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Supporting Information

HFIP-Promoted Michael Reactions: Direct *para*-Selective C-H Activation of Anilines with Maleimides

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1. General Information

^{1}H NMR spectra were recorded on 400 or 600 MHz (100 or 150 MHz for ^{13}C NMR) agilent NMR spectrometer with $CDCl_3$ as the solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts were reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the $CDCl_3$ at 7.26 ppm (for ^{1}H NMR) or 77.16 ppm (for ^{13}C NMR). HRMS was recorded on a GCT PremierTM (CI) Mass Spectrometer. Column chromatography was carried out on silica gel (200−300 mesh). All reactions were monitored using thin layer chromatography (TLC) on silica gel plates. All commercially available reagents, unless otherwise indicated, were used without further purification. The uncommercial 1-phenylpyrrolidines **1a**, **1f**-**1k** were readily prepared from tetrahydrofuran and the corresponding anilines (*Catal. Comm*. **2017**, *94*, 56-59), while the uncommercial maleimides **4a**-**4b** were readily prepared from *cis*-butenedioic anhydride and the corresponding alkylamines (*J. Agric. Food Chem.* **2016**, *64*, 4876−4881).

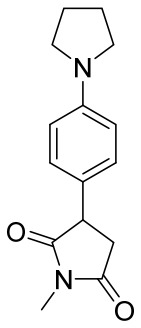
2. General Procedures (GP)

Coupling reaction of aromatic and hetro-aromatic compounds with maleimides

A 15 mL pressure tube equipped with screw cap and stirring was charged with aromatic amines or hetro-aromatic compounds **1** (0.5 mmol) and dissolved in HFIP (4 mL). Subsequently maleimides **2a** or **4** (2.0 mmol) were added. The reaction mixture was stirred under nitrogen at 100 °C for 24 h. The reaction mixture was cooled to room temperature. After removal of the solvent, the residue was purified by column chromatography on silica gel (PE : EA = 5 : 1) to afford corresponding products **3** or **5**.

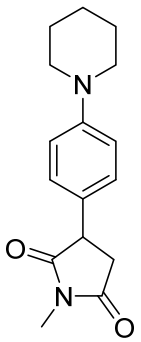
3. Characterization of Synthesized Compounds 3a-3z and 5a-5j

1-Methyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (3a)



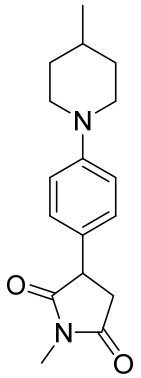
According to **GP**, 1-phenylpyrrolidine **1a** (74 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3a** (117 mg, 91%) as a white solid (mp 174.8–175.5 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.4 Hz, 2H), 6.45 (d, *J* = 8.4 Hz, 2H), 3.83 (dd, *J* = 9.1, 4.3 Hz, 1H), 3.20 – 3.15 (m, 4H), 3.14 – 3.04 (m, 1H), 2.97 (s, 3H), 2.71 (dd, *J* = 18.4, 4.2 Hz, 1H), 1.93 – 1.89 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.68, 176.80, 147.50, 128.00, 123.15, 112.02, 47.57, 45.20, 37.27, 25.44, 25.07. HRMS (CI) calcd for $C_{15}H_{19}N_2O_2$ $[M+H]^+$: 259.1447, found 259.1440.

1-Methyl-3-(4-(piperidin-1-yl)phenyl)pyrrolidine-2,5-dione (3b)



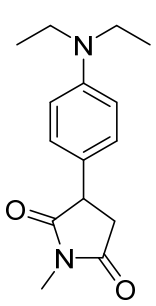
According to **GP**, 1-phenylpiperidine **1b** (81 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3b** (55 mg, 40%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 (d, *J* = 7.7 Hz, 2H), 6.82 (d, *J* = 7.8 Hz, 2H), 3.85 (dd, *J* = 8.9, 4.1 Hz, 1H), 3.11 – 3.04 (m, 5H), 2.97 (s, 3H), 2.72 (dd, *J* = 18.4, 3.8 Hz, 1H), 1.62 – 1.59 (m, 4H), 1.49 (d, *J* = 4.3 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.35, 176.58, 151.72, 127.92, 126.85, 116.73, 50.32, 45.15, 37.12, 25.67, 25.12, 24.22. HRMS (CI) calcd for $C_{16}H_{21}N_2O_2$ $[M+H]^+$: 273.1603, found 273.1605.

1-Methyl-3-(4-(4-methylpiperidin-1-yl)phenyl)pyrrolidine-2,5-dione (3c)



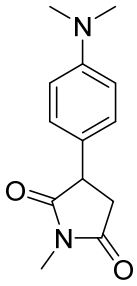
According to **GP**, 4-methyl-1-phenylpiperidine **1c** (87 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3c** (80 mg, 56%) as a colorless oil. ^{1}H NMR (400 MHz, CDCl3) δ 7.08 (d, *J* = 8.3 Hz, 2H), 6.92 (d, *J* = 7.7 Hz, 2H), 3.95 – 3.94 (m, 1H), 3.64 (d, *J* = 11.8 Hz, 2H), 3.17 (dd, *J* = 18.4, 9.5 Hz, 1H), 3.06 (s, 3H), 2.81 (dd, *J* = 18.4, 4.0 Hz, 1H), 2.69 (t, *J* = 12.0 Hz, 2H), 1.73 (d, *J* = 12.6 Hz, 2H), 1.52 – 1.51 (m, 1H), 1.33 (d, *J* = 10.7 Hz, 2H), 0.98 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.36, 176.59, 151.42, 127.94, 126.81, 116.71, 49.69, 45.15, 37.12, 33.91, 30.66, 25.13, 21.85. HRMS (CI) calcd for $C_{17}H_{23}N_2O_2$ $[M+H]^+$: 287.1760, found 287.1756.

3-(4-(Diethylamino)phenyl)-1-methylpyrrolidine-2,5-dione (3d)



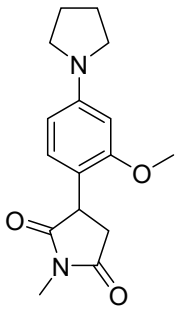
According to **GP**, *N*,*N*-diethylaniline **1d** (75 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3d** (105 mg, 81%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.5 Hz, 2H), 6.66 (d, *J* = 8.6 Hz, 2H), 3.92 (dd, *J* = 9.3, 4.5 Hz, 1H), 3.35 (q, *J* = 7.0 Hz, 4H), 3.17 (dd, *J* = 18.4, 9.5 Hz, 1H), 3.06 (s, 3H), 2.81 (dd, *J* = 18.4, 4.5 Hz, 1H), 1.16 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.70, 176.79, 147.30, 128.17, 123.01, 112.01, 45.07, 44.31, 37.20, 25.07, 12.49. HRMS (CI) calcd for $C_{15}H_{21}N_2O_2$ $[M+H]^+$: 261.1603, found 261.1594.

3-(4-(Dimethylamino)phenyl)-1-methylpyrrolidine-2,5-dione (3e)



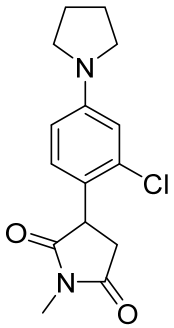
According to **GP**, *N*,*N*-dimethylaniline **1e** (61 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3e** (46 mg, 40%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.4 Hz, 2H), 6.71 (d, *J* = 8.5 Hz, 2H), 3.93 (dd, *J* = 9.3, 4.5 Hz, 1H), 3.16 (dd, *J* = 18.4, 9.5 Hz, 1H), 3.05 (s, 3H), 2.94 (s, 6H), 2.85 – 2.76 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.55, 176.70, 150.10, 127.97, 124.41, 112.97, 45.11, 40.53, 37.17, 25.10. HRMS (CI) calcd for $C_{13}H_{17}N_2O_2$ $[M+H]^+$: 233.1290, found 233.1292.

3-(2-Methoxy-4-(pyrrolidin-1-yl)phenyl)-1-methylpyrrolidine-2,5-dione (3f)



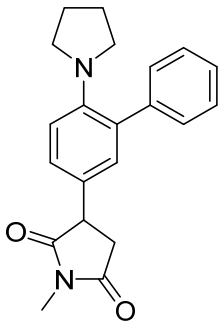
According to **GP**, 1-(3-methoxyphenyl)pyrrolidine **1f** (89 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3f** (125 mg, 87%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 7.9 Hz, 1H), 6.10 (d, *J* = 7.8 Hz, 1H), 6.04 (s, 1H), 3.86 – 3.76 (m, 1H), 3.72 (s, 3H), 3.28 – 3.26 (m, 4H), 3.05 (s, 3H), 3.09 – 2.98 (m, 1H), 2.71 (d, *J* = 18.0, Hz, 1H), 2.01 – 1.99 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 179.62, 177.41, 157.78, 149.20, 131.06, 112.45, 103.78, 95.36, 55.23, 47.70, 43.36, 36.77, 25.43, 24.85. HRMS (CI) calcd for $C_{16}H_{21}N_2O_3$ $[M+H]^+$: 289.1552, found 289.1549.

3-(2-Chloro-4-(pyrrolidin-1-yl)phenyl)-1-methylpyrrolidine-2,5-dione (3g)



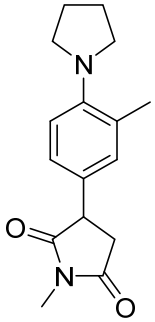
According to **GP**, 1-(3-chlorophenyl)pyrrolidine **1g** (91 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3g** (108 mg, 74%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.4 Hz, 1H), 6.55 (s, 1H), 6.40 (d, *J* = 6.4 Hz, 1H), 4.17 (dd, *J* = 9.4, 5.5 Hz, 1H), 3.26 – 3.23 (m, 4H), 3.17 (dd, *J* = 18.4, 9.6 Hz, 1H), 3.08 (s, 3H), 2.75 (dd, *J* = 18.4, 5.4 Hz, 1H), 2.02 – 1.99 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.14, 176.37, 148.33, 134.12, 130.35, 120.56, 112.60, 110.53, 47.57, 44.22, 36.88, 25.41, 25.08. HRMS (CI) calcd for $C_{15}H_{18}ClN_2O_2$ $[M+H]^+$: 293.1057, found 293.1056.

1-Methyl-3-(6-(pyrrolidin-1-yl)-[1,1'-biphenyl]-3-yl)pyrrolidine-2,5-dione (3h)



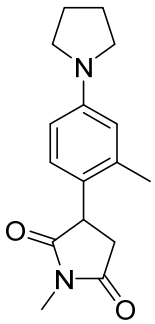
According to **GP**, 1-([1,1'-biphenyl]-2-yl)pyrrolidine **1h** (112 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3h** (134 mg, 80%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.29 – 7.23 (m, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.95 (s, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 3.94 (dd, *J* = 9.2, 4.5 Hz, 1H), 3.16 (dd, *J* = 18.5, 9.5 Hz, 1H), 3.03 (s, 3H), 2.87 – 2.79 (m, 5H), 1.74 – 1.71 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.43, 176.58, 147.49, 142.63, 131.15, 130.29, 129.04, 127.94, 126.68, 126.40, 125.86, 114.90, 50.93, 45.19, 37.23, 25.40, 25.12. HRMS (CI) calcd for $C_{21}H_{23}N_2O_2$ $[M+H]^+$: 335.1760, found 335.1750.

1-Methyl-3-(3-methyl-4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (3i)



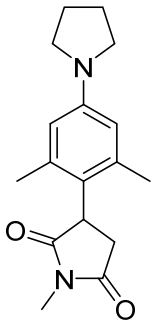
According to **GP**, 1-(*o*-tolyl)pyrrolidine **1i** (81 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3i** (102 mg, 75%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 – 6.92 (m, 2H), 6.84 (d, *J* = 8.7 Hz, 1H), 3.93 (dd, *J* = 9.2, 4.4 Hz, 1H), 3.21 – 3.14 (m, 5H), 3.07 (s, 3H), 2.82 (dd, *J* = 18.5, 4.3 Hz, 1H), 2.32 (s, 3H), 1.95 – 1.92 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.46, 176.67, 149.18, 130.53, 129.09, 128.00, 125.07, 116.07, 50.96, 45.25, 37.24, 25.11, 24.99, 20.74. HRMS (CI) calcd for $C_{16}H_{21}N_2O_2$ $[M+H]^+$: 273.1603, found 273.1605.

1-Methyl-3-(2-methyl-4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (3j)



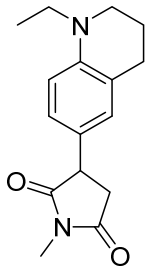
According to **GP**, 1-(*m*-tolyl)pyrrolidine **1j** (81 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3j** (96 mg, 70%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83 (d, *J* = 8.2 Hz, 1H), 6.39 – 6.36 (m, 2H), 4.14 (dd, *J* = 9.0, 4.5 Hz, 1H), 3.26 – 3.24 (m, 4H), 3.16 (dd, *J* = 18.5, 9.6 Hz, 1H), 3.07 (s, 3H), 2.67 (dd, *J* = 18.4, 4.3 Hz, 1H), 2.31 (s, 3H), 2.00 – 1.96 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 179.06, 176.82, 147.41, 136.95, 127.26, 122.42, 113.90, 109.85, 47.53, 42.53, 37.33, 25.42, 25.04, 20.25. HRMS (CI) calcd for $C_{16}H_{21}N_2O_2$ $[M+H]^+$: 273.1603, found 273.1604.

3-(2,6-Dimethyl-4-(pyrrolidin-1-yl)phenyl)-1-methylpyrrolidine-2,5-dione (3k)



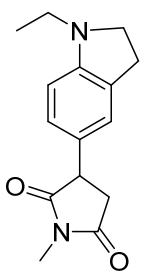
According to **GP**, 1-(3,5-dimethylphenyl)pyrrolidine **1k** (88 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3k** (116mg, 82%) as a white solid (mp: 192.1–193.2 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.24 (d, *J* = 13.6 Hz, 2H), 4.27 (dd, *J* = 9.2, 6.4 Hz, 1H), 3.24 – 3.21 (m, 4H), 3.17 – 3.03 (m, 1H), 3.6 (s, 3H), 2.64 (dd, *J* = 18.5, 6.1 Hz, 1H), 2.32 (s, 3H), 2.00 (s, 3H), 1.97 – 1.94 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 179.42, 176.52, 147.16, 138.08, 136.46, 120.29, 113.05, 111.75, 47.44, 41.16, 36.02, 25.40, 24.97, 21.50, 20.25. HRMS (CI) calcd for $C_{17}H_{23}N_2O_2$ $[M+H]^+$: 287.1760, found 287.1749.

3-(1-Ethyl-1,2,3,4-tetrahydroquinolin-6-yl)-1-methylpyrrolidine-2,5-dione (3l)



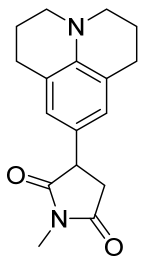
According to **GP**, 1-ethyl-1,2,3,4-tetrahydroquinoline **1l** (81 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3l** (120 mg, 88%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (d, *J* = 8.3 Hz, 1H), 6.75 (s, 1H), 6.54 (d, *J* = 8.4 Hz, 1H), 3.85 (dd, *J* = 9.3, 4.4 Hz, 1H), 3.32 (q, *J* = 7.0 Hz, 2H), 3.25 (t, *J* = 6.1 Hz, 2H), 3.14 (dd, *J* = 18.5, 9.4 Hz, 1H), 3.05 (s, 3H), 2.79 (dd, *J* = 18.5, 4.4 Hz, 1H), 2.71 (t, *J* = 6.1 Hz, 2H), 2.00 – 1.87 (m, 2H), 1.11 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.77, 176.85, 144.66, 127.86, 125.94, 123.10, 122.97, 110.75, 48.27, 45.26, 45.17, 37.30, 28.14, 25.07, 22.04, 10.74. HRMS (CI) calcd for $C_{16}H_{21}N_2O_2$ $[M+H]^+$: 273.1603, found 273.1602.

3-(1-Ethylindolin-5-yl)-1-methylpyrrolidine-2,5-dione (3m)



According to **GP**, 1-ethylindoline **1m** (74 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3m** (121 mg, 94%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.89 – 6.87 (m, 2H), 6.41 (d, *J* = 8.3 Hz, 1H), 3.90 (dd, *J* = 9.1, 4.2 Hz, 1H), 3.34 (t, *J* = 8.2 Hz, 2H), 3.19 – 3.09 (m, 3H), 3.05 (s, 3H), 2.93 (t, *J* = 8.2 Hz, 2H), 2.78 (dd, *J* = 18.4, 4.0 Hz, 1H), 1.17 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.74, 176.77, 152.12, 131.42, 126.51, 125.50, 123.17, 107.03, 52.22, 45.55, 42.88, 37.46, 28.34, 25.09, 11.81. HRMS (CI) calcd for $C_{15}H_{19}N_2O_2$ $[M+H]^+$: 259.1447, found 259.1443.

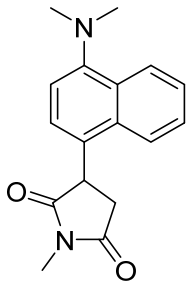
3-(1,2,3,5,6,7-Hexahydropyrido[3,2,1-ij]quinolin-9-yl)-1-methylpyrrolidine-2,5-dione (3n)



According to **GP**, 1,2,3,5,6,7-hexahydropyrido[3,2,1-ij]quinoline **1n** (87 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3n** (84 mg, 59%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59 (s, 2H), 3.80 (dd, *J* = 9.3, 4.4 Hz, 1H), 3.16 – 3.08 (m, 5H), 3.05 (s, 3H), 2.80 – 2.70 (m, 5H), 2.00 – 1.90 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.80, 176.89, 142.60,

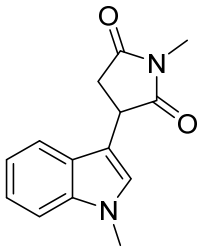
125.68, 123.50, 122.03, 49.84, 45.28, 37.38, 27.62, 25.08, 21.85. HRMS (CI) calcd for $C_{17}H_{21}N_2O_2$ $[M+H]^+$: 285.1603, found 285.1607.

3-(4-(Dimethylamino)naphthalen-1-yl)-1-methylpyrrolidine-2,5-dione (3p)



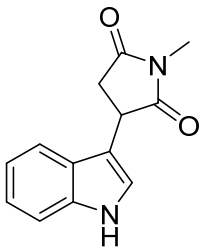
According to **GP**, *N*,*N*-dimethylnaphthalen-1-amine **1p** (86 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3p** (130 mg, 92%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.27 (m, 1H), 7.74 (d, *J* = 5.1 Hz, 1H), 7.58 – 7.48 (m, 2H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.01 (d, *J* = 7.8 Hz, 1H), 4.67 (dd, *J* = 9.3, 4.7 Hz, 1H), 3.34 (dd, *J* = 18.3, 9.6 Hz, 1H), 3.16 (s, 3H), 2.88 (s, 6H), 2.80 (dd, *J* = 18.4, 4.7 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.47, 176.25, 151.17, 132.36, 129.43, 127.92, 126.63, 125.35, 125.28, 124.78, 123.03, 113.53, 45.16, 42.97, 37.71, 25.21. HRMS (CI) calcd for $C_{17}H_{19}N_2O_2$ $[M+H]^+$: 283.1447, found 283.1446.

1-Methyl-3-(1-methyl-1*H*-indol-3-yl)pyrrolidine-2,5-dione (3t)



According to **GP**, 1-methyl-1*H*-indole **1t** (66 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3t** (112 mg, 92%) as a white solid (mp 123.2–125.2 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.2 Hz, 1H), 7.33 (d, *J* = 7.0 Hz, 1H), 7.28 – 7.25 (m, 1H), 7.15 – 7.13 (m, 1H), 7.04 (s, 1H), 4.31 – 4.28 (m, 1H), 3.76 (s, 3H), 3.27 (dd, *J* = 18.1, 9.3 Hz, 1H), 3.12 (s, 3H), 2.92 (d, *J* = 18.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.33, 176.55, 137.35, 126.73, 126.12, 122.25, 119.61, 118.59, 109.85, 109.74, 38.13, 36.67, 32.77, 25.10. HRMS (CI) calcd for $C_{14}H_{15}N_2O_2$ $[M+H]^+$: 243.1134, found 243.1134.

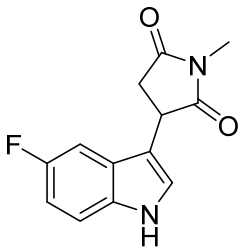
3-(1*H*-indol-3-yl)-1-methylpyrrolidine-2,5-dione(3u)



According to **GP**, 1*H*-indole **1u** (59 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3u** (86 mg, 75%) as a white solid (mp 181.1–182.8 °C). ^{1}H NMR (400 MHz, d^6-DMSO) δ 11.05 (s, 1H), 7.41 – 7.35 (m, 2H), 7.34 (s, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.99 (t, *J* = 7.4 Hz, 1H), 4.36 (dd, *J* = 9.1, 4.9 Hz, 1H), 3.23 (dd, *J* = 18.0, 9.4 Hz, 1H), 2.92 (s, 3H), 2.79 (dd, *J* = 18.0, 4.8 Hz, 1H). ^{13}C NMR (151 MHz, d^6-DMSO) δ 178.86, 177.08, 136.88, 126.35, 123.87, 121.76, 119.20, 118.82, 112.11, 111.16, 38.03, 36.57, 25.03. HRMS (CI) calcd for $C_{13}H_{12}N_2O_2$ $[M+H]^+$: 229.0972, found 229.0962.

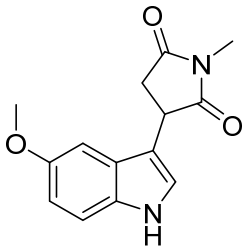
.

3-(5-fluoro-1*H*-indol-3-yl)-1-methylpyrrolidine-2,5-dione(3v)



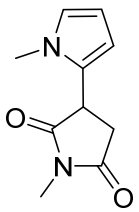
According to **GP**, 5-fluoro-1*H*-indole **1v** (68 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3v** (39 mg, 32%) as a yellow oil. ^{1}H NMR (400 MHz, d^{6}-DMSO) δ 11.16 (s, 1H), 7.42 (s, 1H), 7.37 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.20 (d, *J* = 9.8 Hz, 1H), 6.95 (t, *J* = 8.7 Hz, 1H), 4.35 (dd, *J* = 8.6, 5.3 Hz, 1H), 3.22 (dd, *J* = 17.9, 9.3 Hz, 1H), 2.91 (s, 3H), 2.82 (dd, *J* = 18.0, 4.9 Hz, 1H). ^{13}C NMR (151 MHz, d^{6}-DMSO) δ 178.68, 176.96, 157.94, 156.41, 133.50, 126.82, 126.76, 125.77, 113.09, 113.02, 111.41, 111.38, 110.04, 109.87, 103.85, 103.70, 37.82, 36.25, 25.03. HRMS (CI) calcd for $C_{13}H_{11}FN_2O_2$ $[M+H]^+$: 247.0877, found 247.0877.

3-(5-methoxy-1*H*-indol-3-yl)-1-methylpyrrolidine-2,5-dione(3w)



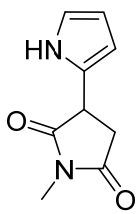
According to **GP**, 5-methoxy-1*H*-indole **1w** (74 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3w** (89 mg, 69%) as a white solid (mp 155.3–156.1 °C). ^{1}H NMR (400 MHz, d^{6}-DMSO) δ 10.89 (s, 1H), 7.27 (s, 2H), 6.87 (s, 1H), 6.75 (d, *J* = 8.7 Hz, 1H), 4.33 (dd, *J* = 8.7, 4.8 Hz, 1H), 3.73 (s, 3H), 3.23 (dd, *J* = 17.9, 9.3 Hz, 1H), 2.92 (s, 3H), 2.79 (dd, *J* = 17.9, 4.5 Hz, 1H). ^{13}C NMR (151 MHz, d^{6}-DMSO) δ 178.68, 176.96, 157.94, 156.41, 133.50, 126.82, 126.76, 125.77, 113.09, 113.02, 111.41, 111.38, 110.04, 109.87, 103.85, 103.70, 37.82, 36.25, 25.03. HRMS (CI) calcd for $C_{14}H_{14}N_2O_3$ $[M+H]^+$: 259.1077, found 259.1078.

1-methyl-3-(1-methyl-1*H*-pyrrol-2-yl)pyrrolidine-2,5-dione(3x)



According to **GP**, 1-methyl-1*H*-pyrrole **1x** (45 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3x** (54 mg, 56%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.66 – 6.61 (m), 6.11 – 6.04 (m), 5.96 (dd, *J* = 3.5, 1.2 Hz), 4.10 (dd, *J* = 9.4, 4.8 Hz), 3.74 (s), 3.16 (dd, *J* = 18.3, 9.4 Hz), 3.01 (s), 2.91 (dd, *J* = 18.3, 4.8 Hz). ^{13}C NMR (151 MHz, $CDCl_3$) δ 178.68, 176.96, 157.94, 156.41, 133.50, 126.82, 126.76, 125.77, 113.09, 113.02, 111.41, 111.38, 110.04, 109.87, 103.85, 103.70, 37.82, 36.25, 25.03. HRMS (CI) calcd for $C_{10}H_{12}N_2O_2$ $[M+H]^+$: 193.0972, found 193.0971.

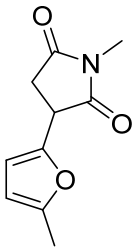
1-methyl-3-(1H-pyrrol-2-yl)pyrrolidine-2,5-dione(3y)



According to **GP**, 1*H*-pyrrole **1y** (34 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3w** (38 mg, 43%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.52 (s, 1H), 6.80 (s, 1H), 6.16 (d, *J* = 2.2 Hz, 1H), 6.02 (s, 1H), 4.09 (dd, *J* = 8.8, 5.0 Hz, 1H), 3.19 (dd, *J* = 18.3, 9.2 Hz, 1H), 2.99 (d, *J* = 10.7 Hz, 4H). ^{13}C NMR (151 MHz, $CDCl_3$ + CD_3OD) δ 177.84, 176.34,

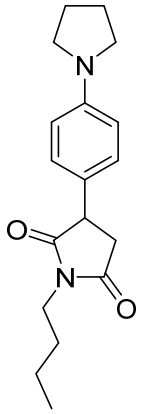
125.31, 118.82, 108.15, 105.45, 38.66, 34.34, 24.92. HRMS (CI) calcd for $C_{14}H_{14}N_2O_3$ $[M+H]^+$: 179.0815, found 179.0812.

1-Methyl-3-(5-methylfuran-2-yl)pyrrolidine-2,5-dione (3z)



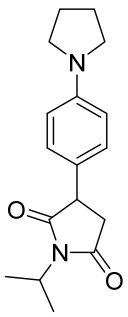
According to **GP**, 2-methylfuran **1z** (41 mg, 0.5 mmol) and 1-methyl-1*H*-pyrrole-2,5-dione **2a** (222 mg, 2.0 mmol) were converted to the desired product **3z** (56 mg, 58%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.50 (d, *J* = 4.1 Hz, 1H), 6.31 (d, *J* = 5.2 Hz, 1H), 5.18 (s, 1H), 2.98 – 2.97 (m, 1H), 2.96 (s, 3H), 2.72 (d, *J* = 6.0 Hz, 1H), 1.73 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.22, 175.01, 140.47, 136.87, 88.08, 80.55, 50.65, 49.44, 24.85, 15.61. HRMS (CI) calcd for $C_{10}H_{12}NO_3$ $[M+H]^+$: 194.0817, found 194.0816.

1-Butyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (5a)



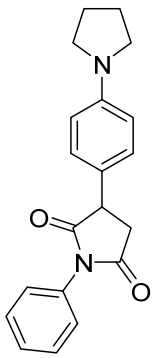
According to **GP**, 1-phenylpyrrolidine **1a** (74 mg, 0.5 mmol) and 1-butyl-1*H*-pyrrole-2,5-dione **4a** (306 mg, 2.0 mmol) were converted to the desired product **5a** (116 mg, 77%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, *J* = 8.4 Hz, 2H), 6.45 (d, *J* = 8.5 Hz, 2H), 3.80 (dd, *J* = 9.4, 4.4 Hz, 1H), 3.47 (t, *J* = 7.3 Hz, 2H), 3.18 (t, *J* = 6.0 Hz, 4H), 3.05 (dd, *J* = 18.4, 9.5 Hz, 1H), 2.67 (dd, *J* = 18.4, 4.4 Hz, 1H), 1.91 (t, *J* = 6.1 Hz, 4H), 1.56 – 1.44 (m, 2H), 1.28 – 1.22 (m, 2H), 0.85 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.55, 176.76, 147.45, 127.94, 123.57, 112.04, 47.57, 45.06, 38.72, 37.32, 29.79, 25.45, 20.06, 13.64. HRMS (CI) calcd for $C_{18}H_{25}N_2O_2$ $[M+H]^+$: 301.1916, found 301.1911.

1-Isopropyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (5b)



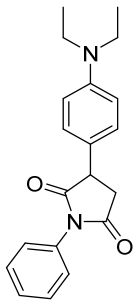
According to **GP**, 1-phenylpyrrolidine **1a** (74 mg, 0.5 mmol) and 1-isopropyl-1*H*-pyrrole-2,5-dione **4b** (278 mg, 2.0 mmol) were converted to the desired product **5b** (116 mg, 81%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (d, *J* = 8.1 Hz, 2H), 6.53 (d, *J* = 8.1 Hz, 2H), 4.46 – 4.39 (m, 1H), 3.82 (dd, *J* = 9.3, 4.1 Hz, 1H), 3.28 – 3.25 (m, 4H), 3.09 (dd, *J* = 18.3, 9.6 Hz, 1H), 2.71 (dd, *J* = 18.3, 4.2 Hz, 1H), 2.01 - 1.97 (m, 4H), 1.41 (t, *J* = 6.5 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.53, 176.75, 147.45, 127.85, 123.78, 112.06, 47.57, 44.83, 43.86, 37.26, 25.43, 19.32, 19.17. HRMS (ESI) calcd for $C_{17}H_{23}N_2O_2$ $[M+H]^+$: 287.1754, found 287.1756.

1-Phenyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (5c)



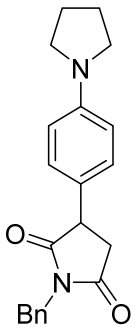
According to **GP**, 1-phenylpyrrolidine **1a** (74 mg, 0.5 mmol) and 1-phenyl-1*H*-pyrrole-2,5-dione **4c** (346 mg, 2.0 mmol) were converted to the desired product **5c** (128 mg, 80%) as a white solid (mp 180.6–181.8 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.31 – 7.29 (m, 1H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 6.55 (d, *J* = 8.1 Hz, 2H), 4.07 (dd, *J* = 9.4, 4.3 Hz, 1H), 3.43 – 3.19 (m, 5H), 2.96 (dd, *J* = 18.5, 4.2 Hz, 1H), 2.01 - 1.97 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.42, 175.70, 147.58, 132.06, 129.12, 128.54, 128.00, 126.49, 123.21, 112.11, 47.59, 45.25, 37.45, 25.45. HRMS (CI) calcd for $C_{20}H_{21}N_2O_2$ 321.1603 $[M+H]^+$, found 321.1602.

3-(4-(Diethylamino)phenyl)-1-phenylpyrrolidine-2,5-dione (5d)



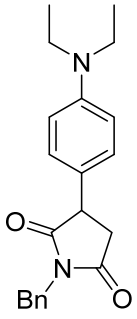
According to **GP**, *N*,*N*-diethylaniline **1d** (75 mg, 0.5 mmol) and 1-phenyl-1*H*-pyrrole -2,5-dione **4d** (346 mg, 2.0 mmol) were converted to the desired product **5d** (126 mg, 78%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 2H), 7.41 – 7.37 (m, 1H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.67 (d, *J* = 8.3 Hz, 2H), 4.08 (dd, *J* = 9.3, 4.3 Hz, 1H), 3.36 – 3.29 (m, 5H), 2.97 (dd, *J* = 18.5, 4.3 Hz, 1H), 1.15 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.42, 175.69, 147.40, 132.05, 129.12, 128.54, 128.17, 126.49, 123.06, 112.08, 45.11, 44.33, 37.38, 12.50. HRMS (ESI) calcd for $C_{20}H_{23}N_2O_2$ $[M+H]^+$: 323.1754, found 323.1753.

1-Benzyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (5e)



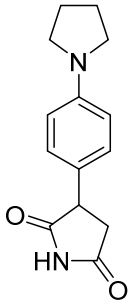
According to **GP**, 1-phenylpyrrolidine **1d** (74 mg, 0.5 mmol) and 1-benzyl-1*H*-pyrrole-2,5-dione **4e** (374 mg, 2.0 mmol) were converted to the desired product **5e** (135 mg, 81%) as a white solid (mp 161.0–161.8 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 6.5 Hz, 2H), 7.33 – 7.22 (m, 3H), 6.98 (d, *J* = 8.6 Hz, 2H), 6.49 (d, *J* = 8.6 Hz, 2H), 4.69 (q, *J* = 14.0 Hz, 2H), 3.89 (dd, *J* = 9.5, 4.6 Hz, 1H), 3.24 (t, *J* = 6.5 Hz, 4H), 3.13 (dd, *J* = 18.5, 9.5 Hz, 1H), 2.76 (dd, *J* = 18.5, 4.6 Hz, 1H), 2.01 – 1.94 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.20, 176.27, 147.49, 135.92, 128.73, 128.61, 127.98, 127.86, 123.27, 112.03, 47.57, 45.14, 42.55, 37.32, 25.43. HRMS (CI) calcd for $C_{21}H_{23}N_2O_2$ $[M+H]^+$: 335.1760, found 335.1758.

1-Benzyl-3-(4-(diethylamino)phenyl)pyrrolidine-2,5-dione (5f)



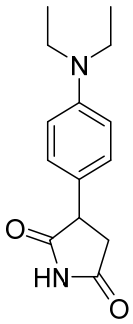
According to **GP**, *N*,*N*-diethylaniline **1d** (75 mg, 0.5 mmol) and 1-phenyl-1*H*-pyrrole-2,5-dione **4f** (346 mg, 2.0 mmol) were converted to the desired product **5f** (126 mg, 78%) as a white solid (mp 99.2–100.2 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 6.9 Hz, 2H), 7.36 – 7.31 (m, 3H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.64 (d, *J* = 8.4 Hz, 2H), 4.74 (q, *J* = 14.0 Hz, 2H), 3.93 (dd, *J* = 9.3, 4.5 Hz, 1H), 3.36 (q, *J* = 7.0 Hz, 4H), 3.17 (dd, *J* = 18.5, 9.5 Hz, 1H), 2.81 (dd, *J* = 18.5, 4.5 Hz, 1H), 1.17 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.21, 176.26, 147.31, 135.92, 128.74, 128.62, 128.15, 127.87, 123.14, 112.04, 45.02, 44.30, 42.57, 37.27, 12.50. HRMS (ESI) calcd for $C_{21}H_{25}N_2O_2$ $[M+H]^+$: 337.1911, found 337.1909.

3-(4-(Pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (5g)



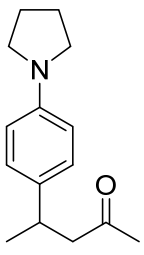
According to **GP**, 1-phenylpyrrolidine **1a** (74 mg, 0.5 mmol) and 1*H*-pyrrole-2,5-dione **4g** (194 mg, 2.0 mmol) were converted to the desired product **5g** (101 mg, 82%) as a white solid (mp 165.8–167.3 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 6.55 (d, *J* = 8.1 Hz, 2H), 3.98 (dd, *J* = 9.3, 4.9 Hz, 1H), 3.38 – 3.16 (m, 5H), 2.85 (dd, *J* = 18.6, 4.7 Hz, 1H), 2.02 – 1.98 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.73, 176.54, 147.58, 128.03, 122.66, 112.07, 47.58, 46.63, 38.40, 25.44. HRMS (CI) calcd for $C_{14}H_{17}N_2O_2$ $[M+H]^+$: 245.1290, found 245.1301.

3-(4-(Diethylamino)phenyl)pyrrolidine-2,5-dione (5h)



According to **GP**, *N*,*N*-diethylaniline **1d** (75 mg, 0.5 mmol) and 1*H*-pyrrole-2,5-dione **4h** (194 mg, 2.0 mmol) were converted to the desired product **5h** (75 mg, 61%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.09 (d, *J* = 8.3 Hz, 2H), 6.68 (d, *J* = 8.1 Hz, 2H), 3.99 (dd, *J* = 9.3, 4.9 Hz, 1H), 3.36 (q, *J* = 6.9 Hz, 4H), 3.22 (dd, *J* = 18.6, 9.6 Hz, 1H), 2.87 (dd, *J* = 18.6, 4.9 Hz, 1H), 1.17 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.96, 176.72, 147.39, 128.22, 122.55, 112.03, 46.51, 44.32, 38.36, 12.49. HRMS (ESI) calcd for $C_{14}H_{19}N_2O_2$ $[M+H]^+$: 247.1441, found 247.1446.

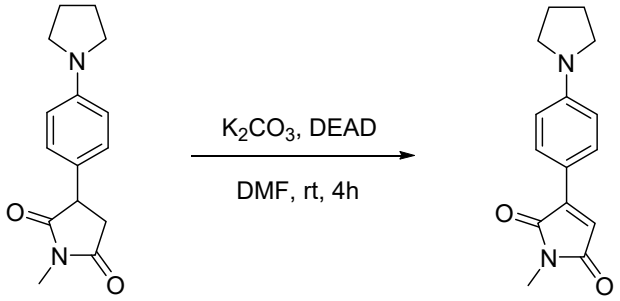
4-(4-(pyrrolidin-1-yl)phenyl)pentan-2-one (5i)



According to **GP**, 1-phenylpyrrolidine **1a** (74 mg, 0.5 mmol) and 3-penten-2-one **4i** (168 mg, 2.0 mmol) were converted to the desired product **5i** (25 mg, 21%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 7.7 Hz, 2H), 6.52 (d, *J* = 7.7 Hz, 2H), 3.32 – 3.17 (m, 5H), 2.66 (ddd, *J* = 23.5, 15.7, 7.2 Hz, 2H), 2.05 (s, 3H), 1.98 (s, 4H), 1.23 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 208.67, 146.60, 132.74, 127.39, 111.72, 52.55, 47.67, 34.84, 30.59, 25.47, 22.32. HRMS (ESI) calcd for $C_{15}H_{21}NO$ $[M+H]^+$: 232.1698, found 232.1696.

4. Synthesis of Succinimides Derivatives 6a-8a

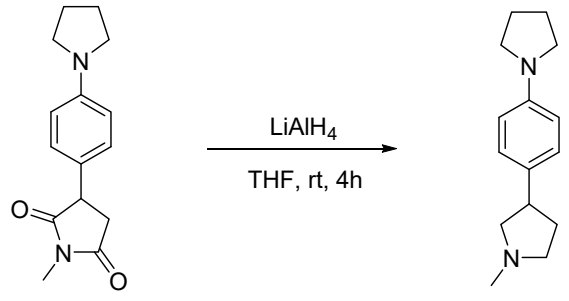
1-Methyl-3-(4-(pyrrolidin-1-yl)phenyl)-1H-pyrrole-2,5-dione (6a)



3a **6a**

The compound **3a** (60 mg, 0.23 mmol 1 equiv), K_2CO_3 (5 equiv) and diethyl azodicarboxylate (1 equiv) were taken in a dried schlenk tube with a magnetic stir bar. Then dry DMF (2 mL) was added and the reaction mixture was allowed to stir for 4 h at room temperature. After completion of the reaction (TLC monitored), the reaction mixture was extracted with EtOAc and washed with brine solution. The organic layer was dried with anhydrous magnesium sulfate and concentrated under reduced pressure. The resulting residue was directly purified by silica gel column chromatography (PE: EA = 5: 1) to provide the product **6a** (40 mg, 69%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.6 Hz, 2H), 6.59 (d, *J* = 8.6 Hz, 2H), 6.43 (s, 1H), 3.41 – 3.39 (m, 4H), 3.07 (s, 3H), 2.09 – 2.05 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.83, 171.64, 149.55, 143.89, 130.32, 115.91, 115.83, 111.75, 47.51, 25.42, 23.58. HRMS (ESI) calcd for $C_{15}H_{17}N_2O_2$ $[M+H]^+$: 257.1285, found 257.1284.

1-Methyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine (7a)

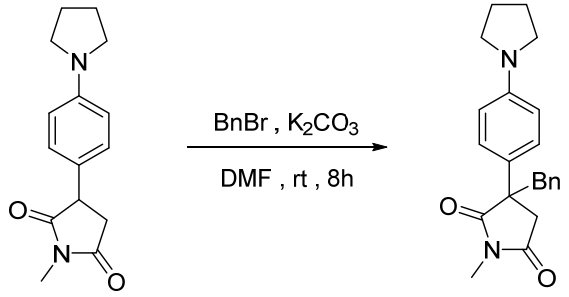


3a **7a**

The compound **3a** (65 mg, 0.25 mmol, 1 equiv) and $LiAlH_4$ (5 equiv) were taken in a dried schlenk tube with a magnetic stir bar. Then dry THF (2 mL) was added and the reaction mixture was allowed to stir for 4 h at room temperature. After completion, the reaction mixture was quenched with 10% NaOH solution. The reaction mixture was extracted with EtOAc (5 mL × 3), dried over anhydrous magnesium sulfate, and concentrated under reduced pressure. The resulting residue was directly purified by silica gel column chromatography (DCM: MeOH = 15: 1) to provide desired product

7a as a colorless oil. (39 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (d, *J* = 8.3 Hz, 2H), 6.53 (d, *J* = 8.3 Hz, 2H), 3.65 – 3.55 (m, 3H), 3.40 – 3.35 (m, 1H), 3.28 – 3.24 (m, 4H), 3.11 – 3.05 (m, 1H), 2.90 (s, 3H), 2.55 – 2.45 (m, 1H), 2.27 – 2.17 (m, 1H), 2.03 – 1.97 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 147.38, 127.78, 124.05, 123.99, 111.92, 70.50, 61.30, 55.50, 47.57, 42.58, 41.47, 25.40. HRMS (ESI) calcd for $C_{15}H_{23}N_2$ $[M+H]^+$: 231.1856, found 231.1863.

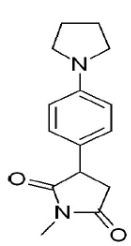
3-Benzyl-1-methyl-3-(4-(pyrrolidin-1-yl)phenyl)pyrrolidine-2,5-dione (8a)



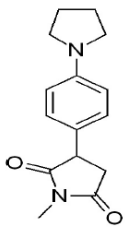
3a **8a**

The compound **3a** (70 mg, 0.27 mmol, 1 equiv) and K_2CO_3 (5 equiv) and benzyl bromide (1.5 equiv) were taken in a dried schlenk tube with a magnetic stir bar. Then dry DMF (2 mL) was added and the reaction mixture was allowed to stir for 8 h at room temperature. After completion of the reaction (TLC monitored), the reaction mixture was extracted with EtOAc and washed with brine solution. The organic layer was dried with anhydrous magnesium sulfate and concentrated under reduced pressure. The resulting residue was directly purified by silica gel column chromatography (PE : EA = 5: 1) to provide the product **8a** (49 mg, 52%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.5 Hz, 2H), 7.26 – 7.23 (m, 3H), 7.08 (d, *J* = 6.4 Hz, 2H), 6.56 (d, *J* = 8.5 Hz, 2H), 3.52 (d, *J* = 13.4 Hz, 1H), 3.31 – 3.26 (m, 4H), 3.06 (d, *J* = 13.5 Hz, 1H), 2.98 (s, 2H), 2.82 (s, 3H), 2.03 – 1.98 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 180.49, 175.67, 135.92, 130.03, 128.47, 127.26, 126.96, 111.74, 52.49, 47.59, 45.09, 39.90, 25.44, 24.70. HRMS (ESI) calcd for $C_{22}H_{25}N_2O_2$ $[M+H]^+$: 349.1911, found 349.1912.

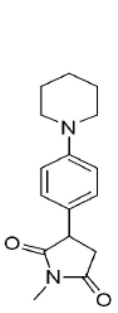
5. ^{1}H and ^{13}C-NMR Spectra



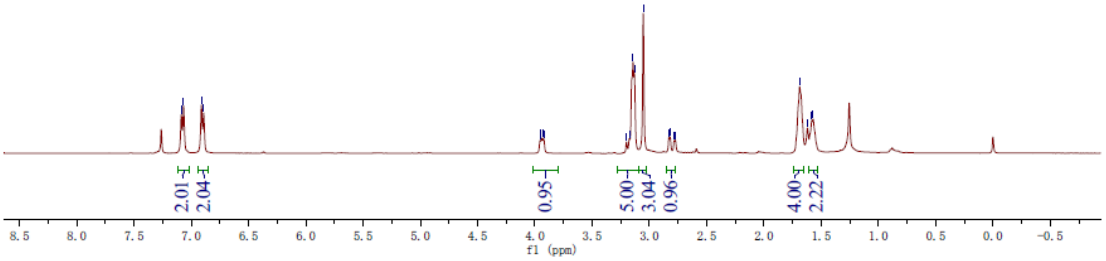
3a

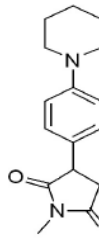


3a

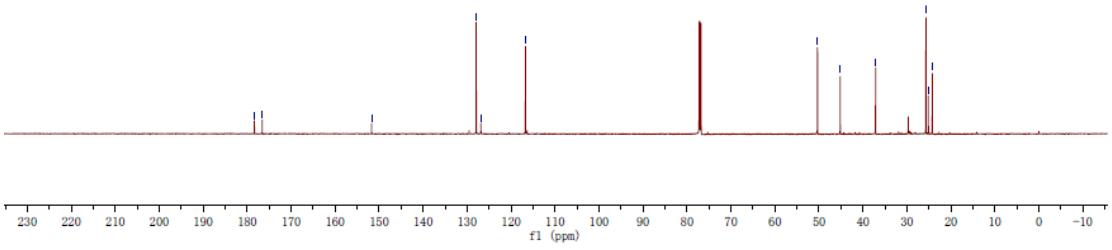


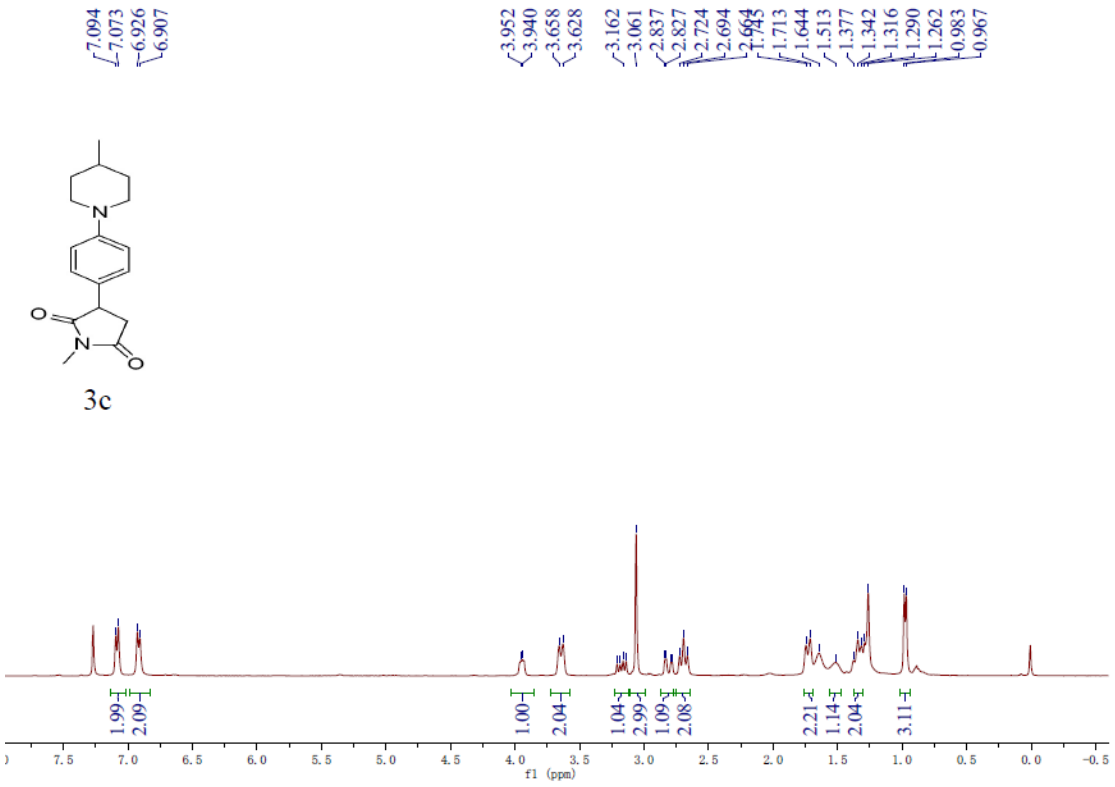
3b





3b

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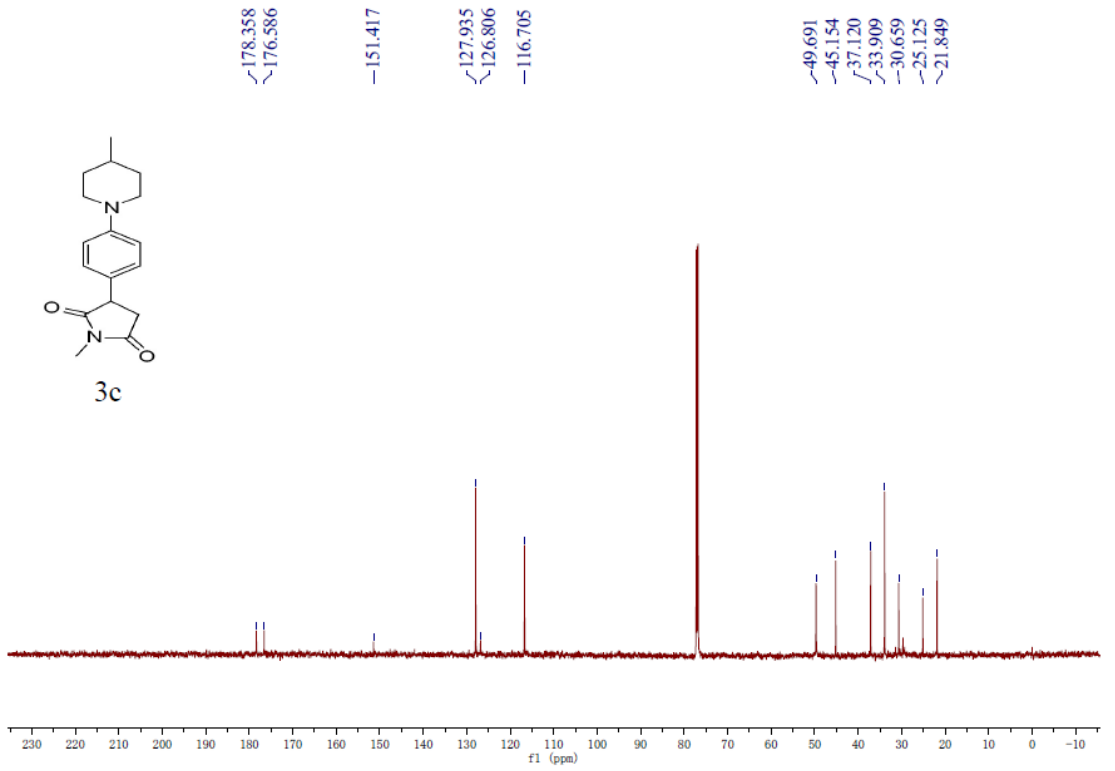
6.907
3.952
3.940
3.658
3.628
3.162
3.061
2.837
2.827
2.724
2.694
1.713
1.644
1.513
1.377
1.342
1.316
1.290
1.262
0.983
0.967
3c
1.99
2.09
1.00
2.04
1.04
2.99
1.09
2.08
2.21
1.14
2.04
3.11
f1 (ppm)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151.417
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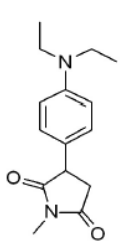
116.705
49.691
45.154
37.120
33.909
30.659
25.125
21.849
3c
f1 (ppm)



3d

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7.042
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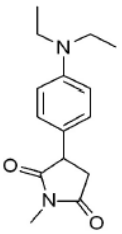
6.646
3.942
3.930
3.918
3.907
3.377
3.360
3.342
3.325
3.159
3.135
3.066
3.047
2.843
1.178
1.160
1.143
2.01
2.06
1.00
4.16
1.12
3.22
1.09
6.05
f1 (ppm)



3d

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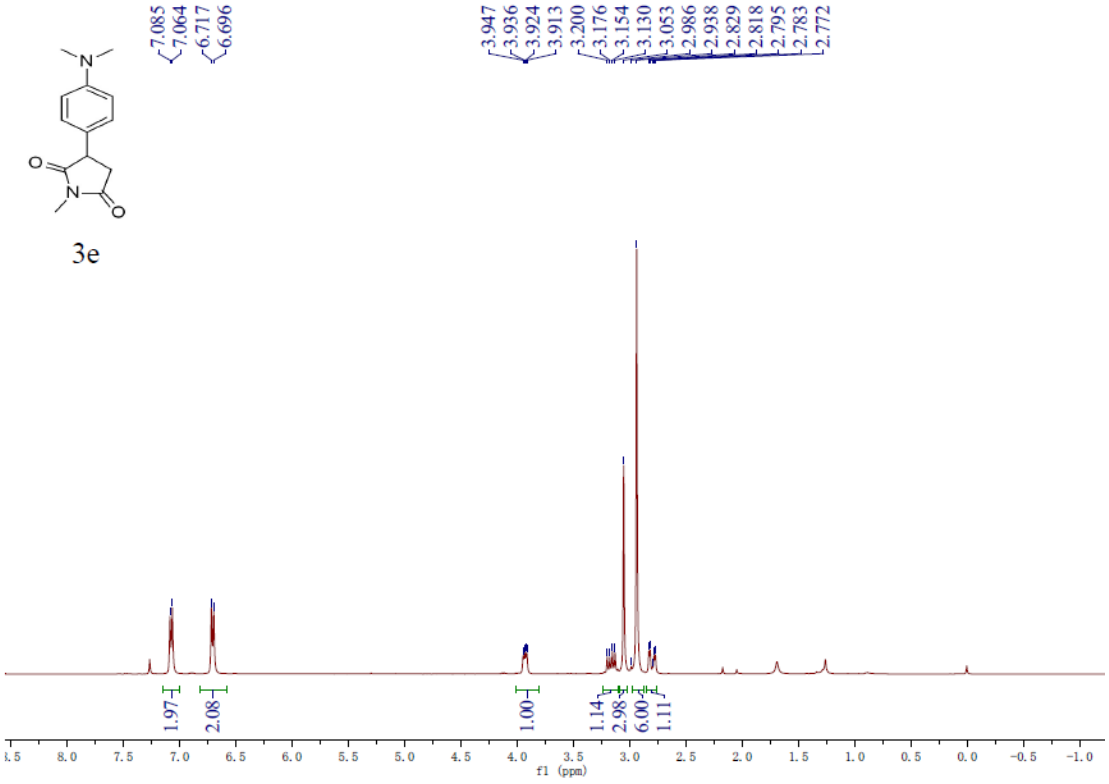
123.008
112.008
45.072
44.308
37.202
25.070
12.491
f1 (ppm)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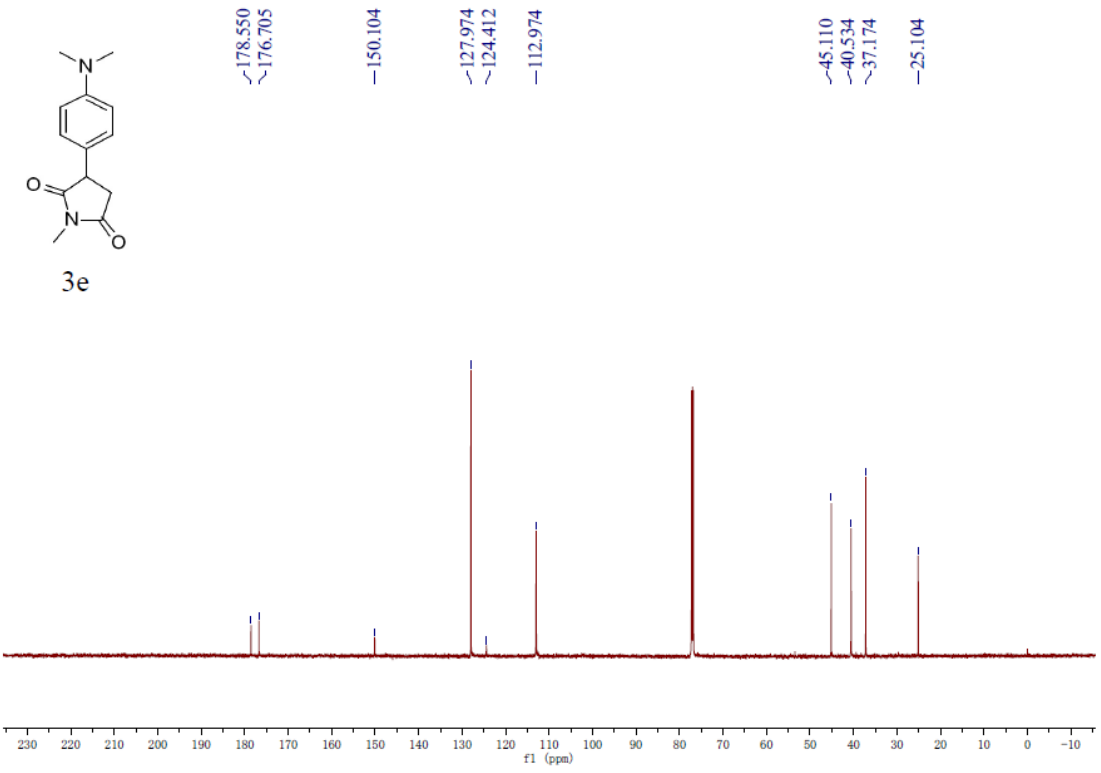
6.717
6.696
3.947
3.936
3.924
3.913
3.200
3.176
3.154
3.130
3.053
2.986
2.938
2.829
2.818
2.795
2.783
2.772
3e
1.97
2.08
1.00
1.14
2.98
6.00
1.11
f1 (ppm)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25.104
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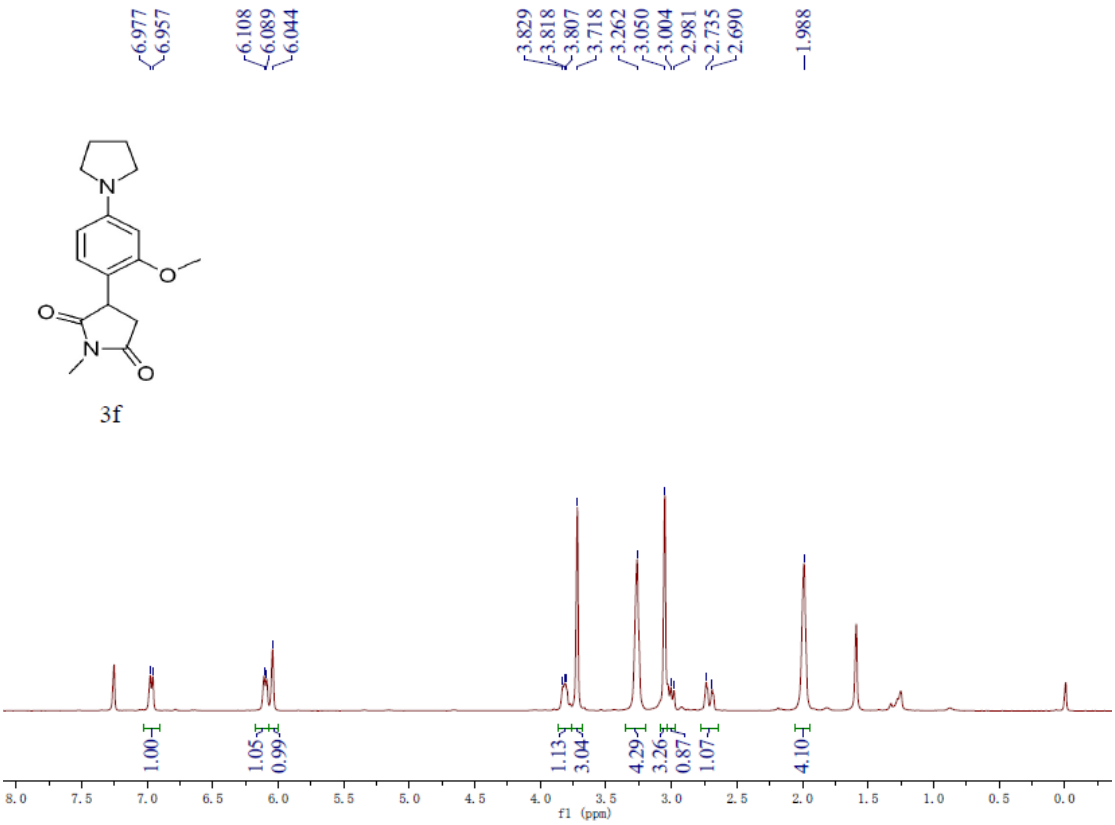
f1 (ppm)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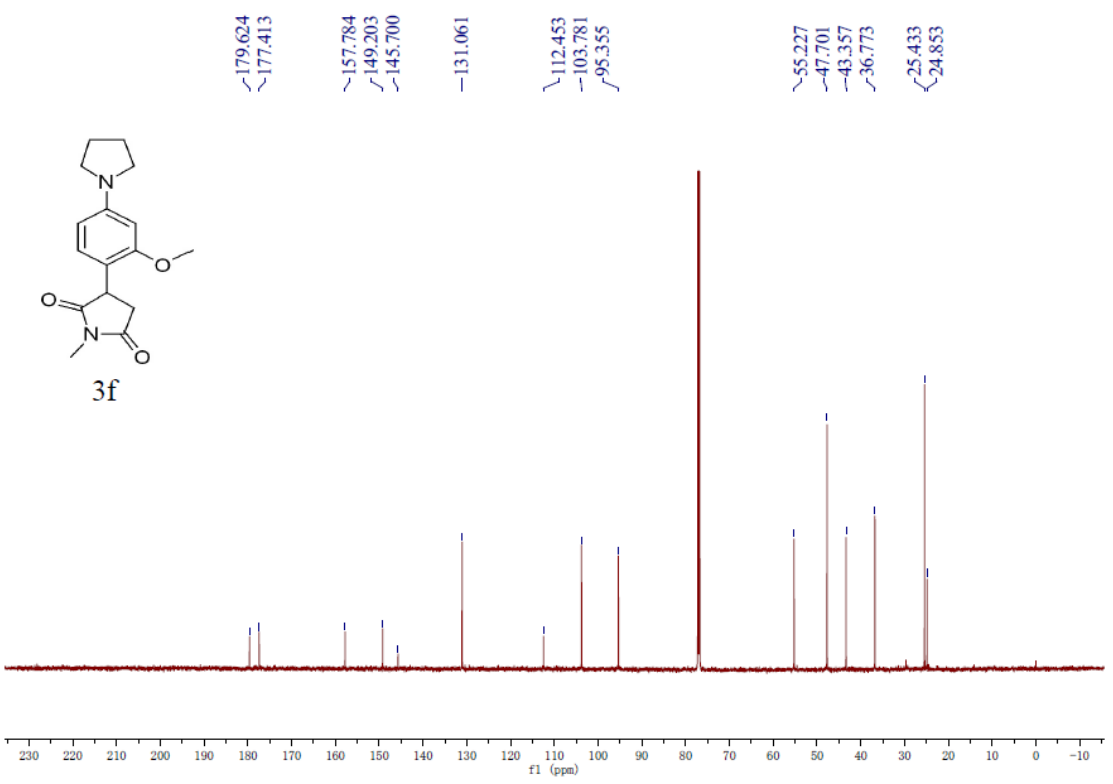
6.108
6.089
6.044
3.829
3.818
3.807
3.718
3.262
3.050
3.004
2.981
2.735
2.690
1.988
1.00
1.05
0.99
1.13
3.04
4.29
3.26
0.87
1.07
4.10
f1 (ppm)

3f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103.781
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55.227
47.701
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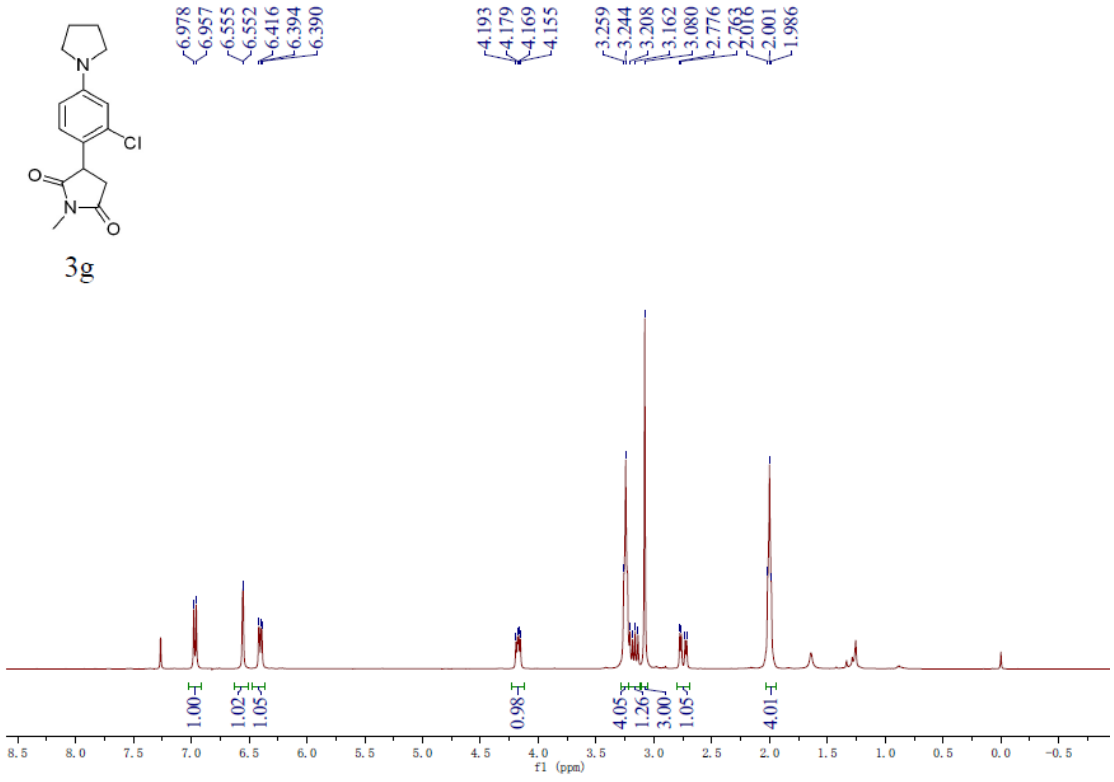
36.773
25.433
24.853
f1 (ppm)

3f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6.390
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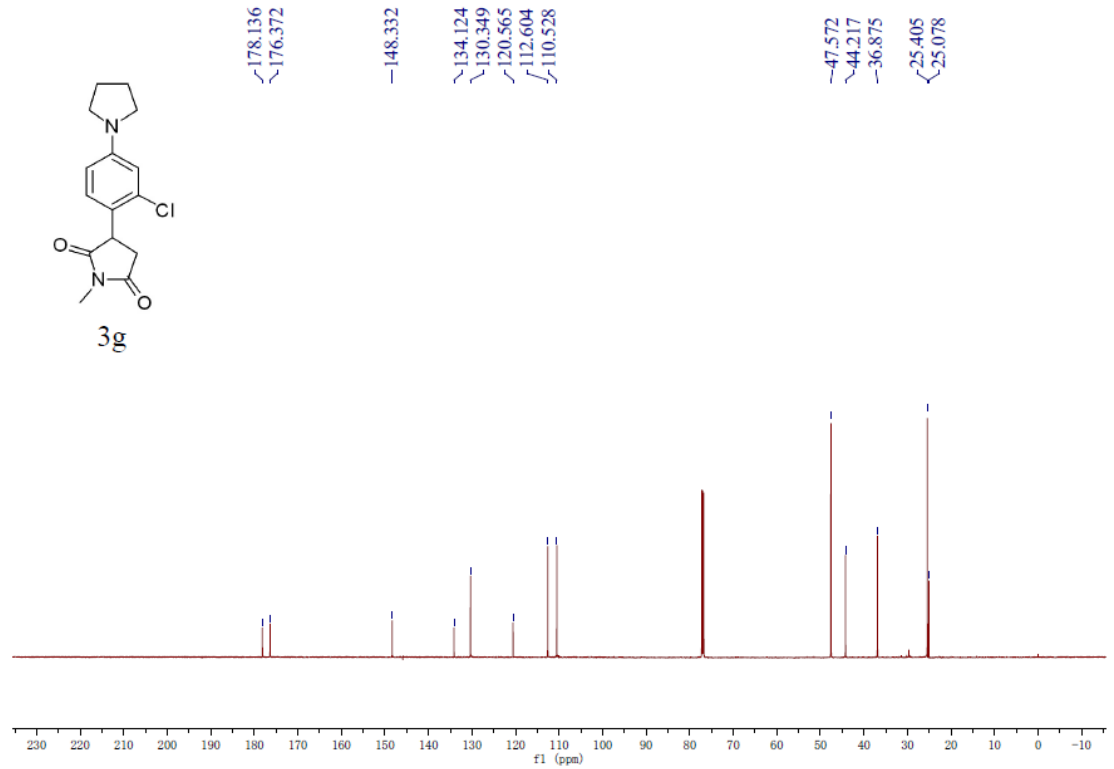
4.179
4.169
4.155
3.259
3.244
3.208
3.162
3.080
2.776
2.763
2.016
2.001
1.986
Cl
O
N
O
N
O
3g
1.00
1.02
1.05
0.98
4.05
1.26
3.00
1.05
4.01
f1 (ppm)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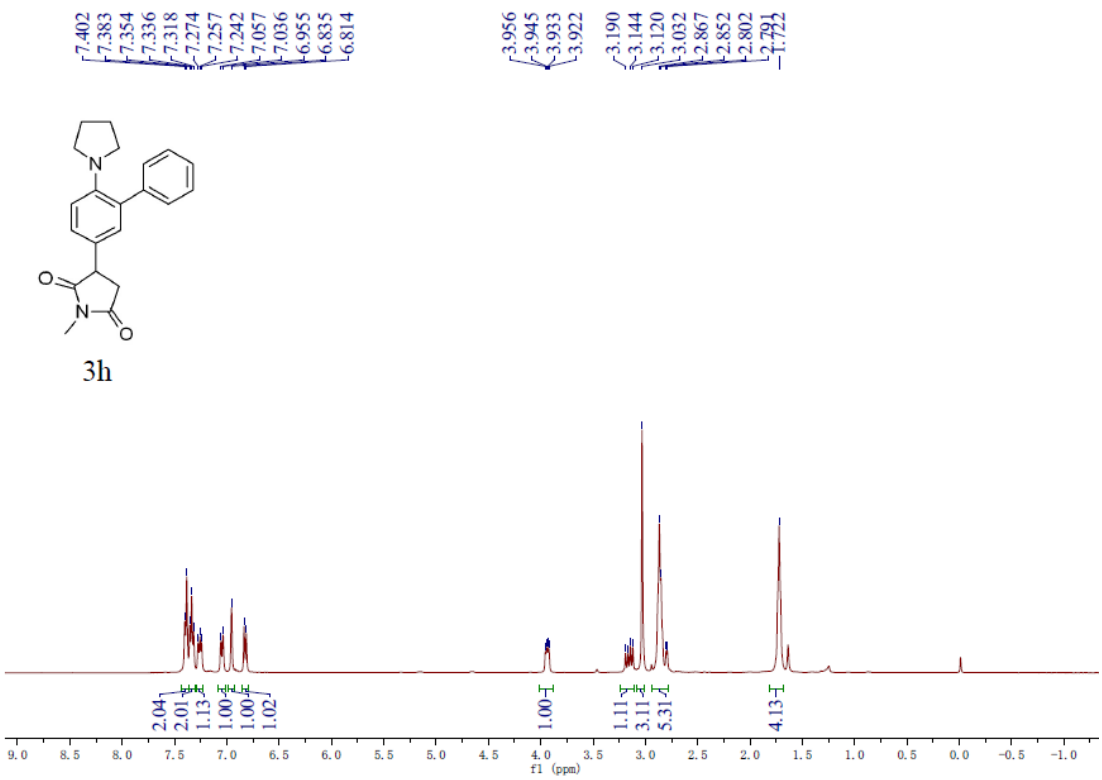
Cl
O
N
O
N
O
3g
f1 (ppm)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7.036
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6.814
3.956
3.945
3.933
3.922
3.190
3.144
3.120
3.032
2.867
2.852
2.802
2.791
1.722
3h
2.04
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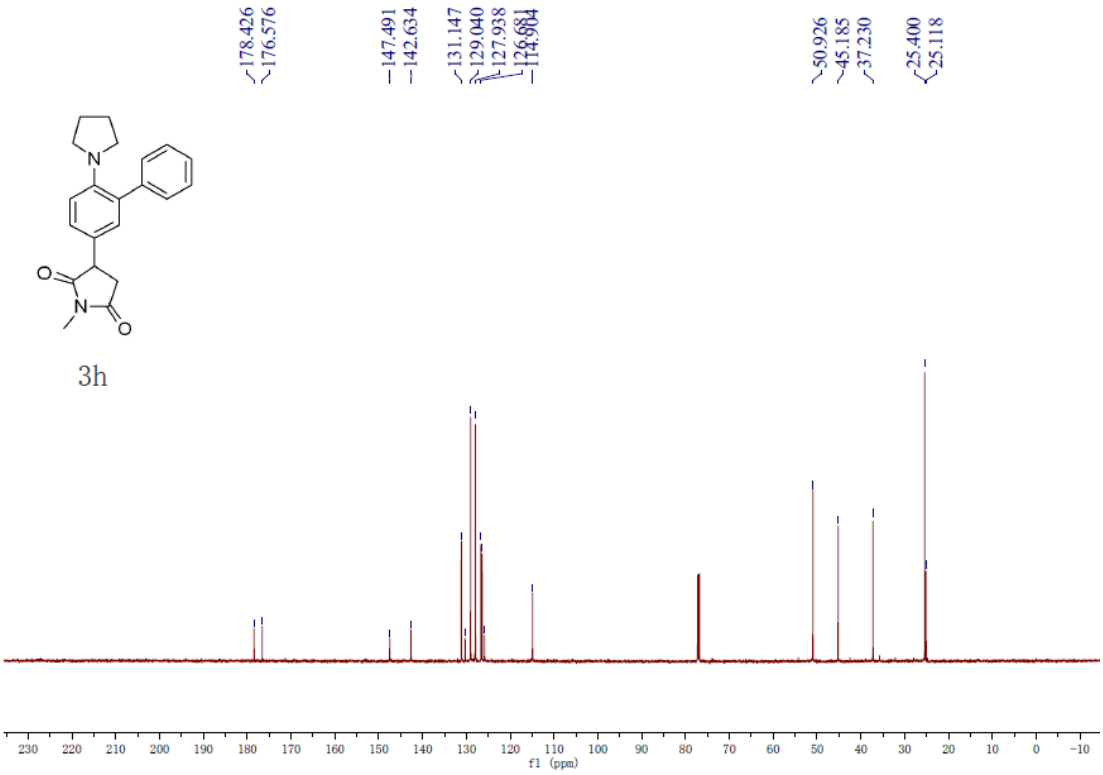
1.11
3.11
5.31
4.13
f1 (ppm)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114.904
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37.230
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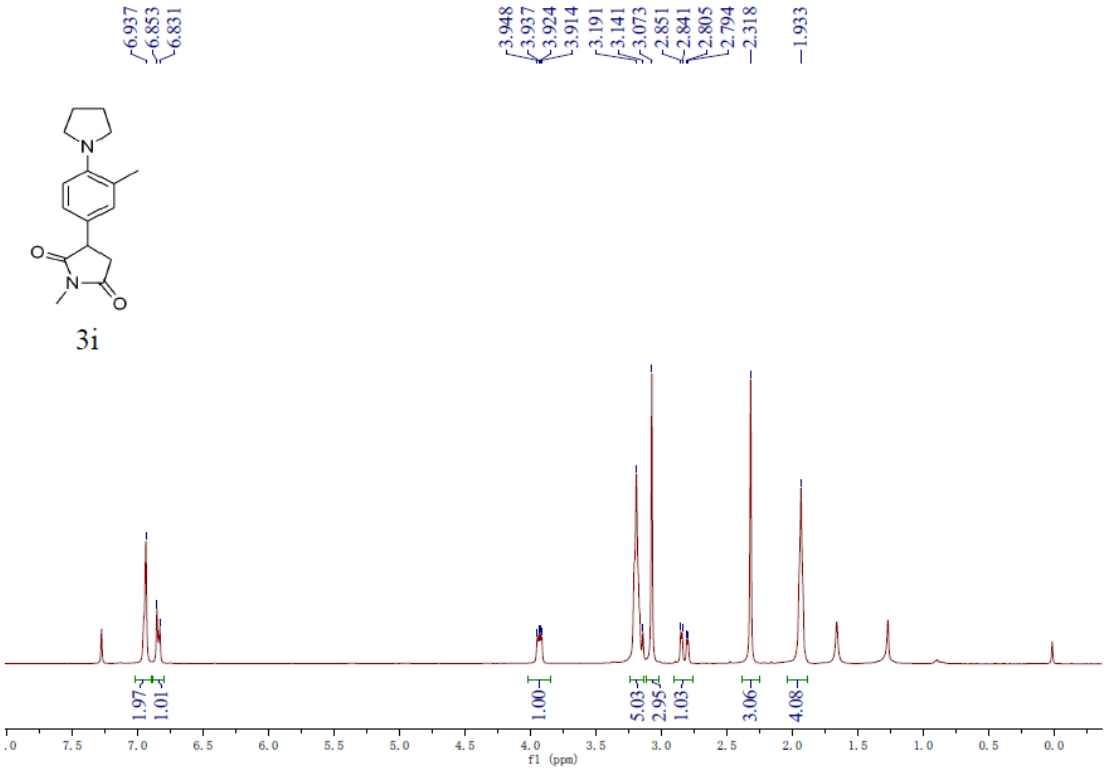
25.118
3h
f1 (ppm)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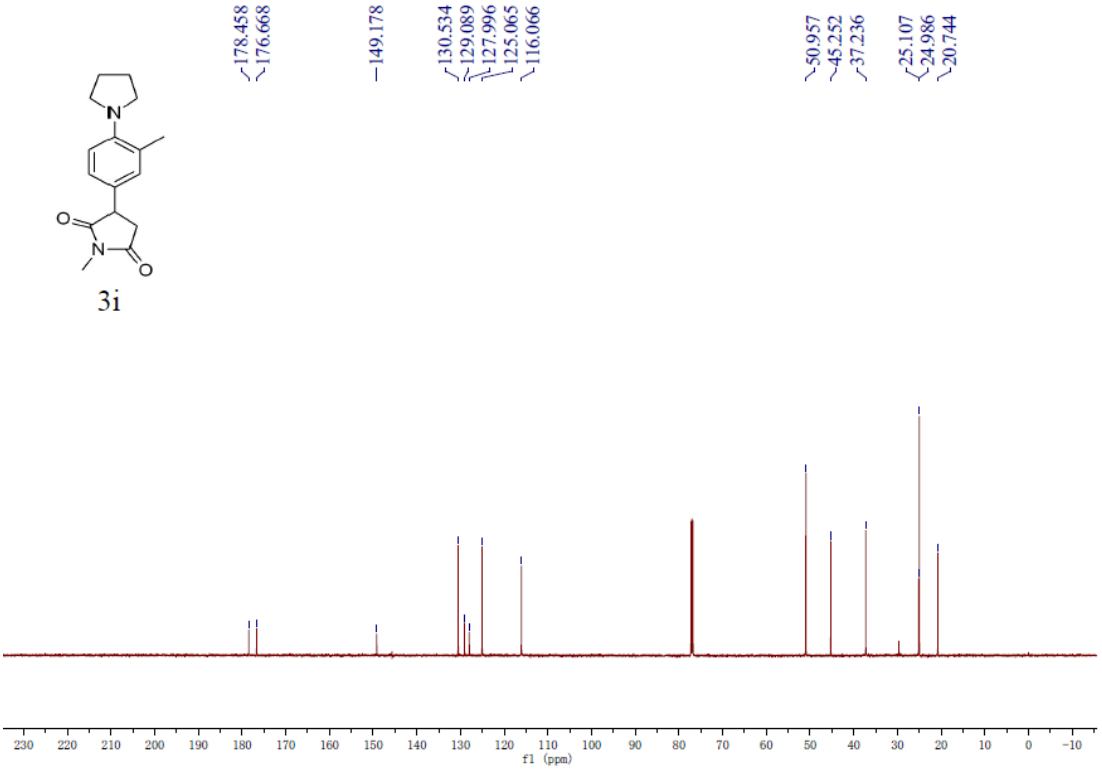
3.924
3.914
3.191
3.141
3.073
2.851
2.841
2.805
2.794
2.318
1.933
3i
1.97
1.01
1.00
5.03
2.95
1.03
3.06
4.08
f1 (ppm)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127.996
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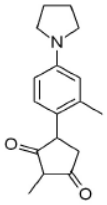
116.066
50.957
45.252
37.236
25.107
24.986
20.744
3i
f1 (ppm)



3j

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6.394
6.362
4.153
4.142
4.130
4.119
3.249
3.195
3.171
3.148
3.125
3.067
3.026
2.696
2.686
2.651
2.640
2.309
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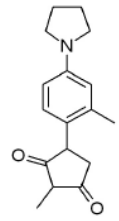
0.96
2.03
1.00
3.34
1.03
2.95
1.05
3.06
4.05
f1 (ppm)



3j

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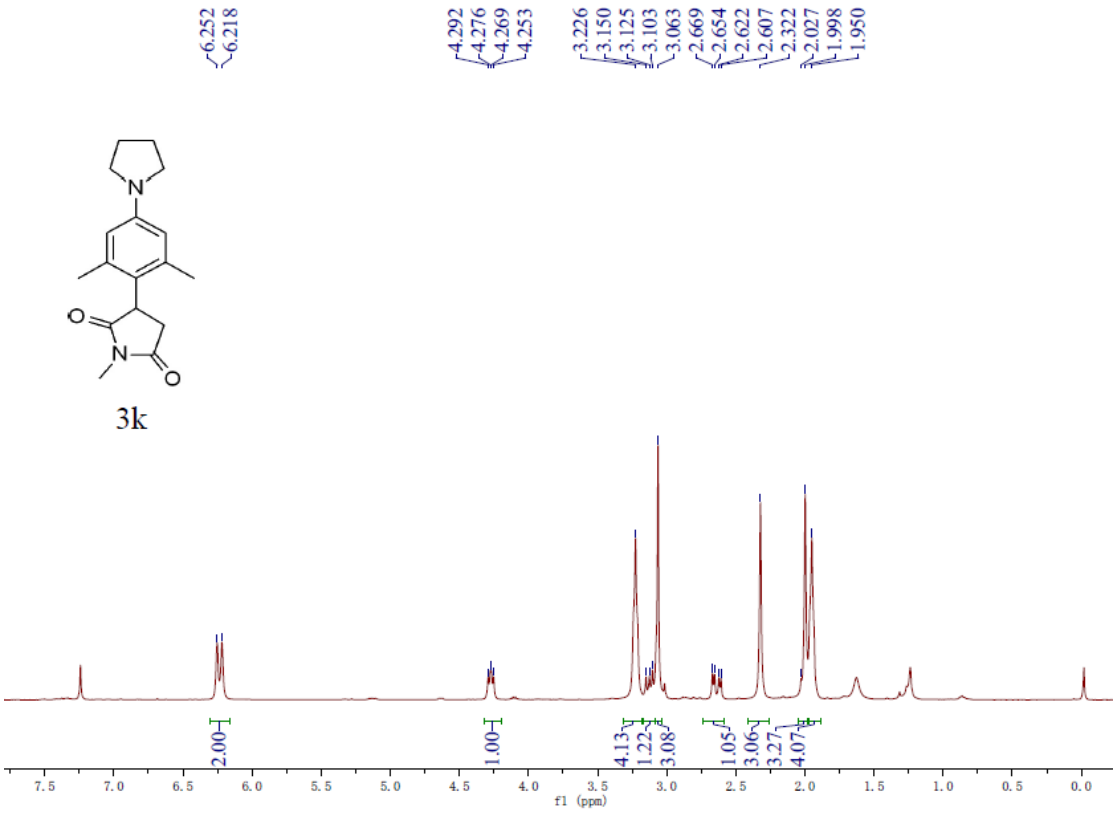
20.253
f1 (ppm)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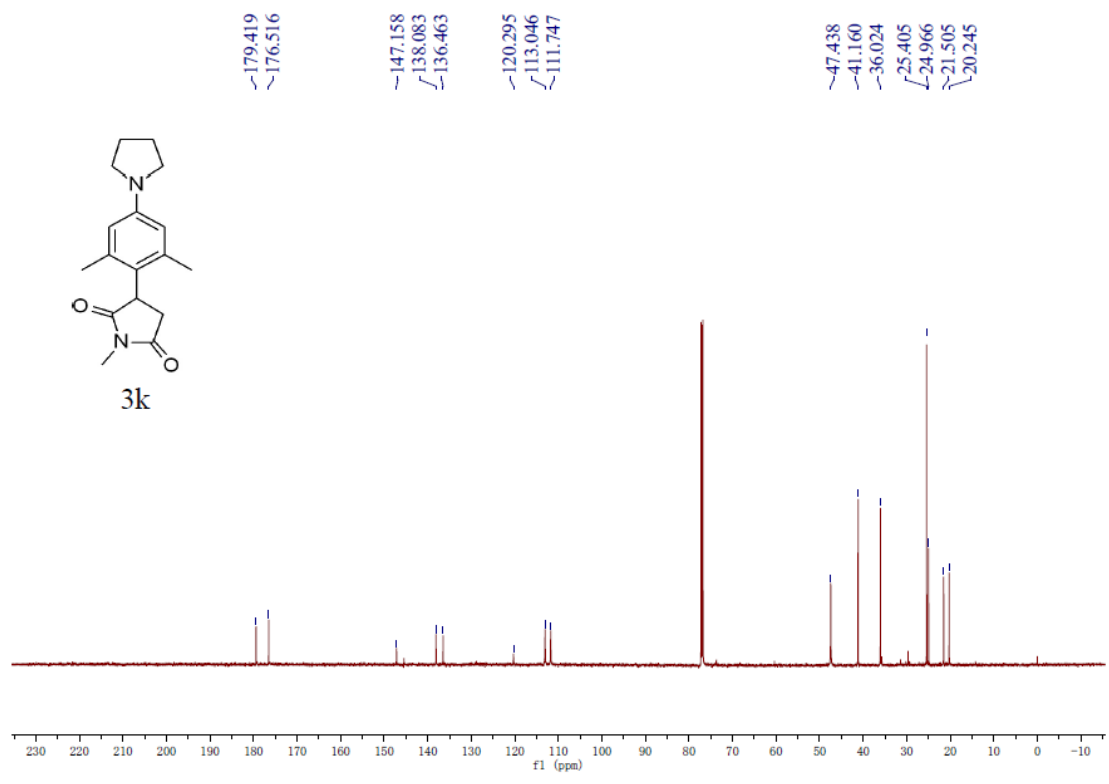
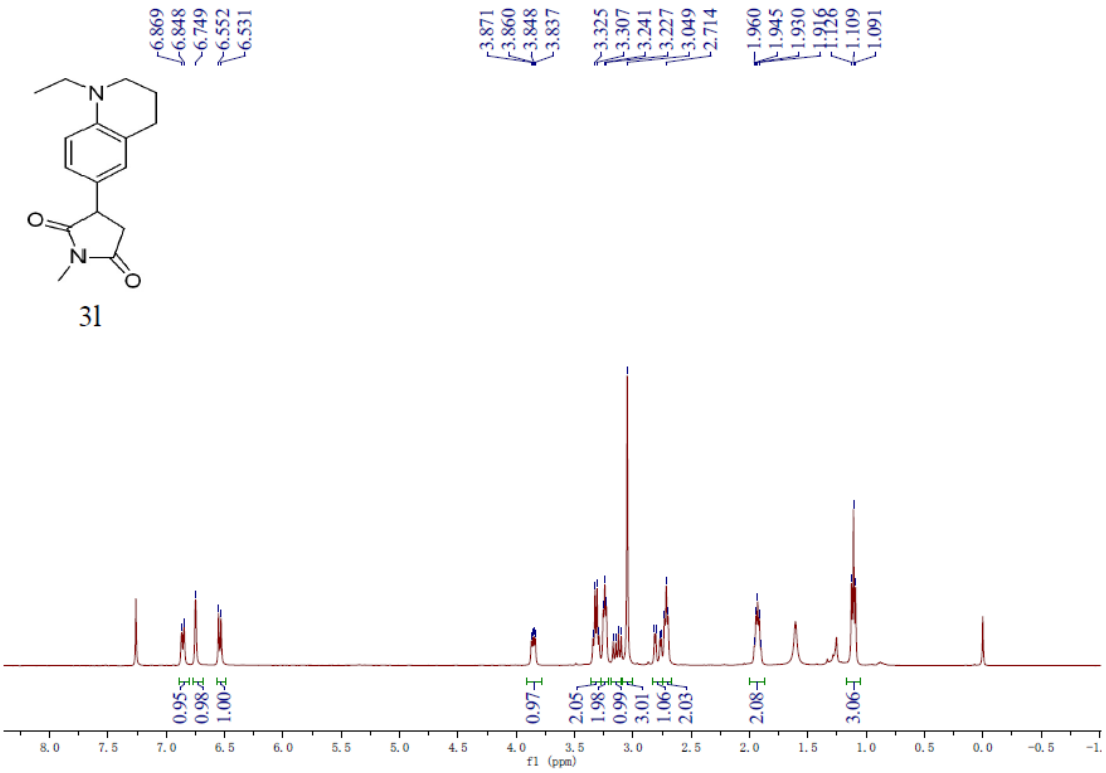
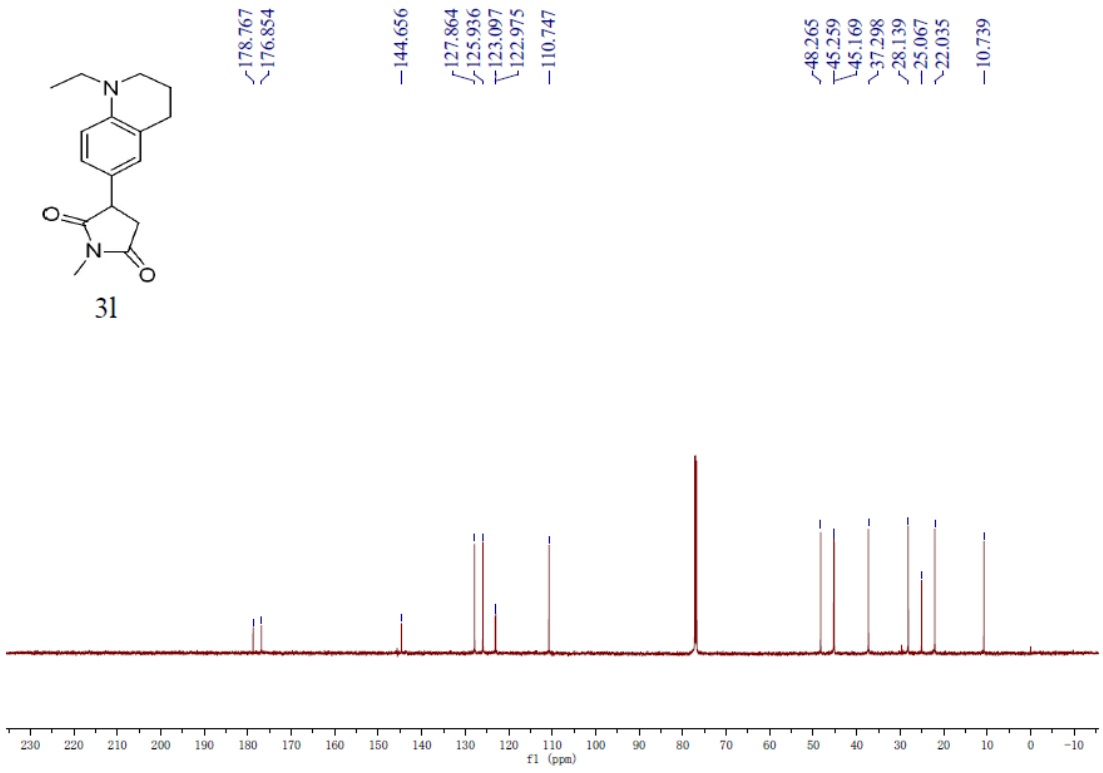
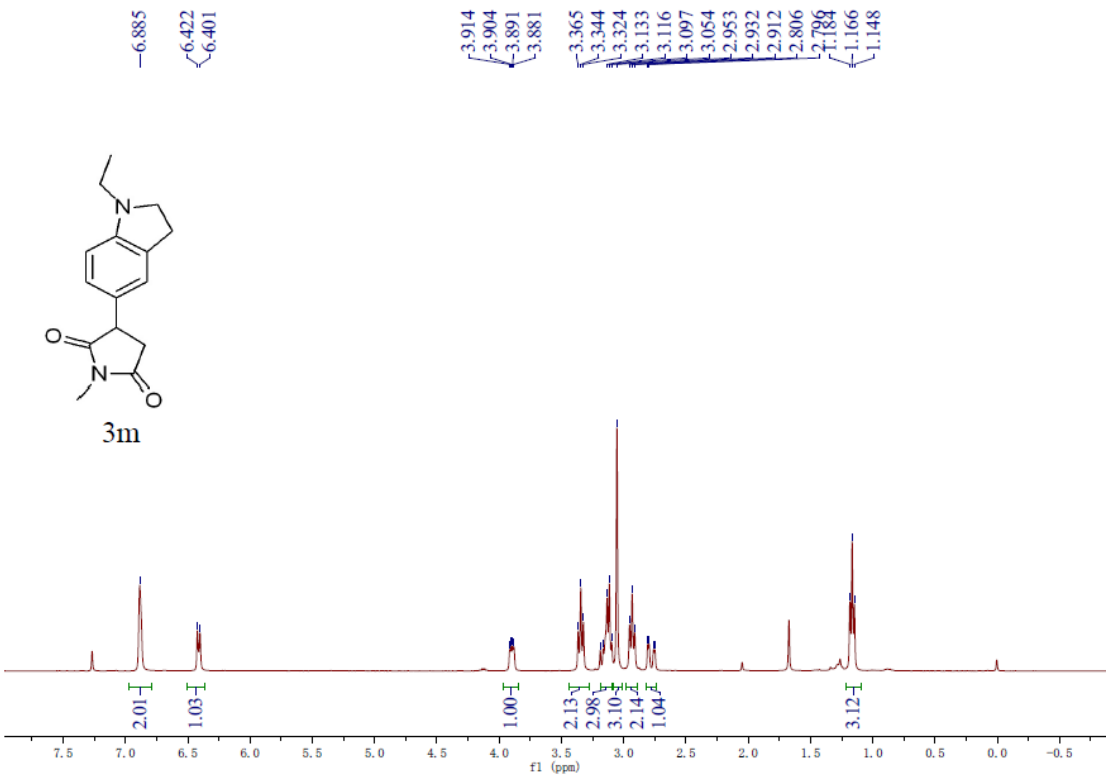
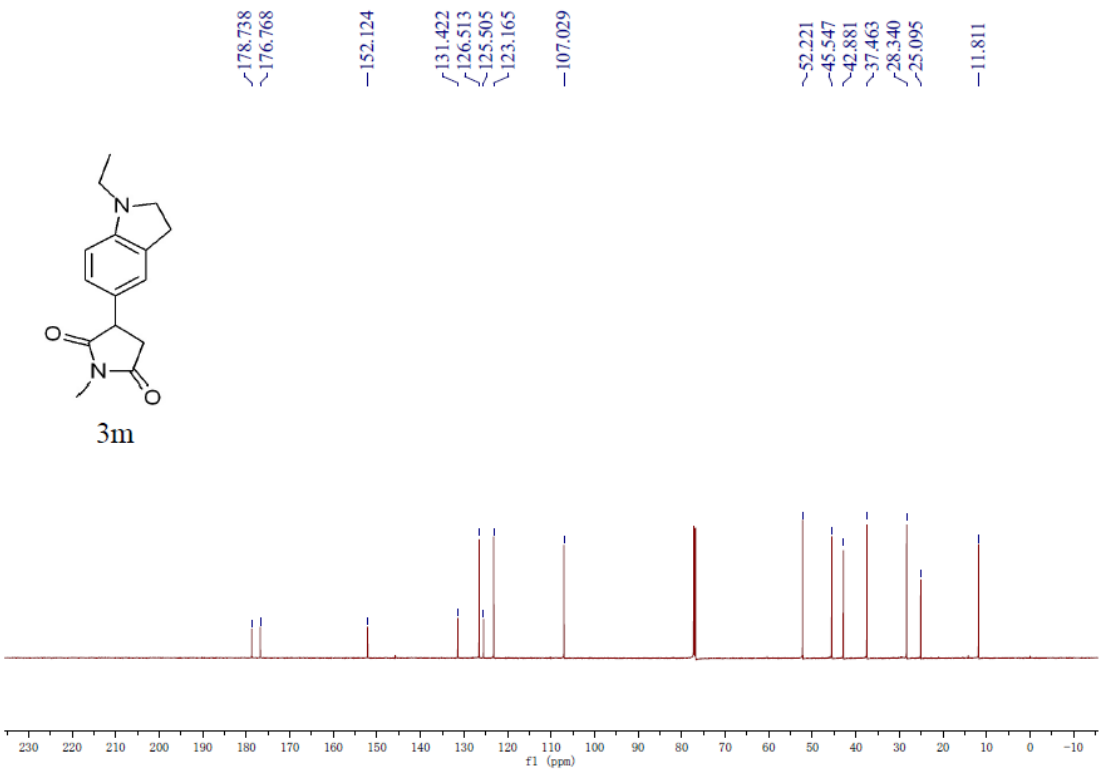
2.622
2.607
2.322
2.027
1.998
1.950
3k
2.00
1.00
4.13
1.22
3.08
1.05
3.06
3.27
4.07
f1 (ppm)

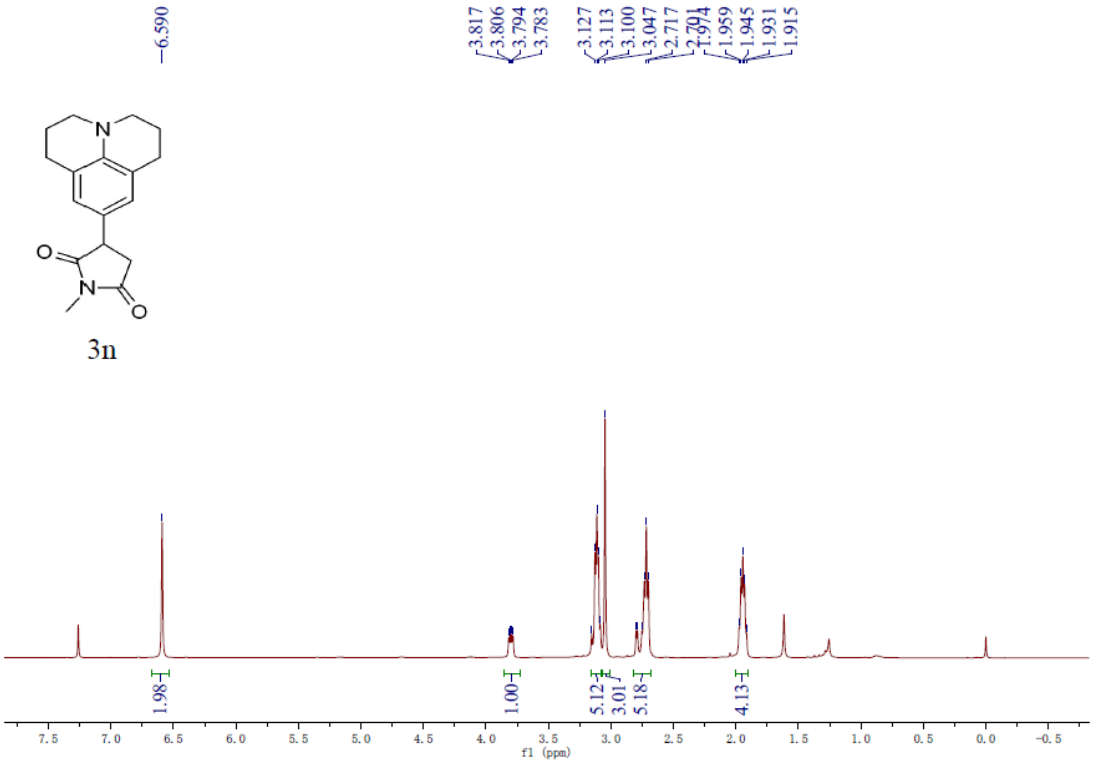

179.419
176.516
147.158
138.083
136.463
120.295
113.046
111.747
47.438
41.160
36.024
25.405
24.966
21.505
20.245
3k
f1 (ppm)


6.869
6.848
6.749
6.552
6.531
3.871
3.860
3.848
3.837
3.325
3.307
3.241
3.227
3.049
2.714
1.960
1.945
1.930
1.916
1.126
1.109
1.091
31
0.95
0.98
1.00
0.97
2.05
1.98
0.99
3.01
1.06
2.03
2.08
3.06
f1 (ppm)

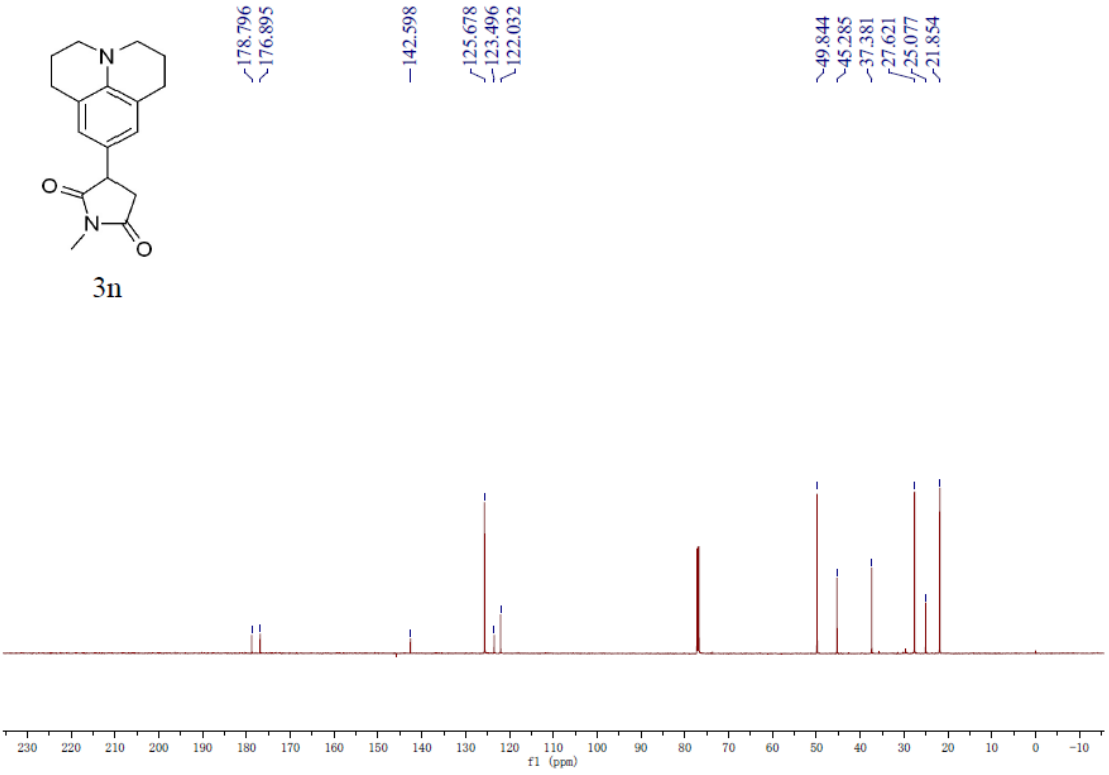

178.767
176.854
144.656
127.864
125.936
123.097
122.975
110.747
48.265
45.259
45.169
37.298
28.139
25.067
22.035
10.739
31
f1 (ppm)


6.885
6.422
6.401
3.914
3.904
3.891
3.881
3.365
3.344
3.324
3.133
3.116
3.097
3.054
2.953
2.932
2.912
2.806
2.796
1.184
1.166
1.148
3m
2.01
1.03
1.00
2.13
2.98
3.10
2.14
1.04
3.12
f1 (ppm)

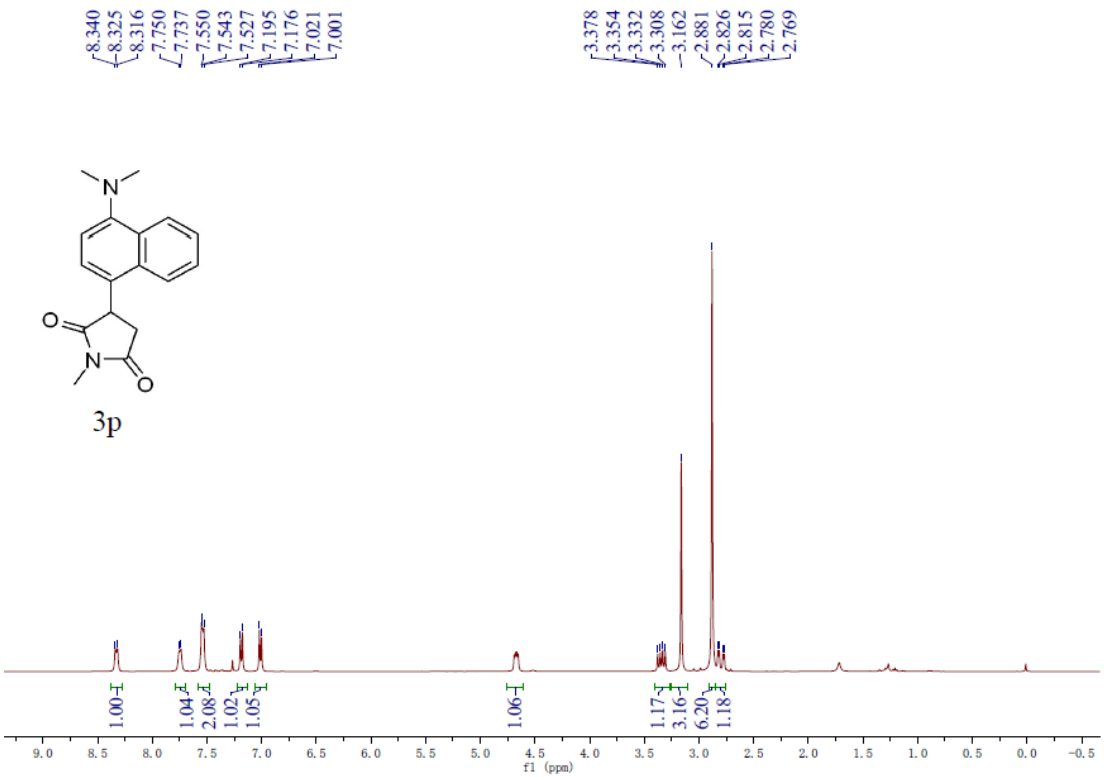

178.738
176.768
152.124
131.422
126.513
125.505
123.165
107.029
52.221
45.547
42.881
37.463
28.340
25.095
11.811
3m
f1 (ppm)

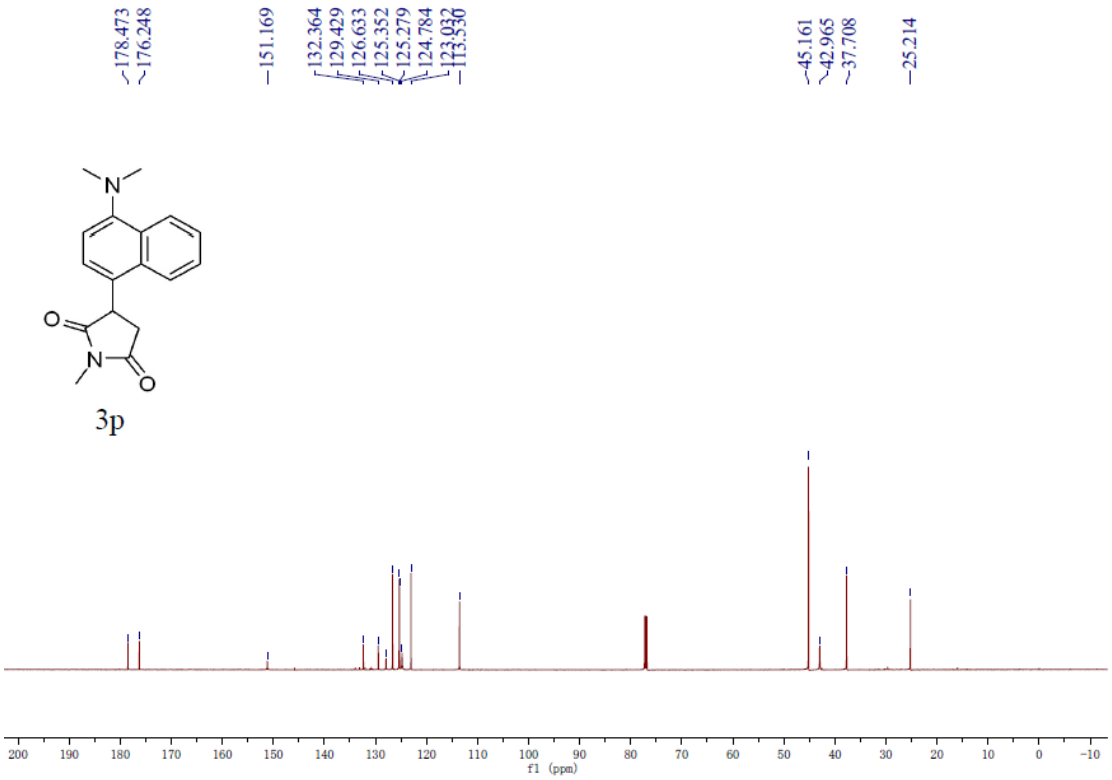

6.590
3.817
3.806
3.794
3.783
3.127
3.113
3.100
3.047
2.717
1.974
1.959
1.945
1.931
1.915
1.98
1.00
5.12
3.01
5.18
4.13
f1 (ppm)

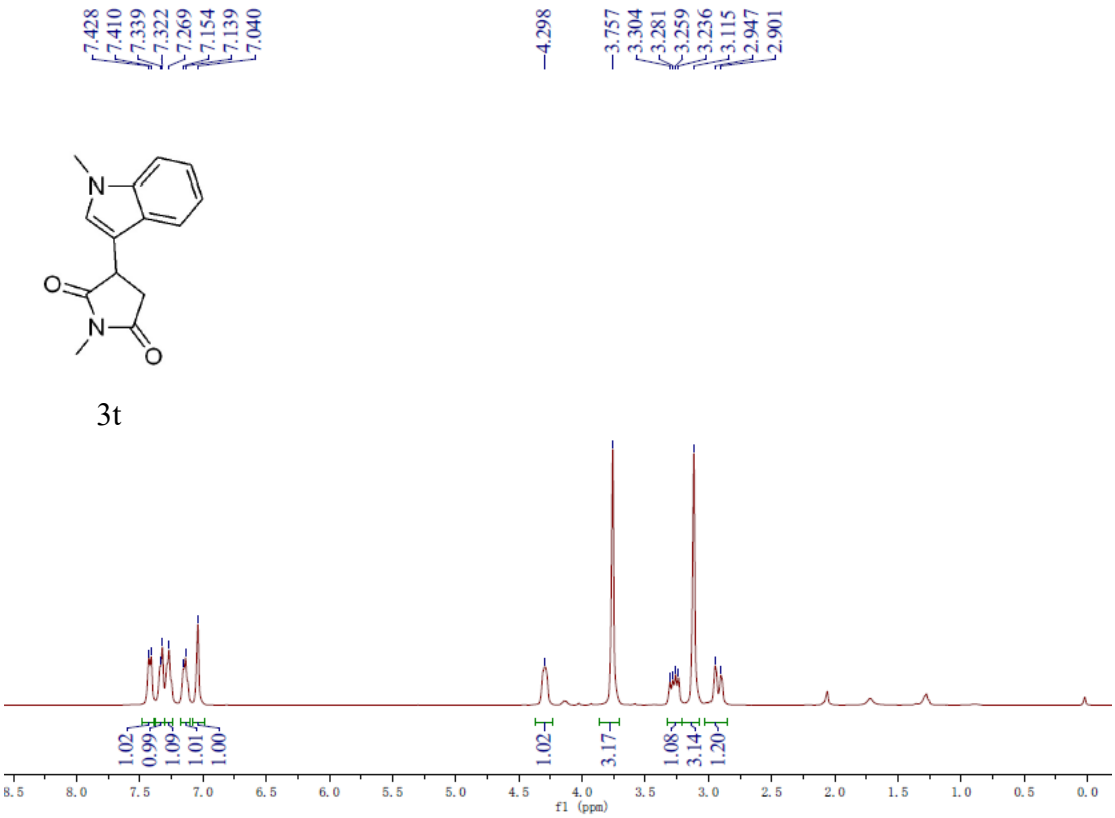
3n


178.796
176.895
142.598
125.678
123.496
122.032
49.844
45.285
37.381
27.621
25.077
21.854
f1 (ppm)

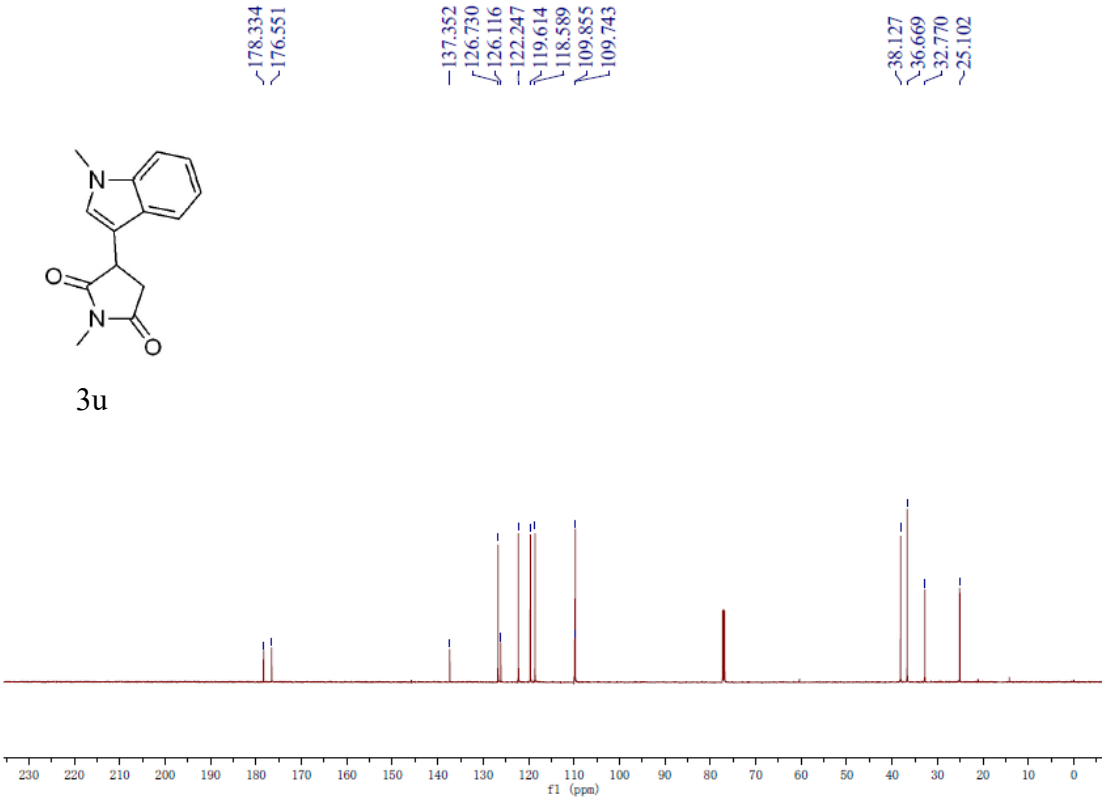
3n

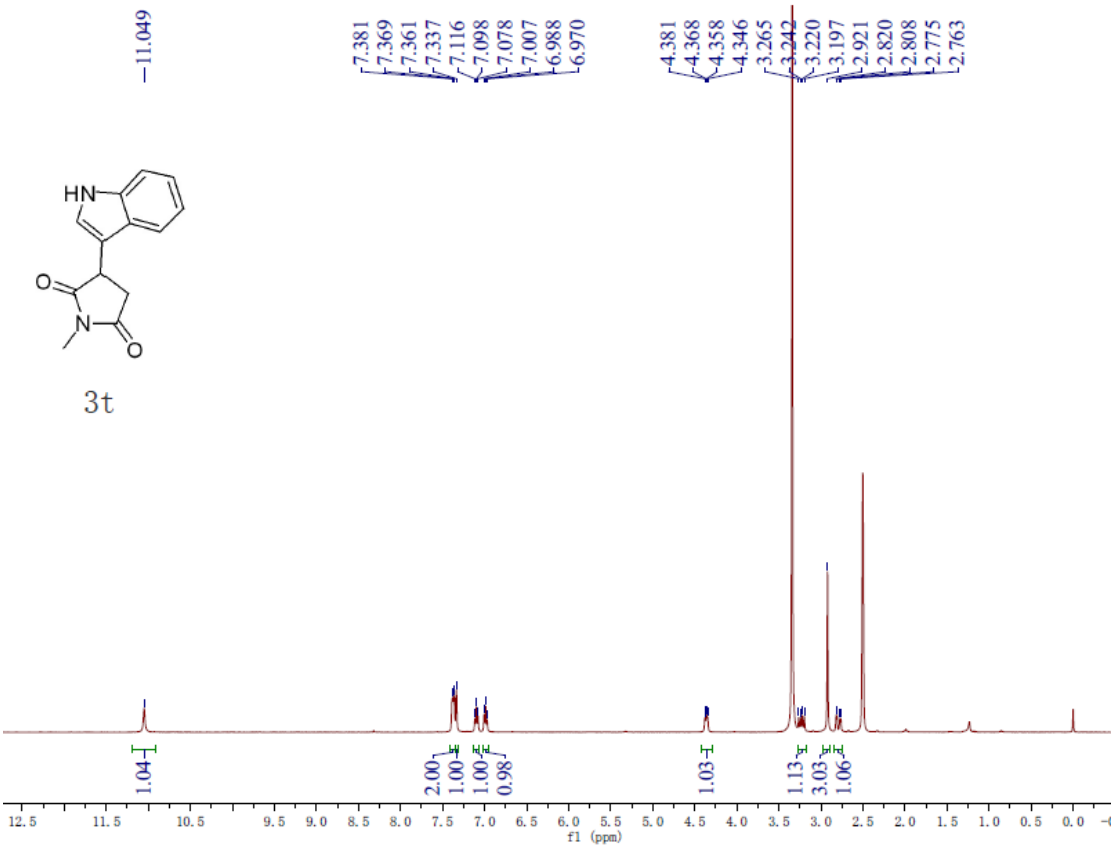

8.340
8.325
8.316
7.750
7.737
7.550
7.543
7.527
7.195
7.176
7.021
7.001
3.378
3.354
3.332
3.308
3.162
2.881
2.826
2.815
2.780
2.769
3p
1.00
1.04
2.08
1.02
1.05
1.06
1.17
3.16
6.20
1.18
f1 (ppm)

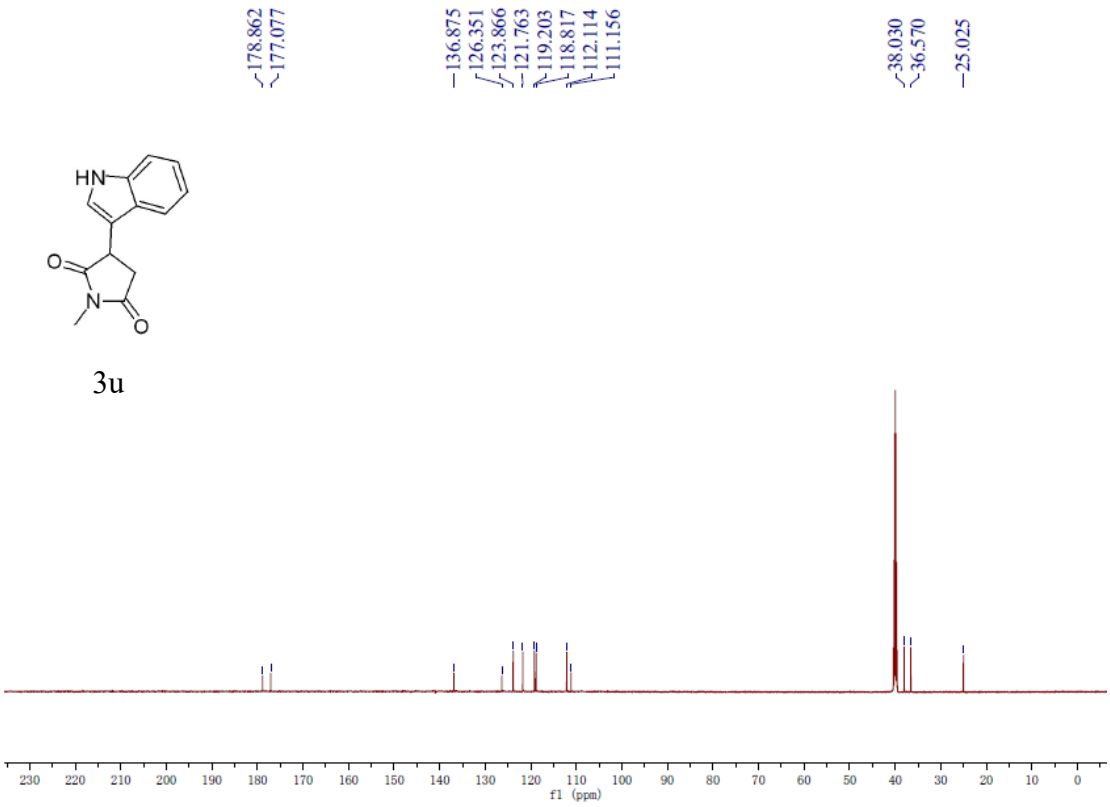

178.473
176.248
151.169
132.364
129.429
126.633
125.352
125.279
124.784
123.032
113.530
45.161
42.965
37.708
25.214
3p
f1 (ppm)


7.428
7.410
7.339
7.322
7.269
7.154
7.139
7.040
4.298
3.757
3.304
3.281
3.259
3.236
3.115
2.947
2.901
N
O
N
O
1.02
0.99
1.09
1.01
1.00
1.02
3.17
1.08
3.14
1.20
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

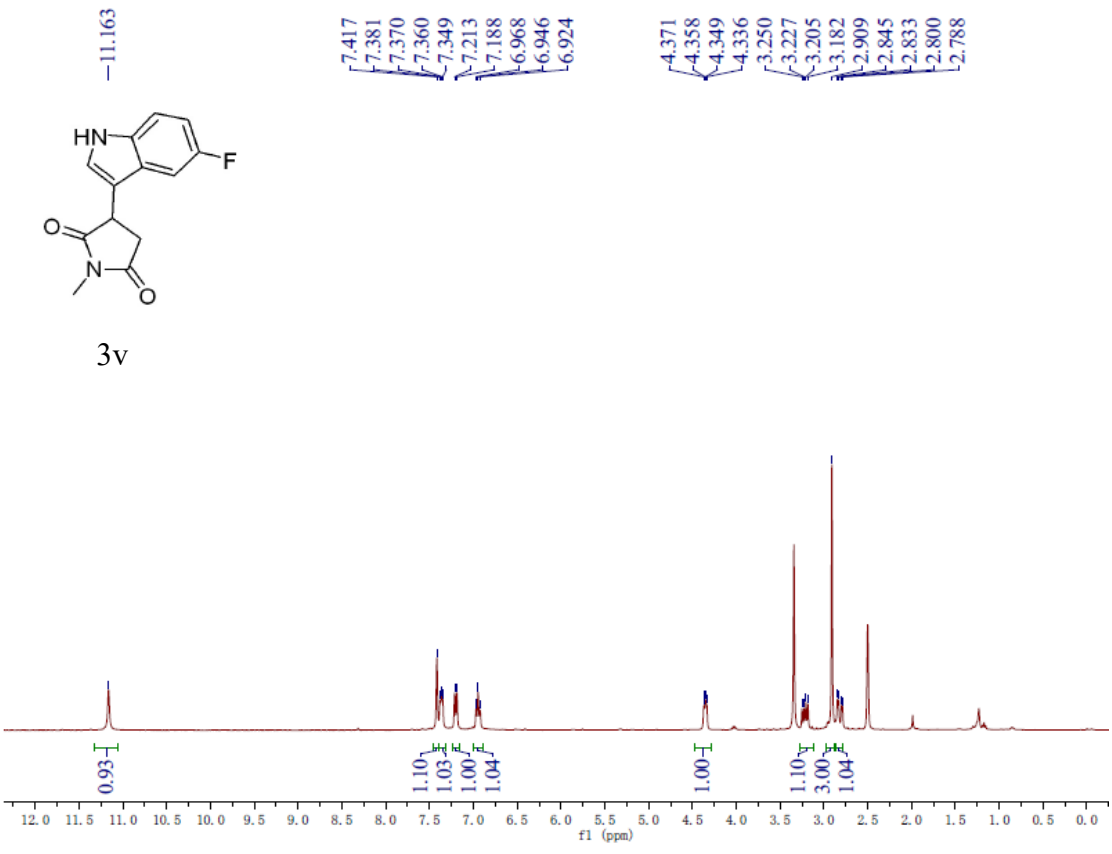
3t


178.334
176.551
137.352
126.730
126.116
122.247
119.614
118.589
109.855
109.743
38.127
36.669
32.770
25.102
N
O
N
O
3u
f1 (ppm)

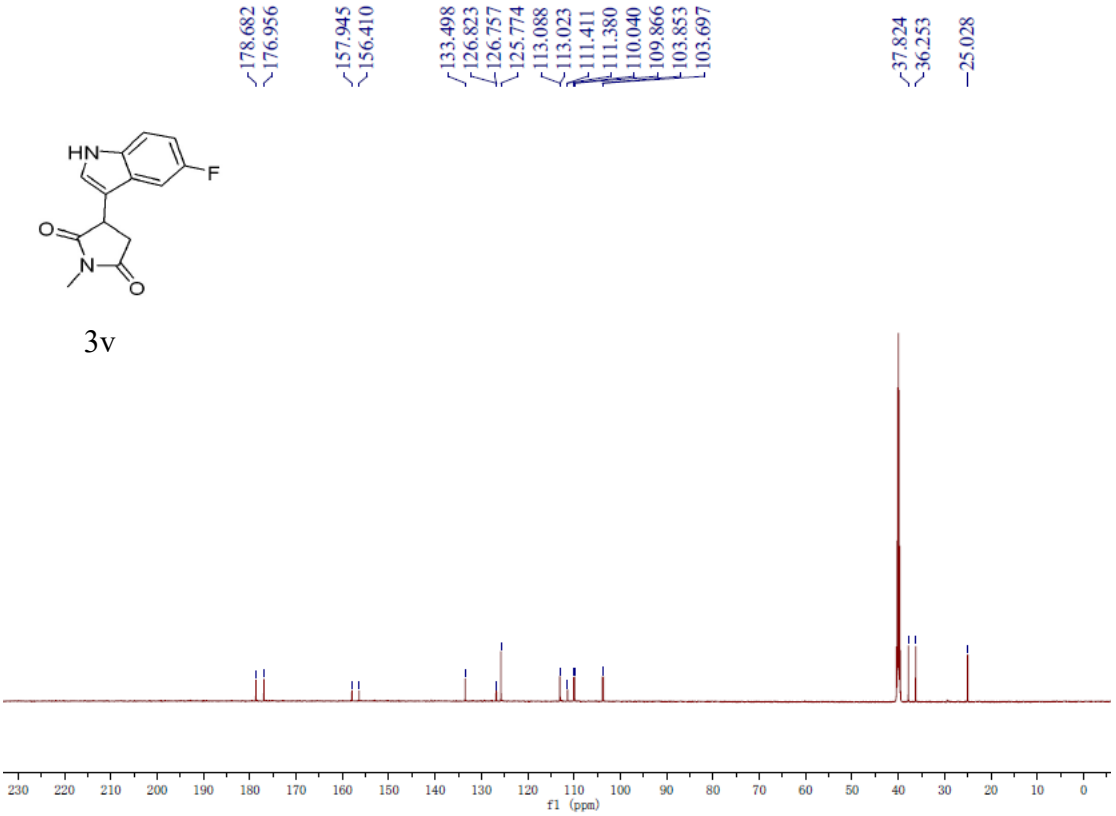

11.049
7.381
7.369
7.361
7.337
7.116
7.098
7.078
7.007
6.988
6.970
4.381
4.368
4.358
4.346
3.265
3.242
3.220
3.197
2.921
2.820
2.808
2.775
2.763
HN
O
N
O
3t
1.04
2.00
1.00
1.00
0.98
1.03
1.13
3.03
1.06
f1 (ppm)


178.862
177.077
136.875
126.351
123.866
121.763
119.203
118.817
112.114
111.156
38.030
36.570
25.025
HN
O
N
O
f1 (ppm)

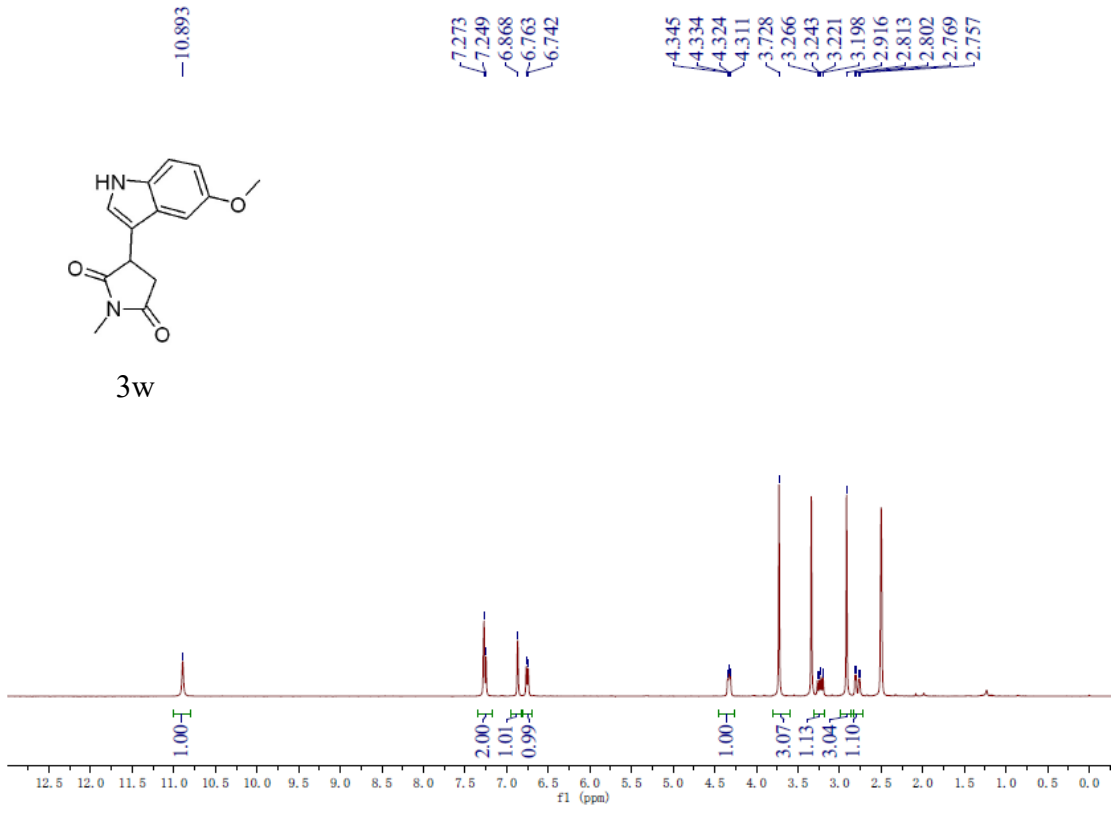
3u


11.163
7.417
7.381
7.370
7.360
7.349
7.213
7.188
6.968
6.946
6.924
4.371
4.358
4.349
4.336
3.250
3.227
3.205
3.182
2.909
2.845
2.833
2.800
2.788
HN
F
O
N
O
0.93
1.10
1.03
1.00
1.04
1.00
1.10
3.00
1.04
f1 (ppm)

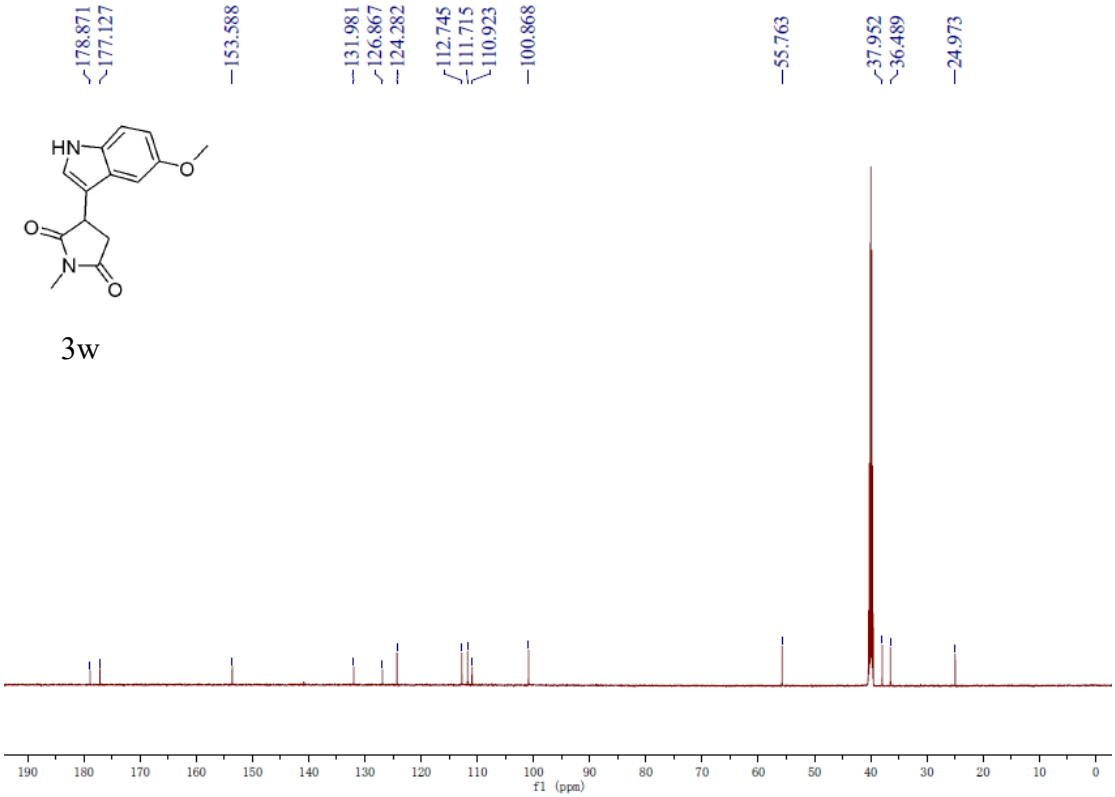
3v


178.682
176.956
157.945
156.410
133.498
126.823
126.757
125.774
113.088
113.023
111.411
111.380
110.040
109.866
103.853
103.697
37.824
36.253
25.028
HN
F
O
N
O
f1 (ppm)

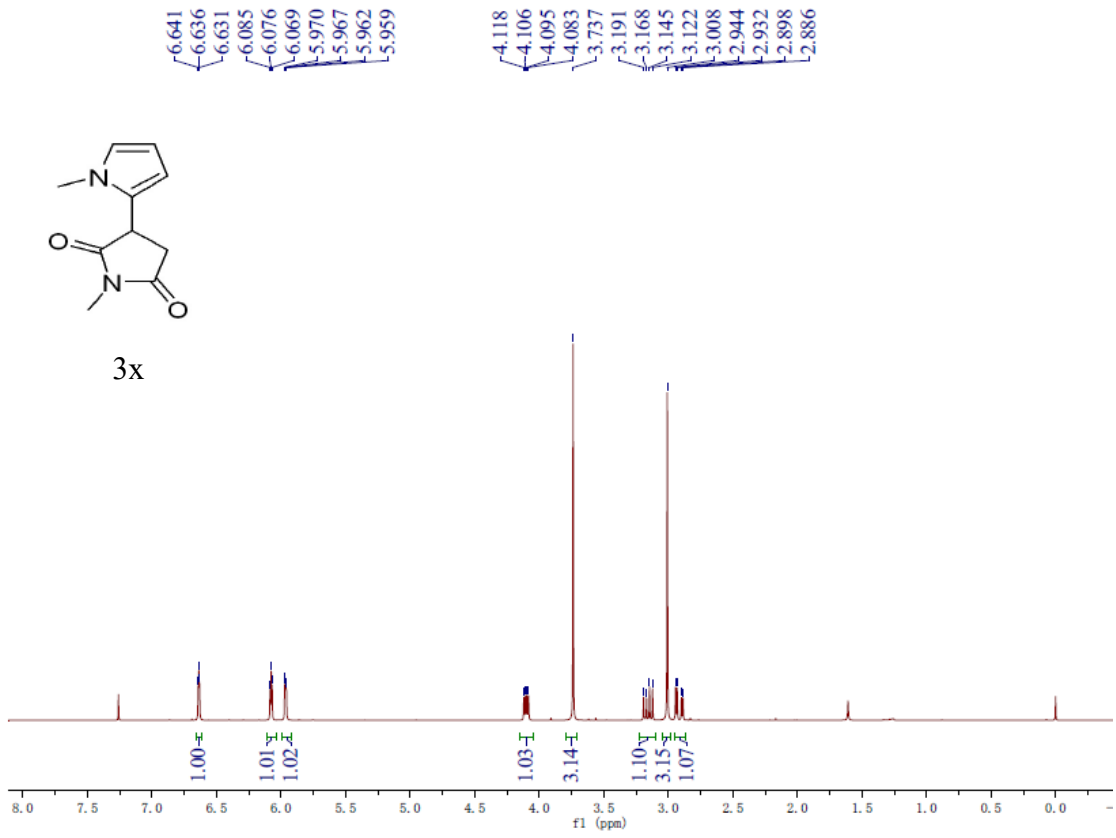
3v


10.893
7.273
7.249
6.868
6.763
6.742
4.345
4.334
4.324
4.311
3.728
3.266
3.243
3.221
3.198
2.916
2.813
2.802
2.769
2.757
HN
O
O
N
O
1.00
2.00
1.01
0.99
1.00
3.07
1.13
3.04
1.10
f1 (ppm)

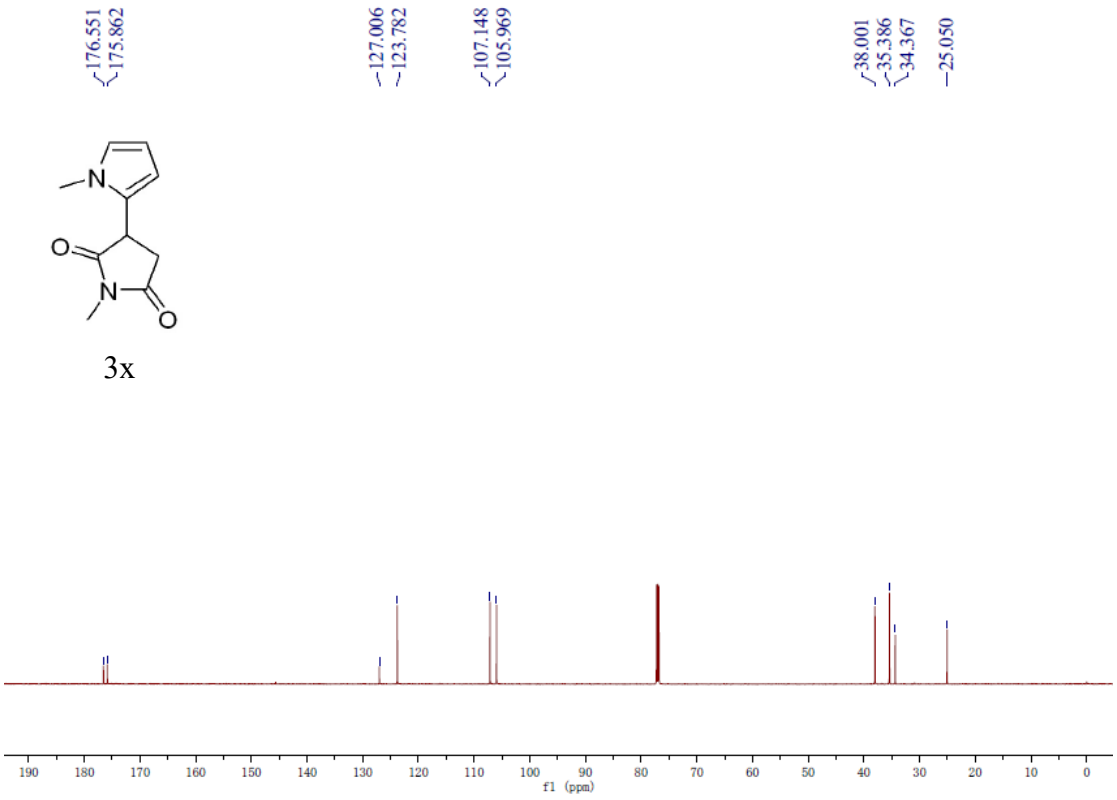
3w


178.871
177.127
153.588
131.981
126.867
124.282
112.745
111.715
110.923
100.868
55.763
37.952
36.489
24.973
HN
O
O
N
O
f1 (ppm)

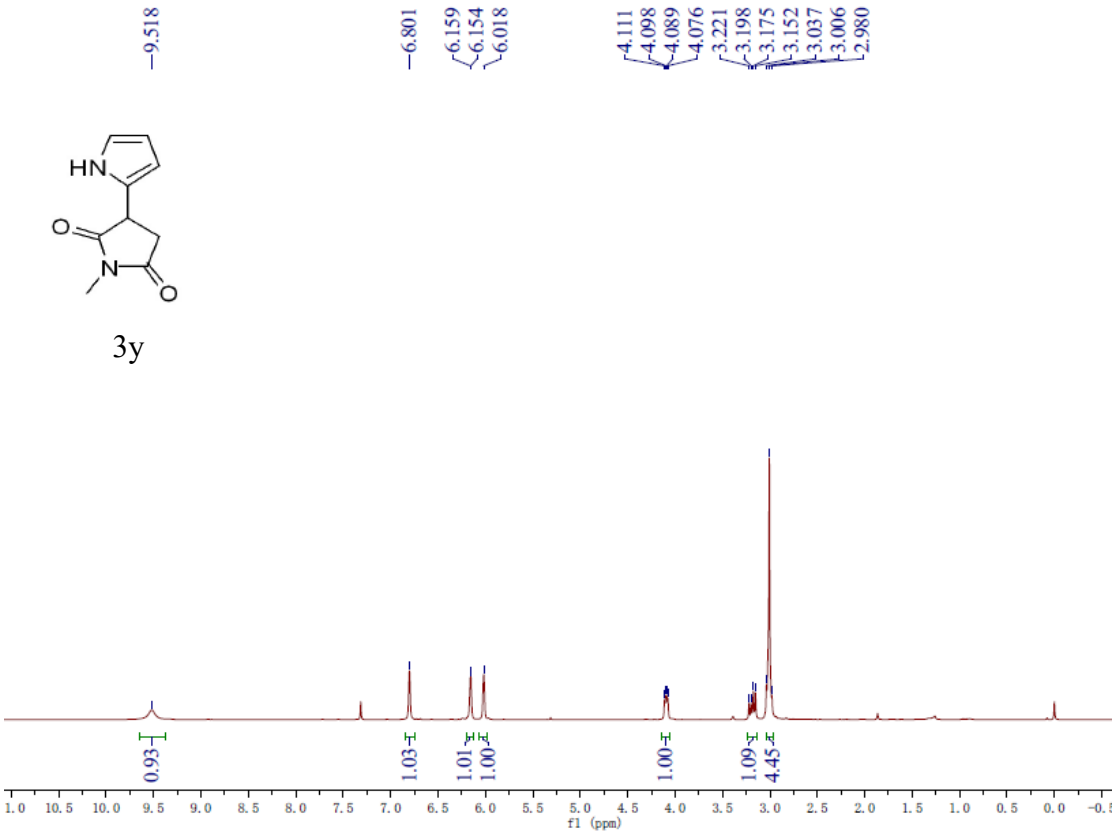
3w


6.641
6.636
6.631
6.085
6.076
6.069
5.970
5.967
5.962
5.959
4.118
4.106
4.095
4.083
3.737
3.191
3.168
3.145
3.122
3.008
2.944
2.932
2.898
2.886
N
O
N
O
1.00
1.01
1.02
1.03
3.14
1.10
3.15
1.07
f1 (ppm)

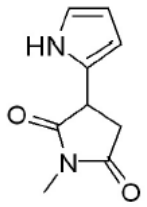
3x


176.551
175.862
127.006
123.782
107.148
105.969
38.001
35.386
34.367
25.050
O
N
O
N
O
f1 (ppm)

3x

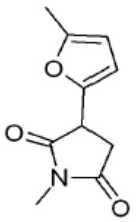

9.518
6.801
6.159
6.154
6.018
4.111
4.098
4.089
4.076
3.221
3.198
3.175
3.152
3.037
3.006
2.980
HN
O
N
O
0.93
1.03
1.01
1.00
1.00
1.09
4.45
f1 (ppm)

3y


HN
O
N
O

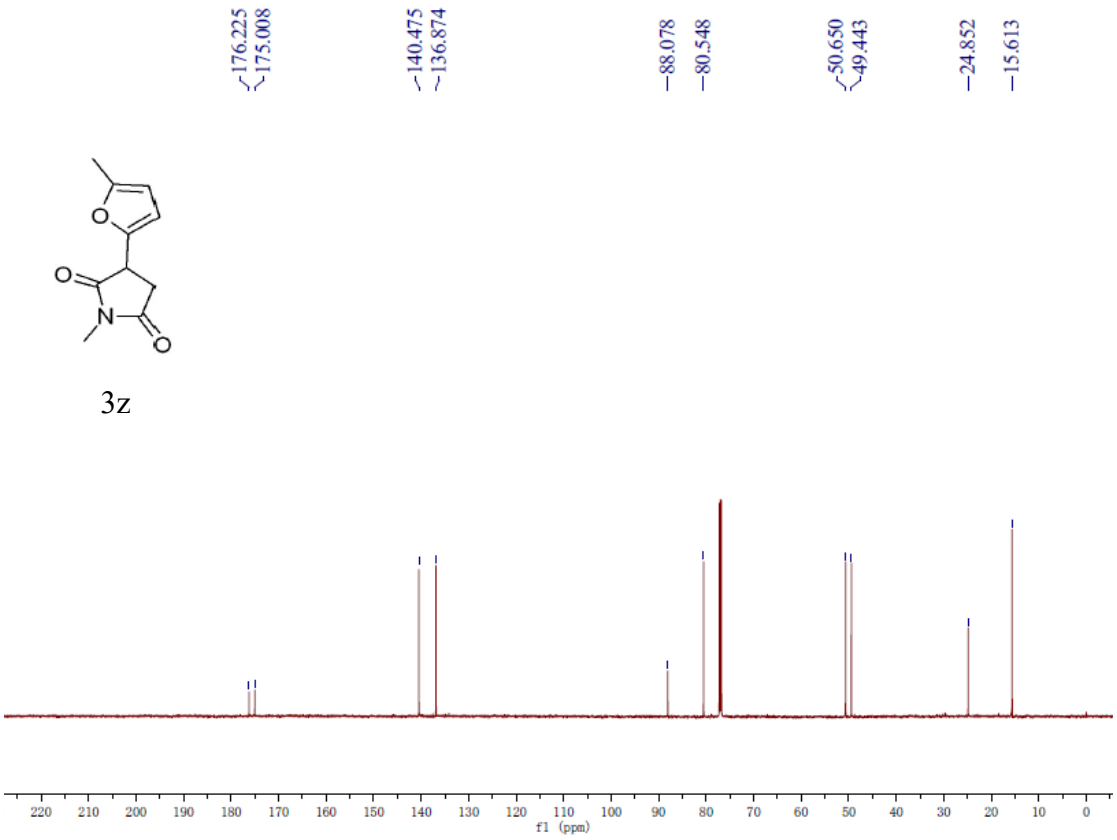
3y

177.836
176.336
125.307
118.820
108.151
105.451
38.662
34.343
24.917
f1 (ppm)

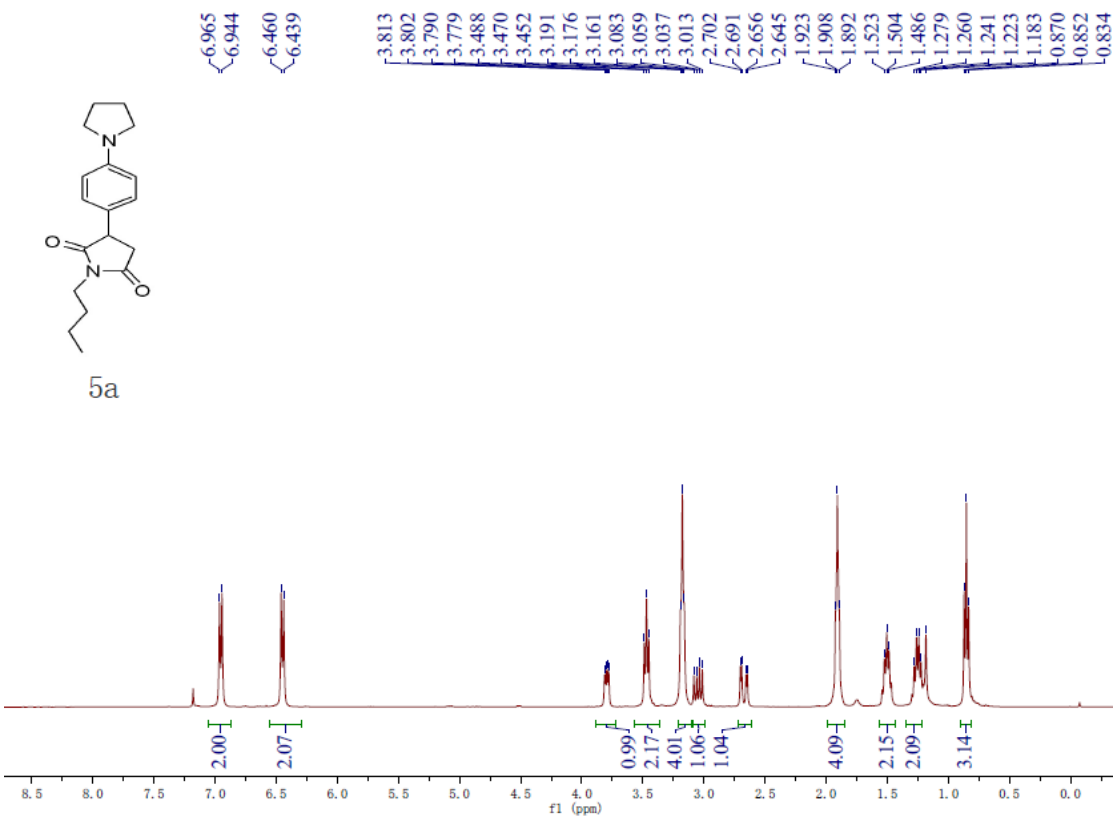

O
O
N
O

3z

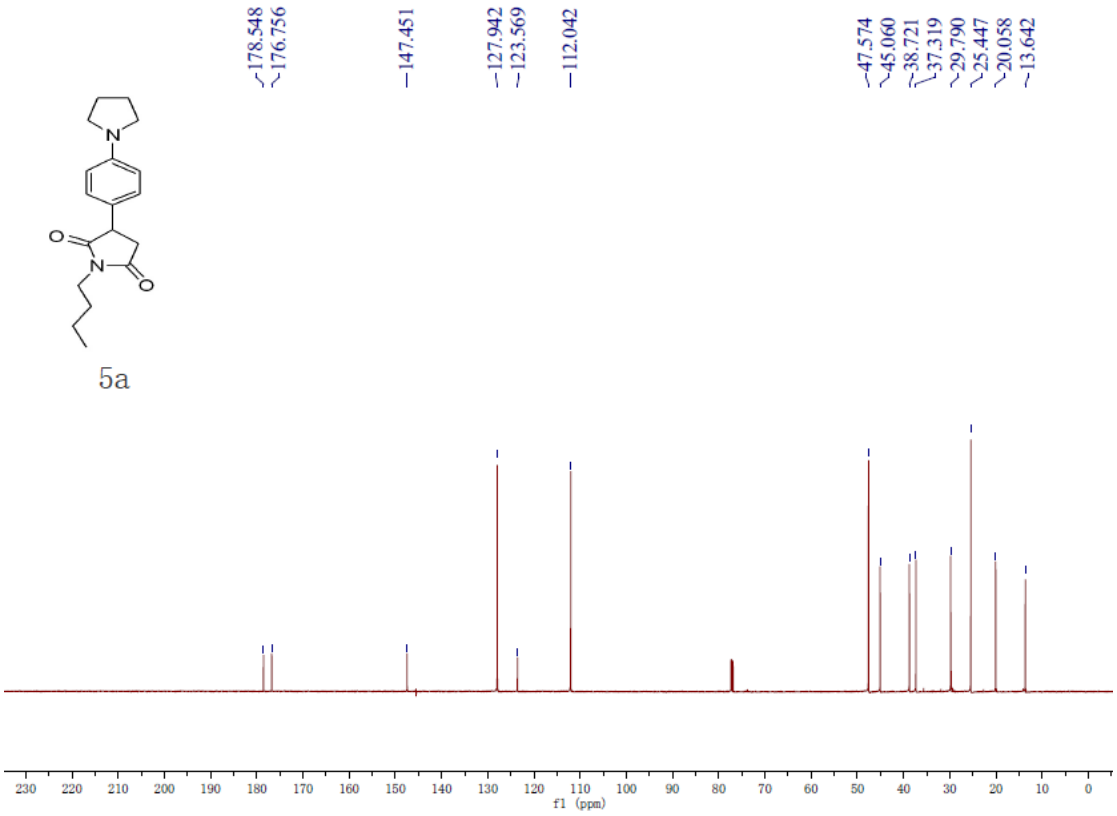
6.508
6.497
6.315
6.302
5.181
2.969
2.727
2.712
1.731
1.00
0.97
0.99
4.05
0.97
3.22
f1 (ppm)

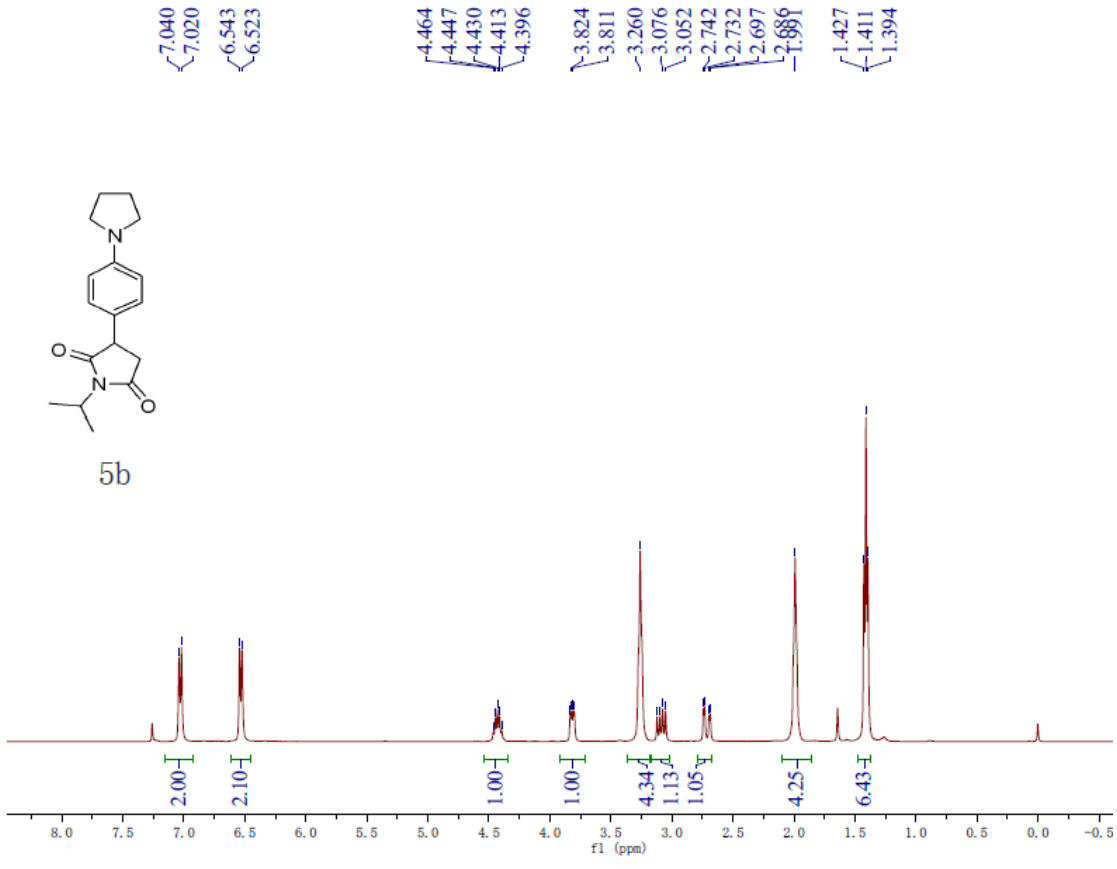

176.225
175.008
140.475
136.874
88.078
80.548
50.650
49.443
24.852
15.613
O
O
N
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

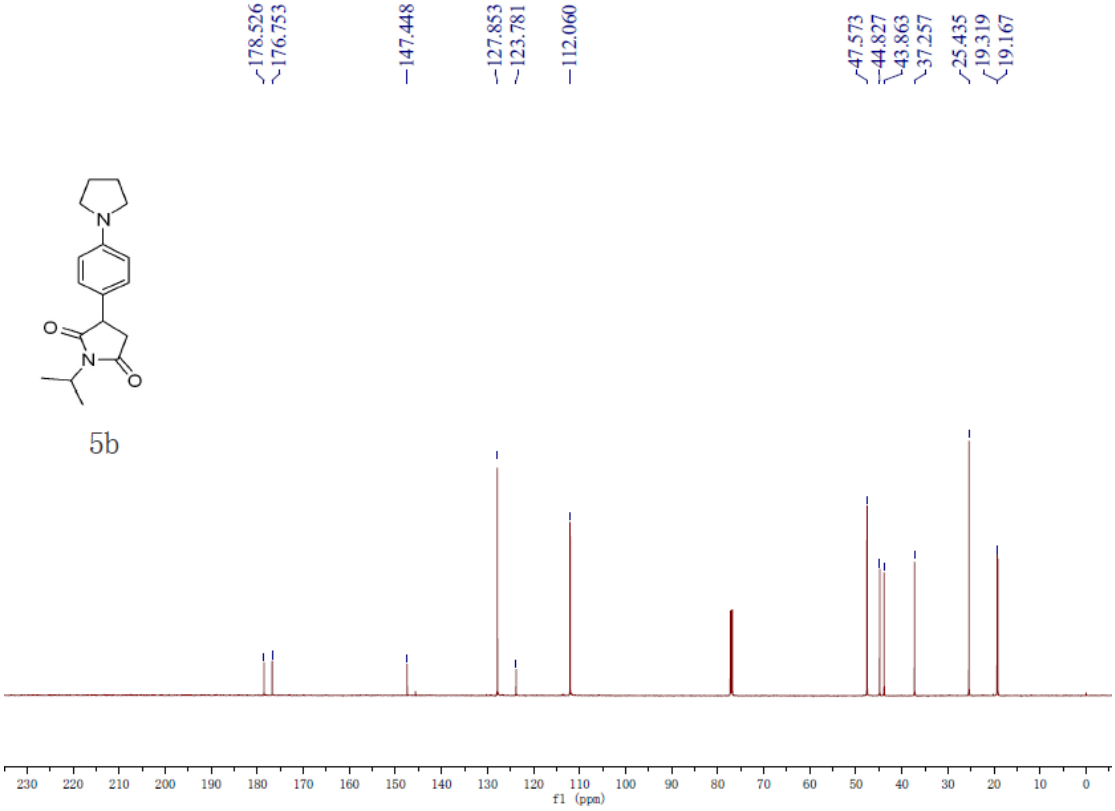
3z

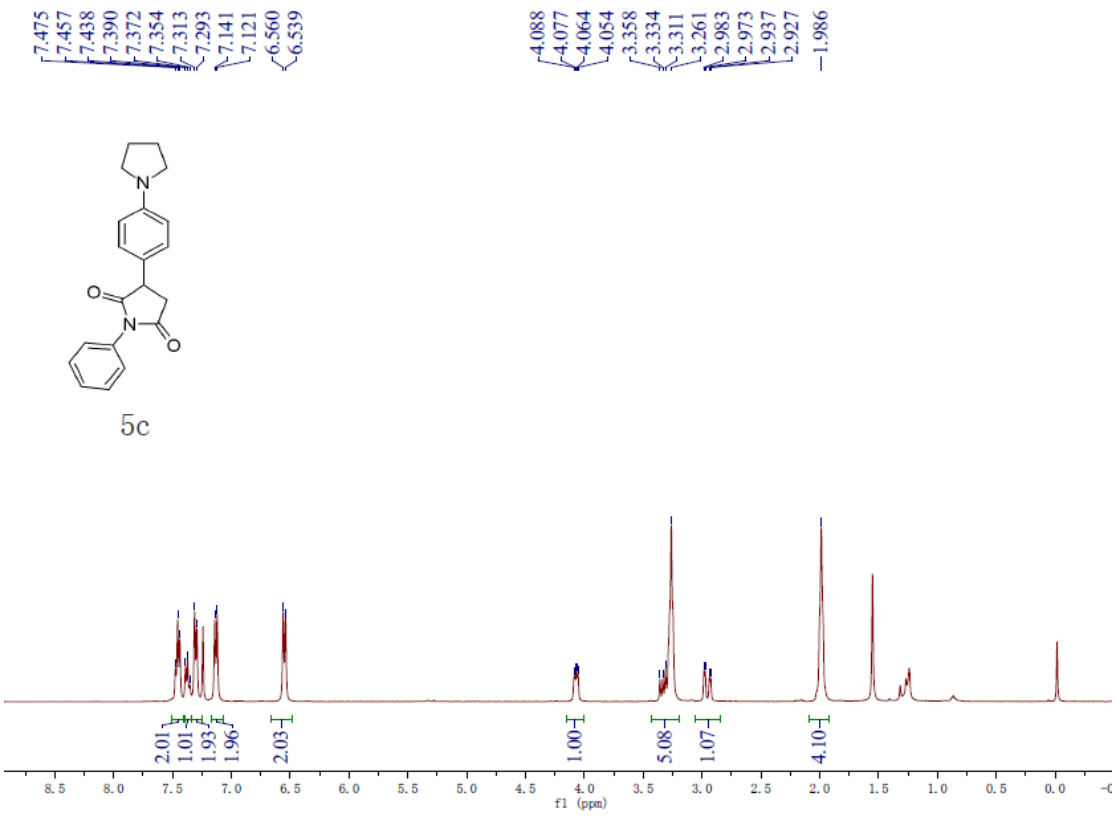

6.965
6.944
6.460
6.439
3.813
3.802
3.790
3.779
3.488
3.470
3.452
3.191
3.176
3.161
3.083
3.059
3.037
3.013
2.702
2.691
2.656
2.645
1.923
1.908
1.892
1.523
1.504
1.486
1.279
1.260
1.241
1.223
1.183
0.870
0.852
0.834
N
O
N
O
2.00
2.07
0.99
2.17
4.01
1.06
1.04
4.09
2.15
2.09
3.14
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

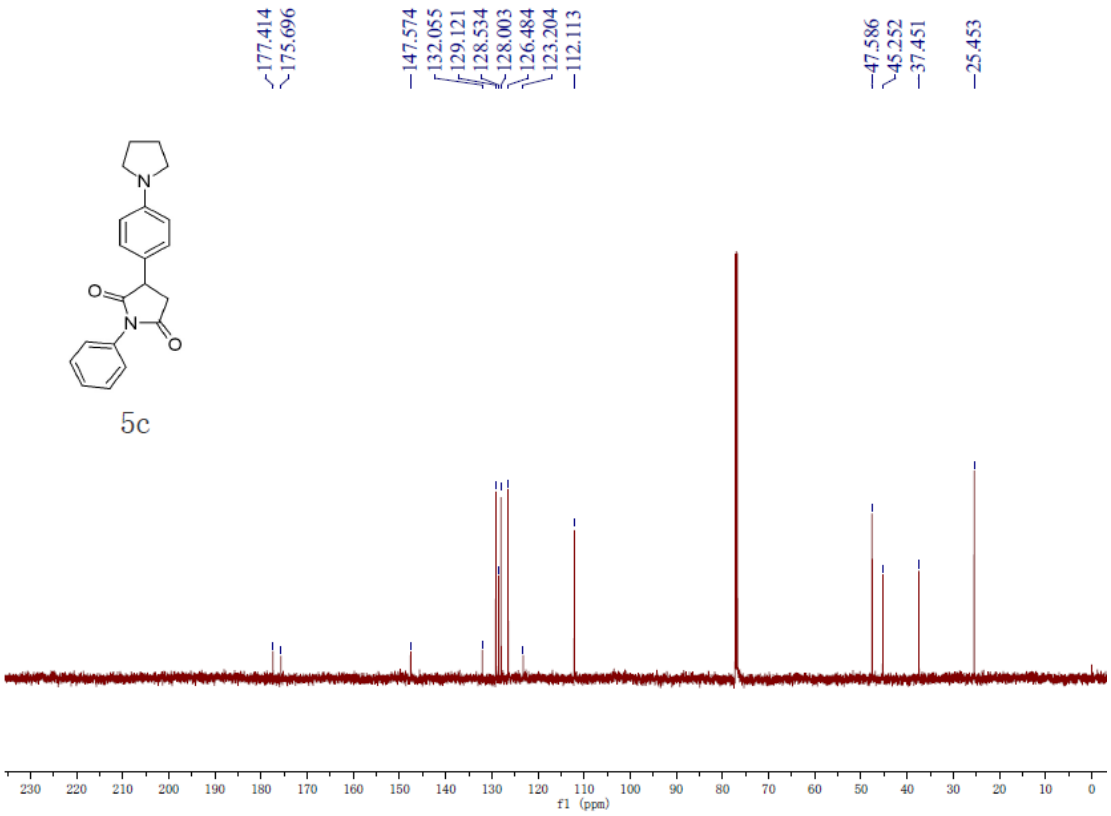
5a

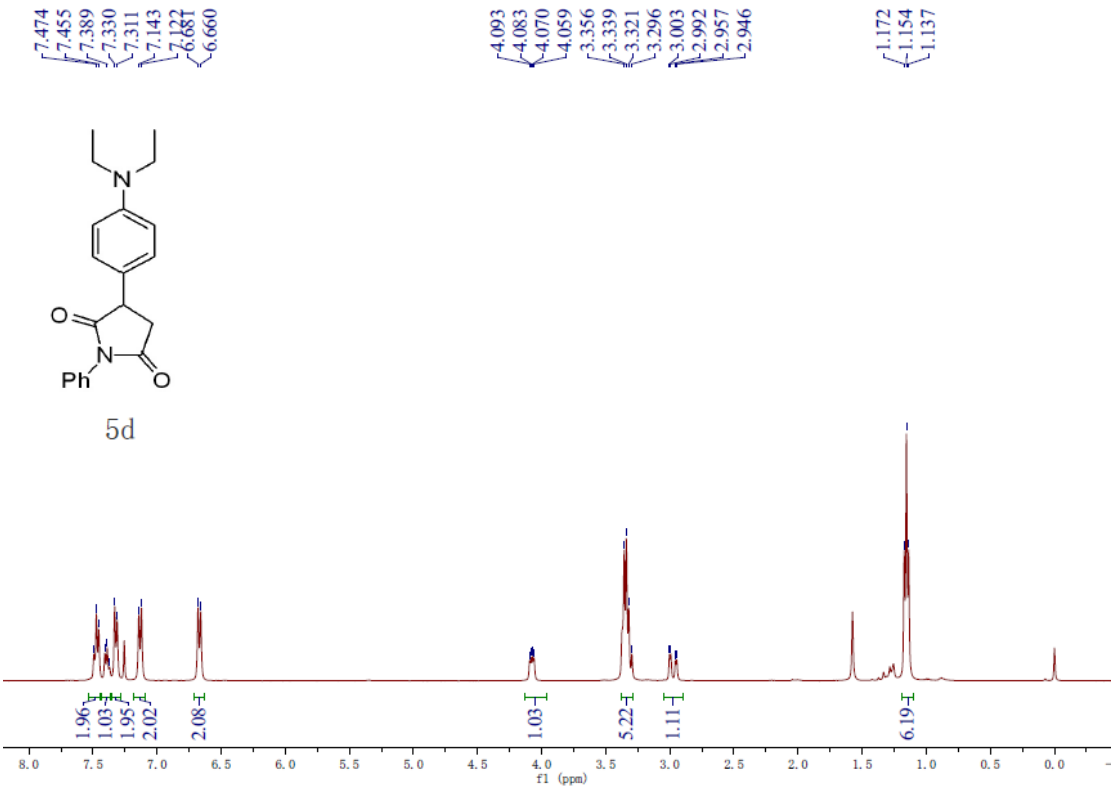

178.548
176.756
147.451
127.942
123.569
112.042
47.574
45.060
38.721
37.319
29.790
25.447
20.058
13.642
5a
f1 (ppm)

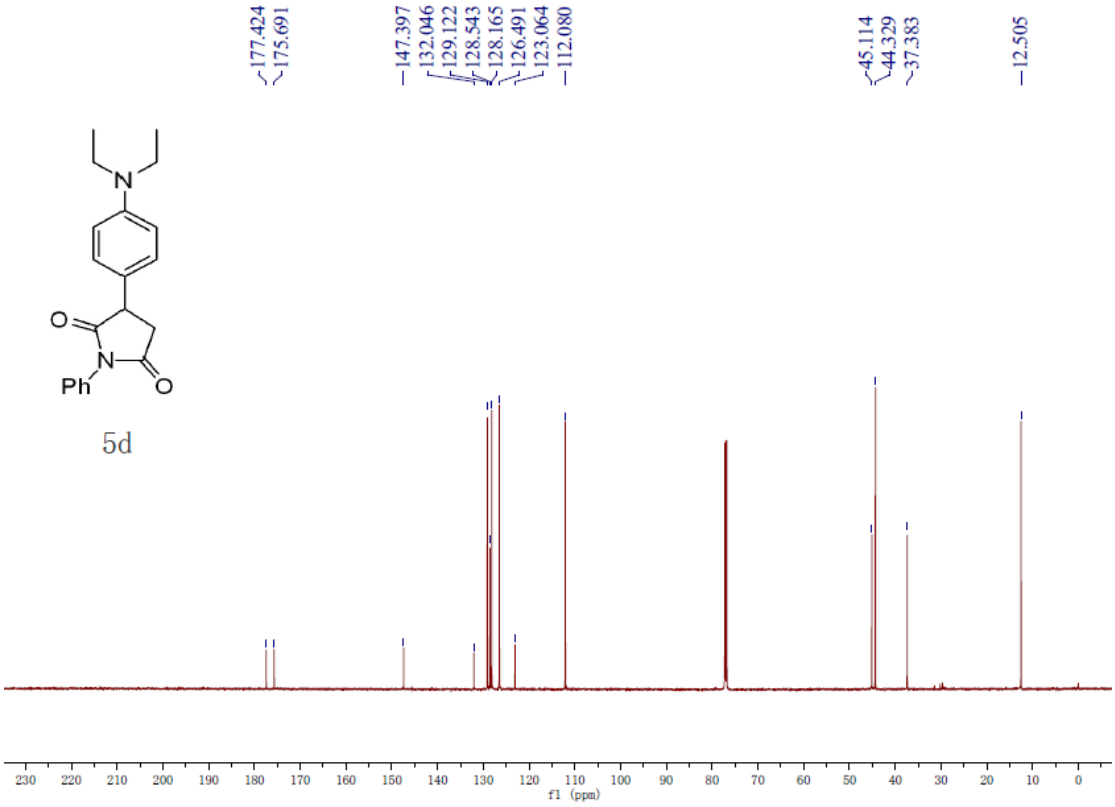

7.040
7.020
6.543
6.523
4.464
4.447
4.430
4.413
4.396
3.824
3.811
3.260
3.076
3.052
2.742
2.732
2.697
1.427
1.411
1.394
5b
2.00
2.10
1.00
1.00
4.34
1.13
1.05
4.25
6.43
f1 (ppm)

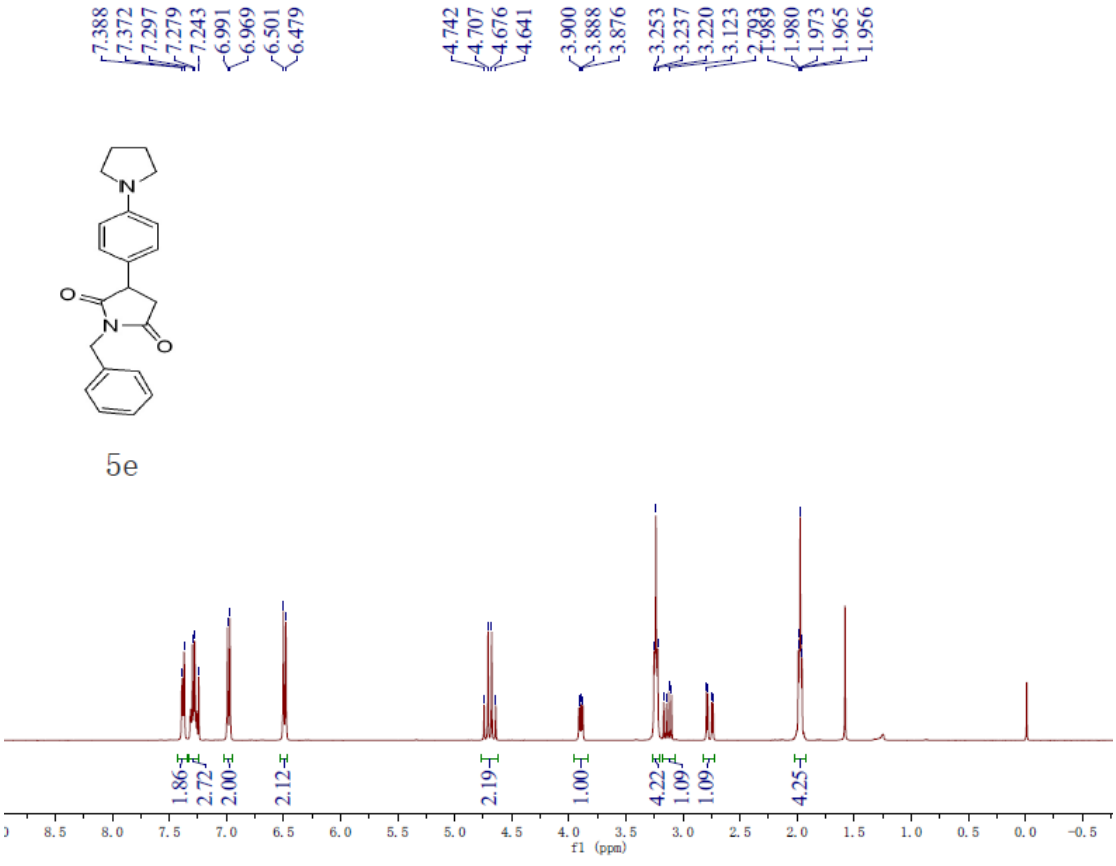

178.526
176.753
147.448
127.853
123.781
112.060
47.573
44.827
43.863
37.257
25.435
19.319
19.167
5b
f1 (ppm)


7.475
7.457
7.438
7.390
7.372
7.354
7.313
7.293
7.141
7.121
6.560
6.539
4.088
4.077
4.064
4.054
3.358
3.334
3.311
3.261
2.983
2.973
2.937
2.927
1.986
5c
2.01
1.01
1.93
1.96
2.03
1.00
5.08
1.07
4.10
f1 (ppm)


177.414
175.696
147.574
132.055
129.121
128.534
128.003
126.484
123.204
112.113
47.586
45.252
37.451
25.453
O
N
O
N
O
5c
f1 (ppm)


7.474
7.455
7.389
7.330
7.311
7.143
7.122
6.681
6.660
4.093
4.083
4.070
4.059
3.356
3.339
3.321
3.296
3.003
2.992
2.957
2.946
1.172
1.154
1.137
N
O
N
Ph
O
5d
1.96
1.03
1.95
2.02
2.08
1.03
5.22
1.11
6.19
f1 (ppm)


177.424
175.691
147.397
132.046
129.122
128.543
128.165
126.491
123.064
112.080
45.114
44.329
37.383
12.505
N
O
N
Ph
O
5d
f1 (ppm)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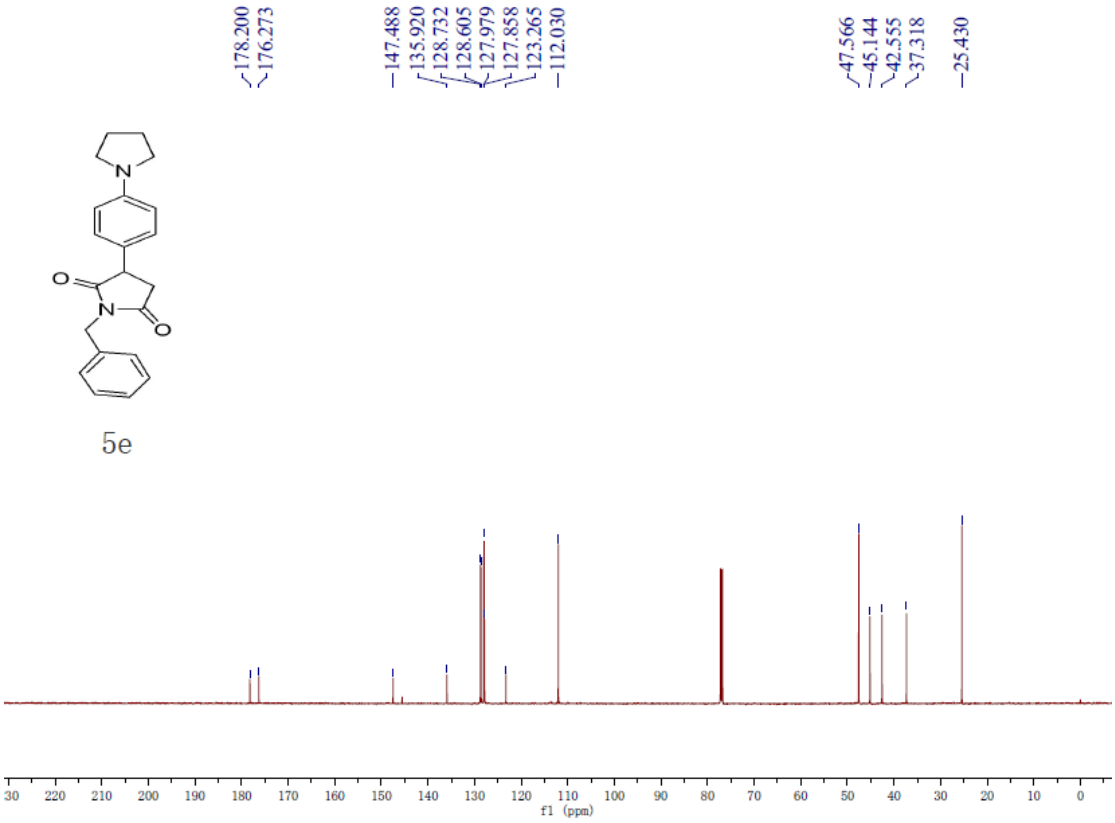
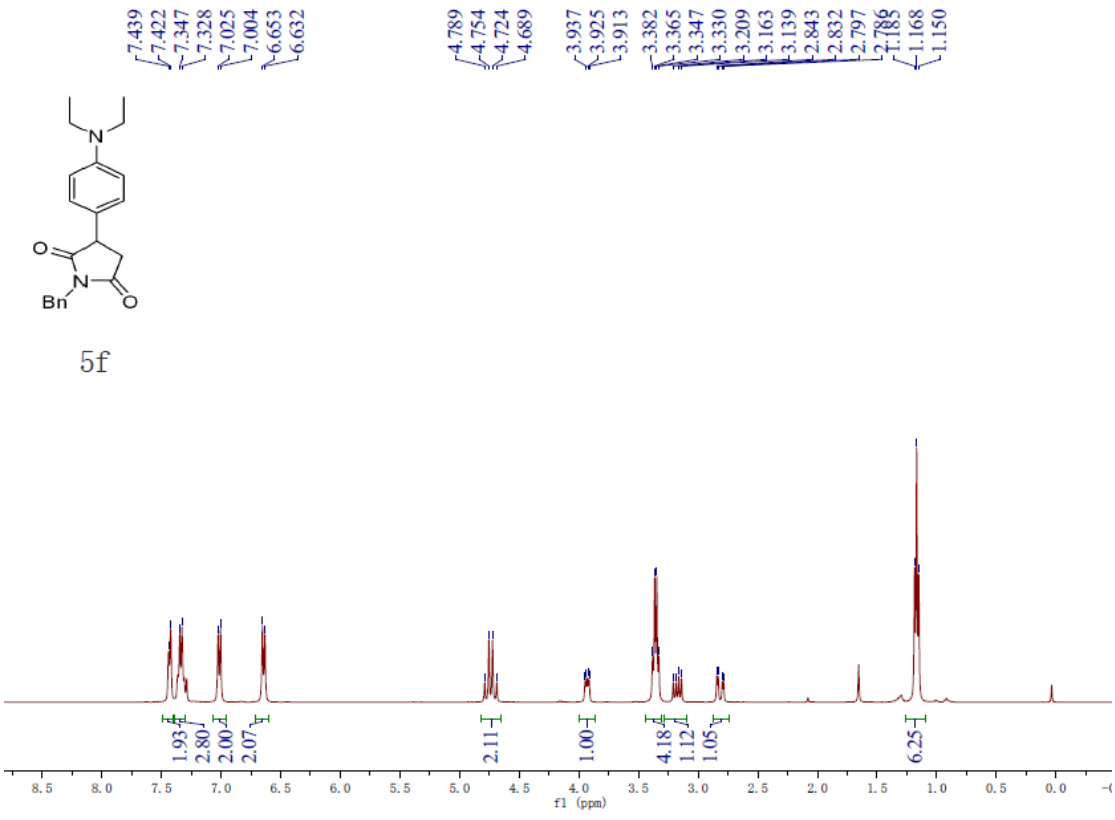
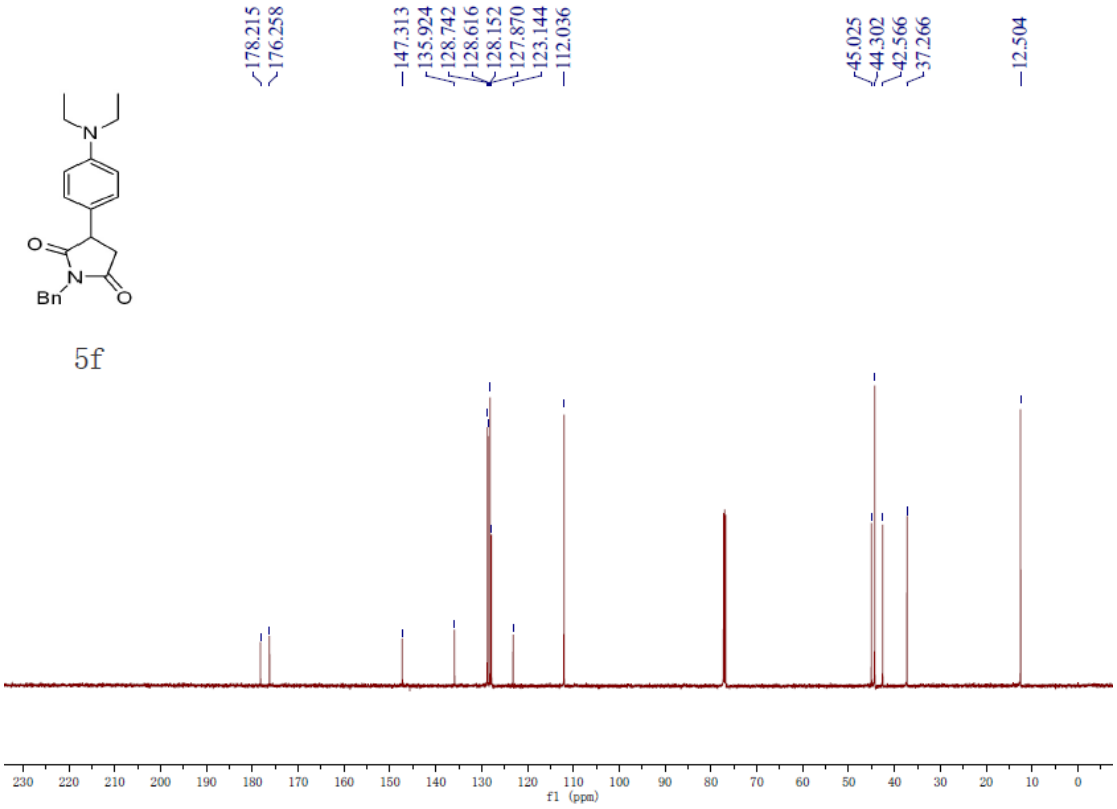
7.372
7.297
7.279
7.243
6.991
6.969
6.501
6.479
4.742
4.707
4.676
4.641
3.900
3.888
3.876
3.253
3.237
3.220
3.123
2.793
1.988
1.980
1.973
1.965
1.956
N
O
N
O
5e
1.86
2.72
2.00
2.12
2.19
1.00
4.22
1.09
1.09
4.25
f1 (ppm)


178.200
176.273
147.488
135.920
128.732
128.605
127.979
127.858
123.265
112.030
47.566
45.144
42.555
37.318
25.430
f1 (ppm)

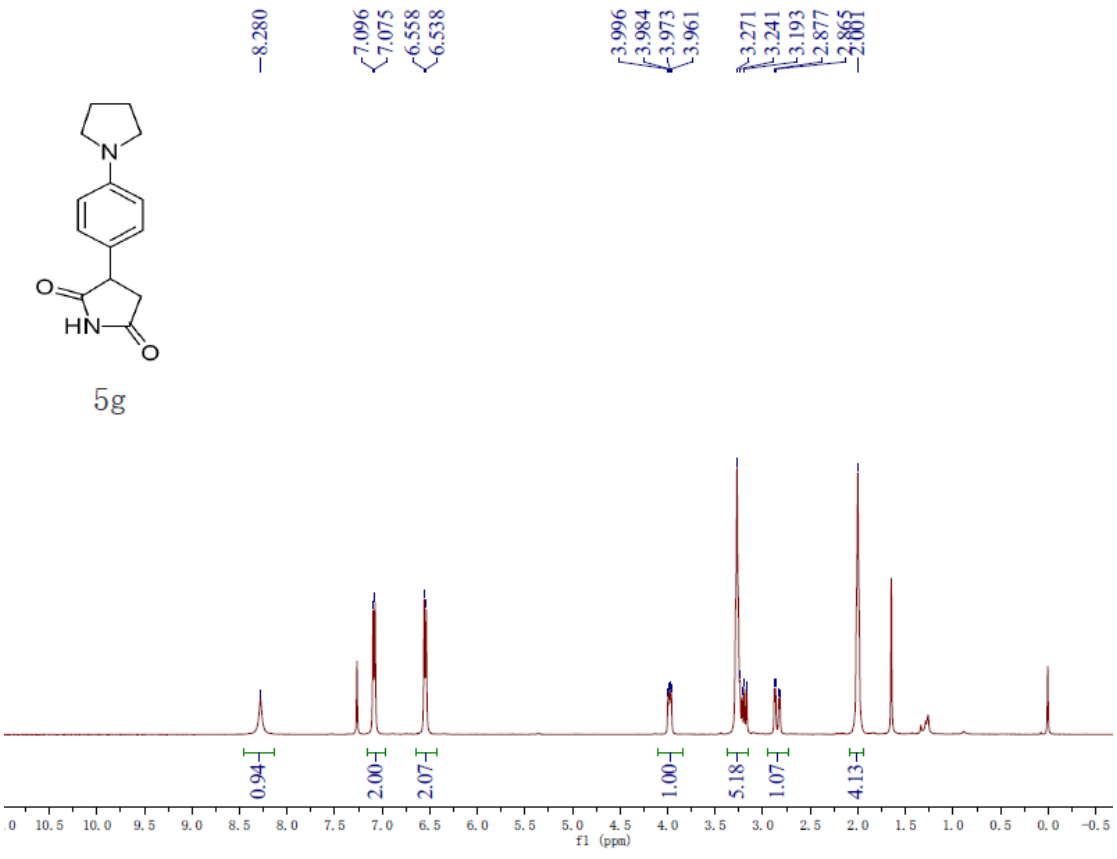
5e


7.439
7.422
7.347
7.328
7.025
7.004
6.653
6.632
4.789
4.754
4.724
4.689
3.937
3.925
3.913
3.382
3.365
3.347
3.330
3.209
3.163
3.139
2.843
2.832
2.797
1.168
1.150
1.93
2.80
2.00
2.07
2.11
1.00
4.18
1.12
1.05
6.25
f1 (ppm)

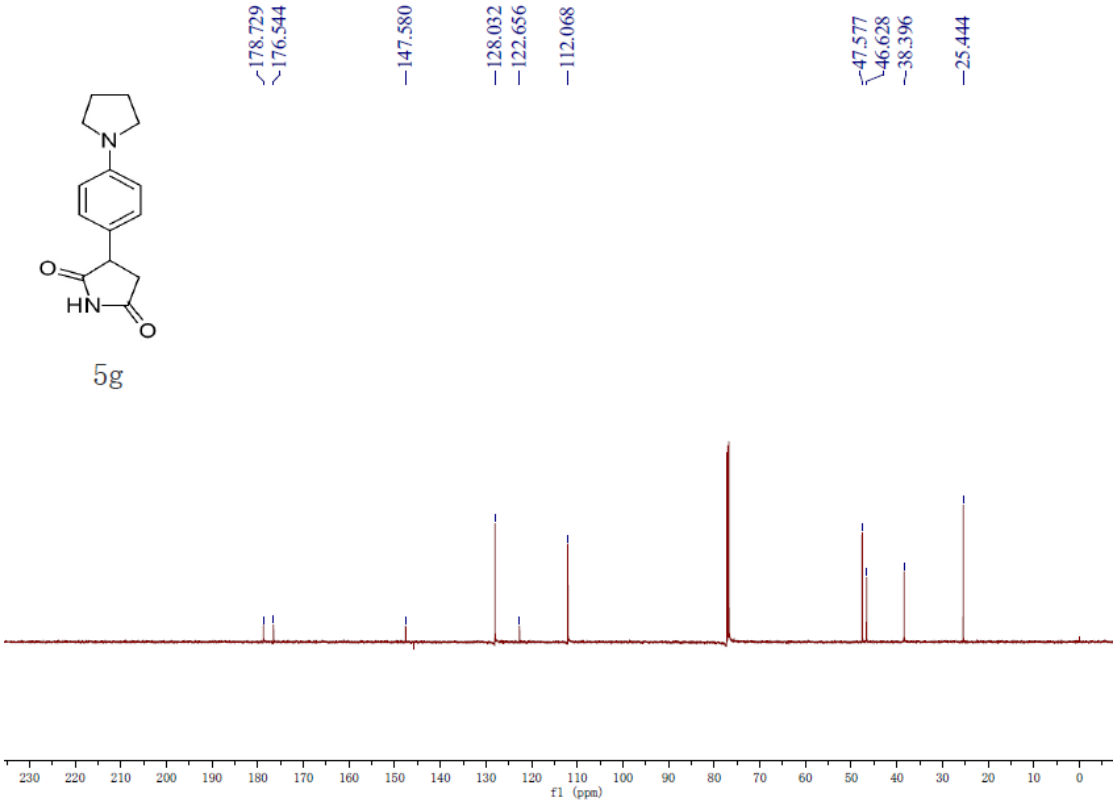
5f

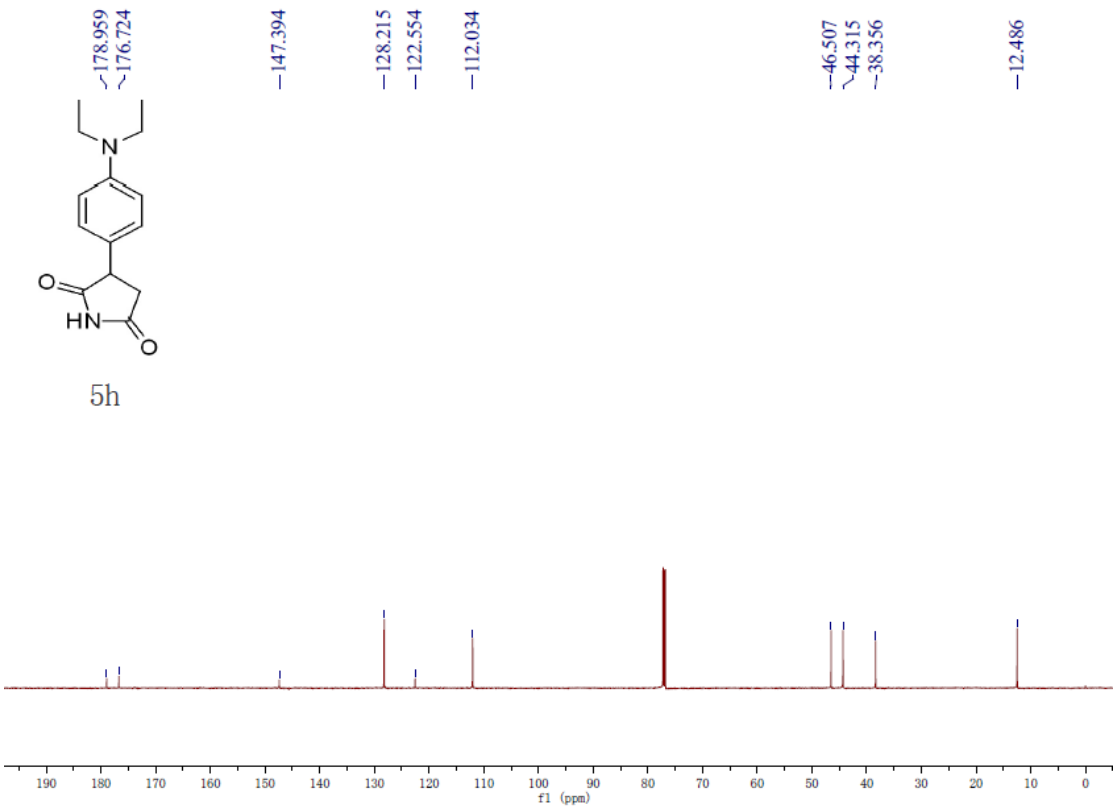

178.215
176.258
147.313
135.924
128.742
128.616
128.152
127.870
123.144
112.036
45.025
44.302
42.566
37.266
12.504
N
O
N
Bn
O
f1 (ppm)

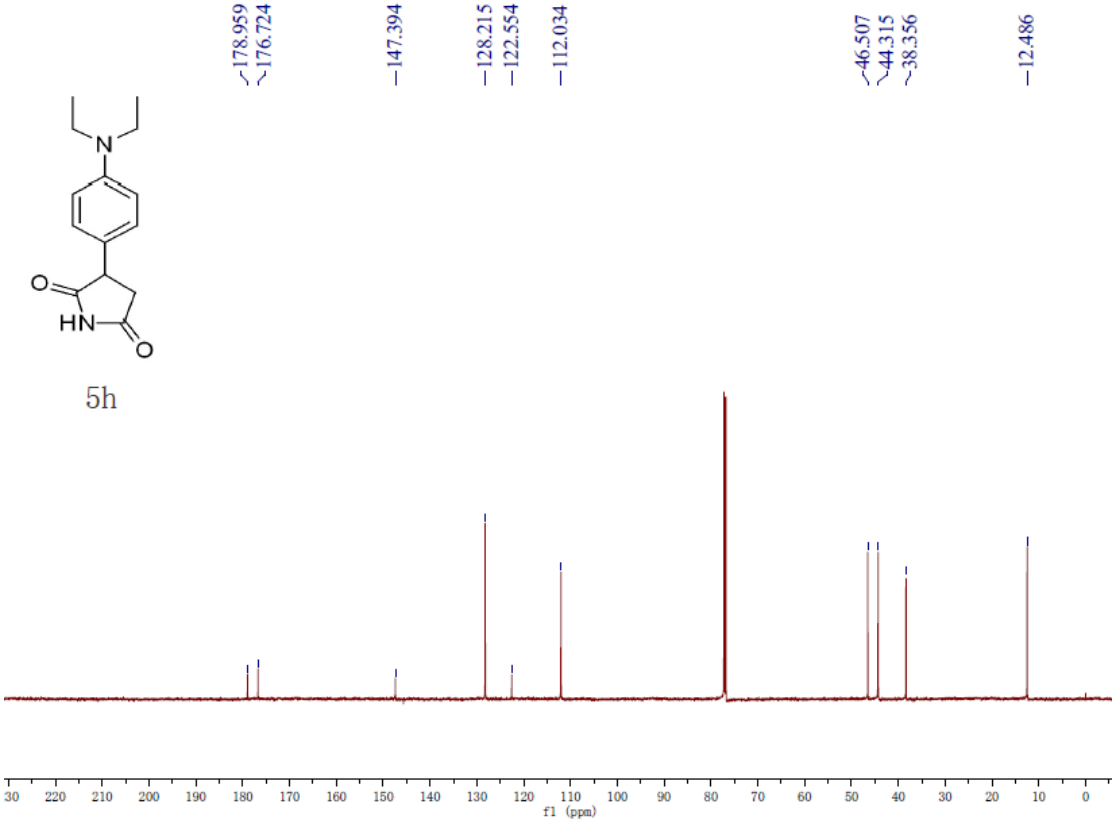
5f


8.280
7.096
7.075
6.558
6.538
3.996
3.984
3.973
3.961
3.271
3.241
3.193
2.877
2.865
2.001
N
O
HN
O
0.94
2.00
2.07
1.00
5.18
1.07
4.13
f1 (ppm)

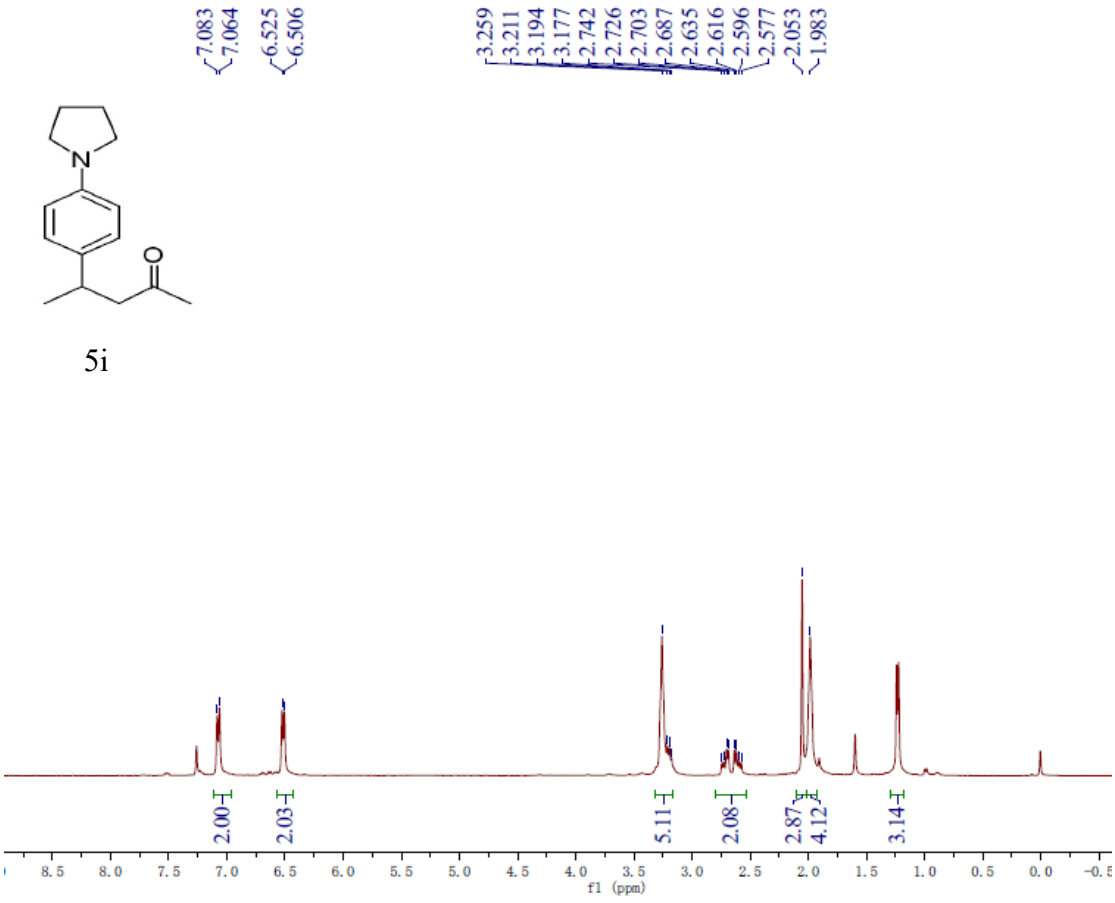
5g


178.729
176.544
147.580
128.032
122.656
112.068
47.577
46.628
38.396
25.444
N
O
HN
O
5g
f1 (ppm)

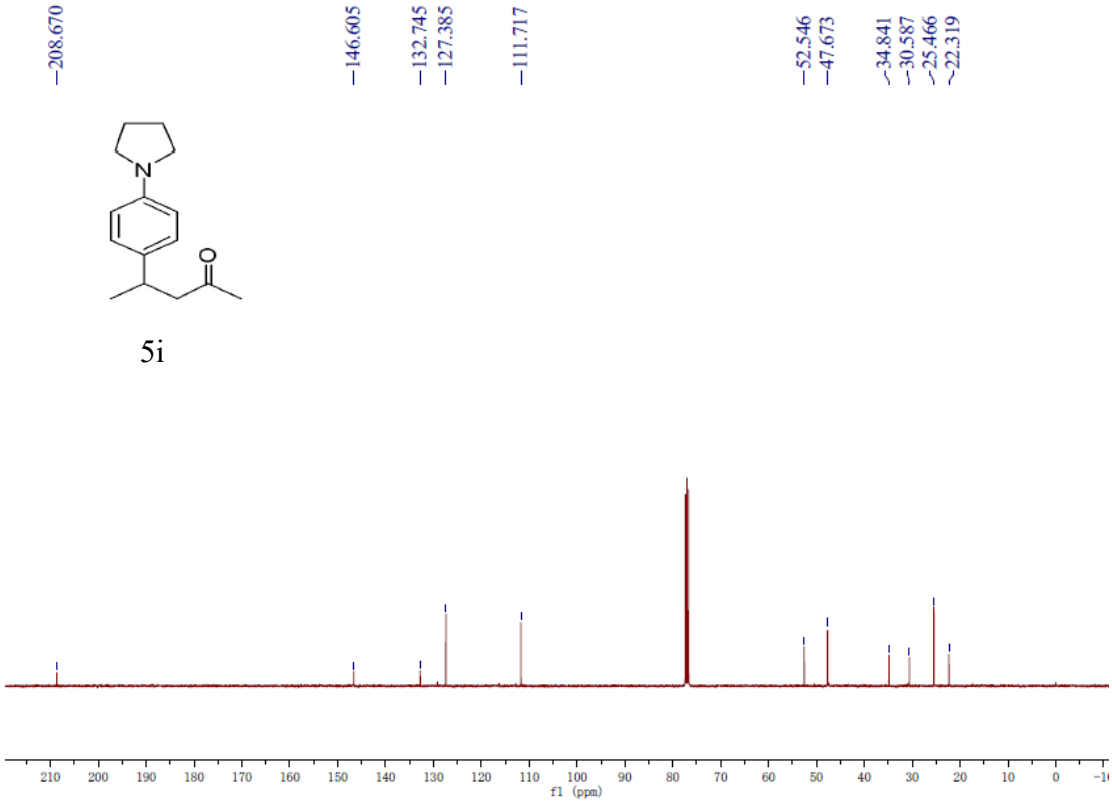

178.959
176.724
147.394
128.215
122.554
112.034
46.507
44.315
38.356
12.486
N
O
HN
O
5h
f1 (ppm)


178.959
176.724
147.394
128.215
122.554
112.034
46.507
44.315
38.356
12.486
O
HN
O
N
f1 (ppm)

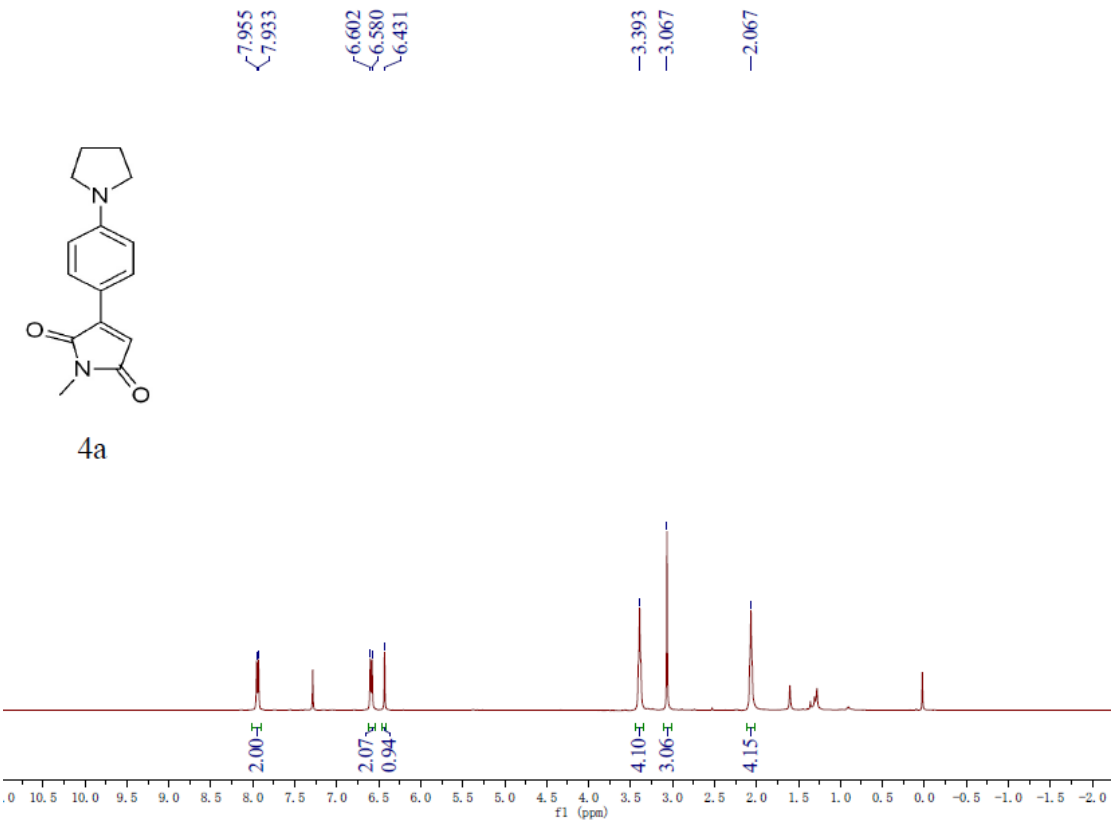
5h


7.083
7.064
6.525
6.506
3.259
3.211
3.194
3.177
2.742
2.726
2.703
2.687
2.635
2.616
2.596
2.577
2.053
1.983
N
O
2.00
2.03
5.11
2.08
2.87
4.12
3.14
f1 (ppm)

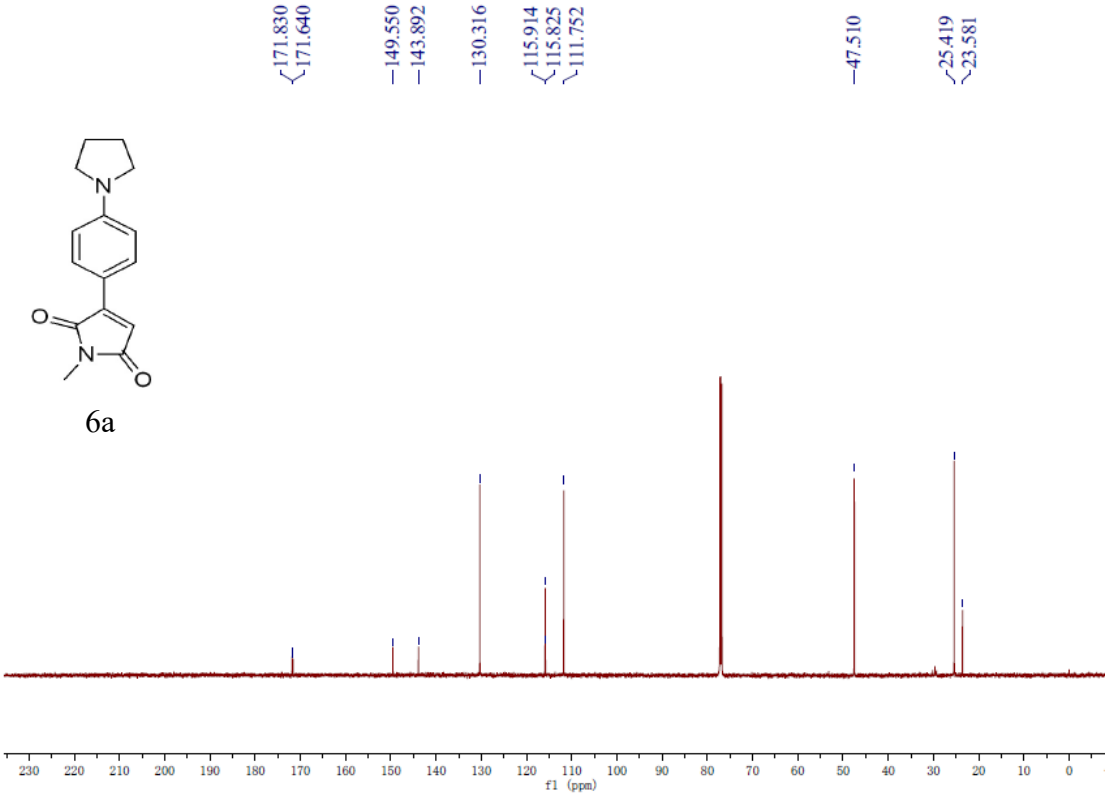
5i


208.670
146.605
132.745
127.385
111.717
52.546
47.673
34.841
30.587
25.466
22.319
N
O
f1 (ppm)

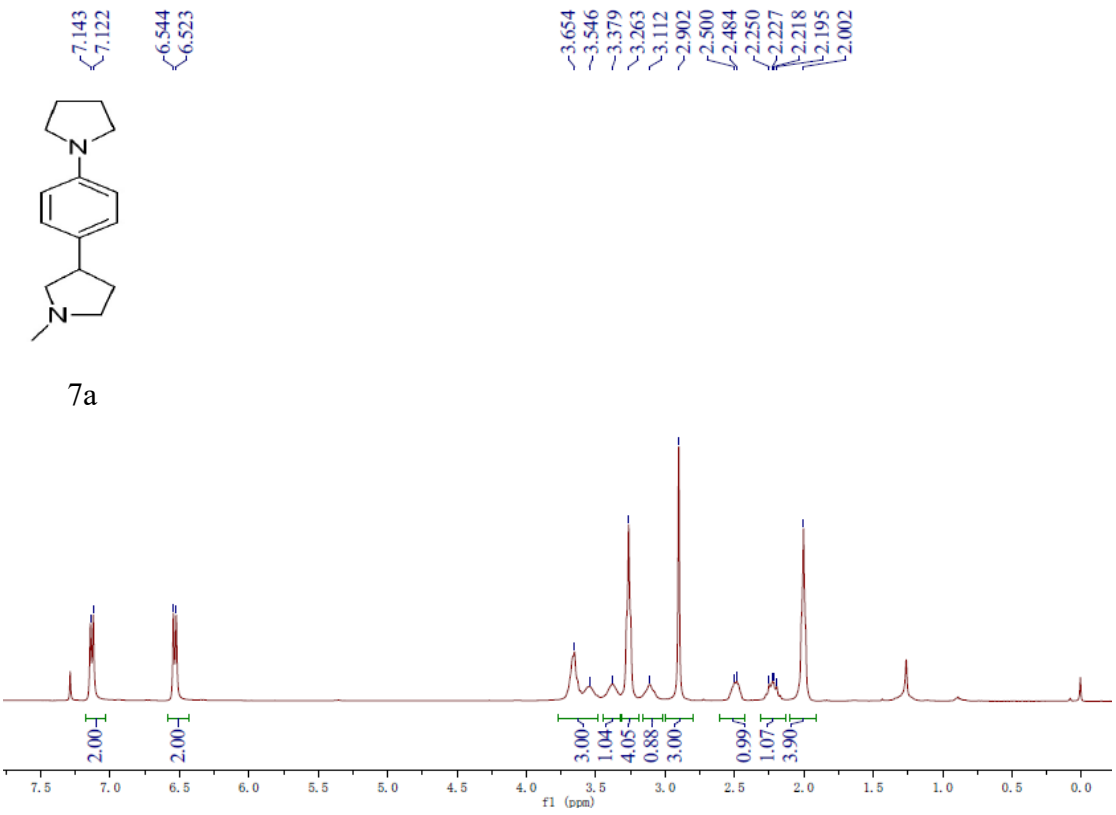
5i


7.955
7.933
6.602
6.580
6.431
3.393
3.067
2.067
N
O
N
O
2.00
2.07
0.94
4.10
3.06
4.15
f1 (ppm)

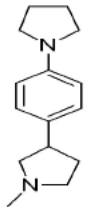
4a


171.830
171.640
149.550
143.892
130.316
115.914
115.825
111.752
47.510
25.419
23.581
f1 (ppm)

6a

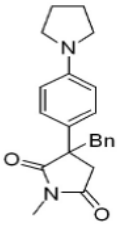

7.143
7.122
6.544
6.523
3.654
3.546
3.379
3.263
3.112
2.902
2.500
2.484
2.250
2.227
2.218
2.195
2.002
2.00
2.00
3.00
1.04
4.05
0.88
3.00
0.99
1.07
3.90
f1 (ppm)

7a

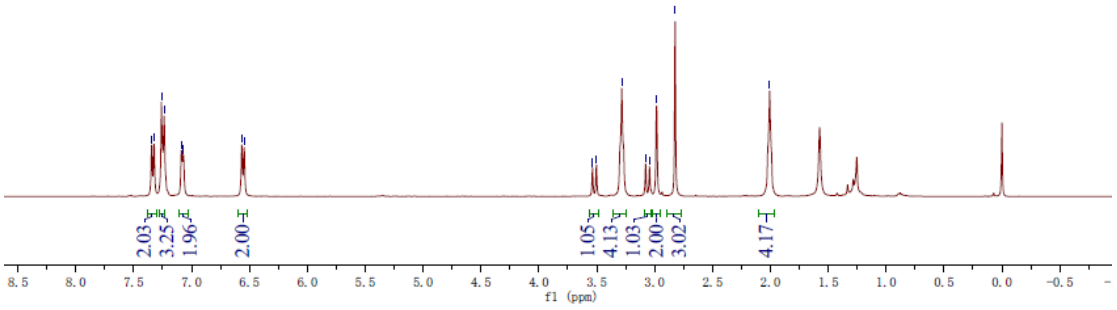


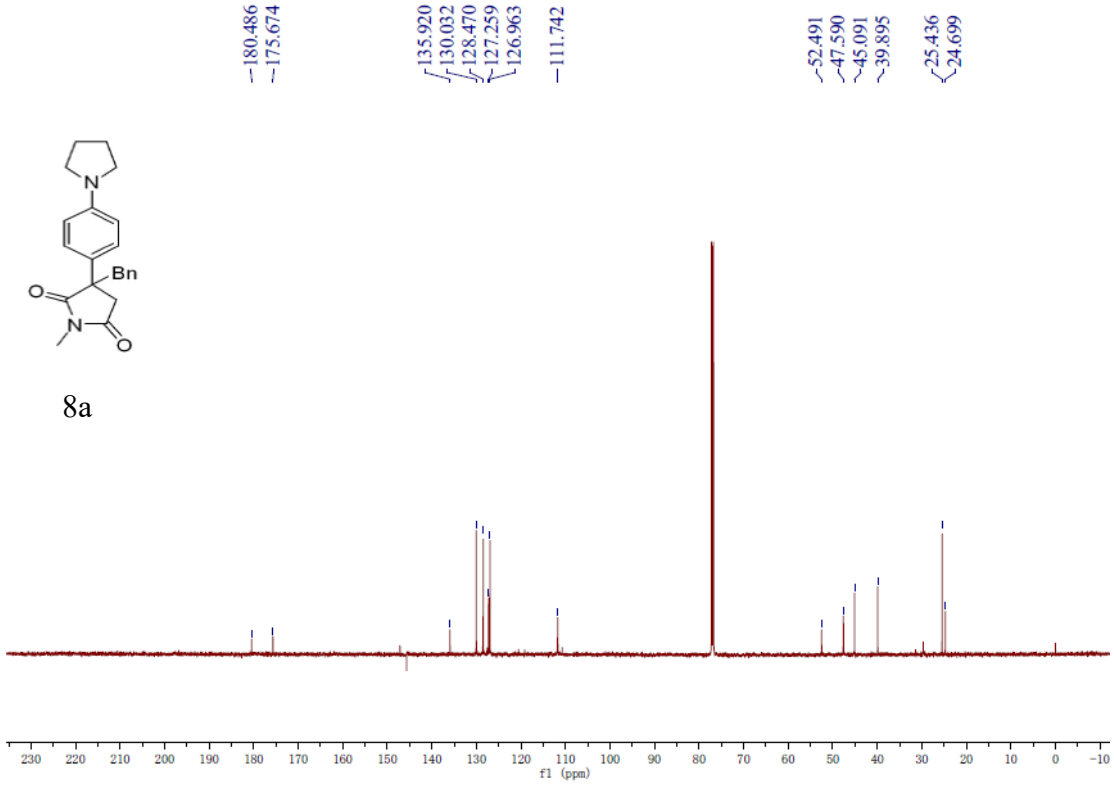
7a

147.379
127.782
124.046
123.993
111.920
70.497
61.303
55.498
47.572
42.579
41.469
25.401
f1 (ppm)


Bn

8a


7.345
7.323
7.260
7.237
7.086
7.070
6.566
6.545
3.536
3.503
3.284
3.078
3.044
2.983
2.823
2.006
2.03
3.25
1.96
2.00
1.05
4.13
1.03
2.00
3.02
4.17
f1 (ppm)


180.486
175.674
135.920
130.032
128.470
127.259
126.963
111.742
52.491
47.590
45.091
39.895
25.436
24.699
Bn
O
N
O
N
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

8a

6. X-ray Crystallography of 3k

Table 1. Crystal data and structure refinement for a.

Identification code	a	
Empirical formula	C17 H22 N2 O2	
Formula weight	286.36	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.8452(14) Å	α= 90°.
	b = 5.9542(4) Å	β= 103.868(2)°.
	c = 27.679(2) Å	γ = 90°.
Volume	3015.3(4) $Å^3$	
Z	8	
Density (calculated)	1.262 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1232	
Crystal size	0.300 x 0.200 x 0.100 mm^3	
Theta range for data collection	3.598 to 27.536°.	
Index ranges	-24<=h<=24, -7<=k<=7, -36<=l<=35	
Reflections collected	36497	
Independent reflections	3460 [R(int) = 0.0426]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	None	
Max. and min. transmission	0.992 and 0.980	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3460 / 0 / 193	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0522, wR2 = 0.1608	
R indices (all data)	R1 = 0.0632, wR2 = 0.1714	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.253 and -0.183 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	974(1)	9096(3)	6583(1)	79(1)
O(2)	2255(1)	2886(2)	7202(1)	57(1)
N(1)	3930(1)	27(2)	5546(1)	44(1)
N(2)	1506(1)	5885(2)	6950(1)	41(1)
C(1)	4779(1)	-2707(4)	5422(1)	70(1)
C(2)	4683(1)	-700(4)	5733(1)	55(1)
C(3)	3614(1)	1508(3)	5820(1)	37(1)
C(4)	2859(1)	1797(3)	5722(1)	37(1)
C(5)	2536(1)	3232(2)	6003(1)	33(1)
C(6)	2969(1)	4468(2)	6395(1)	32(1)
C(7)	2638(1)	5925(2)	6733(1)	35(1)
C(8)	2137(1)	4659(3)	6989(1)	38(1)
C(9)	933(1)	5214(4)	7189(1)	68(1)
C(10)	4043(1)	-3241(4)	5094(1)	59(1)
C(11)	4043(1)	2822(3)	6199(1)	41(1)
C(12)	3733(1)	4278(3)	6483(1)	38(1)
C(13)	2187(1)	7993(3)	6511(1)	42(1)
C(14)	1485(1)	7819(3)	6674(1)	46(1)
C(15)	1710(1)	3301(3)	5879(1)	42(1)
C(16)	4242(1)	5631(4)	6881(1)	58(1)
C(17)	3495(1)	-1800(3)	5275(1)	46(1)

Table 3. Bond lengths [Å] and angles [°] for a.

O(1)-C(14)	1.206(2)
O(2)-C(8)	1.2038(19)
N(1)-C(3)	1.3873(19)
N(1)-C(2)	1.455(2)
N(1)-C(17)	1.457(2)
N(2)-C(8)	1.377(2)
N(2)-C(14)	1.377(2)
N(2)-C(9)	1.452(2)
C(1)-C(10)	1.497(3)
C(1)-C(2)	1.509(3)
C(1)-H(5)	0.9700
C(1)-H(1)	0.9700
C(2)-H(6)	0.9700
C(2)-H(7)	0.9700
C(3)-C(4)	1.395(2)
C(3)-C(11)	1.400(2)
C(4)-C(5)	1.390(2)
C(4)-H(17)	0.9300
C(5)-C(6)	1.401(2)
C(5)-C(15)	1.5117(19)
C(6)-C(12)	1.406(2)
C(6)-C(7)	1.5135(19)
C(7)-C(8)	1.511(2)
C(7)-C(13)	1.538(2)
C(7)-H(13)	0.9800
C(9)-H(10)	0.9600
C(9)-H(11)	0.9600
C(9)-H(2)	0.9600
C(10)-C(17)	1.517(2)
C(10)-H(3)	0.9700
C(10)-H(4)	0.9700
C(11)-C(12)	1.390(2)
C(11)-H(8)	0.9300
C(12)-C(16)	1.510(2)
C(13)-C(14)	1.499(2)
C(13)-H(12)	0.9700

C(13)-H(9)	0.9700
C(15)-H(15)	0.9600
C(15)-H(14)	0.9600
C(15)-H(16)	0.9600
C(16)-H(20)	0.9600
C(16)-H(18)	0.9600
C(16)-H(19)	0.9600
C(17)-H(21)	0.9700
C(17)-H(22)	0.9700

C(3)-N(1)-C(2)	120.25(13)
C(3)-N(1)-C(17)	119.61(13)
C(2)-N(1)-C(17)	109.96(14)
C(8)-N(2)-C(14)	113.35(13)
C(8)-N(2)-C(9)	122.77(15)
C(14)-N(2)-C(9)	123.86(15)
C(10)-C(1)-C(2)	107.08(16)
C(10)-C(1)-H(5)	110.3
C(2)-C(1)-H(5)	110.3
C(10)-C(1)-H(1)	110.3
C(2)-C(1)-H(1)	110.3
H(5)-C(1)-H(1)	108.6
N(1)-C(2)-C(1)	105.79(15)
N(1)-C(2)-H(6)	110.6
C(1)-C(2)-H(6)	110.6
N(1)-C(2)-H(7)	110.6
C(1)-C(2)-H(7)	110.6
H(6)-C(2)-H(7)	108.7
N(1)-C(3)-C(4)	121.57(13)
N(1)-C(3)-C(11)	121.26(13)
C(4)-C(3)-C(11)	117.15(13)
C(5)-C(4)-C(3)	122.03(13)
C(5)-C(4)-H(17)	119.0
C(3)-C(4)-H(17)	119.0
C(4)-C(5)-C(6)	120.32(13)
C(4)-C(5)-C(15)	117.03(13)
C(6)-C(5)-C(15)	122.60(13)
C(5)-C(6)-C(12)	118.25(13)

C(5)-C(6)-C(7)	122.03(13)
C(12)-C(6)-C(7)	119.68(12)
C(8)-C(7)-C(6)	113.50(12)
C(8)-C(7)-C(13)	103.79(12)
C(6)-C(7)-C(13)	118.84(13)
C(8)-C(7)-H(13)	106.7
C(6)-C(7)-H(13)	106.7
C(13)-C(7)-H(13)	106.7
O(2)-C(8)-N(2)	123.89(15)
O(2)-C(8)-C(7)	127.23(15)
N(2)-C(8)-C(7)	108.87(12)
N(2)-C(9)-H(10)	109.5
N(2)-C(9)-H(11)	109.5
H(10)-C(9)-H(11)	109.5
N(2)-C(9)-H(2)	109.5
H(10)-C(9)-H(2)	109.5
H(11)-C(9)-H(2)	109.5
C(1)-C(10)-C(17)	106.58(15)
C(1)-C(10)-H(3)	110.4
C(17)-C(10)-H(3)	110.4
C(1)-C(10)-H(4)	110.4
C(17)-C(10)-H(4)	110.4
H(3)-C(10)-H(4)	108.6
C(12)-C(11)-C(3)	121.76(14)
C(12)-C(11)-H(8)	119.1
C(3)-C(11)-H(8)	119.1
C(11)-C(12)-C(6)	120.36(13)
C(11)-C(12)-C(16)	117.75(14)
C(6)-C(12)-C(16)	121.89(14)
C(14)-C(13)-C(7)	105.54(13)
C(14)-C(13)-H(12)	110.6
C(7)-C(13)-H(12)	110.6
C(14)-C(13)-H(9)	110.6
C(7)-C(13)-H(9)	110.6
H(12)-C(13)-H(9)	108.8
O(1)-C(14)-N(2)	123.96(16)
O(1)-C(14)-C(13)	127.71(16)
N(2)-C(14)-C(13)	108.33(13)

C(5)-C(15)-H(15)	109.5
C(5)-C(15)-H(14)	109.5
H(15)-C(15)-H(14)	109.5
C(5)-C(15)-H(16)	109.5
H(15)-C(15)-H(16)	109.5
H(14)-C(15)-H(16)	109.5
C(12)-C(16)-H(20)	109.5
C(12)-C(16)-H(18)	109.5
H(20)-C(16)-H(18)	109.5
C(12)-C(16)-H(19)	109.5
H(20)-C(16)-H(19)	109.5
H(18)-C(16)-H(19)	109.5
N(1)-C(17)-C(10)	104.37(13)
N(1)-C(17)-H(21)	110.9
C(10)-C(17)-H(21)	110.9
N(1)-C(17)-H(22)	110.9
C(10)-C(17)-H(22)	110.9
H(21)-C(17)-H(22)	108.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	51(1)	69(1)	124(1)	32(1)	34(1)	26(1)
O(2)	79(1)	46(1)	50(1)	16(1)	24(1)	13(1)
N(1)	33(1)	50(1)	49(1)	-15(1)	11(1)	1(1)
N(2)	37(1)	44(1)	44(1)	4(1)	14(1)	-2(1)
C(1)	52(1)	73(1)	85(2)	-28(1)	14(1)	12(1)
C(2)	36(1)	68(1)	61(1)	-17(1)	10(1)	7(1)
C(3)	33(1)	42(1)	36(1)	-4(1)	10(1)	0(1)
C(4)	32(1)	42(1)	35(1)	-6(1)	5(1)	-3(1)
C(5)	28(1)	36(1)	34(1)	2(1)	6(1)	0(1)
C(6)	31(1)	32(1)	33(1)	0(1)	7(1)	1(1)
C(7)	34(1)	34(1)	38(1)	-3(1)	8(1)	2(1)
C(8)	44(1)	38(1)	32(1)	1(1)	10(1)	2(1)
C(9)	55(1)	77(1)	80(1)	17(1)	36(1)	-2(1)
C(10)	54(1)	60(1)	62(1)	-20(1)	14(1)	7(1)
C(11)	26(1)	48(1)	46(1)	-9(1)	7(1)	0(1)
C(12)	32(1)	41(1)	40(1)	-6(1)	5(1)	-2(1)
C(13)	44(1)	31(1)	56(1)	4(1)	20(1)	3(1)
C(14)	38(1)	41(1)	59(1)	5(1)	14(1)	4(1)
C(15)	30(1)	48(1)	45(1)	-5(1)	4(1)	2(1)
C(16)	35(1)	71(1)	64(1)	-30(1)	6(1)	-5(1)
C(17)	42(1)	50(1)	48(1)	-13(1)	14(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for a.

	x	y	z	U(eq)
H(5)	5123	-2364	5221	84
H(1)	4964	-3979	5634	84
H(6)	4772	-1112	6081	66
H(7)	5019	489	5698	66
H(17)	2562	1005	5460	44
H(13)	3046	6480	6995	43
H(10)	850	3627	7147	101
H(11)	491	6007	7040	101
H(2)	1079	5564	7537	101
H(3)	3932	-4821	5119	70
H(4)	4033	-2897	4750	70
H(8)	4550	2717	6263	49
H(12)	2443	9366	6635	51
H(9)	2093	7983	6151	51
H(15)	1521	2687	5552	63
H(14)	1549	4828	5886	63
H(16)	1535	2432	6118	63
H(20)	4739	5349	6868	87
H(18)	4176	5203	7202	87
H(19)	4136	7201	6828	87
H(21)	3123	-1228	4997	55
H(22)	3260	-2652	5492	55

Table 6. Torsion angles [°] for a.

C(3)-N(1)-C(2)-C(1)	165.39(17)
C(17)-N(1)-C(2)-C(1)	20.3(2)
C(10)-C(1)-C(2)-N(1)	-6.0(3)
C(2)-N(1)-C(3)-C(4)	-163.38(16)
C(17)-N(1)-C(3)-C(4)	-21.6(2)
C(2)-N(1)-C(3)-C(11)	18.3(2)
C(17)-N(1)-C(3)-C(11)	160.16(16)
N(1)-C(3)-C(4)-C(5)	178.26(14)
C(11)-C(3)-C(4)-C(5)	-3.4(2)
C(3)-C(4)-C(5)-C(6)	0.8(2)
C(3)-C(4)-C(5)-C(15)	-176.61(14)
C(4)-C(5)-C(6)-C(12)	2.4(2)
C(15)-C(5)-C(6)-C(12)	179.61(14)
C(4)-C(5)-C(6)-C(7)	-175.70(13)
C(15)-C(5)-C(6)-C(7)	1.5(2)
C(5)-C(6)-C(7)-C(8)	57.00(18)
C(12)-C(6)-C(7)-C(8)	-121.05(15)
C(5)-C(6)-C(7)-C(13)	-65.43(19)
C(12)-C(6)-C(7)-C(13)	116.52(16)
C(14)-N(2)-C(8)-O(2)	-177.85(16)
C(9)-N(2)-C(8)-O(2)	3.7(3)
C(14)-N(2)-C(8)-C(7)	3.12(18)
C(9)-N(2)-C(8)-C(7)	-175.32(17)
C(6)-C(7)-C(8)-O(2)	47.2(2)
C(13)-C(7)-C(8)-O(2)	177.59(16)
C(6)-C(7)-C(8)-N(2)	-133.85(13)
C(13)-C(7)-C(8)-N(2)	-3.43(16)
C(2)-C(1)-C(10)-C(17)	-9.4(3)
N(1)-C(3)-C(11)-C(12)	-178.72(15)
C(4)-C(3)-C(11)-C(12)	2.9(2)
C(3)-C(11)-C(12)-C(6)	0.1(2)
C(3)-C(11)-C(12)-C(16)	-179.74(17)
C(5)-C(6)-C(12)-C(11)	-2.8(2)
C(7)-C(6)-C(12)-C(11)	175.31(14)
C(5)-C(6)-C(12)-C(16)	177.06(16)
C(7)-C(6)-C(12)-C(16)	-4.8(2)

C(8)-C(7)-C(13)-C(14)	2.56(17)
C(6)-C(7)-C(13)-C(14)	129.71(15)
C(8)-N(2)-C(14)-O(1)	177.87(19)
C(9)-N(2)-C(14)-O(1)	-3.7(3)
C(8)-N(2)-C(14)-C(13)	-1.4(2)
C(9)-N(2)-C(14)-C(13)	177.05(17)
C(7)-C(13)-C(14)-O(1)	179.9(2)
C(7)-C(13)-C(14)-N(2)	-0.91(19)
C(3)-N(1)-C(17)-C(10)	-171.32(15)
C(2)-N(1)-C(17)-C(10)	-25.9(2)
C(1)-C(10)-C(17)-N(1)	21.2(2)

Symmetry transformations used to generate equivalent atoms: