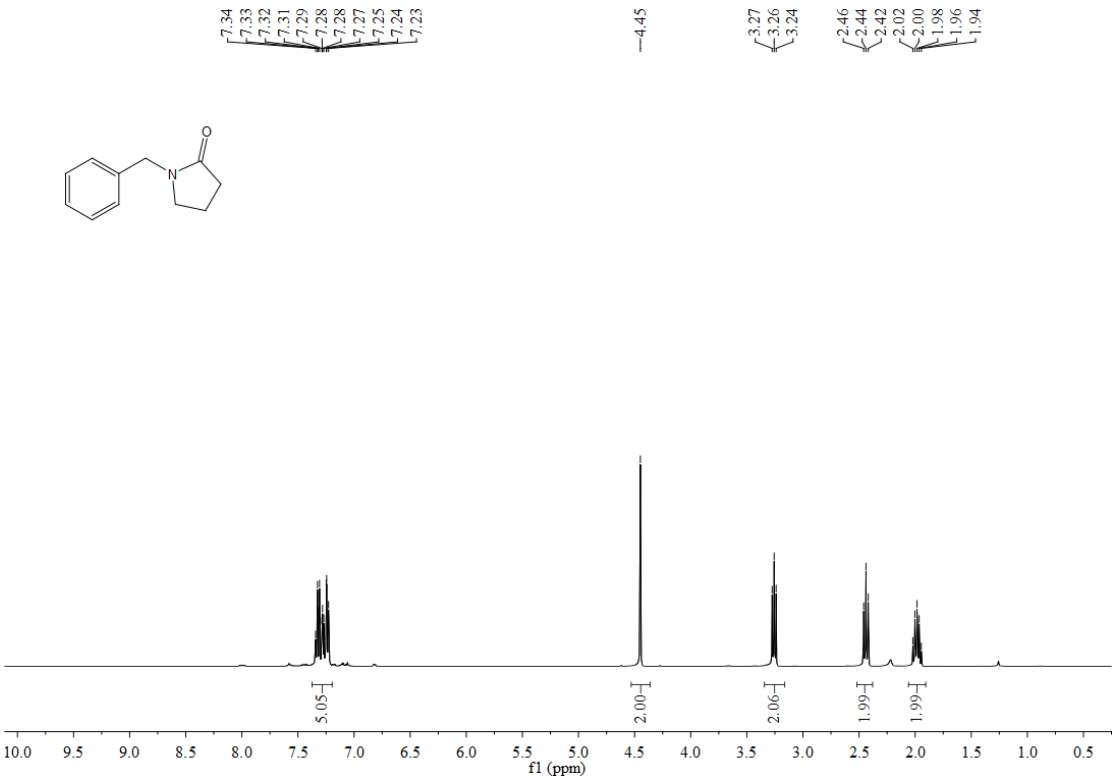
7.36
7.26
6.96
6.94
6.93
6.93
6.92
3.80
3.79
3.77
3.11
2.57
2.56
2.55
2.53
2.53
2.32
2.15
2.13
2.11
2.09
2.07
1.01
2.10
2.00
4.09
6.02
3.10
2.06
f1 (ppm)
174.14
153.62
151.19
140.08
139.99
135.91
135.88
115.99
115.77
113.55
113.48
111.72
111.69
55.05
50.25
50.21
49.16
46.06
32.61
17.93
f1 (ppm)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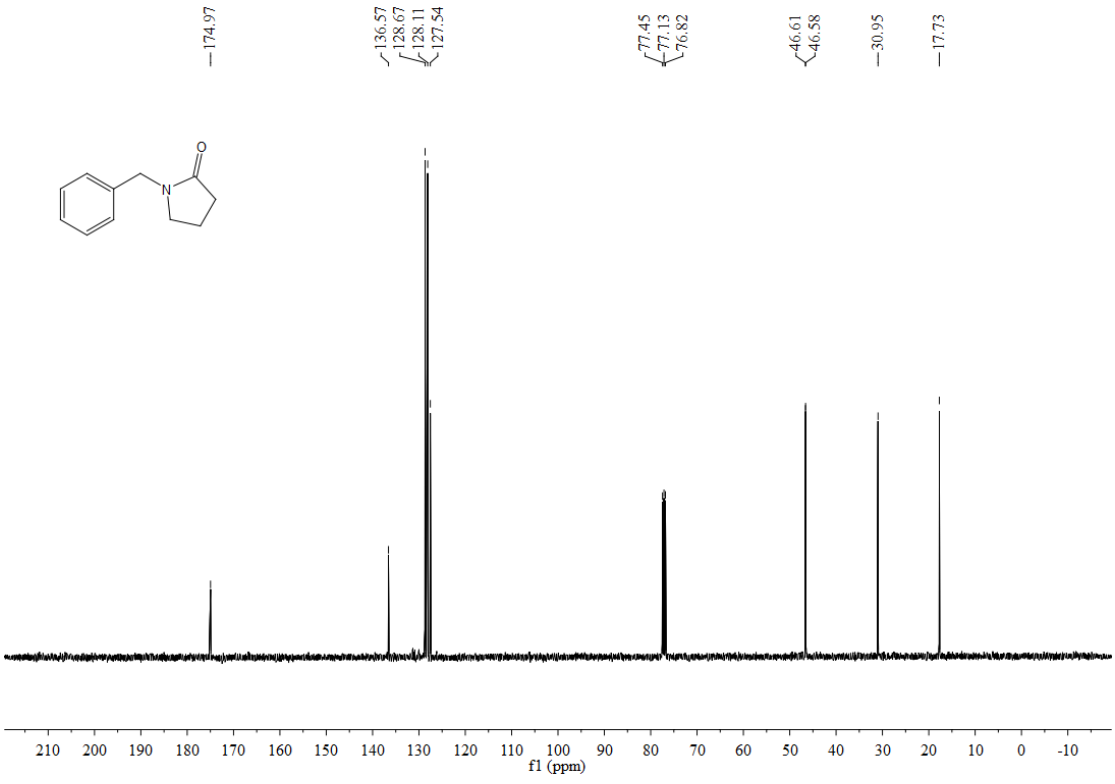
7.33
7.32
7.31
7.29
7.28
7.28
7.27
7.25
7.24
7.23
4.45
3.27
3.26
3.24
2.46
2.44
2.42
2.02
2.00
1.98
1.96
1.94
O
N
5.05
2.00
2.06
1.99
1.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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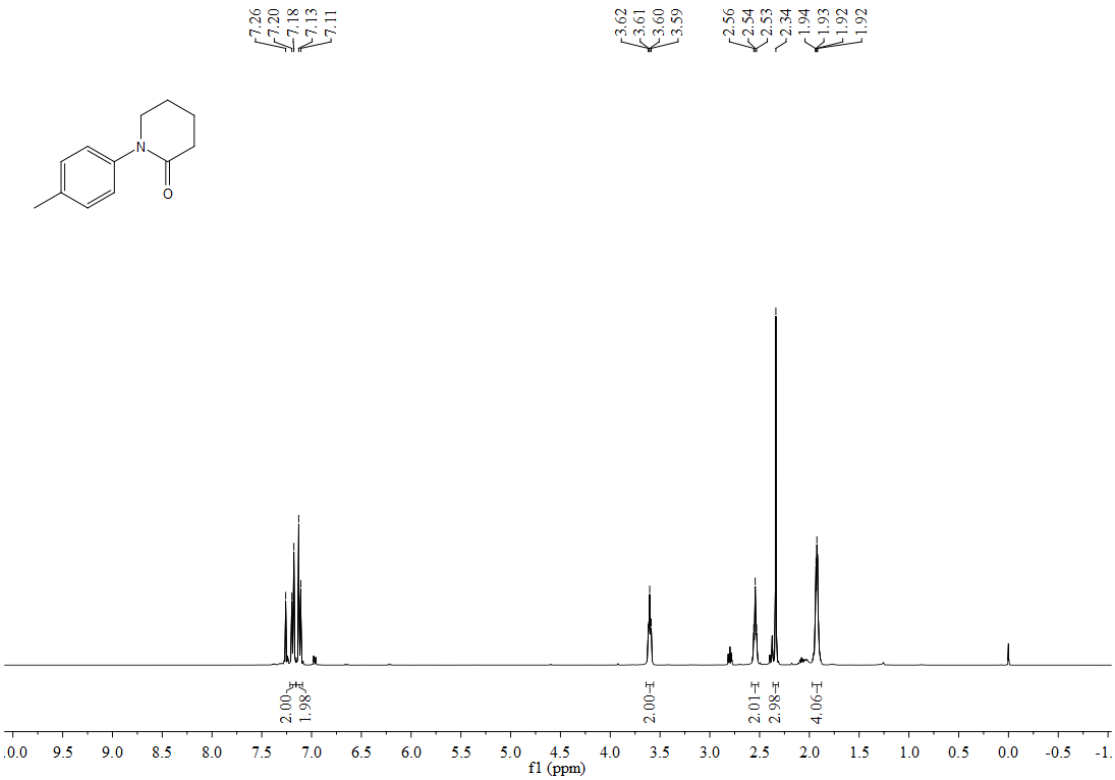
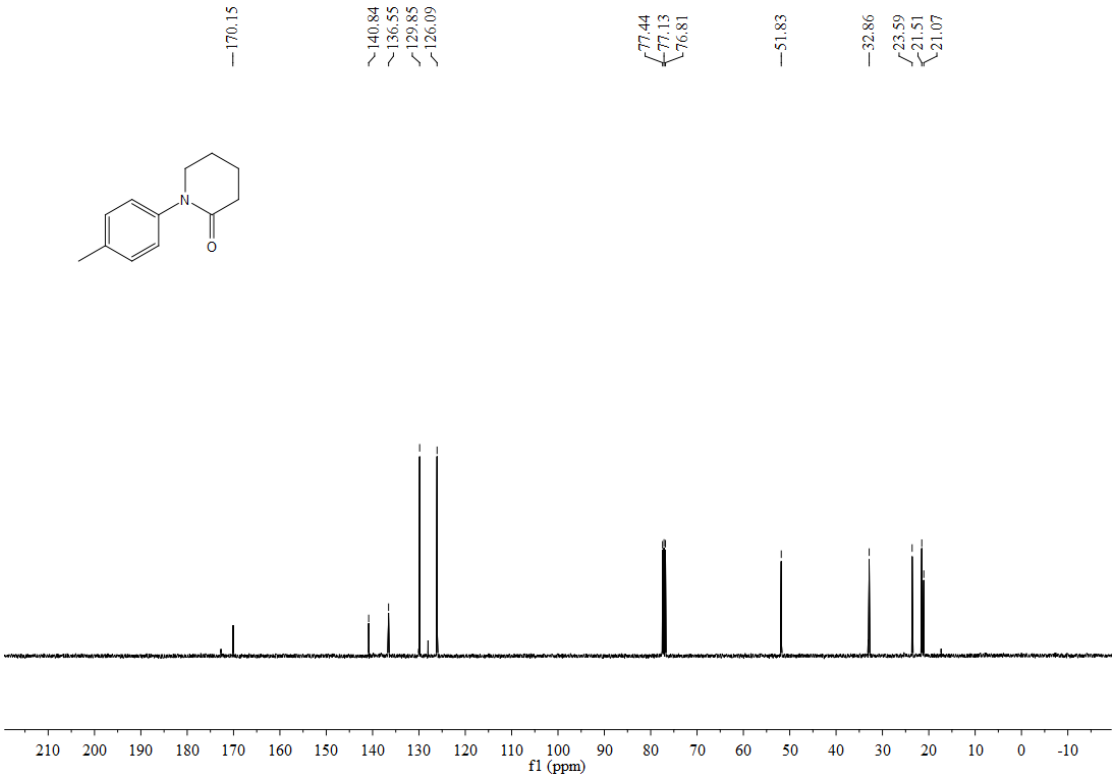
136.57
128.67
128.11
127.54
77.45
77.13
76.82
46.61
46.58
30.95
17.73
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.26
7.20
7.18
7.13
7.11
3.62
3.61
3.60
3.59
2.56
2.54
2.53
2.34
1.94
1.93
1.92
1.92
N
O
2.00
1.98
2.00
2.01
2.98
4.06
f1 (ppm)


170.15
140.84
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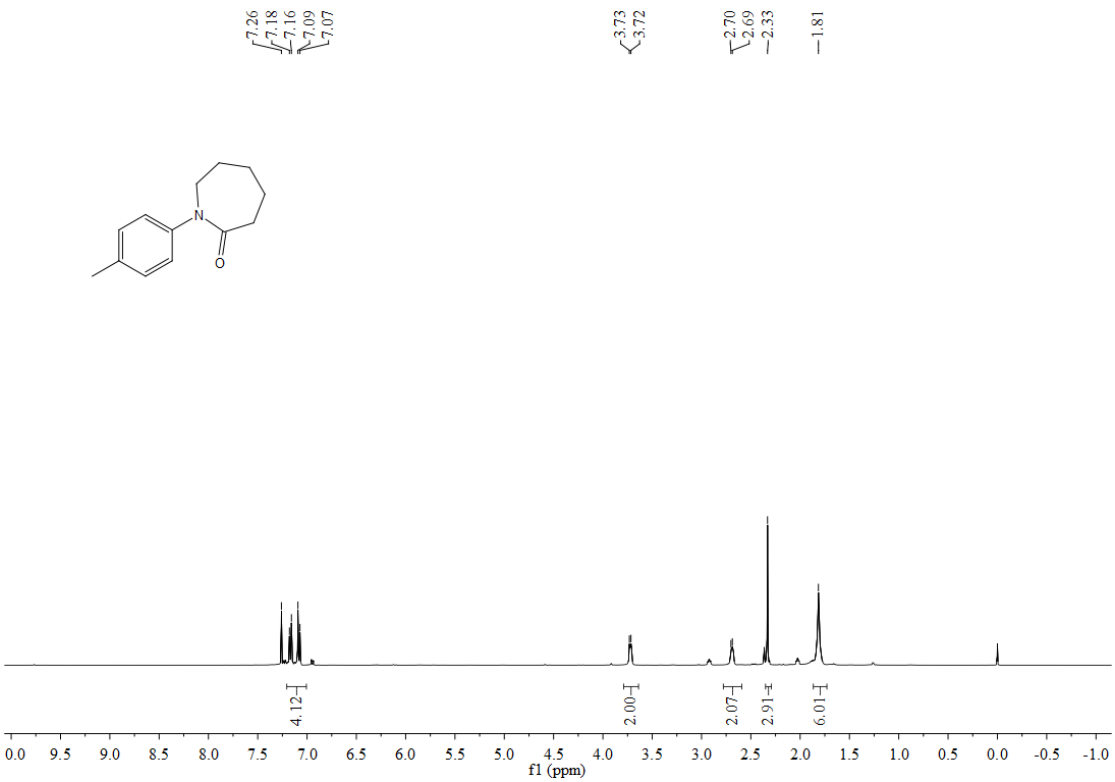
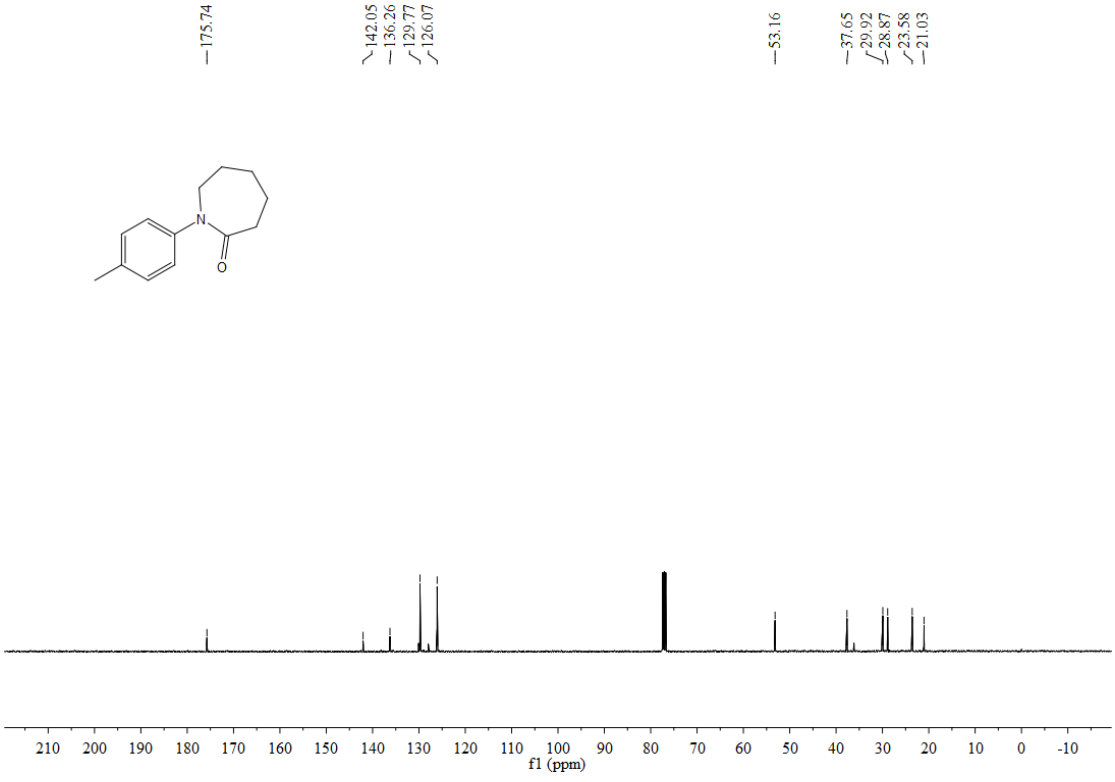
129.85
126.09
77.44
77.13
76.81
51.83
32.86
23.59
21.51
21.07
N
O
f1 (ppm)


7.26
7.18
7.16
7.09
7.07
3.73
3.72
2.70
2.69
2.33
1.81
4.12
2.00
2.07
2.91
6.01
f1 (ppm)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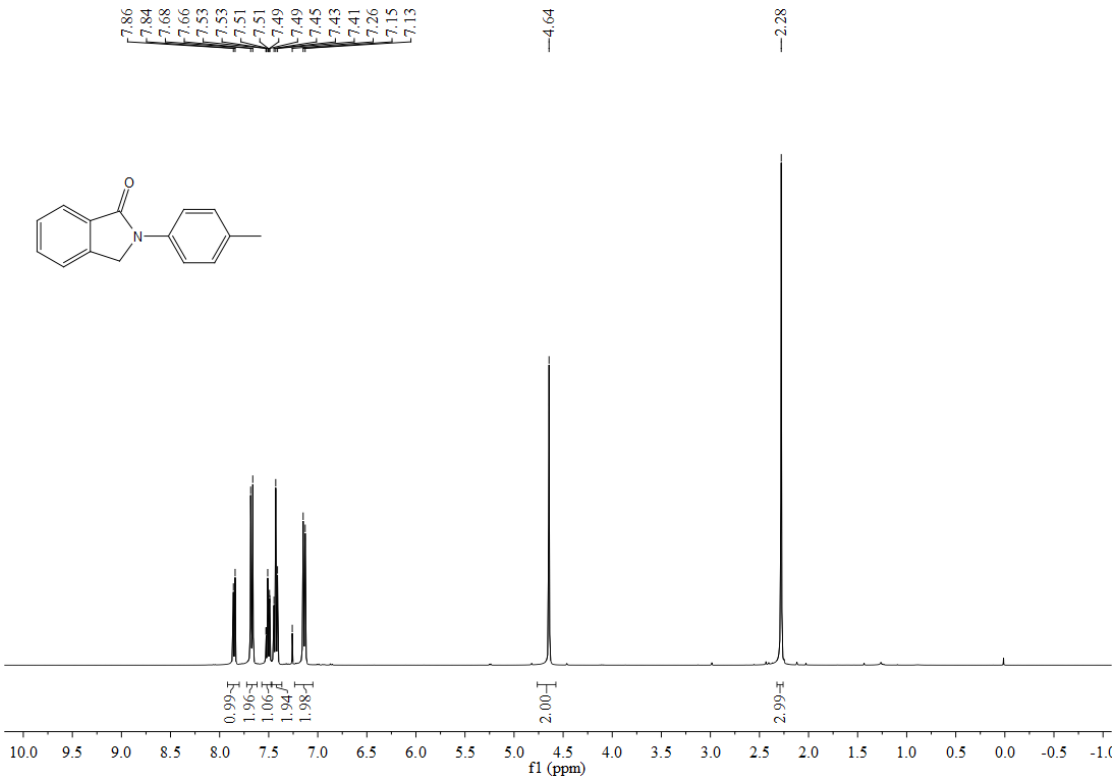
129.77
126.07
53.16
37.65
29.92
28.87
23.58
21.03
f1 (ppm)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7.84
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7.66
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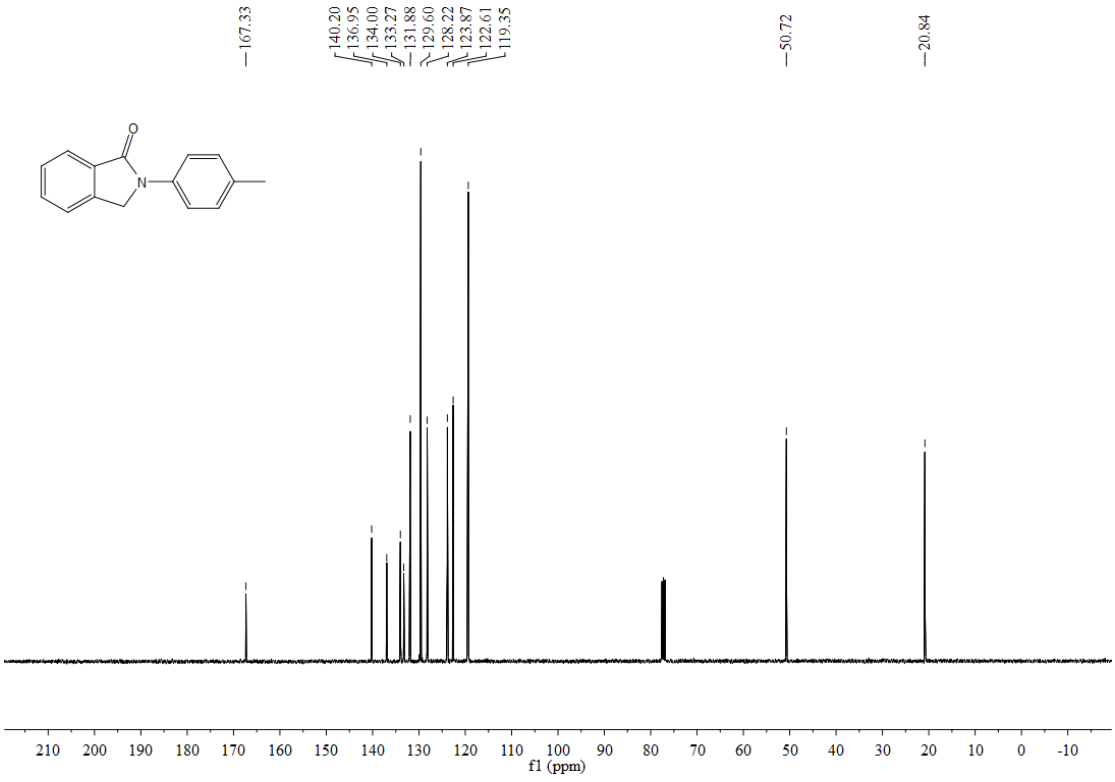
7.53
7.51
7.51
7.49
7.49
7.45
7.43
7.41
7.26
7.15
7.13
4.64
2.28
O
N
0.99
1.96
1.06
1.94
1.98
2.00
2.99
f1 (ppm)


167.33
140.20
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134.00
133.27
131.88
129.60
128.22
123.87
122.61
119.35
50.72
20.84
O
N
f1 (ppm)