

Supporting Information

Nickel-catalyzed Claisen condensation reaction between two different amides.

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Supporting Information

1. General Information
2. General synthetic method for the reaction of *N*-methyl-*N*-phenylbenzamide derivatives (or *N,N*-diphenylbenzamide derivatives) with lactam derivatives (or aliphatic amides)
3. Experiment Data
4. References
5. Copy of NMR Spectra
6. Computational Details
7. Additional Computational Results
8. Calculated Energy Values
9. Cartesian Coordinates for All Species

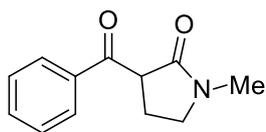
1. General Information

The amides were synthesized from acyl chloride derivatives with amine following the reported method^[1-2] and the acyl chloride derivatives were purchased from supplier or synthesized from corresponding carboxylic acids with oxalyl dichloride according to the literature^[3]. Other reagents include solvents, catalysts, ligand, metal, lactam derivatives and *N,N*-dimethylacetamide were purchased from supplier and used without further purification.

2. General synthetic method for the reaction of *N*-methyl-*N*-phenylbenzamide derivatives (or *N,N*-diphenylbenzamide derivatives) with lactam derivatives (or aliphatic amides)

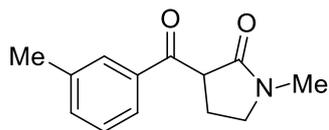
To a 20 mL vial was added *N*-methyl-*N*-phenylbenzamide derivative or *N,N*-diphenylbenzamide derivative (1.0 mmol, 1.0 equiv.), lactam derivative or aliphatic amide (5.0 mmol, 5.0 equiv.), Ni(glyme)Cl₂ (21.8 mg, 0.1 mmol, 0.1 equiv.), terpyridine (23.3 mg, 0.1 mmol, 0.1 equiv.), Mn (137.5 mg, 2.5 mmol, 2.5 equiv), LiCl (42.4 mg, 1.0 mmol, 1.0 equiv) and mesitylene (2.0 mL). The reaction was stirred for 24 h at 170 °C. The reaction was quenched with saturated NH₄Cl and diluted with ethyl acetate (100 mL) and washed with saturated NH₄Cl (50 mL), saturated NaCl (50 mL X 2). The organic layer was dried over anhydrous Mg₂SO₄, filtered and concentrated under vacuum. The crude product was purified through column chromatography with ethyl acetate/hexane 1:1 to 3:1.

3. Experiment Data



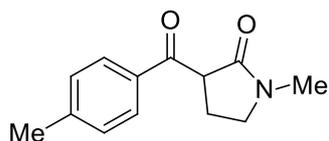
3-Benzoyl-1-methylpyrrolidin-2-one (**3a**)^[4-5]:

N-Methyl-*N*-phenylbenzamide (211 mg, 1.0 mmol) afforded 3-benzoyl-1-methylpyrrolidin-2-one (**3a**) (164 mg, 0.81 mmol, 81% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). *N,N*-Diphenylbenzamide (273 mg, 1.0 mmol) afforded **3a** (160 mg, 0.78 mmol, 78 % yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.57 (d, *J* = 7.4 Hz, 1H), 7.49 (dd, *J* = 8.4, 6.3 Hz, 2H), 4.48 (dd, *J* = 9.3, 5.0 Hz, 1H), 3.64 – 3.54 (m, 1H), 3.44 – 3.35 (m, 1H), 2.89 – 2.82 (m, 3H), 2.67 – 2.56 (m, 1H), 2.32 – 2.19 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 196.4, 170.2, 136.2, 133.5, 129.6, 128.5, 50.5, 48.2, 30.0, 21.9.



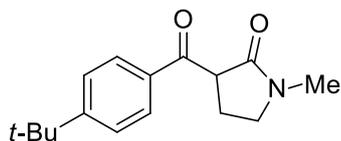
1-Methyl-3-(3-methylbenzoyl)pyrrolidin-2-one (**3b**):

N,3-Dimethyl-*N*-phenylbenzamide (225 mg, 1.0 mmol) afforded 1-methyl-3-(3-methylbenzoyl)pyrrolidin-2-one (**3b**) (136 mg, 0.63 mmol, 63% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 3-Methyl-*N,N*-diphenylbenzamide (287 mg, 1.0 mmol) afforded **3b** (182 mg, 0.84 mmol, 84% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (400 MHz, CDCl_3) δ 7.95 – 7.88 (m, 2H), 7.42 – 7.36 (m, 2H), 4.48 (dd, $J = 9.3, 5.0$ Hz, 1H), 3.65 – 3.56 (m, 1H), 3.43 – 3.36 (m, 1H), 2.87 (s, 3H), 2.64 – 2.54 (m, 1H), 2.42 (s, 3H), 2.31–2.20 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 196.7, 170.4, 138.3, 136.3, 134.3, 129.9, 128.4, 126.8, 50.4, 48.2, 30.0, 22.0, 21.4. HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{16}\text{NO}_2$ 218.1176; Found 218.1175.



1-Methyl-3-(4-methylbenzoyl)pyrrolidin-2-one (**3c**):

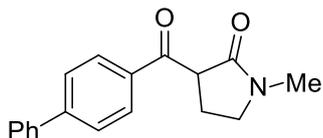
N,4-Dimethyl-*N*-phenylbenzamide (225 mg, 1.0 mmol) afforded 1-methyl-3-(4-methylbenzoyl)pyrrolidin-2-one (**3c**) (72 mg, 0.33 mmol, 33% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 4-Methyl-*N,N*-diphenylbenzamide (287 mg, 1.0 mmol) afforded **3c** (132 mg, 0.61 mmol, 61% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 92 – 94 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.01 (d, $J = 8.3$ Hz, 2H), 7.28 (d, $J = 8.3$ Hz, 2H), 4.44 (dd, $J = 9.3, 4.9$ Hz, 1H), 3.64 – 3.53 (m, 1H), 3.42 – 3.33 (m, 1H), 2.86 (s, 3H), 2.65 – 2.56 (m, 1H), 2.41 (s, 3H), 2.30 – 2.19 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 195.9, 170.3, 144.4, 133.8, 129.7, 129.2, 50.3, 48.2, 30.0, 21.9, 21.7; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{16}\text{NO}_2$ 218.1176; Found 218.1171.



3-(4-(*tert*-Butyl)benzoyl)-1-methylpyrrolidin-2-one (**3d**):

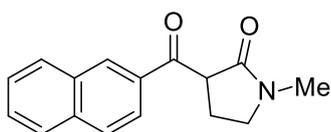
4-(*tert*-Butyl)-*N*-methyl-*N*-phenylbenzamide (267 mg, 1.0 mmol) afforded 3-(4-(*tert*-butyl)benzoyl)-1-methylpyrrolidin-2-one (**3d**) (137 mg, 0.53 mmol, 53% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 4-(*tert*-Butyl)-*N,N*-diphenylbenzamide (329 mg, 1.0 mmol) afforded **3d** (140 mg, 0.54 mmol, 54% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1);

^1H NMR (600 MHz, CDCl_3) δ 8.05 (d, $J = 8.6$ Hz, 2H), 7.49 (d, $J = 8.7$ Hz, 2H), 4.46 (dd, $J = 9.3$, 4.8 Hz, 1H), 3.63 – 3.55 (m, 1H), 3.42 – 3.35 (m 1H), 2.85 (s, 3H), 2.66 – 2.58 (m, 1H), 2.27 – 2.19 (m, 1H), 1.32 (s, 9H); ^{13}C NMR (151 MHz, CDCl_3) δ 195.8, 170.2, 157.2, 133.4, 129.5, 125.4, 50.3, 48.1, 35.1, 31.0, 29.9, 21.8; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{22}\text{NO}_2$ 260.1645; Found 260.1644.



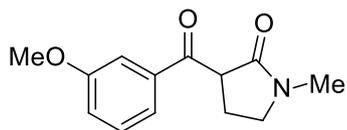
3-([1,1'-Biphenyl]-4-carbonyl)-1-methylpyrrolidin-2-one (**3e**):

N-Methyl-*N*-phenyl-[1,1'-biphenyl]-4-carboxamide (287 mg, 1.0 mmol) afforded 3-([1,1'-biphenyl]-4-carbonyl)-1-methylpyrrolidin-2-one (**3e**) (168 mg, 0.60 mmol, 60% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). *N,N*-Diphenyl-[1,1'-biphenyl]-4-carboxamide (349 mg, 1.0 mmol) afforded **3e** (173 mg, 0.62 mmol, 62% yield) by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 8.23 – 8.18 (m, 2H), 7.74 – 7.69 (m, 2H), 7.65 – 7.61 (m, 2H), 7.50 – 7.45 (m, 2H), 7.43 – 7.37 (m, 1H), 4.51 (dd, $J = 9.2$, 4.9 Hz, 1H), 3.65 – 3.58 (m, 1H), 3.44 – 3.37 (m, 1H), 2.88 (s, 3H), 2.71 – 2.63 (m, 1H), 2.31–2.22 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 195.8, 170.1, 146.1, 139.9, 134.9, 130.2, 128.9, 128.2, 127.3, 127.2, 50.5, 48.2, 30.0, 21.8. HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{18}\text{H}_{18}\text{NO}_2$ 280.1332; Found 280.1333.



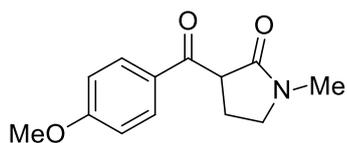
3-(2-Naphthoyl)-1-methylpyrrolidin-2-one (**3f**):

N-Methyl-*N*-phenyl-2-naphthamide (261 mg, 1.0 mmol) afforded 3-(2-naphthoyl)-1-methylpyrrolidin-2-one (**3f**) (198 mg, 0.78 mmol, 78% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). *N,N*-Diphenyl-2-naphthamide (323 mg, 1.0 mmol) afforded **3f** (182 mg, 0.72 mmol, 72% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 8.70 (d, $J = 1.1$ Hz, 1H), 8.11 (dd, $J = 8.6$, 1.8 Hz, 1H), 8.00 (dd, $J = 8.1$, 0.6 Hz, 1H), 7.91 – 7.83 (m, 2H), 7.62–7.51 (m, 2H), 4.62 (dd, $J = 9.3$, 4.9 Hz, 1H), 3.67 – 3.58 (m, 1H), 3.42 (d, $J = 4.5$ Hz, 1H), 2.87 (s, 3H), 2.71 – 2.62 (m, 1H), 2.33–2.24 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 196.2, 170.2, 135.7, 133.5, 132.4, 132.2, 129.9, 128.7, 128.3, 127.6, 126.6, 124.5, 50.5, 48.2, 30.0, 22.0; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{16}\text{NO}_2$ 254.1176; Found 254.1172.



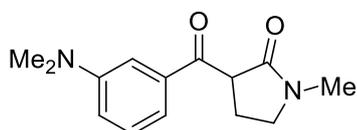
3-(3-Methoxybenzoyl)-1-methylpyrrolidin-2-one (**3g**):

3-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded 3-(3-methoxybenzoyl)-1-methylpyrrolidin-2-one (**3g**) (149 mg, 0.64 mmol, 64% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 3-Methoxy-*N,N*-diphenylbenzamide (303 mg, 1.0 mmol) afforded **3g** (196 mg, 0.84 mmol, 84% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (500 MHz, CDCl₃) δ 7.74 – 7.70 (m, 1H), 7.63 (dd, *J* = 2.6, 1.6 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.13 (ddd, *J* = 8.2, 2.7, 0.9 Hz, 1H), 4.44 (dd, *J* = 9.3, 4.9 Hz, 1H), 3.86 (s, 3H), 3.64 – 3.56 (m, 1H), 3.43 – 3.36 (m, 1H), 2.87 (s, 3H), 2.65 – 2.56 (m, 1H), 2.31 – 2.21 (m, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 196.3, 170.1, 159.7, 137.6, 129.5, 122.4, 120.2, 113.3, 55.4, 50.6, 48.1, 30.0, 22.1; HRMS (FD) *m/z*: [M + H]⁺ Calcd for C₁₃H₁₆NO₃ 234.1125; Found 234.1127.



3-(4-Methoxybenzoyl)-1-methylpyrrolidin-2-one (**3h**):

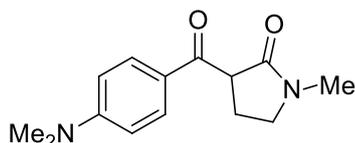
4-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded 3-(4-methoxybenzoyl)-1-methylpyrrolidin-2-one (**3h**) (152 mg, 0.65 mmol, 65% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 4-Methoxy-*N,N*-diphenylbenzamide (303 mg, 1.0 mmol) afforded **3h** (198 mg, 0.85 mmol, 85% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (400 MHz, CDCl₃) δ 8.11 (d, *J* = 9.0 Hz, 2H), 6.96 (d, *J* = 9.0 Hz, 2H), 4.42 (dd, *J* = 9.2, 4.7 Hz, 1H), 3.87 (s, 3H), 3.64 – 3.55 (m, 1H), 3.42 – 3.34 (m, 1H), 2.86 (s, 3H), 2.68 – 2.57 (m, 1H), 2.29 – 2.17 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 194.6, 170.4, 163.9, 132.0, 129.2, 113.7, 55.5, 50.1, 48.2, 30.0, 21.8; HRMS (FD) *m/z*: [M + H]⁺ Calcd for C₁₃H₁₆NO₃ 234.1125; Found 234.1128.



3-(3-(Dimethylamino)benzoyl)-1-methylpyrrolidin-2-one (**3i**):

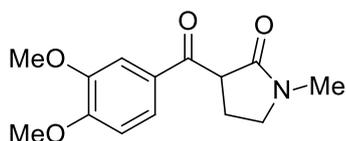
3-(Dimethylamino)-*N*-methyl-*N*-phenylbenzamide (254 mg, 1.0 mmol) afforded 3-(3-(dimethylamino)benzoyl)-1-methylpyrrolidin-2-one (**3i**) (135 mg, 0.55 mmol, 55% yield) as yellow oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 3-(Dimethylamino)-*N,N*-diphenylbenzamide (316 mg, 1.0 mmol) afforded **3i** (99 mg, 0.4 mmol, 40% yield) as yellow oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (500 MHz, CDCl₃) δ 7.47 – 7.41 (m, 2H), 7.36 – 7.31 (m, 1H),

6.94 (ddd, $J = 8.3, 2.7, 0.8$ Hz, 1H), 4.46 (dd, $J = 9.3, 4.8$ Hz, 1H), 3.63 – 3.56 (m, 1H), 3.42 – 3.34 (m, 1H), 2.99 (s, 6H), 2.87 (s, 3H), 2.60 – 2.52 (m, 1H), 2.30 – 2.22 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 197.3, 170.5, 150.6, 137.0, 129.1, 118.0, 117.6, 112.6, 50.6, 48.2, 40.6, 30.0, 22.4; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{19}\text{N}_2\text{O}_2$ 247.1441; Found 247.1446.



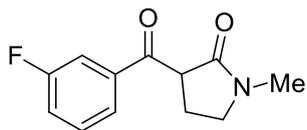
3-(4-(Dimethylamino)benzoyl)-1-methylpyrrolidin-2-one (3j):

4-(Dimethylamino)-*N*-methyl-*N*-phenylbenzamide (254 mg, 1.0 mmol) afforded 3-(4-(dimethylamino)benzoyl)-1-methylpyrrolidin-2-one (**3j**) (148 mg, 0.60 mmol, 60% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 4-(Dimethylamino)-*N,N*-diphenylbenzamide (316 mg, 1.0 mmol) afforded **3j** (138 mg, 56 mmol, 56% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 120 – 121°C; ^1H NMR (500 MHz, CDCl_3) δ 8.00 (d, $J = 9.2$ Hz, 2H), 6.66 (d, $J = 9.2$ Hz, 2H), 4.37 (dd, $J = 9.3, 4.6$ Hz, 1H), 3.64 – 3.55 (m, 1H), 3.40 – 3.32 (m, 1H), 3.05 (s, 6H), 2.85 (s, 3H), 2.63 – 2.54 (m, 1H), 2.26 – 2.16 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 193.9, 171.1, 153.7, 131.8, 124.1, 49.6, 48.3, 40.0, 29.9, 22.1; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{19}\text{N}_2\text{O}_2$ 247.1441; Found 247.1444.



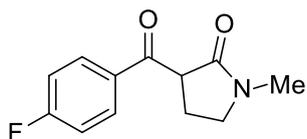
3-(3,4-Dimethoxybenzoyl)-1-methylpyrrolidin-2-one (3k):

3,4-Dimethoxy-*N*-methyl-*N*-phenylbenzamide (271 mg, 1.0 mmol) afforded 3-(3,4-dimethoxybenzoyl)-1-methylpyrrolidin-2-one (**3k**) (13 mg, 0.05 mmol, 5% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 3,4-Dimethoxy-*N,N*-diphenylbenzamide (333 mg, 1.0 mmol) afforded **3k** (39 mg, 0.15 mmol, 15% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 110 – 111 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.80 (dd, $J = 8.5, 2.0$ Hz, 1H), 7.63 (d, $J = 2.0$ Hz, 1H), 6.92 (d, $J = 8.5$ Hz, 1H), 4.41 (dd, $J = 9.2, 4.6$ Hz, 1H), 3.93 (s, 3H), 3.92 (s, 3H), 3.63 – 3.55 (m, 1H), 3.41 – 3.34 (m, 1H), 2.85 (s, 3H), 2.66 – 2.58 (m, 1H), 2.26 – 2.17 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 194.7, 170.3, 153.7, 148.9, 129.4, 125.0, 111.2, 110.0, 56.1, 56.0, 50.2, 48.3, 30.0, 22.0; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_4$ 264.1230; Found 264.1237.



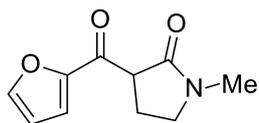
3-(3-Fluorobenzoyl)-1-methylpyrrolidin-2-one (**3l**):

3-Fluoro-*N*-methyl-*N*-phenylbenzamide (229 mg, 1.0 mmol) afforded 3-(3-fluorobenzoyl)-1-methylpyrrolidin-2-one (**3l**) (166 mg, 0.75 mmol, 75% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 3-Fluoro-*N,N*-diphenylbenzamide (291 mg, 1.0 mmol) afforded **3l** (66 mg, 0.30 mmol, 30% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 7.92 (d, $J = 7.8$ Hz, 1H), 7.82 – 7.73 (m, 1H), 7.50 – 7.42 (m, 1H), 7.30 – 7.23 (m, 1H), 4.41 (dd, $J = 9.2, 5.0$ Hz, 1H), 3.63 – 3.55 (m, 1H), 3.43 – 3.35 (m, 1H), 2.86 (s, 3H), 2.68 – 2.56 (m, 1H), 2.31 – 2.19 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 195.1 (d, $J = 2.4$ Hz), 169.8, 162.7 (d, $J = 248.2$ Hz), 138.3 (d, $J = 6.5$ Hz), 130.1 (d, $J = 7.6$ Hz), 125.5 (d, $J = 3.0$ Hz), 120.5 (d, $J = 21.2$ Hz), 116.1 (d, $J = 23.7$ Hz), 50.7, 48.1, 30.0, 21.7; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{13}\text{FNO}_2$ 222.0925; Found 222.0923.



3-(4-Fluorobenzoyl)-1-methylpyrrolidin-2-one (**3m**):

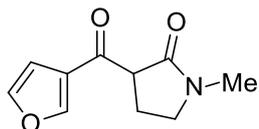
4-Fluoro-*N*-methyl-*N*-phenylbenzamide (229 mg, 1.0 mmol) afforded 3-(4-fluorobenzoyl)-1-methylpyrrolidin-2-one (**3m**) (144 mg, 0.65 mmol, 65% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). 4-Fluoro-*N,N*-diphenylbenzamide (291 mg, 1.0 mmol) afforded **3m** (173 mg, 0.78 mmol, 78% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (400 MHz, CDCl_3) δ 8.17 (dd, $J = 9.0, 5.4$ Hz, 2H), 7.16 (t, $J = 8.7$ Hz, 2H), 4.43 (dd, $J = 9.2, 4.9$ Hz, 1H), 3.65 – 3.55 (m, 1H), 3.44 – 3.36 (m, 1H), 2.87 (s, 3H), 2.70 – 2.60 (m, 1H), 2.29 – 2.19 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 194.5, 169.9, 166.1 (d, $J = 203.6$ Hz), 132.6 (d, $J = 3.0$ Hz), 132.4 (d, $J = 10.1$ Hz), 115.6 (d, $J = 22.2$ Hz), 50.6, 48.2, 30.0, 21.6; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{13}\text{FNO}_2$ 222.0925; Found 222.0926.



3-(Furan-2-carbonyl)-1-methylpyrrolidin-2-one (**3n**):

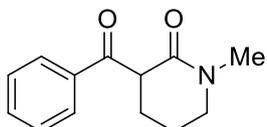
N-Methyl-*N*-phenylfuran-2-carboxamide (201 mg, 1.0 mmol) afforded 3-(furan-2-carbonyl)-1-methylpyrrolidin-2-one (**3n**) (39 mg, 0.20 mmol, 20% yield) as light yellow oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). *N,N*-Diphenylfuran-2-carboxamide (263 mg, 1.0 mmol) afforded **3n** (73 mg, 0.38 mmol, 38% yield) as light yellow oil by

silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, $J = 1.6$ Hz, 1H), 7.41 (dd, $J = 3.6, 0.5$ Hz, 1H), 6.58 (dd, $J = 3.6, 1.7$ Hz, 1H), 4.21 (dd, $J = 9.4, 5.6$ Hz, 1H), 3.62 – 3.54 (m, 1H), 3.45 – 3.34 (m, 1H), 2.87 (s, 3H), 2.65 – 2.55 (m, 1H), 2.28 – 2.18 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 184.7, 170.0, 152.0, 147.5, 120.3, 112.6, 50.8, 48.2, 30.0, 21.2; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_3$ 194.0812; Found 194.0808.



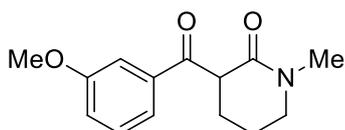
3-(Furan-3-carbonyl)-1-methylpyrrolidin-2-one (3o):

N-Methyl-*N*-phenylfuran-3-carboxamide (201 mg, 1.0 mmol) afforded 3-(furan-3-carbonyl)-1-methylpyrrolidin-2-one (**3o**) (48 mg, 0.25 mmol, 25% yield) as light yellow oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1). *N,N*-Diphenylfuran-3-carboxamide (263 mg, 1.0 mmol) afforded **3o** (70 mg, 0.36 mmol, 36% yield) as light yellow oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 8.27 (dd, $J = 1.3, 0.9$ Hz, 1H), 7.43 – 7.40 (m, 1H), 6.81 (dd, $J = 1.4, 0.5$ Hz, 1H), 3.96 (dd, $J = 9.2, 4.7$ Hz, 1H), 3.59 – 3.49 (m, 1H), 3.37 – 3.29 (m, 1H), 2.83 (s, 3H), 2.68 – 2.60 (m, 1H), 2.21 – 2.13 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 190.1, 169.7, 149.9, 143.9, 127.1, 108.9, 53.0, 48.2, 30.0, 20.8; HRMS (FD) m/z : $[\text{M}]^+$ Calcd for $\text{C}_{10}\text{H}_{11}\text{NO}_3$ 193.0733; Found 193.0731.



3-Benzoyl-1-methylpiperidin-2-one^[5] (4a) [conformer **A**/ conformer **B**/enol = 3/2/1]:

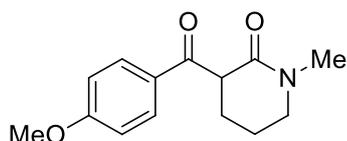
N-Methyl-*N*-phenylbenzamide (211 mg, 1.0 mmol) afforded 3-benzoyl-1-methylpiperidin-2-one (**4a**) (185 mg, 0.85 mmol, 85% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (400 MHz, CDCl_3) δ 8.07 – 7.33 (m, 5H), 4.450 – 4.40 and 2.54 – 2.44 (both m, total 1H), 3.54 – 3.26 (m, 2H), 3.04, 3.00 (both s, total 3H), 2.27 – 1.72 (m, 4H); ^{13}C NMR (101 MHz, CDCl_3) δ 198.5, 170.9, 167.0, 136.4, 135.8, 133.2, 129.1, 129.1, 128.6, 128.1, 128.0, 97.1, 50.0, 49.9, 49.8, 35.0, 34.7, 25.5, 25.3, 22.9, 20.7.



3-(3-Methoxybenzoyl)-1-methylpiperidin-2-one (4b) [conformer **A**/ conformer **B**/enol = 2/2/1]:

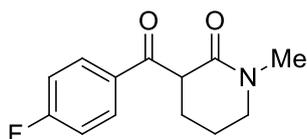
3-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded

3-(3-methoxybenzoyl)-1-methylpiperidin-2-one (**4b**) (124 mg, 0.50 mmol, 50% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 7.59 – 7.26 and 7.12 – 6.89 (both m, 4H), 4.25 – 4.38 and 2.50 – 2.46 (both m, total 1H), 3.90 – 3.77 (m, 3H), 3.45 – 3.28 (m, 2H), 3.10 – 2.95 (m, 3H), 2.21 – 1.73 (m, 4H); ^{13}C NMR (126 MHz, CDCl_3) δ 198.3, 170.8, 166.8, 159.7, 159.2, 137.7, 137.0, 129.5, 128.9, 121.7, 120.6, 119.7, 114.9, 113.5, 113.1, 97.1, 55.4, 55.3, 50.0, 49.9, 49.7, 34.9, 34.6, 25.5, 25.4, 22.8, 20.7; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_3$ 248.1281; Found 248.1282.



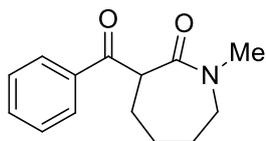
3-(4-Methoxybenzoyl)-1-methylpiperidin-2-one (4c) [conformer **A**/conformer **B**/enol = **12/3/1**]:

4-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded 3-(4-methoxybenzoyl)-1-methylpiperidin-2-one (**4c**) (138 mg, 0.56 mmol, 56% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 7.98 and 7.44 (both d, $J = 8.9$ Hz, total 2H), 6.95 – 6.86 (m, 2H), 4.41-4.36 and 2.53-2.49 (both m, total 1H), 3.85 and 3.81 (both s, total 3H), 3.45 – 3.27 (m, 2H), 3.02 and 2.98 (both s, total 3H), 2.21 – 1.98 (m, 3H), 1.85 – 1.74 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 196.8, 167.1, 163.6, 131.4, 129.7, 129.4, 113.7, 113.25, 55.5, 49.8, 49.5, 35.0, 25.4, 20.7; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_3$ 248.1281; Found 248.1283.



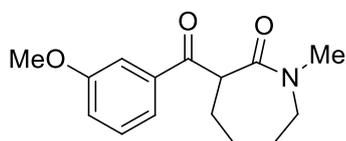
3-(4-Fluorobenzoyl)-1-methylpiperidin-2-one (4d) [conformer **A**/conformer **B**/enol = **2.5/2/1**]:

4-Fluoro-*N*-methyl-*N*-phenylbenzamide (229 mg, 1.0 mmol) afforded 3-(4-fluorobenzoyl)-1-methylpiperidin-2-one (113 mg, 0.48 mmol, 48% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ^1H NMR (500 MHz, CDCl_3) δ 8.06 – 8.00 and 7.49 – 7.44 (both m, total 2H), 7.16 – 7.04 (m, 2H), 4.40 – 4.36 and 2.48-2.45 (both m, total 1H), 3.47 – 3.29 (m, 2H), 3.03 and 2.97 (both s, total 3H), 2.26 – 1.75 (m, 4H); ^{13}C NMR (126 MHz, CDCl_3) δ 196.8, 170.8, 166.4 (d, $J = 93.2$ Hz), 165.7 (d, $J = 233.1$ Hz), 163.0 (d, $J = 249.5$ Hz), 133.0 (d, $J = 2.9$ Hz), 131.8 (d, $J = 9.4$ Hz), 130.2 (d, $J = 8.4$ Hz), 115.6 (d, $J = 22.7$ Hz), 115.0 (d, $J = 21.4$ Hz), 97.1, 50.0, 49.8, 49.7, 35.0, 34.7, 25.6, 25.1, 22.8, 20.8; HRMS (FD) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{15}\text{FNO}_2$ 236.1081; Found 236.1081.



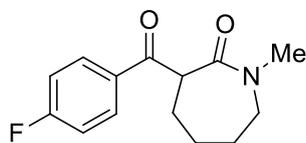
3-Benzoyl-1-methylazepan-2-one (4e)^[6]:

N-Methyl-*N*-phenylbenzamide (211 mg, 1.0 mmol) afforded 3-benzoyl-1-methylazepan-2-one (**4e**) (148 mg, 0.64 mmol, 64% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 137–138 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.92 – 7.85 (m, 2H), 7.54 – 7.48 (m, 1H), 7.46 – 7.39 (m, 2H), 4.46 (dd, *J* = 10.6, 2.0 Hz, 1H), 3.73 (dd, *J* = 15.2, 10.4 Hz, 1H), 3.40 – 3.28 (m, 1H), 2.99 (s, 3H), 2.28 – 2.18 (m, 1H), 2.13 – 2.02 (m, 1H), 1.91 – 1.79 (m, 2H), 1.66 – 1.50 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 196.3, 173.0, 137.1, 132.7, 128.6, 128.1, 52.8, 51.1, 35.7, 28.3, 27.0, 25.2.



3-(3-Methoxybenzoyl)-1-methylazepan-2-one (4f):

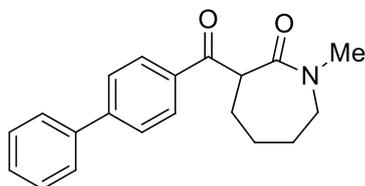
3-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded 3-(3-methoxybenzoyl)-1-methylazepan-2-one (**4f**) (39 mg, 0.15 mmol, 15% yield) as light yellow oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (500 MHz, CDCl₃) δ 7.49 – 7.46 (m, 1H), 7.44 – 7.40 (m, 1H), 7.36 – 7.30 (m, 1H), 7.08 – 7.04 (m, 1H), 4.45 (dd, *J* = 10.6, 2.0 Hz, 1H), 3.84 (s, 3H), 3.75 – 3.66 (m, 1H), 3.40 – 3.30 (m, 1H), 2.99 (s, 3H), 2.26 – 2.20 (m, 1H), 2.12 – 2.05 (m, 1H), 1.90 – 1.80 (m, 2H), 1.64 – 1.49 (m, 2H); ¹³C NMR (126 MHz, CDCl₃) δ 196.0, 172.9, 159.7, 138.4, 129.5, 120.5, 119.1, 112.6, 55.4, 52.8, 51.0, 35.6, 28.3, 26.90, 25.1; HRMS (FD) *m/z*: [*M* + *H*]⁺ Calcd for C₁₅H₂₀NO₃ 262.1438; Found 262.1433.



3-(4-Fluorobenzoyl)-1-methylazepan-2-one (4g) [conformer **A/
conformer **B** = 11/1]:**

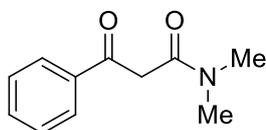
4-Fluoro-*N*-methyl-*N*-phenylbenzamide (229 mg, 1.0 mmol) afforded 3-(4-fluorobenzoyl)-1-methylazepan-2-one (**4g**) (67 mg, 0.27 mmol, 27% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 146 – 147 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.96 – 7.87 and 7.54 – 7.50 (both m, total 2H), 7.45 – 7.41 and 7.14 – 7.07 (both m, total 2H), 4.48 – 4.37 (m, 1H), 3.76 – 3.67 (m, 1H), 3.40 – 3.31 (m, 1H), 3.01 (s, 3H), 2.29 – 2.20 (m, 1H), 2.15 – 2.05 (m, 1H), 1.91 – 1.79 (m, 2H), 1.69 – 1.54 (m, 2H); ¹³C NMR (126 MHz, CDCl₃) δ 194.6,

172.8, 165.4 (d, $J = 254.5$ Hz), 133.5 (d, $J = 3.8$ Hz), 130.6 (d, $J = 8.8$ Hz), 128.3 (d, $J = 61.7$ Hz), 115.6 (d, $J = 21.4$ Hz), 52.8, 51.1, 35.7, 28.3, 26.9, 25.1; HRMS (FD) m/z : $[M + H]^+$ Calcd for $C_{14}H_{17}FNO_2$ 250.1238; Found 250.1232.



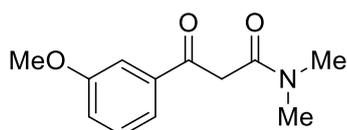
3-([1,1'-Biphenyl]-4-carbonyl)-1-methylazepan-2-one (4h):

N-Methyl-*N*-phenyl-[1,1'-biphenyl]-4-carboxamide (287 mg, 1.0 mmol) afforded 3-([1,1'-biphenyl]-4-carbonyl)-1-methylazepan-2-one (**4h**) (55 mg, 0.18, 18% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 148 – 149 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, $J = 8.5$ Hz, 2H), 7.66 (d, $J = 8.5$ Hz, 2H), 7.61 (d, $J = 7.1$ Hz, 2H), 7.49 – 7.37 (m, 3H), 4.50 (dd, $J = 10.6, 1.9$ Hz, 1H), 3.80 – 3.72 (m, 1H), 3.42 – 3.34 (m, 1H), 3.03 (s, 3H), 2.33 – 2.24 (m, 1H), 2.16 – 2.07 (m, 1H), 1.94 – 1.82 (m, 3.3 Hz, 2H), 1.68 – 1.56 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.8, 173.0, 145.4, 140.1, 135.8, 128.9, 128.6, 128.1, 127.3, 127.3, 52.9, 51.1, 35.7, 28.3, 27.0, 25.1; HRMS (FD) m/z : $[M + H]^+$ Calcd for $C_{20}H_{22}NO_2$ 308.1645; Found 308.1645.



***N,N*-Dimethyl-3-oxo-3-phenylpropanamide^[7] (4i) [ketone/enol = 1.9/1]:**

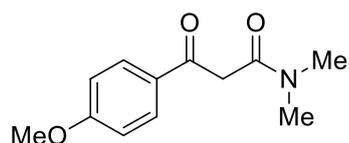
N-Methyl-*N*-phenylbenzamide (211 mg, 1.0 mmol) afforded *N,N*-dimethyl-3-oxo-3-phenylpropanamide (**4i**) (155 mg, 0.81 mmol, 81% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); 1H NMR (400 MHz, $CDCl_3$) δ 8.10 – 7.97 (m, 1.3H), 7.81 – 7.75 (m, 0.7H), 7.64 – 7.53 (m, 0.7H), 7.51 – 7.37 (m, 2.3H), 5.80 (s, 0.35H), 4.12 (s, 1.3H), 3.07 (br, 2.1H), 3.05 (s, 1.95H), 3.0 (s, 1.95 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 172.3, 171.2, 167.2, 136.2, 135.0, 133.7, 130.6, 128.7, 128.7, 128.4, 125.9, 84.6, 45.9, 38.1, 35.6.



3-(3-Methoxyphenyl)-*N,N*-dimethyl-3-oxopropanamide^[7] (4j)
[ketone/enol = 1.5/1]:

3-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded 3-(3-methoxyphenyl)-*N,N*-dimethyl-3-oxopropanamide (**4j**) (173 mg, 0.82 mmol, 82% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); 1H NMR

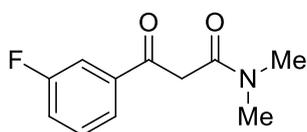
(600 MHz, CDCl₃) δ δ 7.59 (d, *J* = 7.7 Hz, 0.6H), 7.55 – 7.52 (m, 0.6H), 7.41 – 7.29 (m, 1.8H), 7.13 (dd, *J* = 8.2, 2.3 Hz, 0.6H), 6.98 (dd, *J* = 8.0, 1.6 Hz, 0.4H), 5.78 (s, 0.4H), 4.10 (s, 1.2H), 3.88 – 3.81 (m, 3H), 3.07 (br, 2.4H), 3.04 (s, 1.8H), 3.00 (s, 1.8H).; ¹³C NMR (126 MHz, CDCl₃) δ 193.7, 172.3, 171.0, 167.1, 159.8, 159.7, 137.5, 136.5, 129.7, 129.4, 121.4, 120.2, 118.3, 116.4, 112.7, 111.3, 84.8, 55.4, 55.4, 46.0, 38.0, 35.6.



3-(4-Methoxyphenyl)-*N,N*-dimethyl-3-oxopropanamide^[7] (**4k**)

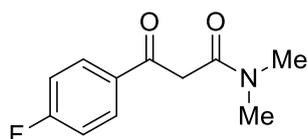
[ketone/enol = 5/1]:

4-Methoxy-*N*-methyl-*N*-phenylbenzamide (241 mg, 1.0 mmol) afforded 3-(4-methoxyphenyl)-*N,N*-dimethyl-3-oxopropanamide (**4j**) (157 mg, 0.71 mmol, 71% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (600 MHz, CDCl₃) δ 8.03 (d, *J* = 8.9 Hz, 1.7H), 7.76 (d, *J* = 8.9 Hz, 0.3H), 6.98 – 6.89 (m, 2H), 5.72 (s, 0.15H), 4.08 (s, 1.7H), 3.92 – 3.83 (m, 3H), 3.13 – 2.97 (m, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 192.3, 172.5, 171.1, 167.2, 163.9, 161.6, 131.1, 129.3, 129.1, 127.5, 113.9, 113.7, 83.1, 55.5, 55.4, 45.9, 38.1, 35.6.



3-(3-Fluorophenyl)-*N,N*-dimethyl-3-oxopropanamide (**4l**) [ketone/enol = 1/1.1]:

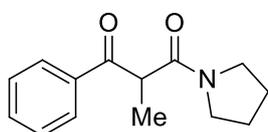
3-Fluoro-*N*-methyl-*N*-phenylbenzamide (229 mg, 1.0 mmol) afforded 3-(3-fluorophenyl)-*N,N*-dimethyl-3-oxopropanamide (**4l**) (115 mg, 0.55 mmol, 55% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (500 MHz, CDCl₃) δ 7.83 – 7.80 (m, 0.45H), 7.72 – 7.68 (m, 0.45H), 7.58 – 7.54 (m, 0.55H), 7.51 – 7.43 (m, 1H), 7.40 – 7.34 (m, 0.55H), 7.31 – 7.27 (m, 0.45H), 5.78 (s, 0.55H), 4.08 (s, 0.9H), 3.16 – 3.02 (m, 4.65H), 3.00 (s, 1.35H); ¹³C NMR (126 MHz, CDCl₃) δ 192.7, 170.9 (d, *J* = 289.8 Hz), 169.8, 166.5, 162.8 (d, *J* = 247.0 Hz), 161.8, 138.28 (d, *J* = 6.3 Hz), 137.35 (d, *J* = 7.5 Hz), 130.40 (d, *J* = 7.7 Hz), 129.95 (d, *J* = 8.2 Hz), 124.60 (d, *J* = 2.9 Hz), 121.50 (d, *J* = 2.9 Hz), 120.7 (d, *J* = 21.4 Hz), 117.3 (d, *J* = 21.42 Hz), 115.3 (d, *J* = 22.7 Hz), 112.9 (d, *J* = 23.9 Hz), 85.2, 46.0, 38.0, 35.6; HRMS (FD) *m/z*: [M + H]⁺ Calcd for C₁₁H₁₃FNO₂ 210.0925; Found 210.0920.



3-(4-Fluorophenyl)-*N,N*-dimethyl-3-oxopropanamide^[7] (**4m**)

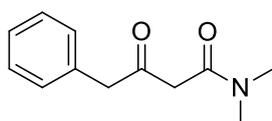
[ketone/enol = **1.7/1**]:

4-Fluoro-*N*-methyl-*N*-phenylbenzamide (229 mg, 1.0 mmol) afforded 3-(4-fluorophenyl)-*N,N*-dimethyl-3-oxopropanamide (**4m**) (169 mg, 0.81 mmol, 81% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (500 MHz, CDCl₃) δ 8.12 – 7.56 (m, 2H), 7.51 – 7.38 and 7.17 – 7.04 (both m, total 2H), 5.73 (s, 0.4 H), 4.07 (s, 1.2H), 3.16 – 2.94 (m, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 192.3, 172.2, 170.3, 166.1 (d, *J* = 235.6 Hz), 165.8 (d, *J* = 209.2 Hz), 132.7 (d, *J* = 3.0 Hz), 131.5 (d, *J* = 9.5 Hz), 128.7 (d, *J* = 4.2 Hz), 128.0 (d, *J* = 8.6 Hz), 115.8 (d, *J* = 22.7 Hz), 115.4 (d, *J* = 22.7 Hz), 84.3, 46.0, 38.1, 35.6.



2-Methyl-1-phenyl-3-(pyrrolidin-1-yl)propane-1,3-dione (**4n**):

N-Methyl-*N*-phenylbenzamide (211 mg, 1.0 mmol) afforded 2-methyl-1-phenyl-3-(pyrrolidin-1-yl)propane-1,3-dione (**4n**) (42 mg, 0.18 mmol, 18% yield) as white solid by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); m.p. 78 – 79 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.98 – 7.92 (m, 2H), 7.57 – 7.53 (m, 1H), 7.47 – 7.42 (m, 2H), 4.32 (q, *J* = 7.1 Hz, 1H), 3.48 (t, *J* = 6.9 Hz, 2H), 3.46 – 3.40 (m, 1H), 3.36 – 3.30 (m, 1H), 1.96 – 1.88 (m, 2H), 1.86 – 1.79 (qd, *J* = 6.9, 1.1 Hz, 2H), 1.49 (d, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 197.0, 169.0, 135.8, 133.3, 128.8, 128.3, 49.0, 46.6, 46.2, 26.2, 24.2, 14.0; HRMS (FD) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₈NO₂ 232.1332; Found 232.1336.



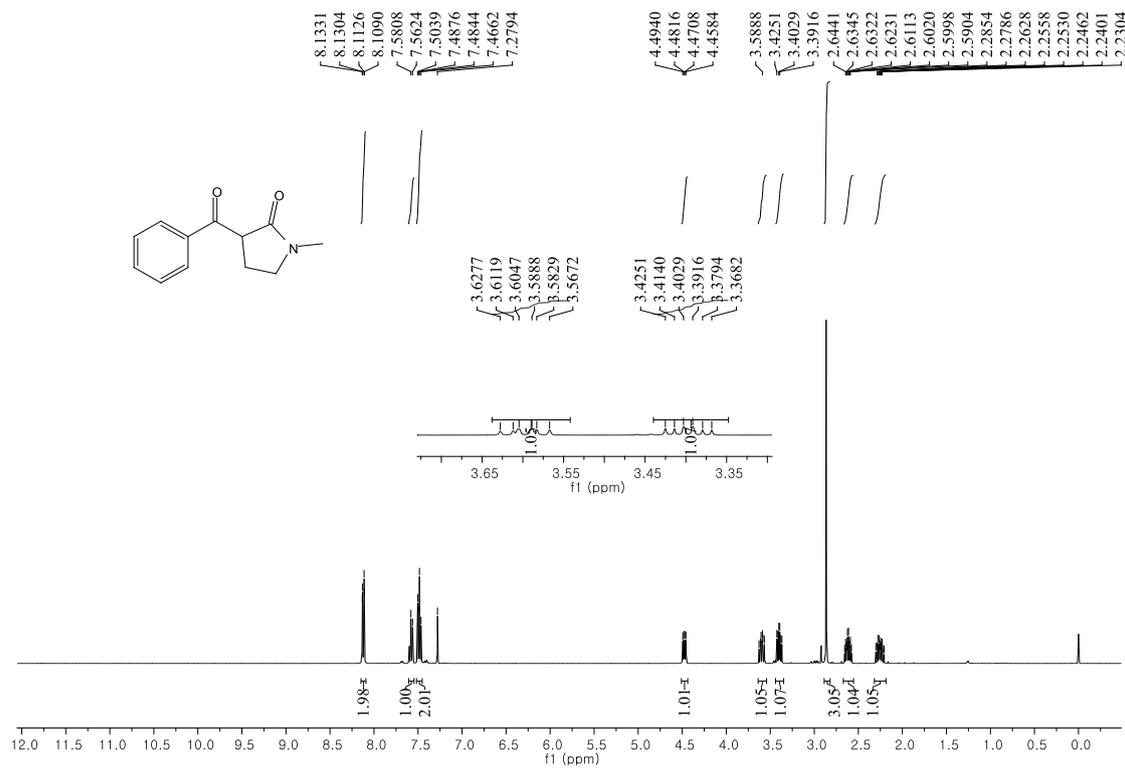
***N,N*-Dimethyl-3-oxo-4-phenylbutanamide**^[8-9] (**4o**) [ketone/enol = **4/1**]:

N-Methyl-*N*-phenylbenzamide (211 mg, 1.0 mmol) afforded *N,N*-dimethyl-3-oxo-4-phenylbutanamide (**4o**) (99 mg, 0.48 mmol, 48% yield) as colorless oil by silica column chromatography (ethyl acetate/hexane 1:1 to 3:1); ¹H NMR (400 MHz, CDCl₃) δ 7.37 – 7.17 (m, 5H), 5.07, 3.85, 3.72 (all s, total 2H), 3.53, 3.50 (both s, total 2 H), 3.00, 2.96, 2.93, 2.84 (all s, total 6H); ¹³C NMR (101 MHz, CDCl₃) δ 202.1, 176.4, 172.0, 171.2, 166.7, 136.4, 135.1, 133.6, 129.6, 129.2, 128.79, 128.75, 128.7, 128.5, 127.3, 127.3, 126.8, 126.7, 87.23, 49.9, 48.2, 42.2, 41.0, 37.8, 35.4.

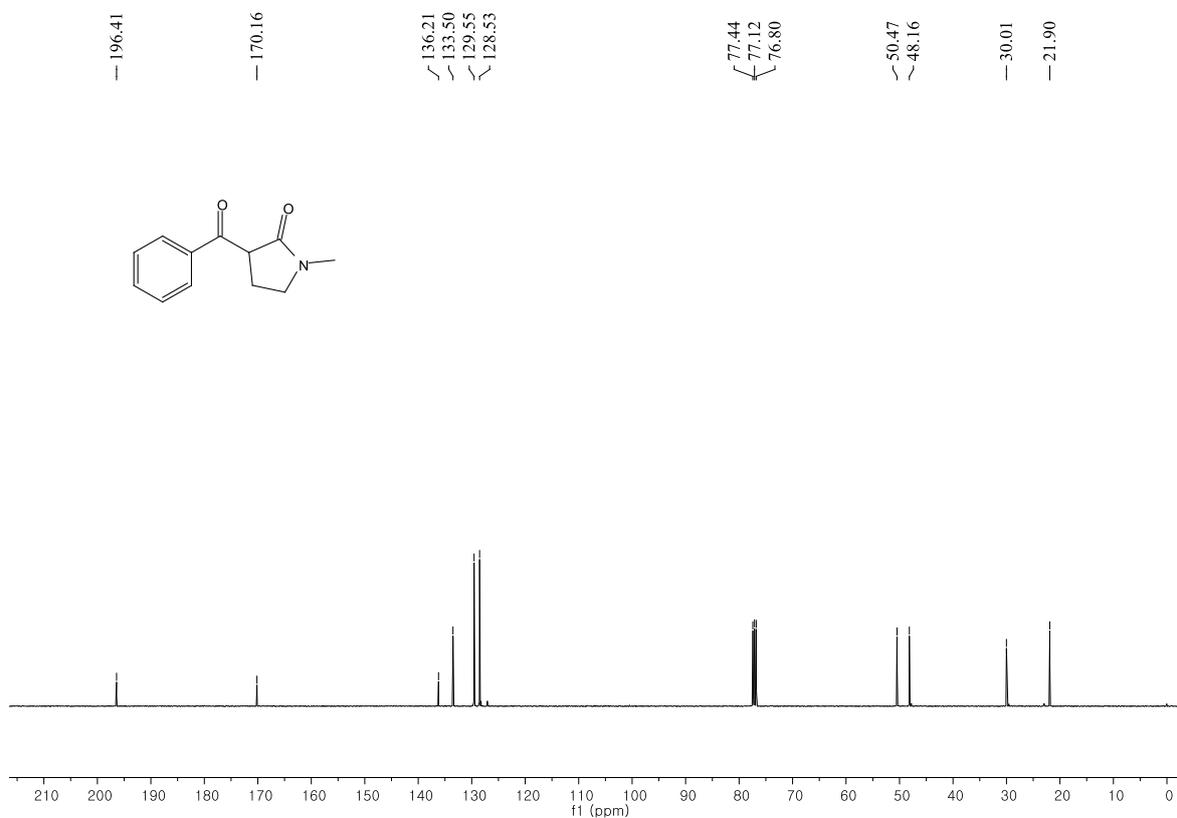
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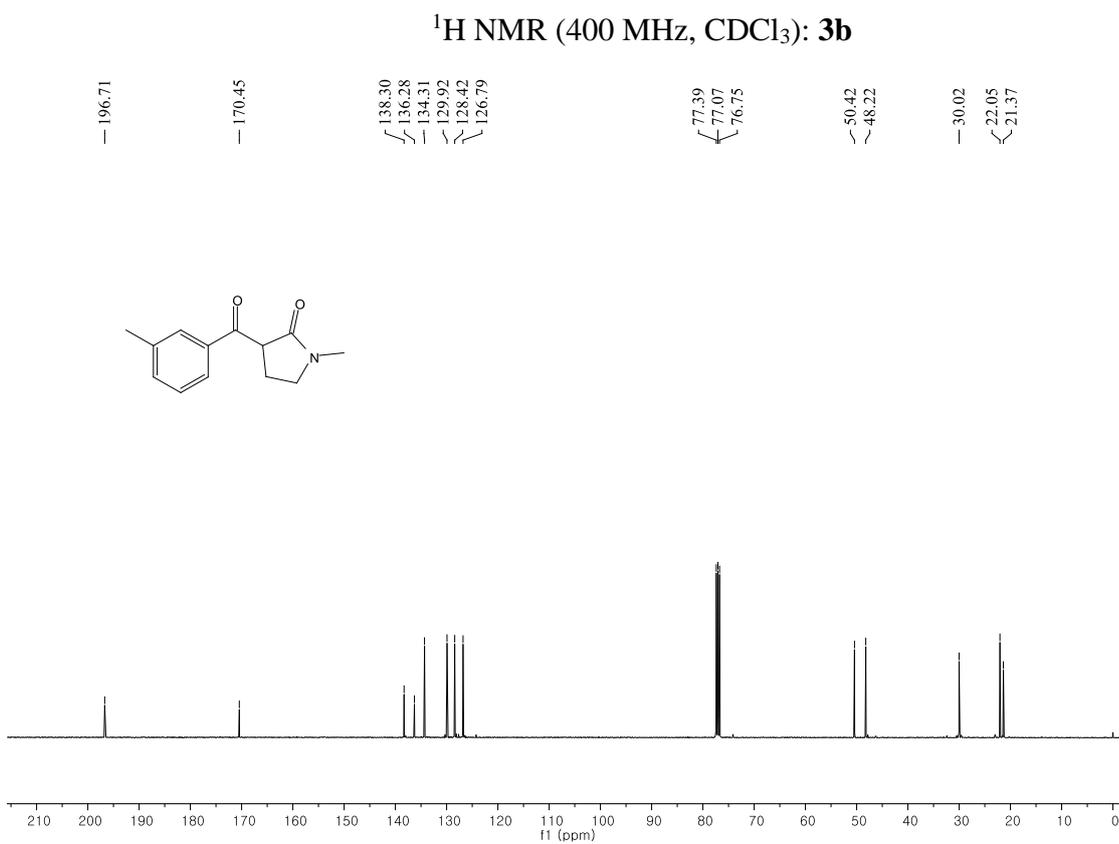
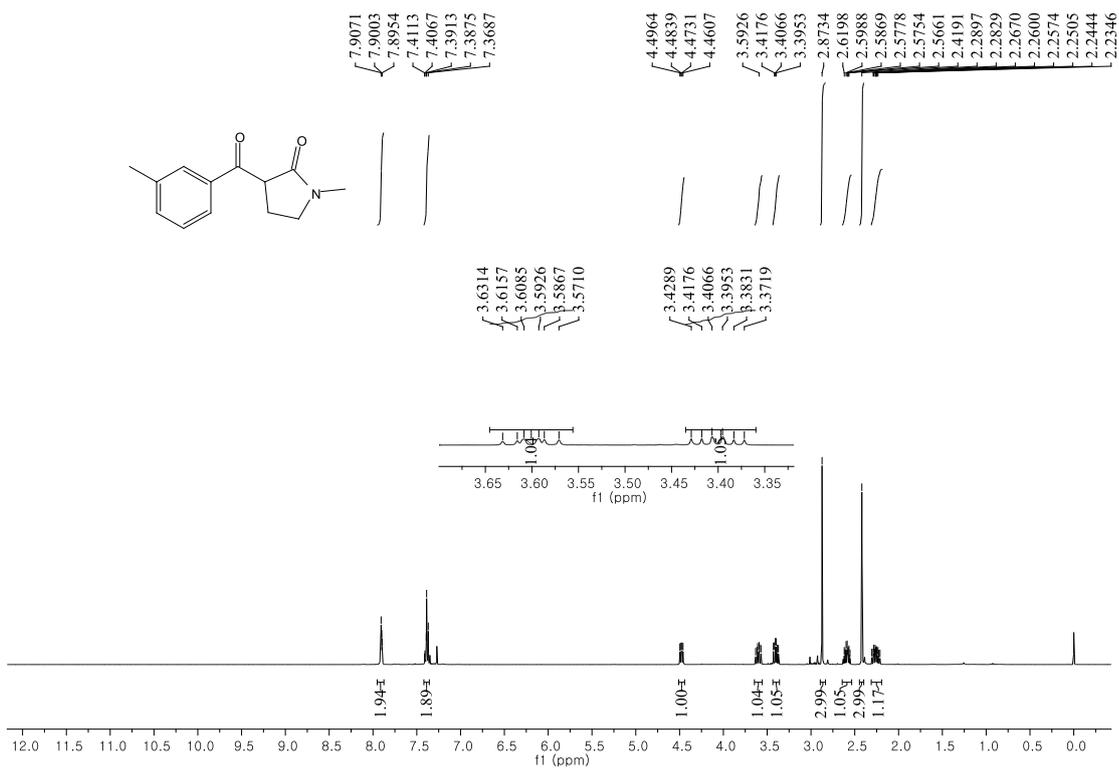
5. Copy of NMR Spectra

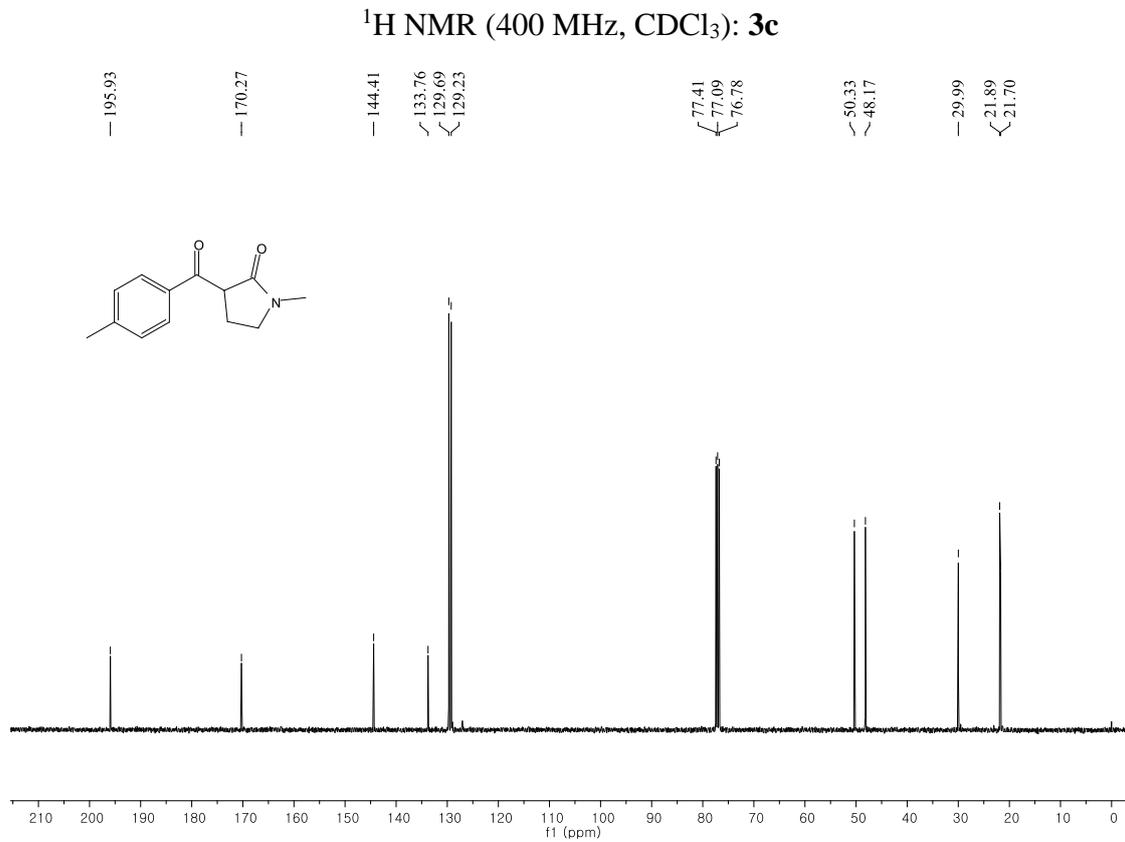
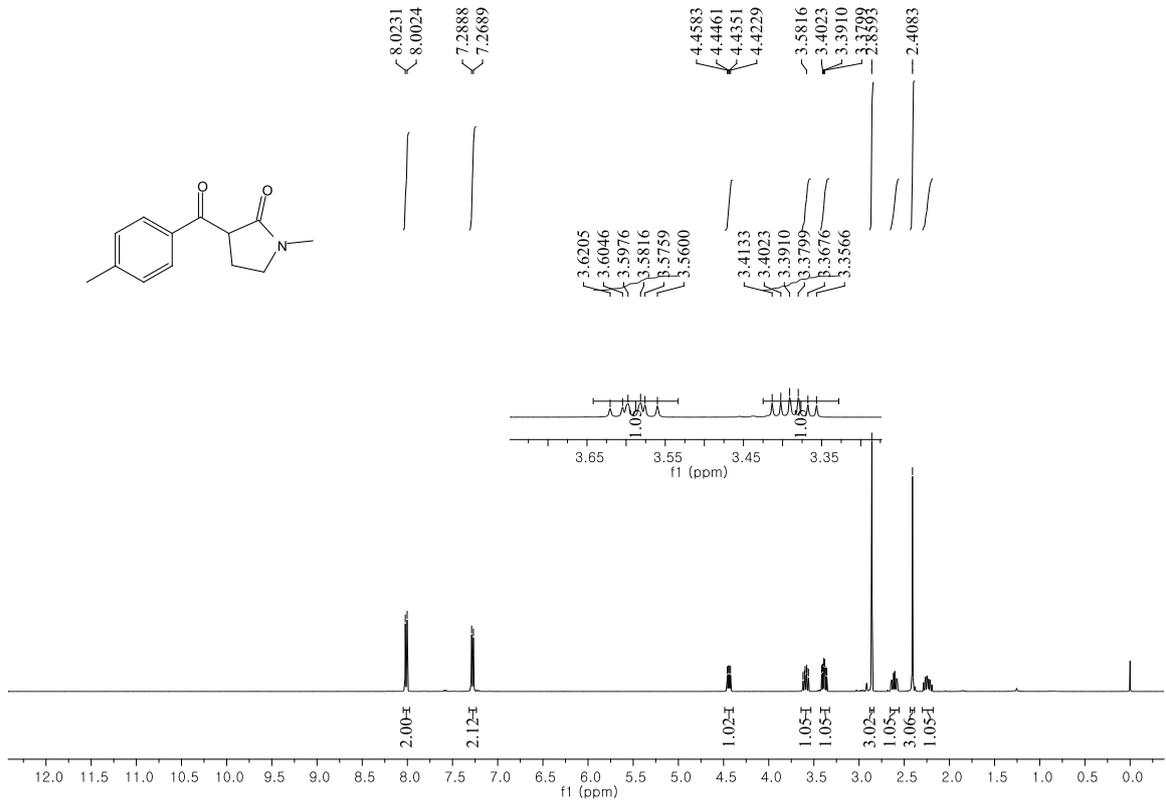


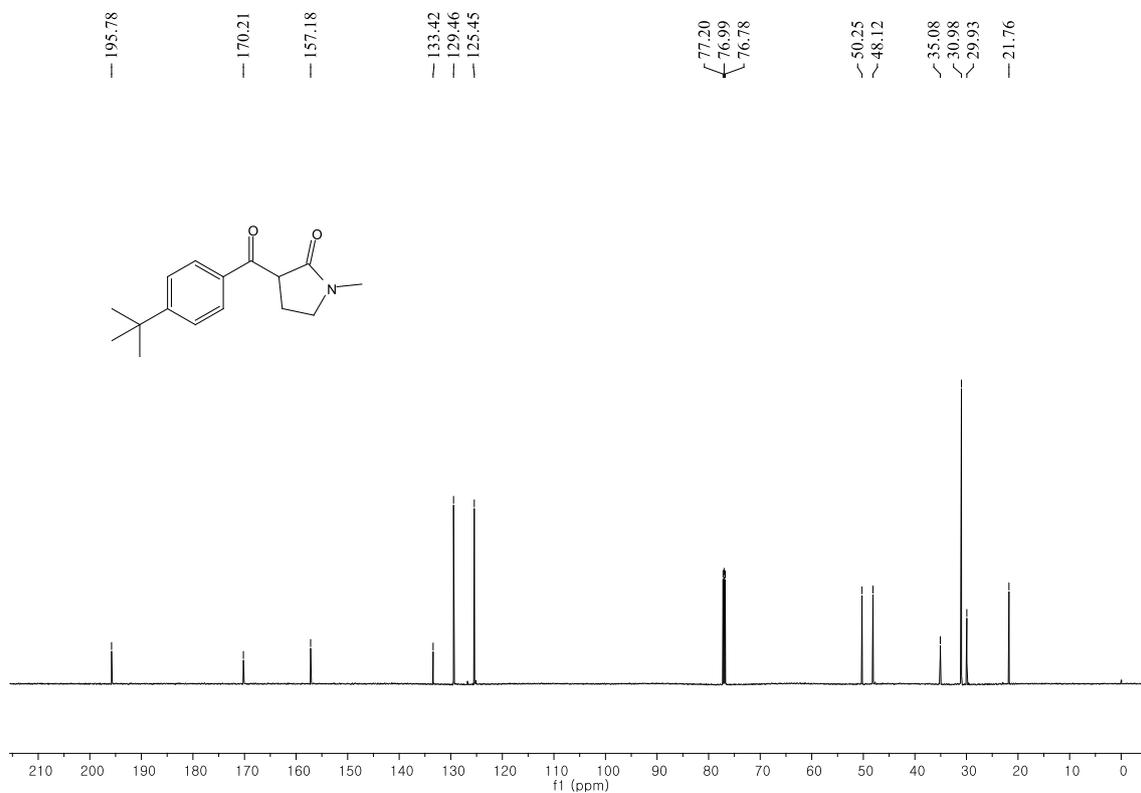
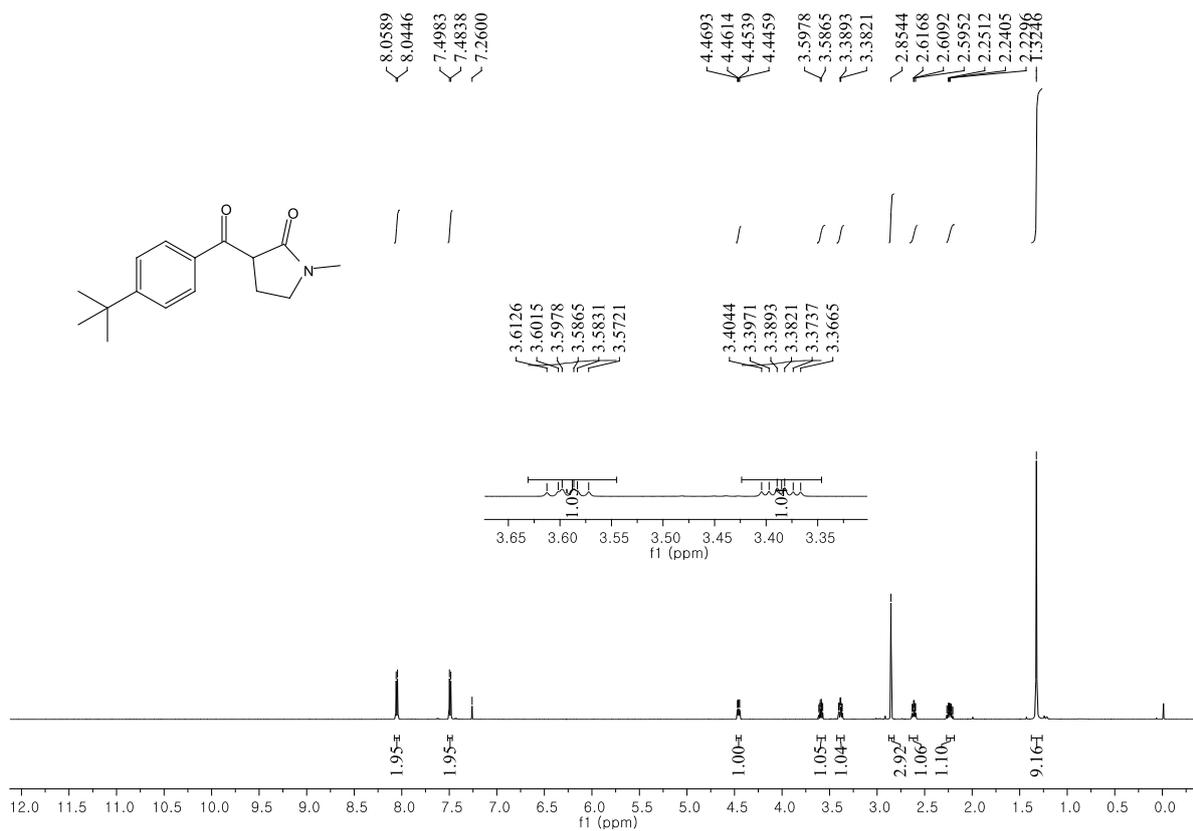
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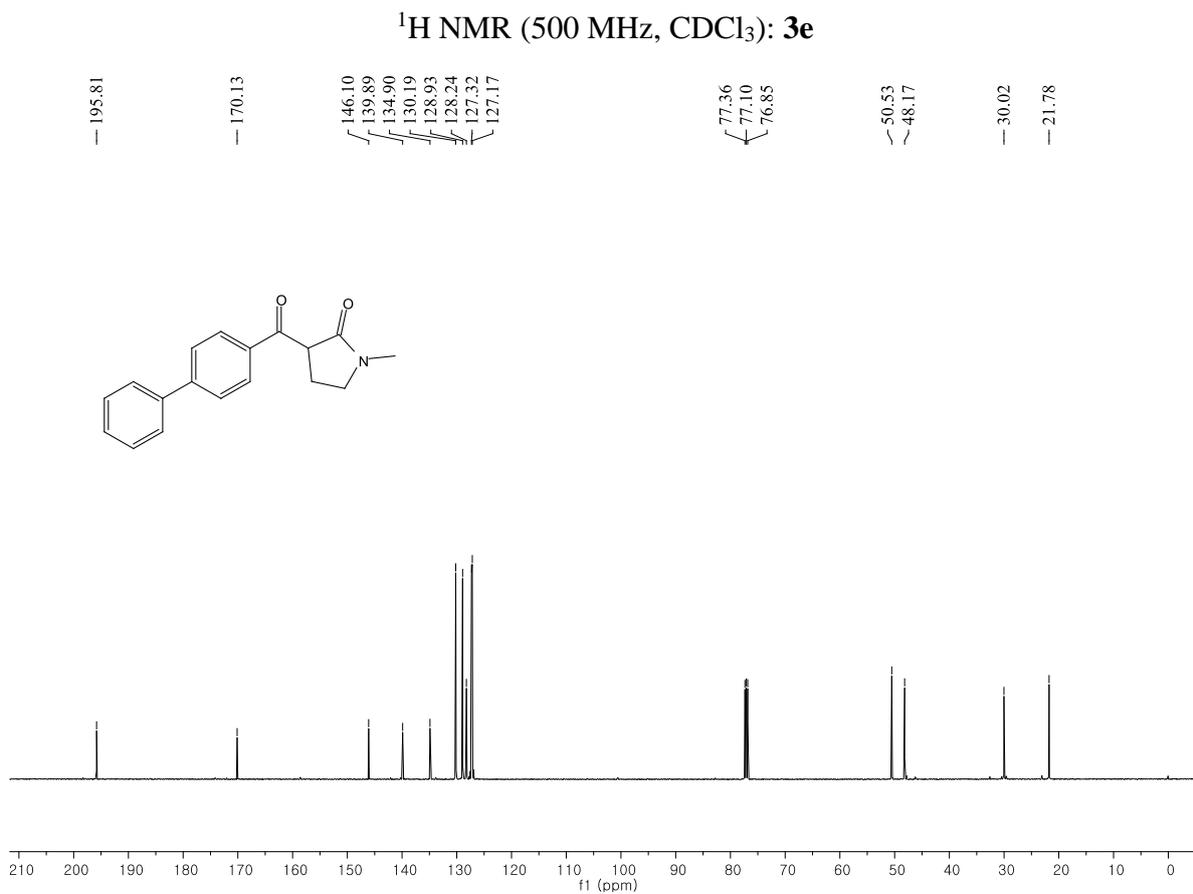
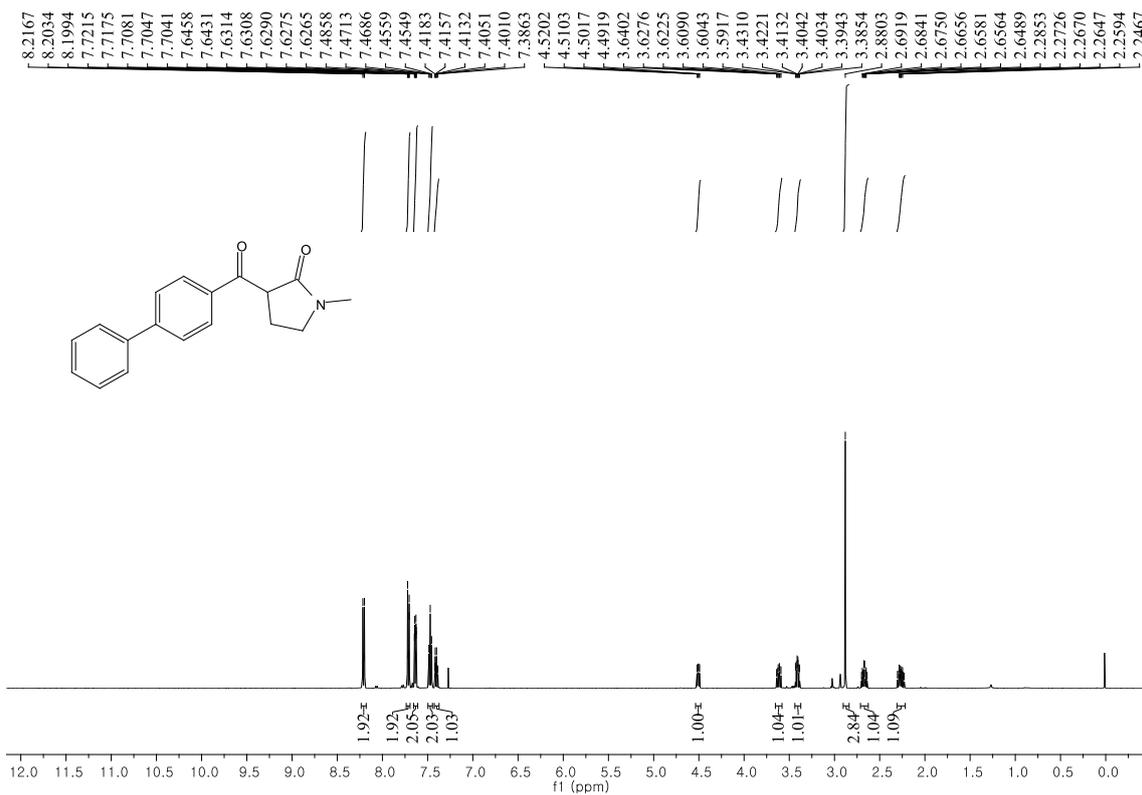


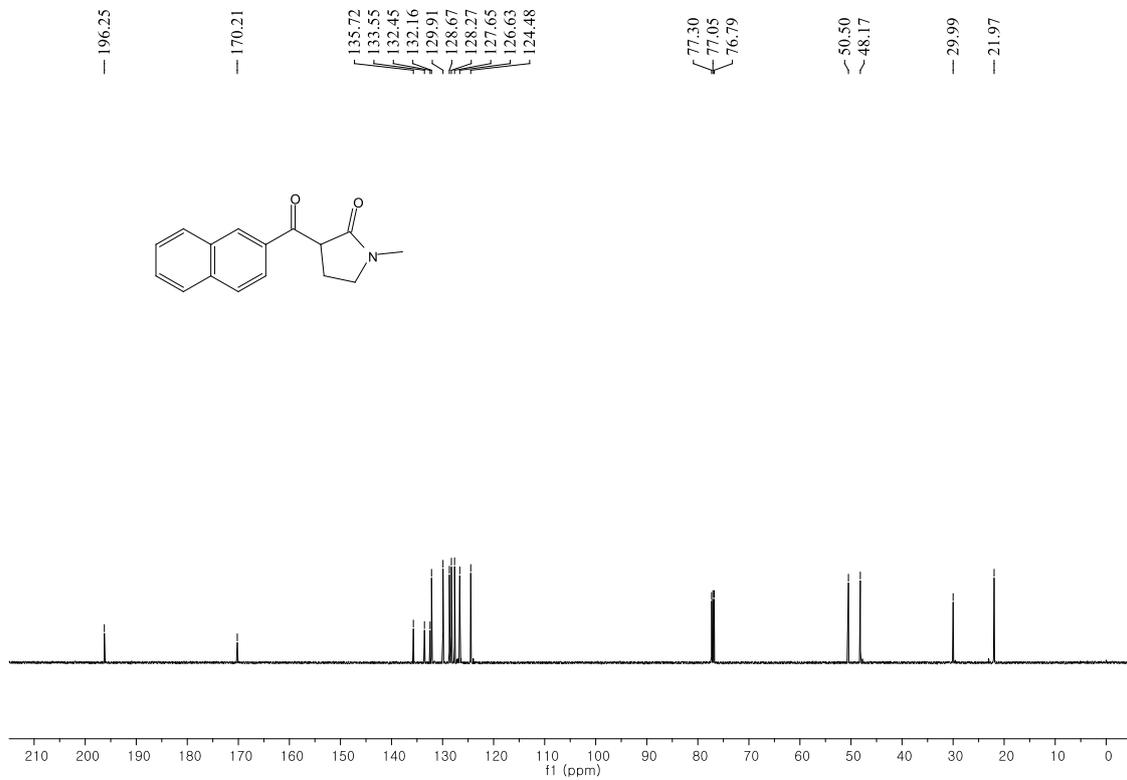
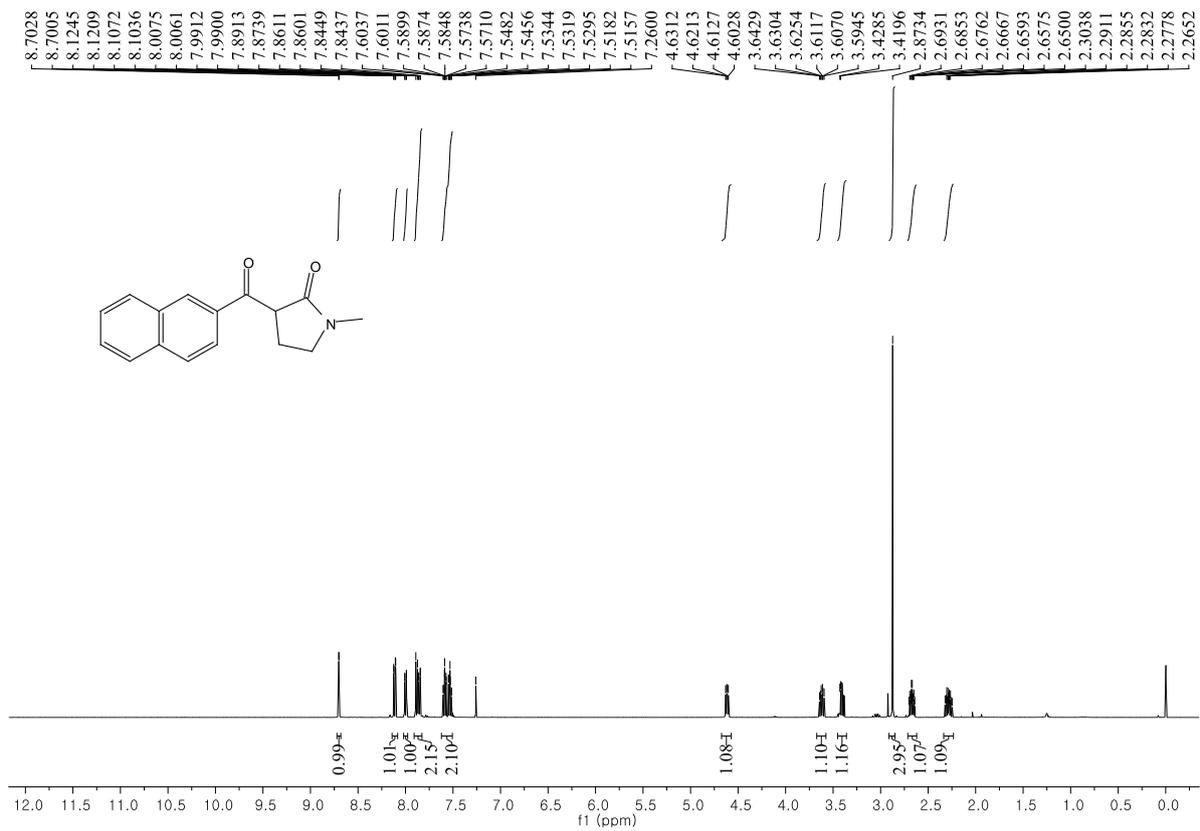
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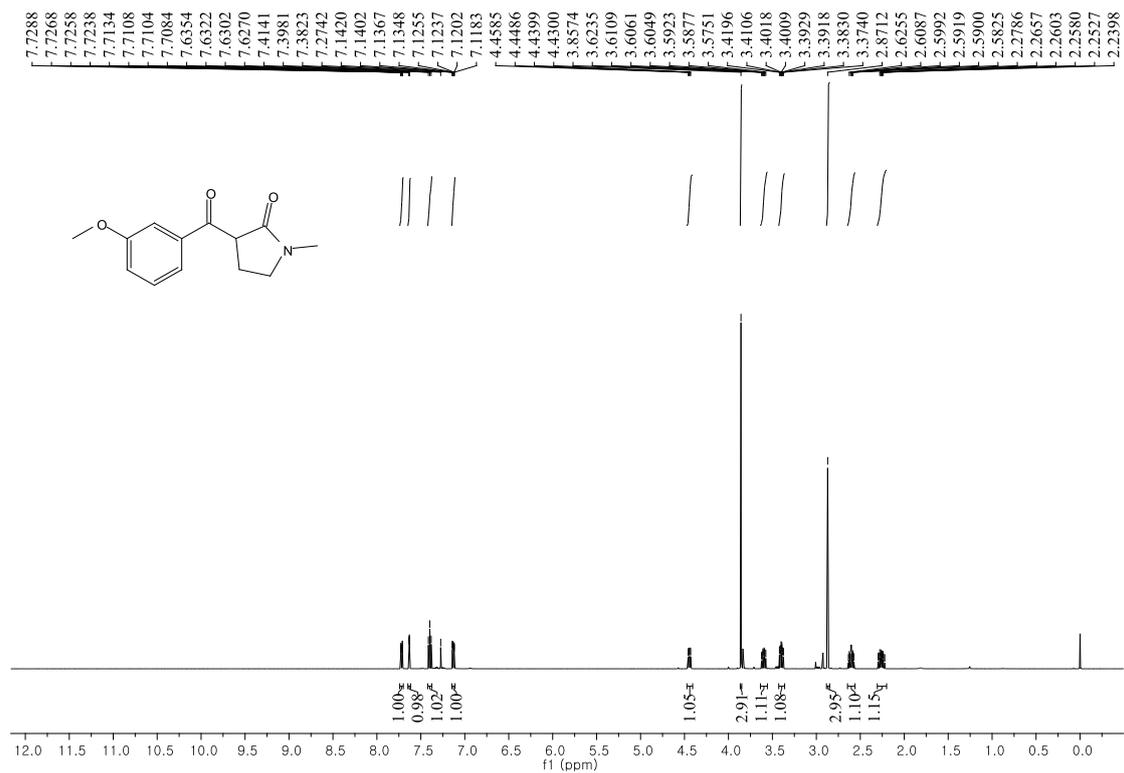




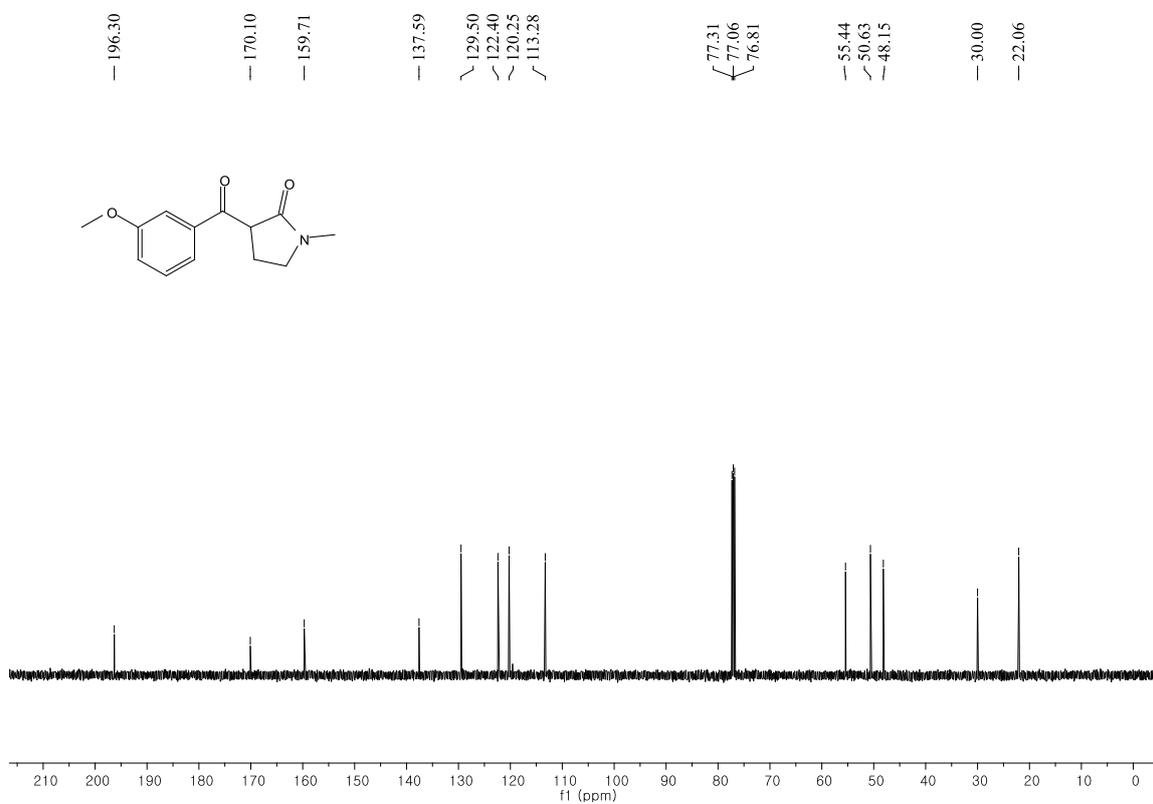




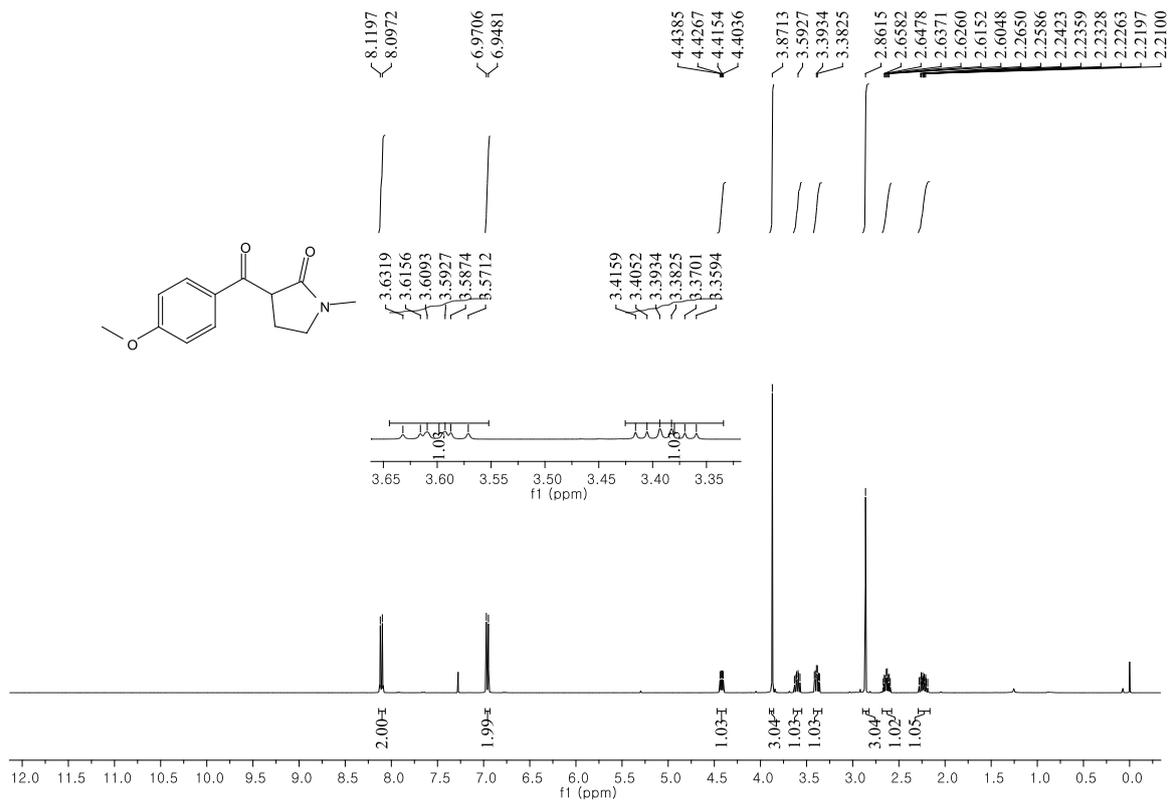




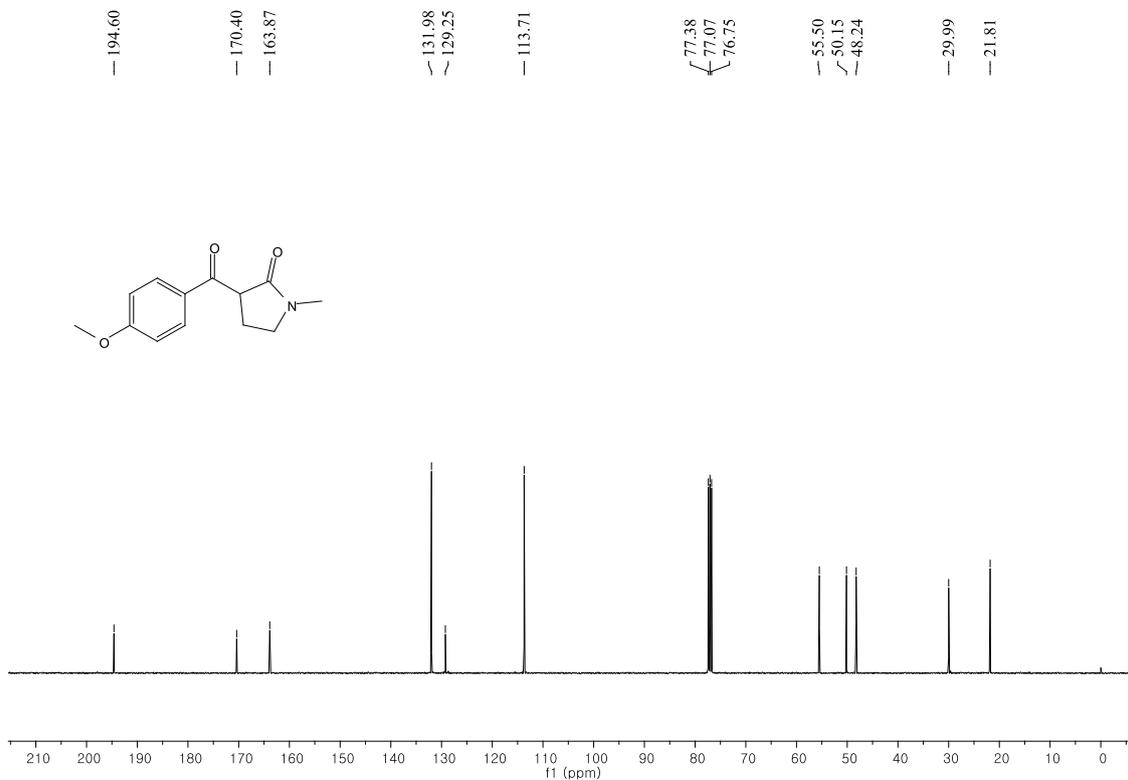
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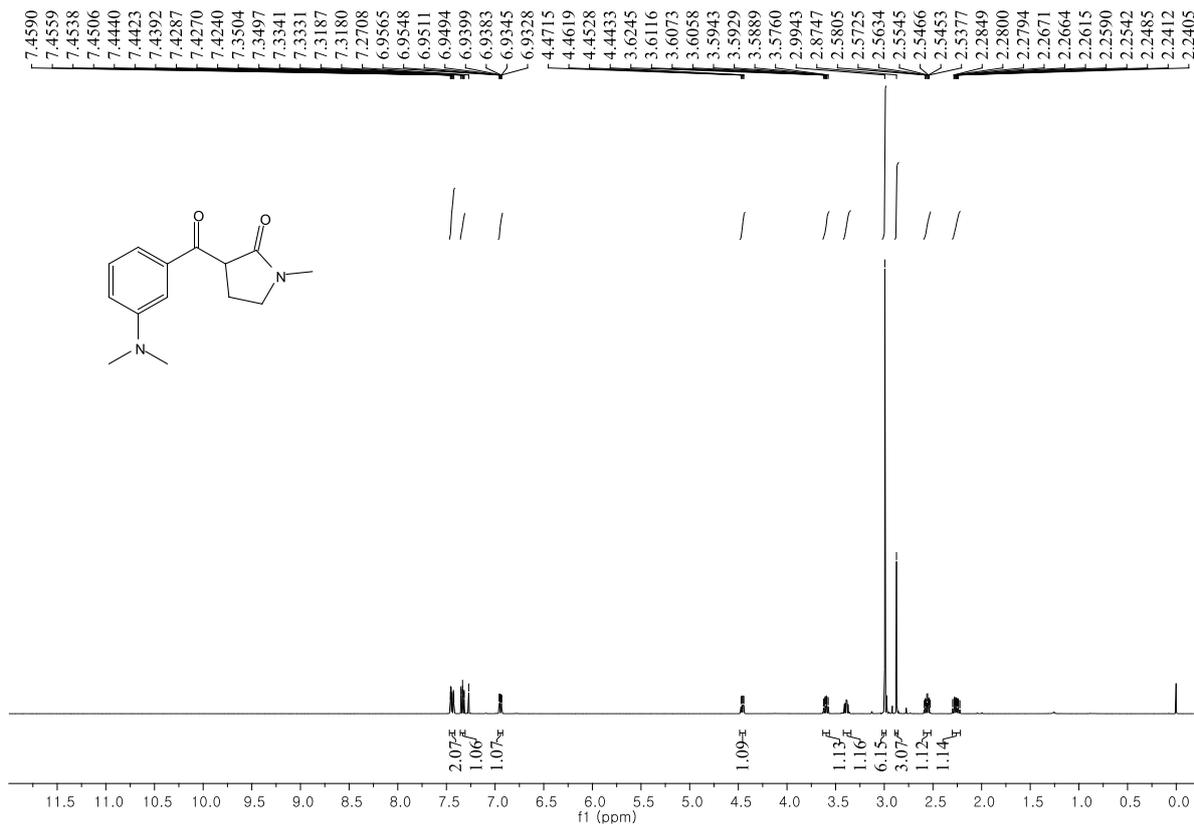
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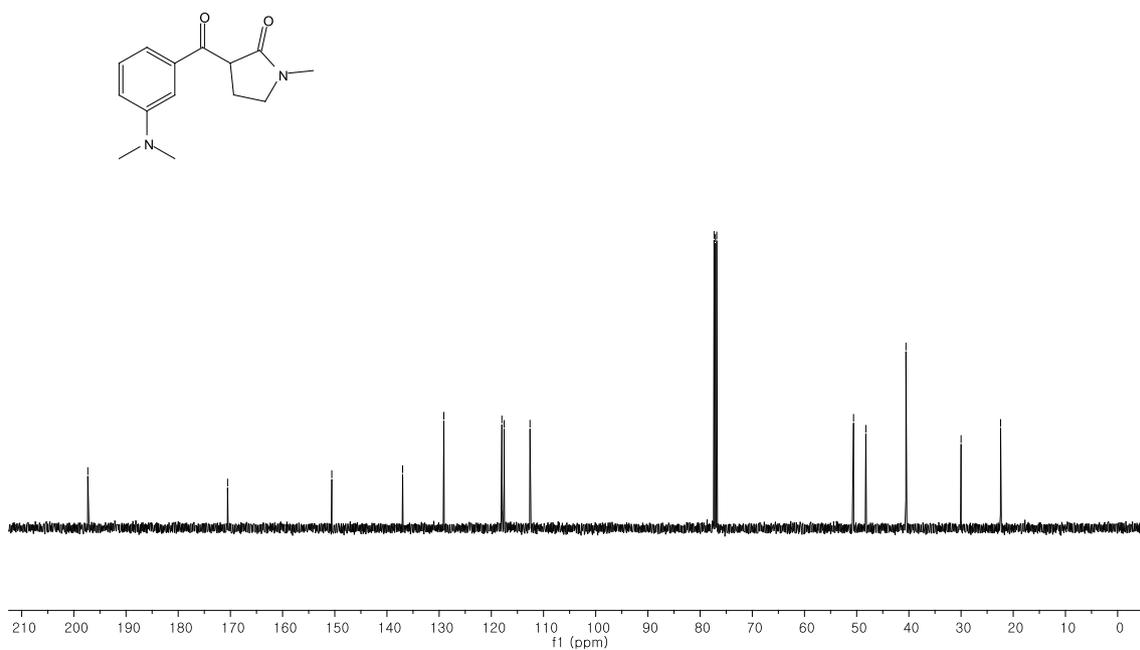
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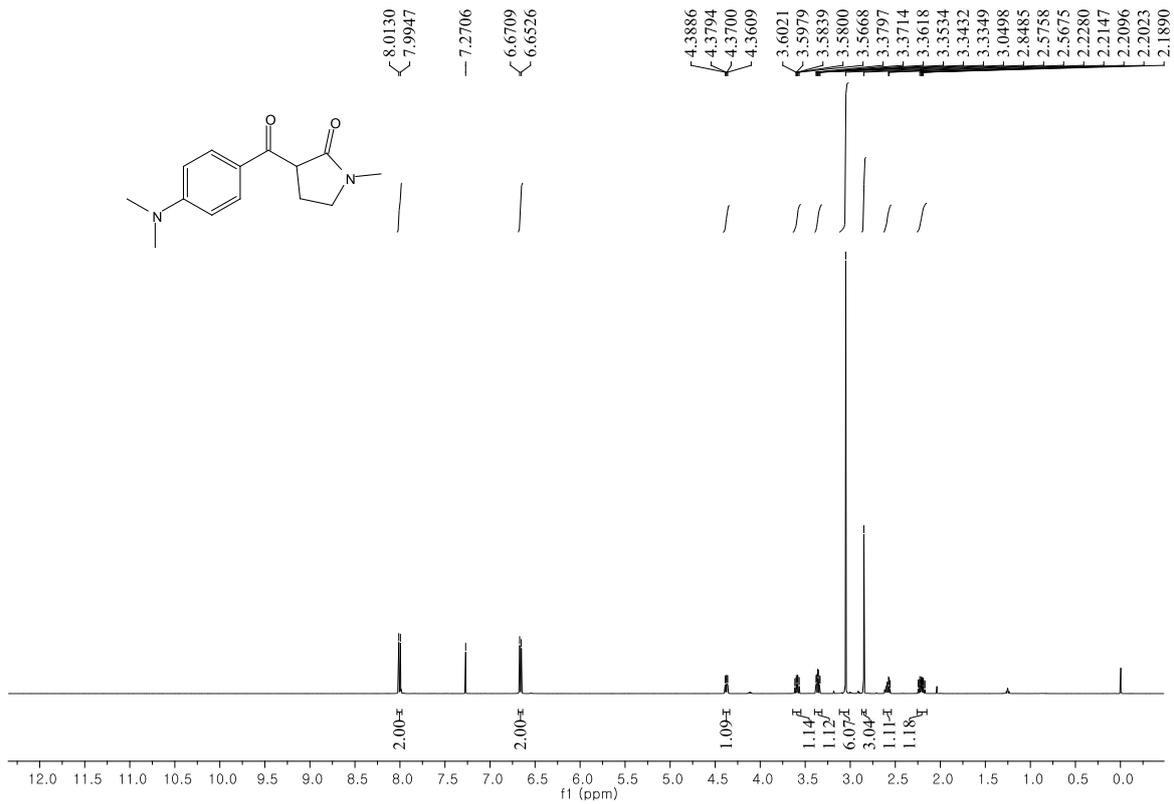
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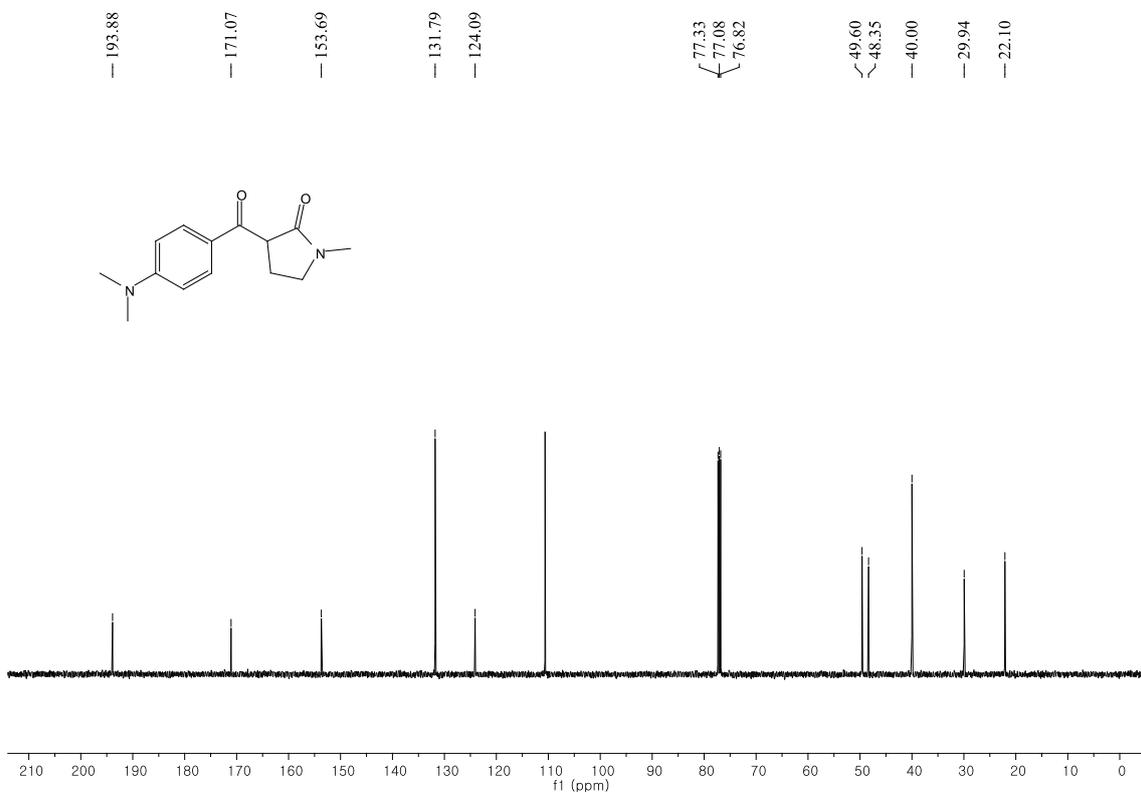
— 197.32
 — 170.54
 — 150.57
 — 137.00
 — 129.10
 — 117.98
 — 117.56
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 — 77.32
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 — 76.81
 — 50.60
 — 48.24
 — 40.56
 — 30.00
 — 22.42



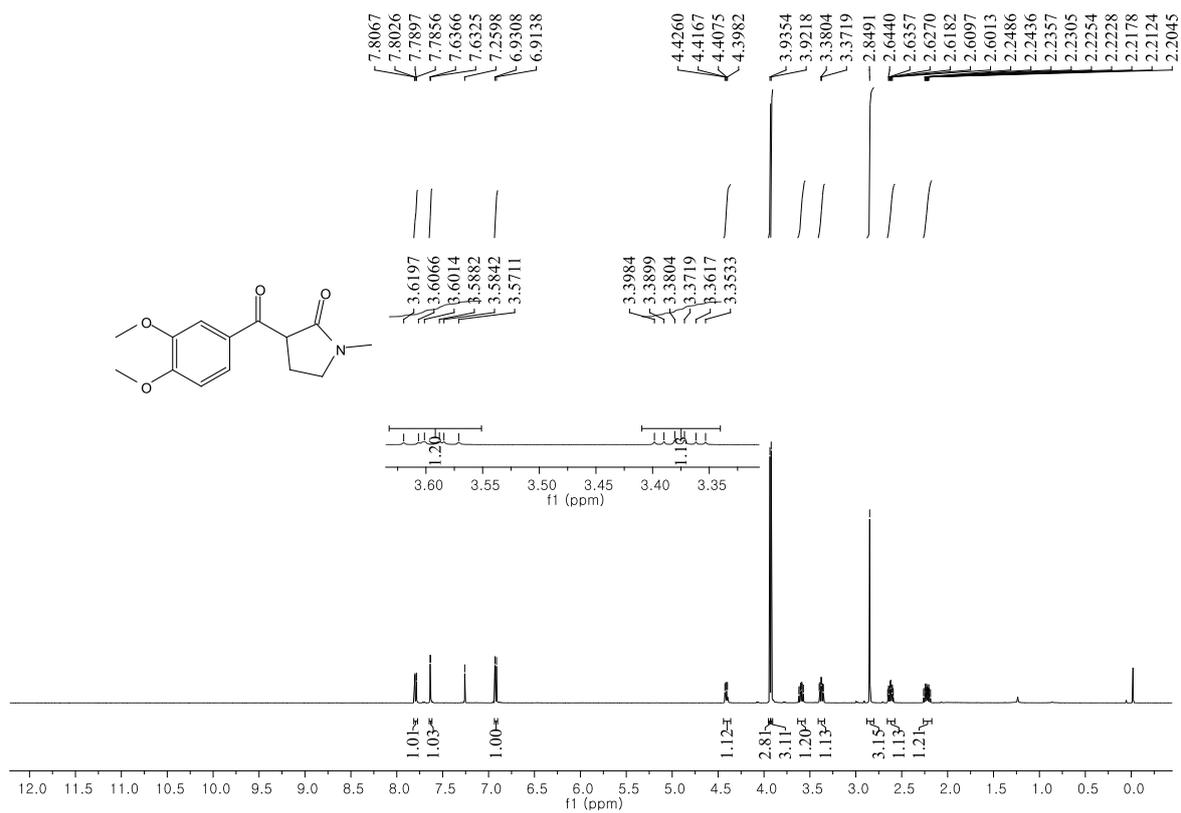
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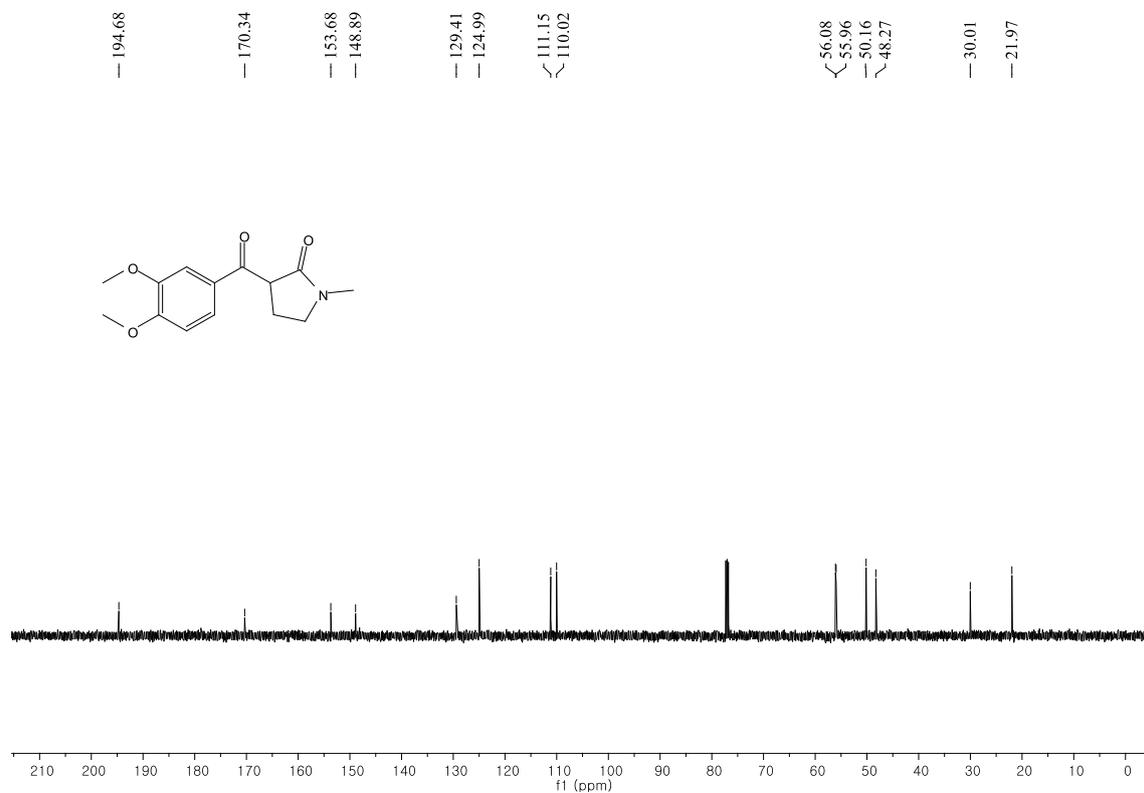
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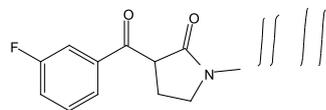
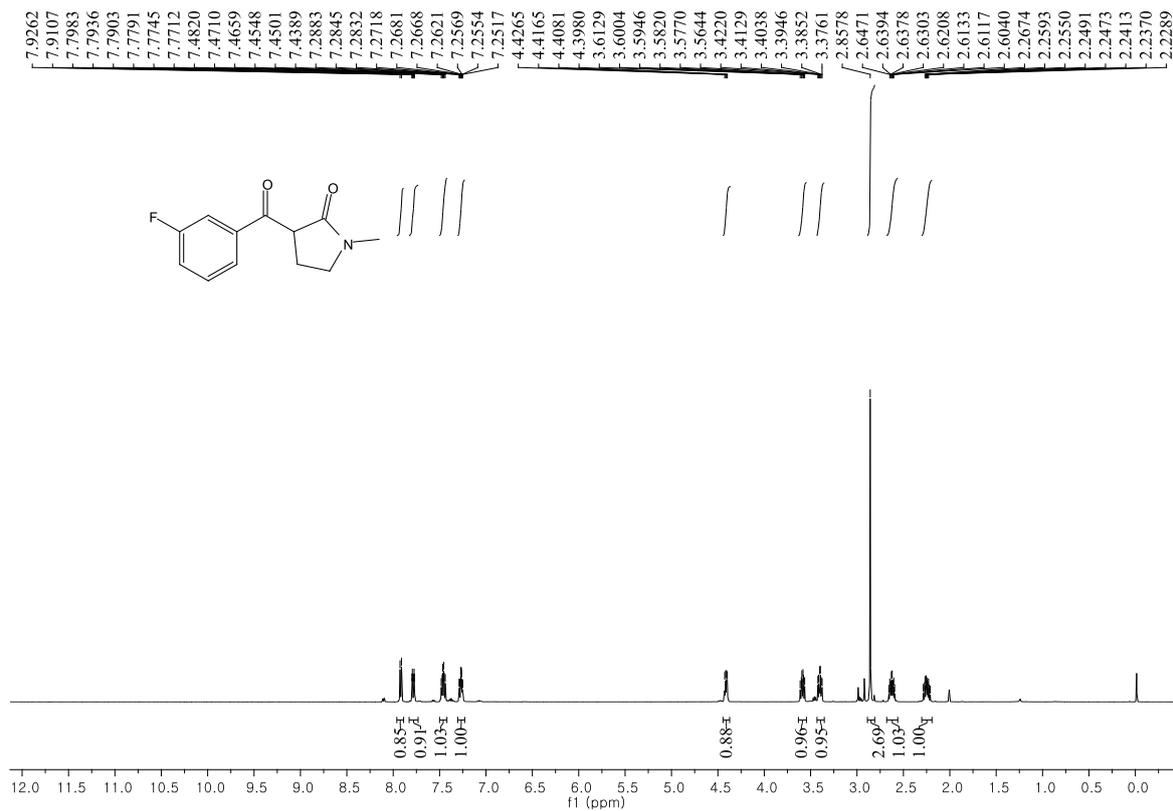
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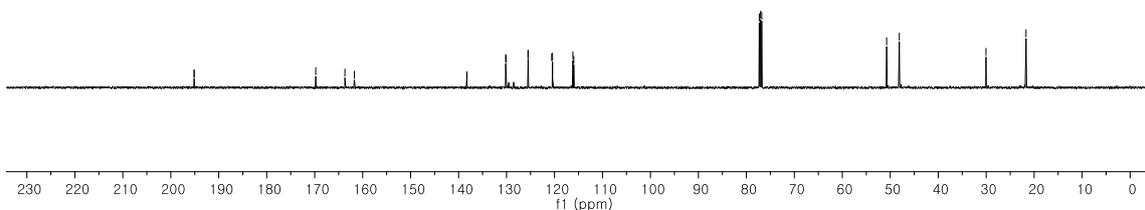
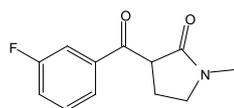
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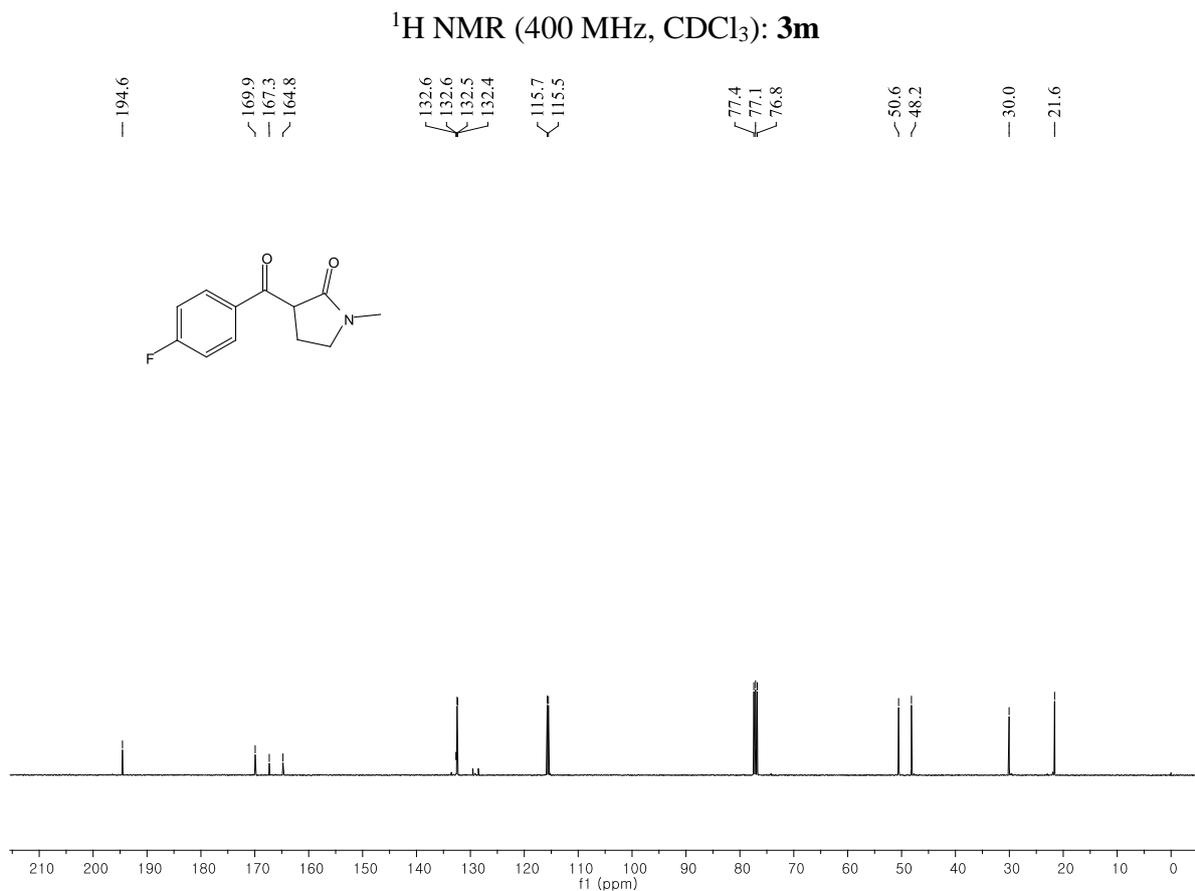
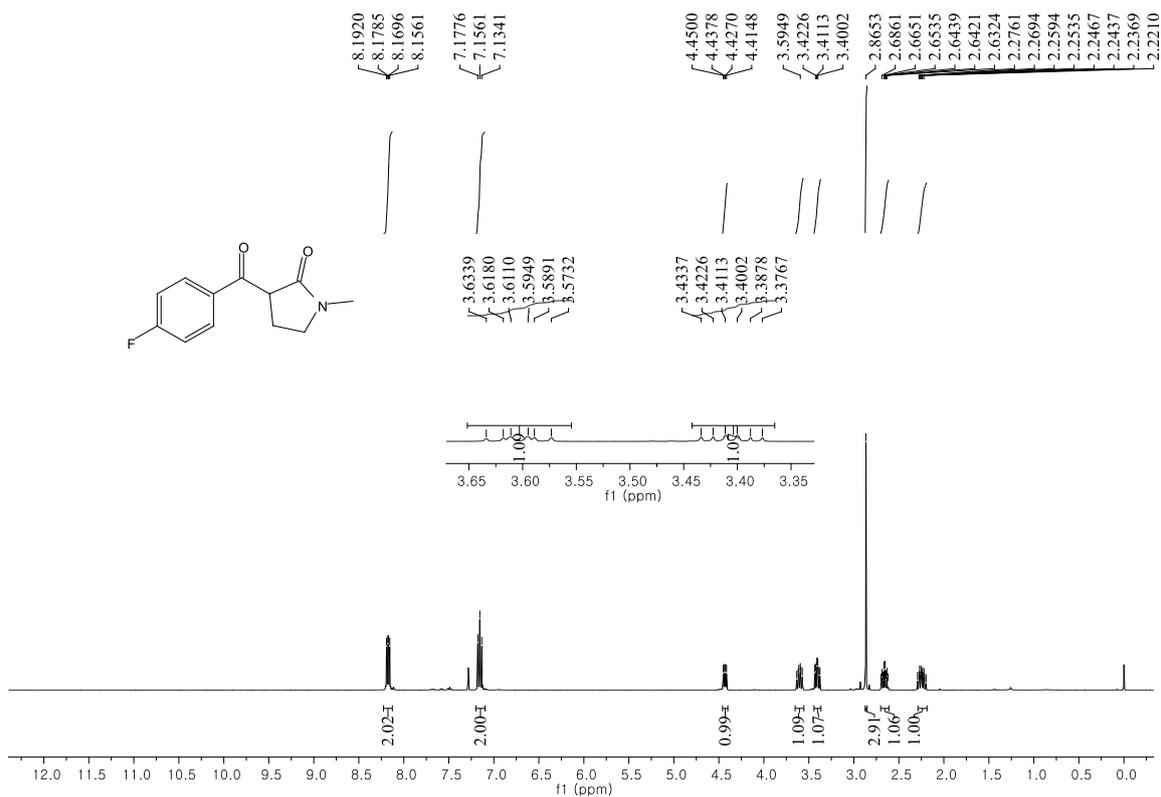
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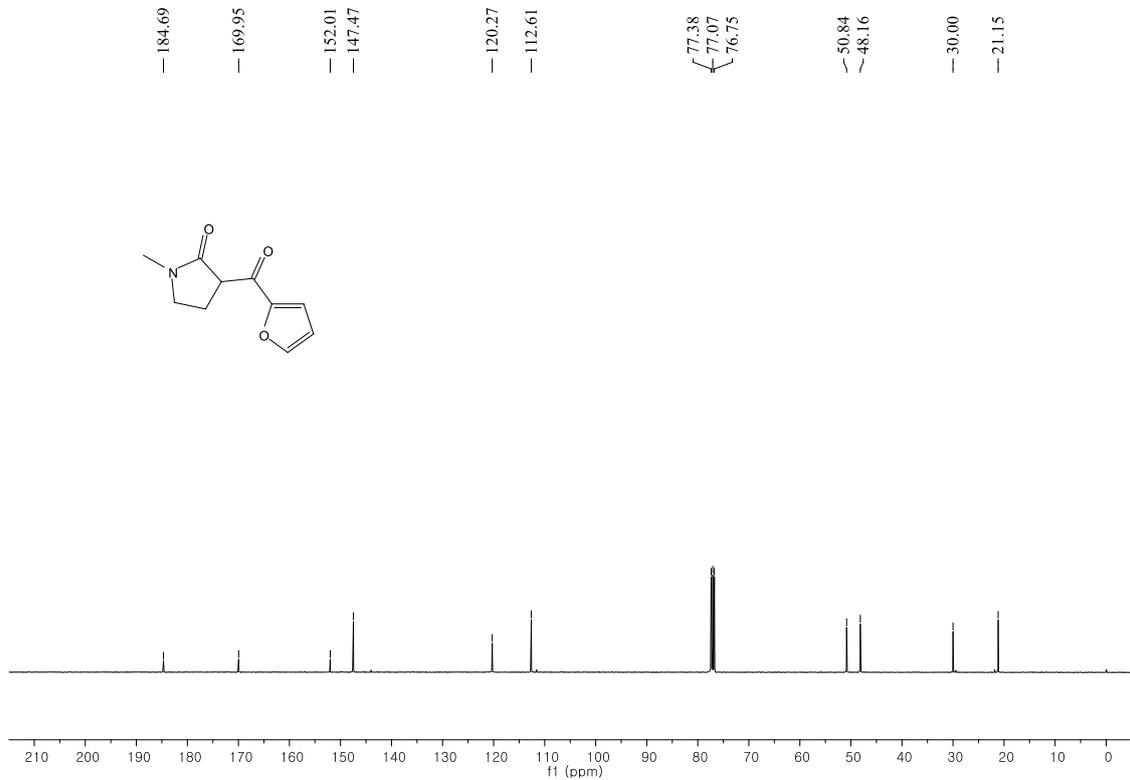
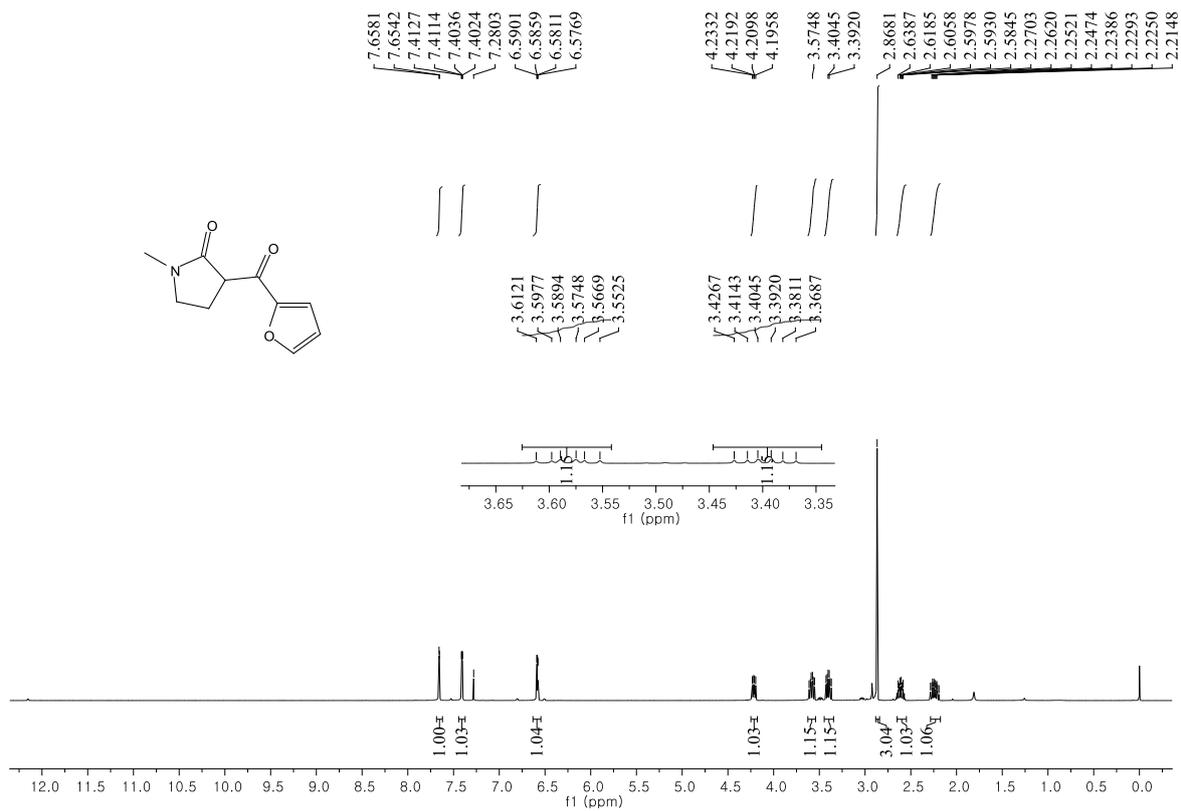


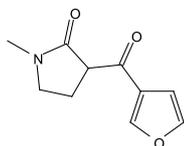
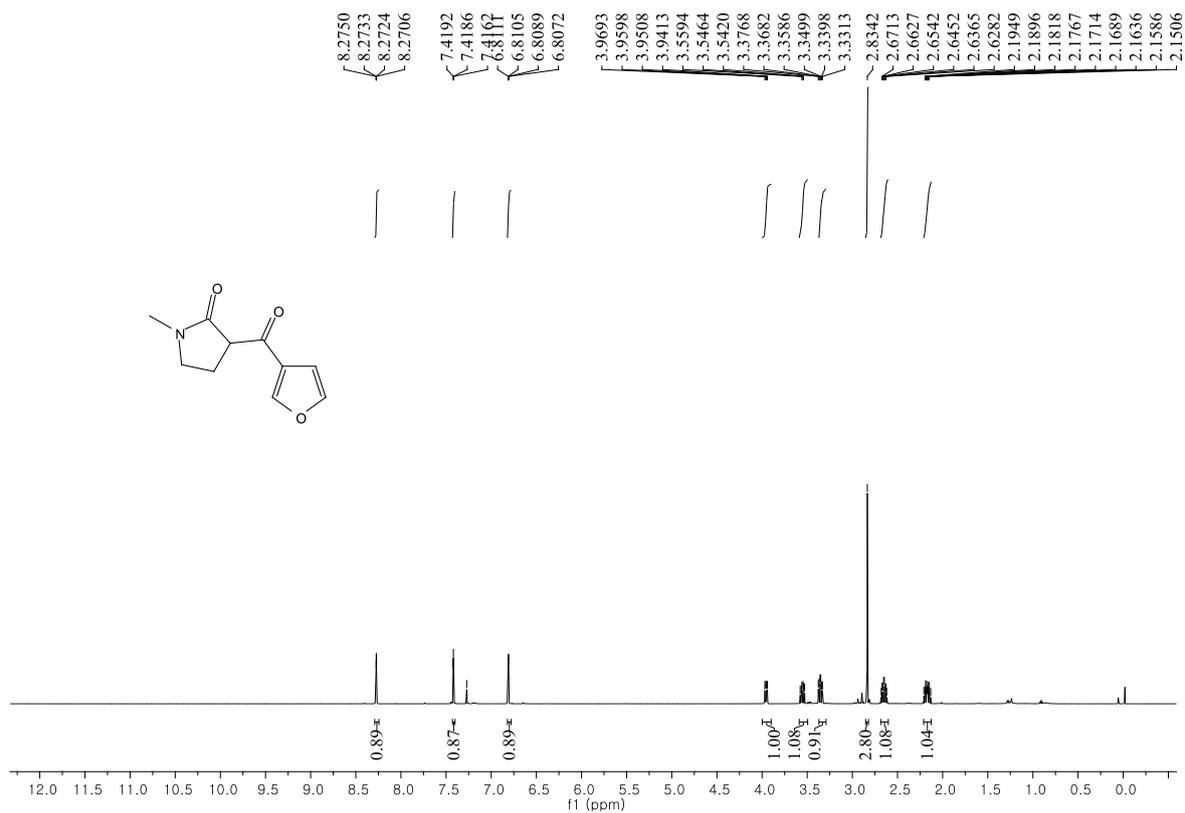
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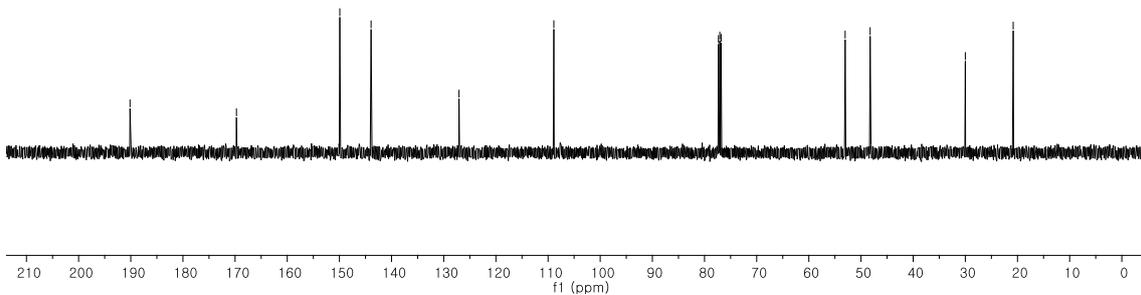
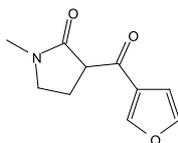
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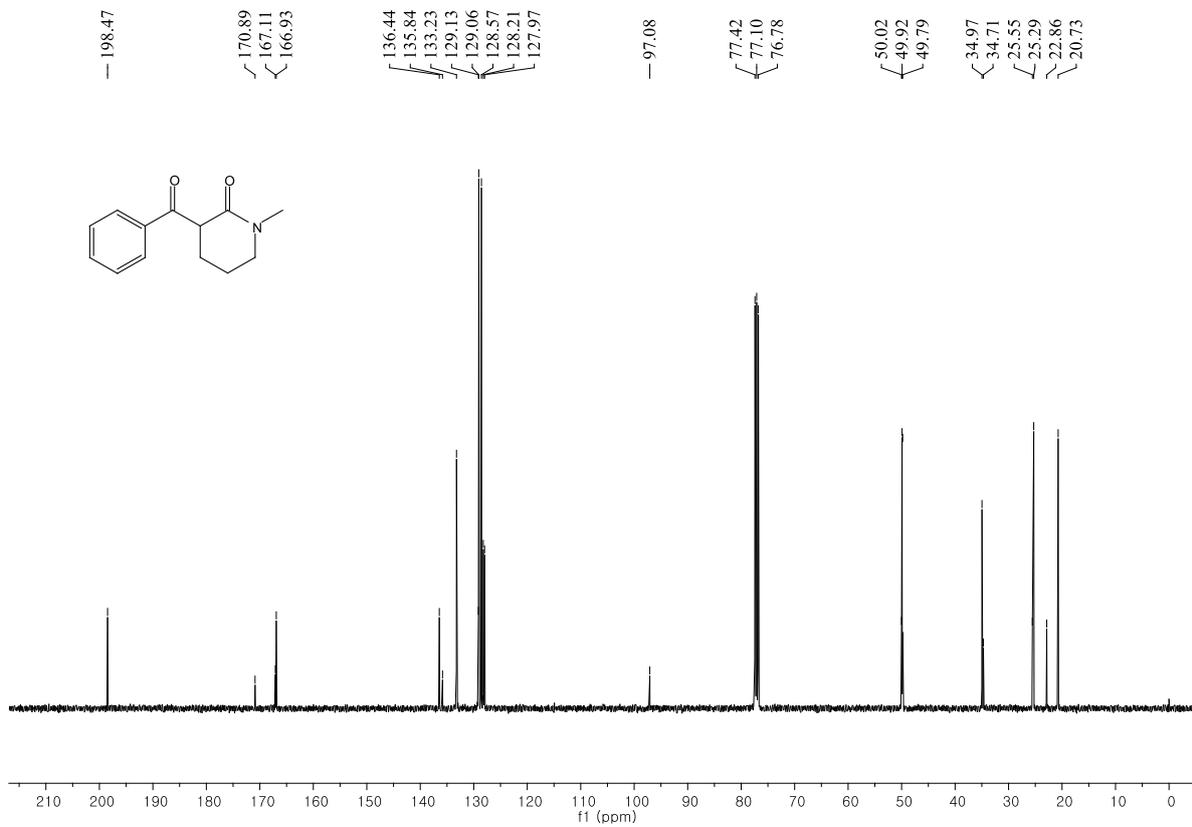
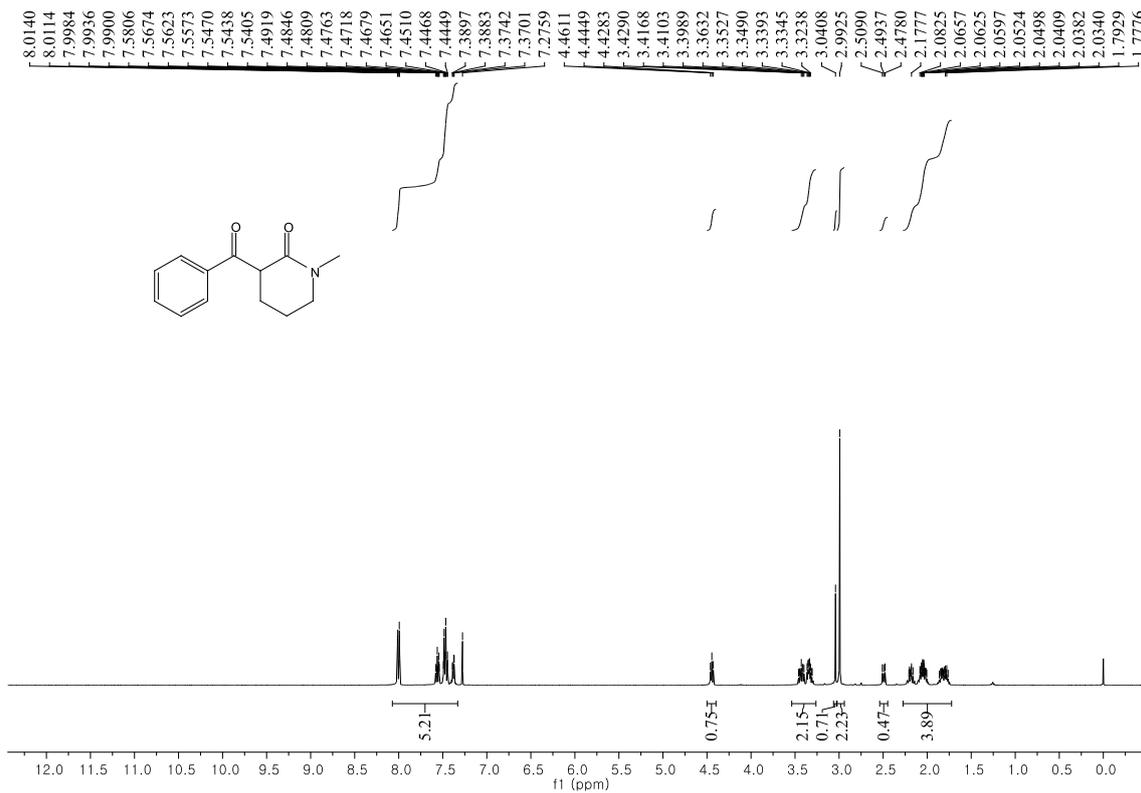


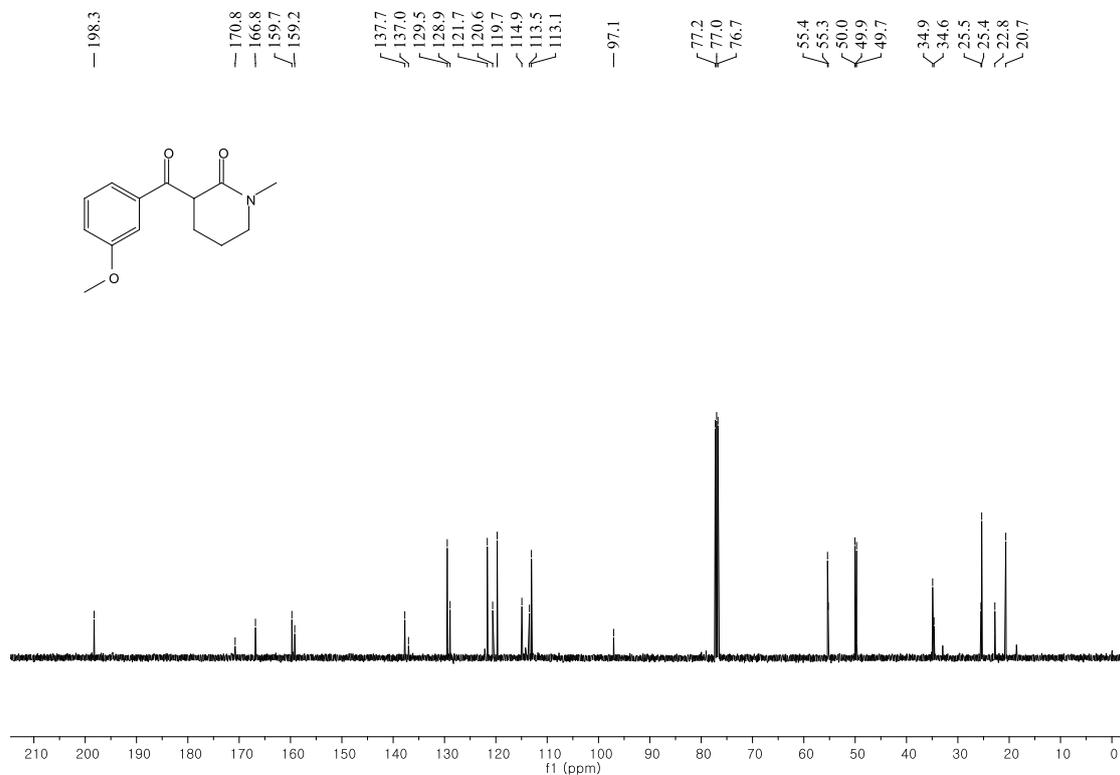
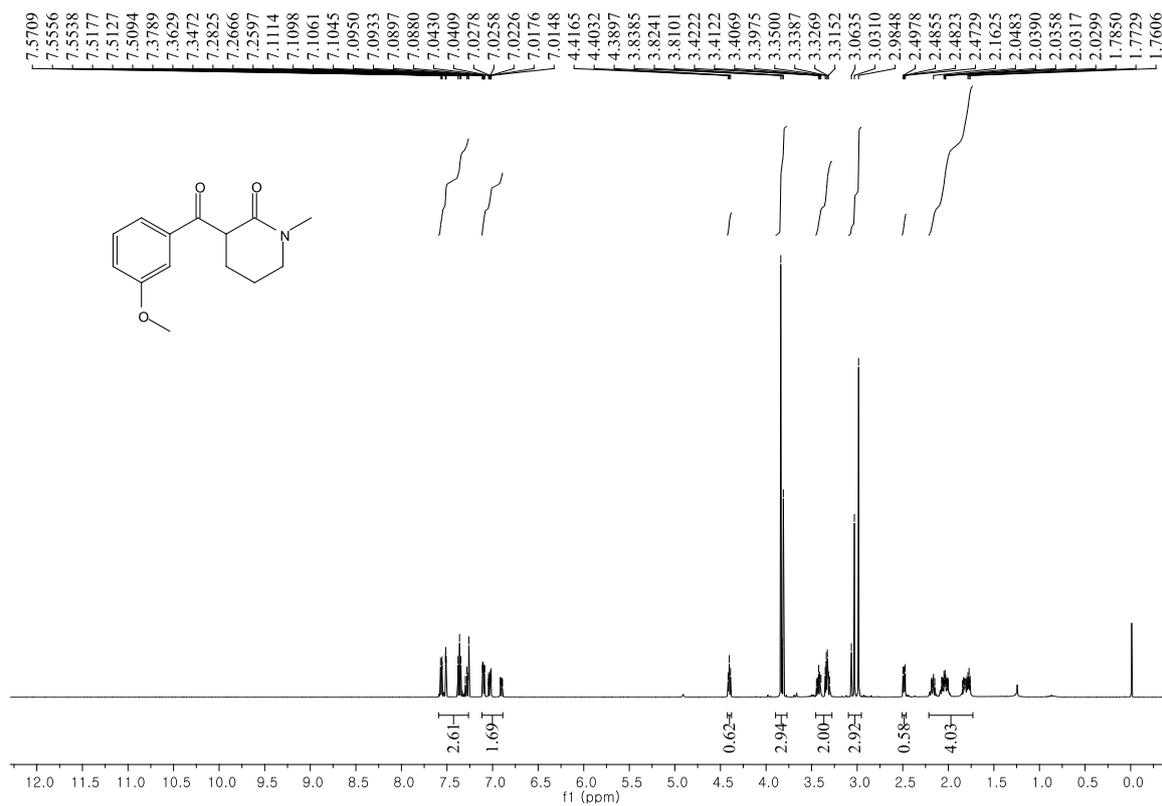


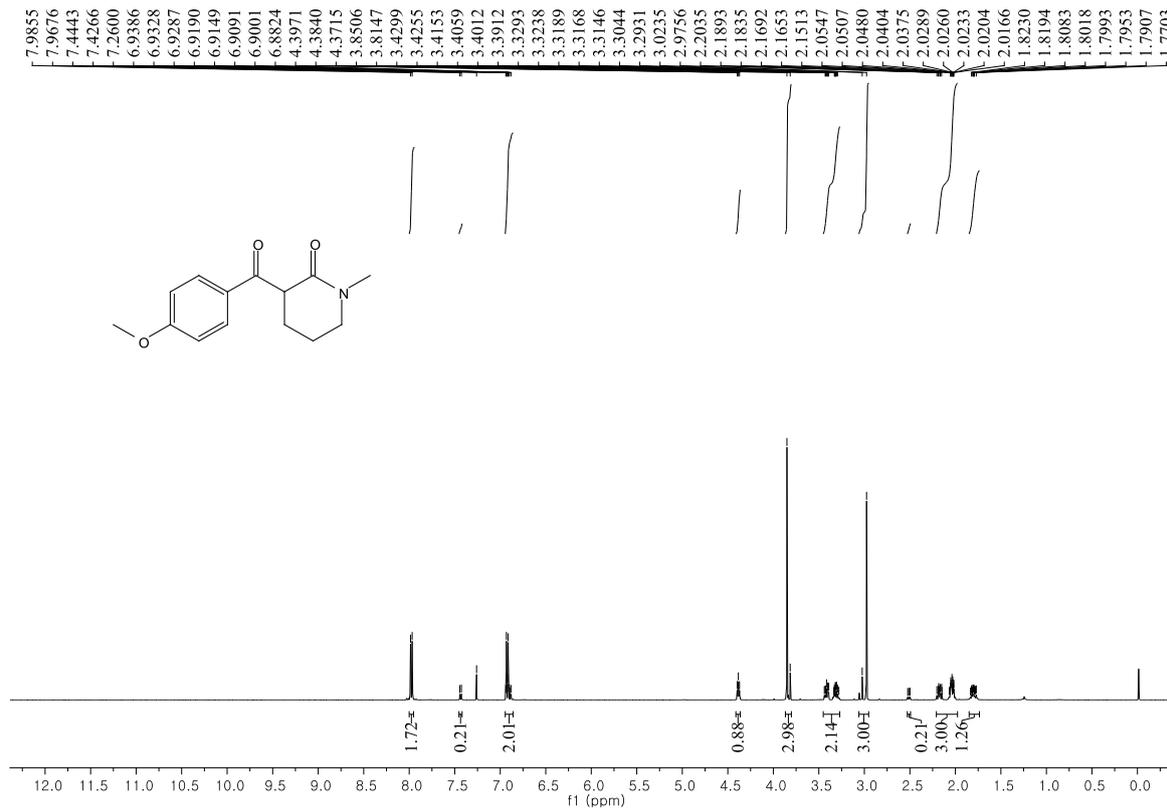
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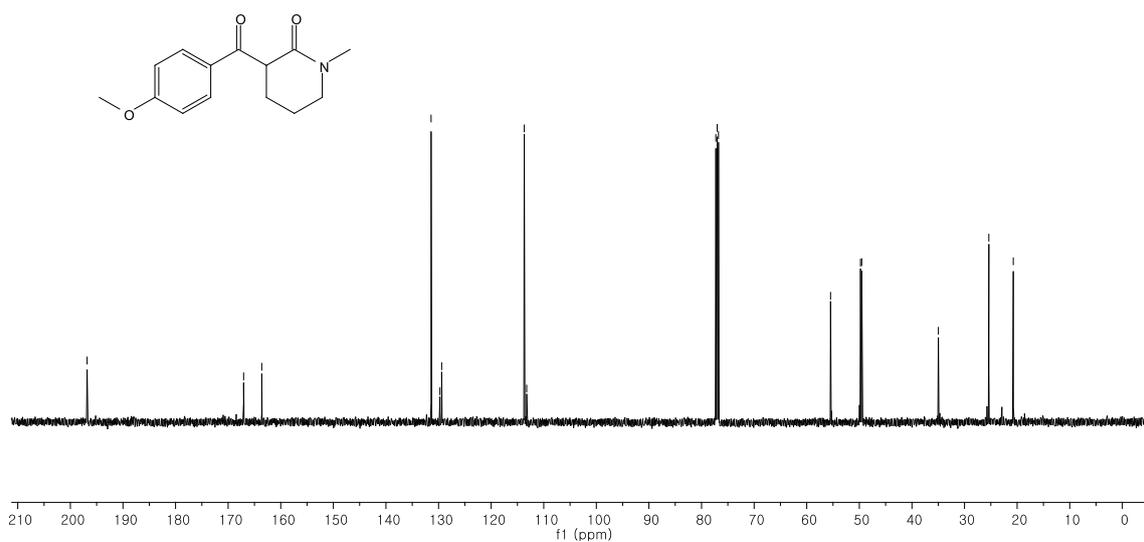
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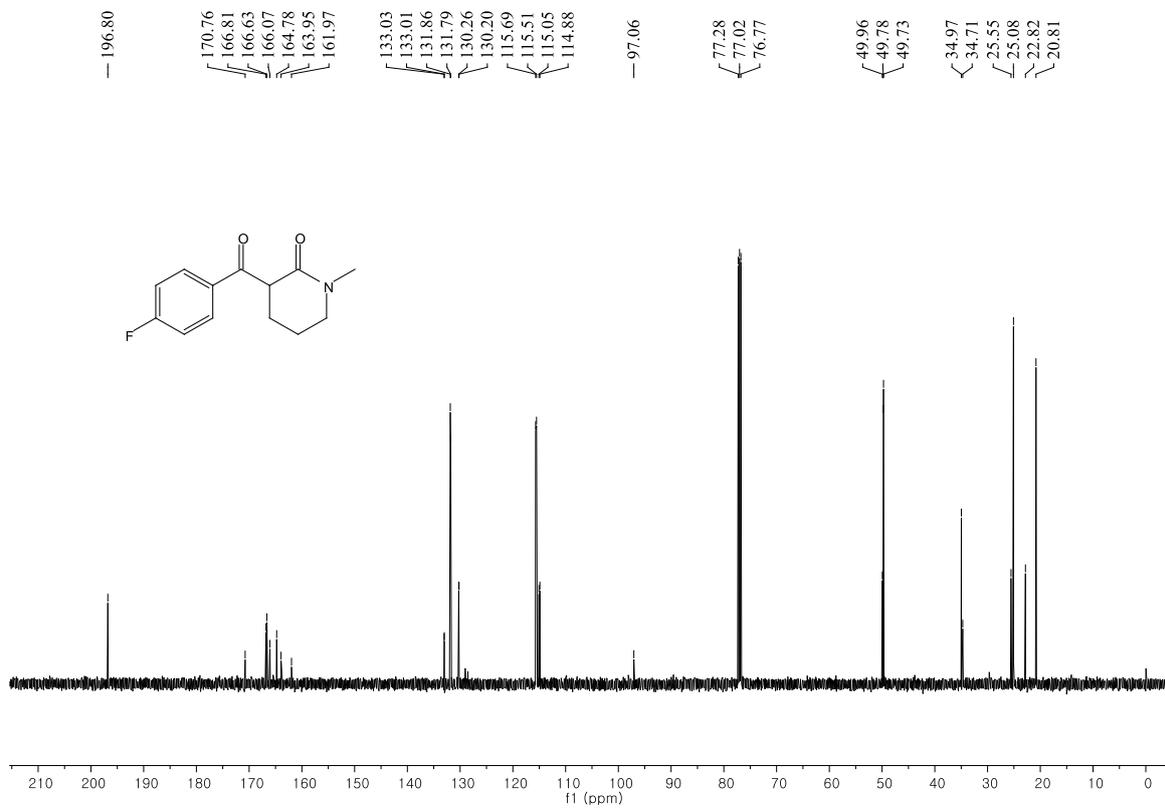
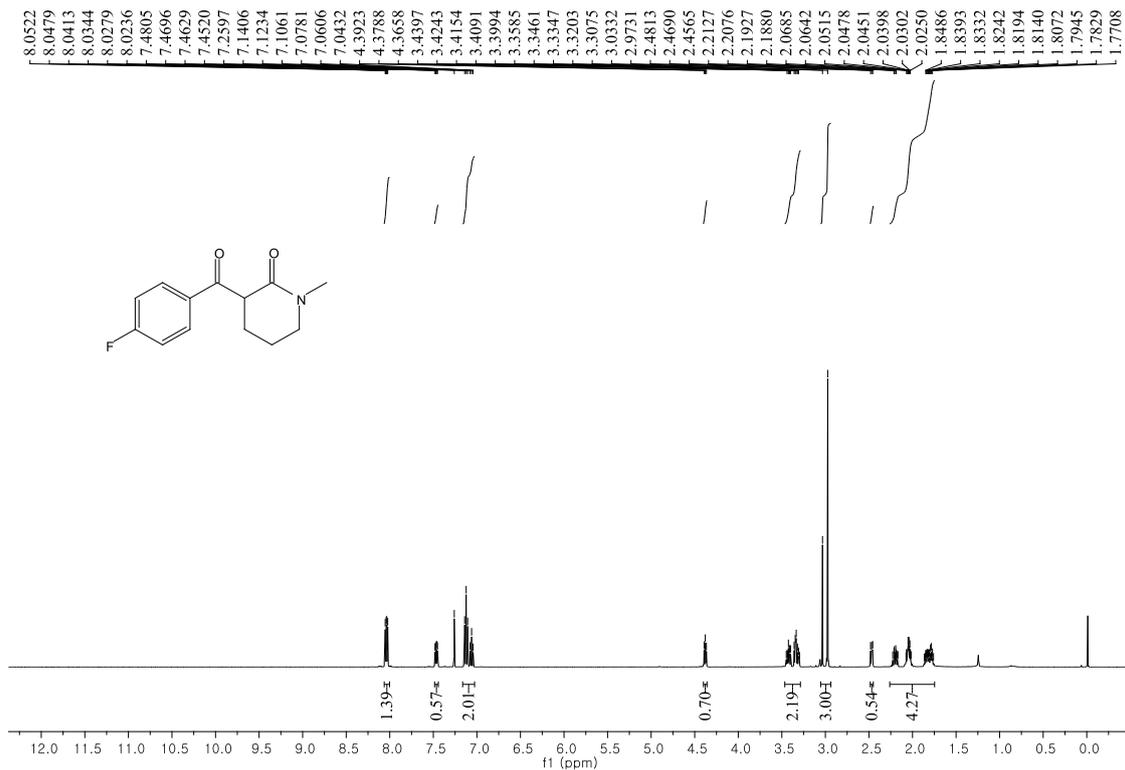


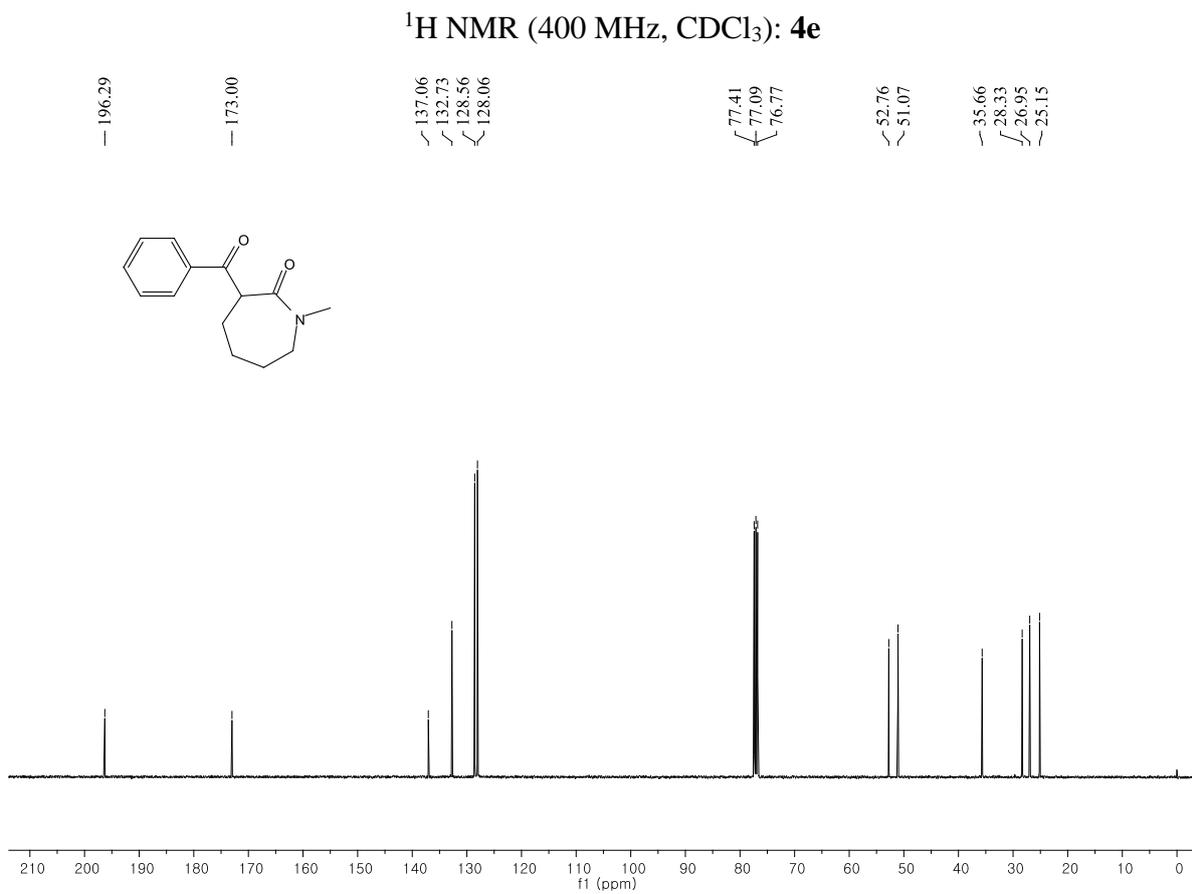
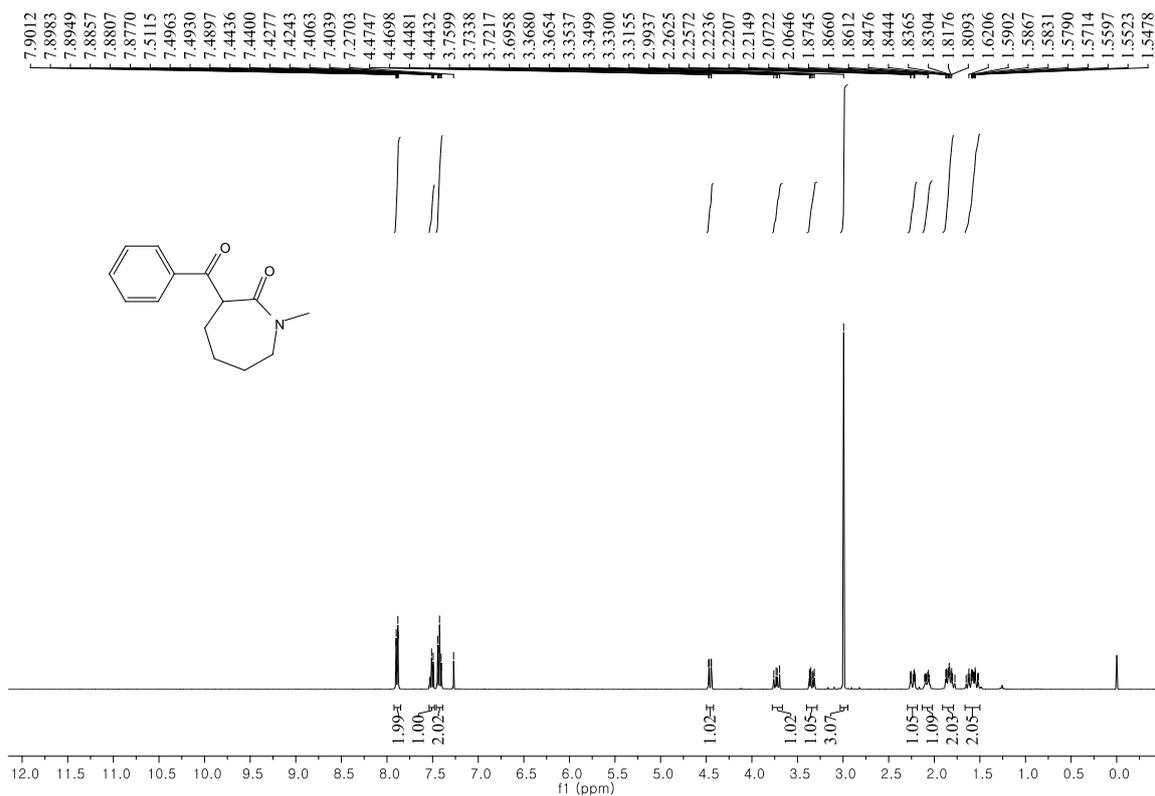


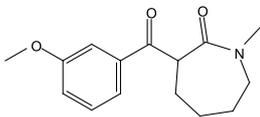
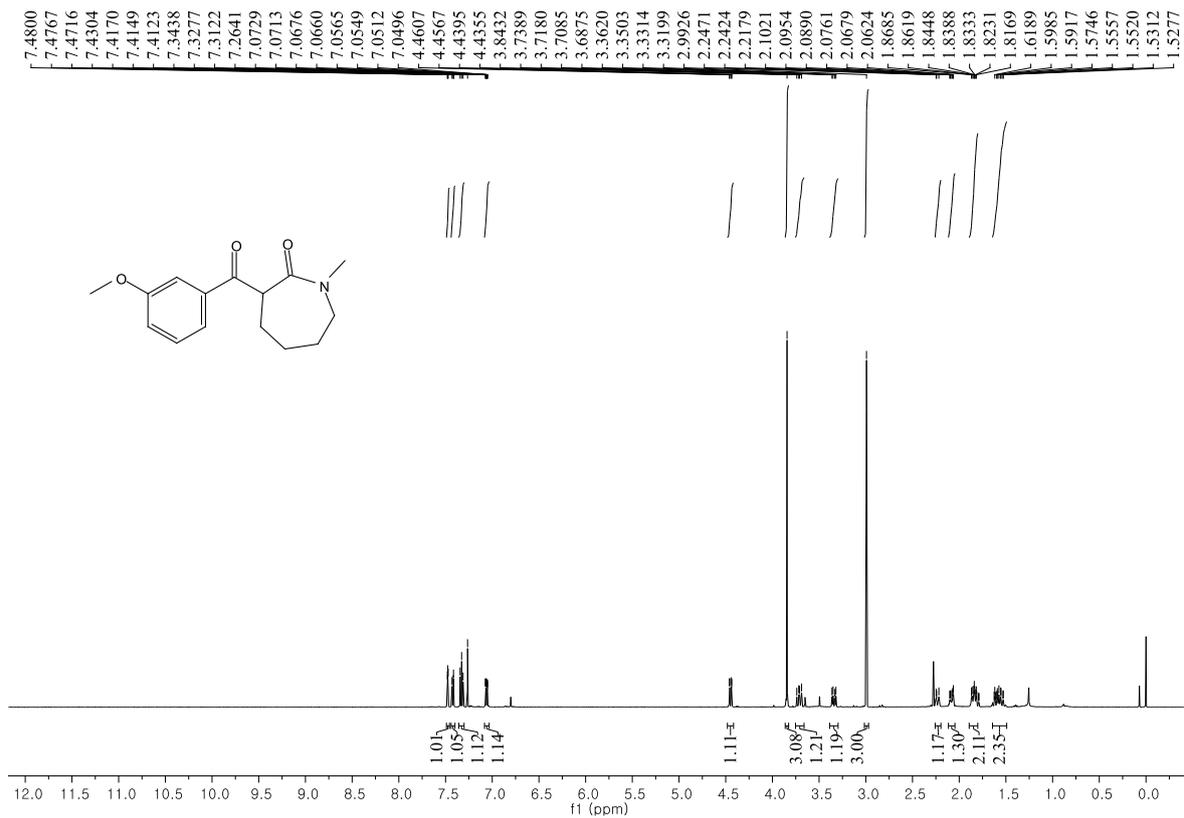
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 { 131.42
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 — 20.73



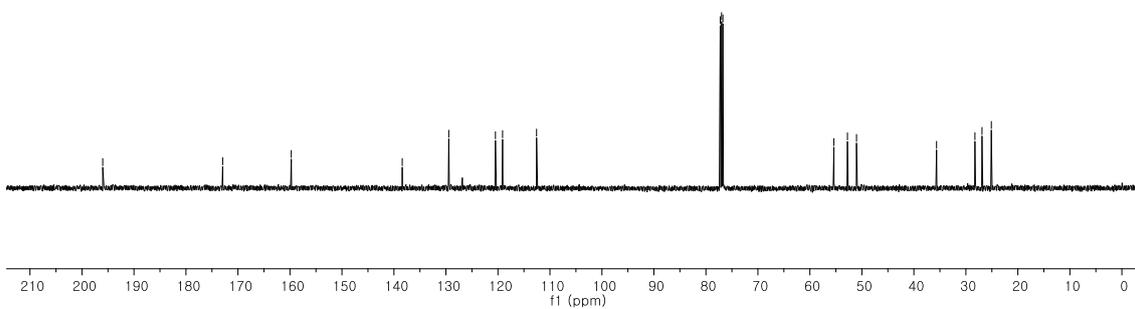
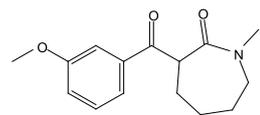
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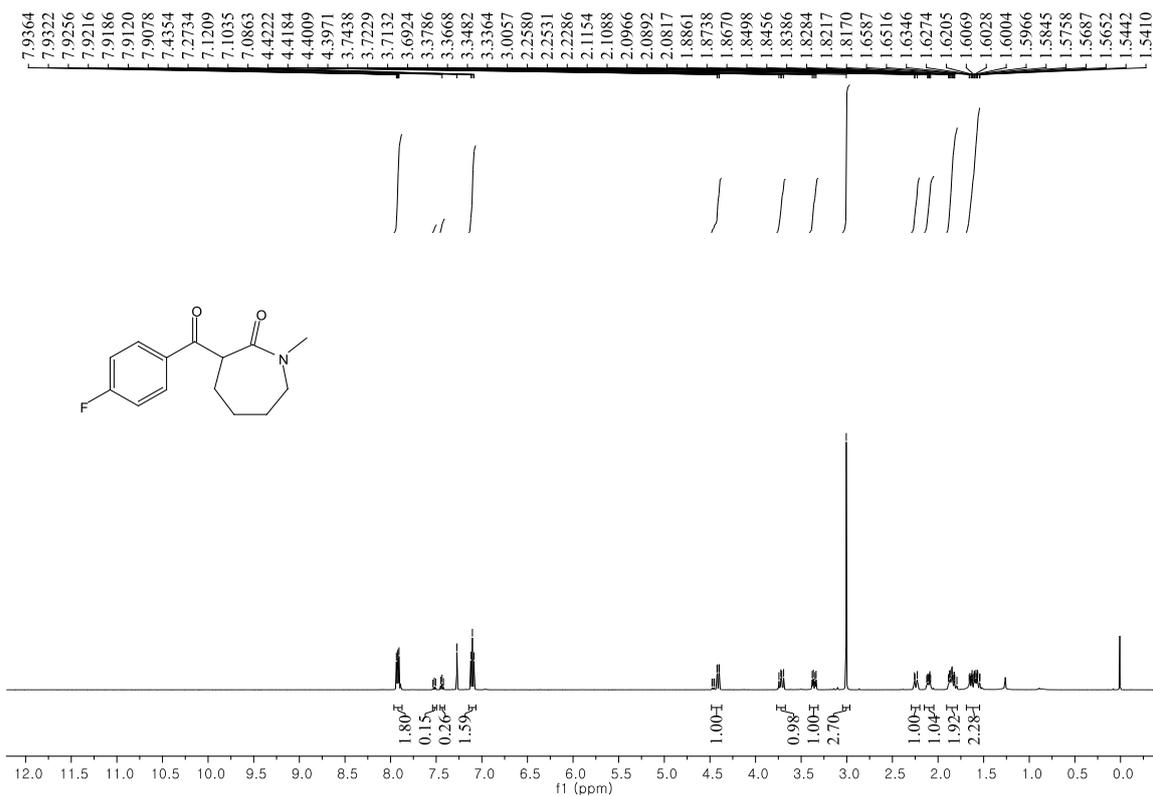




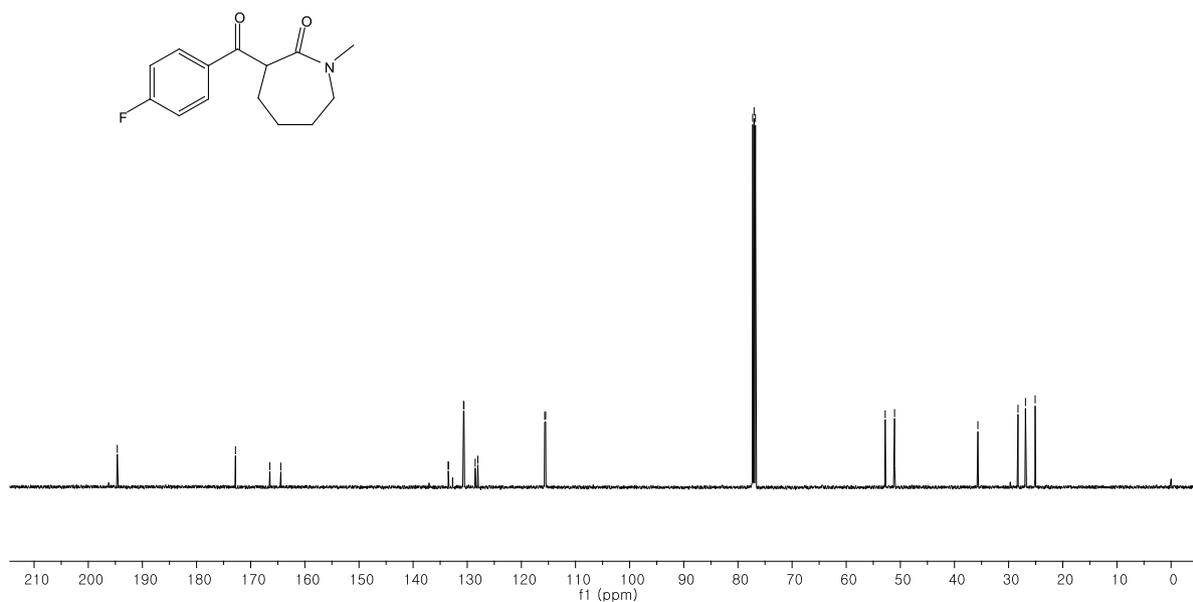
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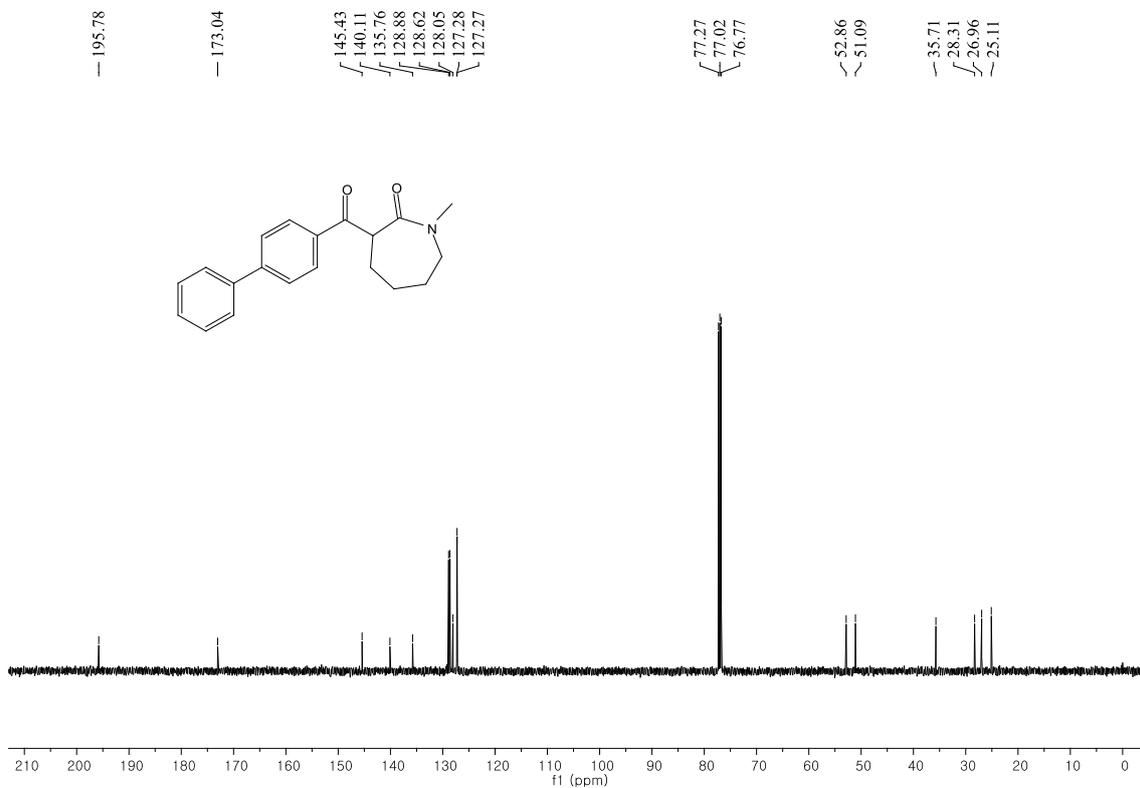
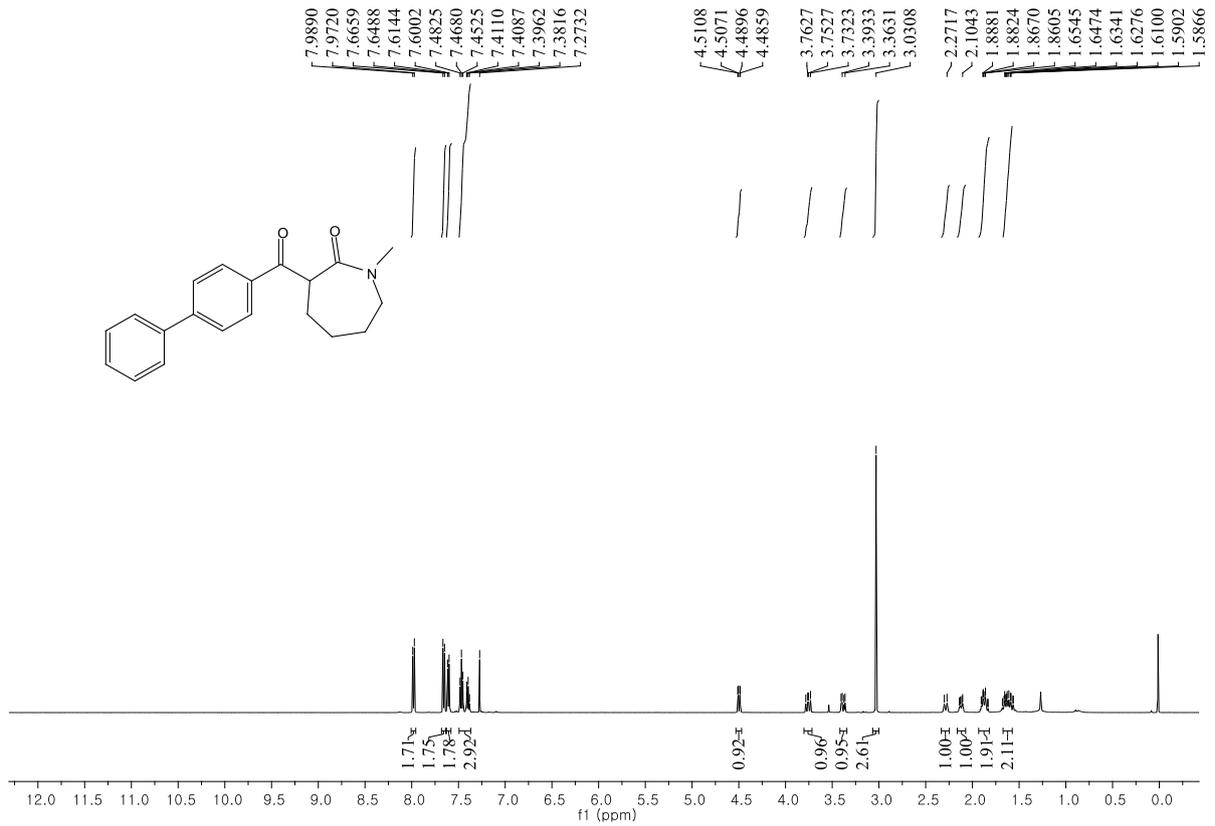
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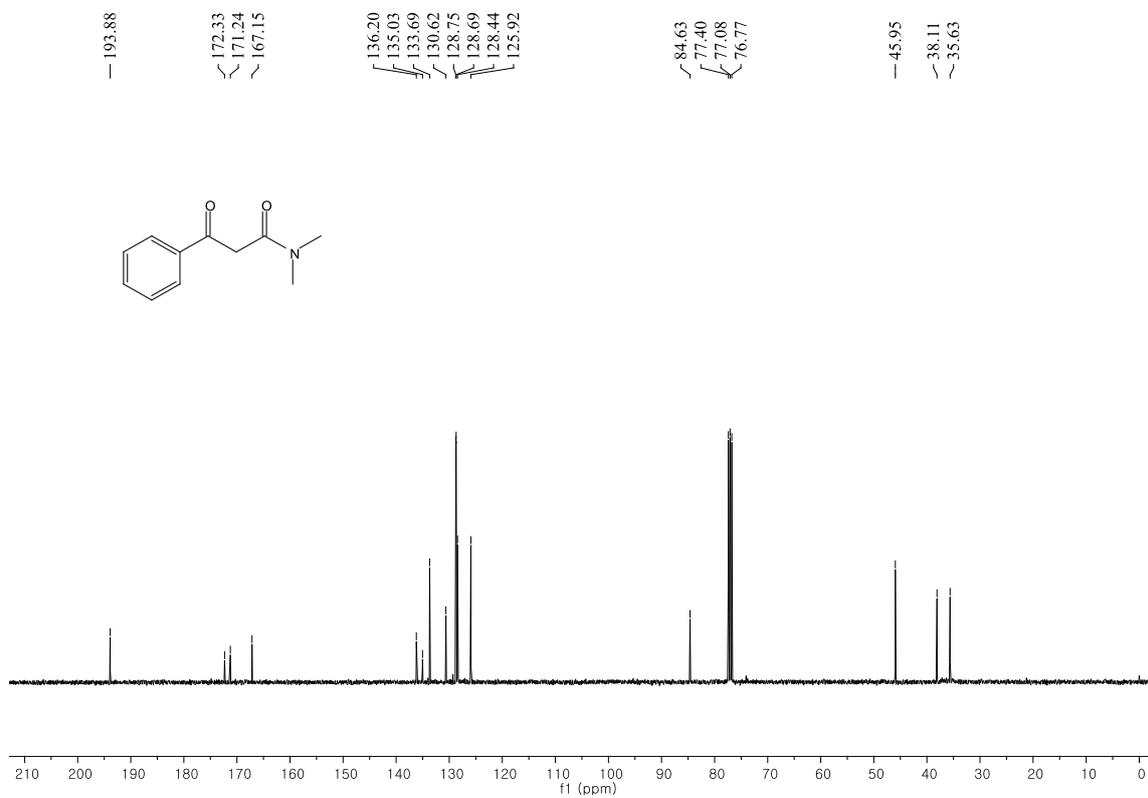
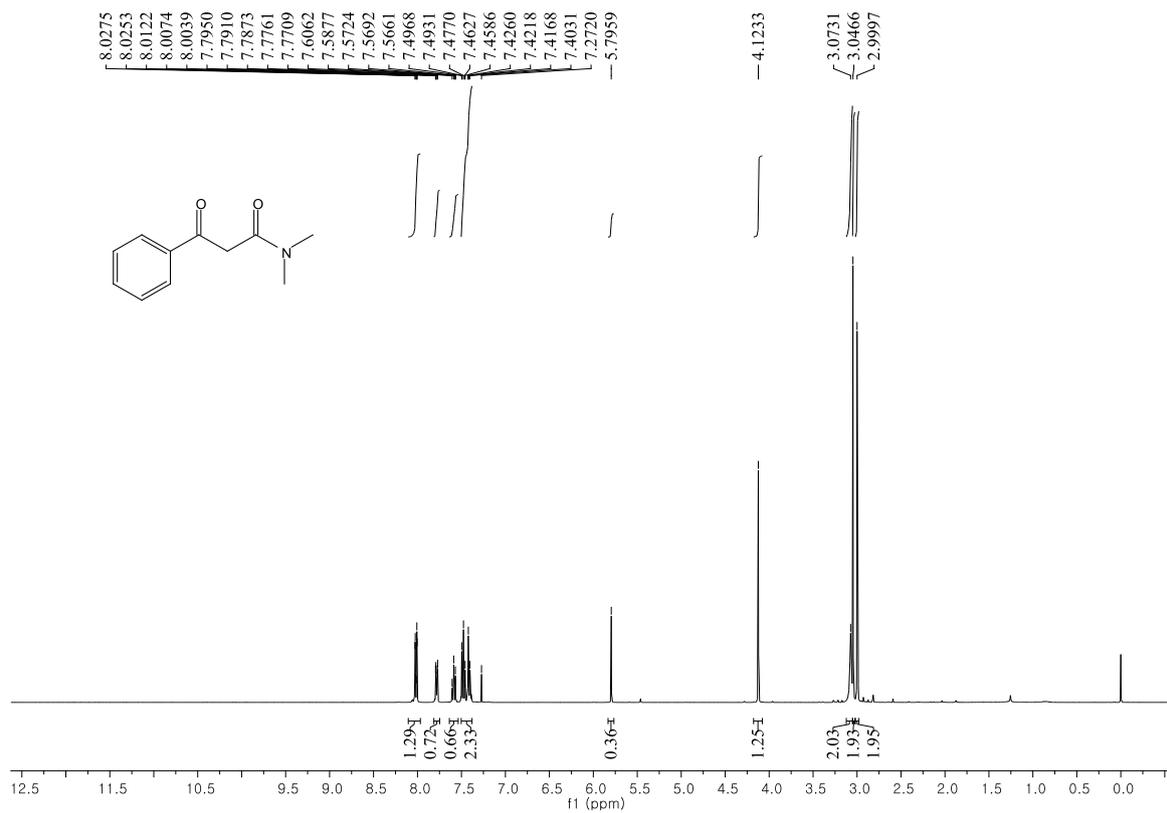


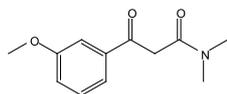
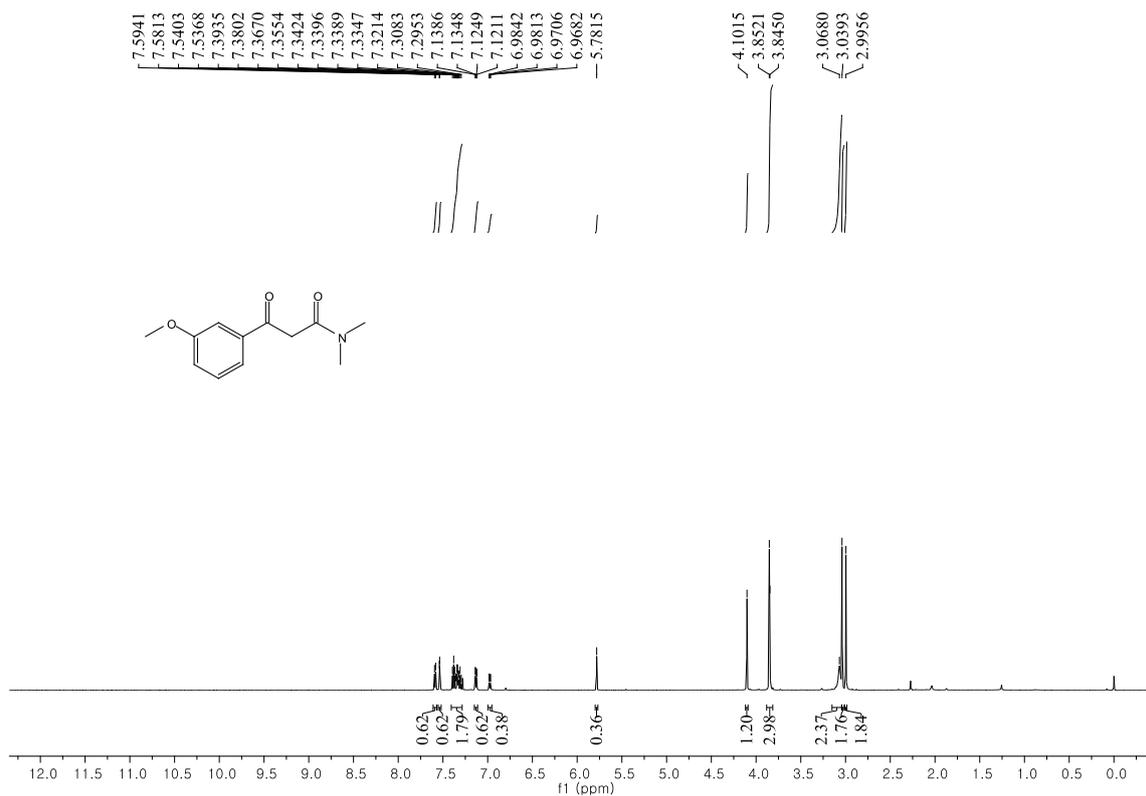
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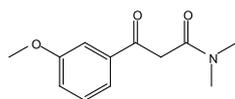
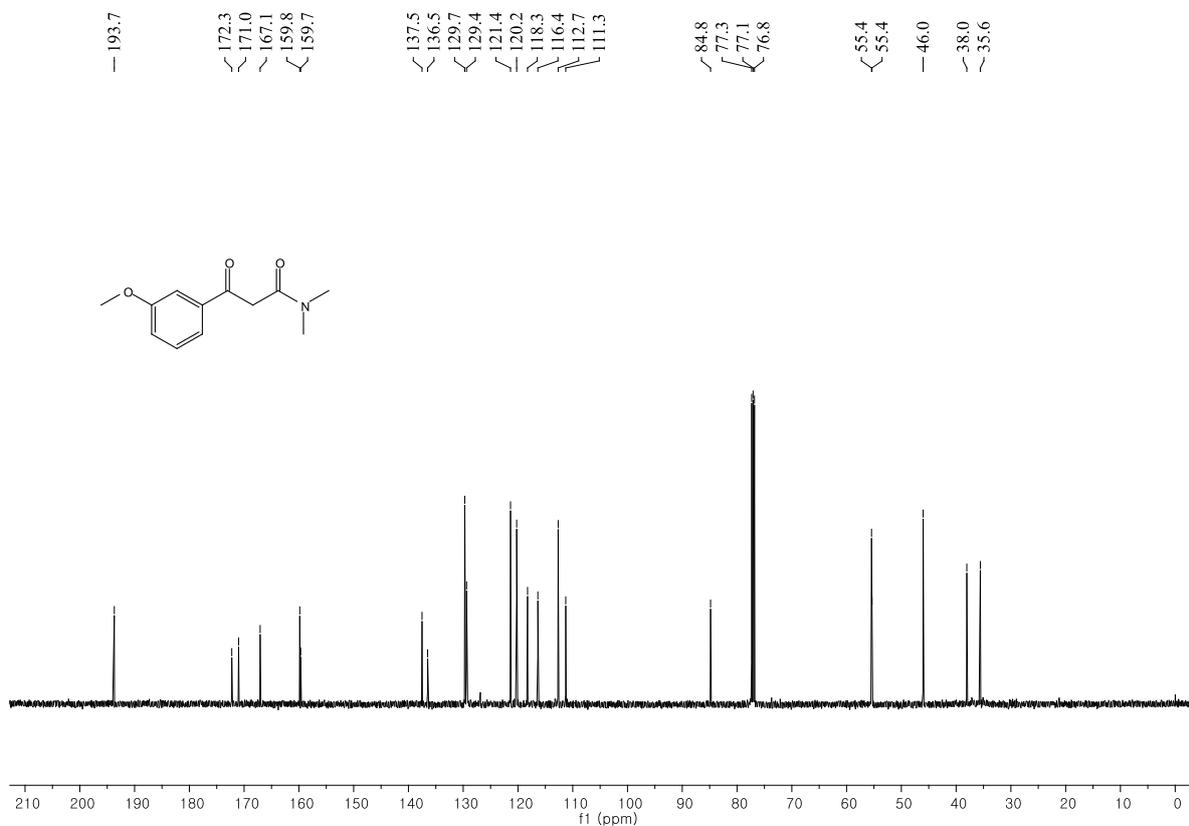
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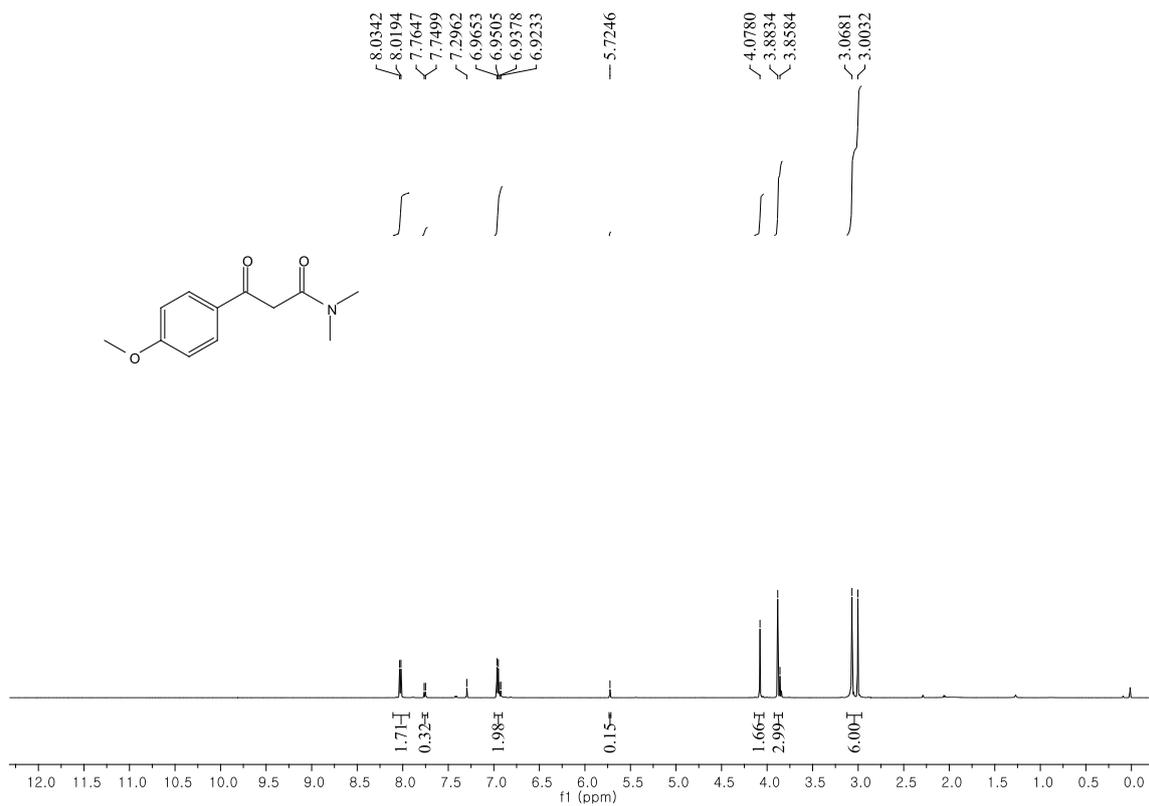




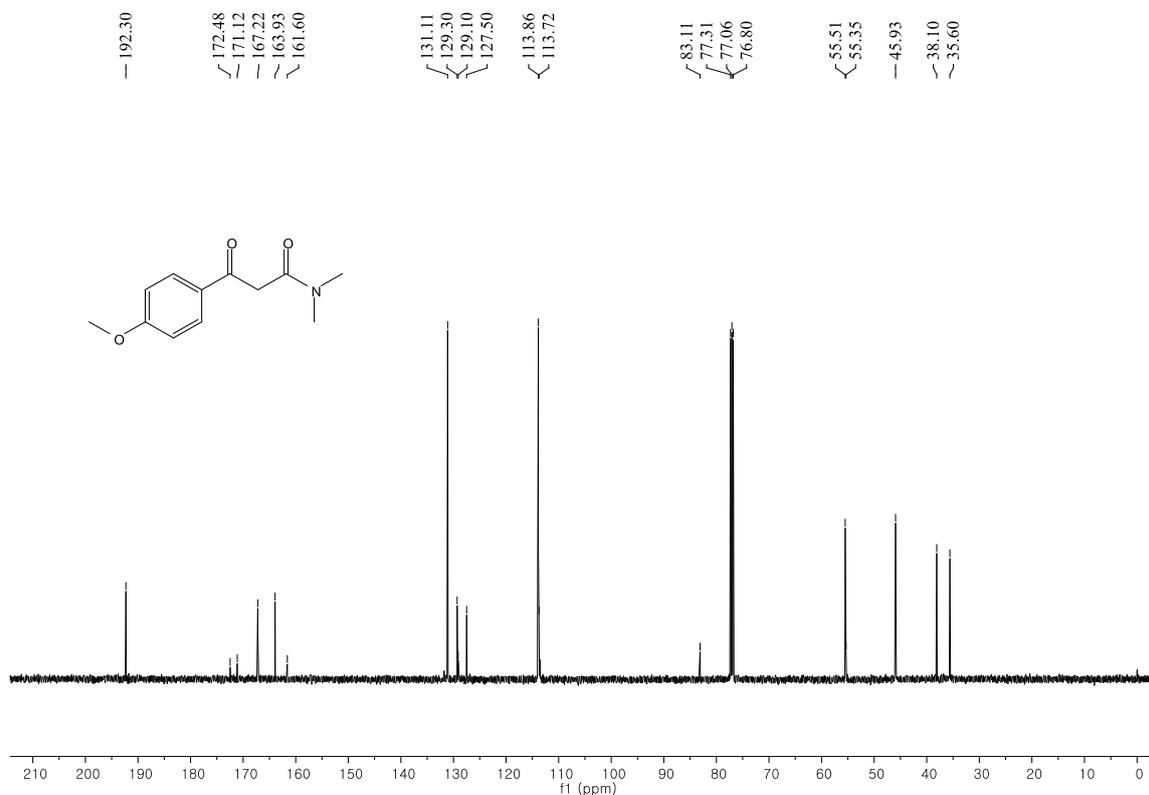
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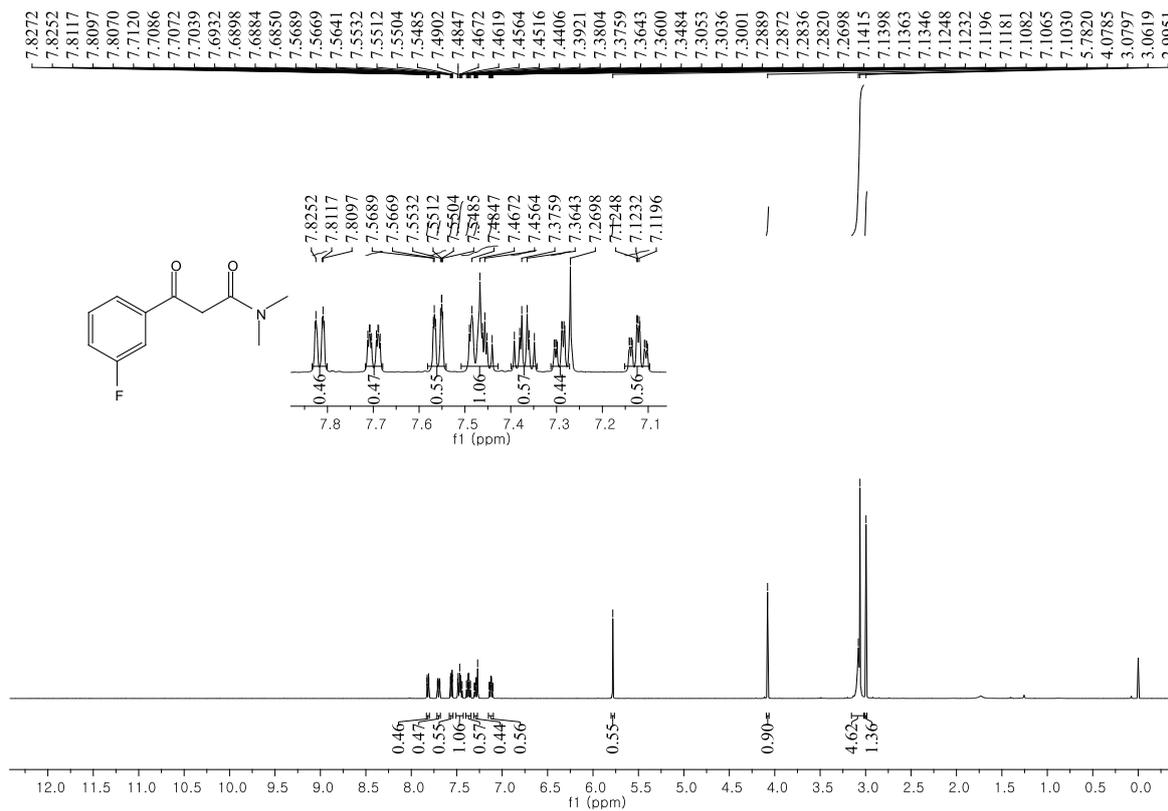
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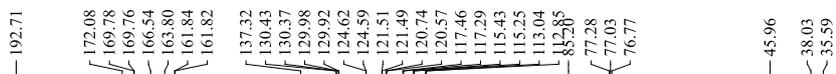
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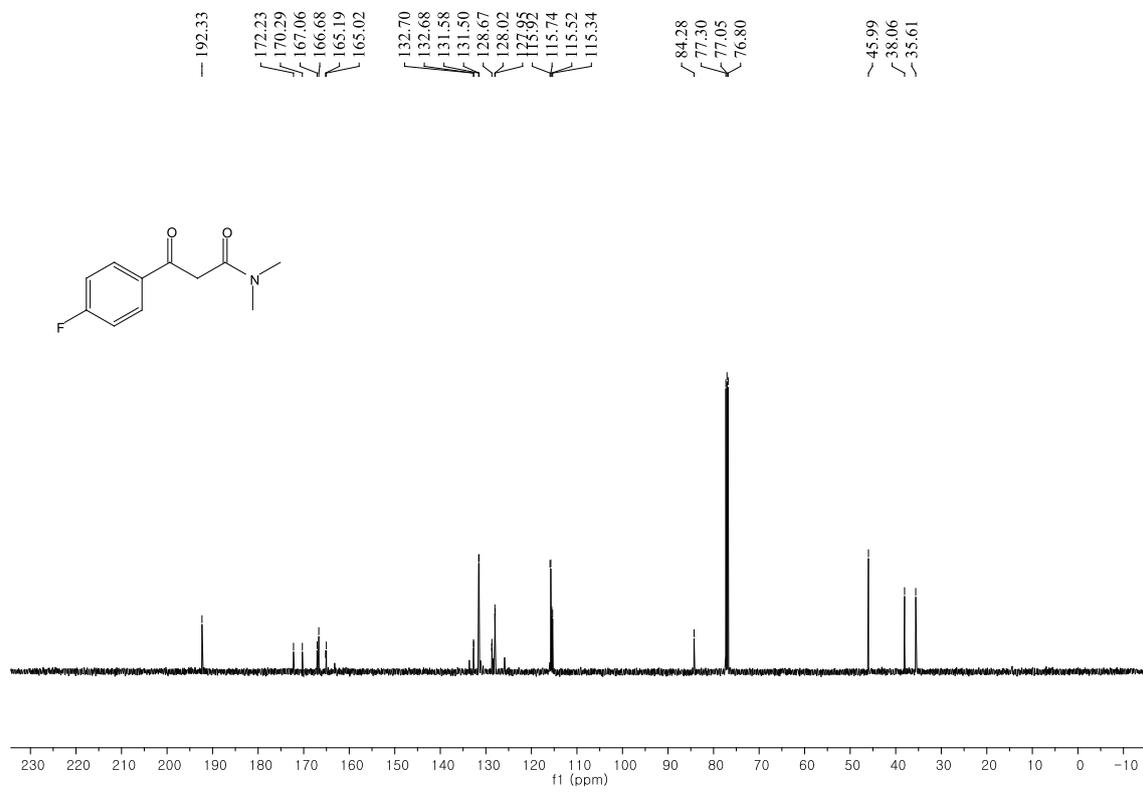
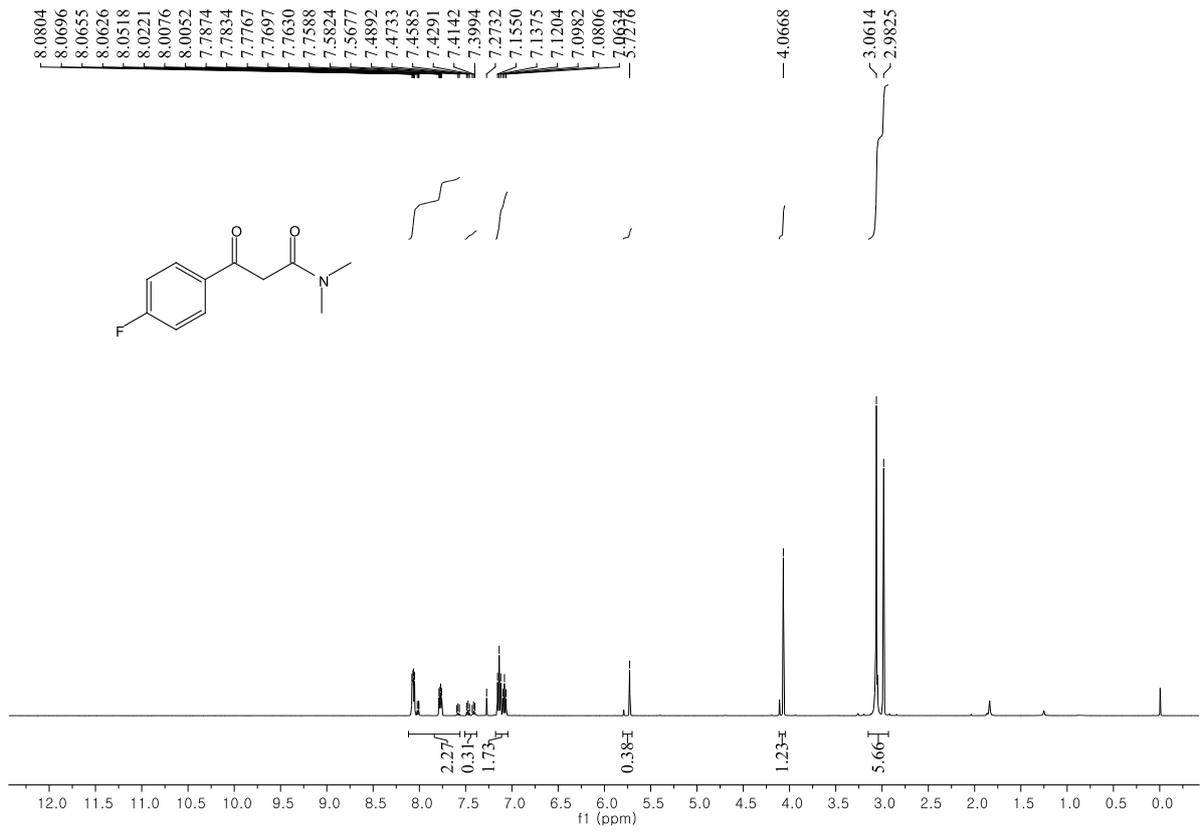
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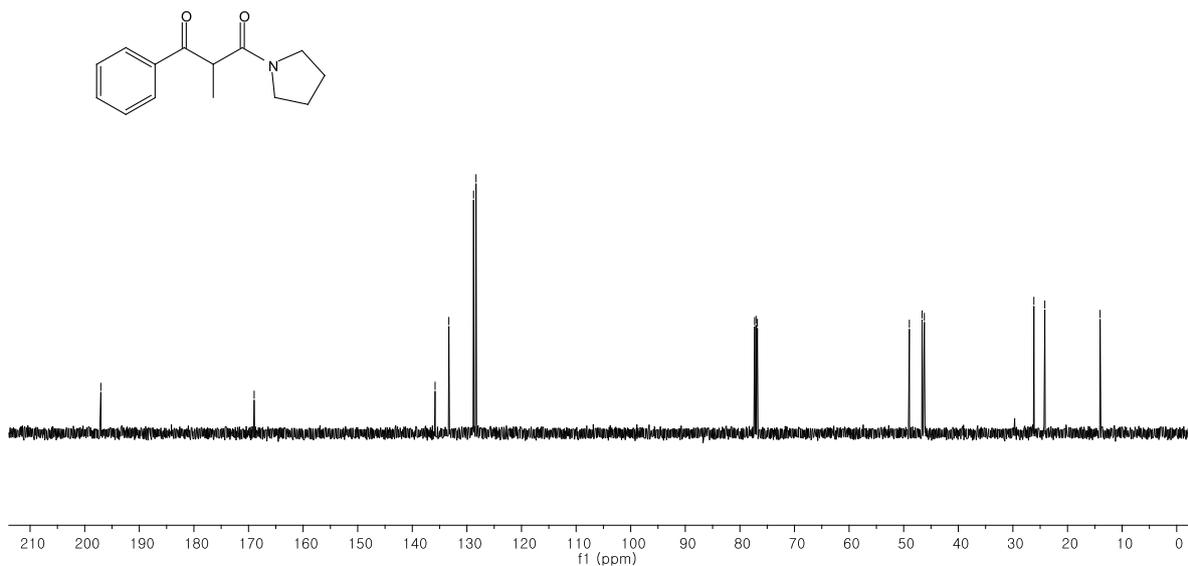
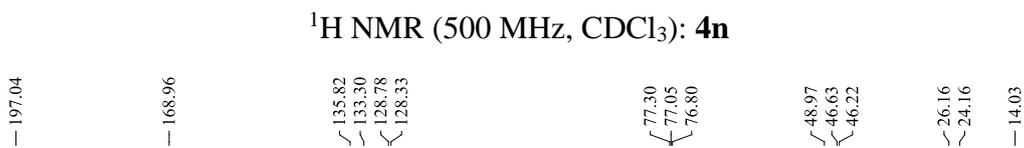
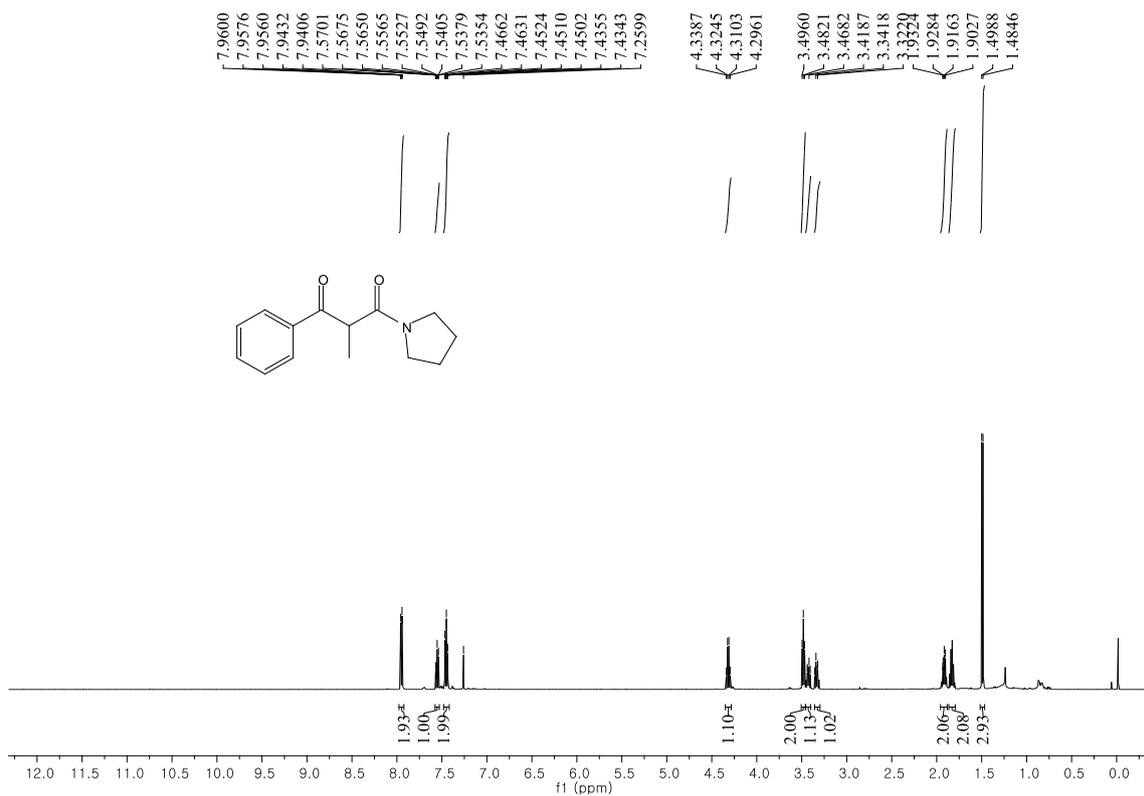


¹H NMR (500 MHz, CDCl₃): 4I

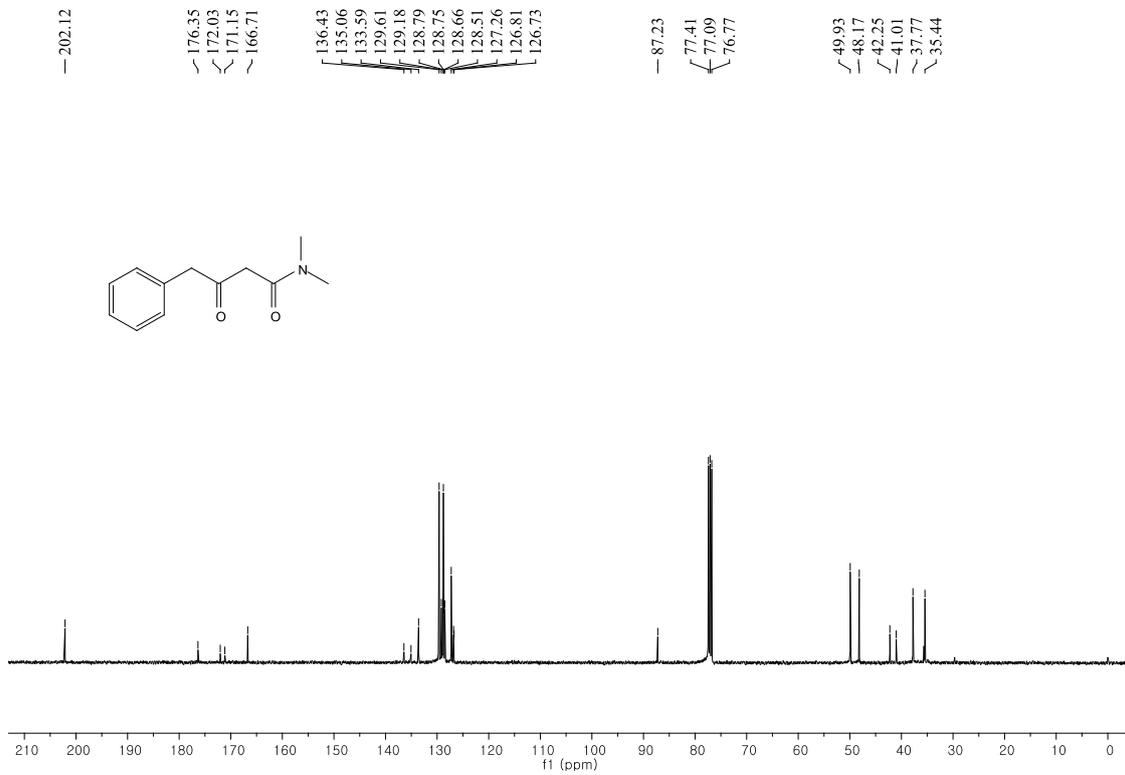
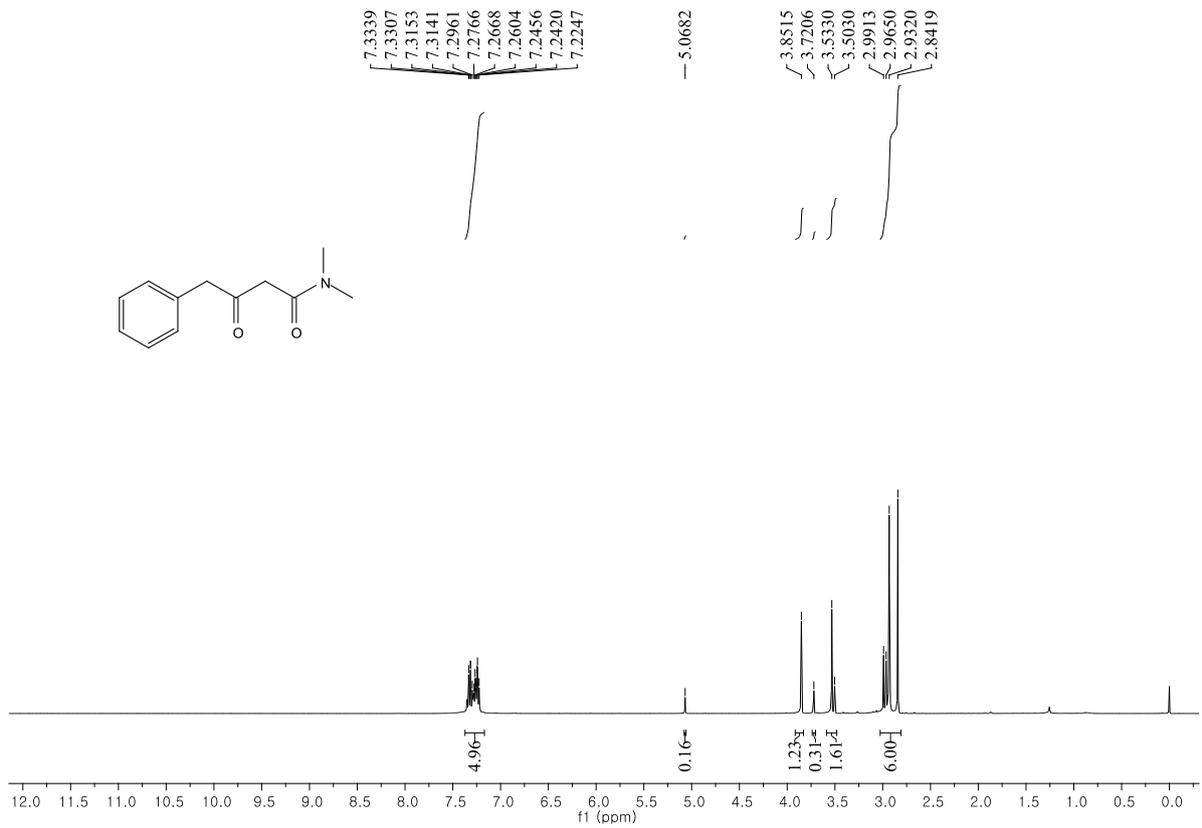


¹³C NMR (126 MHz, CDCl₃): 4I





¹³C NMR (126 MHz, CDCl₃): 4n



6. Computational Details

All calculations were carried out by using the Gaussian 09 suite of computational programs.¹ All stationary points along the reaction coordinate were fully optimized at the DFT level using the B3LYP hybrid functional.² The 6-31G* basis set was applied for all atoms except Ni and Mn, which was described by the LanL2DZ basis set and effective core potential implemented. Frequencies were analytically computed at the same level of theory to get the thermodynamic corrections and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations were carried out to confirm that all transition state structures connect the proposed reactants and products. The solvent effect of mesitylene was evaluated by using the SMD polarizable continuum model. All SCRF calculations were done at the M06 level by using a larger basis set of SDD for Ni, Mn and 6-311+G(d,p) for the rest elements.³ The relative free energies (in kcal/mol) corrected by solvation effects are used for discussion.

The glyme ligand is contained the Ni(II) precatalyst and 10% of terpyridine was added in experiments. Calculations were done to identify which one is the real ligand in the catalytic reaction. It was found that the replacement of glyme with terpyridine is highly energetically favorable for both Ni and Mn complex (see below), suggesting the latter one should be the real ligand in the reaction.

		Exergonicity (kcal/mol)
NiCl ₂ (glyme) + TPY	—————>	NiCl ₂ (TPY) + glyme -33.1
Ni(glyme) + TPY	—————>	Ni (TPY) + glyme -51.7
MnCl ₂ (glyme) + TPY	—————>	MnCl ₂ (TPY) + glyme -55.7

¹ Gaussian 09, Revision A.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

² (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

³ (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.

7. Additional Computational Results

Additional computational results are provided in Figure S1-S8, and all the energies in these figures are much higher than those given in Scheme 5. Accordingly, When only Ni(0) is used without Mn, the results show that quite high energy barrier (36.8 kcal/mol) is needed for the enolization through **TS4** (Figure S1). The possible enolization of **2a** with Ni(0) by C-H insertion was calculated (Figure S2), however, the energies required is more than 40 kcal/mol. As shown in Figure S2, the formation of Ni hydride **IN17** may be possible with a barrier of 28.6 kcal/mol. Further transformation between **IN7** and **IN3** was simulated, but the barrier would be 38 kcal/mol via **TS5** (Figure S3).

If no Ni is used and only Mn(0) is involved (Figure S4), the barrier for C-N bond cleavage of **1a** via **TS8** is more than 40 kcal/mol, and even higher barriers are calculated for the following transformations via **TS9** and **TS10**. The possible enolization of **2a** with Mn(0) was shown in Figure S5. The complexation process is exergonic, however, the following oxidative addition requires a barrier of 35.3 kcal/mol (**TS11**).

The possibility for formation of Mn(I) species is investigated (Figure S6). The formation of **IN31** from **IN3** and LMnCl is exergonic by 20.1 kcal/mol. After formation of **IN32** by dissociation and the incorporation of **2a** to generate **IN33**, the enolate **IN34** could be formed by deprotonation via **TS14**. However, the following transformations are difficult due to high barrier nearly 40 kcal/mol from **IN31** to **TS3**. If **IN37** is involved, even higher barrier is required as determined by **TS5**.

In Scheme 5, the enolization was realized by the first formation of **IN6** from **IN3** and MnCl₂L is required, as the amino group should be involved in the deprotonation step. To test the possibility of direct deprotonation with MnCl₂L (Figure S6), the energies for **TS16** show in Figure S7 is over 40 kcal/mol. If Mn(I) is involved, the oxidative addition via **TS15** is also highly unfavorable. The chloride anion in MnCl was also used as a base for deprotonation, however, even higher barrier was calculated (not shown in the figure).

The interconversion between enolate **IN9** and **IN42** was found to be quite facile (Figure S8), and the intermediacy of **IN43** is involved.

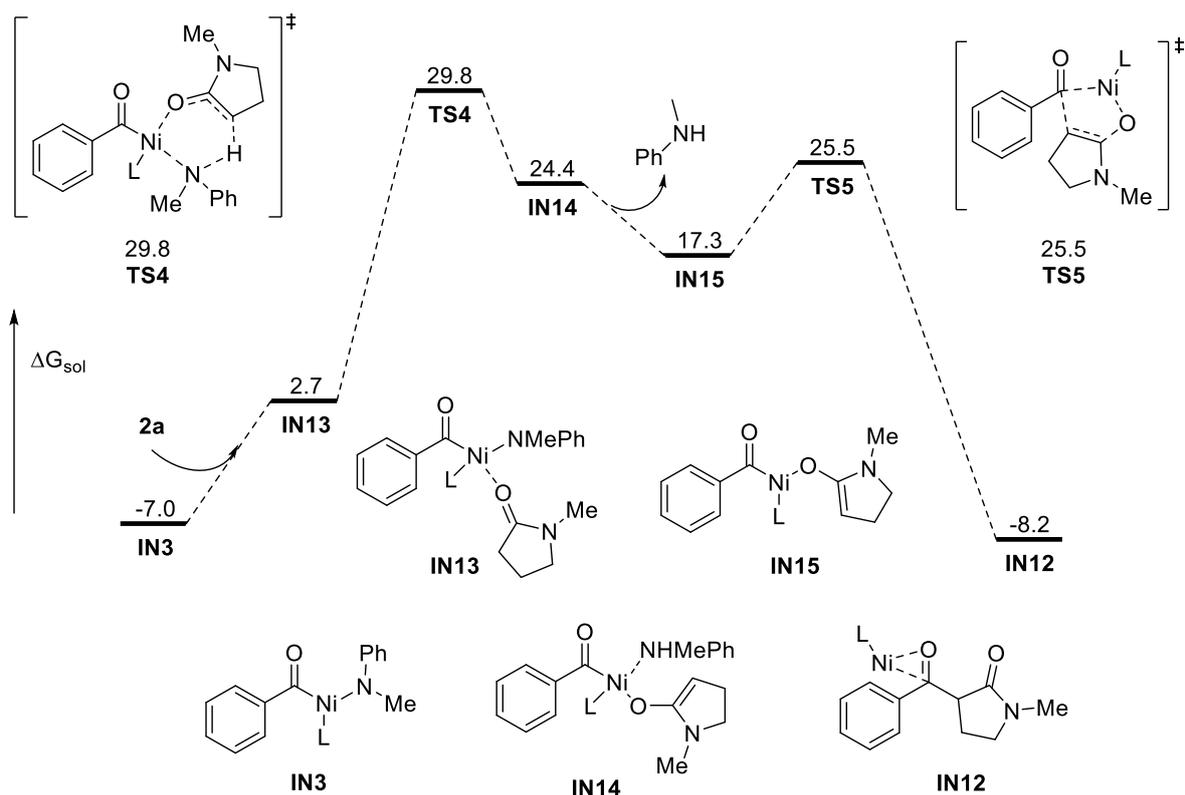
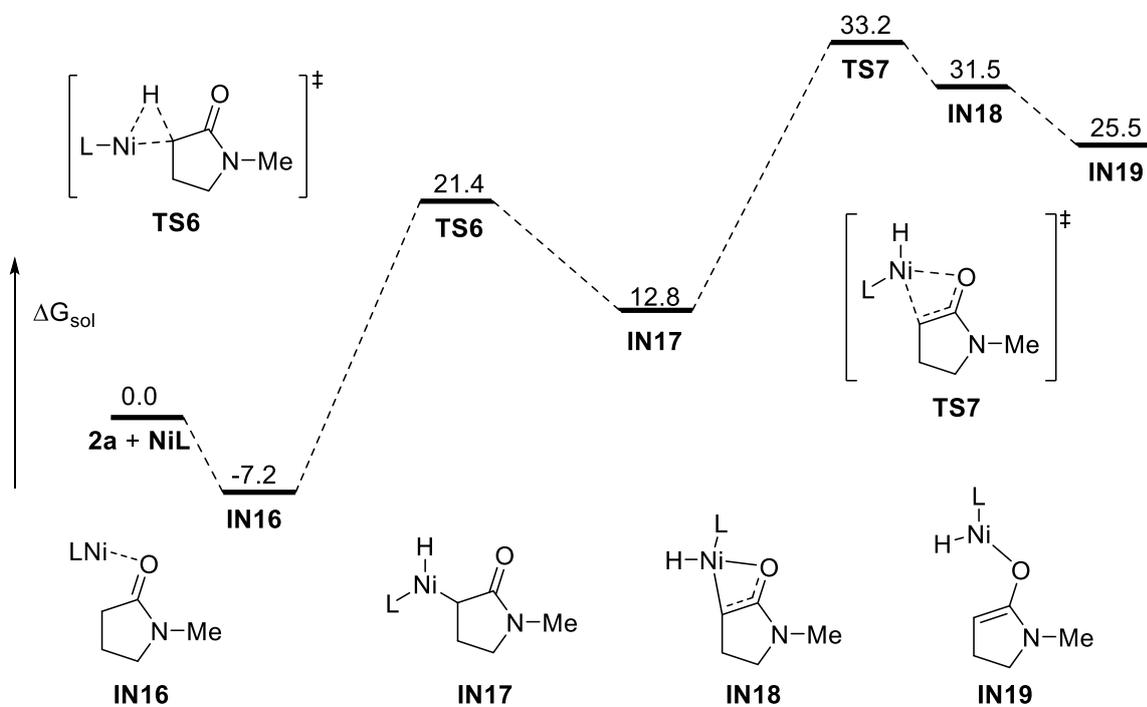


Figure S1. Possible reaction of **IN3** with **2a** in the absence of Mn (L = TPY; relative Gibbs free energies in solution are in kcal/mol).



S2. Possible enolization of **2a** with Ni(0) (L = TPY; relative Gibbs free energies are in kcal/mol).

Figure

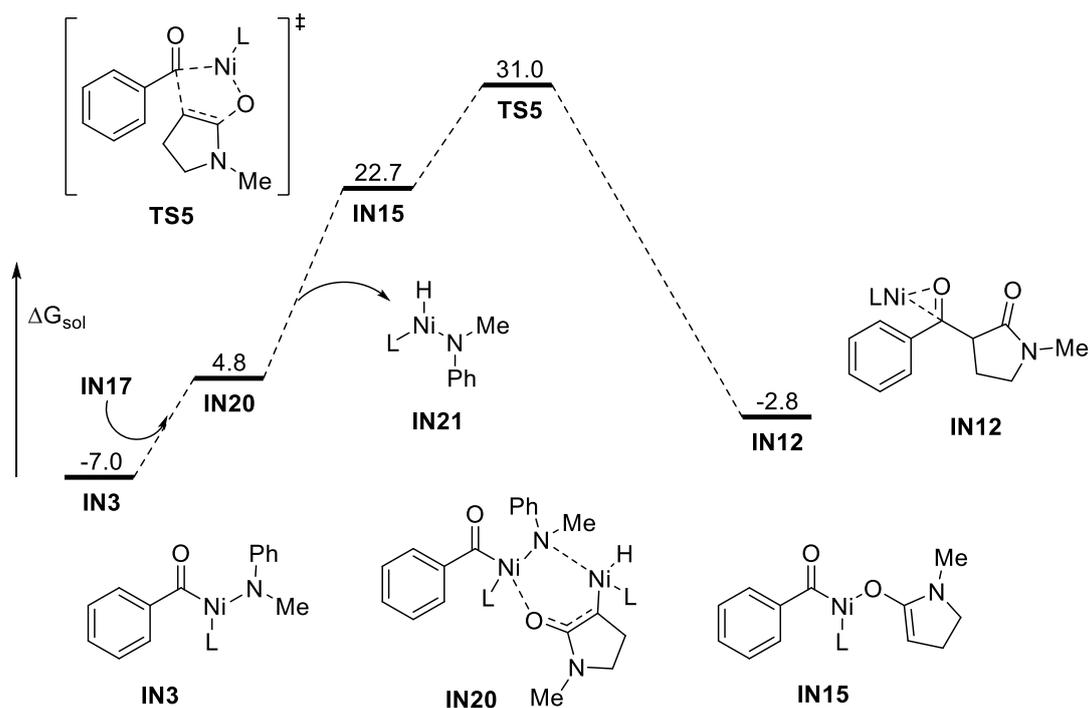


Figure S3. Possible formation of the coupling product from **IN3** and **IN17** (L = TPY; relative Gibbs free energies are in kcal/mol).

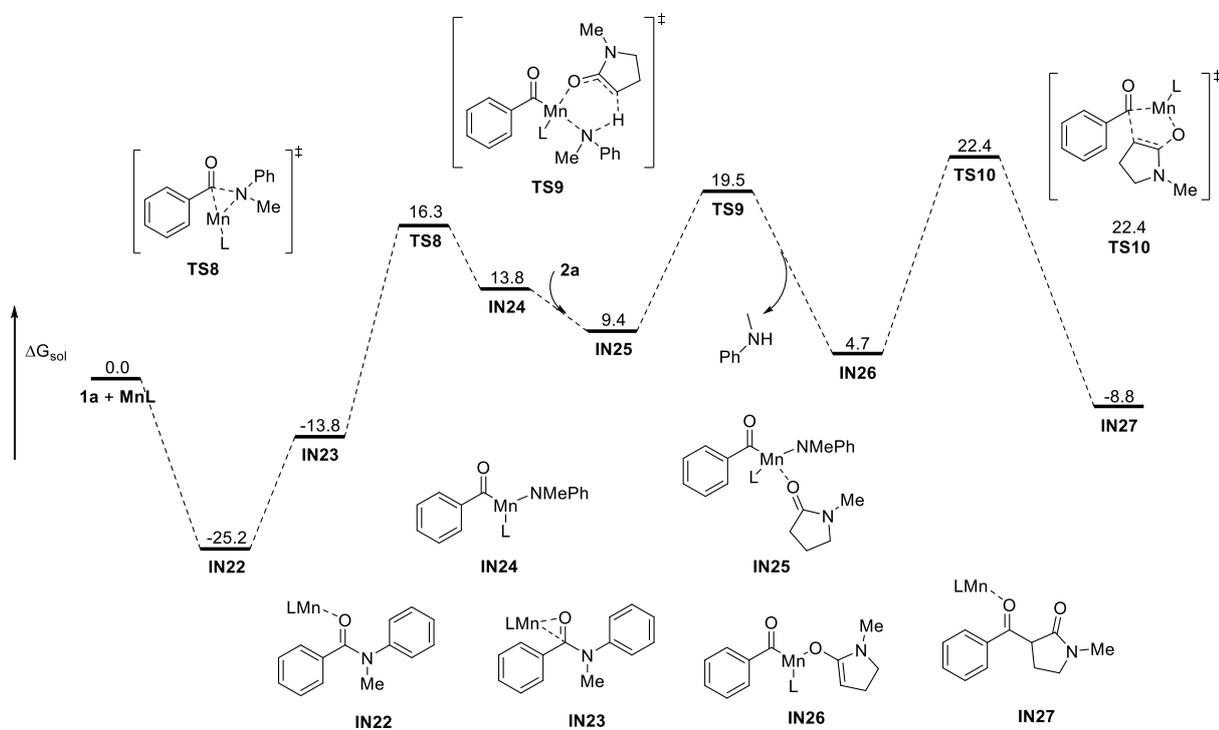


Figure S4. Possible Coupling reaction between **1a** and **2a** catalyzed by Mn in the absence of Ni (L = TPY; relative Gibbs free energies are in kcal/mol).

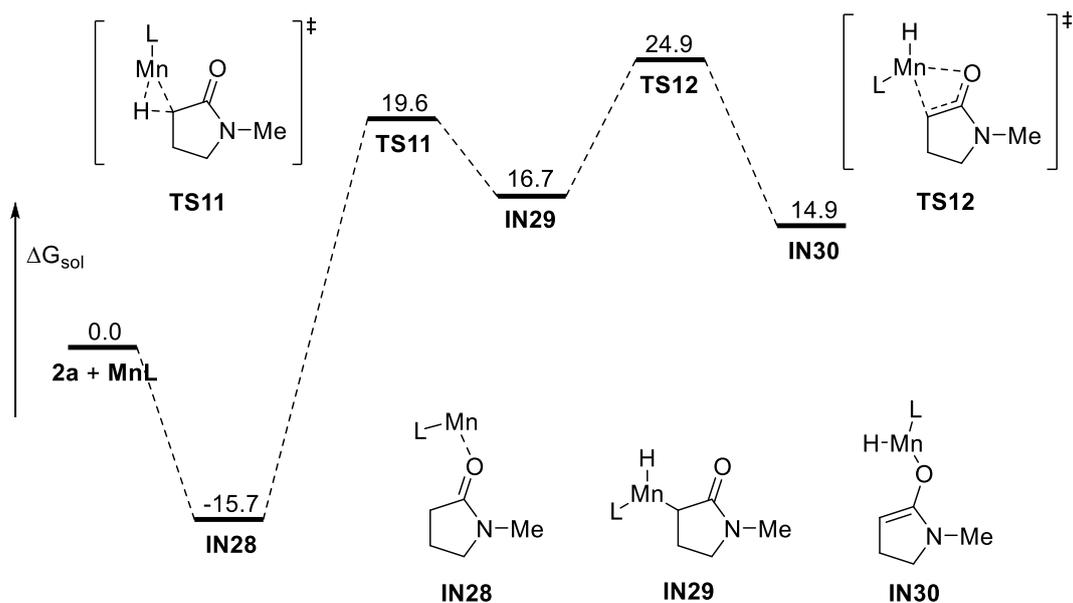


Figure S5. Computed potential energy surface for the Mn(0)-catalyzed reaction of 2a (L = TPY; relative Gibbs free energies are in kcal/mol).

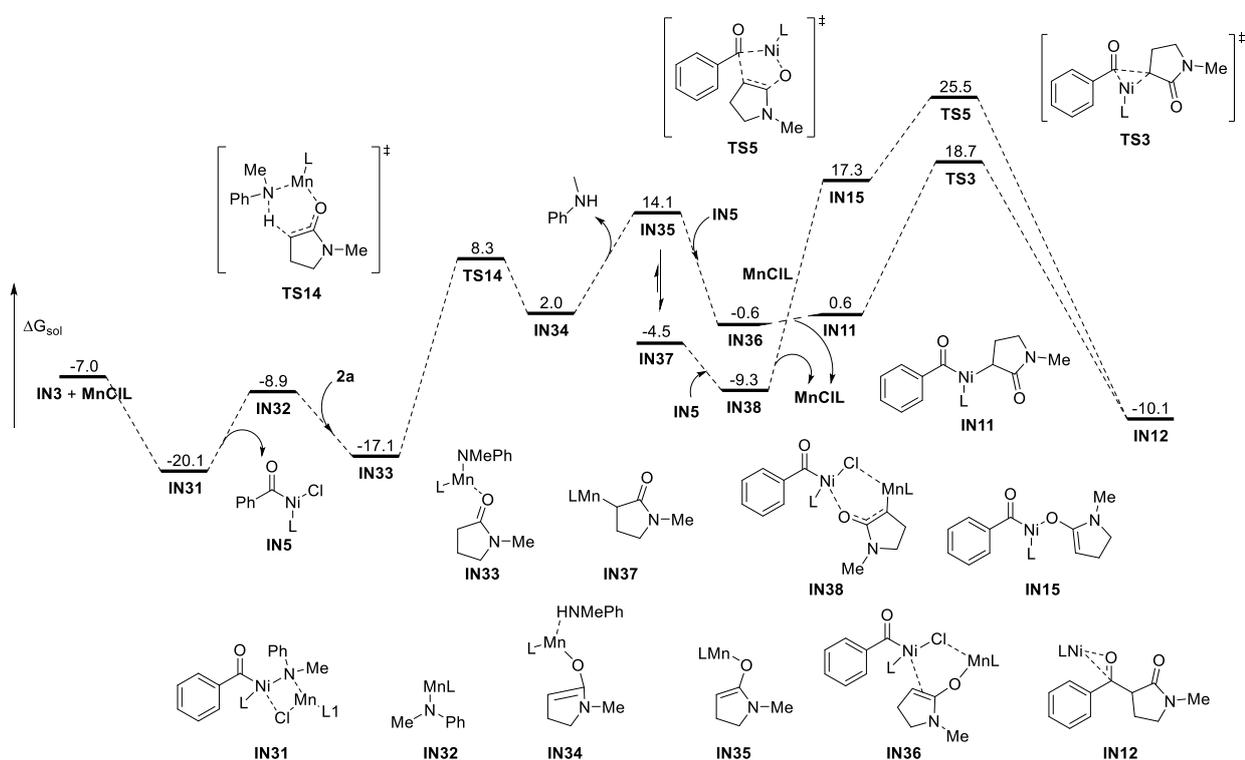


Figure S6. Possible involvement of Mn(I) species in the reaction (L = TPY; relative Gibbs free energies are in kcal/mol).

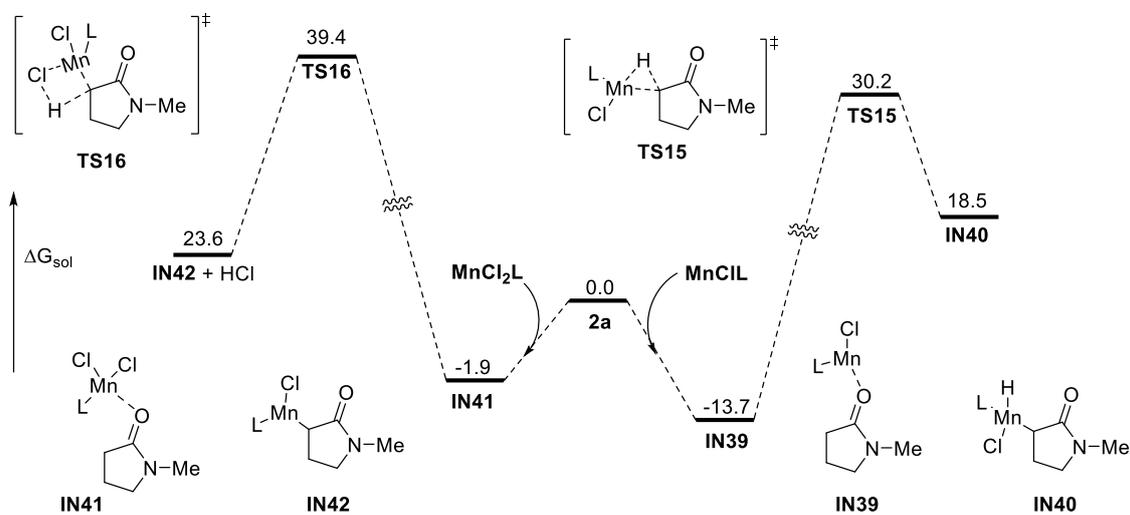


Figure S7. Possible enolization of **2a** with MnCIL or MnCl_2L ($\text{L} = \text{TPY}$; relative Gibbs free energies are in kcal/mol).

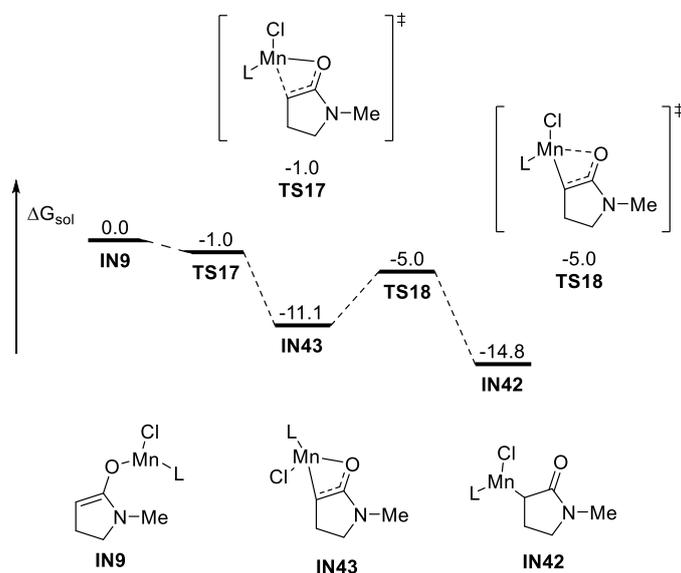


Figure S8. Mechanism and energies for isomerization of the Mn(II) -enolate **IN9** ($\text{L} = \text{TPY}$; relative Gibbs free energies are in kcal/mol).

8. Calculated Energy Values

Table S1. Energies (in Hartree) calculated at M06/6-311+G(d,p)-SDD-SMD(mesitylene) //B3LYP/6-31G*-LANL2DZ level.

Species	G ₂₉₈ ^a	E ^b	G _{sol} ^c
1a	-671.102809	-671.2981054	-670.986928522
2a	-325.835889	-325.944722	-325.818717172
NiL	-911.598982	-911.7859919	-913.093349875
MnL	-846.191894	-846.3764262	-846.4630628
MnClL	-1306.438647	-1306.625144	-1306.680675
MnCl₂L	-1766.731542	-1766.9159612	-1766.98332727
PhNHMe	-326.794978	-326.9096158	-326.746662799
HCl	-460.806911	-460.7956941	-460.7962681
IN1	-1582.691751	-1583.0933015	-1584.10860121
IN2	-1582.671138	-1583.0746291	-1584.10324818
TS1	-1582.66861	-1583.0709034	-1584.09889633
IN3	-1582.678463	-1583.0793151	-1584.11003626
IN4	-3349.394742	-3350.0061954	-3351.12843354
IN5	-1716.743994	-1717.0189035	-1718.20132203
IN6	-1632.669982	-1632.9806553	-1632.90076274
IN7	-1958.480626	-1958.9232594	-1958.7303243
TS2	-1958.447612	-1958.8886638	-1958.69939202
IN8	-1958.457529	-1958.9012574	-1958.71274517
IN9	-1631.68517	-1631.989285	-1631.944218
IN10	-3348.424038	-3349.0278553	-3350.1722971

IN11	-1581.708256	-1582.1034837	-1583.17011587
TS3	-1581.677218	-1582.0714905	-1583.14029934
IN12	-1581.735039	-1582.1338427	-1583.18775409
IN13	-1908.497368	-1909.0251941	-1909.93144306
TS4	-1908.459026	-1908.9869115	-1909.88818556
IN14	-1908.464504	-1908.9966035	-1909.9010191
IN15	-1581.689195	-1582.0844998	-1583.14359595
TS5	-1581.678671	-1582.0741279	-1583.13063411
IN16	-1237.438043	-1237.752598	-1238.9423
TS6	-1237.383381	-1237.69492	-1238.893607
IN17	-1237.394702	-1237.707596	-1238.908788
TS7	-1237.363823	-1237.674224	-1238.873721
IN18	-1237.369994	-1237.679448	-1238.875409
IN19	-1237.382005	-1237.692591	-1238.886132
IN20	-2820.050854	-2820.788737	-2823.024158
IN21	-1238.343074	-1238.660347	-1239.826595
IN22	-1517.320719	-1517.7234294	-1517.51303121
IN23	-1517.303539	-1517.7069971	-1517.49567708
TS8	-1517.264173	-1517.6676689	-1517.4476082
IN24	-1517.268023	-1517.6705532	-1517.4506889
IN25	-1843.097587	-1843.6308105	-1843.29822546
TS9	-1843.074525	-1843.6035572	-1516.53366425
IN26	-1516.324565	-1516.71766	-1516.533664

TS10	-1516.302245	-1516.699322	-1516.509464
IN27	-1516.343871	-1516.742996	-1516.561099
IN28	-1172.051546	-1172.364132	-1172.325998
TS11	-1171.984801	-1172.296789	-1172.269142
IN29	-1172.006474	-1172.318144	-1172.27349
TS12	-1171.991675	-1172.3055	-1172.262521
IN30	-1172.015511	-1172.326911	-1172.276067
IN31	-2889.124829	-2889.736871	-2890.836285
IN32	-1172.382619	-1172.693534	-1172.590859
IN33	-1498.217916	-1498.658424	-1498.443446
TS14	-1498.174978	-1498.61615	-1498.403495
IN34	-1498.185936	-1498.631329	-1498.417843
IN35	-1171.39317	-1171.696871	-1171.624756
IN36	-2888.144533	-2888.749676	-2889.876043
IN37	-1171.407569	-1171.713819	-1171.657066
IN38	-2888.155536	-2888.760502	-2889.889729
IN39	-1632.287181	-1632.601558	-1632.54035
TS15	-1632.200061	-1632.513706	-1632.469658
TS15-1	-1632.200302	-1632.510231	-1632.458088
IN40	-1632.220941	-1632.534736	-1632.488437
IN41	-2092.549812	-2092.865271	-2092.827212
TS16	-2092.483078	-2092.793851	-2092.756815
IN42	-1631.702503	-1632.008918	-1631.970147

TS17	-1631.684282	-1631.98921	-1631.946612
IN43	-1631.695433	-1632.000329	-1631.962706
TS18	-1631.68182	-1631.988472	-1631.954654

^a Sum of electronic and thermal free energies

^b Electronic energies

^c Single point energies in solution

9. Cartesian Coordinates for All Specie

1a

C	-2.26242914	1.28456890	1.20135120
C	-0.86726965	1.28387849	1.20232926
C	-0.16894265	1.17449158	0.00000000
C	-0.86580731	1.06453256	-1.20395399
C	-2.26063211	1.06475280	-1.20481088
C	-2.95902186	1.17517276	-0.00211845
H	-2.81281002	1.37126900	2.14935268
H	-0.31838358	1.37091377	2.15121847
H	-0.31498533	0.97823735	-2.15181717
H	-2.81013213	0.97809930	-2.15350215
H	-4.05862543	1.17552113	-0.00305531
C	1.37105709	1.17460361	0.00088786
O	2.00448982	2.26195522	0.00089099
N	2.10362674	-0.09985353	0.00173461
C	3.54938660	0.16600056	0.00155798
C	4.23502000	0.29505136	1.20974843
C	4.23579640	0.28913630	-1.20642684
C	5.60662997	0.54785132	1.20985725
H	3.69343899	0.19868453	2.16192763
C	5.60800545	0.54103352	-1.20648881
H	3.69559870	0.18727562	-2.15876075
C	6.29345383	0.67053655	0.00137148
H	6.14700676	0.65020650	2.16212446
H	6.14902147	0.63766339	-2.15908451
H	7.37492932	0.86980270	0.00170741
C	1.48598590	-1.43380218	0.00262089
H	0.87793947	-1.54472934	0.87604788
H	0.87887703	-1.54632435	-0.87125415
H	2.25156612	-2.18132190	0.00371404

2a

C	1.30624100	-0.74955900	0.06013700
C	1.79107800	0.71109200	-0.04734100
C	0.50256300	1.58258100	-0.06138500
N	-0.59152100	0.62987900	-0.01294300
C	-1.97373300	1.05038000	-0.00616600
H	-2.22180400	1.60687400	-0.91989900
H	-2.59176300	0.15199600	0.05012800
H	-2.18701900	1.69383700	0.85831900

H	0.43225600	2.20299800	-0.96622600
H	0.45569900	2.26548400	0.79953800
H	2.37301400	0.87427800	-0.95834800
H	2.43141900	0.98722700	0.79455200
C	-0.22159000	-0.68934400	0.07175000
O	-0.99262200	-1.64869700	0.14332900
H	1.64379400	-1.25181200	0.97253100
H	1.62623500	-1.37438900	-0.77982800

NiL

C	2.78221100	-3.70538900	-3.96939600
C	2.82964500	-5.00286400	-4.48186500
C	3.38786300	-6.01088000	-3.69207200
C	3.87305900	-5.72559400	-2.41356600
C	3.80019800	-4.41010700	-1.95235300
N	3.28255000	-3.45689300	-2.74661100
H	3.43409300	-7.02714100	-4.07052600
H	2.43476100	-5.22881100	-5.46603900
H	4.28738800	-6.51203500	-1.79279400
C	4.19014000	-3.87269100	-0.64175500
C	4.73135300	-4.62059100	0.40215100
C	4.21157900	-1.93307100	0.66127100
C	5.01738400	-3.98957100	1.61087000
H	4.91600400	-5.68153700	0.27320100
H	3.98106000	-0.87495500	0.69744900
H	5.43651900	-4.55571200	2.43712400
C	2.20490400	-2.49819100	-4.57568700
C	1.59166400	-2.44426300	-5.82586800
C	1.76112000	-0.23529900	-4.19755700
C	1.04982200	-1.23781000	-6.26373100
H	1.53143000	-3.33488800	-6.44193200
H	1.85990200	0.59483200	-3.50818700
H	0.56589000	-1.17625900	-7.23374300
N	3.94331900	-2.53713000	-0.50409200
N	2.28943400	-1.39311400	-3.77851900
C	4.75114700	-2.62797900	1.74218000
C	1.13372800	-0.11939800	-5.43670300
H	0.72077100	0.83760500	-5.73657500
H	4.95351900	-2.09913900	2.66721300
Ni	3.02718300	-1.74741400	-2.02008000

MnL

Mn	2.28281300	-1.84500600	-1.67232300
C	2.60449600	-3.65949400	-3.86525500
C	2.88428600	-4.87827600	-4.46543800
C	3.52148100	-5.88233900	-3.70908800
C	3.88466200	-5.62787700	-2.38862000
C	3.59245600	-4.38448800	-1.81481100
N	2.91917000	-3.43113800	-2.55147900
H	3.74365400	-6.84390300	-4.16065800
H	2.62319800	-5.06231800	-5.50239400
H	4.39668600	-6.39106600	-1.81061100
C	3.96176700	-3.91444300	-0.50498300
C	4.78532100	-4.61069300	0.40419100
C	3.99140500	-2.03442800	0.91533100
C	5.21716500	-3.99769500	1.56305600
H	5.10028800	-5.62288100	0.17012400
H	3.64875500	-1.01704000	1.07521800
H	5.86042900	-4.52748300	2.25933600
C	2.00805900	-2.48775600	-4.50401600
C	1.64611500	-2.41346600	-5.85792900
C	1.41831800	-0.24656500	-4.20214800
C	1.17129500	-1.21904600	-6.37932200
H	1.75247000	-3.28606900	-6.49358900
H	1.35019900	0.58373500	-3.50864100
H	0.89492400	-1.15028400	-7.42753600
N	3.50908700	-2.62939500	-0.21025700
N	1.86139700	-1.40330200	-3.67359000
C	4.82939700	-2.66043100	1.81486100
C	1.06795300	-0.10203400	-5.53719200
H	0.72057600	0.85681500	-5.90739600
H	5.17124000	-2.12890800	2.69652400

MnCIL

Mn	2.85221100	-1.67511600	-1.90568800
C	2.72220600	-3.64043400	-3.92400400
C	2.92007300	-4.90028200	-4.48574600
C	3.54015200	-5.90078900	-3.73111100
C	3.95249300	-5.62244300	-2.42442400
C	3.74008600	-4.35158700	-1.89369800
N	3.13045600	-3.37407900	-2.64060600

H	3.70021400	-6.88615300	-4.15637000
H	2.59507000	-5.10506100	-5.50072100
H	4.43506100	-6.39113500	-1.82944800
C	4.10252800	-3.86983100	-0.55941200
C	4.73923800	-4.63401800	0.42541800
C	4.05718300	-2.01191800	0.86278000
C	5.03646100	-4.05743700	1.65487500
H	4.99810200	-5.66883600	0.22641600
H	3.76050000	-0.97332300	0.97179900
H	5.53068700	-4.63907400	2.42753200
C	2.09240000	-2.47478500	-4.54727300
C	1.57657100	-2.44018300	-5.84805500
C	1.47506800	-0.24380800	-4.20569300
C	0.99805100	-1.26965000	-6.32501300
H	1.63007900	-3.32334400	-6.47619400
H	1.46662000	0.58758600	-3.50763500
H	0.59401200	-1.22906500	-7.33231300
N	3.76217600	-2.55827100	-0.33536900
N	2.03985000	-1.37301700	-3.72915100
C	4.68904000	-2.72027300	1.87733400
C	0.94619800	-0.15009200	-5.48704600
H	0.50336500	0.78316500	-5.81957800
H	4.90282400	-2.23179100	2.82248400
Cl	2.84023450	0.51070805	-1.13021456

MnCl₂L

Mn	-0.12864700	-7.41603100	-1.93023900
C	-1.13736000	-8.66807000	-4.26134900
C	-2.11549500	-9.22386800	-5.08237000
C	-3.41697100	-9.37500100	-4.59351500
C	-3.71587800	-8.98334000	-3.28372200
C	-2.71342600	-8.43086800	-2.49214600
N	-1.44895700	-8.26796100	-2.98925900
H	-4.18813000	-9.80795600	-5.22215000
H	-1.86885500	-9.54579400	-6.08854400
H	-4.71749900	-9.11564500	-2.88881300
C	-2.81691400	-8.01321500	-1.09720800
C	-3.98512300	-8.03954300	-0.32477600
C	-1.58257100	-7.21642200	0.72899400
C	-3.92990200	-7.63980900	1.00408700
H	-4.92131000	-8.36567600	-0.76489400

H	-0.60147100	-6.91904200	1.08418900
H	-4.82757100	-7.65402200	1.61538500
C	0.27498600	-8.47626700	-4.56977300
C	0.88914000	-8.76867100	-5.79475600
C	2.32226500	-7.77834500	-3.66636500
C	2.25256900	-8.54960100	-5.93957500
H	0.30104700	-9.15552500	-6.62011700
H	2.82828500	-7.39919300	-2.78498900
H	2.74278000	-8.76869800	-6.88369100
N	-1.62961900	-7.59752500	-0.56098900
N	1.00080500	-7.98578900	-3.51910600
C	-2.70699500	-7.22193200	1.54450400
C	2.98521900	-8.04489000	-4.85707100
H	4.05206200	-7.86413600	-4.93284800
H	-2.62461500	-6.90906400	2.57986500
Cl	1.59398300	-7.50717900	-0.38244400
Cl	-0.39848100	-5.66606000	-2.43857900

PhNHMe

N	2.10432400	0.15763600	-0.00808100
C	3.53178800	0.29880300	-0.00693000
C	4.23862600	0.75463300	1.11564200
C	4.24307400	-0.07292800	-1.15721000
C	5.62985500	0.84006000	1.07158800
H	3.69973500	1.05032000	2.00421600
C	5.63473300	0.00866000	-1.18747000
H	3.70907100	-0.41661800	-2.03773800
C	6.33631600	0.46810400	-0.07311700
H	6.16420000	1.19601200	1.94850800
H	6.16694700	-0.28203700	-2.08936500
H	7.42046300	0.53540400	-0.09612900
C	1.57588300	-1.08688100	-0.57956300
H	0.58812700	-1.29373300	-0.16918500
H	1.49338100	-1.05452900	-1.67283000
H	2.24614400	-1.90773200	-0.30971100
H	1.50309333	0.86704430	0.35969821

HCl

Cl	-0.16069221	0.59950555	0.00000000
H	-1.45069221	0.59950555	0.00000000

IN1

C	-1.31062185	5.50796061	-5.82119898
C	-0.44603962	4.88792711	-4.92191936
C	0.50980148	3.96804463	-5.37526005
C	0.61433092	3.71364147	-6.74946382
C	-0.23590787	4.35332534	-7.65224287
C	-1.20706667	5.24241092	-7.18908179
H	-2.05793631	6.20778096	-5.45711414
H	-0.49279004	5.11438094	-3.86137375
H	1.37640311	3.03321837	-7.11834397
H	-0.13648968	4.15948688	-8.71687283
H	-1.87443112	5.73415666	-7.89177777
C	1.47942710	3.41422144	-4.36067663
O	1.98495495	4.17862794	-3.54607190
N	1.77537744	2.05780191	-4.40475253
C	2.85041469	1.50882083	-3.62983473
C	3.10232020	1.90879960	-2.30917981
C	3.64772415	0.50796716	-4.20415637
C	4.14076173	1.31643223	-1.59119879
H	2.49858288	2.68406573	-1.85988953
C	4.67818992	-0.08343757	-3.47431544
H	3.47218406	0.19615239	-5.22912896
C	4.93210554	0.31939671	-2.16346018
H	4.32503770	1.63709004	-0.56922226
H	5.28598130	-0.85565128	-3.93847780
H	5.73672639	-0.13805786	-1.59446618
C	0.95996835	1.09584450	-5.15602484
H	-0.02764700	1.51474812	-5.34574948
H	1.40535821	0.81734904	-6.11891326
H	0.84631827	0.18935061	-4.55501006
C	4.70853045	7.78679151	-1.83313363
C	5.30851706	8.77843516	-1.04014508
C	4.64595324	9.21757186	0.11097449
C	3.40538658	8.68920997	0.48328791
C	2.81971233	7.69788511	-0.32067134
N	3.48756225	7.28019822	-1.44953716
H	5.10430881	9.98493249	0.72869944
H	6.27036144	9.19718822	-1.31569625
H	2.90367649	9.03980391	1.37872829
C	1.56770436	7.00982368	-0.14867969
C	0.66445792	7.21803931	0.90889941

C	0.10875187	5.37626009	-1.04985219
C	-0.51549769	6.50342240	0.98339275
H	0.90883798	7.95253673	1.67071042
H	-0.07949531	4.65460098	-1.84280786
H	-1.21157330	6.66512563	1.80037149
C	5.18722821	7.18024355	-3.04701428
C	6.40064683	7.49047604	-3.68638523
C	4.72025147	5.59261683	-4.74105894
C	6.77034999	6.84962898	-4.85306690
H	7.04616506	8.24575272	-3.24772722
H	4.03085978	4.84592799	-5.13118154
H	7.70693935	7.09052752	-5.34588091
N	1.28583009	6.06501039	-1.15578651
N	4.32181522	6.20668116	-3.58532384
C	-0.79791502	5.55148114	-0.03342293
C	5.89647691	5.86793512	-5.39412556
H	6.14349680	5.33747079	-6.30809701
H	-1.71164085	4.96616528	-0.01797356
Ni	2.69890351	5.95998072	-2.51192503

IN2

Ni	3.44953400	5.48141800	-0.06659300
C	4.44491600	7.10271500	0.06790800
O	3.76299200	8.02870200	0.59504000
C	5.93004100	7.04701700	0.38588200
C	6.57298200	8.26571100	0.65988200
C	6.67707700	5.86517400	0.47510000
C	7.93478100	8.30539700	0.95871300
H	5.98033600	9.17300100	0.63471900
C	8.04023400	5.90159700	0.78157100
H	6.18491600	4.91236200	0.30514600
C	8.67579600	7.12040700	1.01446900
H	8.41831900	9.25830700	1.15347900
H	8.60141300	4.97275900	0.84012000
H	9.73696100	7.14758200	1.24858300
N	4.06560200	6.73400700	-1.43795200
C	5.07073300	6.37527200	-2.40669400
C	5.55645500	5.06274600	-2.47671200
C	5.59178800	7.32560100	-3.29996700
C	6.56188500	4.71765100	-3.38287800
H	5.13271100	4.31328700	-1.81516700

C	6.58376300	6.97466200	-4.21561100
H	5.23177100	8.34850400	-3.27454900
C	7.08238900	5.67010300	-4.25543600
H	6.92620100	3.69362400	-3.41044200
H	6.97553600	7.72988600	-4.89252300
H	7.86283300	5.40176500	-4.96597000
C	3.06688300	7.70234200	-1.94524200
H	3.47300000	8.72136000	-1.96300000
H	2.75430000	7.40457700	-2.95120300
H	2.20745200	7.71405100	-1.27677300
C	2.47299700	2.87503900	-1.62748700
C	2.69389300	1.49352800	-1.74981600
C	3.02357800	0.75643900	-0.62019100
C	3.10638200	1.40792700	0.60991300
C	2.90455800	2.78881500	0.65700500
N	2.63191200	3.52560100	-0.45252200
H	3.19996900	-0.31300600	-0.68985000
H	2.58174300	1.03727800	-2.72568300
H	3.35440800	0.85906200	1.51175600
C	2.99799500	3.56248600	1.91352400
C	2.81292800	3.01734200	3.18908900
C	3.29339400	5.69571000	2.81273100
C	2.87917100	3.85656600	4.30006700
H	2.59317600	1.96284600	3.30714400
H	3.48488900	6.74391900	2.58442900
H	2.73083000	3.45266900	5.29702800
C	1.98191900	3.63625100	-2.80687800
C	1.28701300	4.84497500	-2.66174300
C	1.71455400	3.68181600	-5.09160900
C	0.79689400	5.47626900	-3.80224500
H	1.13615900	5.26539200	-1.67318300
H	1.90540500	3.19031700	-6.04352800
H	0.24615100	6.40916900	-3.71617700
N	3.25015900	4.88130100	1.74293600
N	2.18222200	3.05929200	-4.00813000
C	3.11559300	5.21981600	4.10731100
C	1.01586100	4.89240600	-5.04760600
H	0.65426600	5.35223200	-5.96220700
H	3.16791000	5.90576800	4.94644300

TS1

H	4.86122300	7.53671300	-4.01033300	C	4.47788200	9.09349300	-1.23999000
C	6.90264000	4.83427500	-4.32483400	O	3.44734500	9.64366500	-1.60301500
H	6.98723200	3.19457600	-2.92248800	C	5.72729200	9.89455400	-1.01505100
H	6.55887700	6.61187100	-5.49320900	C	6.89399000	9.31157400	-0.50599100
H	7.65965100	4.42931000	-4.99051000	C	5.71748000	11.26751000	-1.31890000
C	3.34194100	7.66567700	-2.05810400	C	8.03549600	10.08779000	-0.30120100
H	4.08464100	8.48078800	-2.10766300	H	6.90748200	8.25069000	-0.28195200
H	2.82432800	7.63693600	-3.03068800	C	6.85696100	12.03976400	-1.11740800
H	2.60985800	7.94132900	-1.29535800	H	4.80313200	11.70206100	-1.71095800
C	2.56145100	3.09476000	-1.75264400	C	8.01896200	11.44971300	-0.60674000
C	2.88813600	1.74303300	-1.96901500	H	8.93799000	9.62779600	0.09190600
C	3.32564200	0.96997100	-0.90539400	H	6.84485900	13.10050800	-1.35523700
C	3.39733100	1.54291400	0.36668200	H	8.90955300	12.05304500	-0.44900100
C	3.07325900	2.89227600	0.50481100	N	5.05000600	6.76012600	-2.73008800
N	2.70868400	3.66975700	-0.54151800	C	6.46270100	6.54093200	-2.72243200
H	3.59434100	-0.07195100	-1.05389600	C	7.06778900	5.91958300	-1.61178900
H	2.78012200	1.34544600	-2.97016800	C	7.30843000	6.90944700	-3.78796300
H	3.71958700	0.95955300	1.22228200	C	8.43743600	5.68724200	-1.55958000
C	3.07242600	3.58270000	1.81528600	H	6.43537100	5.62016400	-0.78517800
C	2.86815000	2.91351100	3.02534900	C	8.68485700	6.66883200	-3.73415900
C	3.11083800	5.63521100	2.90859400	H	6.90437800	7.38758100	-4.67128000
C	2.79068000	3.64520800	4.20767400	C	9.26523400	6.06129800	-2.62336700
H	2.73904800	1.83712400	3.03323800	H	8.86316400	5.21159900	-0.67880800
H	3.20406400	6.70987300	2.80653000	H	9.30424500	6.97045900	-4.57578600
H	2.62738500	3.14057200	5.15534200	H	10.33635000	5.88311200	-2.58336300
C	1.96576900	3.88620400	-2.85984900	C	4.64584100	7.71483000	-3.78385500
C	2.68156460	4.15802249	-4.03301582	H	5.24447900	8.63432700	-3.74465800
C	0.17044653	5.12784329	-3.57820237	H	4.75853200	7.28064400	-4.78417800
C	2.08333927	4.95336430	-5.00880717	H	3.60177700	7.98614400	-3.64380800
H	3.67938293	3.76060130	-4.16345845	C	7.45659200	7.61928300	3.47745000
H	-0.83009525	5.49828870	-3.36168177	C	7.97827500	6.40641200	2.99852900
H	2.61501515	5.18391542	-5.92768986	C	7.18738400	5.61910100	2.16657100
N	3.21229400	4.93045600	1.76642200	C	5.91385800	6.06197100	1.81338500
N	0.73502465	4.37803415	-2.63145043	C	5.48241400	7.29228900	2.32579700
C	2.90164700	5.03300000	4.14584000	N	6.22715700	8.04005800	3.15225600
C	0.79795138	5.44357077	-4.78632581	H	7.55034700	4.65857800	1.81111500
H	0.29256928	6.06191272	-5.52208028	H	8.96320000	6.07027900	3.30632500
H	2.82809200	5.64868000	5.03596600	H	5.25368000	5.46650500	1.19282100
				C	4.10370800	7.80541000	2.08475900
				C	3.41725500	8.35033400	3.17971900
				C	2.25444200	8.14962100	0.73055300
IN4							
Ni	4.29670500	7.23795300	-0.95105300				

C	2.49895300	4.11304900	-4.14728000
C	0.37710700	5.65357200	-3.39645800
C	1.86969600	4.89823400	-5.11122000
H	3.37194900	3.51794000	-4.39315300
H	-0.46524500	6.25633300	-3.06148800
H	2.23328200	4.90425000	-6.13491100
N	3.28771000	4.84642700	1.76841000
N	0.96859000	4.90775100	-2.45977000
C	3.12274500	4.86966800	4.16397900
C	0.77883700	5.67973800	-4.73479600
H	0.25447900	6.30289400	-5.45302200
H	3.09869800	5.45601300	5.07636100
Cl	3.81603458	6.32983157	-2.01116824

IN6

N	3.23056680	0.10366353	0.47645672
C	3.19054311	-0.58843517	-0.73193655
C	3.35244703	0.11830360	-1.94096680
C	3.02768326	-1.98452958	-0.79210605
C	3.35609067	-0.54913887	-3.16015509
H	3.48141420	1.19878073	-1.91105282
C	3.03851969	-2.64237757	-2.02311163
H	2.89420806	-2.55849015	0.11885568
C	3.20039309	-1.93789744	-3.21516980
H	3.48129394	0.02186244	-4.07697453
H	2.91207497	-3.72222388	-2.04328186
H	3.20373086	-2.45697577	-4.16906532
C	4.48791698	0.48253465	1.09196579
H	4.58966035	-0.05468517	2.03863216
H	5.36862697	0.26089955	0.46647792
H	4.49681005	1.55481489	1.31951055
Mn	1.68772764	0.51654732	1.44912024
C	1.92717173	2.69734187	3.18791222
C	2.06488414	3.31177841	4.44317113
C	2.13883966	2.50818385	5.58583228
C	2.07906103	1.11324486	5.50003637
C	1.94175350	0.51505004	4.23694517
N	1.86997964	1.32353690	3.12518017
H	2.24488321	2.97712387	6.56018658
H	2.11321905	4.39220176	4.52548940
H	2.13767279	0.50329891	6.39500743

C	1.85907721	-0.88039624	3.89572980
C	1.90480875	-1.94546045	4.81291478
C	1.63856292	-2.43775892	2.12508608
C	1.81702194	-3.25513688	4.38214457
H	2.01083720	-1.72284735	5.87063188
H	1.53380077	-2.59646126	1.05324372
H	1.85263990	-4.07612626	5.09125051
C	1.83109242	3.30153242	1.88549878
C	1.85776038	4.68356530	1.62723904
C	1.60425681	2.88950969	-0.43553462
C	1.75731117	5.16472486	0.33615154
H	1.95833638	5.37098955	2.46203834
H	1.50519257	2.15075253	-1.22889766
H	1.77738835	6.23175297	0.13829976
N	1.72272788	-1.12939291	2.51522304
N	1.70096872	2.37734688	0.82933143
C	1.67917992	-3.50392535	2.98967564
C	1.62652368	4.23116152	-0.72755688
H	1.54473786	4.56076291	-1.75829886
H	1.60646766	-4.51548430	2.60342490
Cl	-0.17714351	0.03491713	0.47142502

IN7

C	0.70257372	-1.57050254	0.53285393
C	-0.64897785	-0.88851078	0.39262981
C	-0.27105342	0.60726433	0.22431423
N	1.08390529	0.71404424	0.77431136
H	-0.96114691	1.29139992	0.73207962
H	-0.25215920	0.88540370	-0.84383911
H	-1.25357587	-1.02868586	1.30079607
H	-1.25519971	-1.23816405	-0.45073814
C	1.65393541	-0.54816178	0.79971251
O	2.91502748	-0.76970021	0.82283181
C	1.23909805	-4.05056281	-2.89150056
C	0.58082105	-5.22254481	-3.28171356
C	0.52203505	-6.29046481	-2.39201256
C	1.12973405	-6.16296881	-1.15005456
C	1.77144905	-4.96007381	-0.81705456
N	1.80418505	-3.91558481	-1.67203956
H	0.00945005	-7.20831281	-2.66556356
H	0.09947405	-5.28659281	-4.25088656

H	6.95964824	0.65270906	0.96521419
H	7.23363724	0.74042006	-1.51165381
H	5.35394724	0.25165206	-3.00213981
N	2.81421424	-0.43328394	-2.20084181
H	-0.13617728	0.24288962	-2.35911027
C	2.92271124	-0.09877894	-3.61207581
H	3.57206124	-0.79457694	-4.16834581
H	1.92377124	-0.15358294	-4.05906281
H	3.31267024	0.91810106	-3.79015581
Mn	2.01559855	-2.37116299	-2.07108127
Cl	0.88286716	-4.15525210	-1.62437595

IN8

C	0.41598300	0.43973100	-1.40236000
C	-0.10185800	1.68945000	-0.70065200
C	-0.08476100	1.28542100	0.79410000
N	-0.11279600	-0.17639800	0.76262300
C	-0.01805100	-0.95782500	1.97318200
H	-0.86922300	-0.73795700	2.63020100
H	-0.03828200	-2.01583200	1.70528400
H	0.90684500	-0.74637200	2.53858300
H	-0.93280500	1.68077400	1.36637600
H	0.84033300	1.62993400	1.28858000
H	-1.13143800	1.93690300	-1.00748100
H	0.50339200	2.58811400	-0.86936900
C	0.29002500	-0.63196700	-0.47622200
O	0.60754500	-1.86479300	-0.64181900
H	1.93139700	-0.02947500	-1.79944000
C	2.80153900	-3.42887200	-4.57544000
C	3.72352100	-3.90631500	-5.50796600
C	4.97946500	-4.33197600	-5.07423300
C	5.28379300	-4.30133000	-3.70633100
C	4.33616700	-3.82661000	-2.80674200
N	3.12871200	-3.36502500	-3.24952800
H	5.71131700	-4.69485000	-5.78839300
H	3.46713200	-3.94031200	-6.56166600
H	6.24813600	-4.65032600	-3.35304100
C	4.44051100	-3.81121300	-1.34478000
C	5.47499100	-4.39966000	-0.60864900
C	3.29144100	-3.28247100	0.61241800
C	5.39360600	-4.42151200	0.77871300

H	6.31629700	-4.85567800	-1.11887400
H	2.39503400	-2.83992800	1.03254300
H	6.18472100	-4.88014900	1.36470000
C	1.44565400	-2.96303900	-4.83383000
C	0.77679100	-3.06166200	-6.06148800
C	-0.46531700	-2.07566600	-3.82491600
C	-0.54395500	-2.64640300	-6.15466900
H	1.28470500	-3.48286200	-6.92252400
H	-0.91497900	-1.72127700	-2.90542900
H	-1.07688200	-2.72225800	-7.09781600
N	3.37912400	-3.23241000	-0.72256700
N	0.82685300	-2.43650400	-3.73381400
C	4.27369500	-3.86789700	1.40384300
C	-1.18435500	-2.15538300	-5.00949200
H	-2.22368600	-1.84559000	-5.03167900
H	4.16263700	-3.88319800	2.48281000
C	3.90469500	-0.28234800	-1.37900300
C	3.73152000	-0.14097100	0.01043800
C	4.79865300	0.20230100	0.83551600
C	6.07443700	0.41149900	0.30384300
C	6.25831300	0.27103500	-1.07153700
C	5.19089800	-0.06677200	-1.90620200
H	2.74985200	-0.30466200	0.43825700
H	4.63096600	0.31181100	1.90477300
H	6.90576400	0.68110600	0.94932300
H	7.24243800	0.42760800	-1.50764100
H	5.36917800	-0.16648800	-2.97152600
N	2.76659600	-0.58848800	-2.18838500
H	0.05770700	0.24837300	-2.41331200
C	2.91292600	-0.14051800	-3.58242600
H	3.54652300	-0.80806000	-4.17313200
H	1.92188700	-0.11691400	-4.03923400
H	3.33808800	0.86930500	-3.63175600
Mn	1.90339900	-2.62253500	-2.01872100
Cl	0.85741900	-4.69967100	-1.65855300

IN9

C	-0.25944100	2.67888100	0.57961000
C	0.07350500	3.56053300	1.76898600
C	-1.07144100	3.22682900	2.76824000
N	-1.53274400	1.90557200	2.33474400

H	-1.09623700	4.24648700	-1.37665100
H	-3.11974200	3.88202400	2.40576900
N	3.53070700	0.70617600	-0.69422500
N	-0.59666300	2.59596400	-0.25473700
C	5.71415000	-0.13289300	-1.25122600
C	-2.21005900	4.22686400	0.47571600
H	-2.74174700	5.15036700	0.26745200
H	6.66760800	0.04025900	-1.73948100

IN12

C	2.81983500	-4.39341300	-2.42362700
C	3.81984800	-4.83564600	-3.51091200
C	5.09602900	-4.04999300	-3.13381400
N	4.56186600	-2.82732400	-2.52183700
C	5.35827000	-1.64078500	-2.28513400
H	5.78925200	-1.27186300	-3.22358000
H	4.70908000	-0.87398400	-1.85828000
H	6.17714600	-1.85075700	-1.58489500
H	5.71910100	-3.79360800	-3.99809800
H	5.72386200	-4.59667400	-2.41444500
H	3.48671700	-4.53149500	-4.50615100
H	3.98482600	-5.91539000	-3.52772100
C	3.27839900	-2.97850000	-2.13294400
O	2.55898000	-2.08582600	-1.64113700
C	-2.20825800	-2.48247400	-0.94541500
C	-3.59018100	-2.50808900	-1.08612400
C	-4.15347300	-2.42825700	-2.37059700
C	-3.32050000	-2.24638900	-3.47857800
C	-1.93731300	-2.21679800	-3.30105500
N	-1.39734200	-2.43377900	-2.05405200
H	-5.23129300	-2.45153000	-2.49550400
H	-4.23140800	-2.55843900	-0.21163000
H	-3.74968700	-2.10061300	-4.46504700
C	-0.92748900	-1.86321000	-4.27236700
C	-1.16584800	-1.56500600	-5.62770600
C	1.33117700	-1.31190100	-4.53328900
C	-0.13223500	-1.11820900	-6.42874000
H	-2.16692200	-1.67934800	-6.03115000
H	2.30289600	-1.22144900	-4.05846400
H	-0.30802600	-0.87722100	-7.47307000
C	-1.44743200	-2.41165200	0.29124500

C	-1.97771300	-2.50057600	1.58878200
C	0.70053200	-2.09998100	1.16168200
C	-1.13618800	-2.36829200	2.68202800
H	-3.03981700	-2.67555100	1.72788000
H	1.75326100	-1.96065700	0.93459400
H	-1.53443600	-2.43060800	3.69079900
N	0.34082600	-1.76733100	-3.73487500
N	-0.10483500	-2.21549300	0.09047900
C	1.15086100	-0.97264700	-5.86204600
C	0.23653600	-2.15870900	2.46713600
H	0.92811600	-2.05152500	3.29656400
H	1.98792600	-0.60480100	-6.44700200
C	1.27506900	-4.44009800	-2.51390700
H	3.05242000	-4.96766700	-1.51061600
O	0.74267900	-4.43495500	-1.29159600
C	0.58075600	-5.19989500	-3.58621500
C	-0.42011700	-6.12409800	-3.22534100
C	0.84334400	-5.02262500	-4.95899300
C	-1.10429700	-6.85817000	-4.19137200
H	-0.64273700	-6.24849300	-2.17063700
C	0.15918900	-5.76086700	-5.92496000
H	1.55641200	-4.26944100	-5.28053800
C	-0.81478900	-6.68829300	-5.54870500
H	-1.86603400	-7.57132100	-3.88386600
H	0.37932500	-5.59918900	-6.97789400
H	-1.34759100	-7.26282600	-6.30219900
Ni	0.48986600	-2.60736900	-1.84856300

IN13

Ni	-4.45230800	4.43923200	0.24611100
C	-5.98999100	5.53978900	0.30784300
O	-6.76049800	5.66002700	-0.62311100
C	-6.26562200	6.25977900	1.61349000
C	-7.45971300	6.98726000	1.74636300
C	-5.37342000	6.21443100	2.69086300
C	-7.75198500	7.65194100	2.93434900
H	-8.13824700	7.01773300	0.89935200
C	-5.66027400	6.88528800	3.88062400
H	-4.44832600	5.65297700	2.58529100
C	-6.85183200	7.60324600	4.00469000
H	-8.67982800	8.21076200	3.03017600

C	3.08914300	-6.08095600	-6.11789500
H	1.44912300	-6.99255600	-5.03738400
C	3.37514400	-3.70897000	-5.75725800
H	1.98184400	-2.79131200	-4.38606700
C	3.77803600	-4.89256100	-6.38069200
H	3.39621000	-7.00560700	-6.60161000
H	3.90541400	-2.78107400	-5.95896200
H	4.62058700	-4.88951500	-7.06793300
Ni	-0.40875300	-3.35098900	-2.95740200

IN16

C	-0.20249100	-1.62950100	0.06708300
C	-1.35540000	-0.81883500	0.68948400
C	-0.64315000	0.22746400	1.57489900
N	0.68039100	0.34604100	0.96432900
C	1.63202200	1.36299500	1.36686800
H	1.88142700	1.26563500	2.43166600
H	2.53923900	1.24085800	0.77341900
H	1.21649700	2.36238700	1.19494000
H	-0.54986600	-0.10400000	2.61986800
H	-1.14907200	1.19919000	1.57717200
H	-2.05341600	-1.43340600	1.26246800
H	-1.92314700	-0.31171300	-0.09688800
C	0.98709900	-0.69418000	0.15350300
O	2.09042100	-0.84137800	-0.40494600
H	-0.37373400	-1.93376100	-0.97001900
C	3.13339500	-3.67943200	-4.05808700
C	3.57919300	-4.73326200	-4.87853700
C	4.39837100	-5.72083200	-4.32392000
C	4.77691100	-5.68057000	-2.97886900
C	4.31988600	-4.61724900	-2.17739500
N	3.51791000	-3.65044700	-2.73706400
H	4.74720200	-6.53731000	-4.95115500
H	3.29162300	-4.77901900	-5.92348500
H	5.41083300	-6.45525600	-2.56087600
C	4.57456800	-4.36863900	-0.78510400
C	5.37054100	-5.17178800	0.05479600
C	4.17645200	-2.89912100	1.02800300
C	5.56587100	-4.83502200	1.37897300
H	5.83414300	-6.06335400	-0.35771000
H	3.69315700	-1.98744400	1.36984800

H	6.18113600	-5.45476700	2.02423300
C	2.28929100	-2.56990700	-4.40197900
C	1.74611400	-2.32556900	-5.67896400
C	1.24856900	-0.59762400	-3.60556200
C	0.95450300	-1.22024300	-5.91413500
H	1.96346200	-3.02389900	-6.48220100
H	1.08767300	0.07059800	-2.76302400
H	0.53856800	-1.03418300	-6.89965900
N	3.95321600	-3.20833600	-0.28221700
N	2.02283400	-1.68860800	-3.33244800
C	4.94837000	-3.65353600	1.87814300
C	0.70304500	-0.32345000	-4.83581300
H	0.09885800	0.56786900	-4.97458000
H	5.08110700	-3.34264500	2.90986300
H	0.03028700	-2.53820000	0.63816600
Ni	2.87862600	-2.23996100	-1.63489300

TS6

C	0.36621962	-1.75293640	-0.55737302
C	0.60693833	-0.92441221	0.69360542
C	-0.54619139	0.10432449	0.78990480
N	-1.52798239	-0.44042998	-0.12001037
C	-2.81599658	0.17078308	-0.32471777
H	-2.72081877	1.21451099	-0.66465295
H	-3.33538292	-0.40677836	-1.09237205
H	-3.40808808	0.16858685	0.60088819
H	-0.22672449	1.11143336	0.47076595
H	-0.95578852	0.20028361	1.80526404
H	1.58343586	-0.42846432	0.68625697
H	0.58328191	-1.57491091	1.58330847
C	-1.00487291	-1.39853502	-0.98654844
O	-1.67095257	-1.85445937	-1.92711654
H	1.86379588	-1.33932808	-1.34082277
C	3.50152500	-3.31770900	-4.06271700
C	4.59614300	-3.76871100	-4.80861300
C	5.67189800	-4.35660900	-4.15120600
C	5.63198900	-4.47963100	-2.76651300
C	4.50364400	-4.02699700	-2.07299000
N	3.45734500	-3.46325400	-2.71848300
H	6.53215000	-4.71140900	-4.71074900
H	4.60756300	-3.67118600	-5.88733000

H	6.46938700	-4.91929100	-2.23870100	C	3.59714700	-4.25116800	-4.84745500
C	4.38077100	-4.10912900	-0.60190700	C	4.48280000	-5.17751800	-4.29458900
C	5.34742800	-4.72396600	0.20976300	C	4.68983500	-5.19882800	-2.90246800
C	3.13427800	-3.52952300	1.25470600	C	3.99690700	-4.30520100	-2.09983400
C	5.18186300	-4.72237500	1.58930800	N	3.11591300	-3.40741000	-2.64856300
H	6.21718600	-5.20098100	-0.22667100	H	5.01745300	-5.87168300	-4.93471300
H	2.24334100	-3.04480100	1.63047500	H	3.44347300	-4.21794600	-5.92139300
H	5.92092500	-5.19369100	2.23076600	H	5.38663900	-5.90693200	-2.46651800
C	2.33228600	-2.64960400	-4.67274000	C	4.08305700	-4.17456300	-0.64833900
C	2.29782200	-2.26279000	-6.02029900	C	4.93419900	-4.92160800	0.17603800
C	0.21314100	-1.79269100	-4.31523100	C	3.27553700	-2.98415300	1.20295700
C	1.16749700	-1.61763400	-6.50999300	C	4.94363300	-4.68491600	1.54406800
H	3.14210600	-2.44652200	-6.67483900	H	5.58391400	-5.67357400	-0.25910000
H	-0.60097200	-1.67654300	-3.61166400	H	2.60638900	-2.19959000	1.55530700
H	1.12174500	-1.30711300	-7.55014100	H	5.60113500	-5.25510300	2.19410700
N	3.27732300	-3.53377300	-0.07696200	C	2.00794700	-2.30800200	-4.39471800
N	1.30206400	-2.40907800	-3.83593500	C	1.65819200	-1.97154400	-5.71409200
C	4.05404600	-4.10280300	2.12847800	C	0.74253000	-0.50997000	-3.58514900
C	0.10326500	-1.37947300	-5.64222400	C	0.83207500	-0.88782400	-5.95518800
H	-0.80258000	-0.88596500	-5.97940600	H	2.04971400	-2.55955400	-6.53787700
H	3.88372700	-4.06529000	3.19961500	H	0.43279700	0.05603100	-2.71494700
Ni	1.81387600	-2.75348100	-1.66624700	H	0.55908400	-0.61935000	-6.97133200
H	-0.14930515	-2.54940139	-0.06262284	N	3.25111600	-3.21718700	-0.12708800

IN17

C	0.38252300	-2.02876900	-0.28912900
C	-0.99398800	-1.91557600	-0.97999100
C	-1.48191900	-0.48218800	-0.65340500
N	-0.67869200	-0.09662400	0.48897500
C	-0.87950400	1.14408600	1.19567200
H	-1.89023600	1.19679100	1.62314100
H	-0.14350600	1.18756600	2.00109900
H	-0.74172400	2.01267500	0.53392200
H	-2.55258300	-0.45086600	-0.40683500
H	-1.33163400	0.21373400	-1.49505000
H	-1.69736400	-2.64436000	-0.55578900
H	-0.97584300	-2.08800800	-2.06088600
C	0.38156000	-0.94193400	0.74255200
O	1.15529800	-0.78141000	1.69020600
H	2.58412800	-0.86480100	-1.11006300
C	2.92143800	-3.36138500	-4.01071200

TS7

C	0.70257372	-1.57050254	0.53285393
C	-0.64897785	-0.88851078	0.39262981
C	-0.27105342	0.60726433	0.22431423
N	1.08390529	0.71404424	0.77431136
H	-0.96114691	1.29139992	0.73207962
H	-0.25215920	0.88540370	-0.84383911
H	-1.25357587	-1.02868586	1.30079607
H	-1.25519971	-1.23816405	-0.45073814
C	1.65393541	-0.54816178	0.79971251

H	2.07776300	2.16244300	-0.64857900
H	1.27104300	2.79816300	0.80692700
H	3.80134100	-2.01797600	-1.30505700

IN19

C	-1.90233600	-4.78034100	0.82344800
C	-2.86012100	-4.30773600	-0.24548400
C	-2.63239300	-2.77602300	-0.20960200
N	-1.26760400	-2.62283500	0.31289600
C	-0.92791200	-1.33345100	0.88830300
H	-1.65788800	-1.00882900	1.65284500
H	0.05555500	-1.40214100	1.35797800
H	-0.89706100	-0.56970400	0.10283100
H	-3.35205200	-2.30138700	0.48214300
H	-2.73511900	-2.29402800	-1.18794800
H	-3.90959600	-4.56099800	-0.05291100
H	-2.61118500	-4.71253100	-1.23959400
C	-1.00134000	-3.78322300	1.07975200
O	0.08185900	-3.81179800	1.83608100
H	2.18231500	-5.16963600	2.01381100
C	2.01592400	-7.38322500	-0.43963000
C	2.42845600	-8.64642600	-0.84741800
C	2.20278400	-9.75116200	-0.01403100
C	1.56515100	-9.56847600	1.21972500
C	1.16371700	-8.29326100	1.60311700
N	1.38612700	-7.21704600	0.77232900
H	2.52015600	-10.74151500	-0.32317400
H	2.92151900	-8.77791800	-1.80511300
H	1.38515200	-10.41670700	1.87239200
C	0.49461100	-7.89957500	2.82938600
C	0.13539400	-8.74862600	3.88666300
C	-0.38864600	-6.05231500	3.98116300
C	-0.49741600	-8.22425000	5.00349400
H	0.35796200	-9.80889600	3.82452900
H	-0.56048400	-4.98162000	3.95786400
H	-0.77873900	-8.87224700	5.82828700
C	2.15524100	-6.12679200	-1.15596900
C	2.76626800	-5.96355800	-2.40767500
C	1.69256400	-3.83087300	-1.05389500
C	2.83446100	-4.70238700	-2.97982000
H	3.18411400	-6.82508200	-2.91800200

H	1.24112300	-3.02714500	-0.48497100
H	3.30772700	-4.56380700	-3.94739900
N	0.22265300	-6.55411400	2.88754700
N	1.62036000	-5.05282800	-0.48712000
C	-0.76436400	-6.84594400	5.05329700
C	2.28404000	-3.61228000	-2.28851400
H	2.31291200	-2.60923400	-2.70084200
H	-1.25432000	-6.39683700	5.91073200
H	-1.92587500	-5.74567500	1.31033400
Ni	0.84589000	-5.47830500	1.32340100

IN20

Ni	4.73923000	1.79610000	1.84869200
C	3.39944600	3.11088800	1.79118100
O	2.28945200	2.74049900	2.15163400
C	3.62441400	4.53834500	1.38229900
C	2.52739700	5.41664600	1.33767600
C	4.89970900	5.01585600	1.05787200
C	2.70760700	6.74740500	0.97380000
H	1.54628900	5.02899600	1.59429300
C	5.08071800	6.35129400	0.69616500
H	5.74430100	4.33638200	1.07945400
C	3.98665000	7.21699400	0.65315200
H	1.85621600	7.42279600	0.93992700
H	6.07366300	6.71341800	0.44454900
H	4.12767700	8.25724200	0.37008600
N	4.41534900	1.40299800	-0.30181300
C	5.30239600	2.15697600	-1.10682800
C	6.61329700	2.43836000	-0.65798100
C	4.95562300	2.67607500	-2.37700500
C	7.52750700	3.14624200	-1.43332200
H	6.89413700	2.11388600	0.33701300
C	5.87327000	3.39066200	-3.14974100
H	3.96285300	2.51465700	-2.77734900
C	7.17133500	3.62742800	-2.69728900
H	8.52186300	3.34126000	-1.03618700
H	5.55968200	3.76886900	-4.12062700
H	7.87942100	4.18894300	-3.30061000
C	3.00927200	1.61710900	-0.68513900
H	2.75251200	2.68453100	-0.74303700
H	2.77965700	1.17156700	-1.66185100

H	2.35736000	1.15925100	0.05853700	H	7.63428400	-2.50521300	-0.92209200
C	8.38584200	5.23879300	3.95204300	C	6.54110200	-0.75701000	1.63056800
C	9.16145300	4.65324600	2.93743200	O	5.99668100	0.16097200	2.32191800
C	8.79359700	3.40322300	2.44787900	C	1.73760600	-1.55938400	-0.77088900
C	7.65359600	2.77948500	2.95205900	C	0.57156100	-1.92329900	-1.46244500
C	6.91867400	3.45628100	3.93503200	C	0.62203300	-2.13574600	-2.83170300
N	7.28880400	4.64245000	4.43829500	C	1.84505700	-2.00108800	-3.47918000
H	9.38859800	2.91626800	1.68002700	C	2.97558300	-1.63434800	-2.74225900
H	10.02690400	5.17102800	2.53691200	N	2.91958200	-1.38439500	-1.40806200
H	7.34282700	1.79137700	2.62955600	H	-0.27280900	-2.40497600	-3.38555000
C	5.71046800	2.85177900	4.56591600	H	-0.34628400	-2.02322000	-0.89788300
C	5.53107200	3.02420100	5.94595600	H	1.92664400	-2.14614800	-4.55044700
C	3.76314800	1.59246500	4.45203700	C	4.28995800	-1.49246700	-3.42035800
C	4.44896500	2.43343900	6.58476400	C	4.64084200	-2.28518500	-4.52209300
H	6.25178800	3.62888900	6.48236400	C	6.31904400	-0.39731000	-3.48024300
H	3.04852100	1.09432400	3.80912300	C	5.89097900	-2.10254500	-5.10939300
H	4.30744100	2.55426400	7.65513700	H	3.96397600	-3.04764200	-4.89352800
C	8.75583500	6.56055400	4.54246800	H	6.94476800	0.37255900	-3.03750900
C	10.10077800	6.94931600	4.65312000	H	6.19183100	-2.71027800	-5.95825700
C	8.05397400	8.53087000	5.49051800	C	1.63655500	-1.41407700	0.71257100
C	10.40399600	8.19164900	5.20598700	C	2.72040000	-1.64383600	1.56926700
H	10.89509800	6.28105100	4.33606900	C	0.22054000	-1.04413700	2.49011100
H	7.20898500	9.13725900	5.81450200	C	2.50885400	-1.57059400	2.94571000
H	11.43809800	8.50994500	5.30780700	H	3.69752800	-1.88374200	1.15777700
N	4.81854300	2.15188600	3.82619900	H	-0.78821300	-0.79784200	2.81751800
N	7.74791300	7.34385300	4.96345200	H	3.33168200	-1.75499000	3.62944000
C	3.54961900	1.69078500	5.82123700	N	5.12319700	-0.57339700	-2.90516300
C	9.35933700	9.00849800	5.63394300	N	0.40272600	-1.12869200	1.17235700
H	9.54484400	9.98521600	6.07076900	C	6.74772700	-1.13466700	-4.58385200
H	2.68156000	1.21382200	6.26455500	C	1.23680500	-1.26141400	3.42343000
C	6.95737500	-0.76731400	0.26089700	H	1.02875500	-1.19480900	4.48747500
C	7.77205100	-2.03170800	0.05395200	H	7.72650000	-0.95165700	-5.01679000
C	7.28125600	-2.93506900	1.20038900	H	7.27614000	0.15870000	-0.19838300
N	6.85134700	-1.97590700	2.21323500	Ni	4.72778000	-0.75421700	-0.59982100
C	6.26739300	-2.42236400	3.45359200	H	5.01709300	-2.21298800	-0.58677700
H	7.00417700	-2.97638600	4.04853600				
H	5.94279200	-1.54390100	4.01497200				
H	5.40151700	-3.08596500	3.28626700				
H	8.05228900	-3.60590600	1.59823100				
H	6.42205900	-3.54447400	0.87198500				
H	8.84921000	-1.82984500	0.17806800				
				IN21			
				C	-1.12203000	-8.76952000	-4.24035600
				C	-2.07858200	-9.39743300	-5.03064900
				C	-3.36744900	-9.60467400	-4.52353400
				C	-3.67983900	-9.16329800	-3.23164700

C	-2.70304100	-8.53825100	-2.46418600
N	-1.43507700	-8.35701300	-2.96593400
H	-4.12190300	-10.09236100	-5.13167500
H	-1.83051800	-9.71696600	-6.03744200
H	-4.68056000	-9.30054800	-2.83540000
C	-2.84098100	-7.99244700	-1.12453800
C	-3.99844600	-8.04634700	-0.33568100
C	-1.70229200	-6.84176000	0.57131700
C	-3.98952000	-7.48175100	0.93131000
H	-4.88975100	-8.53264700	-0.71782700
H	-0.76838000	-6.38151800	0.87411300
H	-4.87955300	-7.51836400	1.55312600
C	0.24903300	-8.44479500	-4.59557600
C	0.87503000	-8.76132000	-5.80917600
C	2.20597600	-7.41258500	-3.82036800
C	2.19511900	-8.38891600	-6.01570800
H	0.32633800	-9.29885400	-6.57533800
H	2.67833600	-6.88285800	-3.00061500
H	2.69216600	-8.62981000	-6.95074000
N	-1.69937200	-7.38529000	-0.66416700
N	0.92121900	-7.76808500	-3.60858000
C	-2.81753800	-6.86793400	1.39528600
C	2.87527700	-7.70127200	-5.00025500
H	3.90775700	-7.39149300	-5.12159800
H	-2.76885800	-6.41463000	2.37959300
H	0.29426700	-8.89913300	-1.35363200
Ni	-0.11329500	-7.52912800	-1.89680600
N	-0.59575281	-5.86506066	-2.54535388
C	0.54586016	-4.94575590	-2.43355684
H	0.47287010	-4.19277148	-3.19025156
H	0.53842557	-4.48355512	-1.46856194
H	1.45725449	-5.49178763	-2.56048098
C	-0.99204988	-5.98492803	-3.95584332
C	-0.04026165	-5.82702533	-4.96363165
C	-2.31954988	-6.25662736	-4.28670790
C	-0.41611014	-5.94014446	-6.30197529
H	1.00608123	-5.61206706	-4.70247785
C	-2.69548396	-6.37078856	-5.62538287
H	-3.06980198	-6.38128499	-3.49253456
C	-1.74407176	-6.21246639	-6.63299684
H	0.33392067	-5.81507478	-7.09639827

IN22

H	-3.74215200	-6.58542439	-5.88594323
H	-2.04016746	-6.30167022	-7.68830075
C	0.03282470	5.71045511	-7.10251803
C	0.48551070	5.19999911	-5.89277603
C	0.80585170	3.82186411	-5.75190403
C	0.64815070	2.99402711	-6.89800603
C	0.19528070	3.51827111	-8.10172603
C	-0.12001530	4.87860511	-8.21950403
H	-0.20955030	6.76803511	-7.17742503
H	0.58276570	5.85452211	-5.03198703
H	0.91902670	1.94498611	-6.83000503
H	0.09484370	2.86254011	-8.96357403
H	-0.47489330	5.28266011	-9.16336203
C	1.28143570	3.30143011	-4.49727703
O	1.65195469	4.02720756	-3.58933277
N	1.28238170	1.90023811	-4.26533403
C	2.34801370	1.30971711	-3.55994803
C	2.16065570	0.17899111	-2.74342903
C	3.65736170	1.81736511	-3.69811703
C	3.24432870	-0.41928989	-2.09624303
H	1.17042270	-0.23799589	-2.60097003
C	4.72601970	1.21769511	-3.04185803
H	3.83134870	2.67633111	-4.33632003
C	4.53304770	0.09215411	-2.23355203
H	3.06786270	-1.29329689	-1.47384303
H	5.72373970	1.63011911	-3.17163903
H	5.37197470	-0.37489389	-1.72573403
C	-0.01953130	1.23437211	-4.24220103
H	-0.68809230	1.74156611	-4.93841503
H	0.08161470	0.18979711	-4.55618303
H	-0.48179830	1.25273311	-3.24215703
Mn	2.52639273	5.05937671	-1.82910978
C	4.40615186	6.28123989	-0.05441019
C	4.81983847	6.93566407	1.10254876
C	3.87258819	7.27896003	2.07635776
C	2.52167543	6.96454157	1.88017022
C	2.13388865	6.30579155	0.71629570
N	3.07563650	5.97160100	-0.23268013
H	4.18499206	7.79115203	2.98068905

H	5.86647905	7.18229832	1.24767294	H	2.39516200	0.98303400	2.43271500
H	1.78360021	7.23230503	2.62912545	C	4.13297100	2.43398200	-0.02149900
C	0.80320420	5.88699463	0.32702946	C	5.37944600	2.66178000	0.61174000
C	-0.36854092	6.07244965	1.07654772	C	4.02301700	2.82393700	-1.37929400
C	-0.42843391	4.79462418	-1.35363530	C	6.44144000	3.25402800	-0.07415100
C	-1.58112629	5.60941981	0.59337188	H	5.52768100	2.38206900	1.64697900
H	-0.31381373	6.57790081	2.03545103	C	5.08472200	3.43247900	-2.04275600
H	-0.39190355	4.29026086	-2.31283058	H	3.08418300	2.68116700	-1.89174000
H	-2.49219497	5.74912670	1.16709597	C	6.30791600	3.65035700	-1.40331900
C	5.21311092	5.85881721	-1.18035200	H	7.38139700	3.40818100	0.45023000
C	6.60106965	6.02324344	-1.29873065	H	4.95347900	3.72967700	-3.08006500
C	5.13865750	4.84861855	-3.30338245	H	7.13763300	4.11494700	-1.93085700
C	7.25796247	5.58773865	-2.43794792	Mn	1.28583570	0.38738701	-0.31117624
H	7.15180007	6.49440470	-0.49080817	C	2.56688385	-2.00609265	0.61588197
H	4.52163189	4.40880984	-4.07838971	C	2.72458228	-3.10563742	1.44802522
H	8.33198491	5.71153801	-2.53672165	C	1.66467807	-3.48029179	2.29509678
N	0.76672131	5.24804254	-0.89974194	C	0.43795418	-2.82210857	2.19319214
N	4.47850009	5.25794159	-2.18947159	C	0.32202627	-1.71902452	1.34139119
C	-1.60837585	4.95178211	-0.65245655	N	1.43622000	-1.23068692	0.69557378
C	6.50362308	4.98885568	-3.46553991	H	1.77218879	-4.33686698	2.95422344
H	6.97172182	4.64281149	-4.38105007	H	3.62594769	-3.70699533	1.40426375
H	-2.53515643	4.56880744	-1.06677778	H	-0.42744008	-3.18869045	2.73557707

IN23

C	1.39720400	2.89986300	0.50947500	C	-2.18678812	-1.30846179	1.37597370
O	1.24008100	3.11322000	-0.72851000	C	-1.72333948	0.51269803	-0.62787692
C	1.35638600	3.94706800	1.54672100	C	-3.26380938	-0.66282300	0.79362306
C	1.61962200	5.27691700	1.17752800	H	-2.34067882	-2.02873029	2.17515435
C	1.04901500	3.65426700	2.88543100	H	-1.47908236	1.24956660	-1.38603551
C	1.59963100	6.28959600	2.13543200	H	-4.27555309	-0.86800749	1.12898759
H	1.84724100	5.49616400	0.13991900	C	3.41289240	-1.63329183	-0.51406480
C	1.02526000	4.67300200	3.83992400	C	4.68323236	-2.17114339	-0.77717637
H	0.81668900	2.63275800	3.16884600	C	3.46492652	-0.44735371	-2.51799648
C	1.30614200	5.98845400	3.46985400	C	5.33124273	-1.84140186	-1.96103187
H	1.81447200	7.31406300	1.84287300	H	5.14625095	-2.84107268	-0.06277673
H	0.78403100	4.43610000	4.87306400	H	2.95276587	0.24730135	-3.17779019
H	1.28940600	6.78098500	4.21402000	H	6.31157816	-2.25380692	-2.18185626
N	3.04270700	1.86591700	0.65186700	N	-0.65901911	-0.10807744	-0.06858367
C	3.30202800	1.42478600	2.01720700	N	2.82718147	-0.74264917	-1.37465415
H	4.08648400	0.65202600	2.03885000	C	-3.02689326	0.26139450	-0.24435996
H	3.61507400	2.24546500	2.67929800	C	4.70156581	-0.97667197	-2.86288243
				H	5.16721222	-0.70371079	-3.80478674

H	-3.84390832	0.78273845	-0.72903447
TS8			
C	1.33733700	3.06004200	0.56027900
O	1.11146800	3.12395500	-0.67220100
C	1.40768800	4.19157300	1.49098600
C	1.61461300	5.48468100	0.97501500
C	1.24595200	4.01911300	2.87505700
C	1.67242300	6.57924200	1.83455900
H	1.73240500	5.60844400	-0.09695100
C	1.30164300	5.11857900	3.72945300
H	1.05914400	3.02527600	3.26825800
C	1.51750500	6.39887000	3.21252000
H	1.83941500	7.57467200	1.43113900
H	1.17080400	4.97868500	4.79904900
H	1.56052700	7.25477600	3.88092000
N	3.00795500	1.88283900	0.72067500
C	3.21995000	1.46744100	2.09931500
H	3.99427700	0.68845500	2.16240100
H	3.52314900	2.29634900	2.75911400
H	2.29264700	1.04186000	2.49058100
C	4.10469400	2.46856000	0.07961400
C	5.35373700	2.66204200	0.71960300
C	4.00168200	2.90577600	-1.26464800
C	6.42885700	3.24433700	0.04756600
H	5.49422200	2.35196900	1.74822000
C	5.07631100	3.50114100	-1.91685600
H	3.05463800	2.80230600	-1.77818500
C	6.30636900	3.67161200	-1.27447400
H	7.37338700	3.36696900	0.57350700
H	4.95077200	3.83098400	-2.94623500
H	7.14665300	4.12566600	-1.79240000
Mn	1.12438300	1.01067400	-0.08805800
C	1.76910300	-1.81393100	0.37373600
C	1.64768000	-3.04634700	0.99840500
C	0.57224500	-3.26998300	1.88131000
C	-0.40484000	-2.28862000	2.02427700
C	-0.25354700	-1.06076500	1.37048200
N	0.90246600	-0.79430000	0.66616100
H	0.46564600	-4.22802500	2.37974000
H	2.34166500	-3.84903200	0.77215400

H	-1.29899600	-2.48977400	2.60572800
C	-1.24311400	-0.01921400	1.23917500
C	-2.49244200	0.01385500	1.89114000
C	-1.78004400	1.96218500	0.09261000
C	-3.39029900	1.02484100	1.61003800
H	-2.74293700	-0.76156600	2.60808600
H	-1.43858100	2.72436400	-0.60088000
H	-4.35802800	1.05230000	2.10221900
C	2.69632100	-1.49808000	-0.71732700
C	3.76664100	-2.31596500	-1.10801200
C	3.12735900	-0.03716300	-2.47403600
C	4.51244800	-1.97556100	-2.22816500
H	4.00537600	-3.20818300	-0.53869500
H	2.84601100	0.87670400	-2.98575100
H	5.34091100	-2.60198300	-2.54606300
N	-0.89006400	0.97692700	0.35035600
N	2.40100500	-0.34642400	-1.38777200
C	-3.03091700	2.02139300	0.67686600
C	4.17788100	-0.81820700	-2.94006400
H	4.72549300	-0.51910300	-3.82750100
H	-3.70887800	2.82967200	0.42441700

IN24

C	1.21834400	2.99721900	0.59629700
O	1.20570200	3.26311900	-0.62276300
C	1.24764500	3.98961400	1.67399600
C	1.40223100	5.35518000	1.37337100
C	1.10925500	3.58346500	3.01050400
C	1.41854700	6.29580800	2.39867100
H	1.51574900	5.65187100	0.33538400
C	1.12292000	4.52923400	4.03419900
H	0.98764700	2.52718900	3.23135400
C	1.27801100	5.88430300	3.72899400
H	1.54376700	7.35004400	2.16648100
H	1.01427200	4.21296200	5.06804600
H	1.29099300	6.62133400	4.52778400
N	3.21578200	1.63343000	0.58890300
C	3.97129571	2.55719424	-0.24325202
H	4.33741295	3.42569366	0.32842177
H	4.85043261	2.08609816	-0.71487625
H	3.33228540	2.93725629	-1.04257553

C	3.89906714	1.08304925	1.65517808
C	5.25352019	1.40473991	1.95452967
C	3.26781678	0.15864559	2.53284299
C	5.90614070	0.85566811	3.05555070
H	5.80040030	2.09333349	1.32186387
C	3.93808411	-0.39007511	3.62089408
H	2.24915519	-0.14329129	2.33182858
C	5.26290170	-0.04641591	3.90508719
H	6.93981356	1.13801514	3.24656356
H	3.41277517	-1.09843867	4.25908076
H	5.77920753	-0.47253641	4.76089088
Mn	1.33983100	1.20957400	-0.02736800
C	1.90236200	-1.50979900	0.66344800
C	1.78369600	-2.65767300	1.43390500
C	0.71029100	-2.76940400	2.33915800
C	-0.29294500	-1.79896800	2.32650500
C	-0.13564600	-0.66337200	1.52674000
N	1.05731700	-0.44739000	0.87156200
H	0.60731500	-3.65591700	2.95644700
H	2.46522500	-3.49036300	1.29250400
H	-1.20875700	-1.95072900	2.88961400
C	-1.14468300	0.29660000	1.13878400
C	-2.46282000	0.35234100	1.62649300
C	-1.61522400	2.00922700	-0.39101500
C	-3.36391200	1.24009200	1.06535700
H	-2.76680400	-0.31109600	2.42999200
H	-1.22189900	2.66882900	-1.15784100
H	-4.38785600	1.28388300	1.42472000
C	2.71988200	-1.34247900	-0.53897900
C	3.75228400	-2.20650200	-0.93039800
C	2.91731600	-0.14511500	-2.52257100
C	4.35947100	-2.02496900	-2.16653400
H	4.06759400	-3.00917700	-0.27182800
H	2.56534900	0.68676800	-3.12354300
H	5.15950600	-2.68686500	-2.48573900
N	-0.71945800	1.15521900	0.14861200
N	2.32900400	-0.29578500	-1.32712600
C	-2.93555500	2.07901800	0.01956900
C	3.92260500	-0.98563100	-2.99256700
H	4.36127600	-0.81406800	-3.96967200
H	-3.61300100	2.78206500	-0.45348500

IN25

C	0.46318000	0.30200500	-1.40827600
C	-0.11690900	1.47833700	-0.61214700
C	-0.08588700	0.97527300	0.85060800
N	-0.06927000	-0.48235200	0.71351500
C	0.02270800	-1.34061900	1.87511600
H	-0.81612400	-1.14295400	2.55214900
H	-0.02614900	-2.38015000	1.54597000
H	0.95891100	-1.17963700	2.43006100
H	-0.94699600	1.30125300	1.44673700
H	0.82788000	1.30430000	1.36615600
H	-1.15271200	1.69225000	-0.90999500
H	0.45444000	2.40406100	-0.72294500
C	0.34087700	-0.85571500	-0.53166200
O	0.69003900	-2.04325900	-0.78940900
H	1.60793700	0.19884200	-1.66192200
C	3.03948600	-3.07216300	-4.83764600
C	4.06594700	-3.31133100	-5.74361500
C	5.33687700	-3.66968100	-5.27395300
C	5.55417200	-3.76884600	-3.89562900
C	4.50529200	-3.53831000	-3.01100500
N	3.25035300	-3.21742200	-3.48514600
H	6.14802100	-3.84997500	-5.97129100
H	3.88968000	-3.19548000	-6.80795900
H	6.53911700	-4.01885900	-3.51511000
C	4.53933900	-3.63176700	-1.56343000
C	5.63486200	-4.04900500	-0.79208600
C	3.20693200	-3.49493400	0.35772400
C	5.49175800	-4.19624100	0.57862500
H	6.58220000	-4.26494400	-1.27433600
H	2.22786300	-3.25460500	0.75500300
H	6.33182800	-4.52107200	1.18512200
C	1.69242700	-2.61677300	-5.13817100
C	1.13911800	-2.49268500	-6.42059000
C	-0.32613500	-1.93712300	-4.16826300
C	-0.17416600	-2.06819500	-6.56109600
H	1.73549500	-2.74218700	-7.29178000
H	-0.87237500	-1.77630000	-3.24754400
H	-0.61469700	-1.96773200	-7.54864600
N	3.33760200	-3.33659900	-0.97271300

N	0.95852000	-2.31382200	-4.02274200	C	-0.15003300	-0.59262000	1.75016600
C	4.24601000	-3.92854400	1.16613900	H	-0.96693700	-0.24759600	2.39429600
C	-0.92669800	-1.79238000	-5.41083700	H	-0.28576600	-1.65557100	1.54431200
H	-1.96331900	-1.47928300	-5.47489900	H	0.79746800	-0.44906700	2.29330200
H	4.08937400	-4.03974800	2.23381300	H	-0.81309800	2.08442300	1.03325200
C	3.98067300	-0.19273100	-1.37457700	H	0.94845900	1.85582400	0.98153300
C	3.81005800	-0.30136700	0.03185300	H	-0.95728700	2.26689900	-1.35680200
C	4.84759500	-0.02911300	0.91655700	H	0.72719300	2.77629900	-1.21193400
C	6.10737000	0.36032300	0.44866000	C	0.19472900	-0.39870800	-0.70474300
C	6.29978400	0.47104500	-0.92868100	O	0.38583800	-1.65331900	-0.84158300
C	5.26549800	0.20510100	-1.82492600	H	1.75134800	0.24719700	-1.90680900
H	2.84386600	-0.61366100	0.41720300	C	2.74754100	-3.42667100	-4.57370300
H	4.67099200	-0.12103900	1.98656700	C	3.70047500	-3.96804100	-5.42955900
H	6.91598300	0.57372700	1.14239100	C	4.91171900	-4.44006100	-4.90841900
H	7.27081200	0.77027600	-1.31856900	C	5.12910100	-4.39057400	-3.52620000
H	5.45391600	0.29918400	-2.88861300	C	4.15308300	-3.85068900	-2.69480600
N	2.90199100	-0.44606900	-2.21699600	N	2.99430100	-3.33625800	-3.22441200
H	0.02936100	0.15244900	-2.39933000	H	5.66254300	-4.86476000	-5.56630200
C	3.03727000	0.09732400	-3.56145900	H	3.50377600	-4.03229000	-6.49473000
H	3.72027500	-0.48051300	-4.20708500	H	6.04414500	-4.79179900	-3.10297000
H	2.05582600	0.09494300	-4.04713800	C	4.16212900	-3.81246000	-1.24365900
H	3.40485700	1.13797500	-3.55708300	C	5.20535300	-4.25758600	-0.41777200
Mn	1.90549300	-2.71924000	-2.25064700	C	2.85115000	-3.32575000	0.63211800
C	0.77327100	-4.39352500	-2.27383600	C	5.04502600	-4.23636700	0.95894100
O	-0.42351900	-4.15387600	-2.17607900	H	6.12746000	-4.61838700	-0.86056900
C	1.17552400	-5.82965900	-2.54105000	H	1.89985800	-2.95225400	0.99260500
C	2.45898900	-6.33598800	-2.30223200	H	5.84486400	-4.58098300	1.60777000
C	0.19331400	-6.69762300	-3.05227300	C	1.44445900	-2.89927700	-4.93596200
C	2.75566500	-7.67557200	-2.56196500	C	0.91482100	-2.84866200	-6.23506200
H	3.22459600	-5.68997100	-1.89531800	C	-0.51139600	-1.93733400	-4.07952800
C	0.49220400	-8.02868000	-3.32945600	C	-0.35231000	-2.32662700	-6.44052100
H	-0.80297200	-6.30042500	-3.21860100	H	1.49799400	-3.22247000	-7.06982800
C	1.77694400	-8.52331400	-3.08267500	H	-1.03934300	-1.61006700	-3.19043900
H	3.75384600	-8.05587200	-2.35915200	H	-0.77241500	-2.28708800	-7.44120700
H	-0.27522800	-8.68475800	-3.73320500	N	2.99967000	-3.32977100	-0.70424700
H	2.01161400	-9.56363700	-3.29406400	N	0.72525900	-2.42563000	-3.87049300
TS9				C	3.83726200	-3.77164800	1.49930700
C	0.45850500	0.62958200	-1.67514100	C	-1.08731800	-1.86132400	-5.33827500
C	0.03901400	1.94660300	-1.02037800	H	-2.08934800	-1.46206100	-5.45316900
C	0.00017000	1.59417400	0.48573500	H	3.66681700	-3.75083500	2.57033100
N	-0.16816600	0.13823500	0.50081800	C	3.89758200	-0.24551800	-1.42333200

C	0.15397467	0.96678227	1.20714995
H	-0.09227944	-0.99826836	0.34923627
C	1.86370504	2.34975447	0.20418090
H	2.90105439	1.46830098	-1.47498630
C	0.86358693	2.16791450	1.16483620
H	-0.63005390	0.82490087	1.94704832
H	2.41838079	3.28404436	0.16495110
H	0.63876350	2.96031091	1.87451660

TS10

C	2.88508000	-4.50258000	-1.94497200
C	4.05937600	-5.24349000	-2.58507000
C	5.11684000	-4.13900800	-2.87192500
N	4.39031800	-2.88515500	-2.66354100
C	4.97836400	-1.59021200	-2.92920100
H	5.28247400	-1.51032700	-3.98042400
H	4.23150800	-0.82704300	-2.70372000
H	5.86366000	-1.42580300	-2.30026000
H	5.50854200	-4.17674800	-3.89588000
H	5.97696500	-4.19311900	-2.18849100
H	3.76144600	-5.73959100	-3.51454400
H	4.46489400	-6.01608600	-1.92584300
C	3.17833100	-3.06789200	-2.08846600
O	2.39012700	-2.09423400	-1.78053000
C	-2.32168200	-2.10624100	-0.70522000
C	-3.69712800	-1.90259100	-0.70890700
C	-4.35968300	-1.68372700	-1.92577800
C	-3.61933100	-1.62273800	-3.11271000
C	-2.24216600	-1.82736800	-3.07607800
N	-1.61608400	-2.12881000	-1.88720300
H	-5.43301900	-1.52467500	-1.94245800
H	-4.25288400	-1.89069800	0.22348800
H	-4.11513100	-1.39765000	-4.05181300
C	-1.30452500	-1.69379900	-4.17268600
C	-1.64548100	-1.38220500	-5.50117800
C	0.96665200	-1.67121700	-4.73472900
C	-0.65006800	-1.20209100	-6.44532800
H	-2.69002100	-1.27743600	-5.77635300
H	1.98493400	-1.79581600	-4.38302900
H	-0.90391800	-0.95652200	-7.47242600
C	-1.45938200	-2.24838100	0.45457200

C	-1.88590100	-2.30560500	1.79223200
C	0.77486600	-2.39996700	1.13849100
C	-0.94807500	-2.40432200	2.80734600
H	-2.94590900	-2.27523000	2.02272500
H	1.81254900	-2.43083400	0.82060300
H	-1.26712900	-2.44699900	3.84487700
N	0.01247100	-1.85964000	-3.79977400
N	-0.12372600	-2.30532600	0.14118400
C	0.69395100	-1.33896100	-6.05033000
C	0.41764000	-2.44859900	2.47714000
H	1.18249800	-2.52033700	3.24349900
H	1.50707200	-1.19632400	-6.75472500
Mn	0.25296800	-2.56418200	-1.86883700
C	1.00549100	-4.61844900	-2.55662300
H	2.64812600	-4.78078200	-0.91900400
O	0.24568900	-4.62522700	-1.53488500
C	0.77520800	-5.35619700	-3.79547000
C	-0.34812300	-6.20678300	-3.89224100
C	1.60058000	-5.20716100	-4.92900900
C	-0.61788300	-6.89295400	-5.07224500
H	-0.99065600	-6.31291600	-3.02398700
C	1.32624500	-5.90016300	-6.10607400
H	2.44322600	-4.52342200	-4.88840200
C	0.21884700	-6.74983800	-6.18495200
H	-1.48392700	-7.54862300	-5.12615500
H	1.97430300	-5.77082100	-6.96979900
H	0.00673100	-7.28919100	-7.10428000

IN27

C	2.90592500	-4.64096200	-2.30037400
C	4.02481600	-5.15954300	-3.19434200
C	5.02060600	-3.96763200	-3.27521400
N	4.20300600	-2.81788800	-2.89013100
C	4.80629200	-1.52023500	-2.67268700
H	5.23055300	-1.12578400	-3.60245200
H	4.03641600	-0.83756000	-2.30675500
H	5.61331900	-1.57321300	-1.92374200
H	5.44178000	-3.82280500	-4.27744500
H	5.86096000	-4.08928300	-2.57132000
H	3.65042400	-5.40886700	-4.19987700
H	4.51073400	-6.06030500	-2.80453600

C	3.10000200	-3.24093800	-2.16331900
O	2.34454600	-2.39195900	-1.58387200
C	-2.27069800	-2.22067300	-0.82582900
C	-3.64421600	-2.03117300	-0.90407000
C	-4.23775100	-1.80970600	-2.15952900
C	-3.42898900	-1.68794900	-3.29159800
C	-2.05081600	-1.87727300	-3.17187200
N	-1.50948200	-2.26113100	-1.96820300
H	-5.31072200	-1.66679500	-2.23673900
H	-4.24991500	-2.01508800	-0.00360500
H	-3.86481300	-1.41516700	-4.24769400
C	-1.02490500	-1.60516000	-4.15281400
C	-1.24661800	-1.19451200	-5.47972700
C	1.28920600	-1.39614700	-4.45514500
C	-0.17436900	-0.86554800	-6.28801000
H	-2.26422300	-1.13238200	-5.85741500
H	2.27250200	-1.51089600	-4.01805300
H	-0.33398800	-0.54162500	-7.31162600
C	-1.45627600	-2.27613000	0.38204800
C	-1.93741500	-2.33403800	1.69827200
C	0.75215500	-2.22183900	1.15414000
C	-1.03496900	-2.31779300	2.75273700
H	-3.00472500	-2.39531900	1.88471500
H	1.79949400	-2.19648300	0.87139600
H	-1.39231800	-2.35675400	3.77778200
N	0.25454600	-1.72827200	-3.65150200
N	-0.11333300	-2.22880700	0.12640100
C	1.12673900	-0.95647600	-5.75798400
C	0.33941200	-2.25370500	2.47961100
H	1.07329600	-2.23742100	3.27868900
H	1.99763000	-0.70071400	-6.35346400
Mn	0.35433400	-2.67744800	-1.84515000
C	0.66661900	-4.46743200	-2.58124800
H	2.58126600	-5.21569400	-1.42998000
O	0.24833600	-4.64136400	-1.39302500
C	0.43026000	-5.39947900	-3.69526000
C	-0.21412100	-6.63039400	-3.46581400
C	0.84456300	-5.07770800	-4.99980600
C	-0.41733200	-7.52272500	-4.51773600
H	-0.54029000	-6.87048500	-2.45837400
C	0.63390900	-5.97280500	-6.04695200

IN28

H	1.33671400	-4.12763700	-5.17712600
C	0.00788400	-7.20070600	-5.80974700
H	-0.91048000	-8.47285200	-4.33050000
H	0.96291500	-5.71364300	-7.05080200
H	-0.14995500	-7.89878300	-6.62682400
C	0.73950579	-1.70893857	-0.19544826
C	-0.60278870	-1.38510903	0.48831422
C	-0.25257799	-0.26113831	1.48805314
N	0.94761330	0.34455654	0.91247019
C	1.52478512	1.56833288	1.43311963
H	1.81516710	1.44724314	2.48503440
H	2.40937428	1.81118733	0.84267074
H	0.80287960	2.38972296	1.36181700
H	-0.03506117	-0.65028149	2.49391117
H	-1.04726548	0.48679282	1.58429977
H	-1.05282599	-2.24845986	0.98358970
H	-1.31872415	-1.01195523	-0.25066960
C	1.56167722	-0.45152356	0.00530505
O	2.64319736	-0.17441547	-0.54628382
H	0.65801409	-1.94522135	-1.26081371
Mn	2.60271500	-2.15564900	-1.61968400
C	2.96480700	-3.63094500	-4.00747200
C	3.44411000	-4.69815600	-4.79087700
C	4.22921500	-5.68252200	-4.18376600
C	4.54165800	-5.62600400	-2.82235100
C	4.05239700	-4.54926600	-2.05876100
N	3.28455100	-3.58596000	-2.66969600
H	4.60345500	-6.50922600	-4.78230200
H	3.20817700	-4.75628200	-5.84807900
H	5.14941900	-6.39827800	-2.36313400
C	4.24037100	-4.28294800	-0.65906200
C	4.99112700	-5.07786300	0.22887000
C	3.76076900	-2.78831900	1.11316700
C	5.12338400	-4.72433300	1.55652800
H	5.47051900	-5.97639700	-0.14901200
H	3.26509500	-1.87067500	1.41952900
H	5.70413200	-5.33756500	2.23891900
C	2.14531800	-2.52181400	-4.40710300
C	1.66520900	-2.29275700	-5.71196500

C	1.07992400	-0.53274600	-3.68912400
C	0.89247300	-1.18664200	-6.00015200
H	1.91622800	-3.00386200	-6.49392300
H	0.88313200	0.14858900	-2.86491600
H	0.52495300	-1.01254000	-7.00687400
N	3.60114100	-3.11338100	-0.20246600
N	1.83361000	-1.62385500	-3.36404400
C	4.48690700	-3.53450100	2.00969600
C	0.59550000	-0.27312000	-4.94774400
H	0.00406600	0.61940000	-5.12764500
H	4.57005800	-3.21083600	3.04268100
H	1.26514509	-2.54575366	0.28358456

TS11

C	0.69324957	-1.49295772	-0.36272300
C	0.43458958	-1.19025193	1.12297902
C	-0.63501814	-2.21549434	1.55384792
N	-0.41643509	-3.31630641	0.62846829
C	-1.12946622	-4.56844575	0.73915167
H	-2.21815217	-4.41515093	0.69707105
H	-0.82665039	-5.20070843	-0.09764172
H	-0.88859847	-5.07059490	1.68434769
H	-1.65796489	-1.81645806	1.44907000
H	-0.51512234	-2.54981163	2.59213090
H	0.11756597	-0.15922371	1.29997819
H	1.34113874	-1.35850313	1.71090055
C	0.23694841	-2.94124512	-0.52020077
O	0.38863250	-3.67695538	-1.49381617
H	1.78447600	-0.66952600	-1.10852100
Mn	2.20555900	-2.08756000	-1.70863100
C	2.90908200	-3.51927700	-4.08831400
C	3.43546500	-4.59036200	-4.81958100
C	4.17301700	-5.57676900	-4.16860300
C	4.38696300	-5.48746300	-2.77858500
C	3.84925200	-4.41405400	-2.08336300
N	3.11569800	-3.45281900	-2.72596000
H	4.58096700	-6.41218600	-4.72865400
H	3.26659000	-4.65757300	-5.88973000
H	4.95485200	-6.25557100	-2.26446700
C	3.98453200	-4.14724500	-0.65134600
C	4.78861000	-4.89453100	0.22018400

C	3.42056200	-2.67896500	1.08599100
C	4.91008600	-4.50696100	1.54749400
H	5.32613000	-5.76051400	-0.15098000
H	2.84484500	-1.80590400	1.38380600
H	5.53558300	-5.07697300	2.22878000
C	2.15458700	-2.39913900	-4.59399000
C	1.90621900	-2.15134000	-5.95920000
C	1.14133100	-0.35861000	-4.03939000
C	1.27020500	-0.99078200	-6.35309500
H	2.23869800	-2.87184300	-6.69981900
H	0.87807800	0.33941600	-3.25290700
H	1.08337500	-0.79321200	-7.40449800
N	3.28518800	-3.05152900	-0.20533400
N	1.72191800	-1.50844800	-3.61802600
C	4.22320700	-3.36868200	1.98673000
C	0.89372800	-0.05547300	-5.36363500
H	0.42101500	0.88561700	-5.62439600
H	4.29648200	-3.02326200	3.01265200
H	-0.22701209	-0.96299030	-0.49369246

IN29

C	0.77482400	-0.66790200	0.25267000
C	-0.55018400	-0.14015100	-0.31846200
C	-0.39460300	1.40769000	-0.31572300
N	1.04474600	1.60780400	-0.18950200
C	1.62827800	2.92690700	-0.09485200
H	1.17877200	3.51188800	0.72402500
H	2.69580300	2.80734000	0.10596200
H	1.49011300	3.48716900	-1.02833300
H	-0.92154600	1.87491500	0.53465300
H	-0.77328600	1.87618100	-1.23236900
H	-1.41373100	-0.44682000	0.28104500
H	-0.73692500	-0.48813400	-1.34095300
C	1.66884700	0.49655700	0.36057200
O	2.84373300	0.50076500	0.77746300
Mn	2.17414900	-1.89250300	-0.76595300
C	1.78779500	-3.81188300	-2.78493100
C	1.70354900	-5.10261600	-3.30221800
C	2.01471100	-6.19792600	-2.49083200
C	2.40216800	-5.98518500	-1.15967700
C	2.48285900	-4.69213500	-0.66391800

H	1.43416350	2.31408484	-0.27244473
H	0.04464772	2.63947021	-1.35116299
H	-1.89055010	0.54075769	0.45990467
H	-1.81520950	0.60328273	-1.31339147
H	-1.80590978	-1.85551219	0.08254020
H	-1.10511093	-1.64579735	-1.51806254
C	0.94165267	-0.15078599	0.12567314
O	2.18480954	-0.00933618	0.17649186
Mn	2.29305600	-1.80314900	-0.66912700
C	1.79814200	-3.64438500	-2.71284600
C	1.71021400	-4.91823900	-3.26979200
C	1.98989900	-6.04251500	-2.48545600
C	2.36809500	-5.87347800	-1.14824900
C	2.45758700	-4.59979100	-0.61278200
N	2.15996200	-3.49690900	-1.39133000
H	1.92144900	-7.03325500	-2.91084000
H	1.41888700	-5.03069000	-4.30792700
H	2.59802900	-6.73852000	-0.53222300
C	2.83237900	-4.22445100	0.73949600
C	3.17449000	-5.10208700	1.77814800
C	3.16668300	-2.38383800	2.15571900
C	3.51997800	-4.60122800	3.02192000
H	3.17099100	-6.17224900	1.59639100
H	3.16532300	-1.30387400	2.23400200
H	3.79007800	-5.27400900	3.83511300
C	1.55203400	-2.37034100	-3.35784600
C	1.15669000	-2.18077200	-4.68924600
C	1.56217000	-0.05561800	-3.01006700
C	0.97369400	-0.89785700	-5.17853200
H	1.00344500	-3.04504400	-5.33077700
H	1.72462800	0.75137500	-2.30694400
H	0.67168900	-0.74193900	-6.20658000
N	2.82153700	-2.87258100	0.94208400
N	1.74205900	-1.30102800	-2.52117700
C	3.52057700	-3.21076500	3.21180400
C	1.18544800	0.19226500	-4.31820700
H	1.05506900	1.21185000	-4.65778000
H	3.79408800	-2.77339600	4.16262100
H	0.43235278	-2.00504898	1.05215044
H	3.78387600	-1.67309700	-1.09691600

IN31

Ni	4.40551000	7.18334700	-0.85000500
C	4.61642200	9.01776900	-1.22097500
O	3.59712000	9.58420400	-1.58855000
C	5.89769200	9.78387300	-1.06042300
C	7.07262900	9.16860200	-0.61114900
C	5.91104100	11.15615000	-1.36712500
C	8.24507600	9.91197200	-0.46926500
H	7.06956200	8.10765100	-0.38716600
C	7.08033100	11.89642400	-1.22462600
H	4.99080000	11.61564900	-1.71431400
C	8.25053900	11.27412600	-0.77458700
H	9.15423100	9.42512800	-0.12700900
H	7.08539000	12.95723000	-1.46237300
H	9.16466400	11.85237300	-0.66461000
N	5.10374900	6.66152300	-2.81537100
C	6.51160800	6.43717000	-2.82666700
C	7.11624400	5.74910400	-1.75379300
C	7.35829200	6.86668200	-3.86889900
C	8.48463200	5.50642400	-1.71990000
H	6.48092400	5.40352400	-0.94645600
C	8.73422500	6.61948500	-3.83055200
H	6.95385400	7.39823700	-4.72139000
C	9.31310600	5.94217600	-2.76009200
H	8.91056900	4.97219100	-0.87319800
H	9.35433900	6.96959300	-4.65272200
H	10.38337200	5.75663900	-2.73273600
C	4.68432000	7.65779600	-3.81720500
H	5.28899600	8.57214500	-3.75950600
H	4.77072100	7.26181500	-4.83731200
H	3.64593200	7.93120200	-3.64141700
C	7.44341000	7.84526500	3.63425100
C	8.09558700	6.73618400	3.07087000
C	7.40420000	5.94685100	2.15644500
C	6.09886000	6.28811400	1.80656600
C	5.53801700	7.42763600	2.39765900
N	6.18817900	8.17266300	3.30295900
H	7.86868300	5.05996500	1.73460600
H	9.10322000	6.47468200	3.37759200
H	5.51039000	5.67356500	1.13539900
C	4.13509000	7.85587800	2.13310800

C	3.39320000	8.36159400	3.21094800	H	1.44145300	6.18484500	-1.52774200
C	2.31714800	8.15184000	0.72060300	H	-1.11769700	7.40928900	-4.78056300
C	2.07110200	8.74161400	3.02557500	N	5.37456100	3.51559100	-3.09349100
H	3.88739900	8.45069800	4.17078600	N	2.17369900	5.83984300	-3.41910100
H	1.95028300	8.11652900	-0.29730300	C	6.87938300	1.79171500	-2.33754500
H	1.48586200	9.12461400	3.85671000	C	0.02575900	6.85821600	-3.02190200
C	8.11506700	8.70187300	4.65723200	H	-0.70542000	7.20862300	-2.30045200
C	9.49513200	8.95006400	4.59815600	H	7.29569100	1.23867500	-1.50146200
C	7.91081300	9.97700900	6.55522100	Cl	3.61256300	4.86033700	-0.37581500
C	10.08167000	9.74951700	5.57702900				
H	10.09177100	8.54546000	3.78661800				
H	7.24715100	10.37019400	7.32439800				
H	11.14681300	9.96286700	5.54710200				
N	3.59709600	7.76169200	0.89400700				
N	7.33417000	9.21395100	5.62441100				
C	1.51751800	8.62759300	1.75076100				
C	9.27533600	10.27653400	6.58387500				
H	9.68544000	10.90530800	7.36846000				
H	0.49296900	8.91865000	1.54401800				
Mn	3.93454000	4.93533500	-2.96140100				
C	2.97144300	5.27533000	-5.57407000				
C	3.04480700	5.20718700	-6.96358400				
C	4.09694500	4.51415800	-7.56977200				
C	5.03617100	3.86161400	-6.76476100				
C	4.93297300	3.93670300	-5.37807500				
N	3.93958300	4.68903800	-4.78369900				
H	4.17259000	4.46636600	-8.65111400				
H	2.28861200	5.69299700	-7.57239800				
H	5.84031900	3.29118100	-7.21884100				
C	5.72865900	3.22617900	-4.38935800				
C	6.70093500	2.25961700	-4.68399400				
C	5.93702300	2.78259400	-2.10737000				
C	7.28747100	1.53824100	-3.65448500				
H	6.97383200	2.06661000	-5.71646900				
H	5.60246000	3.02953800	-1.10531800				
H	8.03699000	0.78222200	-3.86968600				
C	1.93141200	5.90004200	-4.77148100				
C	0.75549900	6.47350700	-5.27660800				
C	1.21531300	6.29482600	-2.58287700				
C	-0.20262900	6.96427100	-4.40096300				
H	0.59575100	6.51897600	-6.34900500				
				IN32			
				Mn	3.24931200	-1.69590000	-1.72555300
				C	2.84776000	-3.53177100	-3.79965800
				C	2.97798700	-4.77408500	-4.40780400
				C	3.41246000	-5.88341500	-3.66923600
				C	3.71151500	-5.71880600	-2.31169500
				C	3.57815100	-4.47336800	-1.70730900
				N	3.15223700	-3.36331800	-2.44529200
				H	3.52338400	-6.85231000	-4.14461800
				H	2.74771700	-4.88226600	-5.46399800
				H	4.05560400	-6.56596900	-1.72493600
				C	3.81947600	-4.12895000	-0.33108400
				C	4.12642500	-5.03205200	0.70582000
				C	3.77865000	-2.36210900	1.20616000
				C	4.25010800	-4.57763400	2.00589500
				H	4.25139200	-6.08588400	0.47635700
				H	3.64603300	-1.29406500	1.35583000
				H	4.48526700	-5.26748100	2.81138900
				C	2.40594400	-2.29641700	-4.39952500
				C	1.89330800	-2.15246600	-5.70323800
				C	2.02425500	-0.02649600	-3.98193500
				C	1.43492300	-0.91975400	-6.13159300
				H	1.85090600	-3.01568400	-6.36034100
				H	2.12280500	0.79516800	-3.28004500
				H	1.03657400	-0.79849800	-7.13505100
				N	3.67634600	-2.77771700	-0.07842500
				N	2.48635400	-1.21850400	-3.54311900
				C	4.05583100	-3.20583800	2.26688700
				C	1.49144200	0.17121500	-5.24411800
				H	1.14542300	1.15699400	-5.53821700
				H	4.13291500	-2.80623600	3.27326500

N	3.34797368	-0.00122827	-0.99404996	H	3.73291500	-6.17754300	-1.86725800
C	2.24138947	0.63034763	-0.35259991	C	3.87317600	-3.75461500	-0.41210700
C	2.26288817	2.01092623	-0.08918648	C	4.33560700	-4.69694500	0.52057800
C	1.08849628	-0.09353750	-0.00197377	C	4.21640800	-2.02331800	1.12331200
C	1.17732134	2.64366421	0.51985752	C	4.73420600	-4.27536000	1.78035100
H	3.14875181	2.57816045	-0.36625224	H	4.38347900	-5.74706200	0.25004200
C	0.00619007	0.53821763	0.61097244	H	4.18355500	-0.95215100	1.29230700
H	1.06424085	-1.16088521	-0.20517018	H	5.09438500	-4.99390000	2.51117200
C	0.04304653	1.91033803	0.87467177	C	2.35026800	-1.68195600	-4.32290900
H	1.21917044	3.71238400	0.71953154	C	1.94243700	-1.43050900	-5.64292300
H	-0.87153745	-0.04374870	0.88335866	C	2.28213500	0.60501000	-3.83507400
H	-0.80154861	2.40093789	1.35174685	C	1.69499400	-0.12706800	-6.04678600
C	4.42335862	0.97845245	-1.18165637	H	1.82902100	-2.25484000	-6.33998700
H	5.29926276	0.51303359	-1.63370989	H	2.46918500	1.37085700	-3.08981500
H	4.10381611	1.81172480	-1.83014814	H	1.37980000	0.08168900	-7.06520100
H	4.72679803	1.42260115	-0.21945607	N	3.80785400	-2.41850700	-0.10034400

IN33

C	-0.10652500	-3.02323100	-1.26606200	C	4.67537900	-2.90781700	2.08873400
C	-1.63196000	-3.12501800	-1.07878800	C	1.87007500	0.91465600	-5.12303900
C	-1.93822300	-2.13847000	0.06835500	H	1.70014200	1.94970400	-5.40192100
N	-0.82540400	-1.19376500	0.00793400	H	4.99084800	-2.53437200	3.05776800
C	-0.79194900	0.01661100	0.80542500	H	0.44238600	-3.78712700	-0.70102000
H	-0.82689600	-0.22030200	1.87705400	H	0.22395600	-3.09774100	-2.30416200
H	0.13496700	0.54877100	0.58680900	N	4.54410482	-0.07638160	-1.53863990
H	-1.64745100	0.65619700	0.56013000	C	5.09098533	0.10541760	-2.89096041
H	-1.96260900	-2.63502200	1.05028600	C	4.83764644	1.28405084	-3.59318154
H	-2.89128300	-1.61369000	-0.06257000	C	5.86324621	-0.90030586	-3.47206418
H	-1.97137200	-4.13804800	-0.84993700	C	5.35592870	1.45655662	-4.87647691
H	-2.14303700	-2.79888700	-1.99030600	H	4.22813274	2.07643512	-3.13507457
C	0.24056300	-1.66647600	-0.68342000	C	6.38258244	-0.72749657	-4.75535554
O	1.31867000	-1.05748400	-0.77429500	H	6.06316318	-1.82924250	-2.91867558
Mn	3.10966400	-1.27439600	-1.60220900	C	6.12895050	0.45063086	-5.45765434
C	2.66758200	-2.98901700	-3.77068100	H	5.15576347	2.38528105	-5.43028313
C	2.63820700	-4.21888900	-4.42248100	H	6.99178482	-1.52046753	-5.21311502
C	3.01120800	-5.38231500	-3.74013900	H	6.53753997	0.58689560	-6.46947591
C	3.42389100	-5.28683600	-2.40606000	C	5.59011364	-0.61086579	-0.65484569
C	3.44660900	-4.04890900	-1.77066000	H	5.60686362	-0.05125654	0.25699690
N	3.05399600	-2.90147400	-2.44196800	H	5.38393268	-1.63838450	-0.43898760
H	2.99345700	-6.34378700	-4.24252600	H	6.54092491	-0.53200248	-1.13924069
H	2.33152400	-4.27239300	-5.46279500				

TS14

C	5.25776000	-4.39110900	-3.61348900
C	4.32541300	-3.84918500	-2.73337600
N	3.14926300	-3.29573500	-3.20089600
H	5.71578100	-4.82051600	-5.68199200
H	3.53303800	-3.94794400	-6.51007900
H	6.18882500	-4.80062800	-3.23408500
C	4.38649200	-3.82068400	-1.28139400
C	5.38792100	-4.41864300	-0.50233600
C	3.20942200	-3.22325400	0.64451900
C	5.27780000	-4.41760400	0.88008900
H	6.23620000	-4.89141700	-0.98669400
H	2.32784000	-2.73443800	1.04619100
H	6.04496300	-4.88085500	1.49364900
C	1.50704500	-2.90337600	-4.82644400
C	0.86255800	-2.98233600	-6.07066000
C	-0.44709700	-2.07744800	-3.84315500
C	-0.46490200	-2.59788600	-6.18684700
H	1.40323700	-3.35951400	-6.93282600
H	-0.92392000	-1.72933100	-2.93352800
H	-0.97353200	-2.65763600	-7.14458400
N	3.30623200	-3.19778100	-0.70224100
N	0.85685400	-2.41312500	-3.71444600
C	4.15329800	-3.81857300	1.46660000
C	-1.14069800	-2.15020800	-5.04123600
H	-2.18511300	-1.85747200	-5.07966000
H	4.01888300	-3.80512000	2.54365500
C	3.96542300	-0.21172700	-1.48031200
C	3.86295000	-0.04289600	-0.08754700
C	4.98148700	0.26473200	0.68198300
C	6.23767000	0.41107700	0.08630500
C	6.35125900	0.24455600	-1.29379000
C	5.23176500	-0.05845900	-2.07163200
H	2.89382700	-0.15470900	0.38725900
H	4.87057000	0.39649100	1.75602700
H	7.10971200	0.65244300	0.68793600
H	7.31970500	0.35205800	-1.77718100
H	5.35029400	-0.18383700	-3.14263100
N	2.78083200	-0.49868300	-2.22951000
H	0.05800200	0.24650900	-2.35567900
C	2.83829600	0.00077700	-3.61557400
H	3.42672200	-0.65193300	-4.26620200

IN35

H	1.81926400	0.03890400	-4.00583700
H	3.26584100	1.01023000	-3.65457100
Mn	2.00314300	-2.43339600	-2.04566700
C	-1.90679405	1.77106279	2.41749987
C	-2.35754888	3.14933085	2.84950676
C	-1.95903191	4.01314023	1.62298906
N	-1.95475574	3.05817141	0.50919142
C	-1.33986187	3.44081332	-0.74469812
H	-0.30334630	3.79913797	-0.61132292
H	-1.32543440	2.57273721	-1.40706890
H	-1.91874636	4.24031722	-1.22094279
H	-0.95075422	4.44425945	1.76112894
H	-2.65408869	4.83704397	1.42805220
H	-1.87243986	3.50259876	3.76575138
H	-3.44319962	3.19671611	3.02658774
C	-1.69051800	1.79295900	1.05738000
O	-1.47991100	0.74977500	0.29261200
Mn	0.33304100	0.33443300	-0.14601900
C	-0.44268600	-1.63082600	-1.99790000
C	-0.84156500	-2.90427200	-2.39369800
C	-0.83273100	-3.95266300	-1.46681100
C	-0.42874000	-3.70219700	-0.14908000
C	-0.04005700	-2.41889400	0.21847400
N	-0.03988100	-1.40166000	-0.70547900
H	-1.14041800	-4.94931600	-1.76474100
H	-1.16030400	-3.08431500	-3.41509100
H	-0.42651100	-4.50436400	0.58161100
C	0.39442600	-1.97728600	1.53679700
C	0.57042000	-2.80763400	2.65483800
C	1.11046700	-0.12025900	2.76780200
C	1.02629700	-2.25992800	3.84464300
H	0.36070700	-3.86922500	2.58119300
H	1.32253200	0.94186900	2.74918500
H	1.17125800	-2.89266600	4.71561100
C	-0.37192200	-0.43651700	-2.82594900
C	-0.65781400	-0.39484600	-4.20057000
C	0.23607700	1.81714300	-2.85965900
C	-0.49122600	0.79015600	-4.89884700
H	-0.99597200	-1.29066100	-4.70997700

C	9.38673300	-0.31569300	-2.03578300
H	10.32765200	0.19733200	-1.86599300
H	2.36004100	-2.01757400	4.03112600
H	4.33968900	1.22820000	2.10100600
Cl	4.67271600	0.83700400	-0.57589900
C	4.64520800	3.68653600	-1.13190000
O	3.57693600	4.28034700	-1.02545600
C	5.35546500	3.72749800	-2.46891400
C	4.99682100	4.72212700	-3.39374400
C	6.38069800	2.83050900	-2.80023500
C	5.65647900	4.82500700	-4.61654700
H	4.19302700	5.40265400	-3.12956800
C	7.03230000	2.92365900	-4.03145200
H	6.63656900	2.04095700	-2.10176100
C	6.67658500	3.92422400	-4.93901000
H	5.37617600	5.60350600	-5.32208900
H	7.81333900	2.21024400	-4.28366900
H	7.18933900	4.00152000	-5.89474700

IN37

C	0.63281200	-1.26712900	-0.89554400
C	-0.09972600	-0.04800800	-1.50428600
C	0.29339700	1.13535700	-0.59074800
N	0.63919100	0.48795100	0.66196200
C	0.95084200	1.23060500	1.85763900
H	0.09417300	1.84003400	2.17742400
H	1.19537900	0.51200900	2.64243800
H	1.80998800	1.90086400	1.69956500
H	-0.53112700	1.84549700	-0.44127800
H	1.15035100	1.69247300	-0.99358400
H	-1.18945900	-0.18168600	-1.46891200
H	0.17176900	0.15070000	-2.54562800
C	0.84865400	-0.86692300	0.54403400
O	1.13276800	-1.59777000	1.49908700
Mn	1.42523200	-2.85083400	-1.92193200
C	2.77576700	-2.79713500	-4.39221800
C	3.88270400	-2.85843200	-5.24304600
C	5.12089600	-3.23206300	-4.72494800
C	5.23558200	-3.55350600	-3.36785800
C	4.10749600	-3.48040200	-2.55585900
N	2.90485000	-3.08219700	-3.06004300

H	5.99227300	-3.27600100	-5.37043000
H	3.78024400	-2.61379600	-6.29437500
H	6.19427500	-3.85118900	-2.95613100
C	4.02210700	-3.81464500	-1.12681900
C	5.08443500	-4.32715000	-0.38048500
C	2.60006300	-3.96052300	0.71181100
C	4.87847300	-4.67916200	0.95113100
H	6.05914700	-4.45757900	-0.83842100
H	1.62778100	-3.72346400	1.12213100
H	5.69478200	-5.08108200	1.54429900
C	1.40464500	-2.44886400	-4.74179200
C	0.95907900	-2.17543400	-6.03882400
C	-0.76293400	-2.20616100	-3.91579300
C	-0.38692800	-1.91826500	-6.27001300
H	1.66729400	-2.17251200	-6.86085400
H	-1.41307500	-2.21516700	-3.04710500
H	-0.74482300	-1.70567500	-7.27256800
N	2.78456200	-3.61328300	-0.57653200
N	0.54909200	-2.44138200	-3.66126100
C	3.61071600	-4.50395400	1.50247700
C	-1.26761400	-1.94875300	-5.18160800
H	-2.33000300	-1.76757600	-5.30778900
H	3.40157200	-4.75978300	2.53583200
H	-0.04223300	-2.18453700	-0.85083600

IN38

Ni	4.60971800	2.41577000	1.33318100
C	3.35877400	3.41300700	0.34161200
O	2.20100300	3.05206900	0.49174300
C	3.70069200	4.56286100	-0.55926800
C	2.66204300	5.26165200	-1.19663300
C	5.02647100	4.96514000	-0.76203700
C	2.94761500	6.34570300	-2.02160900
H	1.64084800	4.93379600	-1.02818000
C	5.31237800	6.05119100	-1.58955300
H	5.82688800	4.41519400	-0.27779600
C	4.27479100	6.74229100	-2.21896900
H	2.14052200	6.88436900	-2.51193200
H	6.34345600	6.35792100	-1.74432000
H	4.49827600	7.58974600	-2.86235500
C	7.46372800	6.68307500	2.84933500

C	8.43252200	5.89352900	2.20726700	O	5.52874600	1.12473200	2.60902200
C	8.18813600	4.53350500	2.04329300	Mn	5.39628600	-1.09402400	-0.23789900
C	6.98193700	3.99566800	2.48929500	C	4.84864800	-1.42650800	-3.03822500
C	6.05128800	4.86760000	3.07383600	C	4.06851600	-1.49665500	-4.19392800
N	6.29937300	6.17065400	3.26922600	C	2.68003300	-1.44485000	-4.08345400
H	8.92839700	3.89342500	1.57120000	C	2.09860900	-1.32579000	-2.81743200
H	9.35119500	6.33823200	1.83868500	C	2.91840500	-1.27010200	-1.69291800
H	6.77543200	2.93415200	2.41909200	N	4.27216700	-1.32084800	-1.81026100
C	4.72821700	4.40161800	3.58151000	H	2.05668700	-1.48442100	-4.97087400
C	4.19501700	5.01252100	4.72534300	H	4.53694800	-1.57144800	-5.16924900
C	2.86315400	3.01840000	3.42940500	H	1.02049800	-1.26923100	-2.71664800
C	2.97560900	4.58512700	5.23450200	C	2.46314300	-1.17677800	-0.30330800
H	4.75422400	5.82107000	5.17929400	C	1.12073200	-1.26995500	0.08510400
H	2.34565100	2.26991100	2.84107100	C	3.13338600	-1.02925100	1.91439800
H	2.55909700	5.04762300	6.12491000	C	0.79393100	-1.23694200	1.43399600
C	7.69141800	8.13926800	3.09346900	H	0.34507600	-1.38256500	-0.66374400
C	8.98351200	8.63609900	3.32995500	H	3.95658300	-0.94400100	2.60853900
C	6.79005400	10.24202500	3.29165400	H	-0.24274800	-1.30961200	1.74950800
C	9.15550700	10.00142100	3.54739300	C	6.30604100	-1.41836800	-2.98376000
H	9.83401300	7.96293300	3.36839600	C	7.14232600	-1.64004100	-4.08661600
H	5.88955100	10.85461600	3.26917200	C	8.15355300	-1.14793100	-1.59525600
H	10.14542300	10.40670400	3.73926900	C	8.51903500	-1.60886100	-3.92053700
N	4.05271500	3.41977800	2.93917600	H	6.71080800	-1.84678300	-5.05978100
N	6.60928400	8.93662700	3.08207200	H	8.51574900	-0.95557000	-0.59419300
C	2.29664300	3.55972600	4.57650100	H	9.17881600	-1.78252500	-4.76548000
C	8.03577400	10.83043900	3.52522000	N	3.45944900	-1.03358800	0.61341700
H	8.11872500	11.90078300	3.68843100	N	6.81716500	-1.16975500	-1.74189700
H	1.33666600	3.19440200	4.92628100	C	1.82307700	-1.12717400	2.37131900
C	6.81733000	-0.53344700	1.30561300	C	9.03725400	-1.35840900	-2.64528400
C	7.73838200	-1.62839700	1.88223100	H	10.10648500	-1.32692600	-2.46404900
C	7.04937500	-2.01398200	3.20430900	H	1.62177500	-1.11684700	3.43748400
N	6.32128300	-0.79445900	3.55749400	H	7.32853600	0.24779800	0.73922100
C	5.67193000	-0.62010100	4.83423600	Cl	5.25356000	1.43963700	-0.59242800
H	6.40493000	-0.66584100	5.65043600				
H	5.18694100	0.35787600	4.84292300	IN39			
H	4.91799400	-1.40154600	5.01474200	C	1.30856992	-0.84535438	-0.35052525
H	7.75075400	-2.28291000	4.00417000	C	-0.10994342	-0.49824998	0.13908942
H	6.35018300	-2.84771400	3.05560800	C	0.10174683	0.69680569	1.09304971
H	8.74264200	-1.22991500	2.09842000	N	1.35700761	1.28221951	0.62818911
H	7.84306700	-2.50357300	1.23785300	C	1.85858387	2.54431405	1.13579114
C	6.17233400	0.03944900	2.48318600	H	2.02386186	2.49155671	2.22005938

H	2.80512276	2.76433409	0.63999300
H	1.14224154	3.34768570	0.92946317
H	0.19540218	0.38084952	2.14316753
H	-0.70629370	1.43503726	1.03879636
H	-0.61163283	-1.33358160	0.63338880
H	-0.73174775	-0.18771775	-0.70669737
C	2.08928070	0.43777672	-0.13888597
O	3.22652206	0.70903977	-0.55666900
Mn	3.10966400	-1.27439600	-1.60220900
C	2.66758200	-2.98901700	-3.77068100
C	2.63820700	-4.21888900	-4.42248100
C	3.01120800	-5.38231500	-3.74013900
C	3.42389100	-5.28683600	-2.40606000
C	3.44660900	-4.04890900	-1.77066000
N	3.05399600	-2.90147400	-2.44196800
H	2.99345700	-6.34378700	-4.24252600
H	2.33152400	-4.27239300	-5.46279500
H	3.73291500	-6.17754300	-1.86725800
C	3.87317600	-3.75461500	-0.41210700
C	4.33560700	-4.69694500	0.52057800
C	4.21640800	-2.02331800	1.12331200
C	4.73420600	-4.27536000	1.78035100
H	4.38347900	-5.74706200	0.25004200
H	4.18355500	-0.95215100	1.29230700
H	5.09438500	-4.99390000	2.51117200
C	2.35026800	-1.68195600	-4.32290900
C	1.94243700	-1.43050900	-5.64292300
C	2.28213500	0.60501000	-3.83507400
C	1.69499400	-0.12706800	-6.04678600
H	1.82902100	-2.25484000	-6.33998700
H	2.46918500	1.37085700	-3.08981500
H	1.37980000	0.08168900	-7.06520100
N	3.80785400	-2.41850700	-0.10034400
N	2.51029000	-0.65875600	-3.42055600
C	4.67537900	-2.90781700	2.08873400
C	1.87007500	0.91465600	-5.12303900
H	1.70014200	1.94970400	-5.40192100
H	4.99084800	-2.53437200	3.05776800
H	1.78235237	-1.63477268	0.24651895
H	1.35760588	-1.16386980	-1.39386817
Cl	5.28894593	-0.89520956	-2.25575604

TS15

C	0.56814700	-1.45850100	-0.53511800
C	-0.75207500	-1.16742800	-1.26869600
C	-1.72082500	-0.69504800	-0.16451700
N	-0.82168000	-0.14827600	0.83971000
C	-1.30676900	0.52697300	2.02176100
H	-1.97609200	-0.12069700	2.60745500
H	-0.44255900	0.79173000	2.63390600
H	-1.85732600	1.43655300	1.75135800
H	-2.31081700	-1.52790300	0.25368200
H	-2.42752500	0.06913800	-0.51203600
H	-1.13583700	-2.03185500	-1.81673300
H	-0.61784400	-0.35679300	-1.99025300
C	0.46165100	-0.62833800	0.74161000
O	1.33909600	-0.41452500	1.57622300
H	1.78447600	-0.66952600	-1.10852100
Mn	2.20555900	-2.08756000	-1.70863100
C	2.90908200	-3.51927700	-4.08831400
C	3.43546500	-4.59036200	-4.81958100
C	4.17301700	-5.57676900	-4.16860300
C	4.38696300	-5.48746300	-2.77858500
C	3.84925200	-4.41405400	-2.08336300
N	3.11569800	-3.45281900	-2.72596000
H	4.58096700	-6.41218600	-4.72865400
H	3.26659000	-4.65757300	-5.88973000
H	4.95485200	-6.25557100	-2.26446700
C	3.98453200	-4.14724500	-0.65134600
C	4.78861000	-4.89453100	0.22018400
C	3.42056200	-2.67896500	1.08599100
C	4.91008600	-4.50696100	1.54749400
H	5.32613000	-5.76051400	-0.15098000
H	2.84484500	-1.80590400	1.38380600
H	5.53558300	-5.07697300	2.22878000
C	2.15458700	-2.39913900	-4.59399000
C	1.90621900	-2.15134000	-5.95920000
C	1.14133100	-0.35861000	-4.03939000
C	1.27020500	-0.99078200	-6.35309500
H	2.23869800	-2.87184300	-6.69981900
H	0.87807800	0.33941600	-3.25290700
H	1.08337500	-0.79321200	-7.40449800

N	3.28518800	-3.05152900	-0.20533400	H	6.17085900	-5.03185700	1.47963900
N	1.72191800	-1.50844800	-3.61802600	C	1.24944600	-2.40023500	-4.33690300
C	4.22320700	-3.36868200	1.98673000	C	0.70802700	-1.96786500	-5.55324500
C	0.89372800	-0.05547300	-5.36363500	C	-0.85285300	-2.29306000	-3.33520500
H	0.42101500	0.88561700	-5.62439600	C	-0.64989400	-1.69479100	-5.65096500
H	4.29648200	-3.02326200	3.01265200	H	1.35579600	-1.84491800	-6.41472600
H	0.59790100	-2.51138700	-0.18901800	H	-1.44136400	-2.43720900	-2.43618700
Cl	4.08110073	-1.10323739	-2.13177664	H	-1.07920400	-1.35700500	-6.58932100

TS15-1

C	1.08426300	-1.62923500	-0.28702500
C	0.44628900	-0.22238000	-0.41513300
C	-0.94956200	-0.35197900	0.23886200
N	-1.23830100	-1.78342900	0.11942000
C	-2.53478600	-2.36583200	0.38793500
H	-3.29612800	-1.95691600	-0.28880200
H	-2.46073900	-3.44529800	0.23934700
H	-2.85070200	-2.16542100	1.42069400
H	-1.72272300	0.23042200	-0.27640900
H	-0.95383700	-0.05170600	1.29820800
H	0.33417500	0.04667100	-1.47080600
H	1.04918500	0.55631100	0.05384300
C	-0.10605700	-2.50212100	-0.08507100
O	-0.06105400	-3.75375600	-0.22552500
H	2.37066700	-1.31669100	-1.28402300
Mn	1.51473800	-3.16235300	-1.59387000
C	2.65270200	-2.74276300	-4.13126400
C	3.66852900	-2.75758500	-5.08768700
C	4.95685100	-3.13964400	-4.71208700
C	5.20342400	-3.52059500	-3.38950700
C	4.16354000	-3.49106600	-2.46514200
N	2.90813800	-3.08685400	-2.83303400
H	5.75876600	-3.15235200	-5.44314600
H	3.46015300	-2.47688200	-6.11484700
H	6.19602600	-3.83878100	-3.08845300
C	4.21730600	-3.89717000	-1.06056800
C	5.36954900	-4.31273400	-0.38623100
C	2.92636800	-4.26655400	0.84922700
C	5.28258100	-4.71122800	0.94346800
H	6.32527500	-4.31577600	-0.89965500
H	1.93226500	-4.24583100	1.28422500

N	2.99693200	-3.86229100	-0.43531300
N	0.46960200	-2.55120100	-3.21111600
C	4.03343500	-4.69296200	1.57256400
C	-1.44860000	-1.86921200	-4.51405400
H	-2.51735400	-1.68134200	-4.54015200
H	3.91680900	-5.00389000	2.60591200
Cl	3.46531500	-0.31826300	-1.58498900
H	1.74047200	-1.68652300	0.59232500

IN40

C	0.38252300	-2.02876900	-0.28912900
C	-0.99398800	-1.91557600	-0.97999100
C	-1.48191900	-0.48218800	-0.65340500
N	-0.67869200	-0.09662400	0.48897500
C	-0.87950400	1.14408600	1.19567200
H	-1.89023600	1.19679100	1.62314100
H	-0.14350600	1.18756600	2.00109900
H	-0.74172400	2.01267500	0.53392200
H	-2.55258300	-0.45086600	-0.40683500
H	-1.33163400	0.21373400	-1.49505000
H	-1.69736400	-2.64436000	-0.55578900
H	-0.97584300	-2.08800800	-2.06088600
C	0.38156000	-0.94193400	0.74255200
O	1.15529800	-0.78141000	1.69020600
Mn	2.04553800	-2.26054800	-1.48377300
C	2.92143800	-3.36138500	-4.01071200
C	3.59714700	-4.25116800	-4.84745500
C	4.48280000	-5.17751800	-4.29458900
C	4.68983500	-5.19882800	-2.90246800
C	3.99690700	-4.30520100	-2.09983400
N	3.11591300	-3.40741000	-2.64856300
H	5.01745300	-5.87168300	-4.93471300
H	3.44347300	-4.21794600	-5.92139300

H	5.38663900	-5.90693200	-2.46651800	H	-3.10249200	3.29452200	4.55339400
C	4.08305700	-4.17456300	-0.64833900	H	-2.74994000	3.94888600	8.81472500
C	4.93419900	-4.92160800	0.17603800	C	-3.63616900	8.86745100	2.47345600
C	3.27553700	-2.98415300	1.20295700	C	-3.70080000	10.02532800	1.70084600
C	4.94363300	-4.68491600	1.54406800	C	-3.32909200	7.53639300	0.61140000
H	5.58391400	-5.67357400	-0.25910000	C	-3.54895800	9.90635900	0.31693000
H	2.60638900	-2.19959000	1.55530700	H	-3.85374300	10.99667700	2.15607700
H	5.60113500	-5.25510300	2.19410700	H	-3.18147200	6.52629900	0.23768600
C	2.00794700	-2.30800200	-4.39471800	H	-3.58864900	10.79281900	-0.31049900
C	1.65819200	-1.97154400	-5.71409200	N	-3.39286600	5.21272000	5.21359200
C	0.74253000	-0.50997000	-3.58514900	N	-3.48835200	7.64621200	1.92847700
C	0.83207500	-0.88782400	-5.95518800	C	-2.90426600	3.41876400	6.71820400
H	2.04971400	-2.55955400	-6.53787700	C	-3.33930100	8.64587000	-0.23872900
H	0.43279700	0.05603100	-2.71494700	H	-3.19577600	8.51525000	-1.30578500
H	0.55908400	-0.61935000	-6.97133200	H	-2.70077700	2.36056700	6.84990600
N	3.25111600	-3.21718700	-0.12708800	Cl	-6.13417400	6.70172400	2.89318300
N	1.51283700	-1.58938600	-3.32508400	C	-5.55494300	3.39644700	0.68797600
C	4.10080100	-3.69571800	2.06529500	C	-6.70804400	2.38344400	0.58960600
C	0.37303700	-0.12792400	-4.86257700	C	-7.44452800	2.56166800	1.93085100
H	-0.25000900	0.74860500	-5.00538800	N	-6.40701800	3.07577000	2.82581200
H	4.08489900	-3.46840600	3.12607400	C	-6.64573500	3.18954500	4.24727000
H	0.50579900	-3.00015700	0.21457700	H	-6.94818700	2.21489700	4.64942000
Cl	1.01050034	-4.15527828	-1.54930317	H	-5.73090800	3.51441100	4.73437300
H	2.97809919	-1.38971861	-2.21376327	H	-7.42948300	3.93143900	4.43166600

IN41

Mn	-3.74550600	6.08073300	3.36347800
C	-3.69403800	8.86967900	3.96262100
C	-3.71702200	10.00745600	4.75747200
C	-3.72073300	9.86507200	6.15367600
C	-3.64781900	8.59141900	6.70274400
C	-3.57158000	7.48954700	5.83867500
N	-3.61776100	7.64340300	4.50580800
H	-3.75986900	10.74237200	6.79007600
H	-3.74133400	10.98977500	4.30002500
H	-3.63484300	8.44370600	7.77653700
C	-3.39867500	6.08484000	6.25080400
C	-3.17128900	5.65263300	7.56515000
C	-3.13095800	3.91757100	5.44526200
C	-2.93159600	4.30478100	7.80562400
H	-3.16283300	6.37036700	8.37839700

H	-3.10249200	3.29452200	4.55339400
H	-2.74994000	3.94888600	8.81472500
C	-3.63616900	8.86745100	2.47345600
C	-3.70080000	10.02532800	1.70084600
C	-3.32909200	7.53639300	0.61140000
C	-3.54895800	9.90635900	0.31693000
H	-3.85374300	10.99667700	2.15607700
H	-3.18147200	6.52629900	0.23768600
H	-3.58864900	10.79281900	-0.31049900
N	-3.39286600	5.21272000	5.21359200
N	-3.48835200	7.64621200	1.92847700
C	-2.90426600	3.41876400	6.71820400
C	-3.33930100	8.64587000	-0.23872900
H	-3.19577600	8.51525000	-1.30578500
H	-2.70077700	2.36056700	6.84990600
Cl	-6.13417400	6.70172400	2.89318300
C	-5.55494300	3.39644700	0.68797600
C	-6.70804400	2.38344400	0.58960600
C	-7.44452800	2.56166800	1.93085100
N	-6.40701800	3.07577000	2.82581200
C	-6.64573500	3.18954500	4.24727000
H	-6.94818700	2.21489700	4.64942000
H	-5.73090800	3.51441100	4.73437300
H	-7.42948300	3.93143900	4.43166600
H	-7.86062700	1.62836200	2.32549100
H	-8.25302700	3.30232500	1.86240200
H	-6.31422100	1.36456900	0.51268600
H	-7.36690500	2.55475900	-0.26504900
C	-5.38579500	3.63583800	2.17114100
O	-4.37538800	4.20322200	2.66810100
H	-5.81235500	4.37077100	0.25665600
H	-4.61602400	3.06563200	0.23574800
Cl	-1.47549300	5.55187900	2.72052900

TS16

C	0.36724696	-1.20800557	-1.17226284
C	-0.08760139	0.20830415	-0.75602987
C	-1.52988634	0.01399152	-0.23106776
N	-1.95059815	-1.22784850	-0.85453767
C	-3.28926168	-1.74788096	-0.71380744
H	-4.02671788	-1.05002225	-1.13238362

H	-3.33685076	-2.69377715	-1.25693294
H	-3.53841515	-1.92332315	0.34262646
H	-2.19688166	0.83710771	-0.52137156
H	-1.55394765	-0.07139869	0.86395715
H	-0.10224130	0.88917250	-1.61781990
H	0.54124298	0.66387317	0.01375738
C	-0.92166693	-1.95666867	-1.39758599
O	-1.08022603	-3.03472375	-1.97525113
H	1.95571432	-0.54702115	-1.45477772
Mn	1.40272800	-2.96373000	-1.91664900
C	2.82037700	-2.78535400	-4.36858300
C	3.93562600	-2.82401300	-5.20961100
C	5.16195600	-3.21728500	-4.68064100
C	5.25747800	-3.56825300	-3.33157000
C	4.11480300	-3.51420500	-2.53569900
N	2.93120100	-3.12486400	-3.06362600
H	6.04389600	-3.24556000	-5.31260700
H	3.85185600	-2.54102100	-6.25279200
H	6.21091300	-3.86537400	-2.91029500
C	4.02819800	-3.85761900	-1.10487100
C	5.07130100	-4.43808600	-0.38222800
C	2.62126700	-3.94729500	0.74754400
C	4.86151100	-4.78352100	0.95108600
H	6.02580600	-4.63426200	-0.85745900
H	1.65547800	-3.69456100	1.15891200
H	5.66012600	-5.23988600	1.52867700
C	1.45463200	-2.40775800	-4.73652500
C	1.03081500	-2.13498600	-6.04158900
C	-0.71327300	-2.14419700	-3.93207500
C	-0.31036400	-1.86181500	-6.27954300
H	1.74250200	-2.15399600	-6.85953200
H	-1.36982800	-2.17284900	-3.07069500
H	-0.65757000	-1.65168900	-7.28656200
N	2.82031400	-3.60261900	-0.53218400
N	0.58668700	-2.38375900	-3.68500000
C	3.61548900	-4.54350200	1.52279100
C	-1.20341300	-1.88065800	-5.20476200
H	-2.26260400	-1.69414000	-5.34617300
H	3.40590600	-4.80061100	2.55530700
Cl	0.98852937	-5.21478964	-2.32235528
Cl	3.10153500	0.07737700	-2.05720300

IN42

H	0.29715197	-1.43591340	-0.12916902
C	-1.39928200	0.70759100	0.72196600
C	-2.48048200	1.33511900	-0.16765500
C	-2.24371400	2.85008600	-0.01447900
N	-1.68469800	2.94804300	1.32142900
C	-1.42228800	4.21233300	1.96584900
H	-2.35087500	4.77930600	2.11392000
H	-0.96839000	3.99982800	2.93581600
H	-0.72917100	4.82634300	1.37214400
H	-3.16760500	3.43722100	-0.09578800
H	-1.53611300	3.23471100	-0.76685900
H	-3.47470400	1.09127200	0.23562900
H	-2.46821700	1.01660000	-1.21140800
C	-1.16649600	1.75803500	1.78476100
O	-0.61715600	1.62734100	2.87754000
Mn	0.41938100	0.22450700	-0.14377700
C	-0.60645600	-1.81451100	-1.83597800
C	-1.04562800	-3.10156500	-2.14159800
C	-0.93209900	-4.11676800	-1.18969700
C	-0.36655400	-3.83053600	0.06533500
C	0.06191600	-2.54240400	0.34545500
N	-0.06133900	-1.54655500	-0.59760600
H	-1.27451100	-5.12071000	-1.41688100
H	-1.47515300	-3.31228300	-3.11546800
H	-0.26798300	-4.61324300	0.80972600
C	0.69400300	-2.06487400	1.56950700
C	1.03191200	-2.86536400	2.66733900
C	1.59073900	-0.17447100	2.61910500
C	1.66974700	-2.28858200	3.75789100
H	0.80306900	-3.92554200	2.65772400
H	1.77355000	0.88907500	2.55414500
H	1.94127300	-2.89645700	4.61615400
C	-0.60906900	-0.64971500	-2.69464000
C	-1.02004400	-0.62830000	-4.03790800
C	-0.02165800	1.61706500	-2.81397200
C	-0.93065200	0.54732600	-4.76422400
H	-1.39785000	-1.53450500	-4.49948200
H	0.40054100	2.46557500	-2.28764200
H	-1.24581400	0.57559900	-5.80310300

N	0.97754300	-0.72598400	1.55647200
N	-0.12365000	0.48465300	-2.08599800
C	1.95783100	-0.92079400	3.73249800
C	-0.41466700	1.69527800	-4.14034500
H	-0.31380900	2.63247800	-4.67686000
H	2.45136500	-0.43135000	4.56473700
H	-1.69824000	-0.23977500	1.17730300
Cl	2.48447304	0.99675321	-0.66883173

TS17

C	2.21587698	0.41040350	0.38854165
C	2.04943514	1.79047647	1.02861648
C	0.56218738	1.84291949	1.48133451
N	-0.05989484	0.69807676	0.82415012
C	-1.42207383	0.30093360	1.09854143
H	-2.13170365	1.05262483	0.73081238
H	-1.60256004	-0.64934759	0.59151838
H	-1.59081786	0.16825203	2.17797477
H	0.06375854	2.77785020	1.19305487
H	0.46323604	1.74274413	2.57268929
H	2.24658505	2.58052192	0.29340690
H	2.72039399	1.97428837	1.87463209
C	0.86057064	-0.14584044	0.25672150
O	0.61284654	-1.32682895	-0.17024324
Mn	2.70008700	-1.71989100	-0.74376700
C	1.57604600	-3.50688000	-2.60527900
C	1.10129100	-4.74047400	-3.04306200
C	1.20756000	-5.86115200	-2.21452200
C	1.80291900	-5.73025900	-0.95061700
C	2.26568100	-4.49102800	-0.53077000
N	2.14189800	-3.39076400	-1.35304000
H	0.84191100	-6.82600200	-2.54895700
H	0.65826300	-4.82966700	-4.02969500
H	1.90536400	-6.59431900	-0.30232200
C	2.91824300	-4.15992300	0.72669500
C	3.23940000	-5.05486200	1.75614200
C	3.85267900	-2.37639000	1.93092900
C	3.87952400	-4.57924600	2.89247300
H	2.99157800	-6.10657400	1.65839400
H	4.06135300	-1.31298700	1.93698500
H	4.13742300	-5.25972200	3.69866000

C	1.59786300	-2.25167300	-3.33076100
C	1.16284600	-2.05034300	-4.65025300
C	2.30593500	-0.02051500	-3.19260200
C	1.30083800	-0.79930200	-5.23091900
H	0.73359900	-2.87530800	-5.20910300
H	2.80125600	0.73011200	-2.58650200
H	0.97089500	-0.63039300	-6.25164900
N	3.23075100	-2.83427100	0.82906700
N	2.14616200	-1.22452000	-2.60837000
C	4.19121300	-3.21599000	2.98400300
C	1.89092100	0.23755500	-4.49042300
H	2.03938300	1.22329100	-4.91795200
H	4.69273000	-2.80936200	3.85556900
Cl	4.84773000	-0.90803500	-1.08582700
H	2.63020104	0.96358578	-0.42829673

IN43

C	1.05176900	-0.56843800	-1.70483500
C	2.01571400	0.49043800	-1.16171300
C	1.76921400	0.51127100	0.37836100
N	0.64858800	-0.40348400	0.58944900
C	0.24176700	-0.82260300	1.90927600
H	-0.18158100	0.02003800	2.47150900
H	-0.51917400	-1.59870700	1.79976200
H	1.08765700	-1.22620200	2.48579700
H	1.53139900	1.51293400	0.76238400
H	2.64346400	0.14637200	0.93683200
H	1.80625900	1.47638700	-1.59374300
H	3.06679600	0.26812900	-1.37785900
C	0.29680100	-1.04852700	-0.56352200
O	-0.43943700	-2.08641900	-0.60768700
Mn	1.22312700	-2.64350900	-1.90624300
C	2.34772600	-2.78002200	-4.45705300
C	3.39331700	-2.77772000	-5.37525600
C	4.71805400	-2.78211500	-4.92122100
C	4.97144600	-2.80826200	-3.54646400
C	3.90703500	-2.82439700	-2.64652000
N	2.60210100	-2.78407000	-3.09862000
H	5.53975200	-2.77121800	-5.62984200
H	3.18219600	-2.76426600	-6.44031200
H	5.99392000	-2.82415800	-3.18096400

C	3.95548000	-2.93873500	-1.20053400	C	1.26338100	-5.84348100	-2.25576300
C	5.12018300	-3.10164200	-0.43568300	C	1.85648600	-5.73314100	-0.98888500
C	2.64003800	-3.18795000	0.71997200	C	2.30586400	-4.49796900	-0.54273300
C	5.02943400	-3.31789300	0.93139200	N	2.17296000	-3.38289400	-1.34231400
H	6.08879200	-3.07373300	-0.92507400	H	0.90850900	-6.80488800	-2.61108500
H	1.63725900	-3.21703800	1.13385300	H	0.70163700	-4.77891100	-4.04801100
H	5.92575700	-3.44981500	1.53008000	H	1.96493400	-6.60900200	-0.35755800
C	0.91879800	-2.75742300	-4.72444700	C	2.93733600	-4.18295900	0.72976500
C	0.32050500	-2.80357200	-5.99113600	C	3.26424800	-5.09368300	1.74366900
C	-1.19084300	-2.65626600	-3.70566100	C	3.81616900	-2.40881800	1.98667500
C	-1.06332000	-2.78080100	-6.10122900	C	3.87684200	-4.63009700	2.89996600
H	0.94294300	-2.85912400	-6.87869100	H	3.04373900	-6.14847000	1.61760800
H	-1.73284500	-2.57376000	-2.76845800	H	4.01157300	-1.34273000	2.01658200
H	-1.53704000	-2.81983100	-7.07783300	H	4.13946800	-5.32321000	3.69372900
N	2.70423700	-2.94005800	-0.61090600	C	1.61689400	-2.20650800	-3.29478800
N	0.15541500	-2.68929800	-3.57899500	C	1.17740700	-1.97770300	-4.60844500
C	3.75514400	-3.38215600	1.51895200	C	2.32087600	0.02282200	-3.11060200
C	-1.83613300	-2.70401200	-4.93227200	C	1.31191100	-0.71390600	-5.16201300
H	-2.92045500	-2.67716000	-4.97464300	H	0.74893000	-2.79127600	-5.18436900
H	3.63227300	-3.57393300	2.58035500	H	2.81365600	0.76092800	-2.48724500
H	0.47093700	-0.27378700	-2.57824700	H	0.97904000	-0.52389300	-6.17808300
Cl	1.16398006	-4.80269353	-1.91112125	N	3.21706600	-2.85373800	0.86817800
				N	2.15883600	-1.19170500	-2.55185800
				C	4.15767700	-3.26288500	3.02680800
				C	1.90414000	0.30775800	-4.40245100
				H	2.05350800	1.30122600	-4.81130700
				H	4.64089100	-2.86599700	3.91303600
				H	0.83648700	-1.83495300	1.11917700
				Cl	4.93449600	-1.20291700	-1.14841000
TS18							
C	0.78409300	-1.27437700	0.18731000				
C	-0.58396900	-1.19973700	-0.48463900				
C	-0.73629200	0.29343300	-0.90590000				
N	0.39666900	0.97454900	-0.28323100				
C	0.73540700	2.34309500	-0.60227900				
H	-0.02788100	3.03343100	-0.22205500				
H	1.69497400	2.57188800	-0.13341800				
H	0.82243700	2.49260500	-1.68907000				
H	-1.68671000	0.73361600	-0.57604600				
H	-0.68071800	0.41602000	-1.99774500				
H	-1.38060200	-1.48136600	0.21463700				
H	-0.68333700	-1.85814400	-1.35555300				
C	1.28769000	0.09079900	0.26860600				
O	2.45206000	0.37166700	0.61430200				
Mn	2.70458200	-1.72031100	-0.69609700				
C	1.60786700	-3.47766900	-2.59638700				
C	1.14447900	-4.70630600	-3.05988500				