Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Pd-Catalyzed C-H Alkylation with Maleimide Occurs Preferentially at the *ortho*-Methyl C-H Bond *over* the *ortho*-C-H Bond

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Contents

I. General Information.

^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer in $CDCl_3$ with tetramethylsilane as the internal standard. Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, and m = multiplet), coupling constant (Hz), and integration. In some cases, some peaks in the ^{13}C NMR spectra cannot be analyzed because of overlapping peaks. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra and high resolution mass spectra (HRMS) were obtained using a JEOL JMS-700 spectrometer. Melting points were determined using a Yamato melting point apparatus. Column chromatography was performed with SiO_2 (Silicycle SiliaFlash F60 (230-400 mesh)). Some compounds were purified by LC-908 HPLC (GPC).

II. Materials.

8-Aminoquinoline (CAS 578-66-5), *N*-Methylmaleimide (CAS 930-88-1), *N*-Ethylmaleimide (CAS 128-53-0), *N*-Cyclohexylmaleimide (CAS: 1631-25-0), *N*-Phenylmaleimide (CAS: 941-69-5), *N*-(2-Hydroxyethyl)maleimide (CAS: 1585-90-6), Pivalic acid (CAS: 75-98-9) were purchased from Tokyo Chemical Industry Co., Ltd. Silver acetate (CAS: 563-63-3) was purchased from FUJIFILM Wako Pure Chemical Co. Palladium pivalate (CAS: 106224-36-6) was purchased from Sigma-Aldrich Co.

III. Synthesis of Starting Materials.

All amides bearing an 8-aminoquinoline moiety were prepared by reacting the corresponding acid or the corresponding acid chlorides with 8-aminoquinoline.[1]

General Procedure for the Preparation of Stating Amides.

(1) Synthesis of amides from acid chlorides.

The acid chloride (15 mmol) was dissolved in CH_2Cl_2 (20 mL). After cooling the reaction mixture to 0 °C, a solution of 8-aminoquinoline (15 mmol) and triethylamine (36 mmol) in 10 mL of CH_2Cl_2 was added dropwise. The resulting mixture was allowed to warm to rt and was then stirred overnight. The crude mixture was then washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x20 mL). The combined organic layers were washed with 1 M HCl aq. (20 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solution taken to dryness.The resulting crude amide was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc = 5/1).

(2) Synthesis of amides from carboxylic acid.

To a stirred solution of carboxylic acid (15 mmol) and DMF (5 drops) in CH_2Cl_2 (10 mL), $(COCl)_2$

[1] Shibata, K.; Chatani, N. *Org. Lett*. **2014**, *16*, 5148.

(1.5 mL, 18 mmol) was added dropwise. The solution was magnetically stirred at room temperature for 2 h. The solvent was then eliminated under reduced pressure, and the resulting residue was dissolved in CH_2Cl_2 (15 mL). After cooling the reaction mixture to 0 °C, a solution of 8-Aminoquinoline (15 mmol) and triethylamine (36 mmol) in 10 mL of the same solvent were added dropwise. The resulting mixture was allowed to warm to rt and stirred overnight. The crude product was washed with saturated aqueous $NaHCO_3$ (20 mL), and CH_2Cl_2 (3x20 mL). The organic phase was washed with 1 M HCl aq. (20 mL).The organic phase was dried over anhydrous Na_2SO_4 and the solvent removed by evaporation of the solvent. The resulting crude amide was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc = 5/1).

IV. Synthesis of target materials

(I) General procedure for the Palladium-catalyzed alkylation of aromatic amides with *N*-methylmaleimide.

To an oven-dried 5 mL screw-capped vial, 2-methyl-*N*-(quinolin-8-yl)benzamide (78.7mg, 0.3 mmol), *N*-methylmaleimide (165.2mg, 1.5 mmol), $Pd(OPiv)_2$ (13.89mg, 0.045mmol), AgOAc (60.1mg, 0.36 mmol) and PivOH (1 mL) were added. The mixture was stirred for 24 hours at 160°C and then cooled to room temperature. The resulting mixture was diluted with 1 mL EtOAc. The mixture was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 1.5:1) to afford a 7:1 mixture of the alkylation product **2a** and the annulation byproduct **3a** (106.2 mg, 91%). The ratio of **2** and **3** was determined from an ^1H NMR spectrum of the mixture. Products **2a** and **3a** were separated by Gel Permeation Chromatography giving **2a** as a pale yellow powder and **3a** as a pale yellow colloid.

(2) Synthesis of five-member palladacycle.

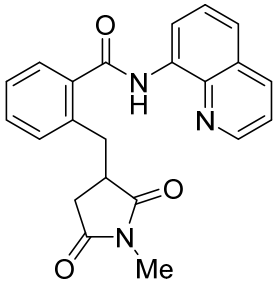
To an oven-dried 100 mL flask, 2-methyl-*N*-(quinolin-8-yl)benzamide (1.3g, 5.0 mmol), $Pd(OAc)_2$ (1.12, 5.0 mmol), MeCN (10 mL) were added. The mixture was stirred for 4 hours at 60°C and then cooled to room temperature. The resulting mixture was filtered and removed insoluble substance, then solvent concentrated in vacuo. The residue was washed by 5 mL cold MeCN and dried. Finally observer palladacycle as deep yellow solid. The crystal was obtained from saturated palladacycle-MeCN solvent.

(3) Synthesis of alkylation product from five-member palladacycle.

To an oven-dried 5 mL screw-capped vial, palladacycle (122.3mg, 0.3 mmol), *N*-methylmaleimide (165.2mg, 1.5 mmol), AgOAc (60.1mg, 0.36 mmol) and PivOH (1 mL) were added. The mixture was stirred for 24 hours at 160°C and then cooled to room temperature. The resulting mixture was diluted with 1 mL EtOAc. The solvent was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 1.5:1) to afford product (25.8 mg, 23 %) as a pale yellow colloid.

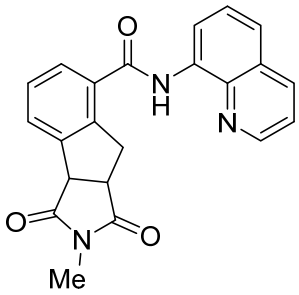
V. Spectroscopic Data.

2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-*N*-(quinolin-8-yl)benzamide (2a)



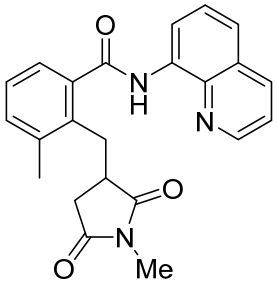
92.9mg, 83% yield. R_f 0.23 (hexane/ EtOAc = 1.5:1). Pale Yellow powder. m.p. 64.8-65.1 °C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.72-2.76 (m, 1H), 2.96 (s, 3H), 3.15 (dd, J = 13.8, 9.3 Hz, 1H), 3.33-3.37 (m, 1H), 3.59 (dd, J = 13.8, 5.5 Hz, 1H), 7.35 (d, J = 7.7 Hz, 1H), 7.42 (dd, J = 7.7, 6.4 Hz, 1H), 7.46-7.50 (m, 2H), 7.56-7.62 (m, 2H), 7.74 (dd, J = 7.7, 1.3 Hz, 1H), 8.19 (dd, J = 8.3, 1.3 Hz, 1H), 8.78 (q, J = 1.9 Hz, 1H), 8.88 (dd, J = 7.1, 1.9 Hz, 1H), 10.25 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 33.7, 33.7, 41.7, 116.9, 121.9, 122.2, 127.5, 127.5, 127.7, 128.1, 130.9, 131.0, 134.5, 136.7, 136.9, 137.3, 138.5, 148.4, 167.7, 176.9, 179.7. MS: *m*/*z* 374, 307, 230, 155, 154, 144, 136, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{22}H_{20}N_3O_3$: 374.1504; Found: 374.1507.

2-methyl-1,3-dioxo-N-(quinolin-8-yl)-1,2,3,3a,8,8a-hexahydroindeno[1,2-c]pyrrole-7-carboxamide (3a)



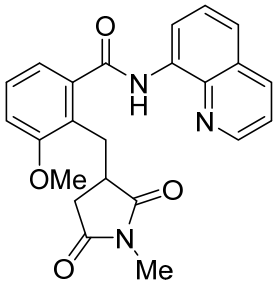
13.3mg, 8% yield. R_f 0.23 (hexane/ EtOAc = 1.5:1). Pale Yellow powder. m.p. 156.5-157.0 °C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.96 (s, 1H), 3.73 (q, J = 7.1 Hz, 1H), 3.90 (d, J = 6.6 Hz, 3H), 4.41 (d, J = 8.0 Hz, 1H), 7.46-7.51 (m, 2H), 7.56-7.63 (m, 2H), 7.79 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 7.8 Hz, 1H), 8.21 (dd, J = 8.2, 1.4 Hz, 1 H), 8.83 (dd, J = 4.1, 1.6 Hz, 1H), 8.89 (dd, J = 7.2, 1.7 Hz, 1H), 10.52 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.3, 35.3, 43.9, 51.6, 117.5, 121.8, 122.3, 127.7, 127.8, 128.3, 128.4, 132.9, 134.2, 137.4, 139.3, 141.7, 148.1, 165.9, 177.4, 179.7. MS: *m*/*z* 372, 326, 307, 289, 228, 154, 138, 136, 115, 107, 89, 77. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{22}H_{18}N_3O_3$: 372.1348; Found: 372.1344.

3-methyl-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2b)



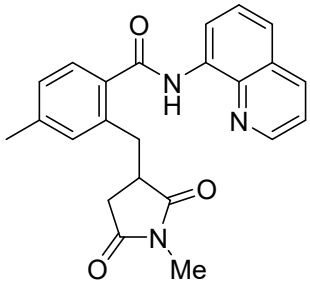
46.2mg, 40% yield. R_f 0.31 (hexane/ EtOAc = 1.5:1). Pale yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.46 (s, 3H), 2.65 (t, J = 9.2 Hz, 1H), 2.89 (dd, J = 18.6, 4.4 Hz, 1H), 2.95 (s, 3H), 3.21-3.28 (m, 2H), 3.51 (d, J = 8.7 Hz, 1H), 7.30-7.37 (m, 2H), 7.46 (q, J = 4.1 Hz, 1H), 7.53-7.59 (m, 3H), 8.18 (dd, J = 8.3, 1.8 Hz, 1H). 8.76 (q, J = 2.0 Hz, 1H), 8.86 (dd, J = 6.6, 2.1 Hz, 1H), 10.17 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.2, 24.9, 30.8, 34.2, 40.3, 116.8, 121.9, 122.2, 125.4, 127.3, 127.5, 128.1, 133.1, 134.6, 135.5, 136.5, 137.7, 138.2, 138.6, 148.5, 168.6, 177.1, 179.7. MS: *m*/*z* 388, 307, 244, 154, 136. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{22}N_3O_3$: 388.1661; Found: 388.1656.

3-methoxy-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2c)



79.5mg, 66% yield. R_f 0.20 (hexane/ EtOAc = 1.5:1). Pale yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.61 (q, J = 9.0 Hz, 1H), 2.91 (dd, J = 18.3, 5.0 Hz, 1H), 2.96 (s, 3H), 3.13-3.16 (m, 1H), 3.45-3.52 (m, 2H), 3.88(s, 3H), 7.04 (d, J = 8.3 Hz, 1H), 7.29-7.31 (m, 1H), 7.39 (t, J = 7.8 Hz, 1H), 7.46 (q, J = 4.1 Hz, 1H), 7.55-7.61 (m, 2H), 8.18 (dd, J = 8.5, 1.6 Hz, 1H), 8.77 (q, J = 2.0 Hz, 1H), 8.87 (dd, J = 7.1, 2.1 Hz, 1H), 10.18 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.8, 28.3, 33.9, 40.0, 55.8, 112.4, 116.9, 119.5, 121.8, 122.2, 125.7, 127.5, 128.1, 128.5, 134.6, 136.6, 138.6, 138.7, 148.4, 158.4, 167.7, 177.6, 180.1. MS: *m*/*z* 404, 307, 289, 260, 154, 136, 120, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{22}N_3O_4$: 404.1610; Found: 404.1617.

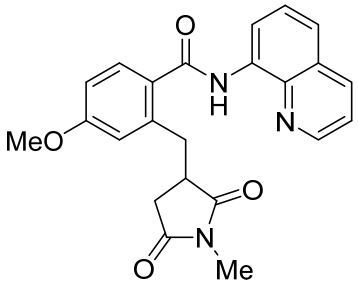
4-methyl-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2d)



95.0mg, 82% yield. R_f 0.26 (hexane/ EtOAc = 1.5:1). Yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.41 (s, 3H), 2.66-2.83 (m, 2H), 2.97 (s, 3H), 3.12 (dd, J = 13.5, 9.4 Hz, 1H), 3.35 (s, 1H), 3.57

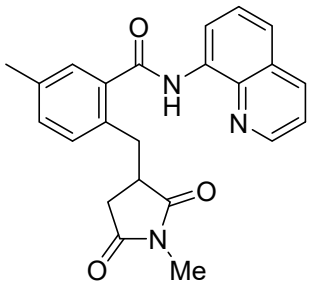
(dd, J = 13.5, 5.3 Hz, 1H), 7.21-7.26 (m, 1H), 7.46 (q, J = 4.1 Hz, 1H), 7.56-7.59 (m, 2H), 7.65 (d, J = 7.8 Hz, 1H), 8.18 (dd, J = 8.3, 1.4 Hz, 1H), 8.78 (t, J = 2.1 Hz, 1H), 8.87 (d, J = 6.9 Hz, 1H), 10.25 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.5, 24.9, 33.6, 33.7, 41.8, 116.7, 121.9, 122.1, 127.5, 127.8, 128.2, 131.8, 134.0, 134.7, 136.6, 137.5, 138.7, 141.3, 148.5, 167.8, 177.1, 179.8. MS: *m*/*z* 388, 307, 289, 244, 154, 144, 136, 107. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{22}N_3O_3$: 388.1661; Found: 388.1666.

4-methoxy-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2e)



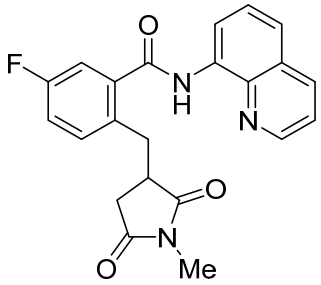
76.7mg, 64% yield. R_f 0.21 (hexane/ EtOAc = 1.5:1). Yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.71-2.78 (m, 2H), 2.97 (s, 3H), 3.19 (dd, J = 13.5, 8.9 Hz, 1H), 3.34 (q, J = 4.6 Hz, 1H), 3.59 (dd, J = 13.5, 5.3 Hz, 1H), 3.86 (d, J = 0.7 Hz, 3H), 6.86 (d, J = 2.3 Hz, 1H), 6.91 (d, J = 8.7 Hz, 1H), 7.44-7.47 (m, 1H), 7.56 (dd, J = 10.8, 8.5 Hz, 2H), 7.73 (d, J = 8.7 Hz, 1H), 8.18 (d, J = 8.3 Hz, 1H), 8.79 (t, J = 2.1 Hz, 1H), 8.85 (d, J = 6.9 Hz, 1H), 10.24 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 33.7, 41.8, 55.6, 112.4, 116.6, 116.7, 121.8, 121.9, 127.5, 128.1, 129.1, 129.5, 134.8, 136.5, 138.7, 140.0, 148.4, 161.4, 167.4, 177.0, 179.8. MS: *m*/*z* 404, 307, 289, 260, 154, 137, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{22}N_3O_4$: 404.1610; Found: 404.1608.

5-methyl-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2f)



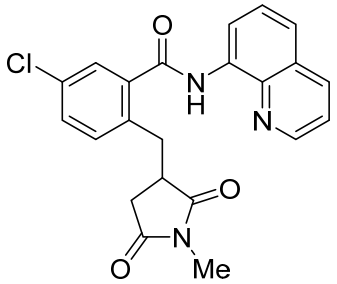
84.3mg, 73% yield. R_f 0.26 (hexane/ EtOAc = 1.5:1). Brown colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.43 (s, 3H), 2.66-2.82 (m, 2H), 2.95 (s, 3H), 3.10 (dd, J = 13.8, 8.7 Hz, 1H), 3.28-3.34 (m, 1H), 3.53 (dd, J = 13.8, 5.5 Hz, 1H), 7.21-7.29 (m, 2H), 7.47 (q, J = 4.3 Hz, 1H), 7.52 (s, 1H), 7.55-7.62 (m, 2H), 8.20 (dd, J = 8.5, 1.6 Hz, 1H), 8.80 (q, J = 2.0 Hz, 1H), 8.88 (dd, J = 6.9, 1.8 Hz, 1H), 10.21 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.2, 24.9, 33.3, 33.7, 41.8, 116.9, 121.9, 122.2, 127.5, 128.2, 130.8, 131.6, 134.1, 134.7, 136.6, 136.9, 137.3, 138.7, 148.5, 168.0, 177.0, 179.8. MS: *m*/*z* 388, 307, 289, 244, 154, 144, 137, 120, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{22}N_3O_3$: 388.1661; Found: 388.1655.

5-fluoro-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2g)



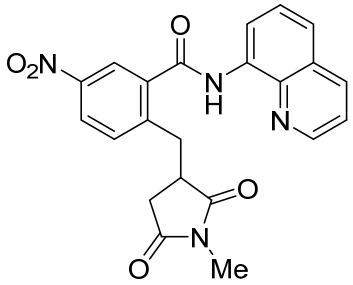
85.6mg, 73% yield. R_f 0.20 (hexane/ EtOAc = 1.5:1). Yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.73 (d, J = 7.3 Hz, 2H), 2.96 (s, 3H), 3.13 (dd, J = 13.8, 9.2 Hz, 1H), 3.29-3.33 (m, 1H), 3.51 (dd, J = 13.8, 5.5 Hz, 1H), 7.19 (td, J = 8.5, 2.8 Hz), 7.34 (dd, J = 8.5, 5.3 Hz, 1H), 7.44 (dd, J = 8.5, 2.5 Hz, 1H), 7.47-7.51 (m, 1H), 7.59-7.60 (m, 2H), 8.21 (d, J = 8.3 Hz, 1H), 8.80-8.81 (m, 1H), 8.85 (dd, J = 5.3, 3.4 Hz, 1H), 10.24 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 33.1, 33.8, 41.7, 116.3 (dd, J = 317, 21 Hz), 117.0, 122.0, 122.6, 127.5, 128.2, 132.8 (d, J = 8 Hz), 133.1 (d, J = 3 Hz), 134.3, 136.7, 138.4 (d, J = 6 Hz), 138.6, 160.3, 162.7, 166.3, 176.7, 179.5. MS: *m*/*z* 392, 307, 289, 248, 154, 136, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{19}FN_3O_3$: 392.1410; Found: 392.1406.

5-chloro-2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2h)



91.0mg, 75% yield. R_f 0.25 (hexane/ EtOAc = 1.5:1). Deep yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.73 (d, J = 6.9 Hz, 2H), 2.96 (s, 3H), 3.12 (dd, J = 13.8, 8.7 Hz, 1H), 3.30 (d, J = 6.4 Hz, 1H), 3.50 (dd, J = 13.8, 5.5 Hz, 1H), 7.30 (d, J = 8.3 Hz, 1H), 7.44-7.51 (m, 2H), 7.60 (d, J = 4.6 Hz, 2H), 7.70 (d, J = 1.8 Hz, 1H), 8.21 (d, J = 8.3 Hz, 1H), 8.81-8.85 (m, 2H), 10.22 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 33.2, 33.7, 41.6, 117.0, 122.6, 127.4, 127.6, 128.1, 130.9, 132.4, 133.2, 134.2, 135.7, 136.7, 138.4, 138.6, 148.6, 166.3, 176.7, 179.4. MS: *m*/*z* 408, 307, 264, 154, 137, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{23}H_{19}ClN_3O_3$: 408.1115; Found: 408.1113.

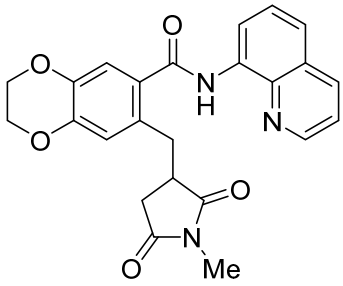
2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-5-nitro-N-(quinolin-8-yl)benzamide (2i)



94.2mg, 75% yield. R_f 0.20 (hexane/ EtOAc = 1:1). Yellow powder. m.p. 190.5-190.9 °C. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.74-2.80 (m, 2H), 2.97 (s, 3H), 3.28-3.37 (m, 2H), 3.57 (t, J = 6.6 Hz, 1H),

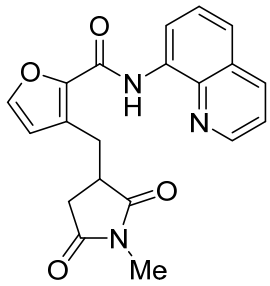
7.51 (q, J = 4.3 Hz, 1H), 7.58-7.63 (m, 3H), 8.22 (dd, J = 8.3, 1.4 Hz, 1H), 8.33 (dd, J = 8.5, 2.5 Hz, 1H), 8.59 (d, J = 2.3 Hz, 1H), 8.59 (d, J = 2.3 Hz, 1H), 8.80-8.85 (m, 2H), 10.35 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.1, 34.0, 34.1, 41.3, 117.2, 122.1, 122.7, 123.0, 125.4, 127.4, 128.1, 132.3, 133.9, 136.7, 138.0, 138.5, 145.0, 146.9, 148.8, 165.3, 176.2, 178.9. MS: *m*/*z* 419, 307, 289, 154, 137, 120, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{22}H_{19}N_4O_5$: 419.1355; Found: 419.1358.

7-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)-2,3-dihydrobenzo[b][1,4]dioxine-6-carboxamide (2j)



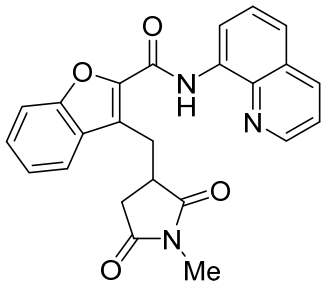
84.4mg, 65% yield. R_f 0.18 (hexane/ EtOAc = 1:1). Yellow powder. m.p. 78.9-79.2 ℃. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.68-2.80 (m, 2H), 2.97 (s, 3H), 3.05-3.11 (m, 1H), 3.27-3.32 (m, 1H), 3.49 (dd, J = 13.8, 5.4 Hz, 1H), 4.32 (s, 4H), 6.82 (s, 1H), 7.27 (s, 1H), 7.47 (q, J = 4.2 Hz, 1H), 7.54-7.60 (m, 2H), 8.18 (dd, J = 8.2, 1.4 Hz, 1H), 8.78-8.84 (m, 2H), 10.21 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 32.9, 33.6, 41.8, 64.5, 64.7, 116.7, 116.9, 119.6, 121.8, 122.0, 127.5, 128.1, 129.6, 131.3, 134.7, 136.6, 138.6, 142.2, 145.6, 148.4, 166.9, 177.1, 179.8.

3-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)furan-2-carboxamide (2k)



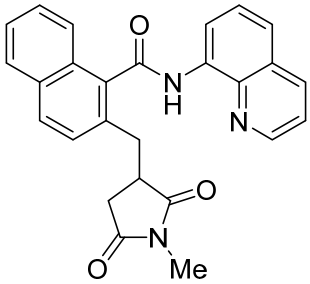
41.9mg, 39% yield. R_f 0.18 (hexane/ EtOAc = 1.5:1). Pale yellow powder. m.p. 66.2-66.5 ℃. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.77 (q, J = 3.4 Hz, 2H), 2.98 (s, 3H), 3.24-3.27 (m, 1H), 3.36 (q, J = 7.1 Hz, 1H), 3.60 (dd, J = 13.5, 5.1 Hz, 1H), 6.44 (d, J = 1.9 Hz, 1H), 7.49 (q, J = 4.1 Hz, 1H), 7.54-7.57 (m, 3H), 8.19 (dd, J = 8.3, 1.3 Hz, 1H), 8.81 (q, J = 3.0 Hz, 1H), 8.88-8.90 (m, 1H), 10.80 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 26.1, 33.3, 40.5, 114.6, 116.8, 121.9, 122.1, 127.5, 128.2, 128.4, 134.2, 136.5, 138.8, 143.7, 143.8, 148.6, 157.4, 176.9, 179.6. MS: *m*/*z* 364, 307, 171, 154, 136, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{20}H_{18}N_3O_4$: 364.1297; Found: 364.1306.

3-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzofuran-2-carboxamide (2l)



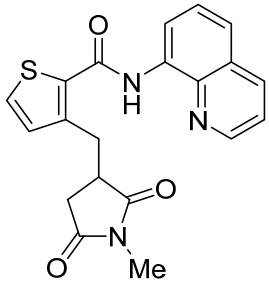
67.0mg, 58% yield. R_f 0.29 (hexane/ EtOAc = 1.5:1). yellow powder. m.p. 154.3-154.8 ℃. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.70 (q, J = 9.1 Hz, 1H), 2.91 (dd, J = 18.5, 4.8 Hz, 1H), 2.95 (s, 3H), 3.36-3.40 (m, 1H), 3.64-3.70 (m, 1H), 3.76-3.81 (m, 1H), 7.35 (t, J = 7.5 Hz, 1H), 7.48-7.52 (m, 2H), 7.57 (d, J = 4.6, 2H), 7.70 (q, J = 7.9 Hz, 2H), 8.19-8.21 (m, 1H), 8.85-8.87 (m , 1H), 8.94 (dd, J = 4.1, 1.4 Hz, 1H), 11.06 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.98, 25.0, 33.5, 40.3, 112.5, 117.1, 121.1, 121.9, 122.5, 123.5, 123.8, 127.4, 127.9, 128.2, 128.4, 134.0, 136.5, 138.8, 144.2, 148.7, 153.8, 158.0, 176.8, 179.6.

2-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)-1-naphthamide (2m)



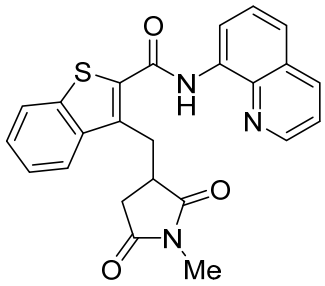
79.2mg, 62% yield. R_f 0.14 (hexane/ EtOAc = 1.5:1). Pale yellow powder. m.p. 96.3-96.7 ℃. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.62-2.87 (m, 2H), 2.94 (s, 3H), 3.09 (t, J = 9.8 Hz, 1H), 3.22-3.44 (m, 1H), 3.60 (dd, J = 14.0, 4.8 Hz, 1H), 7.43 (q, J = 4.1 Hz, 2H), 7.48-7.54 (m, 2H), 7.60-7.68 (m, 2H), 7.87-7.94 (m, 2H), 7.97-8.00 (m, 1H), 8.19 (dd, J = 8.2, 1.8 Hz, 1H), 8.66 (q, J = 2.0 Hz, 1H), 9.07 (dd, J = 7.6, 1.6 Hz, 1H), 10.13 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 33.7, 34.4, 41.6, 117.3, 121.9, 122.6, 125.2, 126.5, 127.5, 127.7, 128.2, 128.3, 130.1, 130.3, 132.5, 134.3, 135.4, 136.6, 138.6, 148.6, 167.9, 176.6, 179.5. MS: *m/z* 424, 307, 289, 167, 154, 137, 107, 89, 77. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{26}H_{22}N_3O_3$: 424.1661; Found: 424.1658.

3-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)thiophene-2-carboxamide (2n)



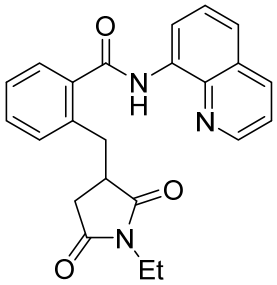
77.1mg, 68% yield. R_f 0.13 (hexane/ EtOAc = 2:1). Brown colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.76-2.78 (m, 2H), 2.98 (d, J = 3.7 Hz, 3H), 3.29-3.33 (m, 1H), 3.46 (dd, J = 13.8, 8.3 Hz, 1H), 3.70 (dd, J = 13.8, 5.5 Hz, 1H), 7.02 (d, J = 5.0 Hz, 1H), 7.42 (d, J = 5.0 Hz, 1H), 7.46 (q, J = 4.1 Hz, 1H), 7.52-7.57 (m, 2H), 8.16 (dd, J = 8.3, 1.8 Hz, 1H), 8.76 (dd, J = 6.6, 2.1 Hz, 1H), 8.82 (q, J = 2.0 Hz, 1H), 10.43 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 29.7, 33.5, 41.0, 116.6, 121.8, 122.0, 127.4, 127.7, 128.0, 131.1, 132.6, 134.4, 136.5, 138.6, 143.3, 148.5, 160.8, 176.8, 190.5. MS: *m*/*z* 380, 307, 236, 154, 137, 107, 89. HRMS (FAB+) m/z ([M+H]$^+$) Calcd for $C_{20}H_{18}N_3O_3S$: 380.1069; Found: 380.1064.

3-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzo[b]thiophene-2-carboxamide (2o)



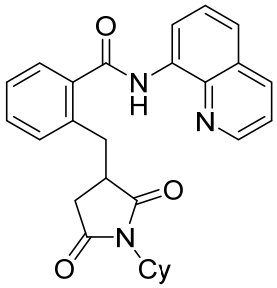
108.8mg, 85% yield. R_f 0.25 (hexane/ EtOAc = 1.5:1). Pale yellow powder. m.p. 84.6-85.3 ℃. . ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.64 (q, J = 9.1 Hz, 1H), 3.01 (s, 3H), 3.05-3.13 (m, 1H), 3.36-3.40 (m, 1H), 3.83 (d, J = 7.8 Hz, 2H), 7.48-7.52 (m , 3H), 7.54-7.58 (m, 2H), 7.91-7.97 (m, 2H), 8.19 (d, J = 8.2 Hz, 1H), 8.81 (q, J = 3.0 Hz, 1H), 8.87 (t, J = 2.1 Hz, 1H), 10.60 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 28.1, 33.7, 40.7, 116.9, 121.9, 122.4, 123.1, 123.3, 125.4, 127.3, 127.4, 128.1, 132.1, 134.3, 136.6, 138.5, 138.6, 138.9, 139.4, 148.6, 161.2, 177.0, 179.5.

3-((1-methyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzo[b]thiophene-2-carboxamide (2aa)



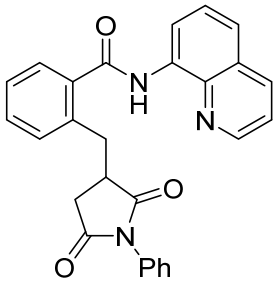
99.6mg, 86% yield. R_f 0.33 (hexane/ EtOAc = 1.5:1). Pale yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.14 (t, J = 7.1 Hz, 3H), 2.71-2.74 (m, 2H), 3.16 (dd, J = 13.8, 8.7 Hz, 1H), 3.32-3.36 (m, 1H), 3.51-3.61 (m, 3H), 7.35 (d, J = 7.3 Hz, 1H), 7.40-7.49 (m, 3H), 7.59 (q, J = 7.8 Hz, 2H), 7.74 (d, J = 7.3 Hz, 1H), 8.20 (d, J = 8.3 Hz, 1H), 8.79 (d, J = 4.1 Hz, 1H), 8.89 (dd, J = 6.6, 1.1 Hz, 1H), 10.26 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.2, 33.6, 33.7, 33.8, 41.6, 116.8, 121.9, 122.3, 127.5, 127.7, 128.1, 130.9, 131.0, 134.6, 136.6, 136.9, 137.3, 138.7, 148.5, 167.7, 176.7, 179.5. MS: *m*/*z* 388, 307, 289, 154, 136, 107, 89. HRMS (FAB+) m/z ([M+H]$^+$) Calcd for $C_{23}H_{22}N_3O_3$: 388.1661; Found: 388.1662.

2-((1-cyclohexyl-2,5-dioxopyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2ab)



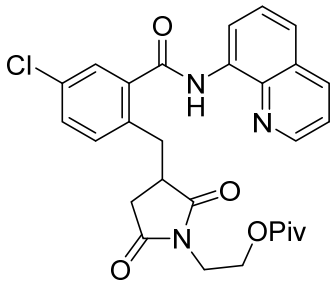
112.2mg, 85% yield. R_f 0.37 (hexane/ EtOAc = 1.5:1). Yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.15-1.31 (m, 3H), 1.53 (d, J = 11.0 Hz, 2H), 1.62 (d, J = 11.9 Hz, 1H), 1.77 (t, J = 10.1 Hz, 2H), 2.11 (qd, J = 12.7, 3.3 Hz, 2H), 2.67 (d ,J = 6.9 Hz, 2H), 3.15 (dd, J = 13.8, 8.3 Hz, 1H), 3.25 (td, J = 7.1, 5.5 Hz, 1H), 3.56 (dd, J = 13.8, 5.5 Hz, 1H), 3.92 (qd, J = 8.3, 4.0 Hz, 1H), 7.35 (dd, J = 7.6, 1.1 Hz, 1H), 7.39-7.49 (m, 3H), 7.56-7.62 (m, 2H), 7.73 (dd, J = 7.6, 1.1 Hz, 1H), 8.20 (dd, J = 8.5, 1.6 Hz, 1H), 8.79 (q, J = 2.0 Hz, 1H), 8.89 (dd, J = 6.9, 1.8 Hz, 1H), 10.25 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.1, 26.0, 28.8, 28.9, 33.6, 33.7, 41.1, 51.7, 117.0, 121.9, 122.3, 127.4, 127.5, 127.6, 128.2, 130.8, 131.1, 134.6, 136.7, 137.0, 137.3, 138.6, 148.4, 167.8, 176.9, 179.8. MS: *m/z* 442, 307, 298, 216, 154, 136, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{27}H_{28}N_3O_3$: 442.2130; Found: 442.2139.

2-((2,5-dioxo-1-phenylpyrrolidin-3-yl)methyl)-N-(quinolin-8-yl)benzamide (2ac)



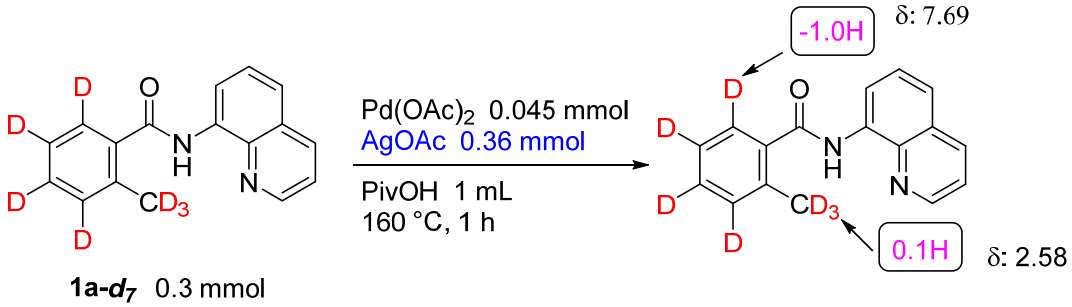
87.0mg, 67% yield. R_f 0.25 (hexane/ EtOAc = 1.5:1). Yellow powder. m.p. 183.7-184.1 ℃. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 2.86-3.01 (m, 2H), 3.31 (dd, J = 13.5, 8.5 Hz, 1H), 3.52-3.56 (m, 1H), 3.67 (dd, J = 13.8, 5.5 Hz, 1H), 7.25-7.27 (m, 1H), 7.34-7.52 (m, 8H), 7.56-7.63 (m, 2H), 7.76-7.78 (m, 1H), 8.19 (dd, J = 8.3, 1.4 Hz, 1H), 8.78 (q, J = 2.0 Hz, 1H), 8.90 (dd, J = 7.1, 1.6 Hz, 1H), 10.30 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 33.7, 33.9, 41.8, 116.9, 121.9, 122.3, 126.6, 127.5, 127.6, 127.7, 128.1, 128.6, 129.2, 131.0, 131.2, 132.1, 134.6, 136.7, 136.9, 137.2, 138.6, 148.5, 167.7, 175.8, 178.6. MS: *m/z* 436, 292, 171, 144, 136, 120, 115, 107, 89. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{27}H_{22}N_3O_3$: 436.1661; Found: 436.1657.

2-(3-(4-chloro-2-(quinolin-8-ylcarbamoyl)benzyl)-2,5-dioxopyrrolidin-1-yl)ethyl pivalate (2ad)

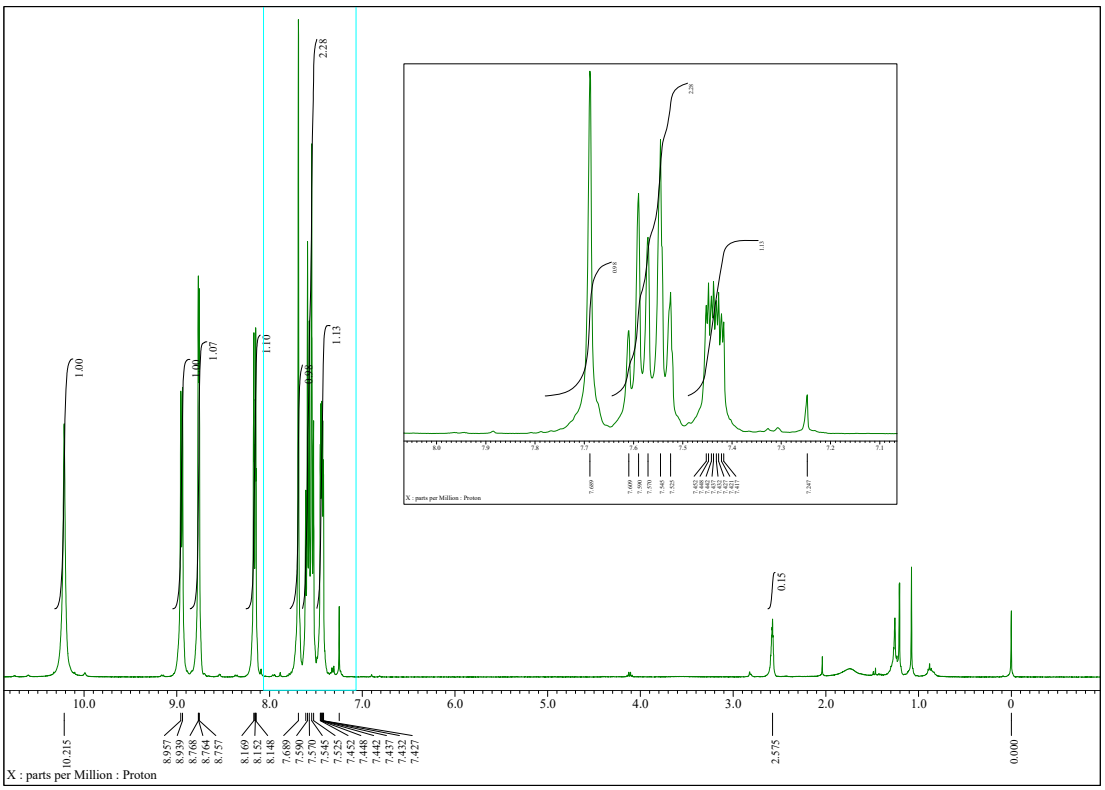


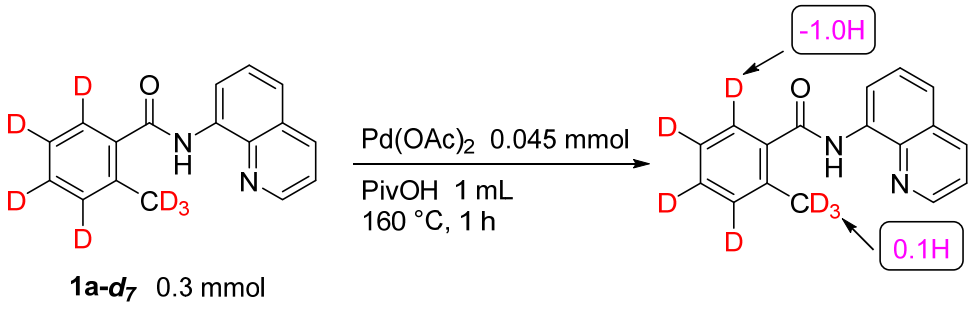
66.5mg, 43% yield. R_f 0.33 (hexane/ EtOAc = 1.5:1). Yellow colloid. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 1.12 (s, 9H), 2.73 (d, J = 7.8 Hz, 2H), 3.11 (dd, J = 14.0, 8.9 Hz, 1H), 3.30-3.33 (m, 1H), 3.50 (dd, J = 13.5, 5.3 Hz, 1H), 3.76 (t, J = 4.1 Hz, 2H), 4.22 (d, J = 5.5 Hz, 2H), 7.32 (d, J = 8.3 Hz, 1H), 7.44-7.50 (m, 2H), 7.59 (t, J = 2.3 Hz, 2H), 7.70 (d, J = 2.3 Hz, 1H), 8.20 (dd, J = 8.3, 1.8 Hz, 1H), 8.80-8.85 (m, 2H), 10.22 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 27.2, 33.3, 33.7, 38.1, 38.8, 41.4, 60.9, 117.0, 122.0, 122.6, 127.4, 127.6, 128.1, 130.9, 132.4, 133.3, 134.3, 135.7, 136.7, 138.4, 138.6, 148.6, 166.2, 176.2, 178.4, 179.0. MS: *m/z* 522, 328, 154, 144, 136, 129, 107, 89, 57. HRMS (FAB+) m/z ($[M+H]^+$) Calcd for $C_{28}H_{29}ClN_3O_3$: 522.1795; Found: 522.1792.

VI. Deuterium Labeling Experiments.



1a-d_7 0.3 mmol




D
O
D
N
H
D
CD3
N
D
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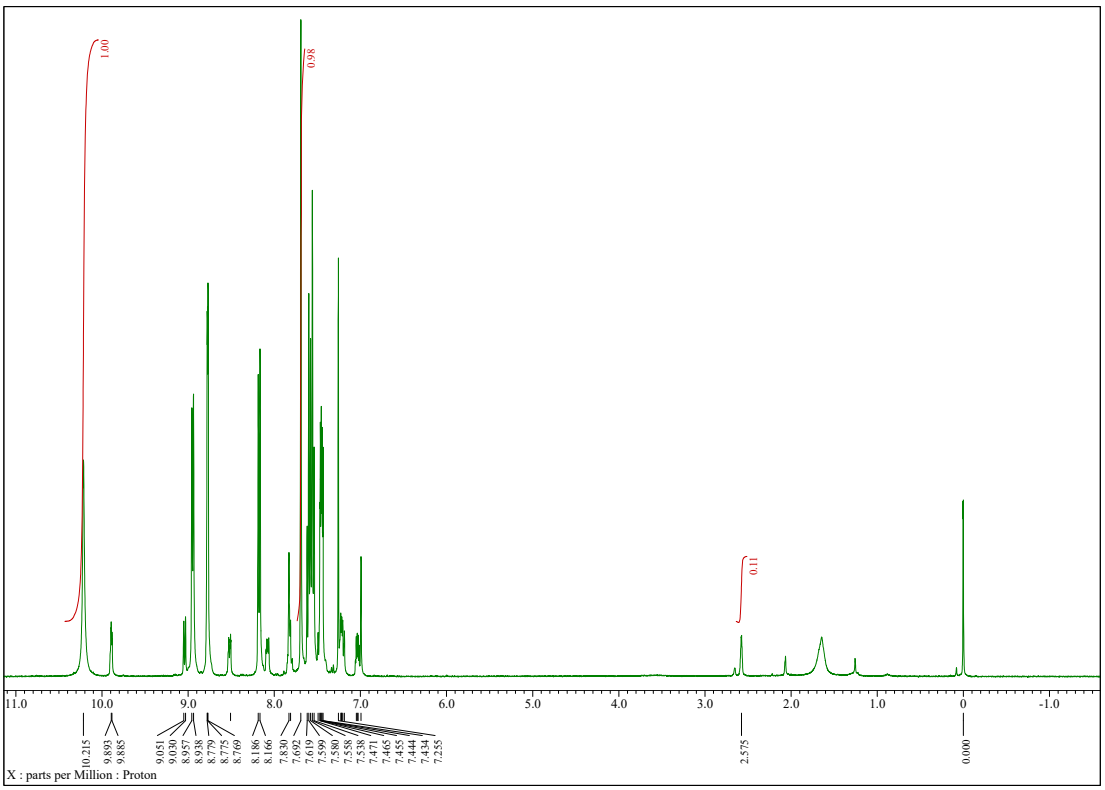
PivOH 1 mL
160 °C, 1 h
-1.0H
0.1H

1a-d_7 0.3 mmol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11.0
10.0
9.0
8.0
7.0
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5.0
4.0
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2.0
1.0
0
-1.0
10.215
9.893
9.885
9.051
9.030
8.957
8.938
8.779
8.775
8.769
8.186
8.166
7.830
7.692
7.619
7.589
7.580
7.558
7.538
7.471
7.465
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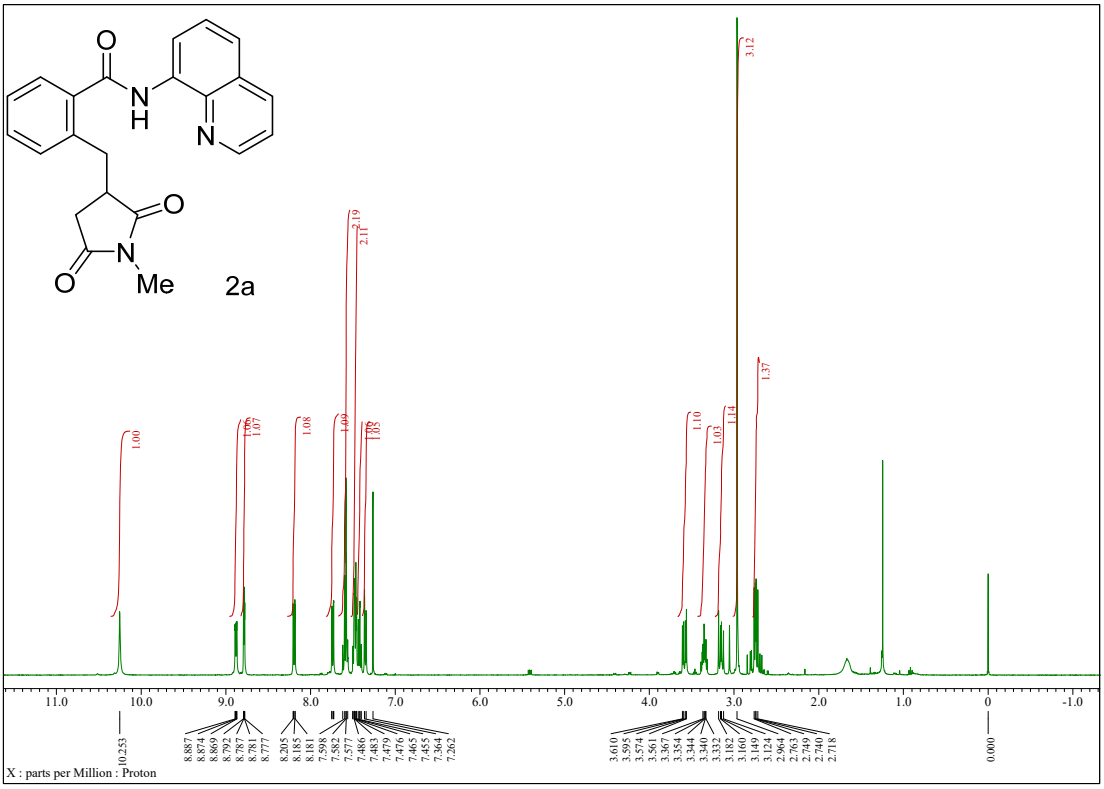
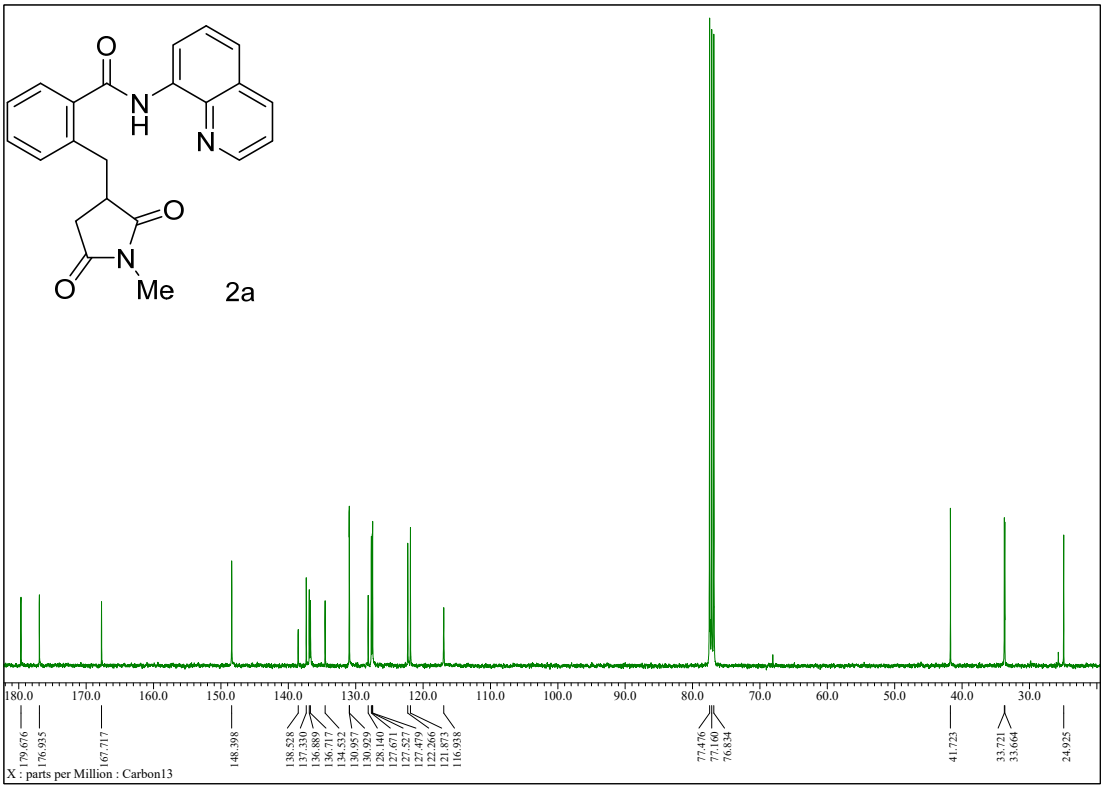
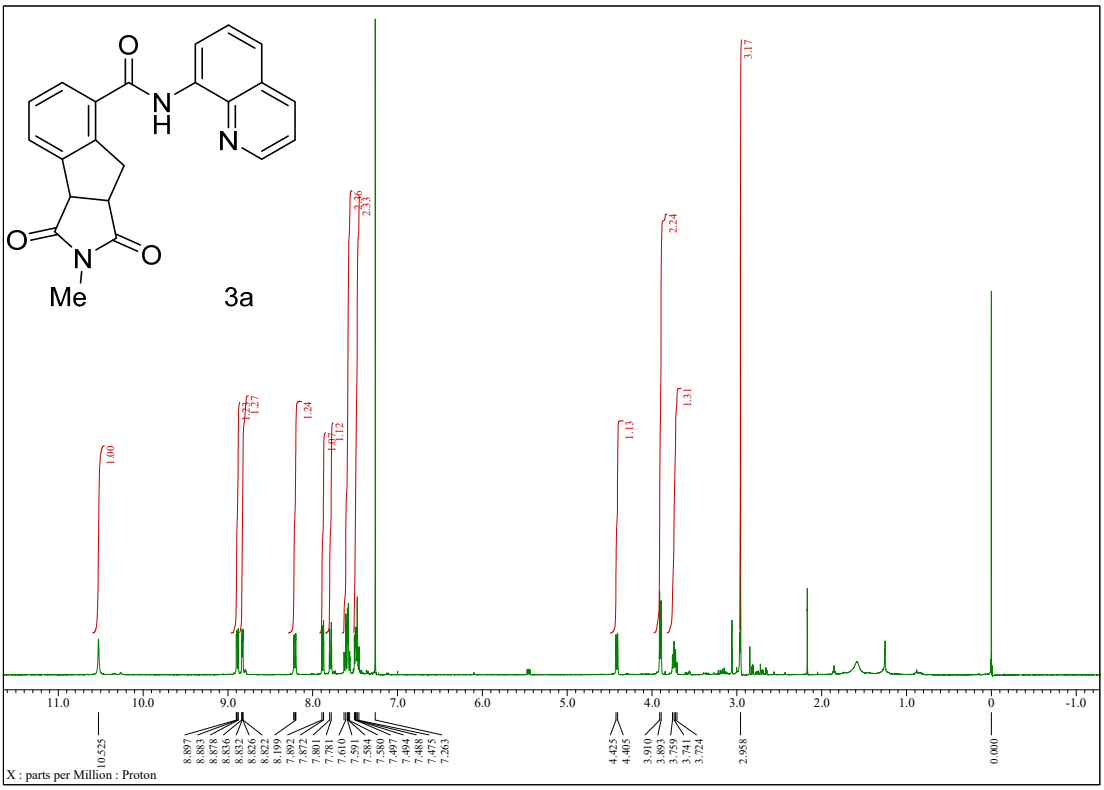
7.434
7.255
2.575
0.000
X : parts per Million : Proton

VII. Copies of ^{1}H and ^{13}C NMR Spectra



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N
H
N
O
N
O
Me
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2.36
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1.13
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1.27
1.23
1.07
1.12
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
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8.897
8.883
8.878
8.836
8.832
8.826
8.822
8.199
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7.872
7.801
7.781
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7.584
7.580
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7.494
7.484
7.475
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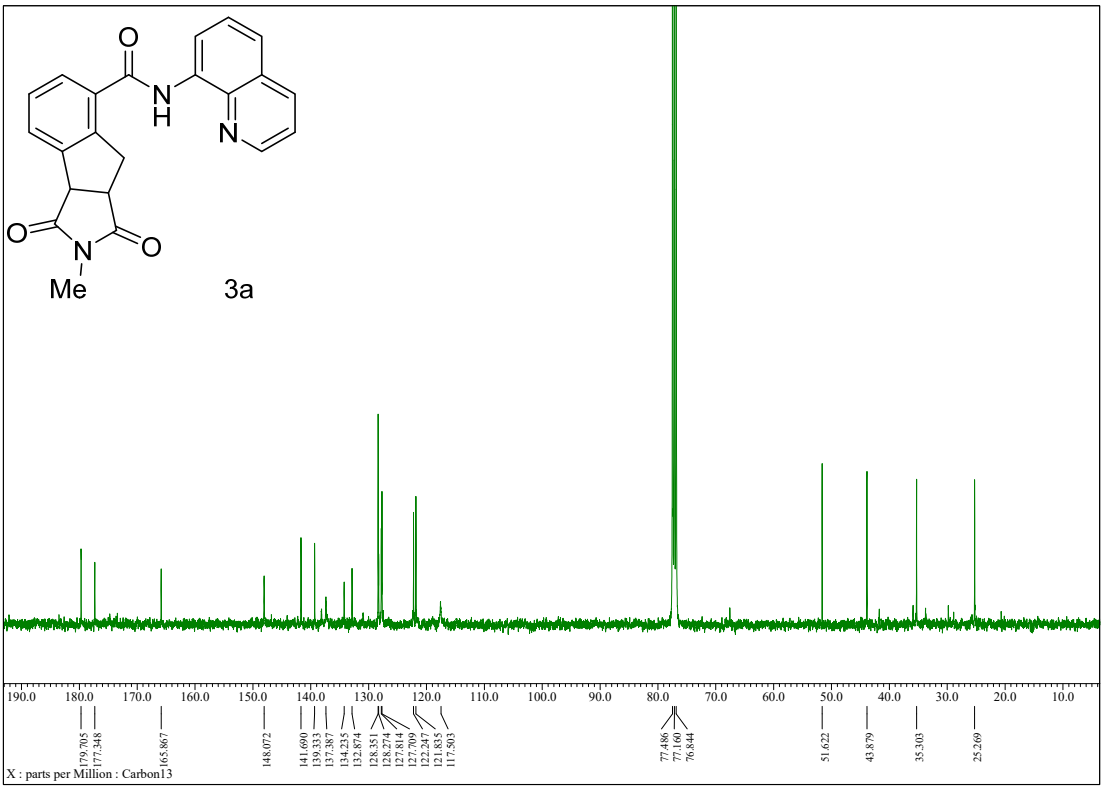
3.759
3.741
3.724
2.958
0.000
X : parts per Million : Proton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H
N
O
N
O
Me
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120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
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177.348
165.867
148.072
141.690
139.333
137.387
134.235
132.874
128.351
128.274
127.814
127.709
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76.844
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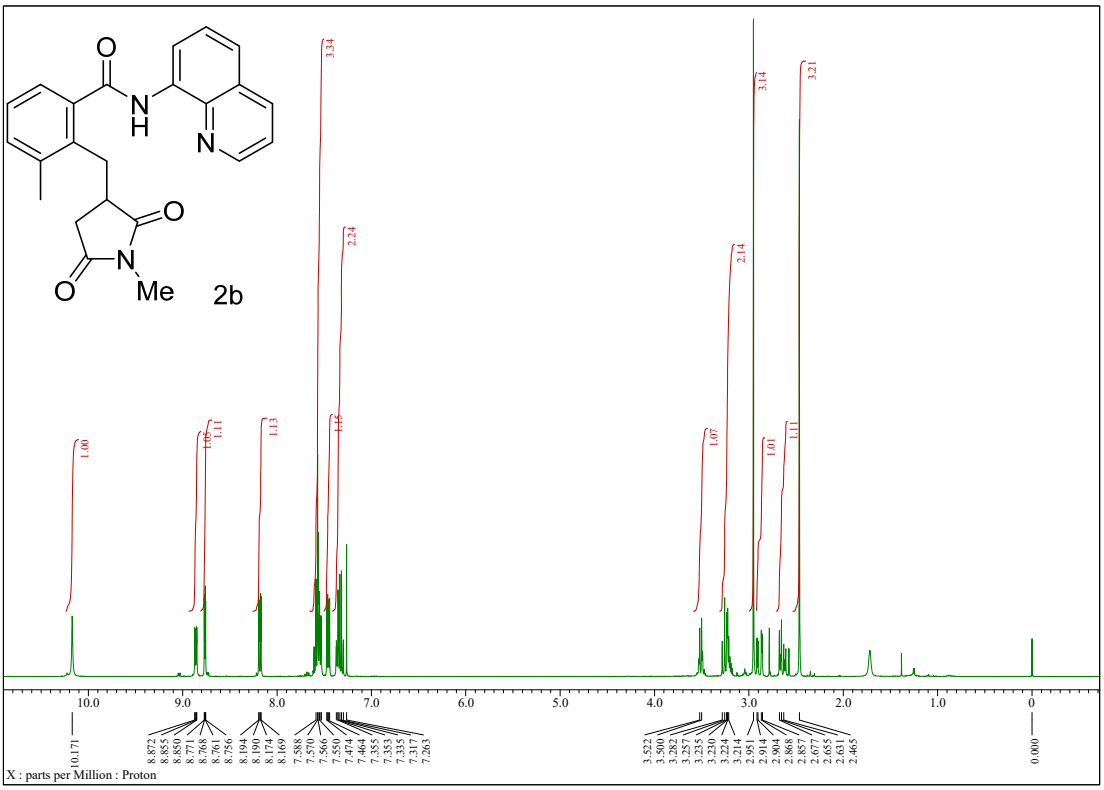
43.879
35.303
25.269
X : parts per Million : Carbon13


O
N
H
N
O
O
N
Me
2b
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3.14
3.21
2.24
2.14
1.00
1.07
1.01
1.11
1.13
1.16
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8.850
8.771
8.768
8.761
8.756
8.194
8.190
8.174
8.169
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7.570
7.566
7.550
7.474
7.464
7.355
7.353
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7.317
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3.500
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3.257
3.255
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3.224
3.214
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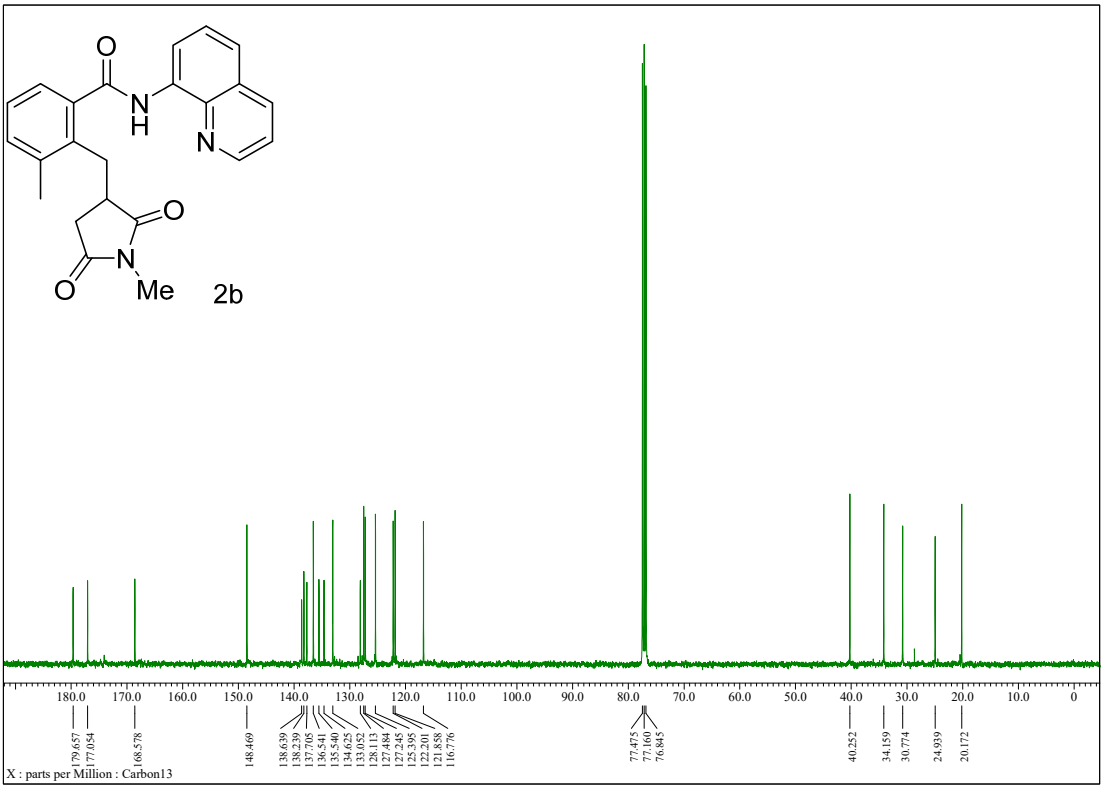
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O
O
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Me
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133.052
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127.245
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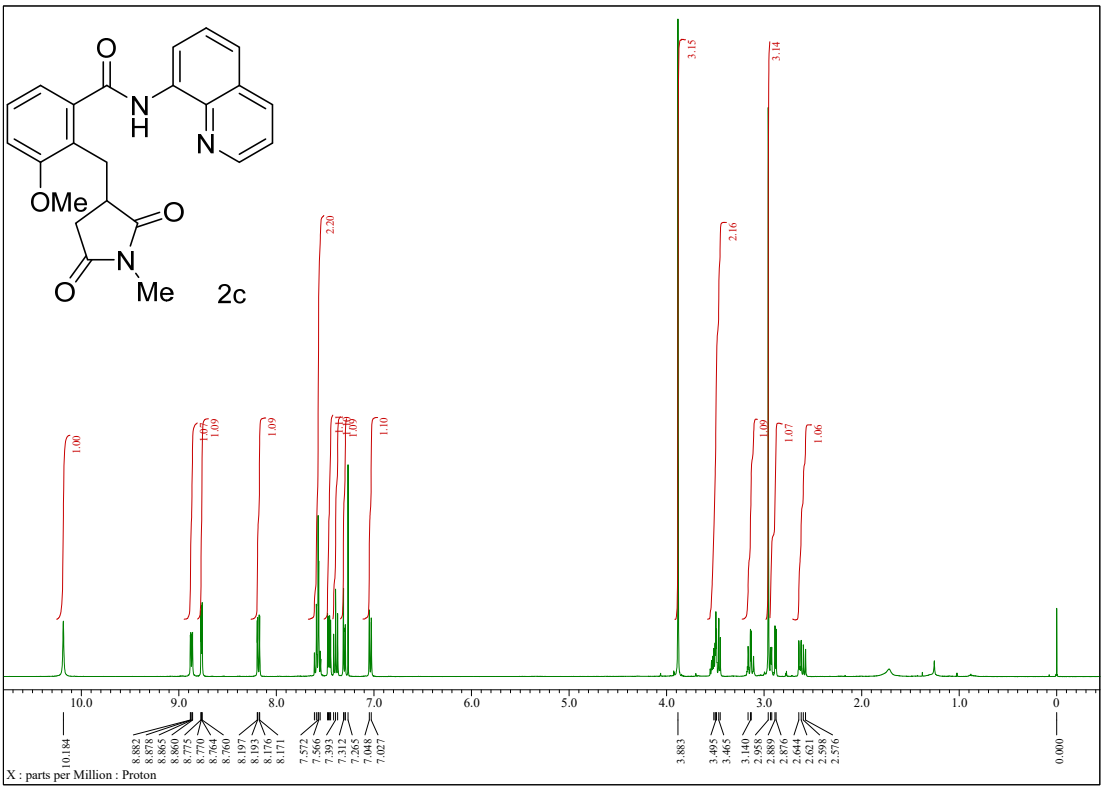
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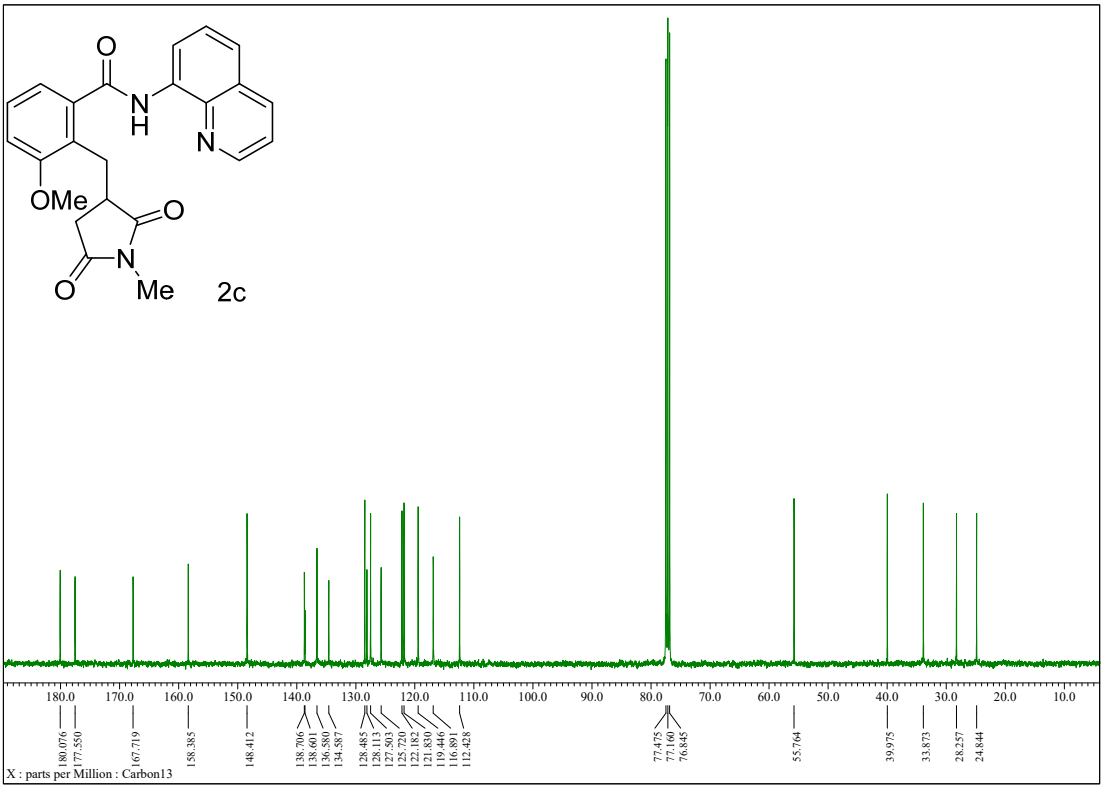
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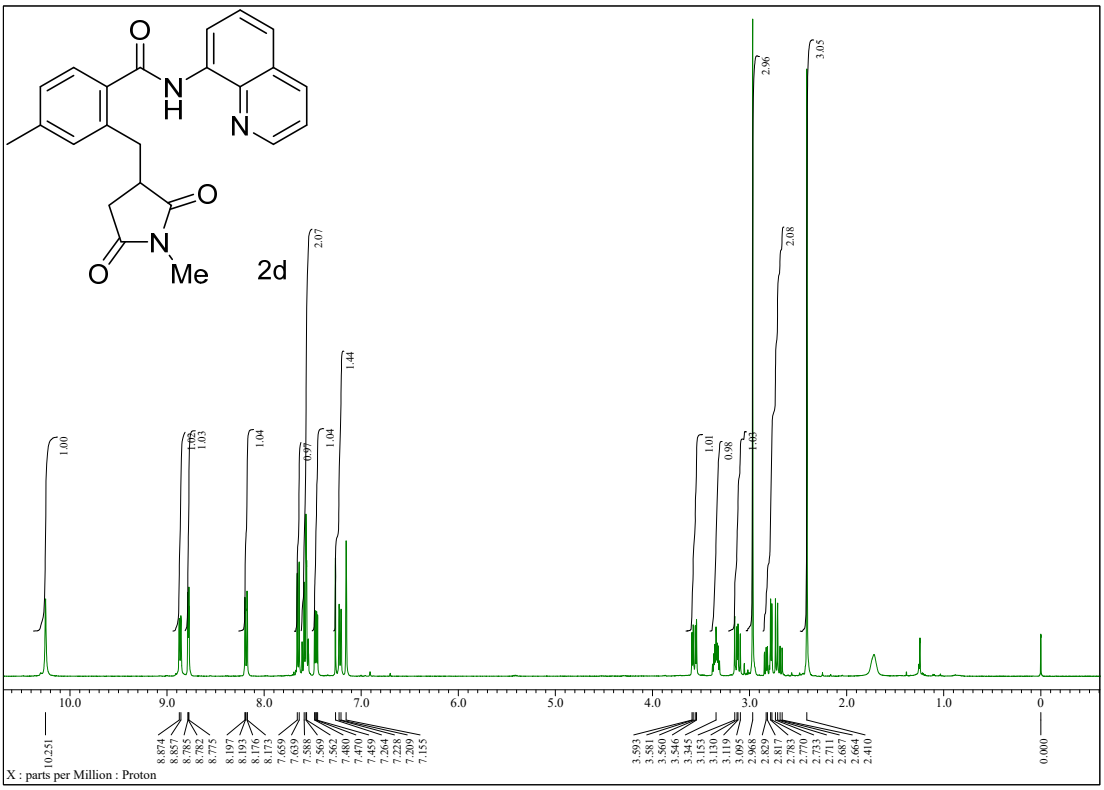
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0.97
1.04
1.01
0.98
1.03
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8.857
8.785
8.782
8.775
8.197
8.193
8.176
8.173
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7.598
7.569
7.562
7.480
7.470
7.459
7.264
7.228
7.209
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3.581
3.560
3.546
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3.110
3.119
3.095
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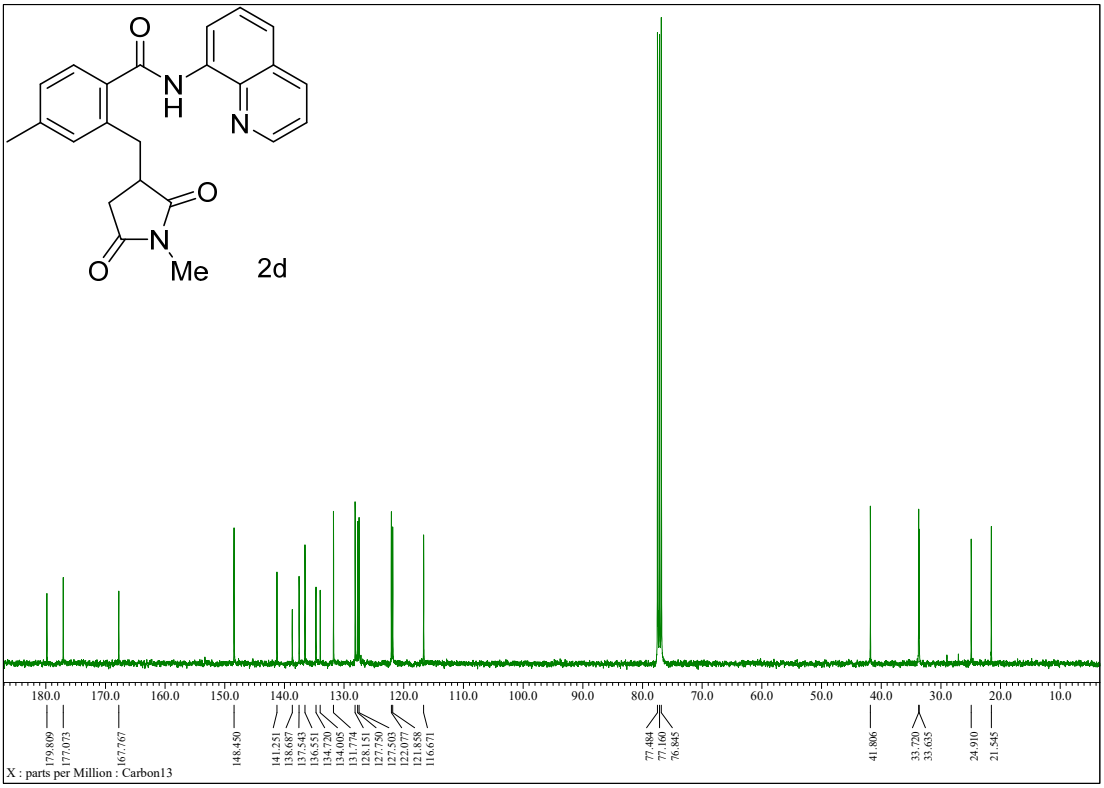
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134.005
131.774
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127.730
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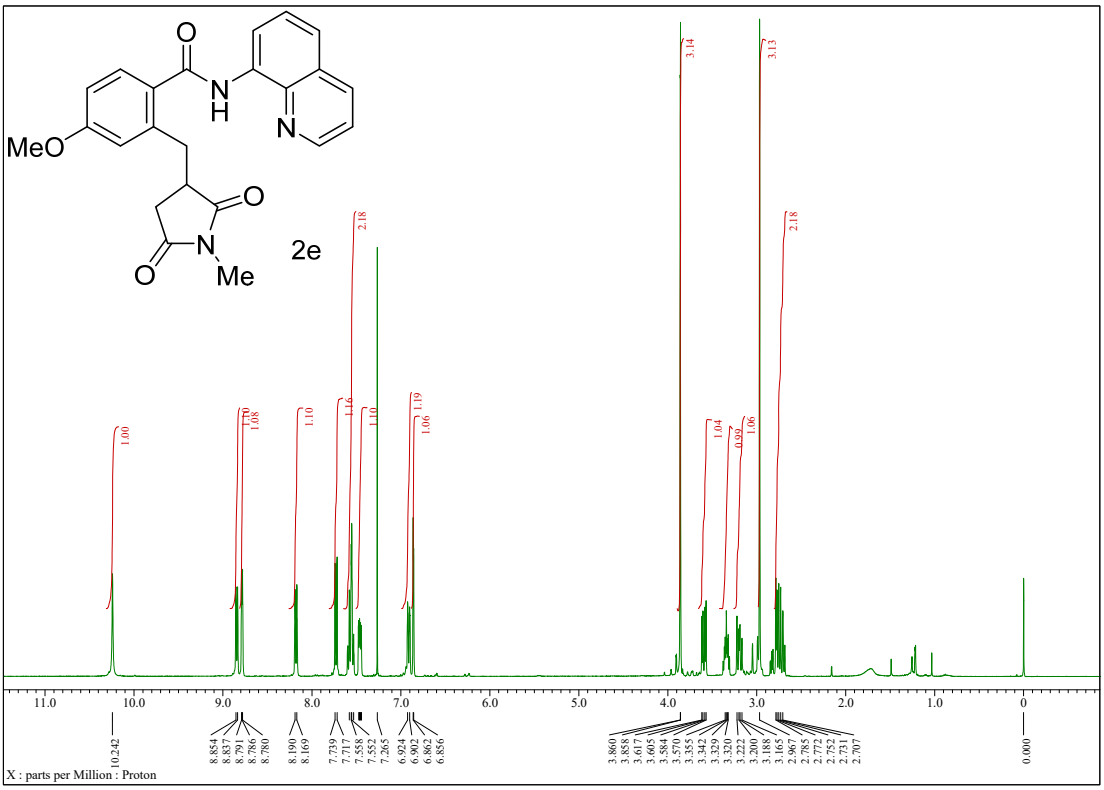
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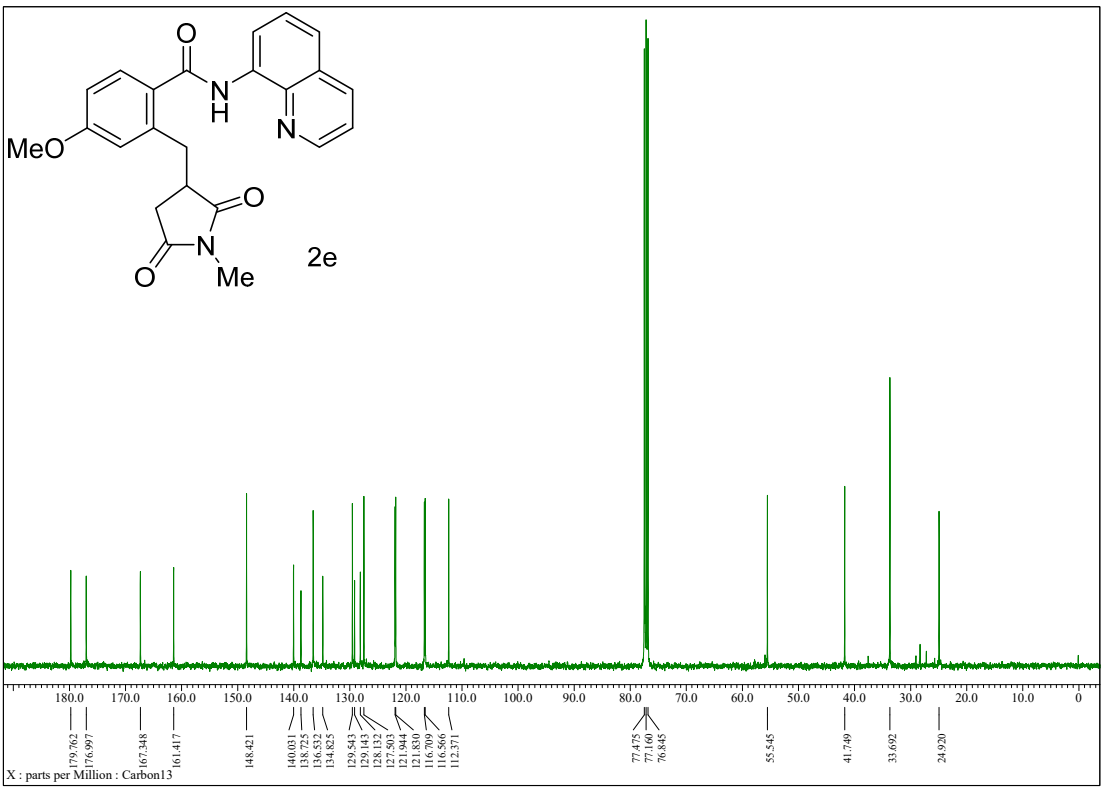
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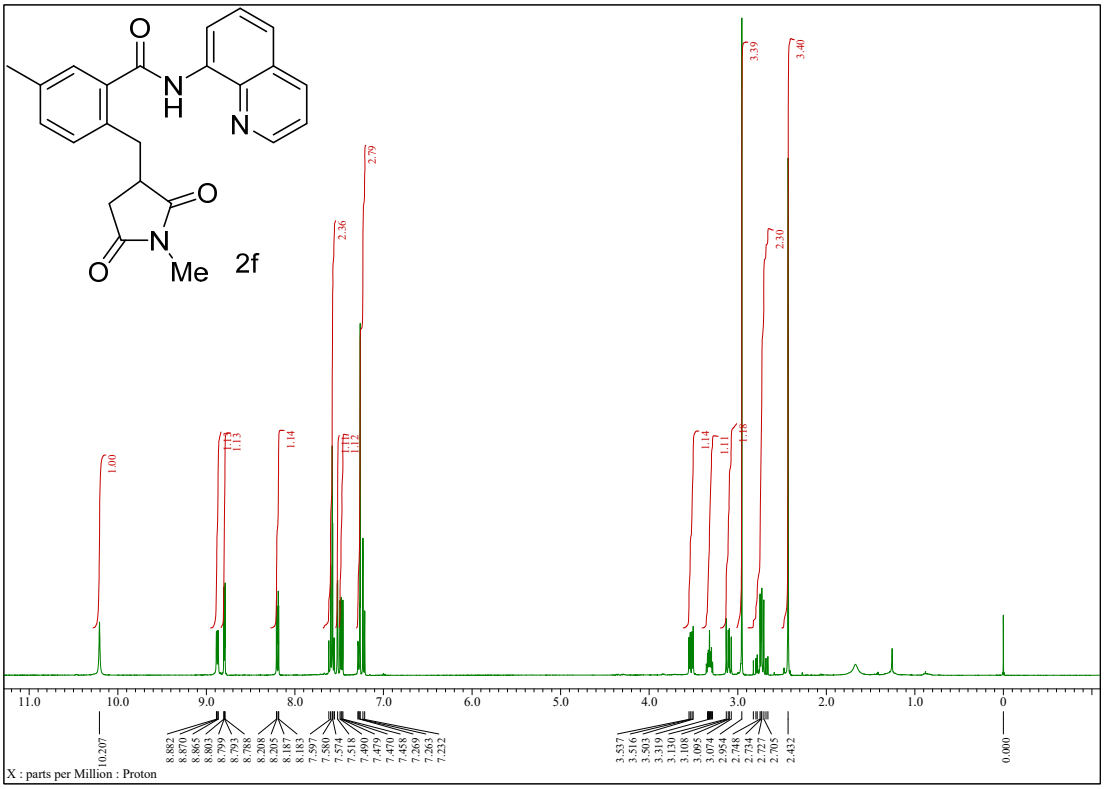
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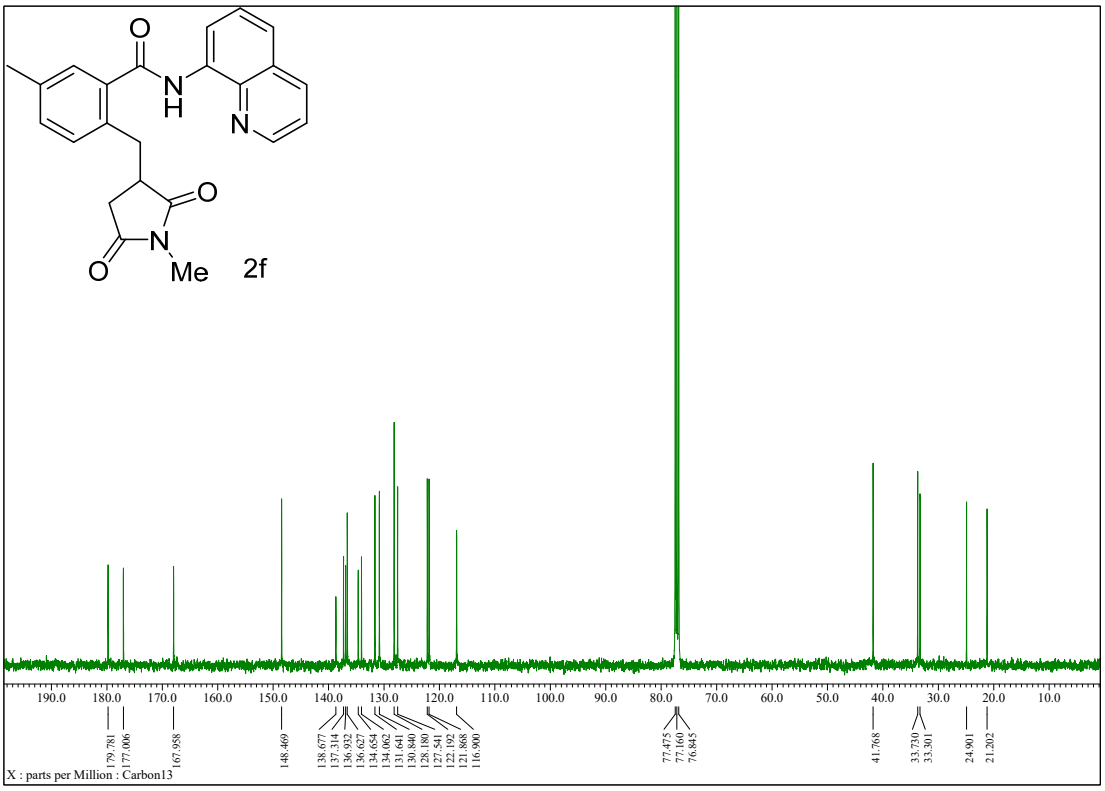
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10.0
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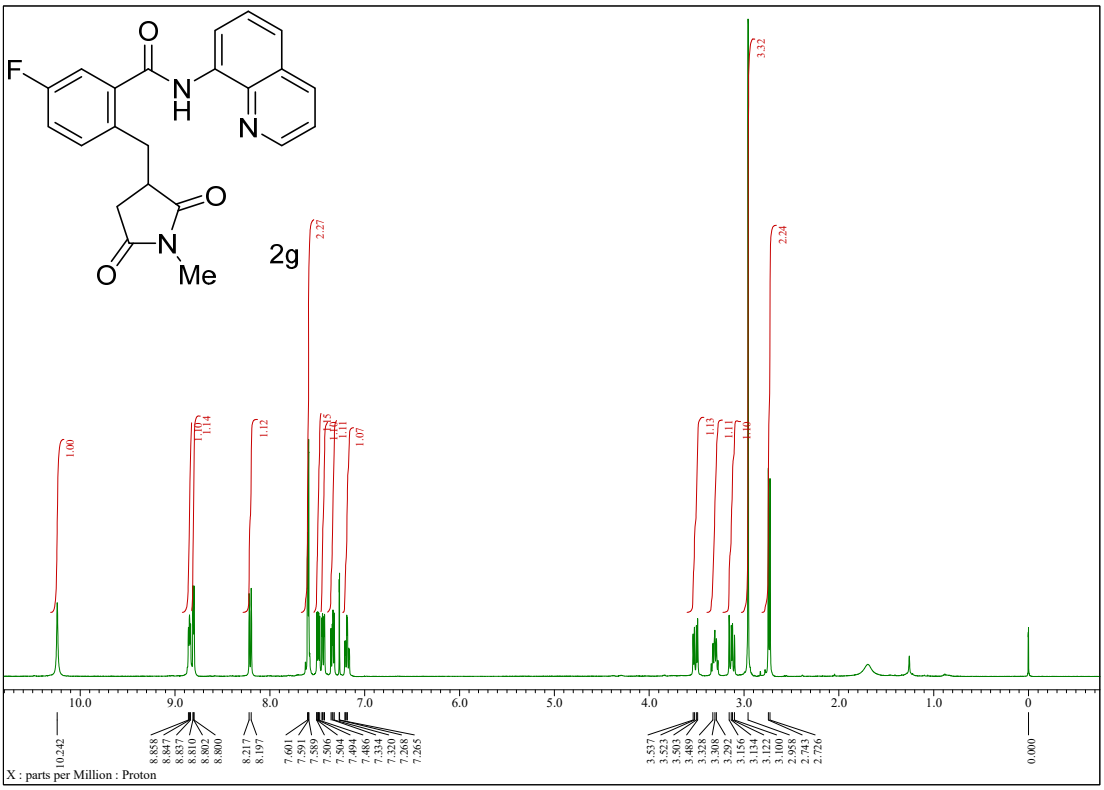
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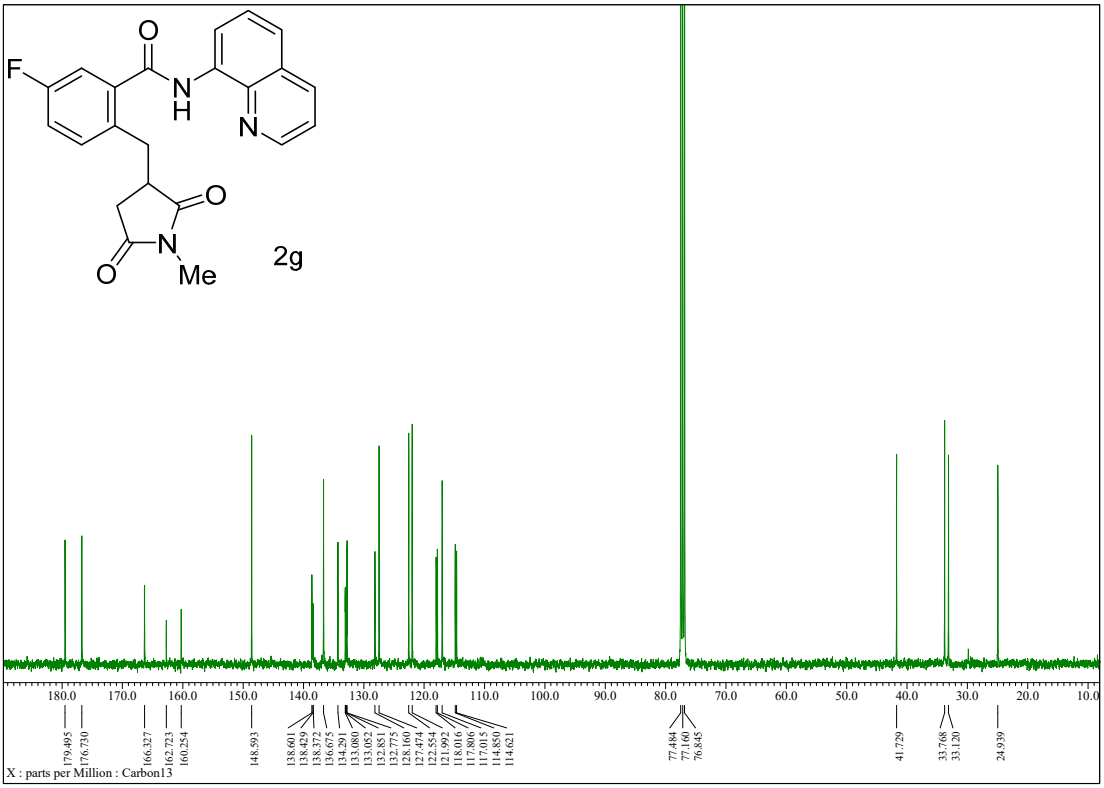
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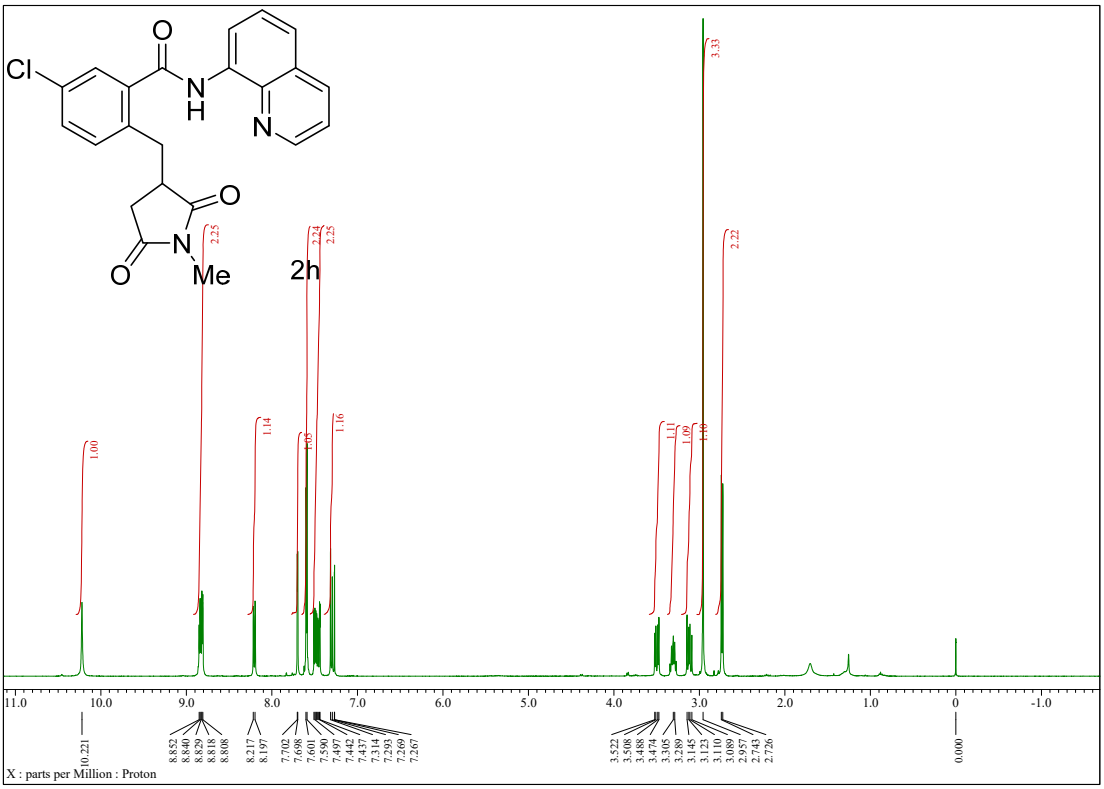
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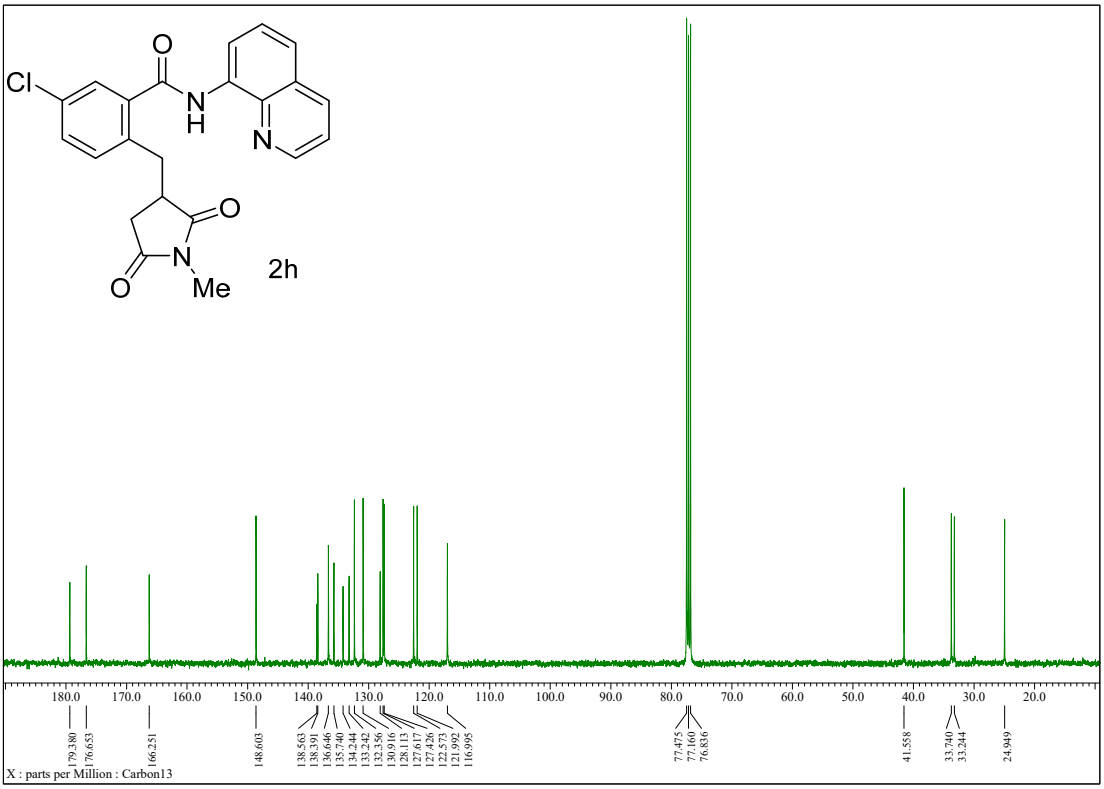
O
Me
2h
X : parts per Million : Proton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2h
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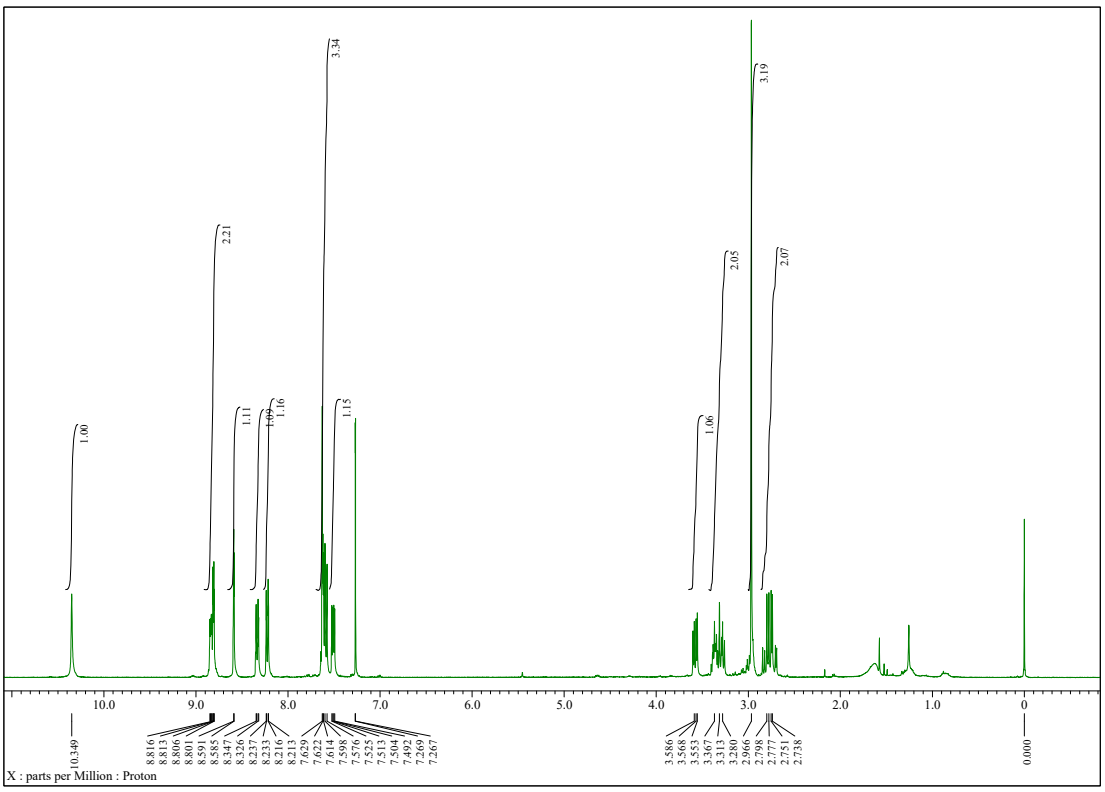
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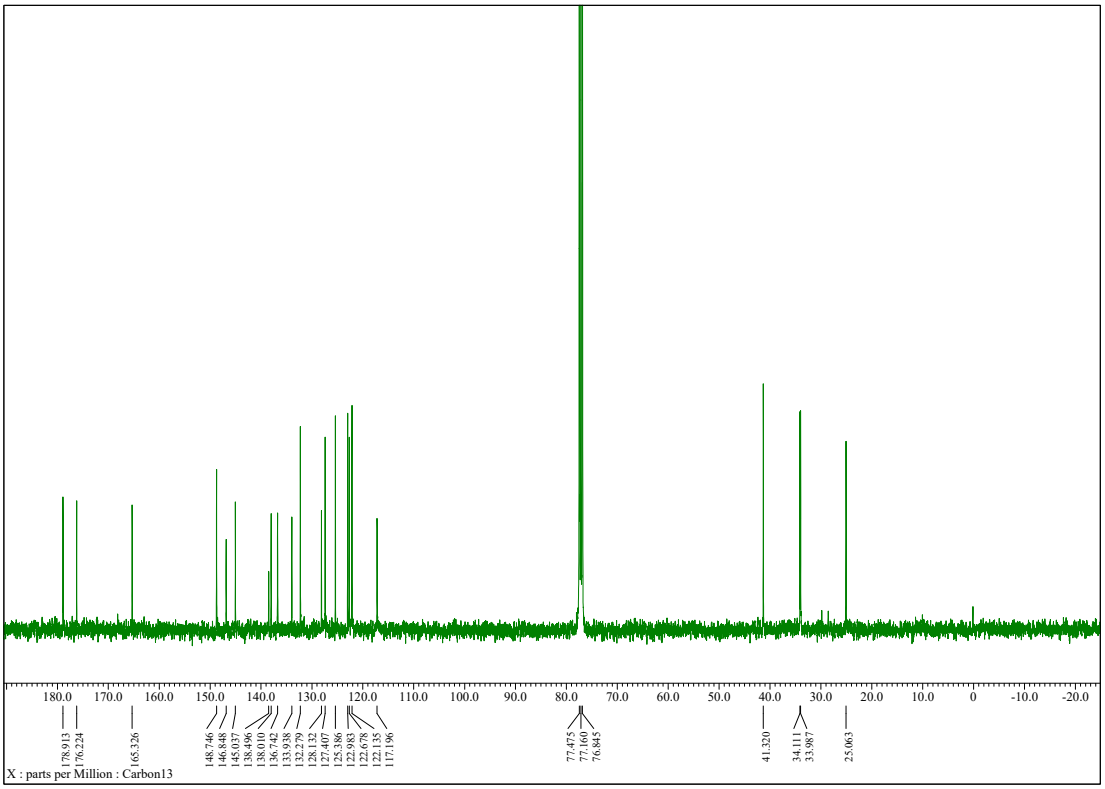
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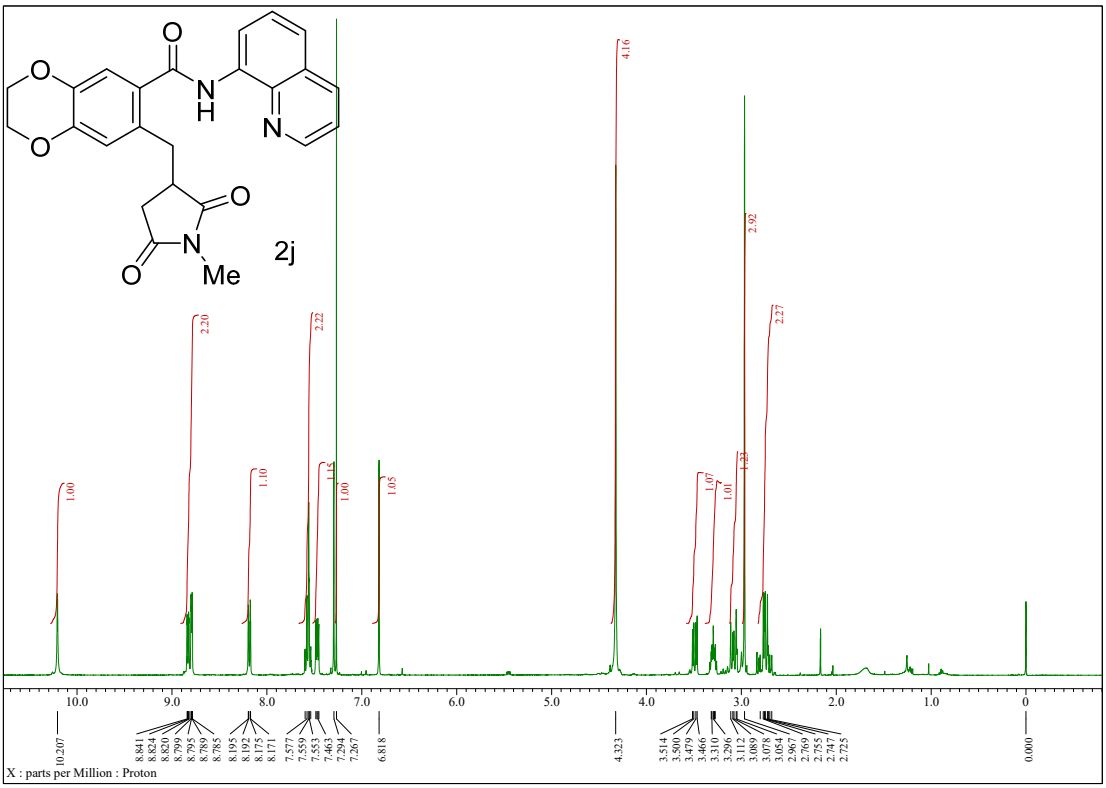
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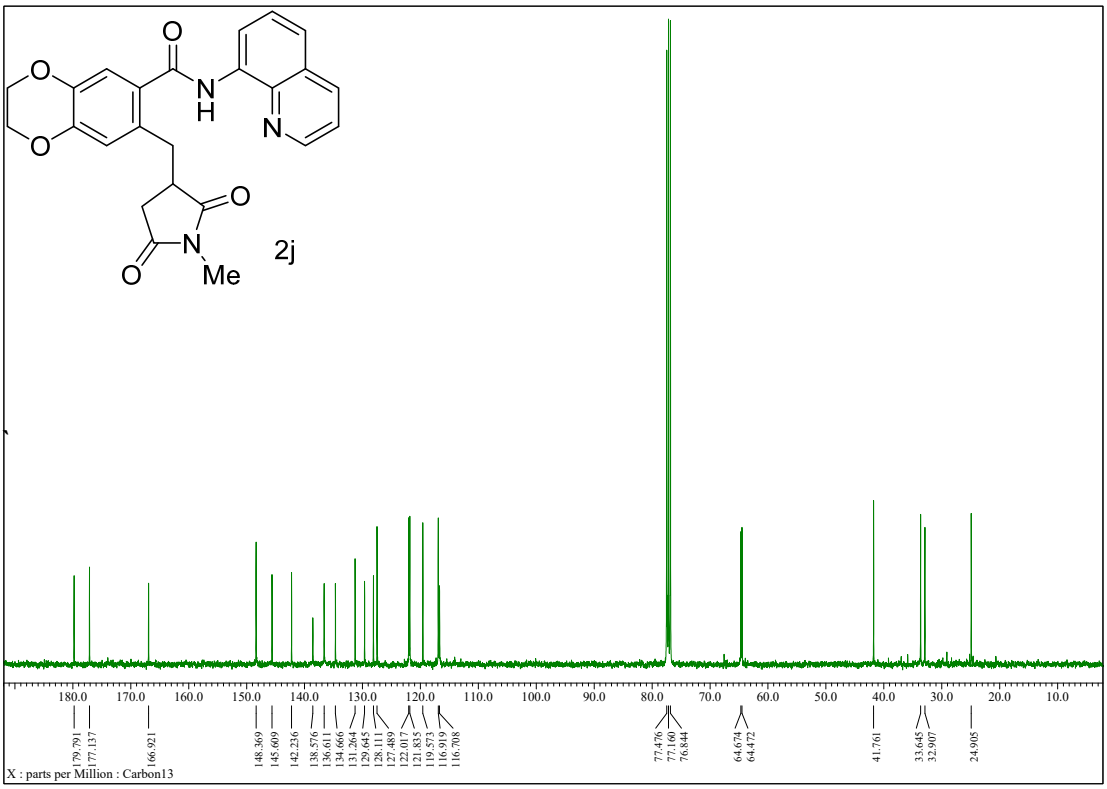
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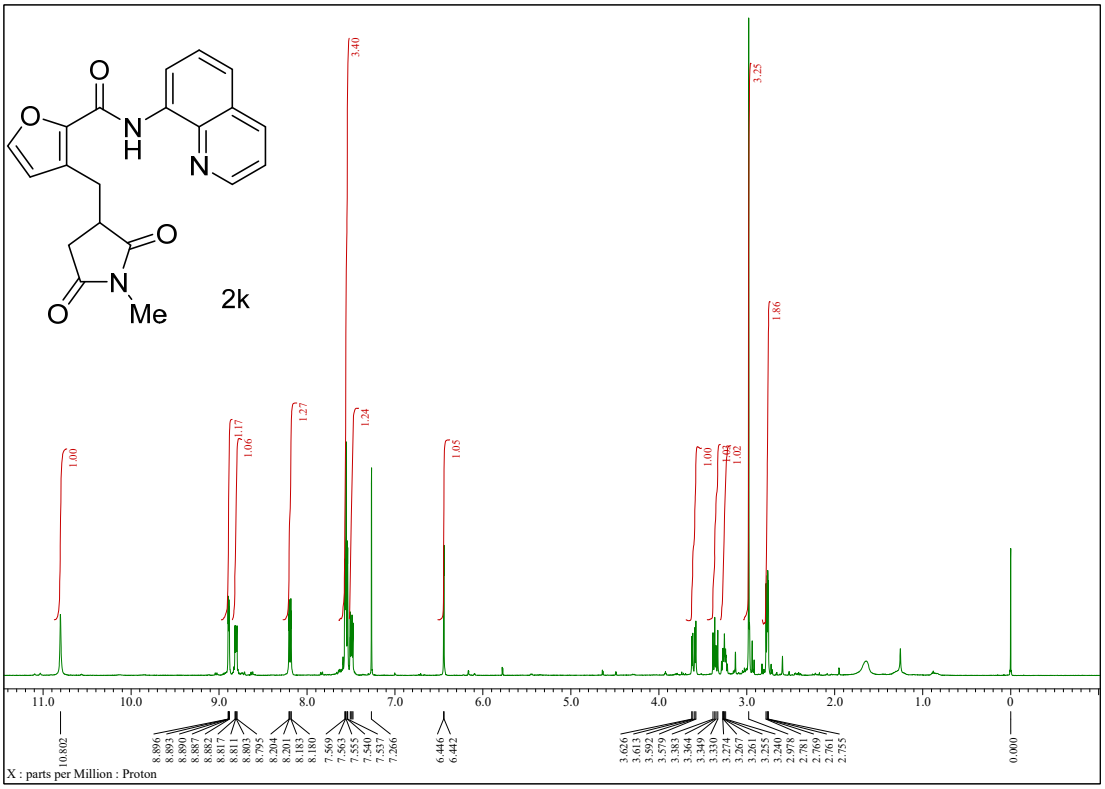
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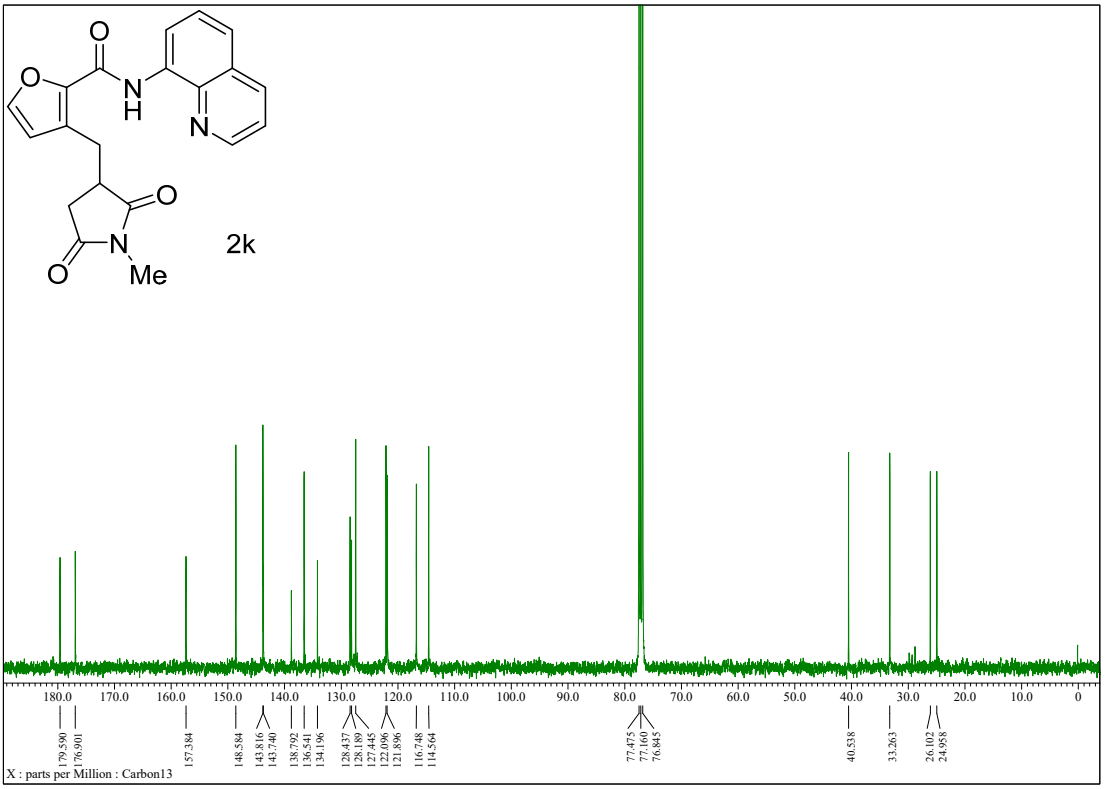
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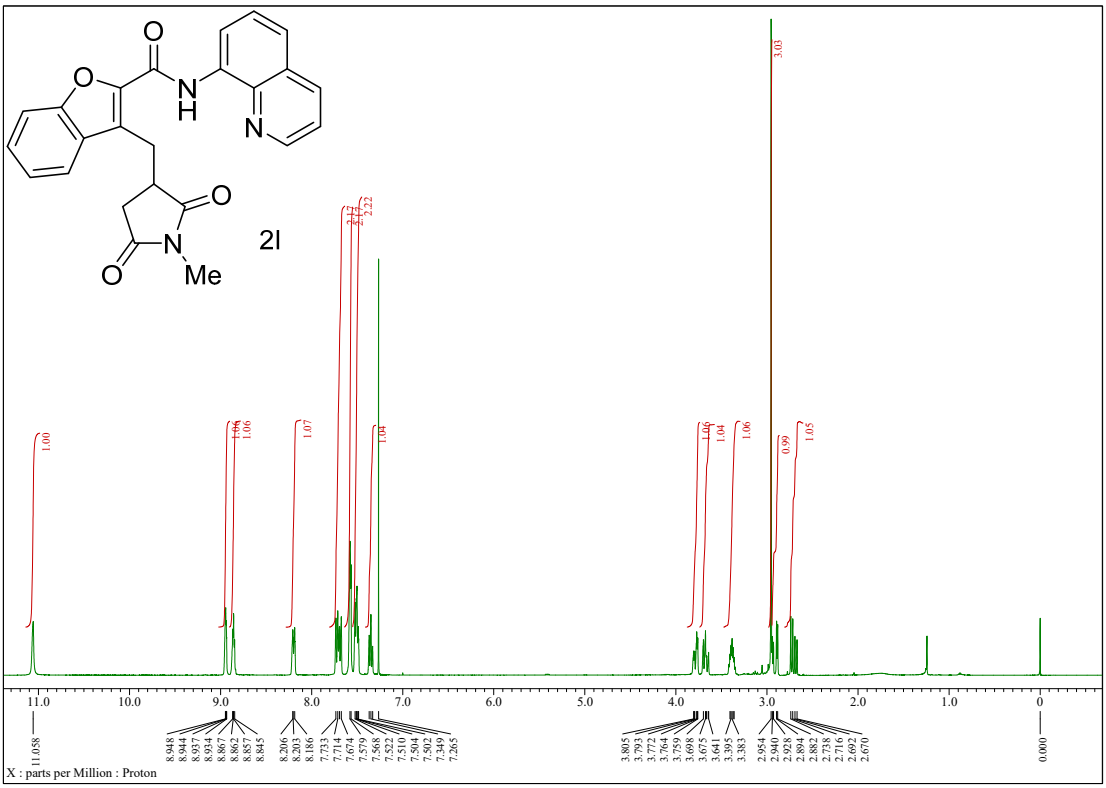
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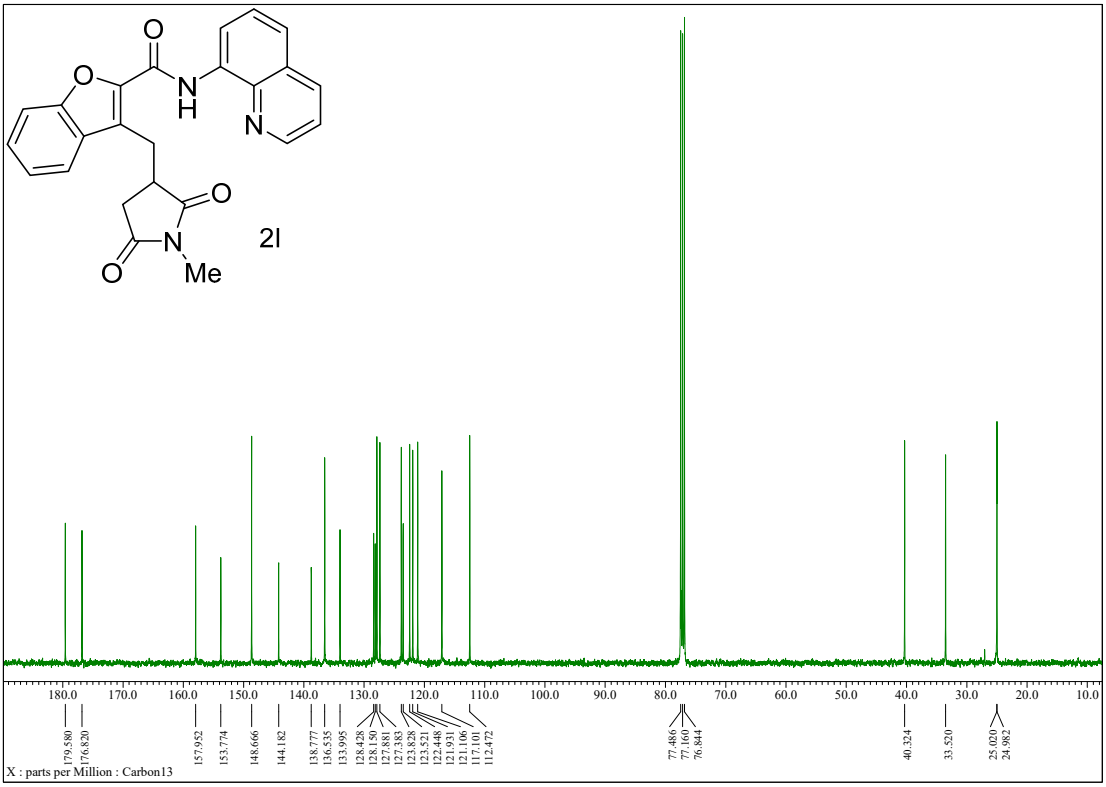
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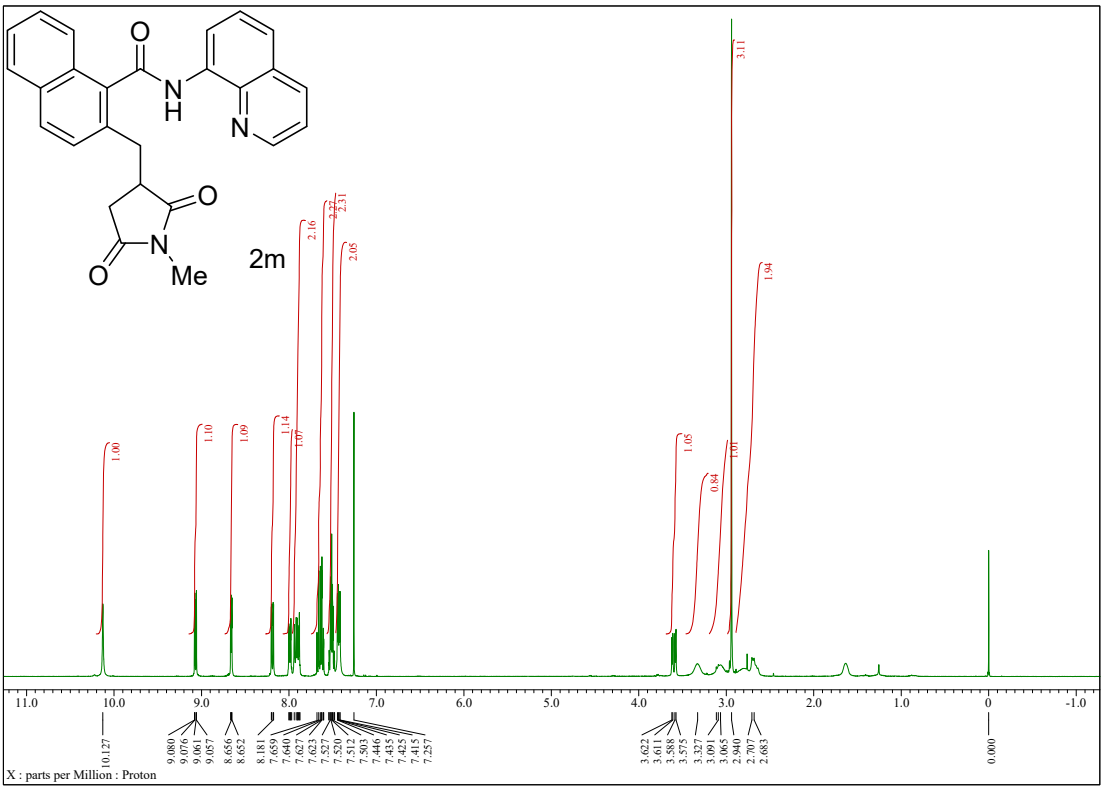
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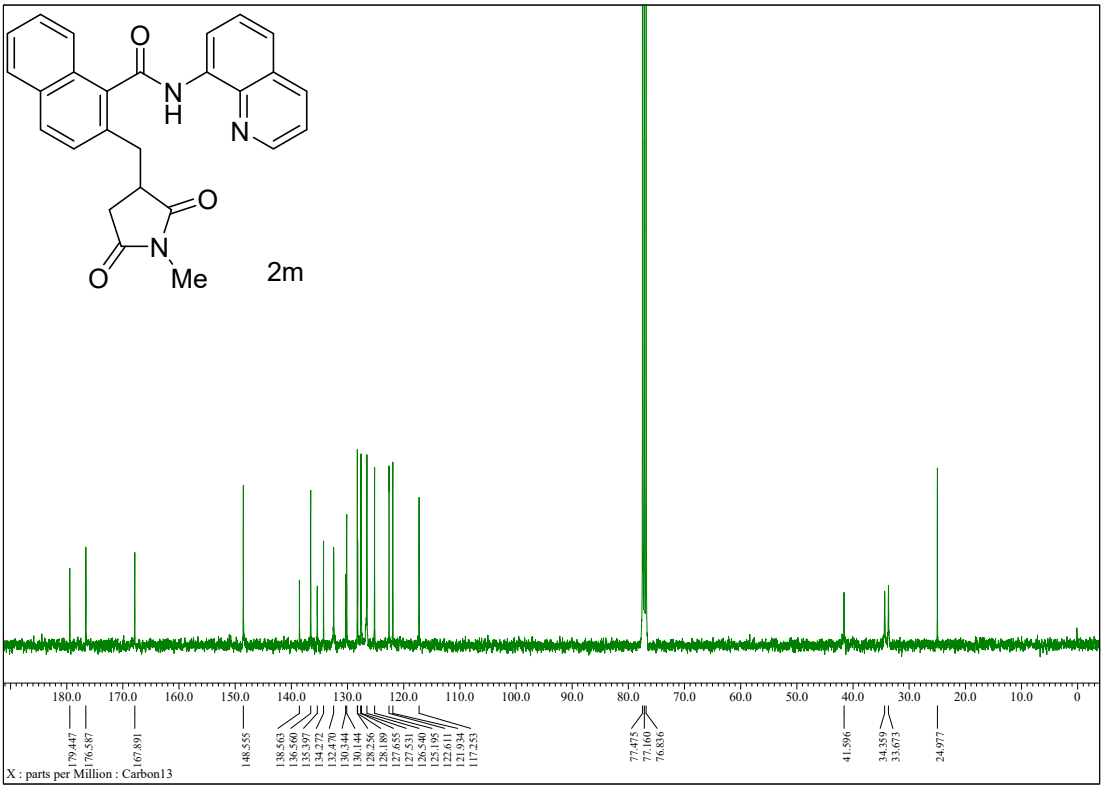
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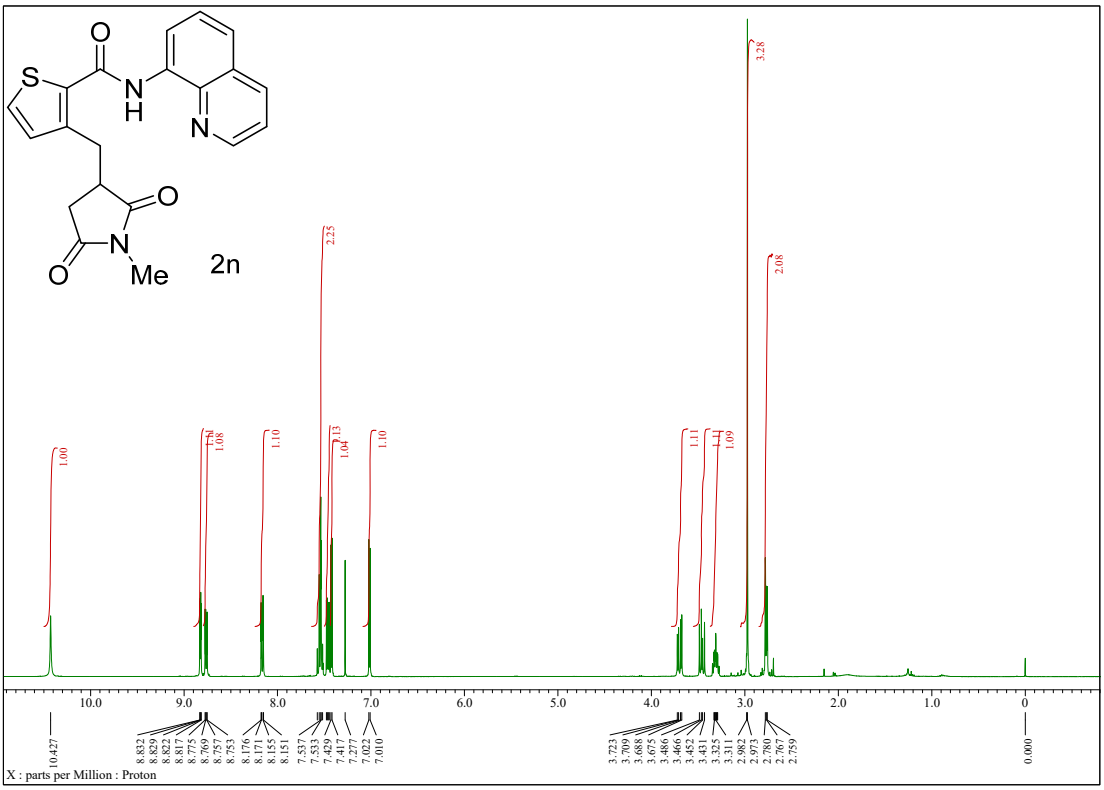
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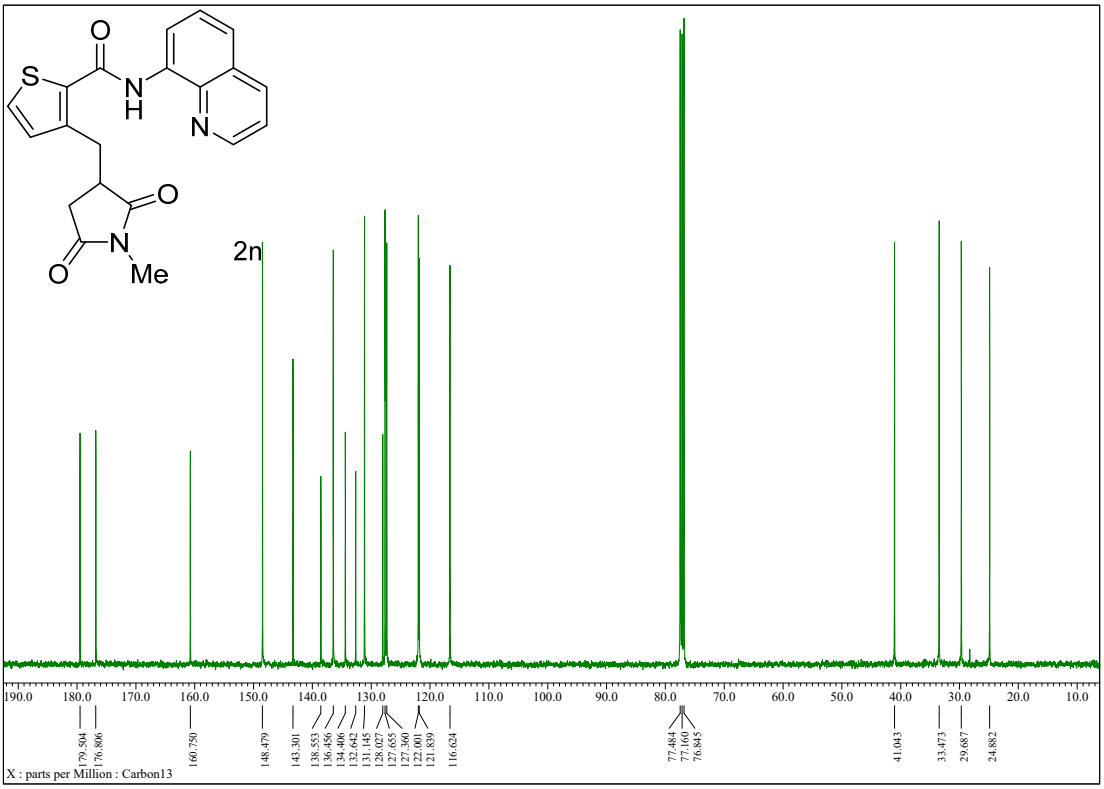
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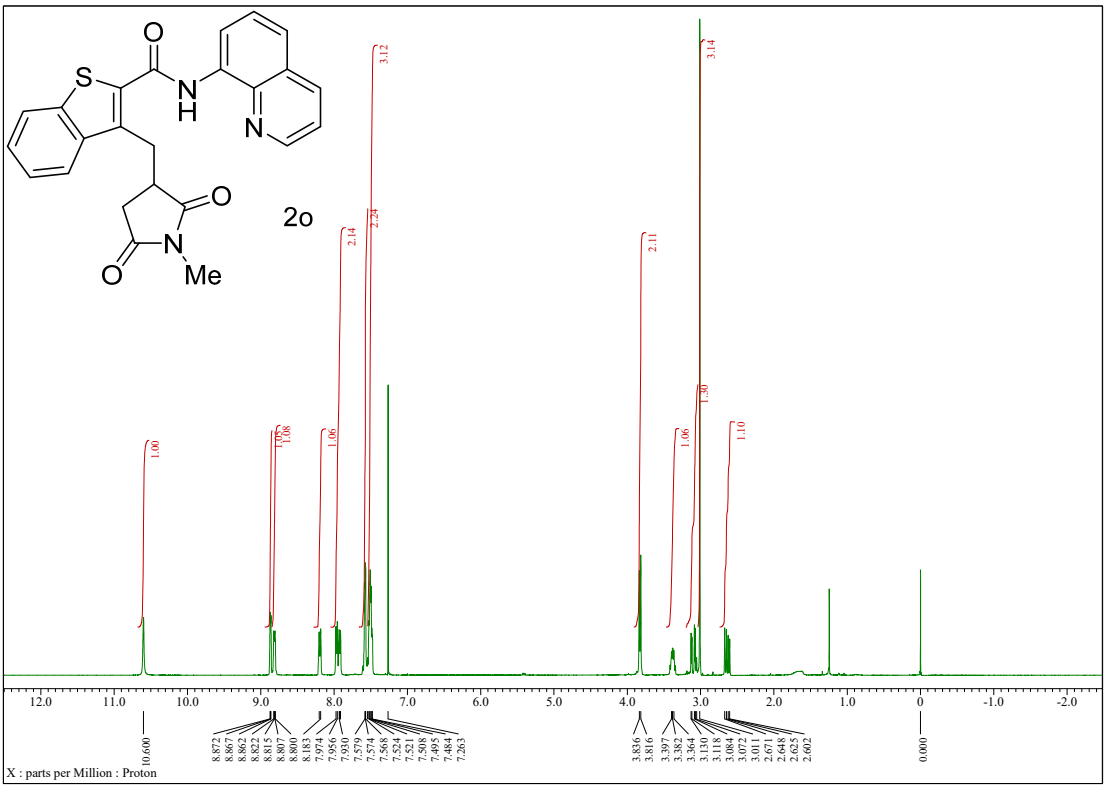
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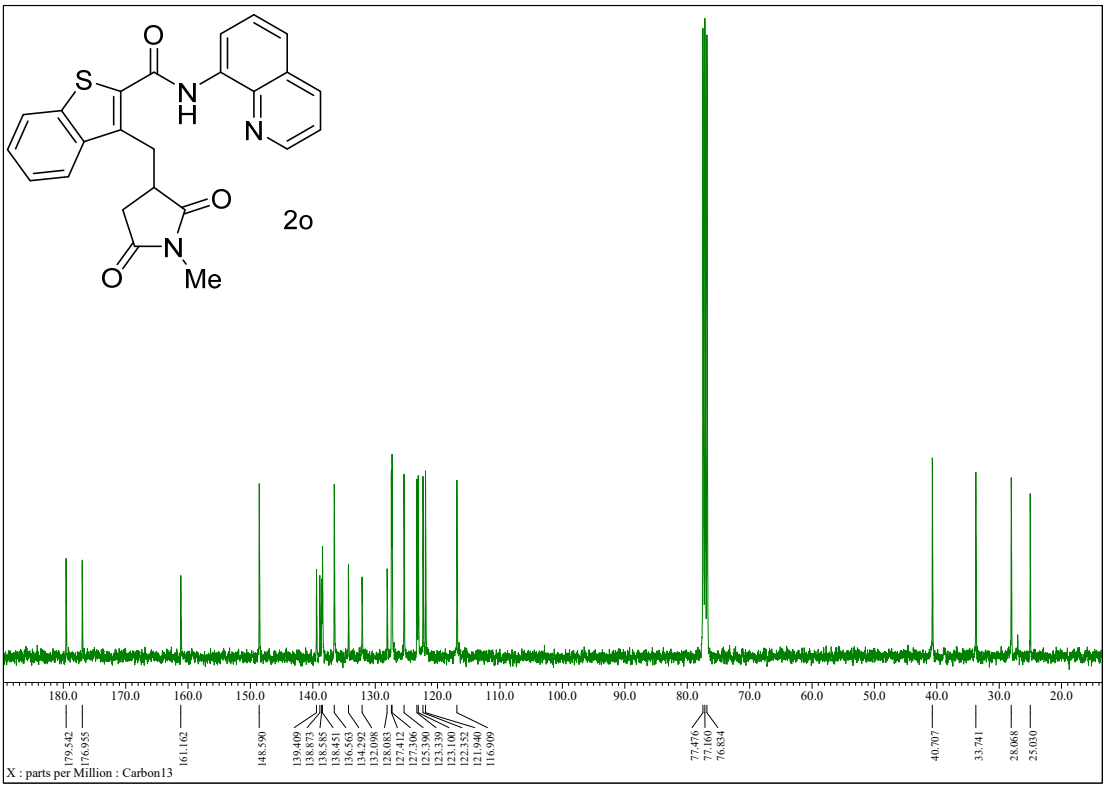
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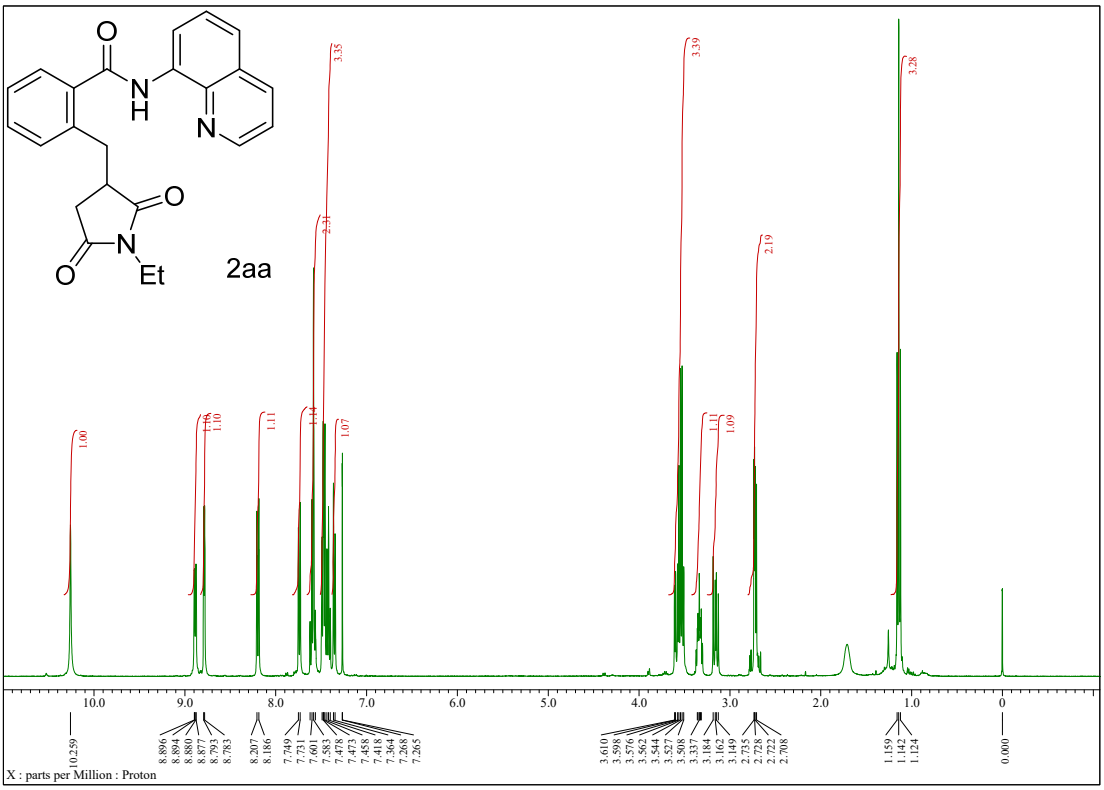
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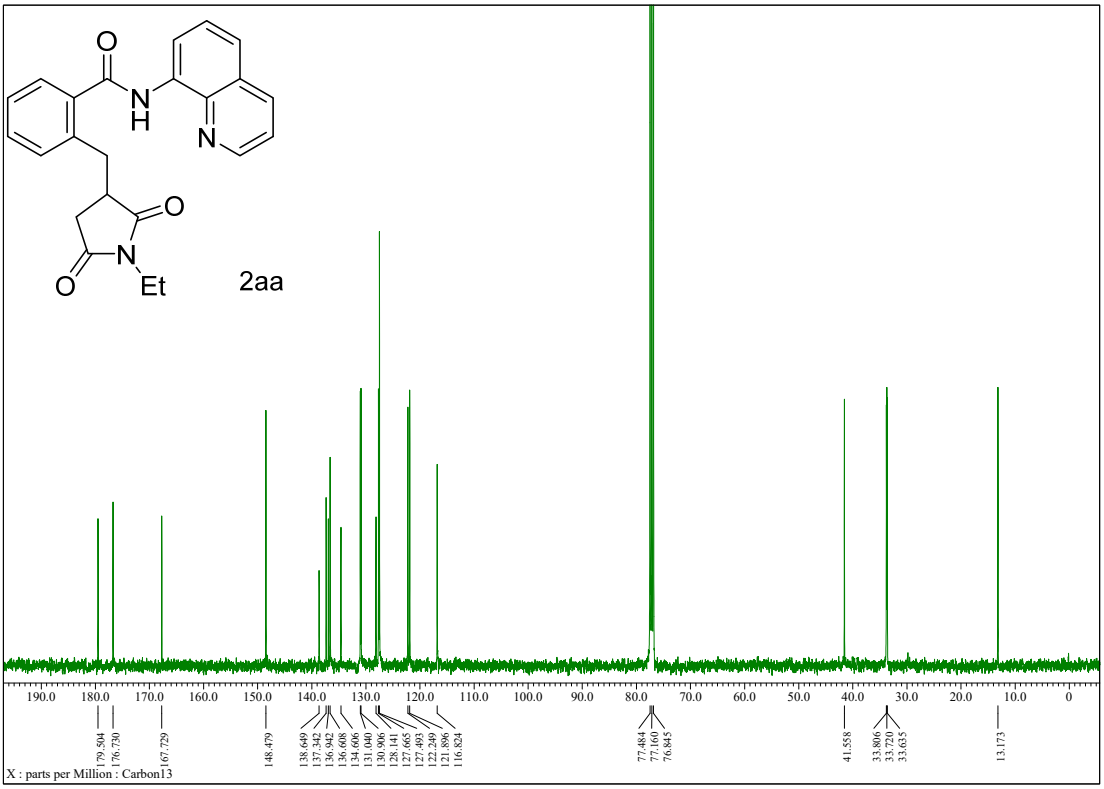
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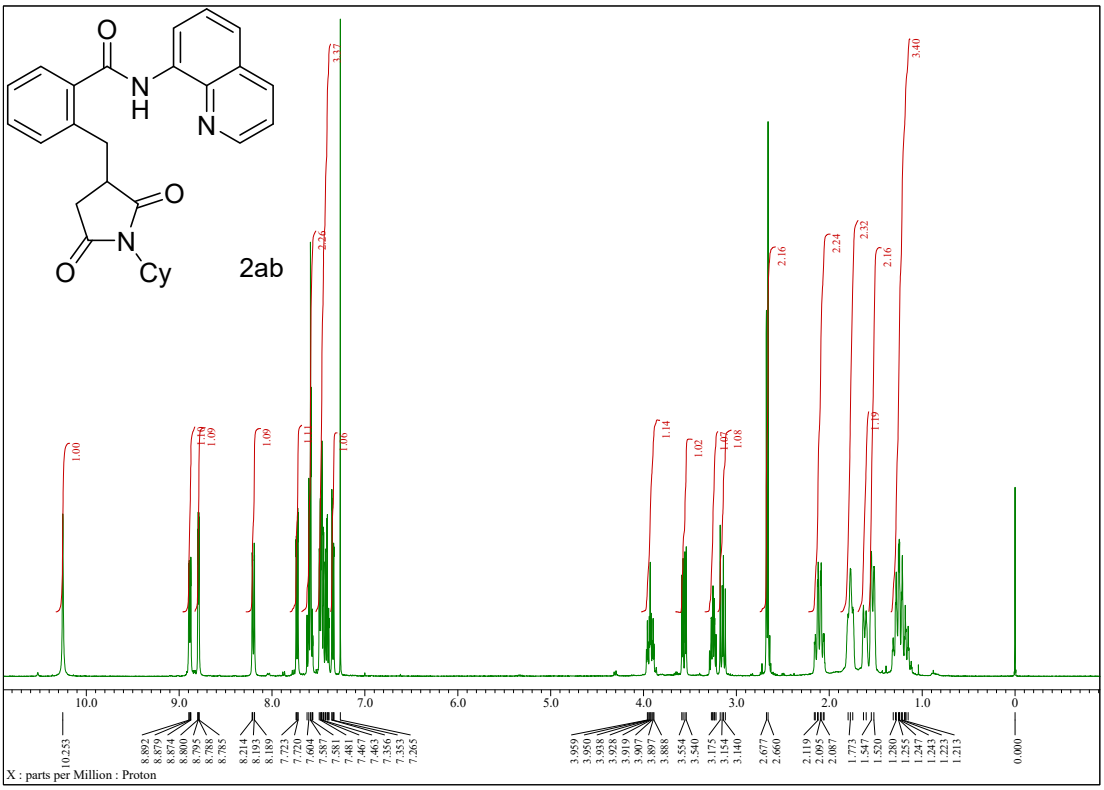
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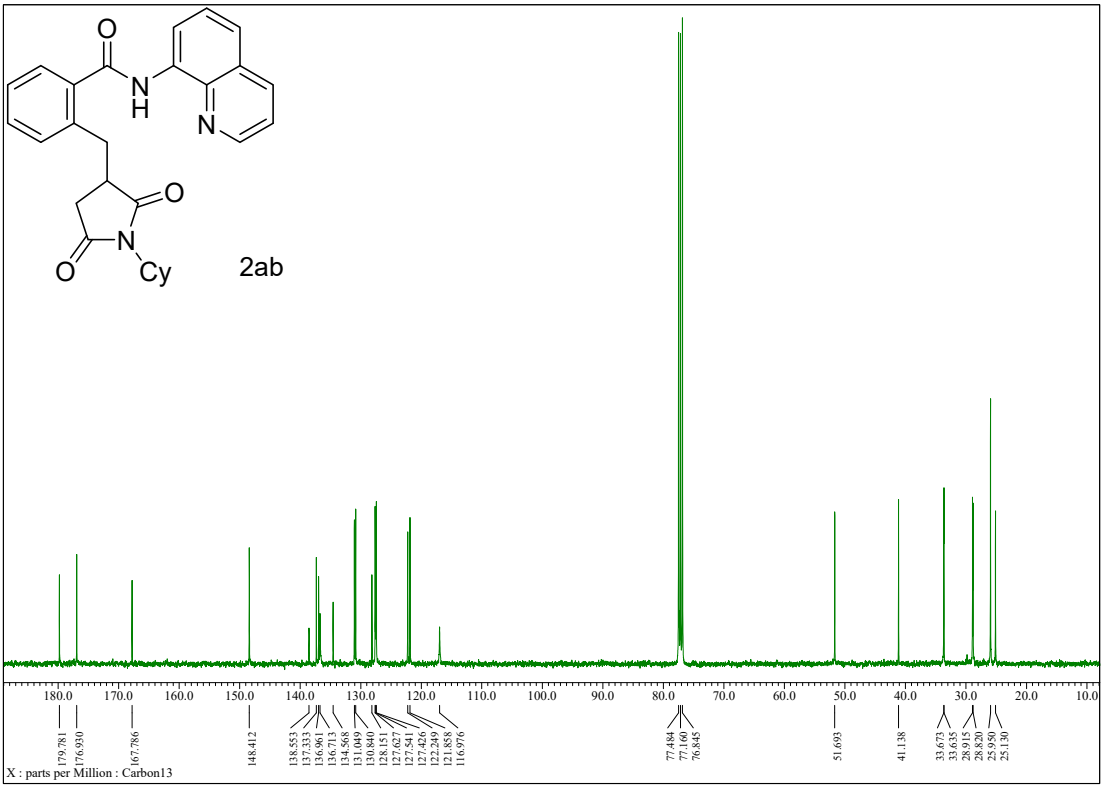
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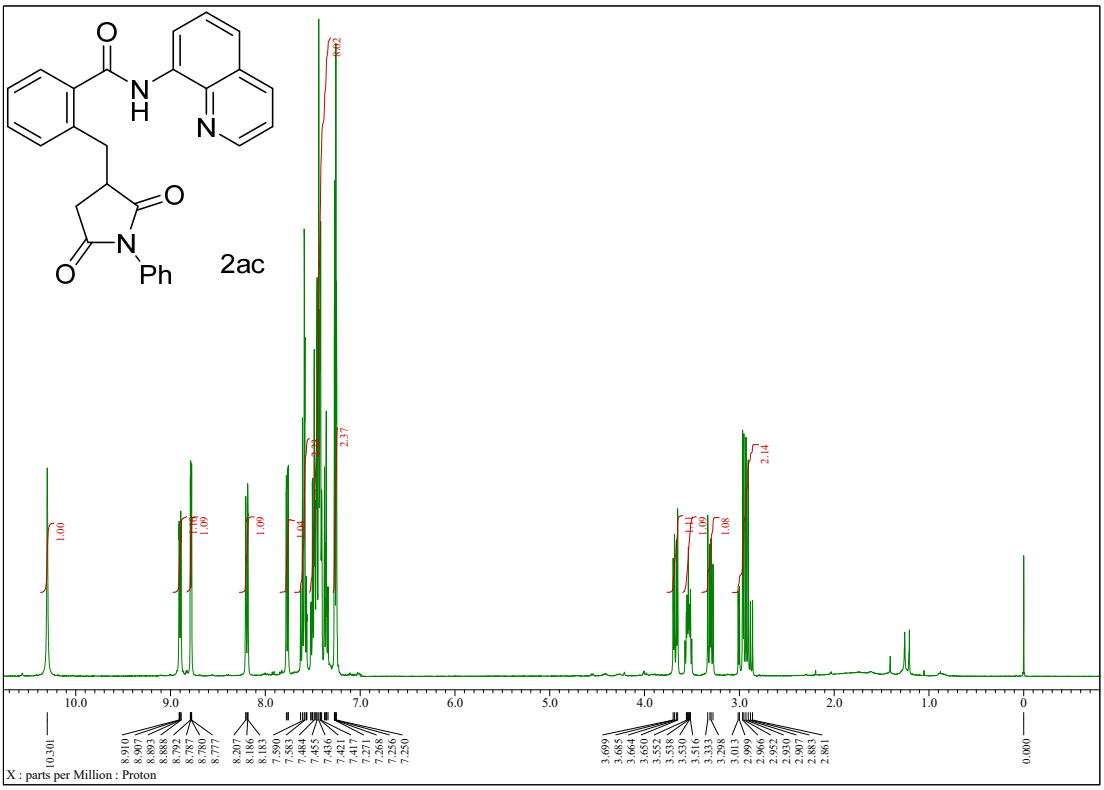
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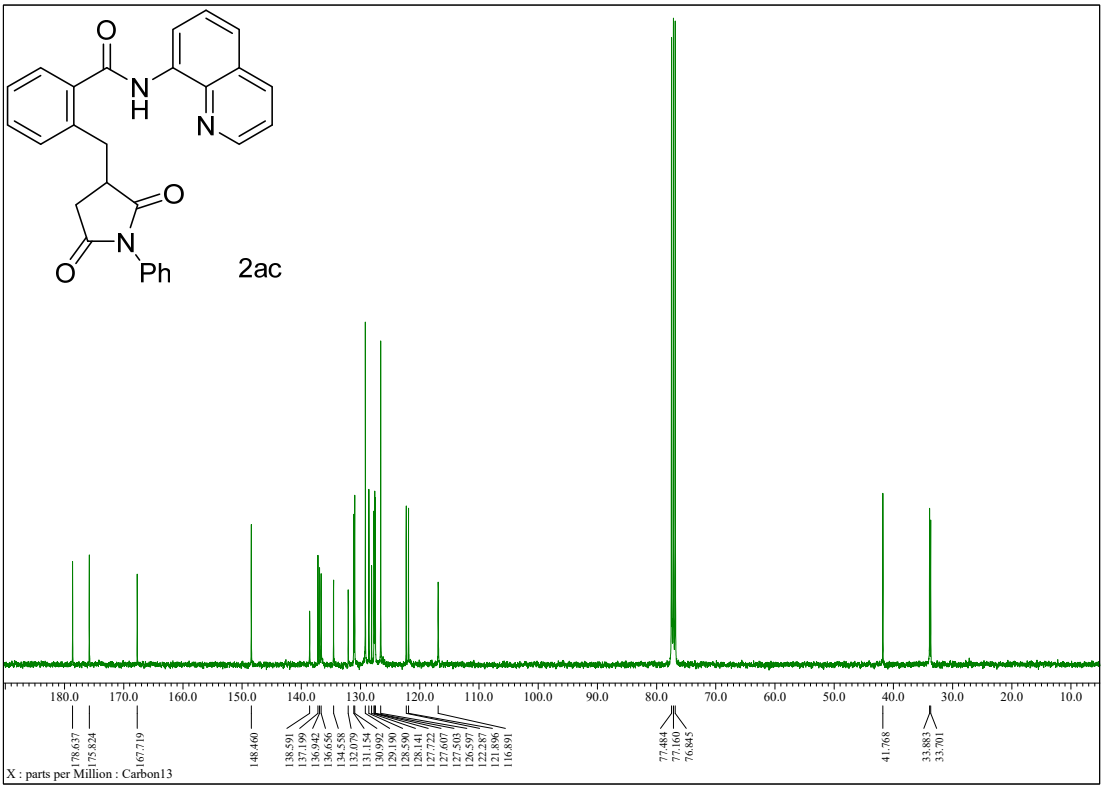
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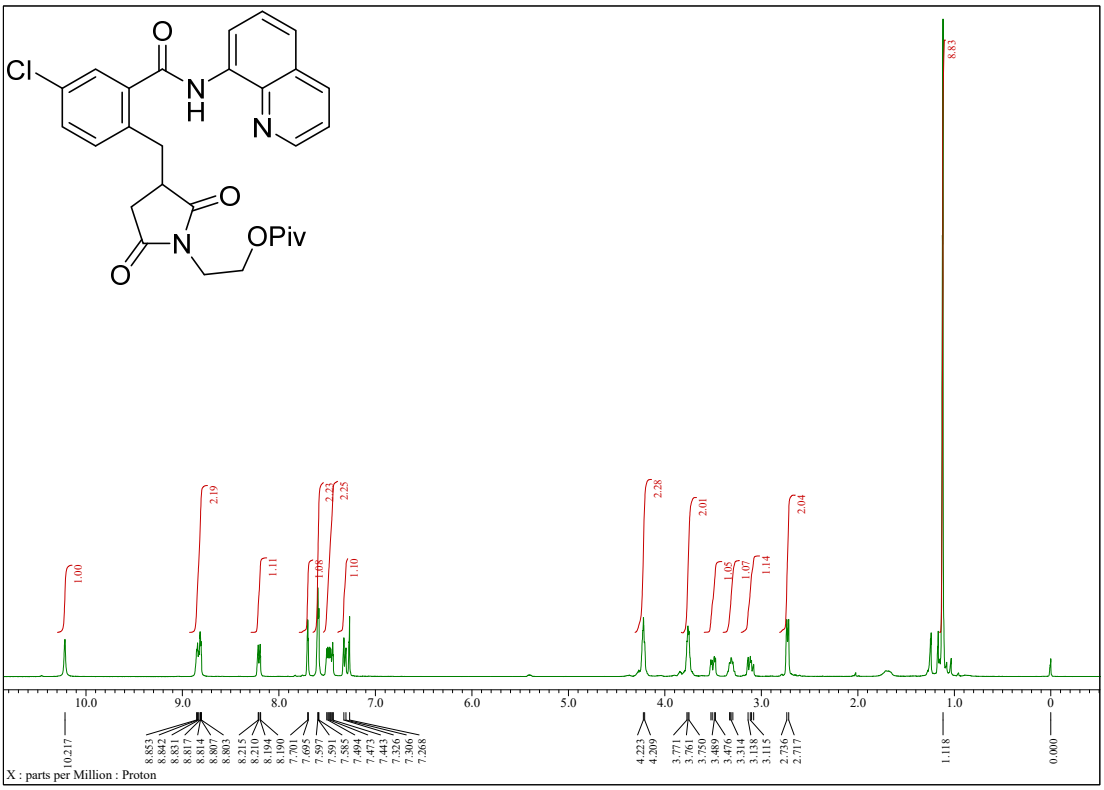
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H
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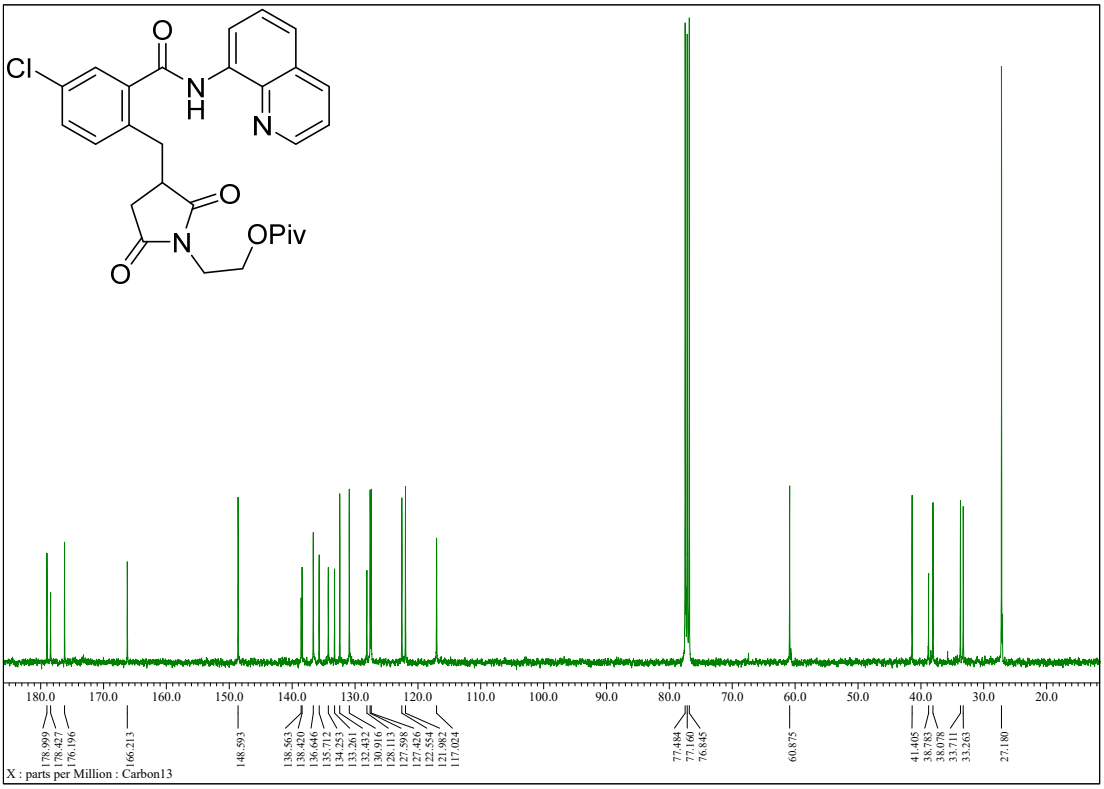
O
N
OPiv
O
X : parts per Million : Proton


Cl
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H
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O
N
OPiv
O
X : parts per Million : Carbon13

VIII. Theoretical Calculations.

Computational method.[1]

All calculations were performed with the Gaussian 09 program.[2] All geometry optimizations and normal coordinate analyses at stationary points were performed using B3LYP functional[3] with the LANL2DZ effective core potential for Pd[4] and the 6-31G(d) basis set for the others.[5] Each reported minimum has no imaginary frequency and each transition state structure has one imaginary frequency. Intrinsic reaction coordinate (IRC) analyses[6] from transition states to minima were used for confirming the reaction pathways. For single-point energy calculations, the M06L functional[7] was conducted using the quasi-relativistic Stuttgart-Dresden-Cologne (SDD) effective core potential and the corresponding basis set for Pd[8] and the 6-311+G(d,p) basis set for the others.[9] For both optimization and single-point energy calculation, the solvation effects of acetic acid (ε = 6.2528) were added using the integral equation formalism model (IEFPCM) calculation with radii and non-electrostatic terms for Truhlar and coworkers' solvation model based on density (SMD).[10] Energy values were shown by the used of Gibbs' free energies (T = 298.15 K and p = 1 atm).

Calculated energy profiles.

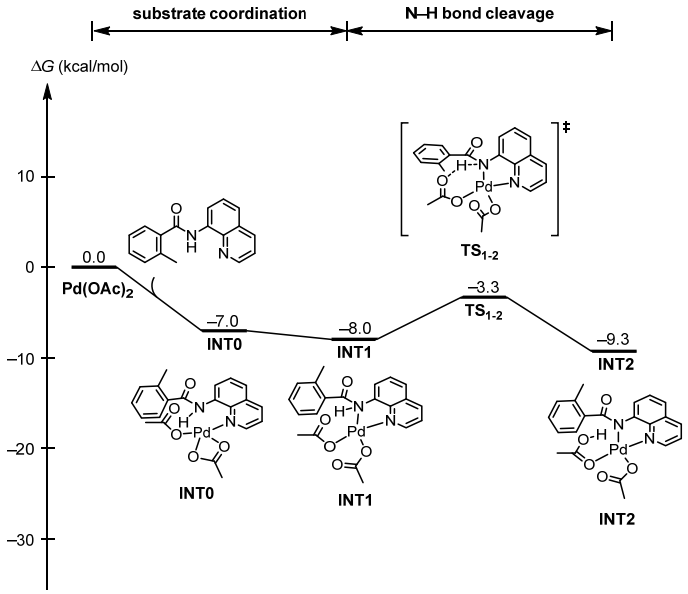


Figure S1. Gibbs energy profiles for the cleavage of N–H bond leading to the formation of **INT2**.

We initially examined a scenario in which one of the acetate ligands on **Pd(OAc)$_2$** is replaced by the amide substrate. This process occurs as the result of the coordination of a quinolone nitrogen to **Pd(OAc)$_2$** to form **INT0**, followed by an interaction between a N–H bond and an acetate ligand to form **INT1** with a total energy release of 8.0 kcal/mol. The concerted deprotonation of the amide nitrogen by the acetate ligand then affords the more stable intermediate **INT2** by 1.3 kcal/mol, through **TS1-2** with an energy barrier of 4.7 kcal/mol.

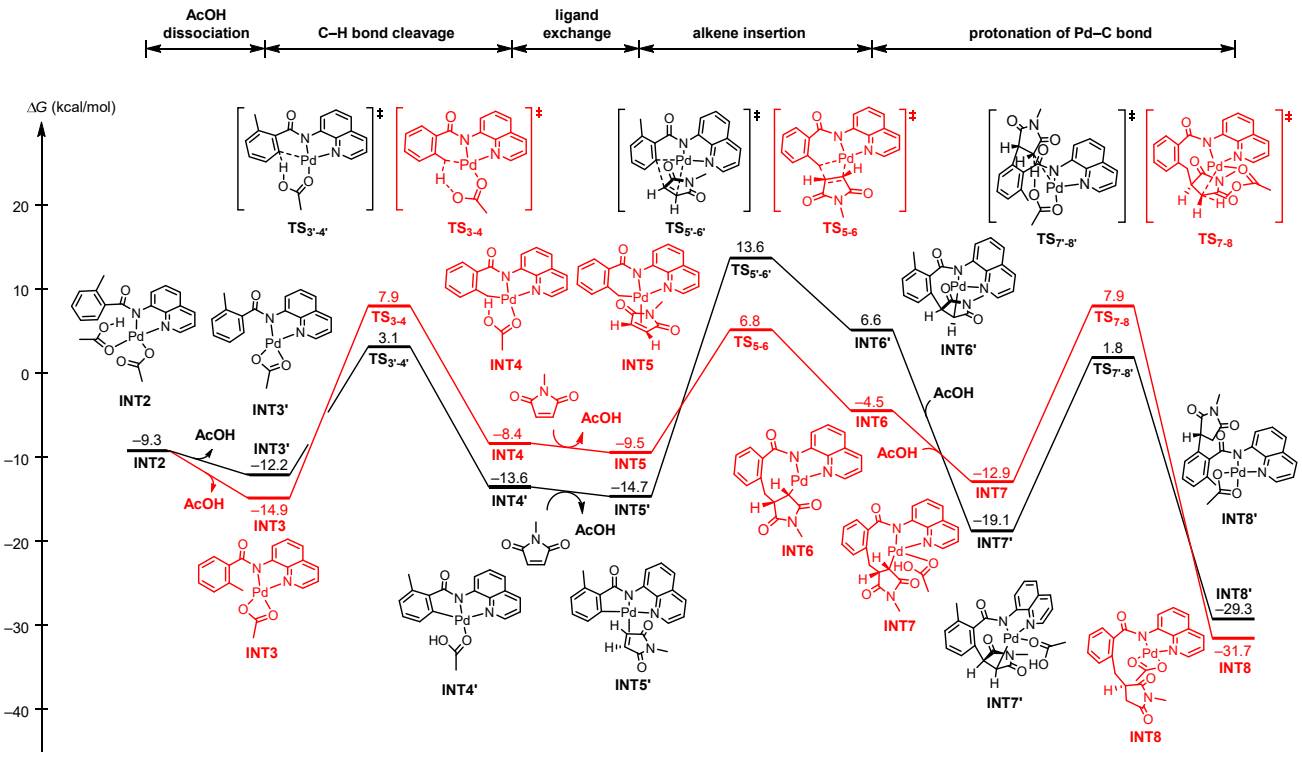


Figure S2. Comparison of Gibbs energy profiles for the pathways involving the cleavage of a C(sp^3)–H bond (red line) and a C(sp^2)–H bond (black line), alkene insertion and protonation of Pd–C bond, leading to **INT8** and **INT8'**, respectively. Values are relative to the separated catalyst and reagents.

The release of the coordinating AcOH from **INT2** gives **INT3** or **INT3'** with a loss of energy of 2.9 or 5.6 kcal/mol, respectively. The generation of a five-membered palladacycle **INT4'** from **INT3'** through $\mathbf{TS_{3'\text{-}4'}}$ requires only 15.3 kcal/mol, which is lower than the energy barrier for generating the six-membered palladacycle **INT4** from **INT3** (22.8 kcal/mol). In addition, the resulting five-membered palladacycle **INT4'** is more stable than **INT4**. The results of the DFT calculations are consistent with the deuterium labeling results. Thus, H/D exchange at the ortho C-H bond is very fast and the ortho C-D bond is completely converted into a C-H bond, even within 1 h. In sharp contrast, the insertion of the maleimide group into the Pd–C(sp^2) bond of the five-membered palladacycle **INT5'** through $\mathbf{TS_{5'\text{-}6'}}$ requires 28.3 kcal/mol, but the insertion of the maleimide into the Pd–C(sp^3) bond of the six-membered palladacycle INT5, leading to the generation of the eight-membered palladacycle **INT6** through $\mathbf{TS_{5\text{-}6}}$ requires only 16.3 kcal/mol. These results indicate that, while both five-membered and six-membered palladacycles can be generated, the formation of the five-membered palladacycle is the kinetically favorable step, but the insertion of the maleimide into the six-membered palladacycyle is energetically favored. The subsequent protonation of the Pd–C bond results in the formation of the more stable intermediates **INT8** and **INT8'**, with relatively lower energy barriers for $\mathbf{TS_{7\text{-}8}}$ and $\mathbf{TS_{7'\text{-}8'}}$.

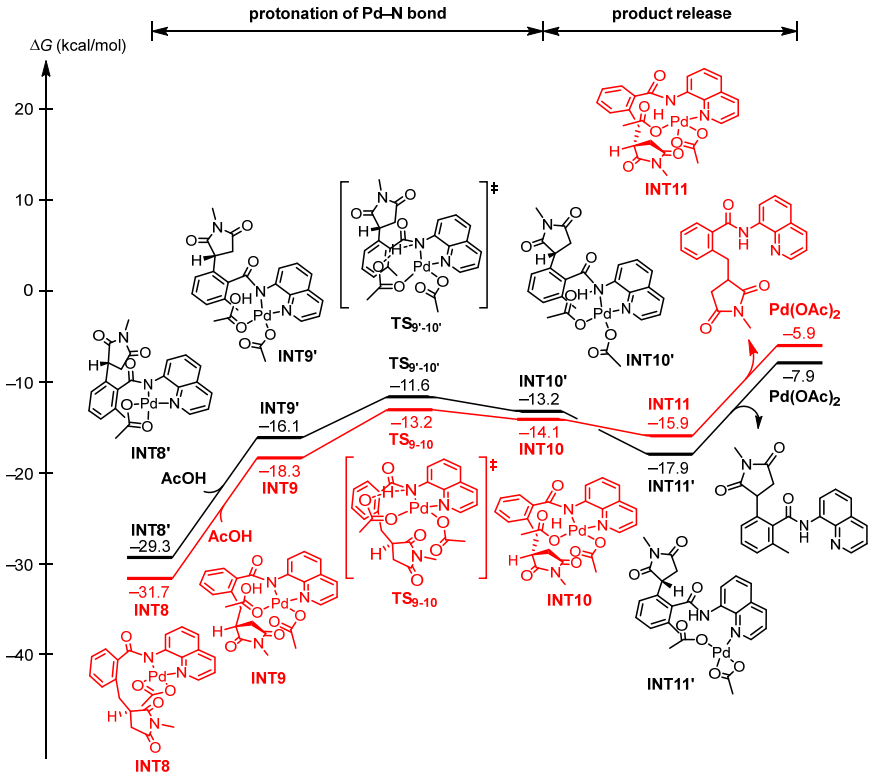


Figure S3. Comparison of Gibbs energy profiles for the pathways involving the protonation of Pd–N bond of **INT8** (red line, via **INT9**) and **INT8'** (black line, via **INT9'**), followed by the regeneration of $Pd(OAc)_2$. Values are relative to the separated catalyst and reagents.

Although the ligation of AcOH to **INT8** is thermodynamically uphill (13.4 kcal/mol), the energy barrier for the concerted protonation of the Pd–N bond via $\mathbf{TS_{9\text{-}10}}$ is relatively low (4.5 kcal/mol), leading to the formation of **INT10**. After the release of the alkylation product, $\mathbf{Pd(OAc)_2}$ is regenerated. The energy profile for the protonation of the Pd–N bond in **INT8'** is much the same.

Evaluation of calculated energy profiles by energetic span model.

Based on the energetic span model,[11] **INT8** is a turnover frequency determining intermediate (TDI) for the C(sp^3)–H alkylation, and $\mathbf{TS_{3\text{-}4}}$ is a turnover frequency determining transition structure (TDTS). The energy gap for these two structures was evaluated to be 33.7 kcal/mol. On the other hand, **INT8'** and $\mathbf{TS_{5'\text{-}6'}}$ are found to be a TDI and TDTS for the C(sp^2)–H alkylation, respectively, which provides a 35.0 kcal/mol energy gap. These results indicate that the C(sp^3)–H alkylation is the more favorable pathway than (sp^2)–H alkylation.

Calculated energy profiles for the formation of palladacycle in MeCN.

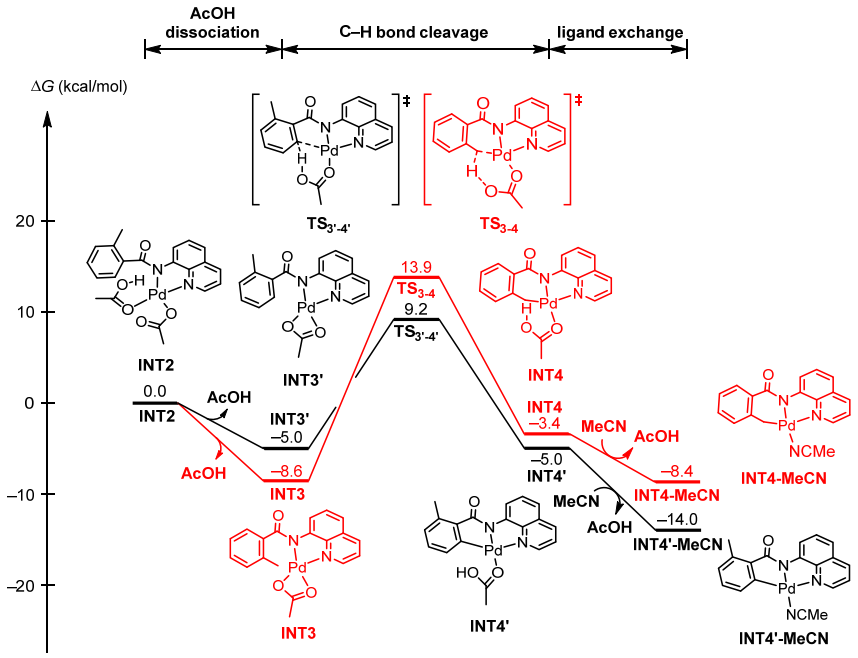


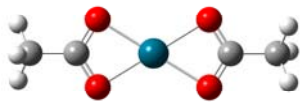
Figure S4. Comparison of Gibbs energy profiles for the formation of six- and five-membered palladacycle in MeCN by using SMD(MeCN)/M06L/6-311G++(d,p)-SDD(Pd)//SMD(MeCN)/B3LYP/6-31(d)-LANL2DZ(Pd) level of theory (T = 298.15 K, P = 1 atm).

We also conducted calculations concerning the formation **INT4** and **INT4'** in MeCN. The energy profiles are much the same as was the case in AcOH where the formation of a five-membered palladacycle is kinetically and thermodynamically favored. The ligand exchange between AcOH and MeCN leads to the generation of the Pd-MeCN complexes, **INT4-MeCN** and **INT4'-MeCN**. The latter intermediate **INT4'-MeCN** is more stable than **INT4-MeCN** by 5.6 kcal/mol, which is in agreement with the experimental result showing that the five-membered palladacycle is produced selectively.

Cartesian coordinates (Å) and energies (hartrees) of all the optimized structures in Figures S1-S3.

Electronic energies (E), as well as zero-point energy (E_{ZPE}), enthalpy (H), Gibbs free energy (G), and imaginary frequency (Im. Freq.) for all structures calculated at B3LYP/6-31G(d)-LANL2DZ level of theory are provided. SMD solvent effects were incorporated for all calculations with acetic acid as the solvent.

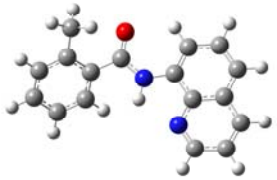
$Pd(OAc)_2$



E = -583.732028256
E_{ZPE} = -583.629096
H = -583.617405
G = -583.667351
Im. Freq.; 0

Pd	0.000000	0.000000	-0.000013
O	1.776947	-1.087786	0.018925
O	1.776947	1.087786	0.018929
O	-1.776947	1.087786	-0.018923
O	-1.776948	-1.087786	-0.018919
C	3.945922	-0.000001	-0.014787
H	4.275846	0.000033	-1.061357
H	4.334086	0.899319	0.470423
H	4.334085	-0.899351	0.470367
C	2.456781	-0.000000	0.018568
C	-3.945921	0.000000	0.014828
H	-4.334093	0.899347	-0.470325
H	-4.334094	-0.899323	-0.470368
H	-4.275828	-0.000025	1.061404
C	-2.456781	0.000000	-0.018551

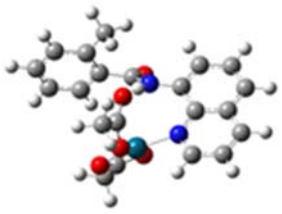
SM-amide



E = -841.019772737
E_{ZPE} = -840.747099
H = -840.73032
G = -840.791522
Im. Freq.; 0

C	4.738021	1.630428	-0.236531
C	3.580107	2.031360	-0.901363
C	2.455919	1.208990	-0.868969
C	2.475831	-0.019408	-0.188445
C	3.650490	-0.439306	0.479206
C	4.761567	0.413305	0.445290
H	5.622984	2.261557	-0.246060
H	3.549830	2.972600	-1.443163
H	1.560582	1.512427	-1.404747
H	5.666128	0.112023	0.968219
C	1.257242	-0.896394	-0.217548
C	-1.238435	-0.714283	-0.153550
C	-2.266090	0.267566	0.062523
C	-1.594786	-2.030388	-0.398107
C	-3.636154	-0.129944	0.024338
C	-2.959155	-2.403034	-0.433670
H	-0.827001	-2.773253	-0.560236
C	-2.817938	2.461941	0.495423
C	-4.606455	0.881224	0.244294
C	-3.965543	-1.487151	-0.227857
H	-3.203955	-3.443623	-0.629194
C	-4.202011	2.174992	0.479989
H	-2.477509	3.479785	0.679081
H	-5.661357	0.618673	0.223448
H	-5.010439	-1.784486	-0.255702
H	-4.919861	2.971129	0.651559
O	1.327433	-2.123401	-0.340677
N	-1.879550	1.553441	0.296339
C	3.750774	-1.745718	1.230872
H	2.877944	-1.926219	1.866844
H	3.820634	-2.596862	0.544593
H	4.642851	-1.749397	1.865740
N	0.070527	-0.220562	-0.102011
H	0.102573	0.777615	0.089366

INT0



E = -1424.75746014

E_{ZPE} = -1424.379875

H = -1424.350916

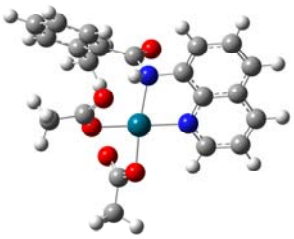
G = -1424.440006

Im. Freq.; 0

C	-5.022547	0.721592	0.594673
C	-4.564227	0.368259	-0.676269
C	-3.279952	0.739505	-1.063366
C	-2.433055	1.433873	-0.184625
C	-2.894255	1.818909	1.093074
C	-4.199013	1.448039	1.453636
H	-6.025704	0.447042	0.911082
H	-5.203015	-0.182736	-1.361161
H	-2.914754	0.496011	-2.056884
H	-4.575989	1.749014	2.428404
C	-2.072291	2.639119	2.063020
H	-1.428455	2.003082	2.681763
H	-1.429987	3.364095	1.552760
H	-2.731285	3.194955	2.738714
C	-1.076033	1.786786	-0.728063
O	-0.951691	2.310704	-1.838837
N	-0.006071	1.444301	0.059122
H	-0.170183	0.868299	0.896410
C	1.336323	1.750518	-0.249854
C	2.364362	0.772278	-0.064824
C	1.690878	3.026206	-0.661357
C	3.734668	1.181690	-0.178060
C	3.036643	3.393744	-0.858316
H	0.909920	3.763296	-0.806349
C	3.054867	-1.392376	0.533667
C	4.749355	0.243971	0.136055
C	4.047790	2.500106	-0.591406
H	3.266427	4.405036	-1.180402
C	4.412952	-1.029182	0.528518
O	2.757175	-2.407470	0.772110
H	5.789022	0.552181	0.066512
H	5.091742	2.784801	-0.685974
H	5.161312	-1.767316	0.794798
N	2.077222	-0.544450	0.225084
Pd	0.284383	-1.484892	-0.240703
O	-1.362698	-2.386382	-1.209686
C	-0.998147	-1.863764	-2.320980
O	0.045903	-1.119214	-2.302310

O	0.165904	-2.197486	1.650262
C	-0.081825	-1.358170	2.614236
O	-0.218614	-0.131942	2.479569
C	-1.733049	-2.140301	-3.591567
H	-2.781007	-2.369681	-3.382084
H	-1.654149	-1.288063	-4.271618
H	-1.278686	-3.012146	-4.079497
C	-0.229920	-2.016199	3.971825
H	-0.063293	-1.283887	4.765601
H	-1.251059	-2.406504	4.065791
H	0.460707	-2.856979	4.080831

INT1



E = -1424.75746014

E_{ZPE} = -1424.379875

H = -1424.350916

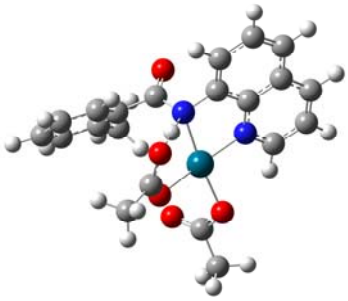
G = -1424.440006

Im. Freq.; 0

C	4.961435	-1.573039	-0.586825
C	4.189468	-2.219414	0.378341
C	2.800277	-2.152167	0.297837
C	2.176829	-1.462512	-0.754720
C	2.950442	-0.815872	-1.750404
C	4.343389	-0.878669	-1.628608
H	6.046431	-1.606864	-0.531543
H	4.660353	-2.768332	1.188617
H	2.202882	-2.663246	1.046478
H	4.955057	-0.371454	-2.370289
C	2.335973	-0.050293	-2.897448
H	1.825566	-0.718492	-3.599258
H	1.598586	0.682702	-2.548944
H	3.112312	0.491711	-3.446300
C	0.693829	-1.486630	-0.868297
O	0.089183	-1.683826	-1.905907
N	-0.063846	-1.237796	0.346847

H	0.474799	-1.299526	1.231100
C	-1.387907	-1.839446	0.367806
C	-2.484782	-1.007327	0.045617
C	-1.585464	-3.176642	0.626698
C	-3.793622	-1.556911	-0.047961
C	-2.889762	-3.724220	0.565802
H	-0.738890	-3.813668	0.865396
C	-3.265609	1.134805	-0.468133
C	-4.849787	-0.676348	-0.396319
C	-3.968811	-2.939038	0.223678
H	-3.028821	-4.779379	0.779655
C	-4.584162	0.656731	-0.615116
H	-3.025510	2.185098	-0.590452
H	-5.860654	-1.064938	-0.482901
H	-4.966731	-3.363469	0.162034
H	-5.369631	1.354788	-0.882967
N	-2.259025	0.334269	-0.149438
Pd	-0.352947	0.890533	0.374050
O	-0.819122	2.873049	0.425636
C	-0.275413	3.586675	-0.528305
O	0.401454	3.130534	-1.456079
O	1.501408	1.367295	1.099842
C	1.974982	0.661398	2.079027
O	1.455520	-0.376387	2.539748
C	-0.543264	5.075732	-0.389251
H	0.033368	5.469546	0.456351
H	-0.243219	5.599703	-1.299696
H	-1.601625	5.263858	-0.180989
C	3.289617	1.175315	2.633605
H	3.472517	0.753384	3.624923
H	4.100069	0.862537	1.963530
H	3.295314	2.268118	2.679023

$TS_{1\text{-}2}$



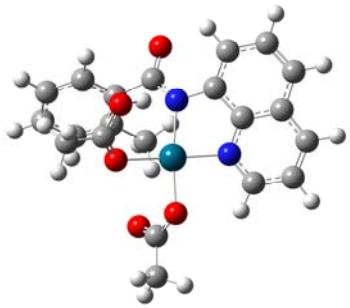
E = -1424.75206307

E_{ZPE} = -1424.379273
H = -1424.350936
G = -1424.438153
Im. Freq.; 1 (-1038.8346 cm^{-1})

C	4.825586	-1.515448	-0.908101
C	4.166716	-2.240100	0.084333
C	2.771903	-2.238624	0.120487
C	2.031618	-1.528799	-0.835634
C	2.688597	-0.811462	-1.861940
C	4.088882	-0.811516	-1.862969
H	5.911894	-1.500422	-0.945568
H	4.728189	-2.804967	0.823552
H	2.255083	-2.806502	0.888035
H	4.610659	-0.250744	-2.634574
C	1.934532	-0.034186	-2.914849
H	1.198543	-0.659640	-3.429341
H	1.398357	0.815748	-2.473074
H	2.625825	0.368183	-3.662095
C	0.536225	-1.665849	-0.830730
O	-0.056806	-2.145765	-1.790742
N	-0.153376	-1.254715	0.343113
H	0.543866	-1.148004	1.475244
C	-1.525359	-1.702207	0.374509
C	-2.531138	-0.784234	-0.015029
C	-1.885008	-2.989223	0.713572
C	-3.892725	-1.185954	-0.104899
C	-3.241767	-3.391715	0.659848
H	-1.118878	-3.700828	1.007095
C	-3.054704	1.401673	-0.676360
C	-4.833587	-0.214656	-0.533078
C	-4.226237	-2.519458	0.248740
H	-3.498873	-4.409984	0.936083
C	-4.415074	1.064085	-0.828459
H	-2.694240	2.409517	-0.849390
H	-5.881018	-0.490642	-0.619495
H	-5.264239	-2.834895	0.195267
H	-5.111507	1.826899	-1.159022
N	-2.154572	0.510974	-0.285748
Pd	-0.245732	0.866142	0.333448
O	-0.544216	2.887457	0.405518
C	0.253637	3.600714	-0.347355
O	1.083763	3.134896	-1.135661
O	1.550225	1.095966	1.375528

C	1.841091	0.239561	2.260022
O	1.238597	-0.889644	2.402382
C	0.084852	5.097635	-0.154370
H	0.511596	5.386679	0.813831
H	0.603123	5.641762	-0.947531
H	-0.974617	5.372678	-0.142406
C	2.984746	0.523323	3.192130
H	2.733373	0.193918	4.204471
H	3.854850	-0.054484	2.856655
H	3.238081	1.584745	3.186696

INT2



E = -1424.75640533

E_{ZPE} = -1424.379283

H = -1424.350296

G = -1424.439818

Im. Freq.; 0

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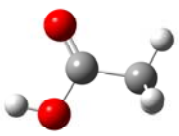
C	4.219234	-2.035606	-0.219743
C	2.882570	-2.324337	0.046129
C	1.856947	-1.763144	-0.732481
C	2.170490	-0.951515	-1.839456
C	3.524421	-0.680882	-2.094522
H	5.577731	-0.970724	-1.518734
H	5.003420	-2.469691	0.395154
H	2.622732	-2.987708	0.867030
H	3.780261	-0.055593	-2.947141
C	1.119516	-0.389544	-2.769144
H	0.167699	-0.923909	-2.695675
H	0.932283	0.669312	-2.553973
H	1.457642	-0.454176	-3.810251
C	0.446643	-2.199904	-0.420648
O	0.129694	-3.371209	-0.669180
N	-0.403512	-1.284315	0.162256

H	0.607208	-1.074011	1.906714
C	-1.791609	-1.584060	0.226952
C	-2.665562	-0.486931	-0.015147
C	-2.365042	-2.822977	0.484178
C	-4.079469	-0.648104	-0.055459
C	-3.771037	-2.983709	0.470941
H	-1.735608	-3.677438	0.686541
C	-2.850104	1.810584	-0.467369
C	-4.862030	0.499562	-0.338816
C	-4.620402	-1.934376	0.196695
H	-4.179221	-3.969077	0.678003
C	-4.252434	1.716344	-0.553313
H	-2.330260	2.754521	-0.583173
H	-5.943862	0.405710	-0.380045
H	-5.697512	-2.071712	0.177067
H	-4.827288	2.609607	-0.772522
N	-2.097562	0.748867	-0.209700
Pd	-0.129079	0.771883	0.256568
O	-0.112977	2.815830	0.413081
C	0.716677	3.444488	-0.378060
O	1.401443	2.905957	-1.256053
O	1.789859	0.831740	1.194692
C	2.075510	0.118123	2.168905
O	1.342989	-0.912829	2.555370
C	0.790518	4.939169	-0.115431
H	1.329540	5.114703	0.823697
H	1.321330	5.441909	-0.927351
H	-0.211226	5.366739	-0.003532
C	3.303378	0.347455	2.989007
H	3.090597	0.170897	4.046985
H	4.069182	-0.370954	2.672113
H	3.677291	1.360014	2.832035

AcOH



E = -229.085373302

E_{ZPE} = -229.023565

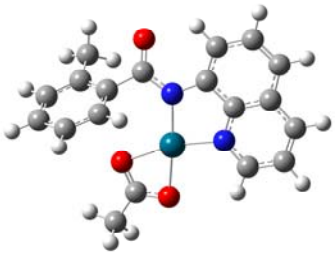
H = -229.018097

G = -229.050695

Im. Freq.; 0

C	1.393656	-0.117376	-0.000438
H	1.673597	-0.744482	-0.853709
H	1.682178	-0.654809	0.909985
H	1.922273	0.835552	-0.048649
C	-0.089051	0.121185	-0.001423
O	-0.636258	1.208539	0.000257
O	-0.784880	-1.039114	-0.000221
H	-1.736571	-0.814507	0.003256

INT3

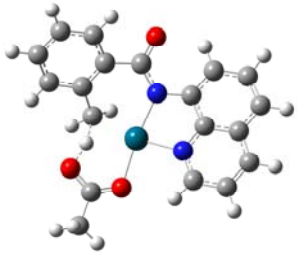


E = -1195.66832927
E_{ZPE} = -1195.354451
H = -1195.331387
G = -1195.406803
Im. Freq.; 0

C	4.447366	-1.324095	-0.085508
C	3.178568	-1.686725	-0.553741
C	2.073689	-1.482142	0.300869
C	2.262015	-0.946027	1.582647
C	3.537913	-0.611406	2.036928
C	4.634082	-0.799209	1.195364
H	5.306722	-1.459894	-0.738436
H	1.401891	-0.808739	2.232321
H	3.671700	-0.208247	3.037399
H	5.634404	-0.536896	1.530877
C	3.023490	-2.267060	-1.940224
H	2.185422	-1.812793	-2.481627
H	3.932543	-2.106076	-2.528986
H	2.830158	-3.345443	-1.903895
C	0.701208	-1.950960	-0.093212
O	0.545069	-3.132982	-0.442269
N	-0.315166	-1.039917	0.014639
C	-1.669889	-1.409941	-0.018541

C	-2.584767	-0.319792	0.065393
C	-2.217698	-2.692168	-0.067078
C	-3.995786	-0.503368	0.103544
C	-3.618747	-2.879140	-0.029088
H	-1.567130	-3.550265	-0.137046
C	-2.818112	2.015595	0.198060
C	-4.802735	0.659066	0.191902
C	-4.503713	-1.825258	0.052152
H	-3.997860	-3.896844	-0.069143
C	-4.220656	1.908076	0.242252
H	-2.313657	2.975832	0.225537
H	-5.883643	0.551406	0.220682
H	-5.577131	-1.987949	0.075676
H	-4.816681	2.811554	0.311269
N	-2.047228	0.938502	0.113695
Pd	-0.046066	0.991268	-0.062110
O	0.381735	3.038842	-0.227755
C	1.633183	2.807574	-0.419910
O	2.010662	1.592858	-0.418557
C	2.589200	3.940653	-0.618099
H	2.184360	4.645976	-1.351112
H	2.711268	4.478723	0.329807
H	3.562008	3.569442	-0.948212

TS_{3-4}



E = -1195.62640672

E_{ZPE} = -1195.317118

H = -1195.295239

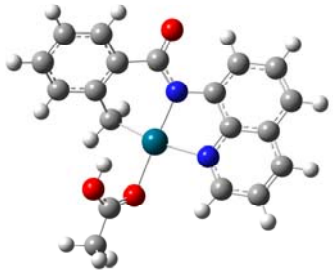
G = -1195.367645

Im. Freq.; 1 (-1449.8954 cm^{-1})

C	4.147113	-0.543921	-0.099822
C	2.784740	-0.722034	-0.393497
C	2.135694	-1.875839	0.095959
C	2.873906	-2.819586	0.829878
C	4.220211	-2.621482	1.123113
C	4.860673	-1.472192	0.655443

H	4.651641	0.341188	-0.480864
H	2.365295	-3.714606	1.172192
H	4.764021	-3.358704	1.707635
H	5.912755	-1.301582	0.869740
C	2.080183	0.310594	-1.209551
H	2.031674	1.488235	-0.481295
H	2.799325	0.907654	-1.787802
H	1.428838	-0.117860	-1.979702
C	0.688114	-2.232558	-0.129732
O	0.383831	-3.440706	-0.119745
N	-0.240828	-1.233195	-0.257459
C	-1.622367	-1.514481	-0.250494
C	-2.471921	-0.414944	0.094370
C	-2.246615	-2.732516	-0.520202
C	-3.882070	-0.564699	0.234973
C	-3.649025	-2.873467	-0.407922
H	-1.651674	-3.584475	-0.807315
C	-2.601483	1.866466	0.634142
C	-4.628563	0.580016	0.612260
C	-4.463121	-1.830981	-0.024940
H	-4.084006	-3.844616	-0.628914
C	-3.994680	1.785644	0.818962
H	-2.061391	2.798750	0.757319
H	-5.705257	0.491819	0.731310
H	-5.538179	-1.954617	0.067661
H	-4.544225	2.675139	1.107999
N	-1.883386	0.807752	0.284849
Pd	0.094551	0.788031	-0.275680
O	0.176174	2.880519	-0.200154
C	1.331607	3.379596	-0.007746
O	2.390293	2.674528	-0.023764
C	1.449940	4.853866	0.267434
H	1.636293	4.996710	1.338972
H	2.304600	5.265565	-0.276596
H	0.534040	5.380454	-0.007254

INT4



E = -1195.65854835

E_{ZPE} = -1195.344177

H = -1195.321622

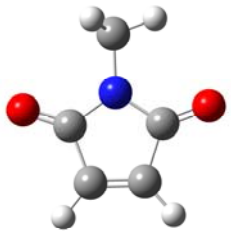
G = -1195.395742

Im. Freq.; 0

C	4.039707	-0.584783	-0.100226
C	2.689941	-0.795575	-0.433620
C	2.060863	-1.974581	0.030950
C	2.808649	-2.918923	0.749710
C	4.147109	-2.694543	1.067725
C	4.762818	-1.514048	0.646997
H	4.529921	0.319855	-0.453782
H	2.314170	-3.829439	1.072414
H	4.700551	-3.431537	1.643657
H	5.804865	-1.320459	0.890088
C	1.964036	0.189800	-1.276910
H	1.858415	1.837057	1.113492
H	2.565446	1.082342	-1.479654
H	1.641650	-0.242421	-2.233677
C	0.602124	-2.307081	-0.165991
O	0.276029	-3.511621	-0.157937
N	-0.291481	-1.272501	-0.243467
C	-1.682317	-1.477847	-0.173780
C	-2.488552	-0.320252	0.125637
C	-2.357059	-2.689146	-0.341151
C	-3.903106	-0.427012	0.292346
C	-3.758434	-2.780822	-0.187710
H	-1.793790	-3.575789	-0.583513
C	-2.565625	1.982785	0.522457
C	-4.622014	0.757199	0.597004
C	-4.530692	-1.687515	0.131764
H	-4.227062	-3.751452	-0.329524
C	-3.960719	1.958601	0.716383
H	-2.007389	2.912280	0.593954
H	-5.699551	0.699249	0.729267

H	-5.607669	-1.766916	0.250506
H	-4.488014	2.878746	0.946366
N	-1.865366	0.894188	0.241072
Pd	0.188863	0.705443	-0.421423
O	0.602579	2.811987	-0.585541
C	1.405730	3.404487	0.147965
O	2.095168	2.794321	1.101391
C	1.680171	4.869231	0.036553
H	1.425209	5.361788	0.981537
H	2.749684	5.027643	-0.140118
H	1.097807	5.299510	-0.778718

_N_-methylmaleimide



E = -398.746971301
E_{ZPE} = -398.650206
H = -398.642216
G = -398.681676
Im. Freq.; 0

C	0.709167	-1.611760	-0.000000
C	-0.626636	-1.645399	-0.000001
H	1.420201	-2.428448	-0.000001
H	-1.295404	-2.496928	-0.000001
N	-0.013344	0.591869	0.000001
C	-1.133288	-0.234535	0.000001
C	1.148977	-0.177610	0.000000
O	-2.289082	0.154603	-0.000000
O	2.287781	0.257743	0.000000
C	-0.066164	2.044438	-0.000001
H	-0.586102	2.407431	0.891384
H	0.958867	2.417852	0.000011
H	-0.586081	2.407431	-0.891397

INT5

E = -1365.30486600

E_{ZPE} = -1364.955039

H = -1364.929799

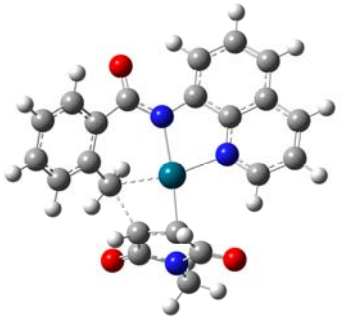
G = -1365.009760

Im. Freq.; 0

C	-4.191408	0.140213	-0.117400
C	-2.943980	-0.391648	0.251434
C	-2.674554	-1.748539	-0.033653
C	-3.660104	-2.541651	-0.630805
C	-4.893722	-1.999172	-0.993391
C	-5.157553	-0.651666	-0.738523
H	-4.408211	1.181859	0.108331
H	-3.441821	-3.587696	-0.820510
H	-5.642274	-2.624620	-1.472334
H	-6.115942	-0.219069	-1.014320
C	-1.952674	0.447639	0.955802
H	-2.322631	1.446666	1.170907
H	-1.558704	-0.006032	1.868506
C	-1.360100	-2.401922	0.289642
O	-1.333650	-3.639350	0.442127
N	-0.252974	-1.602497	0.342161
C	1.020190	-2.153323	0.550799
C	2.116309	-1.482654	-0.083880
C	1.301148	-3.292957	1.301266
C	3.436672	-2.023107	-0.012276
C	2.615330	-3.799268	1.399079
H	0.496757	-3.809611	1.804238
C	2.851060	0.280698	-1.418413
C	4.467639	-1.341013	-0.705155
C	3.668576	-3.196838	0.748357
H	2.784674	-4.690552	1.997488
C	4.174882	-0.202485	-1.417980
H	2.614549	1.187943	-1.959381
H	5.481422	-1.731009	-0.664919
H	4.677123	-3.595218	0.813780
H	4.937375	0.339705	-1.967337

N	1.861792	-0.318585	-0.768470
Pd	-0.171934	0.421438	-0.184447
N	0.528414	3.732853	0.626044
C	1.108152	4.538158	1.689908
H	0.429271	5.360182	1.926968
H	1.273848	3.935630	2.589115
H	2.061484	4.936346	1.338775
C	1.245905	3.158485	-0.419927
C	-0.819881	3.395859	0.550755
C	-0.981377	2.512465	-0.655628
H	-1.949006	2.351959	-1.112648
C	0.261350	2.358461	-1.231127
H	0.480315	2.058724	-2.249027
O	2.435827	3.323642	-0.630451
O	-1.682310	3.785937	1.320258

$TS_{5\text{-}6}$



E = -1365.28500859

E_{ZPE} = -1364.935408

H = -1364.911063

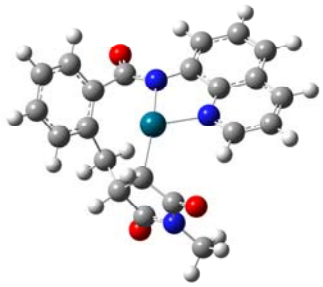
G = -1364.988660

Im. Freq.; 1 (-281.4419 cm^{-1})

C	3.640227	1.869719	-0.545611
C	2.384248	1.642029	0.046455
C	1.438770	2.696088	0.062145
C	1.800674	3.938175	-0.479331
C	3.040349	4.138436	-1.083820
C	3.966881	3.095197	-1.120612
H	4.377991	1.070468	-0.530753
H	1.082195	4.749597	-0.428275
H	3.282276	5.105829	-1.515676
H	4.942907	3.238873	-1.576342
C	2.164797	0.337940	0.723840
H	3.103291	-0.078053	1.078775
H	1.482608	0.351907	1.578236

C	0.036042	2.631442	0.631428
O	-0.419750	3.662790	1.165698
N	-0.658916	1.484870	0.415079
C	-2.045592	1.402190	0.564336
C	-2.657968	0.262888	-0.062742
C	-2.890940	2.309671	1.206001
C	-4.074996	0.095568	-0.069236
C	-4.291489	2.126512	1.211539
H	-2.462768	3.170767	1.695888
C	-2.371371	-1.722151	-1.281293
C	-4.604852	-1.039652	-0.731899
C	-4.887903	1.054389	0.586582
H	-4.904898	2.861967	1.725819
C	-3.760532	-1.940330	-1.339509
H	-1.681686	-2.431162	-1.722640
H	-5.681636	-1.186664	-0.748772
H	-5.965935	0.921606	0.591664
H	-4.136209	-2.818844	-1.853185
N	-1.844491	-0.667299	-0.668880
Pd	0.170463	-0.323090	-0.280296
N	1.667159	-3.394361	0.678149
C	1.608192	-4.474729	1.649732
H	2.602831	-4.909789	1.777205
H	1.251562	-4.105246	2.616814
H	0.919109	-5.231116	1.271673
C	0.787033	-3.243069	-0.405961
C	2.592827	-2.371898	0.733498
C	2.280261	-1.412504	-0.402005
H	3.121851	-1.009040	-0.955104
C	1.139103	-1.972494	-1.087591
H	1.027644	-1.930946	-2.168518
O	-0.080389	-4.055496	-0.697108
O	3.486231	-2.283670	1.562746

INT6



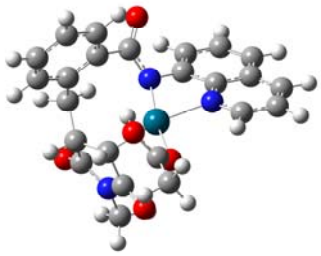
E = -1365.30472587

E_{ZPE} = -1364.953320
H = -1364.928612
G = -1365.007294
Im. Freq.; 0

C	3.676305	0.928254	-0.523483
C	2.501375	1.005506	0.267026
C	1.782737	2.243229	0.244123
C	2.293609	3.328160	-0.493506
C	3.458331	3.218190	-1.240254
C	4.145411	1.998776	-1.269612
H	4.257885	0.010833	-0.504264
H	1.742637	4.264382	-0.476545
H	3.828140	4.072035	-1.801176
H	5.056978	1.895224	-1.851490
C	2.259289	-0.165193	1.236585
H	3.061486	-0.164128	1.985534
H	1.329736	-0.030557	1.799206
C	0.403564	2.514328	0.839234
O	0.220414	3.406856	1.680657
N	-0.519129	1.750487	0.220592
C	-1.890325	1.698174	0.425485
C	-2.522090	0.547857	-0.146336
C	-2.681043	2.634655	1.084363
C	-3.936324	0.390534	-0.087604
C	-4.080508	2.460583	1.158869
H	-2.211895	3.499530	1.535739
C	-2.285524	-1.467232	-1.328537
C	-4.498585	-0.751161	-0.713620
C	-4.707542	1.375837	0.582246
H	-4.670272	3.212194	1.676793
H	-3.681501	-1.664879	-1.338683
H	-1.614270	-2.193237	-1.775036
H	-5.576063	-0.891638	-0.691852
H	-5.786360	1.259706	0.629334
H	-4.082102	-2.545702	-1.828973
N	-1.728857	-0.408951	-0.753815
Pd	0.294190	0.056754	-0.605169
N	0.822475	-3.412901	0.686012
C	0.130007	-4.570679	1.228095
H	0.846617	-5.248541	1.700007
H	-0.609501	-4.261609	1.973833
H	-0.371739	-5.080220	0.404375
C	0.696102	-2.960484	-0.639835

C	1.678376	-2.630926	1.434301
C	2.262938	-1.557550	0.526663
H	3.304762	-1.847895	0.331483
C	1.433570	-1.693908	-0.775107
H	1.985007	-1.632529	-1.715852
O	0.044822	-3.571479	-1.488105
O	1.900483	-2.800552	2.626779

INT7

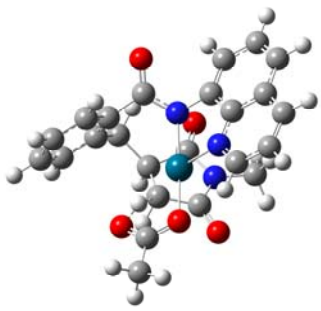


E = -1594.42167626
E_{ZPE} = -1594.005568
H = -1593.975354
G = -1594.066940
Im. Freq.; 0

C	-3.901667	-2.207758	-2.200371
C	-3.750017	-1.937617	-0.841494
C	-2.486108	-1.942088	-0.230925
C	-1.360390	-2.245047	-1.017632
C	-1.521841	-2.551430	-2.379846
C	-2.779198	-2.512144	-2.976934
H	-4.891421	-2.194080	-2.649582
H	-4.628356	-1.726815	-0.234711
H	-0.647105	-2.823581	-2.964225
H	-2.886318	-2.735776	-4.035142
C	0.030401	-2.392501	-0.455044
O	0.630482	-3.461323	-0.665400
N	0.574712	-1.334269	0.221315
O	1.952909	-1.435889	0.544492
C	2.820459	-0.463716	-0.032076
C	2.505862	-2.420603	1.345131
C	4.227865	-0.513733	0.183714
C	3.900881	-2.463149	1.577797
H	1.862326	-3.171349	1.790607
C	3.009824	1.437491	-1.365700

C	5.016245	0.485291	-0.442589
C	4.753538	-1.539682	1.010924
H	4.299744	-3.246981	2.215868
C	4.413136	1.450381	-1.218996
H	2.503037	2.200191	-1.949490
H	6.093628	0.480055	-0.298736
H	5.823801	-1.578554	1.193618
H	4.991358	2.226371	-1.709641
C	-2.355328	-1.617054	1.235443
H	-3.137082	-2.131584	1.805377
H	-1.396377	-1.965426	1.622209
N	2.244495	0.519272	-0.795251
C	-2.497219	-0.107169	1.514514
H	-3.565092	0.143125	1.412145
C	-1.710102	0.929262	0.693582
H	-2.305730	1.384099	-0.101297
Pd	0.128617	0.604156	-0.292092
C	-2.146940	0.210099	2.962260
C	-1.300802	1.955334	1.704696
O	-2.405028	-0.465347	3.950156
O	-0.858937	3.089791	1.536236
N	-1.490841	1.424726	2.986190
C	-1.071224	2.113393	4.195653
H	0.021006	2.163548	4.247825
H	-1.450609	1.555610	5.053117
H	-1.473830	3.129988	4.204218
O	-1.545508	1.783585	-2.786847
H	-1.417890	0.933879	-2.306807
C	-0.813078	2.736925	-2.223866
O	-0.107041	2.549896	-1.225137
C	-0.916053	4.061578	-2.908032
H	-1.967875	4.360486	-2.970004
H	-0.537344	3.971533	-3.932639
H	-0.343496	4.812141	-2.362523

$TS_{7\text{-}8}$



E = -1594.37813765

E_{ZPE} = -1593.967730

H = -1593.938023

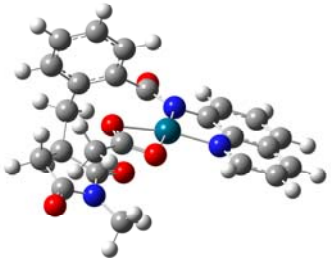
G = -1594.027855

Im. Freq.; 1 (-1565.9650 cm^{-1})

C	-4.251742	-0.726639	-2.142868
C	-3.870362	-1.376539	-0.968963
C	-2.532350	-1.717215	-0.727095
C	-1.572593	-1.391316	-1.700829
C	-1.960891	-0.770334	-2.897456
C	-3.293477	-0.423929	-3.113552
H	-5.295472	-0.470947	-2.306149
H	-4.623375	-1.636561	-0.228127
H	-1.209744	-0.560277	-3.654636
H	-3.584129	0.067554	-4.038238
C	-0.119127	-1.757161	-1.549175
O	0.391994	-2.578248	-2.322431
N	0.569901	-1.093548	-0.563959
C	1.985956	-1.110735	-0.627762
C	2.604961	0.163800	-0.719865
C	2.789916	-2.237113	-0.654116
C	4.011779	0.303678	-0.871948
C	4.194489	-2.107424	-0.781493
H	2.342766	-3.221063	-0.580481
C	2.284150	2.484752	-0.774995
C	4.523039	1.621394	-0.986628
C	4.802487	-0.874844	-0.895891
H	4.799141	-3.009939	-0.794224
C	3.666255	2.701013	-0.948244
H	1.580462	3.307807	-0.711204
H	5.593240	1.768648	-1.105002
H	5.880310	-0.788763	-0.998953
H	4.032427	3.718207	-1.036016
C	-2.141590	-2.438254	0.539223
H	-2.972344	-3.084151	0.838810
H	-1.296735	-3.106157	0.346069
N	1.783230	1.262404	-0.664507
C	-1.778050	-1.532450	1.751005
H	-2.522630	-1.738720	2.533867
C	-1.693448	0.004518	1.653182
H	-2.618666	0.464050	2.025783
Pd	-0.097167	0.747337	0.007287
C	-0.459499	-1.917253	2.415654

C	-0.623575	0.378001	2.647922
O	0.041975	-3.029182	2.488373
O	-0.376356	1.480853	3.124917
N	0.064573	-0.781443	3.010136
C	1.255666	-0.773282	3.844541
H	2.135086	-0.478397	3.261323
H	1.405960	-1.778818	4.240974
H	1.115332	-0.065460	4.664375
O	-2.749825	1.882020	0.065970
H	-2.081376	0.846275	0.573531
C	-1.954670	2.880334	0.103485
O	-0.697247	2.743164	0.250302
C	-2.527023	4.265014	-0.019420
H	-3.205469	4.447777	0.821388
H	-3.117081	4.333634	-0.939595
H	-1.738083	5.018947	-0.025710

INT8



E = -1594.45043924

E_{ZPE} = -1594.034300

H = -1594.004079

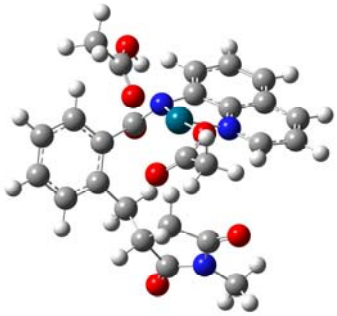
G = -1594.095542

Im. Freq.; 0

C	-3.610503	-1.802700	-2.459473
C	-3.669985	-1.974105	-1.076111
C	-2.513054	-2.058873	-0.286544
C	-1.262622	-1.963418	-0.936642
C	-1.207082	-1.797372	-2.329444
C	-2.370975	-1.715389	-3.092345
H	-4.529247	-1.749607	-3.038051
H	-4.640665	-2.058736	-0.592450
H	-0.237082	-1.747005	-2.816670
H	-2.307954	-1.596965	-4.170896
C	0.040452	-2.183491	-0.212958

O	0.227500	-3.262916	0.372037
N	0.972217	-1.189335	-0.321466
C	2.302089	-1.351565	0.102891
C	3.112053	-0.185841	-0.026317
C	2.926444	-2.504805	0.578774
C	4.499449	-0.176058	0.292024
C	4.303736	-2.498410	0.900063
H	2.353621	-3.410103	0.706023
C	3.169885	2.084024	-0.635931
C	5.201661	1.042391	0.114652
C	5.089524	-1.374083	0.765664
H	4.745005	-3.421377	1.266813
C	4.544794	2.163314	-0.347342
H	2.608365	2.941737	-0.991311
H	6.262167	1.080431	0.348867
H	6.145553	-1.386565	1.018541
H	5.060656	3.106597	-0.490221
C	-2.670509	-2.251370	1.212284
H	-3.581983	-2.834967	1.381642
H	-1.841376	-2.841713	1.609886
N	2.496811	0.950964	-0.477830
C	-2.788199	-0.971865	2.083155
H	-3.134201	-1.309846	3.069831
C	-3.696046	0.173119	1.596768
H	-4.670037	0.211452	2.092942
Pd	0.520124	0.759468	-0.777168
C	-1.456055	-0.284493	2.377193
C	-2.918830	1.440789	1.886431
O	-0.396924	-0.816052	2.667819
O	-3.290740	2.598511	1.755400
N	-1.651980	1.091778	2.326832
C	-0.624586	2.076399	2.632283
H	-0.367026	2.651192	1.737656
H	0.256610	1.543717	2.992086
H	-0.985602	2.761947	3.404322
O	-1.598418	1.119748	-1.072072
H	-3.871829	0.137982	0.516444
C	-1.348618	2.352302	-1.277477
O	-0.119728	2.722962	-1.204560
C	-2.439843	3.331331	-1.569712
H	-3.018442	3.495126	-0.652523
H	-3.117831	2.917952	-2.323150
H	-2.026328	4.282345	-1.913121

INT9

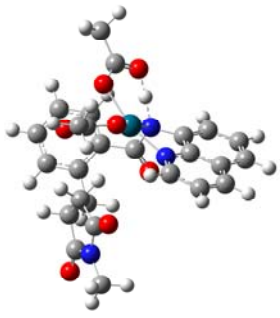


E = -1823.53491996
E_{ZPE} = -1823.055327
H = -1823.019277
G = -1823.124879
Im. Freq.; 0

C	-1.836904	-4.312121	-1.229204
C	-0.492637	-3.944116	-1.253611
C	-0.092785	-2.627877	-1.525816
C	-1.098568	-1.661427	-1.753048
C	-2.449138	-2.041044	-1.749368
C	-2.821551	-3.358458	-1.489275
H	-2.111416	-5.343401	-1.023520
H	0.266203	-4.702200	-1.075218
H	-3.211657	-1.303546	-1.980329
H	-3.871592	-3.638351	-1.498620
C	-0.722168	-0.263272	-2.178855
O	-0.156132	-0.111916	-3.266921
N	-1.031652	0.791157	-1.330755
C	-0.426906	2.044487	-1.664341
C	0.413061	2.612602	-0.671737
C	-0.565461	2.710959	-2.868883
C	1.151066	3.804497	-0.912402
C	0.135747	3.917926	-3.105563
H	-1.205705	2.302044	-3.641778
C	1.291934	2.415441	1.496375
C	2.001643	4.264538	0.125663
C	0.986923	4.454150	-2.162897
H	0.002890	4.418835	-4.060271
C	2.084404	3.566872	1.310844
H	1.288309	1.865009	2.429091
H	2.583073	5.169944	-0.026545
H	1.533139	5.372234	-2.359169
H	2.731838	3.892907	2.117502

N	0.489228	1.968724	0.540843
C	2.201096	-2.667839	-0.341830
H	2.092218	-3.736826	-0.133689
C	3.145571	-1.022770	1.170204
C	3.680217	-2.407560	-0.607716
O	3.325522	-0.154551	2.012362
O	4.372994	-2.922473	-1.471248
N	4.130729	-1.443782	0.286941
C	5.482832	-0.904703	0.297175
H	5.464893	0.165470	0.070806
H	5.937430	-1.052869	1.280665
H	6.061984	-1.430992	-0.462571
O	-0.821130	-1.530747	2.912916
C	-0.841468	-0.413265	3.440971
O	-0.880356	0.720170	2.789037
C	-0.825043	-0.236239	4.949775
H	-1.754072	0.244174	5.278152
H	-0.723199	-1.204326	5.445514
H	0.002951	0.417766	5.244946
Pd	-1.006567	0.611449	0.746714
O	-2.912963	-0.327975	0.995670
C	-3.901789	0.063026	0.352474
C	-5.294523	-0.315861	0.741602
H	-5.982797	0.509853	0.542410
H	-5.605968	-1.172407	0.130387
H	-5.324484	-0.603572	1.793568
O	-3.813448	0.807893	-0.733545
H	-2.850280	0.918858	-1.000112
C	1.884536	-1.813160	0.897494
H	1.048587	-1.123303	0.747738
H	1.641498	-2.408818	1.783003
C	1.390333	-2.304360	-1.610254
H	1.828137	-2.856956	-2.451284
H	1.543544	-1.244673	-1.831545

$TS_{9\text{-}10}$



E = -1823.52980997

E_{ZPE} = -1823.054400

H = -1823.019084

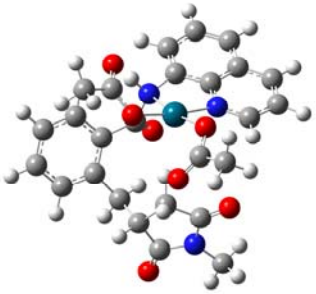
G = -1823.121523

Im. Freq.; 1 (-1123.9844 cm^{-1})

C	-0.229157	4.691957	-1.425139
C	-1.259631	3.759571	-1.522099
C	-1.011103	2.388139	-1.678613
C	0.340012	1.960632	-1.704582
C	1.374608	2.907276	-1.615124
C	1.097661	4.264870	-1.482053
H	-0.462897	5.747998	-1.319159
H	-2.290257	4.104932	-1.496305
H	2.406775	2.582374	-1.679299
H	1.911978	4.982310	-1.431118
C	0.683744	0.523754	-1.965356
O	0.139175	-0.098857	-2.870565
N	1.658638	-0.104685	-1.134166
C	1.848181	-1.497462	-1.480674
C	1.133110	-2.448283	-0.710662
C	2.613032	-1.926071	-2.542858
C	1.144572	-3.826543	-1.057395
C	2.670672	-3.304046	-2.868227
H	3.154184	-1.201849	-3.144300
C	-0.276632	-2.837414	1.121618
C	0.362476	-4.704084	-0.262508
C	1.942382	-4.234542	-2.158815
H	3.285467	-3.619889	-3.705760
C	-0.355776	-4.209871	0.804286
H	-0.786049	-2.420253	1.982462
H	0.341253	-5.763463	-0.503288
H	1.973134	-5.286922	-2.426095
H	-0.966198	-4.856518	1.425092
N	0.444675	-1.998276	0.392753
C	-3.134613	1.423334	-0.581992
H	-3.450059	2.440750	-0.328467
C	-3.437241	-0.516607	0.843946
C	-4.395508	0.633999	-0.922090
O	-3.299974	-1.422973	1.653750
O	-5.198120	0.879246	-1.808891
N	-4.486780	-0.454500	-0.062558
C	-5.543313	-1.454007	-0.119393
H	-5.142599	-2.413670	-0.460067

H	-5.983271	-1.582703	0.872952
H	-6.301853	-1.105028	-0.821071
O	-0.348775	1.598191	2.989928
C	-0.006445	0.524633	3.496712
O	0.620554	-0.435907	2.866688
C	-0.318502	0.186244	4.944893
H	0.567846	-0.207864	5.452290
H	-0.683682	1.072905	5.468543
H	-1.091170	-0.591728	4.975184
Pd	1.095104	-0.127146	0.904304
O	2.271003	1.531581	1.416365
C	3.362623	1.710434	0.802295
C	4.355045	2.687048	1.370629
H	5.367454	2.280442	1.288842
H	4.317939	3.610723	0.780019
H	4.118925	2.918929	2.410514
O	3.675164	1.133385	-0.304792
H	2.735183	0.533306	-0.785886
C	-2.551696	0.692027	0.639651
H	-1.517990	0.361493	0.497044
H	-2.560047	1.295828	1.551873
C	-2.208706	1.462003	-1.823374
H	-2.811475	1.805036	-2.673486
H	-1.894087	0.444506	-2.058990

INT10



E = -1823.53828068

E_{ZPE} = -1823.058269

H = -1823.022166

G = -1823.127656

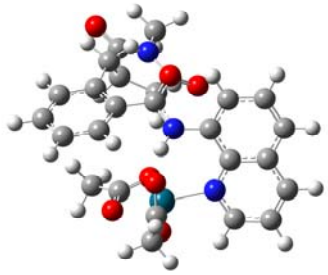
Im. Freq.; 0

C	2.915776	-4.056986	-1.089444
C	3.370985	-2.745971	-1.213085
C	2.500523	-1.668660	-1.428670
C	1.106618	-1.947014	-1.484359

C	0.658400	-3.276756	-1.372730
C	1.550773	-4.326869	-1.182843
H	3.626653	-4.864560	-0.936919
H	4.438362	-2.546052	-1.159924
H	-0.396888	-3.509741	-1.448838
H	1.180442	-5.345621	-1.116042
C	0.114683	-0.866074	-1.748536
O	0.340563	0.121142	-2.426469
N	-1.204853	-0.978138	-1.140553
C	-2.195944	-0.117374	-1.773285
C	-2.419640	1.145038	-1.175357
C	-2.833500	-0.449306	-2.945885
C	-3.250507	2.104098	-1.815417
C	-3.708532	0.480386	-3.560588
H	-2.651859	-1.414305	-3.409966
C	-1.969732	2.598870	0.599911
C	-3.384535	3.370846	-1.189871
C	-3.898292	1.735114	-3.023770
H	-4.213316	0.199113	-4.479562
C	-2.730996	3.621755	-0.003978
H	-1.487855	2.739346	1.560217
H	-4.005482	4.131446	-1.655037
H	-4.547606	2.455763	-3.512619
H	-2.807369	4.582166	0.493815
N	-1.833907	1.406790	0.039259
C	3.518933	0.382651	-0.238864
H	4.194337	-0.278283	0.314008
C	2.358504	2.357594	0.557103
C	4.275218	1.672556	-0.548987
O	1.527582	3.147751	0.981251
O	5.341311	1.775753	-1.135959
N	3.528102	2.748076	-0.084725
C	3.897143	4.143588	-0.271239
H	3.118176	4.664696	-0.834905
H	4.022444	4.632642	0.699154
H	4.836043	4.175237	-0.825304
O	0.727349	0.072596	3.382754
C	-0.413894	0.474222	3.621719
O	-1.414080	0.468350	2.777200
C	-0.780332	1.083903	4.965542
H	-1.778139	0.769963	5.285877
H	-0.039105	0.803098	5.717822
H	-0.787695	2.177173	4.871886
Pd	-1.141319	-0.312789	0.919065

O	-0.702379	-2.124931	1.770701
C	-1.328989	-3.173081	1.341182
C	-1.075868	-4.430475	2.150294
H	-1.916774	-5.121594	2.049583
H	-0.177216	-4.922374	1.756217
H	-0.898728	-4.197430	3.203295
O	-2.058978	-3.213582	0.326083
H	-1.547791	-1.931986	-0.914103
C	2.336759	0.847595	0.627794
H	1.359594	0.484373	0.299676
H	2.434983	0.548209	1.675322
C	3.133983	-0.295422	-1.581483
H	4.058270	-0.414951	-2.157409
H	2.485608	0.372904	-2.146500

INT11



E = -1823.53429817

E_{ZPE} = -1823.054178

H = -1823.018011

G = -1823.123766

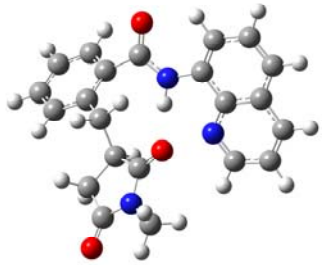
Im. Freq.; 0

C	1.849583	-4.004863	-1.461689
C	2.764249	-2.954776	-1.422273
C	2.376520	-1.610204	-1.546572
C	0.991907	-1.330145	-1.700877
C	0.081053	-2.403232	-1.765626
C	0.496444	-3.725913	-1.646325
H	2.195315	-5.031026	-1.367799
H	3.822163	-3.177611	-1.302956
H	-0.974872	-2.221433	-1.933394
H	-0.233962	-4.527955	-1.705297
C	0.483066	0.083780	-1.801598
O	1.208594	1.031310	-2.125061
N	-0.838907	0.281443	-1.475810
C	-1.463703	1.548359	-1.462036

C	-2.320239	1.927494	-0.375351
C	-1.269132	2.432807	-2.511391
C	-2.961716	3.212941	-0.436215
C	-1.881357	3.700658	-2.543731
H	-0.631370	2.130007	-3.331760
C	-3.377061	1.519572	1.686188
C	-3.831319	3.597977	0.611966
C	-2.721120	4.084948	-1.527317
H	-1.694724	4.358702	-3.387068
C	-4.046183	2.753060	1.672724
H	-3.516540	0.834385	2.515251
H	-4.319573	4.567173	0.558586
H	-3.214887	5.052256	-1.538096
H	-4.705038	3.010406	2.494531
N	-2.548619	1.120197	0.721862
C	3.870341	-0.107212	-0.073523
H	3.878898	-0.978208	0.596328
C	4.032582	1.985676	1.139491
C	5.297246	0.438868	-0.030262
O	3.823266	2.964440	1.839473
O	6.290215	-0.056353	-0.541491
N	5.303320	1.602097	0.725294
C	6.500894	2.363832	1.047052
H	6.387807	3.398032	0.710353
H	6.676019	2.358827	2.127043
H	7.344647	1.898820	0.535456
O	-0.759449	-2.456986	1.850982
C	0.283070	-1.764546	2.136552
O	0.225738	-0.506115	1.911801
C	1.508423	-2.423661	2.679970
H	2.179422	-1.687609	3.128408
H	1.225593	-3.177474	3.420979
H	2.026324	-2.937360	1.860870
Pd	-1.766891	-0.760934	1.177487
O	-3.585987	-1.553604	0.759344
C	-3.879474	-1.756046	-0.493103
C	-5.202758	-2.466218	-0.700793
H	-5.524959	-2.369095	-1.740073
H	-5.077016	-3.530522	-0.466697
H	-5.969085	-2.068025	-0.029218
O	-3.160688	-1.434711	-1.452695
H	-1.463280	-0.506927	-1.292625
C	3.026290	1.022684	0.549364
H	2.449181	1.560737	-0.210014

H	2.320364	0.690097	1.314391
C	3.504028	-0.587889	-1.497069
H	4.399199	-1.074404	-1.899630
H	3.283483	0.273442	-2.125549

sp3-product

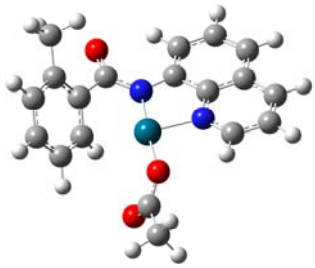


E = -1239.80142571
E_{ZPE} = -1239.426324
H = -1239.402329
G = -1239.480353
Im. Freq.; 0

C	3.144433	3.946593	1.054112
C	1.820600	3.801488	0.653449
C	1.375312	2.619015	0.040434
C	2.285950	1.572975	-0.227055
C	3.623867	1.755972	0.159133
C	4.051254	2.914559	0.803803
H	3.469260	4.860757	1.543326
H	1.108476	4.606051	0.813287
H	4.349428	0.980266	-0.071810
H	5.093867	3.018356	1.092931
C	-0.073486	2.618983	-0.375300
N	-0.821205	1.565261	0.066576
H	-0.383980	0.890406	0.687614
C	-2.164911	1.261746	-0.192685
C	-2.659470	0.082133	0.461965
C	-3.007094	1.990556	-1.015518
C	-4.009109	-0.326416	0.241918
C	-4.342973	1.570419	-1.216732
H	-2.640040	2.881157	-1.505540
C	-2.255733	-1.694265	1.871513
C	-4.443359	-1.502585	0.905077
C	-4.844214	0.441209	-0.610761
H	-4.977596	2.163310	-1.869841
C	-3.570509	-2.189304	1.716766

H	-1.552250	-2.219874	2.515569
H	-5.464662	-1.846846	0.761351
H	-5.871314	0.125485	-0.773407
H	-3.871669	-3.093305	2.236991
N	-1.808731	-0.602457	1.277228
O	-0.536085	3.556395	-1.032555
C	1.899196	0.303090	-0.966046
H	0.937206	0.431118	-1.468572
H	2.638366	0.111640	-1.754156
C	1.801802	-0.957538	-0.075485
C	3.114135	-1.677622	0.288163
H	1.257720	-0.708158	0.844617
H	3.440069	-1.526998	1.320493
H	3.944772	-1.384219	-0.364561
C	1.038943	-4.519927	-1.056794
H	1.663790	-5.333809	-0.687686
H	0.019835	-4.630375	-0.677879
H	1.016885	-4.540513	-2.150549
N	1.606905	-3.264299	-0.587111
C	2.842176	-3.150646	0.041395
C	0.967208	-2.044388	-0.747990
O	3.566727	-4.094439	0.311189
O	-0.103274	-1.908237	-1.317284

INT3’



E = -1195.66345773

E_{ZPE} = -1195.350034

H = -1195.326638

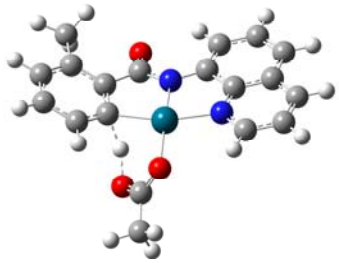
G = -1195.326638

Im. Freq.; 0

C	-3.968252	-1.693735	-0.934588
C	-2.754778	-2.335577	-0.652898
C	-1.885885	-1.714265	0.267990
C	-2.262155	-0.492959	0.892250
C	-3.485481	0.125581	0.575280

C	-4.330597	-0.474763	-0.349189
H	-4.644866	-2.157661	-1.648236
H	-1.719327	-0.147311	1.775393
H	-3.757450	1.051035	1.072546
H	-5.278845	-0.013090	-0.609209
C	-2.407523	-3.629977	-1.348618
H	-2.330372	-4.458528	-0.637243
H	-3.172835	-3.881491	-2.089252
H	-1.442468	-3.564832	-1.864758
C	-0.497450	-2.245564	0.522365
O	-0.244336	-3.440922	0.722474
N	0.403821	-1.230864	0.440425
C	1.794855	-1.338964	0.374525
C	2.455859	-0.145431	-0.045385
C	2.570878	-2.457085	0.660603
C	3.870682	-0.085352	-0.174936
C	3.978166	-2.393802	0.536884
H	2.092181	-3.372964	0.978622
C	2.224207	2.084359	-0.747275
C	4.433296	1.138992	-0.618820
C	4.626956	-1.246376	0.130780
H	4.555770	-3.283936	0.770931
C	3.618413	2.212979	-0.904646
H	1.542642	2.902876	-0.952762
H	5.511191	1.216798	-0.732510
H	5.708370	-1.216202	0.035764
H	4.024706	3.158459	-1.247316
N	1.675777	0.949621	-0.337528
Pd	-0.312957	0.588918	0.007375
O	-0.926443	2.476192	-0.544548
C	-1.486472	3.210062	0.373391
O	-1.692455	2.846426	1.541626
C	-1.888418	4.602835	-0.082382
H	-2.953294	4.757833	0.123881
H	-1.332969	5.345807	0.502015
H	-1.695562	4.762352	-1.145803

$TS_{3'-4'}$



E = -1195.63547097

E_{ZPE} = -1195.326856

H = -1195.304445

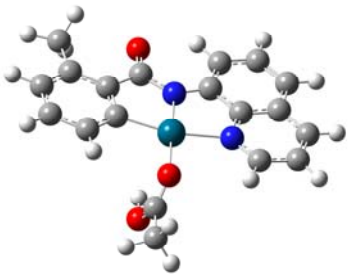
G = -1195.377226

Im. Freq.; 1 (-1411.5632 cm^{-1})

C	-4.331458	-1.571091	-0.741328
C	-3.192630	-2.185334	-0.191797
C	-2.084551	-1.366879	0.113204
C	-2.144115	0.043347	-0.085092
C	-3.288886	0.599414	-0.679264
C	-4.380765	-0.204769	-1.003500
H	-5.191176	-2.191433	-0.983229
H	-1.836581	1.044187	0.814913
H	-3.344876	1.672808	-0.839157
H	-5.270741	0.232364	-1.448791
C	-3.210035	-3.683888	0.002347
H	-3.108876	-3.957704	1.057328
H	-4.152541	-4.098544	-0.370351
H	-2.385253	-4.174088	-0.525398
C	-0.756941	-1.977741	0.475114
O	-0.626875	-3.105251	0.973772
N	0.285492	-1.164845	0.118805
C	1.645727	-1.464867	0.192002
C	2.517925	-0.365989	-0.099662
C	2.225791	-2.697617	0.483987
C	3.932797	-0.522210	-0.103443
C	3.631105	-2.845582	0.481116
H	1.592511	-3.542760	0.714194
C	2.697471	1.905031	-0.655883
C	4.714190	0.620980	-0.412961
C	4.479284	-1.796456	0.194842
H	4.044739	-3.823667	0.712204
C	4.103944	1.824672	-0.689834
H	2.175972	2.836419	-0.853402
H	5.797361	0.532686	-0.427510

H	5.557330	-1.928015	0.192405
H	4.680624	2.712093	-0.928230
N	1.942771	0.852024	-0.375726
Pd	-0.132468	0.746759	-0.228493
O	-0.556920	2.817909	-0.230151
C	-1.340467	3.119721	0.727928
O	-1.945292	2.249617	1.440962
C	-1.571879	4.575168	1.042686
H	-2.646247	4.786470	1.034748
H	-1.204012	4.785019	2.053522
H	-1.058902	5.219354	0.326429

INT4'

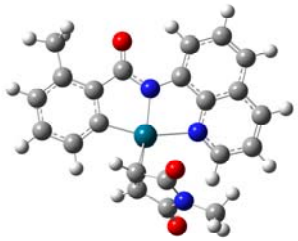


E = -1195.66708655
E_{ZPE} = -1195.353000
H = -1195.329936
G = -1195.404947
Im. Freq.; 0

C	-4.499778	-1.453482	-0.155049
C	-3.320167	-2.198076	-0.000552
C	-2.093922	-1.494894	-0.036061
C	-2.063146	-0.091999	-0.217051
C	-3.255454	0.615530	-0.375480
C	-4.473822	-0.072020	-0.343165
H	-5.455181	-1.972642	-0.129975
H	-1.186499	2.053751	1.662445
H	-3.252310	1.691268	-0.532170
H	-5.408128	0.472216	-0.465896
C	-3.422329	-3.693735	0.190654
H	-2.944871	-4.021183	1.119902
H	-4.474426	-3.998327	0.214890
H	-2.926241	-4.241843	-0.618054
C	-0.762129	-2.166617	0.095042
O	-0.608813	-3.387821	0.255898

N	0.272030	-1.261811	0.008845
C	1.633353	-1.545782	0.080632
C	2.514866	-0.412424	-0.032092
C	2.215822	-2.803989	0.245562
C	3.931358	-0.577248	0.023353
C	3.618411	-2.952331	0.300469
H	1.578401	-3.671586	0.330378
C	2.734460	1.898482	-0.310776
C	4.731892	0.588055	-0.099687
C	4.472970	-1.876050	0.194289
H	4.024276	-3.952523	0.429656
C	4.140978	1.820076	-0.266774
H	2.231793	2.852471	-0.444056
H	5.813925	0.491083	-0.061507
H	5.550909	-2.003658	0.236760
H	4.730883	2.725531	-0.365081
N	1.956066	0.832349	-0.196995
Pd	-0.206699	0.652591	-0.236113
O	-0.702355	2.733057	-0.511970
C	-1.124369	3.462484	0.395310
O	-1.377782	3.019470	1.617884
C	-1.391589	4.920738	0.207538
H	-2.438384	5.135141	0.449362
H	-0.768807	5.497011	0.900944
H	-1.176699	5.212392	-0.820821

INT5’



E = -1365.31326691

E_{ZPE} = -1364.963363

H = -1364.938000

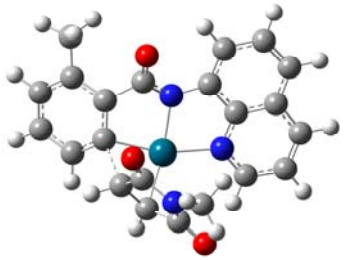
G = -1365.016760

Im. Freq.; 0

C	-4.924637	-1.292493	-0.190622
C	-4.393830	-0.005574	-0.017669
C	-2.985609	0.131571	-0.026664
C	-2.154430	-0.995820	-0.188968

C	-2.710564	-2.260394	-0.365937
C	-4.103070	-2.401690	-0.368994
H	-6.004276	-1.419709	-0.188553
H	-2.098170	-3.146143	-0.500897
H	-4.543493	-3.386429	-0.507132
C	-5.348072	1.151776	0.160955
H	-5.236919	1.899919	-0.631089
H	-6.381087	0.787965	0.147073
H	-5.180303	1.678934	1.105833
C	-2.299320	1.451758	0.105700
O	-2.895897	2.523405	0.276291
N	-0.931075	1.331098	-0.004007
C	-0.019333	2.379217	0.123843
C	1.351532	2.054669	-0.155378
C	-0.317397	3.694387	0.484662
C	2.356612	3.069501	-0.113582
C	0.691655	4.678605	0.554764
H	-1.339978	3.961372	0.704116
C	2.910034	0.467243	-0.845582
C	3.679153	2.704809	-0.465609
C	2.004581	4.391264	0.258126
H	0.408286	5.687646	0.842768
C	3.953381	1.413423	-0.850154
H	3.110420	-0.547945	-1.164565
H	4.460411	3.460278	-0.441867
H	2.775933	5.155147	0.296608
H	4.949400	1.105913	-1.151153
N	1.665041	0.756832	-0.488094
Pd	-0.183609	-0.534201	-0.240080
C	0.240714	-2.491457	0.733549
C	0.547840	-2.670352	-0.605783
H	-0.671731	-2.734597	1.260814
H	-0.078325	-3.053021	-1.401355
C	2.039442	-2.733669	-0.723735
C	1.537641	-2.395032	1.493069
O	1.699777	-2.234420	2.690080
O	2.707964	-2.912045	-1.729521
N	2.556444	-2.565254	0.562263
C	3.971225	-2.513913	0.897307
H	4.541128	-2.707364	-0.012653
H	4.236249	-1.530859	1.297582
H	4.205560	-3.279071	1.642427

$TS_{5'\text{-}6'}$



E = -1365.26771167

E_{ZPE} = -1364.919672

H = -1364.894834

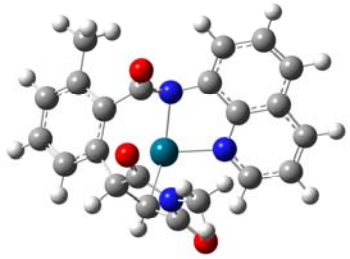
G = -1364.972935

Im. Freq.; 1 (-273.8933 cm^{-1})

C	-4.523854	1.213805	-0.977006
C	-3.568992	1.694255	-0.066036
C	-2.378537	0.956747	0.118023
C	-2.215588	-0.292624	-0.551403
C	-3.159879	-0.698818	-1.506232
C	-4.306228	0.059874	-1.726098
H	-5.439591	1.781045	-1.122428
H	-3.035270	-1.643595	-2.028374
H	-5.043004	-0.267738	-2.454342
C	-3.829204	3.013279	0.625772
H	-3.056382	3.754551	0.393346
H	-4.796104	3.417792	0.310047
H	-3.837676	2.902713	1.714083
C	-1.176231	1.653225	0.732330
O	-1.244856	2.415392	1.706933
N	-0.061767	1.398138	-0.014987
C	1.217112	1.898368	0.205399
C	2.283930	1.093046	-0.319431
C	1.545587	3.098401	0.830057
C	3.638317	1.527975	-0.229547
C	2.890452	3.519054	0.920674
H	0.756317	3.711890	1.244563
C	2.930056	-0.894229	-1.384583
C	4.636965	0.683905	-0.779985
C	3.922920	2.766844	0.400723
H	3.105845	4.465348	1.409986
C	4.287358	-0.516388	-1.356276
H	2.624043	-1.849006	-1.798116
H	5.677080	0.996223	-0.734720
H	4.953478	3.103648	0.466723

H	5.031565	-1.183533	-1.778081
N	1.969441	-0.120109	-0.896471
Pd	-0.101158	-0.497536	-0.798864
C	-1.577926	-1.985439	0.154828
C	-0.511353	-2.579239	-0.658069
H	-2.581932	-2.392068	0.107042
H	-0.707340	-3.148559	-1.561581
C	0.511506	-3.086182	0.280123
C	-1.038562	-1.953432	1.580199
O	-1.548076	-1.432910	2.558719
O	1.517854	-3.743566	0.043987
N	0.139566	-2.680079	1.578560
C	0.975731	-2.860318	2.754068
H	1.570442	-3.765567	2.620541
H	1.644921	-2.003755	2.894560
H	0.335356	-2.962393	3.632511

INT6'

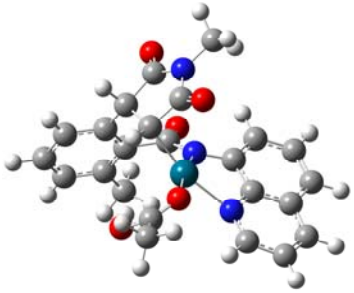


E = -1365.28048440
E_{ZPE} = -1364.931388
H = -1364.906055
G = -1364.985537
Im. Freq.; 0

C	-4.310762	1.496768	-0.927993
C	-3.202146	1.865816	-0.170202
C	-2.274290	0.876482	0.256995
C	-2.501883	-0.505025	-0.074913
C	-3.627676	-0.804290	-0.886279
C	-4.514413	0.167661	-1.308727
H	-5.019595	2.260816	-1.236609
H	-3.819875	-1.843857	-1.137449
H	-5.377120	-0.104653	-1.910059
C	-2.988543	3.323407	0.173412
H	-2.108665	3.729068	-0.342041
H	-3.854933	3.919233	-0.128551

H	-2.829092	3.467515	1.246454
C	-0.999621	1.462079	0.897130
O	-0.945340	1.817969	2.077560
N	-0.036944	1.564694	-0.062389
C	1.307112	1.854624	0.203438
C	2.262738	0.957261	-0.368925
C	1.771498	2.941933	0.930421
C	3.660437	1.205176	-0.242188
C	3.157844	3.176131	1.071245
H	1.057497	3.621125	1.382901
C	2.666583	-1.026563	-1.562908
C	4.551532	0.285678	-0.852476
C	4.089803	2.342061	0.490312
H	3.486570	4.040911	1.641072
C	4.059497	-0.816531	-1.514221
H	2.249856	-1.911069	-2.029866
H	5.621945	0.460492	-0.782536
H	5.154235	2.536523	0.585660
H	4.717243	-1.539864	-1.983881
N	1.806552	-0.172224	-1.023492
Pd	-0.254696	-0.312894	-0.962794
C	-1.778855	-1.816369	0.392742
C	-0.751171	-2.326683	-0.633423
H	-2.577863	-2.555954	0.546572
H	-1.101632	-2.908704	-1.483732
C	0.336027	-2.924327	0.156113
C	-0.993489	-1.801987	1.703886
O	-1.320619	-1.284909	2.760504
O	1.283271	-3.616430	-0.211985
N	0.154472	-2.548765	1.501750
C	1.139391	-2.823238	2.534860
H	1.443077	-3.871481	2.480827
H	2.022945	-2.189035	2.404585
H	0.686687	-2.617317	3.505671

INT7’

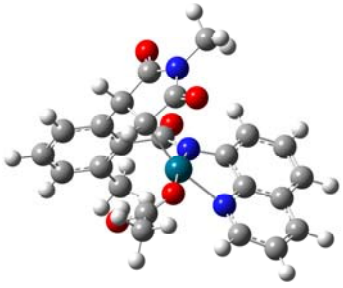


E = -1594.43061010
E_{ZPE} = -1594.015961
H = -1593.985288
G = -1594.077367
Im. Freq.; 0

C	3.574434	-0.982776	-2.919882
C	2.395009	-1.530704	-2.401583
C	2.032184	-1.232039	-1.065618
C	2.859361	-0.410156	-0.277293
C	4.045982	0.097819	-0.823008
C	4.403900	-0.180553	-2.138701
H	3.846738	-1.198630	-3.950348
H	4.688956	0.721223	-0.205931
H	5.323521	0.224434	-2.553145
C	1.549443	-2.414576	-3.291186
H	0.483679	-2.165322	-3.231307
H	1.861497	-2.312421	-4.335757
H	1.642886	-3.468963	-3.009850
C	0.786100	-1.905361	-0.532861
O	0.721302	-3.143543	-0.590463
N	-0.240989	-1.106903	-0.116259
C	-1.552380	-1.626871	-0.031161
C	-2.601237	-0.730584	-0.422839
C	-1.910398	-2.915449	0.348651
C	-3.958009	-1.162788	-0.481002
C	-3.262132	-3.333394	0.310839
H	-1.147872	-3.609889	0.668751
C	-3.186083	1.419574	-1.121740
C	-4.927109	-0.218215	-0.904863
C	-4.271722	-2.493917	-0.103759
H	-3.495757	-4.349691	0.616802
C	-4.545291	1.064183	-1.232190
H	-2.853818	2.430377	-1.340556
H	-5.969928	-0.519585	-0.961933
H	-5.305385	-2.826491	-0.135799
H	-5.266243	1.806297	-1.558747
N	-2.255699	0.558970	-0.735787
C	2.499223	0.011972	1.127431
C	1.398231	1.070726	1.279634
C	3.415006	0.420550	1.583821
H	1.742320	2.102904	1.190215
C	0.790360	0.787720	2.612444
C	2.070353	-1.077872	2.110810

O	2.468132	-2.230777	2.182285
O	0.054269	1.499727	3.292076
N	1.177404	-0.503141	2.998244
C	0.627306	-1.212367	4.142163
H	0.155436	-0.481961	4.801024
H	-0.117615	-1.947058	3.818097
H	1.429423	-1.729764	4.674283
Pd	-0.282176	0.919927	0.063491
O	-0.533451	3.044984	0.219297
C	0.050388	3.849920	-0.519697
O	0.895766	3.473606	-1.468455
H	0.966555	2.490728	-1.475062
C	-0.128550	5.328467	-0.408203
H	0.812261	5.775514	-0.065698
H	-0.357566	5.752319	-1.391052
H	-0.923324	5.557767	0.301997

$TS_{7'-8'}$



E = -1594.39024166

E_{ZPE} = -1593.980785

H = -1593.950841

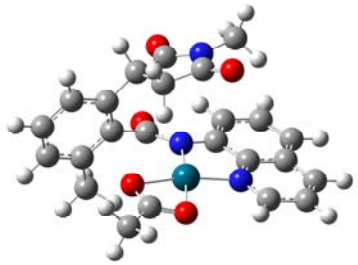
G = -1594.039818

Im. Freq.; 1 (-1461.5149 cm^{-1})

C	3.613738	-1.162286	-2.721100
C	2.321010	-1.556144	-2.359448
C	1.903994	-1.378442	-1.017443
C	2.786403	-0.825788	-0.069569
C	4.082988	-0.470003	-0.464171
C	4.497196	-0.632487	-1.782100
H	3.931982	-1.283007	-3.753735
H	4.766686	-0.054663	0.272143
H	5.503074	-0.345759	-2.077452
C	1.412056	-2.151328	-3.411548
H	0.411245	-1.703691	-3.391789
H	1.831567	-1.994570	-4.410532

H	1.279416	-3.228095	-3.261146
C	0.535702	-1.906331	-0.654571
O	0.284221	-3.100209	-0.872390
N	-0.384707	-1.021714	-0.161267
C	-1.754927	-1.370875	-0.154877
C	-2.641517	-0.318494	-0.521957
C	-2.304661	-2.614405	0.128941
C	-4.041463	-0.528263	-0.660240
C	-3.701574	-2.820282	0.022192
H	-1.663486	-3.433195	0.422859
C	-2.843836	1.939661	-1.124480
C	-4.827173	0.578252	-1.070722
C	-4.560167	-1.817390	-0.373289
H	-4.095495	-3.805701	0.255296
C	-4.232712	1.798319	-1.312495
H	-2.341718	2.890143	-1.266785
H	-5.899995	0.451917	-1.189565
H	-5.628221	-1.993606	-0.461403
H	-4.811810	2.659188	-1.628767
N	-2.089415	0.917804	-0.744286
C	2.385358	-0.498314	1.354022
C	1.600182	0.815709	1.538297
H	3.312074	-0.426868	1.939744
H	2.227073	1.593787	1.995928
C	0.554047	0.508103	2.582405
C	1.553269	-1.533244	2.113811
O	1.712280	-2.742698	2.131835
O	-0.201618	1.286826	3.153368
N	0.609369	-0.852382	2.869477
C	-0.339195	-1.509181	3.757003
H	-0.437488	-0.930908	4.678337
H	-1.319275	-1.591553	3.275624
H	0.039440	-2.507156	3.981527
Pd	-0.173547	1.000788	-0.007505
O	-0.155708	3.094298	-0.069434
C	1.013030	3.583511	-0.211709
O	2.064475	2.872629	-0.104814
H	1.672720	1.732024	0.494905
C	1.154967	5.052758	-0.500615
H	1.684584	5.530834	0.331093
H	1.764308	5.188739	-1.400200
H	0.180263	5.524841	-0.634877

INT8’



E = -1594.44388359

E_{ZPE} = -1594.029210

H = -1593.998450

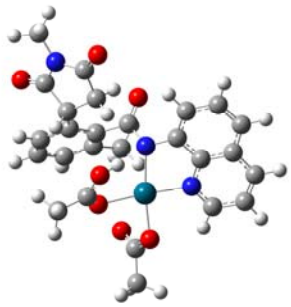
G = -1594.090976

Im. Freq.; 0

C	4.333487	-0.343764	-1.571861
C	2.984398	-0.471528	-1.911408
C	2.079491	-0.990186	-0.954880
C	2.539376	-1.405282	0.312526
C	3.907643	-1.284088	0.602734
C	4.797947	-0.750393	-0.322045
H	5.026817	0.069886	-2.300262
H	4.273015	-1.613219	1.572766
H	5.852315	-0.660139	-0.073621
C	2.519662	-0.055282	-3.289032
H	1.620321	0.571221	-3.248208
H	3.301541	0.512829	-3.803098
H	2.273755	-0.926897	-3.906537
C	0.656930	-1.210270	-1.415061
O	0.447790	-2.080900	-2.271126
N	-0.319538	-0.428710	-0.858265
C	-1.686134	-0.674845	-1.099463
C	-2.565883	0.362794	-0.679073
C	-2.270381	-1.822191	-1.635988
C	-3.981029	0.264876	-0.799690
C	-3.675852	-1.925038	-1.757065
H	-1.648893	-2.641920	-1.961250
C	-2.730657	2.497891	0.290788
C	-4.752734	1.362761	-0.342577
C	-4.527525	-0.916690	-1.359239
H	-4.085012	-2.837552	-2.182284
C	-4.134615	2.469901	0.198853
H	-2.199286	3.345983	0.710227
H	-5.835483	1.318235	-0.422986

H	-5.604330	-1.010513	-1.463998
H	-4.703345	3.320905	0.557318
N	-1.992665	1.480676	-0.135594
C	1.677083	-1.941037	1.451565
C	1.162841	-0.880315	2.454639
H	2.304281	-2.654518	2.002317
H	1.745900	-0.842287	3.379670
C	-0.261689	-1.288037	2.763551
C	0.434153	-2.763730	1.112928
O	0.341121	-3.668477	0.301859
O	-1.033137	-0.771441	3.559023
N	-0.591461	-2.375256	1.971965
C	-1.905138	-3.001494	2.006642
H	-2.084312	-3.439329	2.993301
H	-2.682295	-2.261178	1.799911
H	-1.926199	-3.784595	1.248345
Pd	0.011487	1.430789	-0.048349
O	0.510057	3.322169	0.722987
C	1.766539	3.057419	0.665156
O	2.100200	1.902922	0.240216
H	1.157960	0.127787	2.027905
C	2.788770	4.077852	1.050584
H	3.655193	3.590473	1.506215
H	3.128437	4.598848	0.146496
H	2.358496	4.812572	1.735894

INT9’



E = -1823.52474752

E_{ZPE} = -1823.046116

H = -1823.009739

G = -1823.114433

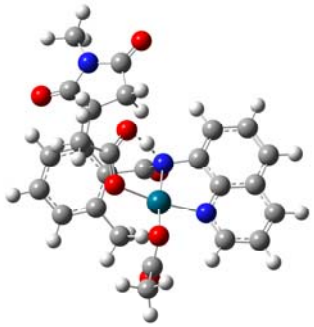
Im. Freq.; 0

C	-1.005054	-2.936257	-2.170522
C	-0.580086	-1.609872	-2.074604
C	-1.254263	-0.730942	-1.191068

C	-2.411348	-1.154094	-0.501324
C	-2.784406	-2.507440	-0.606973
C	-2.085630	-3.392928	-1.419018
H	-0.477836	-3.614179	-2.836639
H	-3.649102	-2.861187	-0.056027
H	-2.396341	-4.432518	-1.481167
C	0.570959	-1.130679	-2.930869
H	1.441961	-0.846302	-2.329401
H	0.891147	-1.920391	-3.616944
H	0.284308	-0.256199	-3.527417
C	-0.696766	0.671970	-1.091786
O	-1.097858	1.542389	-1.876090
N	0.255735	0.897106	-0.114537
C	0.842917	2.198592	-0.092296
C	2.260529	2.259155	-0.096445
C	0.141297	3.393808	-0.071115
C	2.956221	3.501053	-0.142092
C	0.822671	4.633276	-0.086936
H	-0.941396	3.387282	-0.046887
C	4.275788	1.055202	-0.077340
C	4.372747	3.456670	-0.182544
C	2.198536	4.699125	-0.136458
H	0.237447	5.548296	-0.069669
C	5.026467	2.244205	-0.161606
H	4.748406	0.082120	-0.011423
H	4.931284	4.387782	-0.226149
H	2.715514	5.653839	-0.163280
H	6.108798	2.181380	-0.191364
N	2.949955	1.071685	-0.048352
C	-3.339652	-0.298001	0.364675
C	-3.082426	1.194601	0.650342
H	-3.417040	-0.799706	1.340575
H	-2.490053	1.388037	1.546338
C	-4.459529	1.807129	0.775978
C	-4.801564	-0.290721	-0.139545
O	-5.411265	-1.178714	-0.708332
O	-4.753282	2.906738	1.218142
N	-5.375898	0.915745	0.239727
C	-6.787942	1.230221	0.070755
H	-7.146510	1.751665	0.960933
H	-6.938093	1.869789	-0.804699
H	-7.336033	0.296898	-0.064370
C	-0.316519	-1.804222	2.028056
O	0.551334	-2.056971	1.177600

H	-2.615841	1.700745	-0.198225
C	-0.930133	-2.873811	2.872721
H	-1.818025	-3.256441	2.354491
H	-0.224532	-3.696624	3.001063
H	-1.239899	-2.472651	3.840568
Pd	1.749139	-0.505859	0.353626
O	3.351177	-1.680016	0.855278
C	3.508040	-2.748707	0.114609
C	4.625487	-3.660851	0.591212
H	4.864165	-4.396348	-0.180785
H	5.519499	-3.084538	0.850024
H	4.300072	-4.188575	1.496141
O	2.820152	-3.025652	-0.873552
O	-0.784773	-0.586456	2.241350
H	-0.422741	0.046164	1.559614

$TS_{9'\text{-}10'}$



E = -1823.51372085

E_{ZPE} = -1823.039882

H = -1823.003795

G = -1823.108132

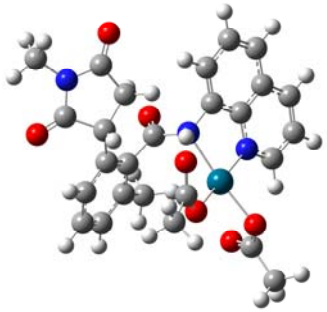
Im. Freq.; 1 (-1606.2558 cm^{-1})

C	-1.000661	-3.115503	-2.087795
C	-0.550258	-1.796404	-2.005145
C	-1.245650	-0.884011	-1.169155
C	-2.435097	-1.271286	-0.512988
C	-2.831131	-2.618100	-0.606592
C	-2.120569	-3.533447	-1.373034
H	-0.459212	-3.819614	-2.714009
H	-3.721646	-2.942002	-0.080453
H	-2.449386	-4.567893	-1.425157
C	0.644009	-1.371872	-2.830579
H	1.417208	-0.878714	-2.231695
H	1.106687	-2.241939	-3.305384

H	0.346631	-0.672097	-3.621070
C	-0.632707	0.493438	-1.077530
O	-0.724809	1.298898	-1.993597
N	0.115975	0.783869	0.096493
C	0.669927	2.121434	0.133759
C	2.064092	2.243994	-0.090310
C	-0.086636	3.261291	0.309003
C	2.673270	3.525672	-0.198535
C	0.519584	4.539470	0.249379
H	-1.155378	3.187437	0.477202
C	4.105638	1.163039	-0.474818
C	4.062139	3.569511	-0.481479
C	1.864315	4.676755	-0.014593
H	-0.098869	5.419612	0.396954
C	4.766780	2.397084	-0.638507
H	4.635360	0.223947	-0.574644
H	4.555967	4.532636	-0.576103
H	2.322630	5.659004	-0.083552
H	5.826332	2.397445	-0.869828
N	2.811311	1.092912	-0.195488
C	-3.374939	-0.377291	0.296213
C	-3.113482	1.126313	0.496003
H	-3.456198	-0.824411	1.297603
H	-2.543094	1.363659	1.394806
C	-4.487709	1.756451	0.561739
C	-4.832425	-0.392832	-0.223190
O	-5.441911	-1.307665	-0.747060
O	-4.773496	2.886305	0.925251
N	-5.404056	0.837675	0.077936
C	-6.814072	1.147419	-0.118925
H	-7.186802	1.690549	0.752394
H	-6.950546	1.764717	-1.012236
H	-7.358739	0.210155	-0.238065
C	-0.326088	-1.674476	2.180540
O	0.635770	-1.998192	1.417926
H	-2.623841	1.584205	-0.367971
C	-0.913228	-2.756491	3.049307
H	-1.581899	-3.370397	2.433270
H	-0.120903	-3.404626	3.432707
H	-1.486814	-2.324962	3.872207
Pd	1.753000	-0.528437	0.464283
O	3.366919	-1.647166	1.019922
C	4.009831	-2.292281	0.083902
C	5.060577	-3.249480	0.621447

H	5.763095	-3.520628	-0.170492
H	5.597709	-2.812169	1.468528
H	4.563158	-4.159923	0.977951
O	3.802972	-2.171526	-1.130228
O	-0.849720	-0.508460	2.241225
H	-0.420948	0.264981	1.221201

INT10’



E = -1823.52582752

E_{ZPE} = -1823.046325

H = -1823.010157

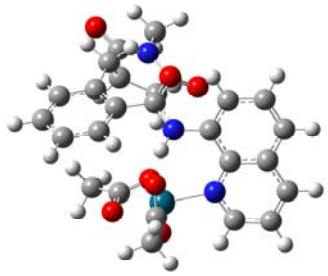
G = -1823.114233

Im. Freq.; 0

C	-1.056193	-3.146916	-2.088551
C	-0.578035	-1.837598	-2.010827
C	-1.257658	-0.907618	-1.177023
C	-2.451600	-1.273138	-0.513798
C	-2.872277	-2.611680	-0.603707
C	-2.182829	-3.540958	-1.372026
H	-0.527861	-3.864059	-2.710769
H	-3.766716	-2.917220	-0.074368
H	-2.532298	-4.568634	-1.422209
C	0.643763	-1.457438	-2.816972
H	1.439128	-1.033284	-2.193662
H	1.056772	-2.340686	-3.312428
H	0.397800	-0.718111	-3.587636
C	-0.596583	0.444306	-1.097488
O	-0.507569	1.195633	-2.048244
N	0.077930	0.783372	0.143310
C	0.619234	2.137818	0.185060
C	2.005415	2.274510	-0.075184
C	-0.153346	3.260645	0.383532
C	2.586955	3.567291	-0.200355
C	0.430980	4.548627	0.311555
H	-1.215402	3.173065	0.580378

C	4.057477	1.234744	-0.497421
C	3.967320	3.638629	-0.517472
C	1.764081	4.704779	0.006132
H	-0.196516	5.418269	0.479733
C	4.690721	2.479769	-0.685566
H	4.604312	0.305985	-0.601146
H	4.438718	4.611280	-0.627090
H	2.204573	5.694135	-0.076791
H	5.744368	2.498870	-0.941526
N	2.771632	1.138012	-0.187827
C	-3.369545	-0.362674	0.299337
C	-3.088711	1.139940	0.456281
H	-3.423941	-0.789755	1.311051
H	-2.505466	1.391461	1.343079
C	-4.452115	1.792098	0.527929
C	-4.840463	-0.375237	-0.183481
O	-5.473413	-1.296552	-0.665397
O	-4.712253	2.937457	0.860110
N	-5.389800	0.871652	0.094581
C	-6.800496	1.196127	-0.072739
H	-7.162625	1.706019	0.823257
H	-6.942565	1.849517	-0.938902
H	-7.350587	0.266640	-0.222341
C	-0.286894	-1.797018	2.142257
O	0.715792	-2.049540	1.366153
H	-2.604206	1.571877	-0.425653
C	-0.824956	-3.012648	2.871321
H	-1.245351	-3.715877	2.143232
H	-0.012117	-3.527739	3.393585
H	-1.599611	-2.721987	3.584312
Pd	1.761078	-0.515843	0.496312
O	3.408466	-1.593199	1.019066
C	4.049160	-2.220300	0.068932
C	5.117092	-3.167947	0.589137
H	5.810270	-3.431751	-0.213390
H	5.662565	-2.726446	1.428695
H	4.632563	-4.082607	0.952404
O	3.829269	-2.091657	-1.141995
O	-0.814997	-0.673194	2.304011
H	-0.419076	0.448324	1.004562

INT11

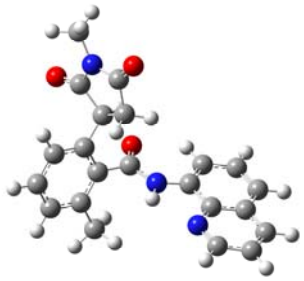


E = -1823.53408307
E_{ZPE} = -1823.055380
H = -1823.018722
G = -1823.125426
Im. Freq.; 0

C	1.423403	3.867111	-0.813802
C	0.792147	2.765977	-1.403306
C	1.313607	1.479042	-1.153764
C	2.475867	1.303057	-0.375663
C	3.092963	2.431620	0.178378
C	2.562030	3.702980	-0.027156
H	1.018592	4.862334	-0.981045
H	3.986157	2.317664	0.784756
H	3.042365	4.568083	0.422421
C	-0.392253	2.976304	-2.318619
H	-1.153405	2.197713	-2.209775
H	-0.860906	3.947050	-2.128356
H	-0.074762	2.960721	-3.369533
C	0.635647	0.311751	-1.835165
O	0.732384	0.152840	-3.054765
N	-0.103391	-0.490371	-1.004712
C	-0.797898	-1.665476	-1.351631
C	-1.794238	-2.175331	-0.450599
C	-0.498129	-2.394990	-2.495513
C	-2.323142	-3.488617	-0.680999
C	-1.100145	-3.642406	-2.755622
H	0.233340	-2.002172	-3.186938
C	-3.031348	-2.028279	1.543218
C	-3.184776	-4.053622	0.291349
C	-1.972756	-4.202282	-1.853706
H	-0.829468	-4.174648	-3.662851
C	-3.504499	-3.345786	1.424318
H	-3.325295	-1.413247	2.386643
H	-3.575459	-5.054123	0.126942
H	-2.399672	-5.187930	-2.014271

H	-4.140892	-3.755198	2.201015
N	-2.242691	-1.454149	0.636803
C	3.106323	-0.071780	-0.233074
C	4.080081	-0.461866	-1.371223
H	2.319201	-0.831315	-0.169834
H	3.632566	-1.099757	-2.137675
C	5.219981	-1.176381	-0.675951
C	3.928174	-0.291495	1.039758
O	3.644502	0.029559	2.180583
O	6.143203	-1.792915	-1.183872
N	5.076627	-0.996239	0.692694
C	6.050038	-1.489082	1.656088
H	6.210886	-2.559762	1.505123
H	7.002956	-0.965184	1.534791
H	5.656581	-1.308899	2.657262
C	-0.233479	0.128880	2.704306
O	-1.454952	0.572156	2.593873
H	4.489290	0.422005	-1.874409
C	0.297626	0.143091	4.123354
H	-0.057466	1.023472	4.666265
H	-0.067092	-0.748011	4.649707
H	1.389663	0.121048	4.105813
Pd	-2.317868	0.627077	0.768633
O	-2.816352	2.664617	0.571642
C	-3.415147	2.419955	-0.533896
C	-4.143314	3.487694	-1.281692
H	-4.112054	3.287924	-2.356034
H	-5.193721	3.486552	-0.963590
H	-3.717044	4.469048	-1.059081
O	-3.387789	1.209046	-0.957749
O	0.456260	-0.298866	1.767809
H	-0.024870	-0.295493	0.005547

sp2-product



E = -1239.80238098

E_{ZPE} = -1239.429113

H = -1239.404345
G = -1239.485827
Im. Freq.; 0

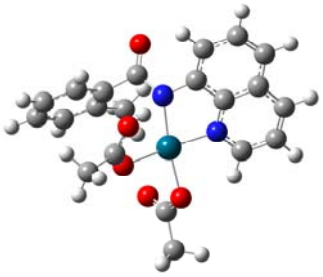
C	2.707032	3.197748	1.057961
C	1.507235	3.766944	0.635862
C	0.555102	3.010618	-0.056784
C	0.842640	1.656473	-0.328487
C	2.063049	1.077419	0.071481
C	2.982210	1.861550	0.778760
H	3.434429	3.798934	1.597021
H	1.303475	4.815128	0.840377
H	3.924829	1.429349	1.103132
C	-0.739296	3.653524	-0.502637
H	-1.012797	3.359326	-1.522249
H	-1.578476	3.381201	0.150652
H	-0.651791	4.744324	-0.481746
C	-0.158585	0.829337	-1.102417
N	-1.264301	0.480916	-0.382444
H	-1.325397	0.804737	0.580407
C	-2.401739	-0.235379	-0.784464
C	-3.425109	-0.358930	0.215954
C	-2.587874	-0.811313	-2.029446
C	-4.620200	-1.075554	-0.090699
C	-3.782117	-1.514699	-2.314616
H	-1.818185	-0.723268	-2.783205
C	-4.139508	0.103184	2.356115
C	-5.595003	-1.171332	0.935441
C	-4.781335	-1.650746	-1.378197
H	-3.899184	-1.954380	-3.301341
C	-5.357696	-0.585902	2.157573
H	-3.934651	0.575218	3.315706
H	-6.519768	-1.709295	0.741382
H	-5.693905	-2.194796	-1.606852
H	-6.083314	-0.641704	2.963153
O	0.033539	0.500094	-2.276713
N	-3.204233	0.219949	1.430169
C	2.356122	-0.388447	-0.194671
C	2.061836	-1.355337	0.976026
H	1.791964	-0.713047	-1.075896
H	1.116612	-1.895132	0.877411
H	2.049849	-0.835868	1.941294
C	3.814866	-0.685518	-0.548771
C	3.224815	-2.327579	0.980862

O	4.535696	-0.064615	-1.310430
O	3.340191	-3.349902	1.636947
N	4.198569	-1.843567	0.116599
C	5.487135	-2.491614	-0.083586
H	5.784606	-2.982091	0.844843
H	5.423977	-3.238844	-0.881296
H	6.220564	-1.732174	-0.359057

Cartesian coordinates (Å) and energies (hartrees) of all the optimized structures of intermediates in Figure S4.

Electronic energies (E), as well as zero-point energy (E_{ZPE}), enthalpy (H), Gibbs free energy (G), and imaginary frequency (Im. Freq.) for all structures calculated at B3LYP/6-31G(d)-LANL2DZ level of theory are provided. SMD solvent effects were incorporated for all calculations with acetonitrile as the solvent.

INT2



E = -1424.77142135

E_{ZPE} = -1424.395021

H = -1424.365783

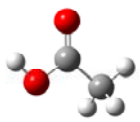
G = -1424.456743

Im. Freq.; 0

C	4.631746	-1.077432	-1.276045
C	4.278231	-1.906121	-0.208472
C	2.932918	-2.200877	0.014631
C	1.933404	-1.654874	-0.804836
C	2.280549	-0.838512	-1.900125
C	3.640218	-0.561506	-2.111401
H	5.676099	-0.844106	-1.466665
H	5.041974	-2.330429	0.437736
H	2.653531	-2.861186	0.831380
H	3.921137	0.065849	-2.954565
C	1.243538	-0.246966	-2.827733
H	0.345011	-0.869193	-2.893797
H	0.940792	0.749869	-2.481617
H	1.650325	-0.135258	-3.839191
C	0.506491	-2.104625	-0.581200

O	0.141166	-3.171706	-1.075271
N	-0.307250	-1.298633	0.206832
H	0.589848	-1.148464	1.826429
C	-1.693593	-1.633219	0.246152
C	-2.602430	-0.572496	-0.012610
C	-2.213846	-2.893889	0.494695
C	-4.007719	-0.793465	-0.077915
C	-3.611415	-3.116848	0.461234
H	-1.546570	-3.719055	0.707144
C	-2.871448	1.712570	-0.478150
C	-4.832134	0.319559	-0.383262
C	-4.497740	-2.101542	0.169774
H	-3.982646	-4.117571	0.663216
C	-4.267726	1.558929	-0.593741
H	-2.392093	2.678360	-0.584680
H	-5.907870	0.180322	-0.445306
H	-5.568017	-2.281631	0.132175
H	-4.873818	2.426670	-0.829645
N	-2.079623	0.685435	-0.200033
Pd	-0.122504	0.774819	0.323785
O	-0.183709	2.810466	0.509705
C	0.476314	3.480134	-0.399772
O	1.046142	2.984964	-1.375680
O	1.758252	0.829918	1.325259
C	1.998315	0.061975	2.273789
O	1.266671	-0.997848	2.553766
C	0.487737	4.981273	-0.142845
H	1.046372	5.196382	0.775781
H	0.956746	5.506325	-0.978362
H	-0.531799	5.355138	0.000690
C	3.153802	0.283936	3.197102
H	2.786761	0.351250	4.227175
H	3.833759	-0.572999	3.142902
H	3.684316	1.198047	2.929670

AcOH



E = -229.090385467

E_{ZPE} = -229.028704

H = -229.023117

G = -229.056864

Im. Freq.; 0

C	1.395124	-0.114355	0.000000
C	1.682809	-0.694972	-0.883286
H	1.682808	-0.694997	0.883270
H	1.921337	0.841105	0.000014
C	-0.090376	0.121695	0.000000
O	-0.640104	1.205043	0.000000
O	-0.782609	-1.041071	0.000000
H	-1.733741	-0.806951	-0.000002

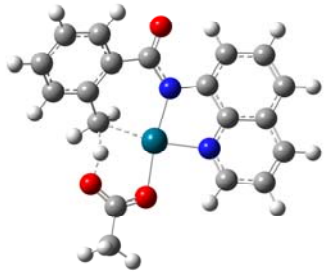
INT3

E = -1195.68047747
E_{ZPE} = -1195.367111
H = -1195.343827
G = -1195.420172
Im. Freq.; 0

C	-3.857715	-1.077398	1.472055
C	-2.488819	-1.268896	1.229880
C	-2.089926	-1.621115	-0.077877
C	-3.053373	-1.795577	-1.082599
C	-4.406704	-1.581302	-0.826426
C	-4.809823	-1.219701	0.461395
H	-4.179556	-0.820993	2.479050
H	-2.730036	-2.104274	-2.073324
H	-5.139100	-1.707298	-1.619431
H	-5.862295	-1.061915	0.683254
C	-1.506215	-1.118623	2.370248
H	-0.959874	-0.168541	2.305627
H	-2.029878	-1.137392	3.331696
H	-0.756733	-1.917986	2.376001
C	-0.669869	-2.003074	-0.417143
O	-0.456261	-3.164128	-0.794023
N	0.301675	-1.048004	-0.270264
C	1.671503	-1.363249	-0.289875

C	2.538735	-0.266034	-0.004332
C	2.275422	-2.603372	-0.507068
C	3.951545	-0.410404	0.092959
C	3.680348	-2.748638	-0.420772
H	1.660308	-3.457949	-0.741692
C	2.675674	2.032027	0.471030
C	4.707434	0.748662	0.403369
C	4.515802	-1.692513	-0.125521
H	4.102584	-3.734642	-0.595752
C	4.076011	1.959220	0.596481
H	2.137613	2.965326	0.597821
H	5.787841	0.667905	0.485550
H	5.592123	-1.819659	-0.060271
H	4.631742	2.859215	0.835437
N	1.952483	0.956894	0.182503
Pd	-0.032067	0.974769	-0.143722
O	-0.517650	3.014239	-0.124103
C	-1.736230	2.761788	-0.444376
O	-2.062775	1.539063	-0.586779
C	-2.712324	3.875019	-0.662296
H	-2.472225	4.384301	-1.603625
H	-3.732382	3.488493	-0.715416
H	-2.629525	4.609518	0.145027

$TS_{3\text{-}4}$



E = -1195.64137486

E_{ZPE} = -1195.332063

H = -1195.310184

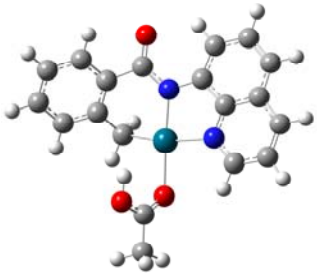
G = -1195.382438

Im. Freq.; 1 (-1428.6267 cm^{-1})

C	4.170133	-0.505190	-0.110336
C	2.805443	-0.686656	-0.396143
C	2.165269	-1.849351	0.085391
C	2.914066	-2.792769	0.810399
C	4.260784	-2.589303	1.100768

C	4.893743	-1.434321	0.634946
H	4.668463	0.383321	-0.491172
H	2.412234	-3.693432	1.146913
H	4.810822	-3.326524	1.679307
H	5.946240	-1.259985	0.843277
C	2.091071	0.355323	-1.192684
H	2.018778	1.504236	-0.426025
H	2.802662	0.969928	-1.760951
H	1.441850	-0.066294	-1.969102
C	0.719735	-2.226720	-0.145838
O	0.440405	-3.436681	-0.168073
N	-0.227485	-1.235918	-0.241607
C	-1.604559	-1.536213	-0.226377
C	-2.470049	-0.438938	0.091095
C	-2.214785	-2.771148	-0.456380
C	-3.878463	-0.603113	0.234886
C	-3.615957	-2.927019	-0.339830
H	-1.604933	-3.622678	-0.711034
C	-2.630281	1.853123	0.579373
C	-4.641548	0.540925	0.582069
C	-4.444170	-1.883467	0.009942
H	-4.038301	-3.910197	-0.529995
C	-4.023487	1.759264	0.761773
H	-2.100797	2.793542	0.683167
H	-5.717097	0.440331	0.699964
H	-5.517798	-2.015552	0.105600
H	-4.584546	2.648484	1.027820
N	-1.898537	0.795372	0.255097
Pd	0.081873	0.791204	-0.282792
O	0.143392	2.878146	-0.227745
C	1.283040	3.385236	0.031562
O	2.346115	2.691072	0.077236
C	1.370948	4.865896	0.291806
H	1.746055	5.029700	1.308121
H	2.090035	5.314381	-0.401546
H	0.397419	5.345544	0.179771

INT4



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E_{ZPE} = -1195.359994

H = -1195.337226

G = -1195.412843

Im. Freq.; 0

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C	2.093117	-1.952680	0.025562
C	2.845730	-2.901086	0.735034
C	4.177983	-2.665767	1.072909
C	4.782546	-1.468261	0.681888
H	4.535369	0.384571	-0.385164
H	2.357932	-3.823222	1.033556
H	4.735079	-3.405858	1.641171
H	5.818546	-1.265049	0.941547
C	1.985048	0.230706	-1.249577
H	1.707622	1.867118	1.136786
H	2.579442	1.132103	-1.430557
H	1.684818	-0.193362	-2.217467
C	0.639943	-2.303122	-0.196845
O	0.333091	-3.507360	-0.236059
N	-0.267906	-1.272540	-0.241652
C	-1.655267	-1.496436	-0.173458
C	-2.478600	-0.348715	0.123316
C	-2.313360	-2.719684	-0.330225
C	-3.890436	-0.476694	0.297775
C	-3.713486	-2.831349	-0.172057
H	-1.732508	-3.597739	-0.562400
C	-2.587445	1.953781	0.518225
C	-4.626144	0.697175	0.605389
C	-4.500784	-1.747266	0.144687
H	-4.168488	-3.809521	-0.306060
C	-3.981597	1.908212	0.720675
H	-2.044849	2.892116	0.586776
H	-5.701687	0.621991	0.743335

H	-5.575972	-1.840027	0.268385
H	-4.520164	2.820647	0.954146
N	-1.873021	0.875374	0.231214
Pd	0.185435	0.712456	-0.424621
O	0.572550	2.816936	-0.633101
C	1.325610	3.424608	0.140983
O	1.949585	2.826865	1.145072
C	1.608393	4.887044	0.020679
H	1.365417	5.388749	0.963260
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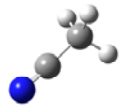
H	1.025841	5.316937	-0.794310

MeCN



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H = -132.714385
G = -132.741833
Im. Freq.; 0

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H	-0.890906	-0.514365	-1.553667
H	0.890906	-0.514365	-1.553667
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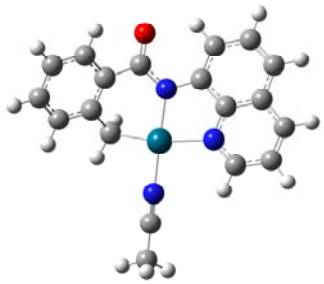
N	0.000000	-0.000000	1.438960

INT4-MeCN



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E_{ZPE} = -1099.055495
H = -1099.033777
G = -1099.106539
Im. Freq.; 0

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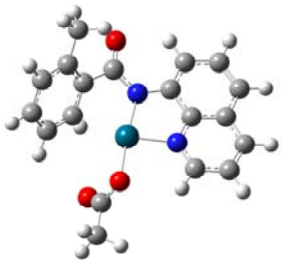
C	2.898919	-0.156281	-0.257586
C	2.471489	-1.476246	0.017257
C	3.341718	-2.363503	0.668183
C	4.601579	-1.954791	1.104845
C	5.013209	-0.639657	0.873972
H	4.505107	1.254851	-0.012087
H	3.003221	-3.379836	0.842206
H	5.251056	-2.653321	1.625739
H	5.989799	-0.302070	1.212254
C	2.056363	0.785122	-1.040570
H	2.511263	1.776139	-1.112624
H	1.850767	0.411766	-2.052684
C	1.104635	-2.024869	-0.320730
O	1.003597	-3.247808	-0.522440
N	0.045471	-1.151399	-0.278615
C	-1.286134	-1.601495	-0.275033
C	-2.286298	-0.642147	0.127957
C	-1.736730	-2.889774	-0.578538
C	-3.658576	-1.016137	0.261567
C	-3.100161	-3.243402	-0.461738
H	-1.019927	-3.630606	-0.894340
C	-2.768562	1.551429	0.778610
C	-4.575559	-0.020217	0.686536
C	-4.053960	-2.343542	-0.042122
H	-3.389271	-4.261022	-0.712430
C	-4.136419	1.257584	0.950061
H	-2.386010	2.550540	0.965191
H	-5.624427	-0.283708	0.795680
H	-5.099905	-2.622036	0.049726
H	-4.815510	2.037676	1.277706
N	-1.887964	0.643719	0.382653
Pd	0.181365	0.897597	-0.234381
N	0.278503	2.957186	-0.197068
C	0.325206	4.113537	-0.180283
C	0.384862	5.565443	-0.158408
H	-0.495711	5.978138	-0.660918
H	0.408313	5.917758	0.877582
H	1.288050	5.904016	-0.676018

INT3’



E = -1195.67482362

E_{ZPE} = -1195.362036

H = -1195.338357

G = -1195.416421

Im. Freq.; 0

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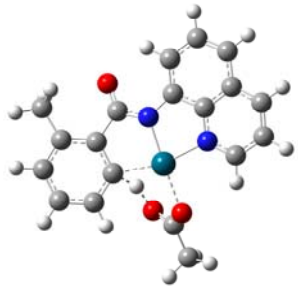
C	-2.809409	-2.305586	-0.631863
C	-1.918536	-1.682187	0.266414
C	-2.267881	-0.443353	0.871255
C	-3.484242	0.190342	0.557117
C	-4.352137	-0.413755	-0.344500
H	-4.710215	-2.117598	-1.605744
H	-1.708618	-0.090344	1.741072
H	-3.729686	1.132437	1.036090
H	-5.295922	0.058522	-0.601314
C	-2.490655	-3.617587	-1.309191
H	-2.388895	-4.428466	-0.581319
H	-3.282002	-3.881921	-2.016983
H	-1.543627	-3.566015	-1.859176
C	-0.535879	-2.235558	0.520425
O	-0.302878	-3.426617	0.746412
N	0.382850	-1.234706	0.409555
C	1.770747	-1.363896	0.355596
C	2.456110	-0.178032	-0.051902
C	2.528232	-2.495761	0.643493
C	3.873234	-0.139337	-0.165121
C	3.938057	-2.453642	0.535243
H	2.028627	-3.404788	0.949353
C	2.266559	2.059270	-0.745290
C	4.460113	1.078950	-0.596298
C	4.609200	-1.313376	0.143348
H	4.499650	-3.353748	0.770086
C	3.665064	2.166897	-0.886969
H	1.598263	2.888456	-0.951189
H	5.540344	1.139485	-0.695832

H	5.691763	-1.296678	0.060437
H	4.090006	3.107189	-1.220678
N	1.696865	0.930757	-0.347013
Pd	-0.299974	0.602218	-0.015522
O	-0.879746	2.500159	-0.542695
C	-1.425420	3.214539	0.404396
O	-1.612782	2.827377	1.563035
C	-1.831346	4.610152	-0.049353
H	-2.584292	4.543745	-0.843541
H	-2.241220	5.180349	0.787581
H	-0.967589	5.140872	-0.465195

$TS_{3'-4'}$



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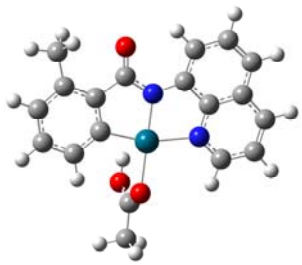
H = -1195.318914
G = -1195.391758
Im. Freq.; 1 (-1382.1005 cm^{-1})

C	-4.315334	-1.600148	-0.756208
C	-3.174283	-2.206471	-0.201082
C	-2.074682	-1.380322	0.116700
C	-2.146727	0.031138	-0.072687
C	-3.293931	0.579834	-0.671067
C	-4.375855	-0.232261	-1.010271
H	-5.166465	-2.227866	-1.008409
H	-1.842213	1.029614	0.819816
H	-3.361822	1.653555	-0.822015
H	-5.265983	0.199876	-1.459606
C	-3.181632	-3.706838	-0.014132
H	-3.094270	-3.982469	1.041480
H	-4.114447	-4.126490	-0.404476
H	-2.342352	-4.186408	-0.527631
C	-0.742633	-1.987257	0.481610
O	-0.607152	-3.112611	0.974180
N	0.296281	-1.162894	0.127576

C	1.657547	-1.455577	0.193078
C	2.522907	-0.349693	-0.096807
C	2.246639	-2.687169	0.475892
C	3.938292	-0.499995	-0.112857
C	3.653124	-2.829042	0.461522
H	1.616458	-3.533895	0.708509
C	2.688494	1.926563	-0.636283
C	4.713454	0.648398	-0.421408
C	4.493841	-1.773813	0.173217
H	4.073549	-3.806051	0.684587
C	4.095560	1.851715	-0.683409
H	2.163387	2.858181	-0.820062
H	5.796489	0.563107	-0.445921
H	5.572594	-1.897514	0.160718
H	4.666111	2.743438	-0.919496
N	1.939933	0.868136	-0.358734
Pd	-0.133134	0.748192	-0.210623
O	-0.574038	2.808070	-0.227006
C	-1.368074	3.110180	0.723135
O	-1.961214	2.245492	1.448426
C	-1.649403	4.569348	0.983253
H	-2.639042	4.814237	0.578636
H	-1.673307	4.761631	2.059568
H	-0.902614	5.204375	0.503117

INT4’



E = -1195.68188760

E_{ZPE} = -1195.368620

H = -1195.345256

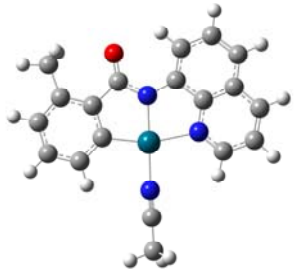
G = -1195.422173

Im. Freq.; 0

C	-4.564371	-1.302834	-0.145808
C	-3.409628	-2.087266	0.005067
C	-2.159606	-1.426520	-0.033039
C	-2.082846	-0.025402	-0.217021
C	-3.251280	0.723225	-0.369642

C	-4.492893	0.077863	-0.332202
H	-5.536079	-1.790444	-0.118985
H	-0.836109	2.063439	1.674670
H	-3.211087	1.798630	-0.523807
H	-5.408332	0.653695	-0.450613
C	-3.564557	-3.578999	0.195404
H	-3.123410	-3.917052	1.138660
H	-4.626217	-3.848397	0.191904
H	-3.060970	-4.143988	-0.595912
H	-0.848218	-2.144438	0.100743
O	-0.732534	-3.362904	0.280378
N	0.215435	-1.270059	-0.006212
C	1.566988	-1.592879	0.079023
C	2.483839	-0.489233	-0.052390
C	2.109737	-2.864796	0.277214
C	3.893861	-0.696226	0.016191
C	3.507567	-3.055074	0.344935
H	1.441684	-3.707424	0.378956
C	2.774618	1.809344	-0.369239
C	4.731130	0.441730	-0.123401
C	4.395315	-2.007514	0.218855
H	3.882075	-4.063570	0.501055
C	4.178606	1.687908	-0.316530
H	2.303940	2.776612	-0.518379
H	5.809084	0.311300	-0.075831
H	5.468821	-2.164182	0.271536
H	4.795991	2.573043	-0.427409
N	1.963549	0.769048	-0.241861
Pd	-0.201623	0.656129	-0.261018
O	-0.649100	2.750270	-0.523227
C	-0.920090	3.487157	0.435752
O	-1.007025	3.038391	1.678999
C	-1.182640	4.950717	0.288146
H	-2.212084	5.165992	0.596240
H	-0.514327	5.514320	0.947478
H	-1.035141	5.256527	-0.747762

INT4'-MeCN



E = -1099.36148370

E_{ZPE} = -1099.063851

H = -1099.041642

G = -1099.115099

Im. Freq.; 0

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C	-3.547643	-1.800403	-0.000404
C	-2.268761	-1.195491	-0.000015
C	-2.129465	0.213307	0.002344
C	-3.266998	1.023389	0.004596
C	-4.536147	0.433459	0.004325
H	-5.660795	-1.400047	0.001546
H	-3.179661	2.106246	0.006712
H	-5.425786	1.059784	0.006114
C	-3.769244	-3.295943	-0.002988
H	-3.317403	-3.776491	0.870835
H	-4.842699	-3.514293	-0.002713
H	-3.318524	-3.773299	-0.879140
C	-0.992933	-1.985853	-0.001676
O	-0.938976	-3.222238	-0.004226
N	0.109910	-1.156439	0.000066
C	1.442208	-1.559409	-0.001189
C	2.415030	-0.496912	0.000505
C	1.919268	-2.872662	-0.003729
C	3.812962	-0.783632	-0.000104
C	3.305602	-3.142301	-0.004549
H	1.208588	-3.685936	-0.005084
C	2.824891	1.805038	0.004659
C	4.708299	0.317866	0.001969
C	4.246348	-2.134179	-0.002707
H	3.627533	-4.180664	-0.006624
C	4.220872	1.605310	0.004405
H	2.406121	2.806666	0.006474
H	5.778174	0.126335	0.001612
H	5.310786	-2.350800	-0.003265

H	4.883639	2.464218	0.006069
N	1.960353	0.800405	0.002707
Pd	-0.213674	0.810140	0.002426
N	-0.571658	2.855801	0.001066
C	-0.727762	4.002266	-0.004567
C	-0.932360	5.440683	-0.012931
H	-0.675684	5.855231	0.967092
H	-0.296533	5.899171	-0.776967
H	-1.981354	5.660648	-0.235645

References

[1] A similar combination of DFT methods and basis set have been used to study Pd-catalyzed cross coupling reaction: (a) Hruszkewycz, D. P.; Balcells, D.; Guard, L. M.; Hazari, N.; Tilset, M. *J. Am. Chem. Soc.* **2014**, *136*, 7300. DFT calculation for Pd-catalyzed C–H arylation using related functionals and basis sets:

[2] 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, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; 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, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09 (Revision D.01)*,Gaussian, Inc., Wallingford CT, 2013.

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