SUPPORTING INFORMATION

Controlling Cyclization Pathways in Palladium(II)-Catalyzed Intramolecular Alkene Hydrofunctionalization via Substrate Directivity

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Table of Contents

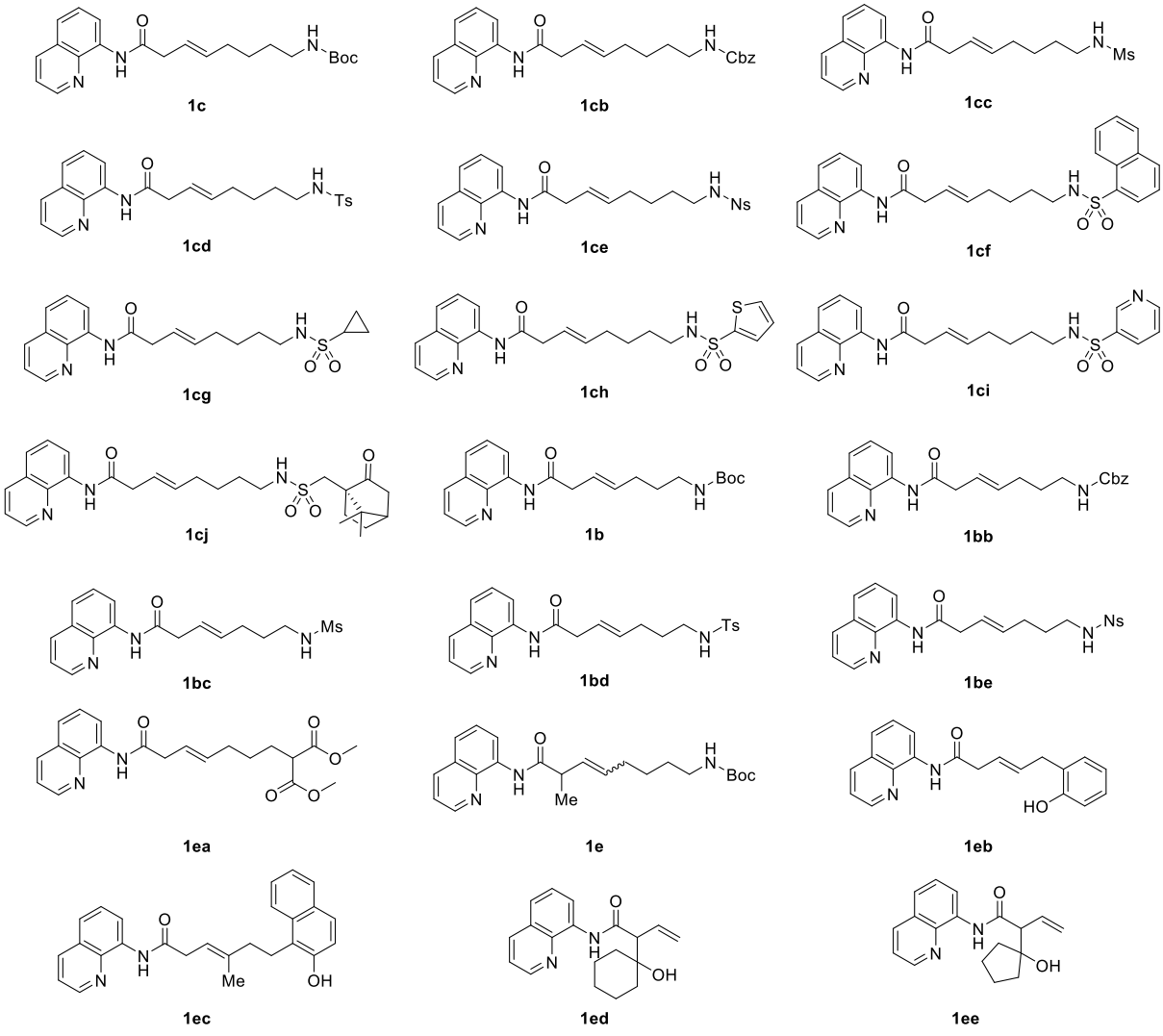
General Information

Unless otherwise noted, all materials were used as received from commercial sources without further purification. All commercial reagents and solvents were purchased from Aldrich, Alfa Aesar, Oakwood, and Combi-Blocks. $Pd(OAc)_2$ was obtained from Johnson Matthey. NMR spectra were recorded on Bruker AV-400, DRX-500 and AV-600 instruments. ^{1}H and ^{13}C spectra were internally referenced to $SiMe_4$ or solvent signals. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on an Agilent LC/MSD TOF mass spectrometer by electrospray ionization time of flight experiments.

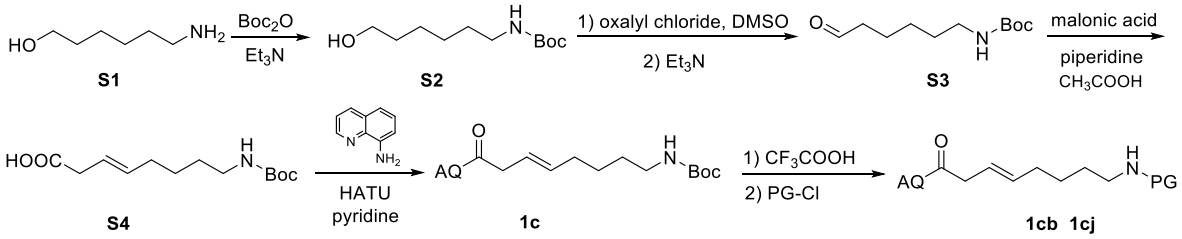
Experimental Procedures

Substrates Synthesis

Table S1. Substrates **1c-1ee**.

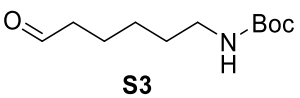


Substrates 1c-1ee were prepared according to adapted literature procedures.[1-7]



Scheme S1: Synthesis of substrates containing a nitrogen nucleophile [N–H] for 6-exo-trig cyclization (**1c–1cj**).

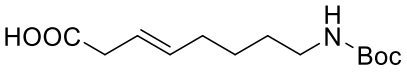
2-(5-hydroxypentyl)isoindoline-1,3-dione (S2): To a 250-mL round-bottom flask equipped with a magnetic stir bar were added commercially available 6-aminohexan-1-ol (2.8 g, 24 mmol) and di-*tert*-butyl dicarbonate (5.2 g, 24 mmol) in CH_2Cl_2 (100 mL). Next, Et_3N (2.7 g, 26 mmol) was added dropwise. The reaction mixture was stirred at room temperature for 2 h. After that time, the solvent was removed *in vacuo*. Purification using silica gel column chromatography with 1:1 hexanes:EtOAc as the eluent gave the product as a colorless oil (5.0 g, 96% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 4.58 (s, 1H), 3.61 (q, *J* = 4.8, 3.3 Hz, 2H), 3.09 (q, *J* = 6.7 Hz, 2H), 1.83 (s, 1H), 1.56–1.52 (m, 2H), 1.48–1.44 (m, 2H), 1.42 (s, 9H), 1.37–1.31 (m, 4H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 156.2, 79.2, 62.7, 40.5, 32.7, 30.2, 28.5, 26.5, 25.4.



S2

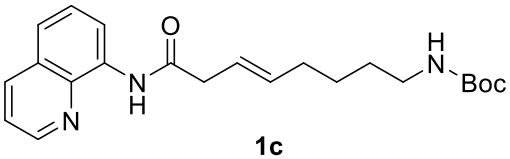
S3

***tert*-butyl (6-oxohexyl)carbamate (S3):** A solution of DMSO (3.4 mL, 48 mmol) in dry DCM (20 mL) was added dropwise to a solution of oxalyl chloride (3.0 mL, 35 mmol) in dry DCM (100 mL) at –78 ºC, and the resulting mixture was stirred for 15 min. To this reaction mixture, was added dropwise a solution of **S2** (5.0 g, 23 mmol) in dry DCM (50 mL) at –78 ºC, and the resulting solution was stirred for another 30 min. Et_3N (12 g, 120 mmol) was then added, and the solution was slowly warmed to room temperature before treated with sat. NH_4Cl. The organic layer was separated, washed with sat. $NaHCO_3$ (100 mL, ×1) and brine (100 mL, ×1), dried over anhydrous Na_2SO_4, and concentrated to afford **S3** as a colorless oil, which was purified quickly by silica gel column chromatography with 1:1 hexanes:EtOAc as eluent. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.74 (t, *J* = 1.7 Hz, 1H), 4.55 (s, 1H), 3.10 (q, *J* = 6.8 Hz, 2H), 2.42 (td, *J* = 7.3, 1.7 Hz, 2H), 1.65–1.61 (m, 2H), 1.48–1.46 (m, 2H), 1.42 (s, 9H), 1.36–1.31 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.6, 156.1, 79.2, 43.9, 40.4, 30.0, 28.5, 26.4, 21.8.



S4

(*E*)-8-((*tert*-butoxycarbonyl)amino)oct-3-enoic acid (S4): To a solution of **S3** (3.4 g, 16 mmol) and malonic acid (1.8 g, 17 mmol) in DMSO (8 mL) were added piperidine (10 µL) and acetic acid (6 µL). The reaction mixture was heated to 100 °C while stirring over 8 h. The reaction solution was cooled to room temperature, quenched with brine, and extracted with EtOAc. The organic layer was separated, dried over anhydrous Na_2SO_4, and concentrated *in vacuo*. Purification using silica gel column chromatography with 1:1 hexanes:EtOAc as the eluent gave the product as a colorless oil (3.1 g, 76% yield). **^{1}H NMR** (500 MHz, DMSO-d_6) δ 12.11 (s, 1H), 6.75 (t, *J* = 6.3 Hz, 1H), 5.53–5.41 (m, 2H), 2.93 (d, *J* = 5.6 Hz, 2H), 2.89 (q, *J* = 6.5 Hz, 2H), 2.00–1.93 (m, 2H), 1.36 (m, 11H), 1.33–1.25 (m, 2H); **^{13}C NMR** (150 MHz, DMSO-d_6) δ 172.9, 155.6, 133.1, 122.9, 77.3, 37.6, 31.6, 29.0, 28.3, 26.0.

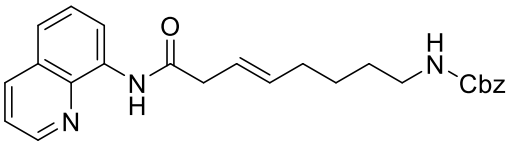


1c

***tert*-butyl (*E*)-(8-oxo-8-(quinolin-8-ylamino)oct-5-en-1-yl)carbamate (1c):** The carboxylic acid **S4** (3.2 g, 12.4 mmol) was charged into a 200-mL round-bottom flask equipped with a Teflon-coated magnetic stir bar containing DCM (80 mL). 8-Aminoquinoline (1.7 g, 12 mmol), pyridine (1.9 mL, 24 mmol), and HATU (6.7 g, 18 mmol) were added sequentially, and the reaction was stirred at ambient temperature for 20 h. The deep brown solution was diluted with

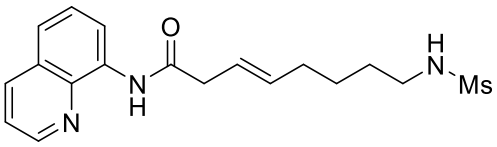
EtOAc (80 mL), washed with sat. $NaHCO_3$ (50 mL, ×2) and brine (50 mL, ×1), and dried over Na_2SO_4. The solvent was removed under vacuum and the resulting residue was purified by column chromatography (10:1 to 5:1 hexanes:EtOAc) to afford the substrate **1a** as a colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.79–8.76 (m, 2H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.55–7.49 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.83–5.72 (m, 2H), 4.51 (s, 1H), 3.29–3.26 (m, 2H), 3.15 (d, *J* = 6.9 Hz, 2H), 2.18 (q, *J* = 6.6 Hz, 2H), 1.58–1.51 (m, 4H), 1.43 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.1, 156.1, 148.3, 138.7, 136.6, 136.5, 134.6, 128.1, 127.5, 122.9, 121.7, 121.7, 116.5, 79.2, 42.3, 40.6, 32.4, 29.7, 28.6, 26.5; **HRMS** (ESI-TOF) Calcd for $C_{22}H_{30}N_3O_3^+$ [M+H] 384.2287, found 384.2288.

General Procedure A for preparation of 1cb–1cj: To a 25-mL round-bottom flask equipped with a magnetic stir bar was added the substrate **1c** (1.0 equiv) in DCM. The reaction mixture was cooled to 0 ºC before treatment with trifluoroacetic acid. After stirring for 1 h, the reaction mixture was concentrated *in vacuo*. The residue was diluted with EtOAc, washed with sat. $NaHCO_3$ and brine, dried over anhydrous Na_2SO_4. The solution was filtered through a plug of celite, and the filtrate was concentrated under vacuum to afford a light-yellow oil, which was carried on to the next step without further purification. The residue was dissolved in THF (10 mL), which was cooled to 0 ºC. Et_3N (1.2 equiv) and benzyl carbonochloridate or RSO_2Cl (1.0 equiv) were added sequentially in a dropwise fashion. The reaction mixture was slowly warmed to room temperature and stirred for an additional 2 h. After removal of the solvent *in vacuo*, purification using silica gel column chromatography with hexanes:EtOAc as the eluent gave the product as a light-yellow solid or oil.



1cb

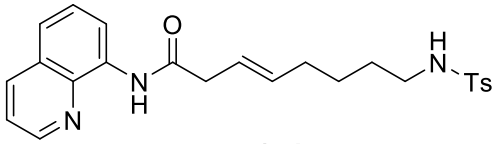
benzyl (*E*)-(8-oxo-8-(quinolin-8-ylamino)oct-5-en-1-yl)carbamate (1cb): The title compound was prepared from substrate **1c** (383 mg, 1.0 mmol) and benzyl carbonochloridate (171 mg, 1.0 mmol) according to General Procedure A. Purification using silica gel column chromatography with 3:1 hexane:EtOAc as the eluent gave the product as a light-yellow oil (293 mg, 70% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.79–8.75 (m, 2H), 8.13 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.54–7.48 (m, 2H), 7.41 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.34 (m, 4H), 7.32–7.28 (m, 1H), 5.77 (dt, *J* = 11.9, 6.4 Hz, 2H), 5.08 (s, 2H), 4.76 (s, 1H), 3.27 (d, *J* = 6.1 Hz, 2H), 3.23 (q, *J* = 6.6 Hz, 2H), 2.18 (q, *J* = 6.8 Hz, 2H), 1.62–1.51 (m, 4H); **^{13}C NMR** (125 MHz, CDCl3) δ 170.1, 156.5, 148.3, 138.7, 136.8, 136.4, 134.6, 128.6, 128.2, 128.2, 128.1, 127.5, 123.0, 121.7, 121.7, 116.5, 66.7, 42.2, 41.1, 32.4, 29.6, 26.4; **HRMS** (ESI-TOF) Calcd for $C_{25}H_{28}N_3O_3^+$ [M+H] 418.2131, found 418.2129.



1cc

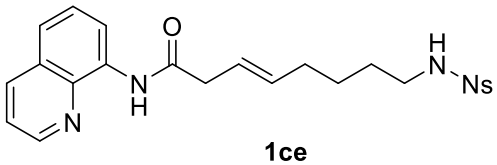
(*E*)-8-(methylsulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1cc): The title compound was prepared from substrate **1c** (383 mg, 1.0 mmol), methanesulfonyl chloride (115 mg, 1.0 mmol) according to General Procedure A. Purification using silica gel column chromatography with 1:1 hexane:EtOAc as the eluent gave the product as a light-yellow solid (224 mg, 62% yield). **^{1}H NMR** (600 MHz, CDCl3) δ 10.00 (s, 1H), 8.80 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.76 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.55–7.49 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.77 (ddd, *J* = 6.2, 4.9, 4.0 Hz, 2H), 4.28 (s, 1H), 3.30–3.27 (m, 2H), 3.16 (q, *J* = 6.7 Hz, 2H), 2.93 (s, 3H), 2.20 (td, *J* = 7.2, 5.1 Hz, 2H), 1.69–1.63 (m, 2H), 1.57 (dq, *J* = 10.0, 7.2 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 148.4, 138.6, 136.5, 135.9, 134.5, 128.1, 127.5,

123.4, 121.8, 121.6, 116.5, 43.3, 42.2, 40.4, 32.2, 29.7, 26.2; **HRMS** (ESI-TOF) Calcd for $C_{18}H_{24}N_3O_3S^+$ [M+H] 362.1538, found 362.1534.



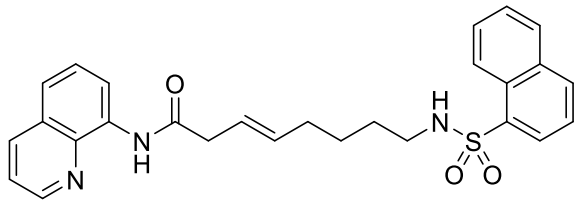
1cd

(*E*)-8-((4-methylphenyl)sulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1cd): The title compound was prepared from substrate **1c** (383 mg, 1.0 mmol), 4-methylbenzenesulfonyl chloride (191mg, 1.0 mmol) according to General Procedure A. Purification using silica gel column chromatography with 3:1 hexane:EtOAc as the eluent gave the product as a light-yellow solid (271 mg, 62% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.78 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.55–7.49 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 5.76–5.65 (m, 2H), 4.43 (t, *J* = 6.2 Hz, 1H), 3.25 (d, *J* = 5.7 Hz, 2H), 2.96 (q, *J* = 6.7 Hz, 2H), 2.41 (s, 3H), 2.11 (td, *J* = 7.0, 5.3 Hz, 2H), 1.55 (dq, *J* = 10.9, 6.8 Hz, 2H), 1.51–1.46 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 148.4, 146.4, 143.5, 138.6, 137.1, 136.5, 136.1, 134.5, 129.8, 127.5, 127.2, 123.2, 121.8, 121.7, 116.5, 43.2, 42.2, 32.1, 29.1, 26.1, 21.6; **HRMS** (ESI-TOF) Calcd for $C_{24}H_{28}N_3O_3S^+$ [M+H] 438.1851, found 438.1849.



1ce

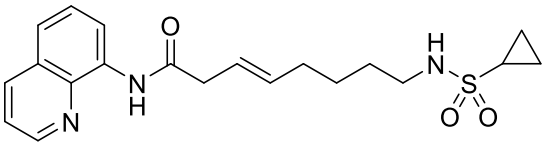
(*E*)-8-((4-methylphenyl)sulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1ce): The title compound was prepared from substrate **1c** (383 mg, 1.0 mmol), 4-nitrobenzenesulfonyl chloride (235 mg, 1.0 mmol) according to General Procedure A. Purification using silica gel column chromatography with 3:1 hexane:EtOAc as the eluent gave the product as a light-yellow oil (271 mg, 62% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.95 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 7.2, 1.8 Hz, 1H), 8.35–8.30 (m, 2H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.05–8.00 (m, 2H), 7.58–7.49 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.75–5.67 (m, 2H), 4.80 (t, *J* = 6.1 Hz, 1H), 3.27 (dd, *J* = 4.9, 1.5 Hz, 2H), 3.04 (q, *J* = 6.7 Hz, 2H), 2.14 (q, *J* = 6.9 Hz, 2H), 1.62–1.57 (m, 2H), 1.55–1.46 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.1, 150.1, 148.4, 146.2, 138.6, 136.6, 135.7, 134.5, 128.4, 128.1, 127.6, 124.5, 123.5, 121.8, 121.8, 116.6, 43.3, 42.0, 32.0, 29.1, 25.8; **HRMS** (ESI-TOF) Calcd for $C_{23}H_{25}N_4O_5S^+$ [M+H] 469.1546, found 469.1542.



1cf

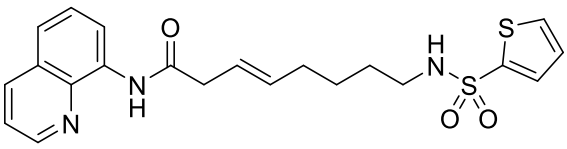
(*E*)-8-(naphthalene-1-sulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1cf): The title compound was prepared from substrate **1c** (500 mg, 1.3 mmol), 4-naphthalene-1-sulfonyl chloride (297 mg, 1.3 mmol) according to General Procedure A. Purification using silica gel column chromatography with 1:1 hexane:EtOAc as the eluent gave the product as a light-yellow oil (500 mg, 81% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.95 (s, 1H), 8.79–8.73 (m, 2H), 8.42 (d, *J* = 1.4 Hz, 1H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 2H), 7.89 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.81 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.61 (dddd, *J* = 24.8, 8.1, 6.9, 1.3 Hz, 2H), 7.56–7.47 (m, 2H), 7.43 (dd, *J* = 8.2, 4.2 Hz, 1H), 5.70–5.60 (m, 2H), 4.60 (t, *J* = 6.2 Hz, 1H), 3.22–3.17 (m, 2H), 3.02 (q, *J* = 6.7 Hz, 2H), 2.08 (td, *J* = 7.3, 5.3 Hz, 2H), 1.59–1.51 (m, 2H), 1.47 (dq, *J* = 9.5, 7.1 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 148.4, 138.6, 136.9, 136.5, 136.0, 134.9, 134.5, 132.3, 129.6, 129.3, 128.9, 128.5,

128.1, 128.0, 127.7, 127.5, 123.2, 122.5, 121.8, 121.7, 116.5, 43.3, 42.1, 32.1, 29.1, 26.1; **HRMS** (ESI-TOF) Calcd for $C_{27}H_{28}N_3O_3S^+$ [M+H] 474.1851, found 474.1847.



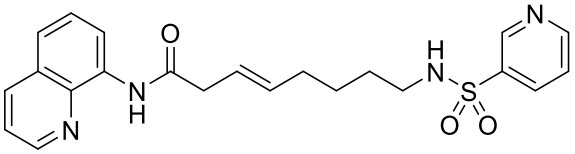
1cg

(*E*)-8-(cyclopropanesulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1cg): The title compound was prepared from substrate **1c** (545 mg, 1.4 mmol), 4-cyclopropanesulfonyl chloride (200 mg, 1.0 mmol) according to General Procedure A. Purification using silica gel column chromatography with 1:1 hexane:EtOAc as the eluent gave the product as a light-yellow solid (512 mg, 93% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.4, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.55–7.49 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.81–5.73 (m, 2H), 4.23 (s, 1H), 3.30–3.26 (m, 2H), 3.18 (q, *J* = 6.8 Hz, 2H), 2.38 (tt, *J* = 8.0, 4.8 Hz, 1H), 2.20 (td, *J* = 7.2, 5.2 Hz, 2H), 1.66 (dtd, *J* = 8.8, 7.4, 7.0, 5.5 Hz, 2H), 1.60–1.54 (m, 2H), 1.17–1.13 (m, 2H), 0.98–0.94 (m, 2H); **^{13}C NMR** (150 MHz, CDCl3) δ 170.0, 148.4, 138.6, 136.5, 136.0, 134.5, 128.1, 127.5, 123.3, 121.8, 121.7, 116.5, 43.4, 42.2, 32.2, 30.1, 29.9, 26.2, 5.4; **HRMS** (ESI-TOF) Calcd for $C_{20}H_{26}N_3O_3S^+$ [M+H] 388.1695, found 388.1693.



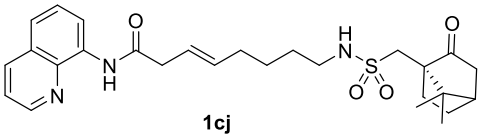
1ch

(*E*)-*N*-(quinolin-8-yl)-8-(thiophene-2-sulfonamido)oct-3-enamide (1ch): The title compound was prepared from substrate **1c** (500 mg, 1.3 mmol), thiophene-2-sulfonyl chloride (238 mg, 1.3 mmol) according to General Procedure A. Purification using silica gel column chromatography with 2:1 hexane:EtOAc as the eluent gave the product as a light-yellow solid (465 mg, 83% yield). **^{1}H NMR** (600 MHz, CDCl3) δ 9.99 (s, 1H), 8.79 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.61–7.53 (m, 2H), 7.57–7.47 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.07 (dd, *J* = 5.0, 3.7 Hz, 1H), 5.79–5.67 (m, 2H), 4.56 (t, *J* = 6.1 Hz, 1H), 3.27 (d, *J* = 5.4 Hz, 2H), 3.07 (q, *J* = 6.7 Hz, 2H), 2.14 (td, *J* = 7.1, 5.2 Hz, 2H), 1.64–1.56 (m, 2H), 1.52 (tdd, *J* = 9.5, 6.8, 5.1 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 148.4, 141.1, 138.6, 136.5, 136.0, 134.5, 132.2, 131.9, 128.1, 127.5, 127.5, 123.3, 121.8, 121.7, 116.5, 43.5, 42.2, 32.1, 29.0, 26.1; **HRMS** (ESI-TOF) Calcd for $C_{21}H_{24}N_3O_3S_2^+$ [M+H] 430.1259, found 430.1262.



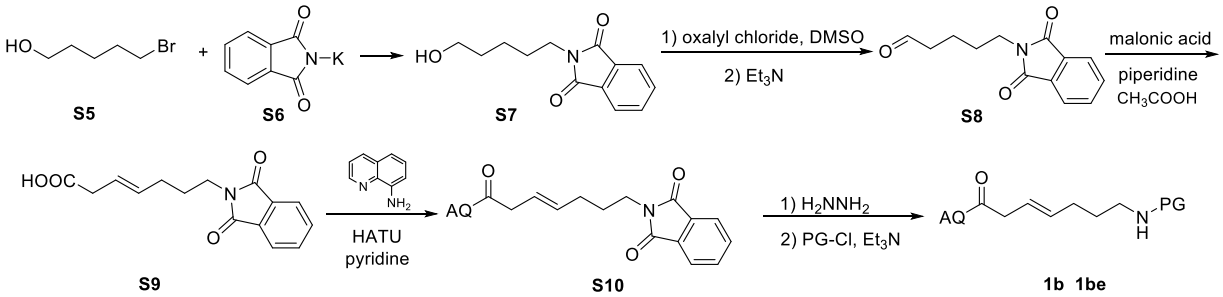
1ci

(*E*)-8-(pyridine-3-sulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1ci): The title compound was prepared from substrate **1c** (547 mg, 1.4 mmol), pyridine-3-sulfonyl chloride (258 mg, 1.4 mmol) according to General Procedure A. Purification using silica gel column chromatography with 2:1 hexane:EtOAc as the eluent gave the product as a light-yellow solid (499 mg, 82% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.97 (s, 1H), 9.07 (dd, *J* = 2.4, 0.8 Hz, 1H), 8.79–8.76 (m, 2H), 8.74 (dd, *J* = 7.3, 1.7 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.12 (ddd, *J* = 8.0, 2.4, 1.7 Hz, 1H), 7.54–7.48 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.42 (ddd, *J* = 8.0, 4.9, 0.9 Hz, 1H), 5.74–5.65 (m, 2H), 5.08 (t, *J* = 6.1 Hz, 1H), 3.27–3.23 (m, 2H), 3.02 (q, *J* = 6.7 Hz, 2H), 2.11 (td, *J* = 7.3, 5.1 Hz, 2H), 1.61–1.54 (m, 2H), 1.52–1.46 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.1, 153.2, 148.4, 148.1, 138.6, 137.0, 136.5, 135.9, 134.8, 134.4, 128.1, 127.5, 123.8, 123.3, 121.8, 121.8, 116.5, 43.2, 42.1, 32.0, 29.1, 26.0; **HRMS** (ESI-TOF) Calcd for $C_{22}H_{25}N_4O_3S^+$ [M+H] 425.1647, found 425.1648.

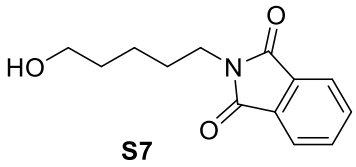


1cj

(*E*)-8-((((1*S*)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methyl)sulfonamido)-*N*-(quinolin-8-yl)oct-3-enamide (1cj): The title compound was prepared from substrate **1c** (535 mg, 1.4 mmol), D(+)-10-Camphorsulfonyl chloride (350 mg, 1.4 mmol) according to General Procedure A. Purification using silica gel column chromatography with 1:1 hexane:EtOAc as the eluent gave the product as a light-yellow solid (440 mg, 63% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.81 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.4, 1.6 Hz, 1H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.56–7.47 (m, 2H), 7.46 (dd, *J* = 8.2, 4.2 Hz, 1H), 5.85–5.73 (m, 2H), 5.16 (dd, *J* = 7.4, 5.0 Hz, 1H), 3.38 (d, *J* = 15.1 Hz, 1H), 3.28 (d, *J* = 6.6 Hz, 2H), 3.26–3.12 (m, 2H), 2.89 (d, *J* = 15.1 Hz, 1H), 2.38 (dt, *J* = 18.6, 4.0 Hz, 1H), 2.20 (m, 3H), 2.12 (t, *J* = 4.5 Hz, 1H), 2.02 (ddt, *J* = 15.8, 12.0, 4.2 Hz, 1H), 1.98–1.87 (m, 2H), 1.69 (dt, *J* = 14.3, 7.3 Hz, 2H), 1.65–1.58 (m, 2H), 1.43 (ddd, *J* = 12.9, 9.3, 4.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 217.3, 170.0, 148.5, 138.7, 136.4, 136.4, 134.6, 128.1, 127.5, 123.1, 121.8, 121.6, 116.5, 59.4, 49.4, 49.0, 43.8, 43.1, 42.9, 42.3, 32.4, 29.7, 27.2, 26.9, 26.4, 20.1, 19.6; **HRMS** (ESI-TOF) Calcd for $C_{27}H_{36}N_3O_4S^+$ [M+H] 498.2427, found 498.2428.

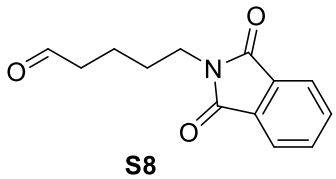


Scheme S2: Synthesis of substrates containing a nitrogen nucleophile [N–H] for 5-*exo-trig* cyclization (**1b–1be**).



S7

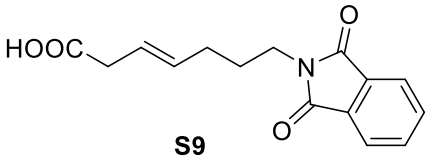
2-(5-hydroxypentyl)isoindoline-1,3-dione (S7): To a 250-mL round-bottom flask equipped with a magnetic stir bar were added commercially available 5-bromopentan-1-ol (5.0 g, 30 mmol), potassium phthalimide (8.3 g, 45 mmol), and DMF (50 mL). The mixture was heated to 70 °C while stirring for 2 h. After this time, the flask was allowed to cool to room temperature, and the reaction mixture was diluted with H_2O (50 mL) and extracted with CH_2Cl_2 (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated *in vacuo*. Purification using silica gel column chromatography with 3:1 to 1:1 hexanes:EtOAc as the eluent gave the product as a colorless oil (5.5 g, 79% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86–7.79 (m, 2H), 7.73–7.67 (m, 2H), 3.72–3.66 (m, 2H), 3.63 (q, *J* = 6.2 Hz, 2H), 1.74–1.68 (m, 2H), 1.65–1.58 (m, 2H), 1.48 (t, *J* = 4.6 Hz, 1H), 1.46–1.38 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.6, 134.0, 132.3, 123.3, 62.8, 38.0, 32.3, 28.5, 23.2.



S8

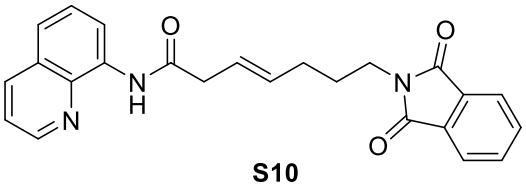
5-(1,3-dioxoisoindolin-2-yl)pentanal (S8): The title compound was prepared from oxalyl chloride (3.3 mL, 38 mmol), DMSO (3.8 mL, 53 mmol), intermediate **S7** (5.9 g, 25 mmol) and Et_3N (18 mL, 130 mmol) using a procedure similar to the one described above for the synthesis of intermediate **S3**. Purification using silica gel column chromatography with 3:1 to 2:1

hexanes:EtOAc as the eluent was performed quickly to afford the product as a colorless oil (5.1 g, 87% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.76 (s, 1H), 7.87–7.80 (m, 2H), 7.71 (dt, *J* = 6.9, 2.0 Hz, 2H), 3.71 (t, *J* = 6.5 Hz, 2H), 2.50 (t, *J* = 7.1 Hz, 2H), 1.71 (dp, *J* = 22.3, 7.2 Hz, 4H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.0, 168.5, 134.1, 132.2, 123.4, 43.3, 37.6, 28.1, 19.3.



S9

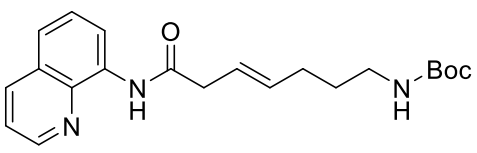
(*E*)-7-(1,3-dioxoisoindolin-2-yl)hept-3-enoic acid (S9): The title compound was prepared from intermediate **S8** (5.1 g, 22 mmol), malonic acid (2.5 g, 24 mmol), piperidine (10 μL), and acetic acid (6 μL) using a procedure similar to the one described above for the synthesis of the intermediate **S4**. Purification using silica gel column chromatography with 2:1 hexanes:EtOAc as the eluent gave the product as a yellow solid (3.6 g, 60% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 7.87–7.81 (m, 4H), 5.56–5.44 (m, 2H), 3.56 (t, *J* = 7.1 Hz, 2H), 2.98–2.86 (m, 2H), 2.01 (dt, *J* = 9.1, 6.0 Hz, 2H), 1.65 (p, *J* = 7.3 Hz, 2H); **^{13}C NMR** (150 MHz, DMSO-d_6) δ 172.8, 167.9, 134.3, 132.1, 131.6, 123.5, 123.0, 37.5, 37.1, 29.3, 27.5.



S10

(*E*)-7-(1,3-dioxoisoindolin-2-yl)-*N*-(quinolin-8-yl)hept-3-enamide (S10): The title compound was prepared from intermediate **S9** (3.6 g, 13 mmol), 8-aminoquinoline (1.7 g, 12 mmol), pyridine (1.9 mL, 24 mmol), and HATU (6.7 g, 18 mmol) using a procedure similar to the one described above for the synthesis of the intermediate **1a**. Purification using silica gel column chromatography with 2:1 hexanes:EtOAc as the eluent gave the product as yellow solid (4.2 g, 88% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.77 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.13 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.84 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.55–7.48 (m, 2H), 7.42 (dd, *J* = 8.2, 4.2 Hz, 1H), 5.85–5.79 (m, 2H), 3.78 (t, *J* = 7.2 Hz, 2H), 3.28–3.24 (m, 2H), 2.24 (ddd, *J* = 8.9, 7.0, 5.2 Hz, 2H), 1.95–1.87 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.9, 168.6, 148.4, 138.7, 136.4, 135.5, 134.6, 134.1, 132.3, 128.1, 127.5, 123.6, 123.4, 121.7, 121.6, 116.5, 42.2, 37.8, 30.2, 28.3.

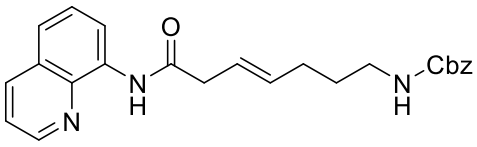
General Procedure B for preparation of 1b–1be: To a 25-mL round-bottom flask equipped with a magnetic stir bar were added intermediate **S10** (1.0 equiv) and 50% hydrazine hydrate (2.3 equiv) in MeOH. The reaction mixture was stirred at ambient temperature for 3 h. The reaction mixture was concentrated *in vacuo*, and the crude product was carried forward to the next step without further purification. The residue was dissolved in DCM (8 mL), and the solution was cooled to 0 ºC before treatment with Et_3N (2.0 equiv). Next, di-*tert*-butyl decarbonate (2 equiv), benzyl carbonochloridate (2 equiv), or RSO_2Cl (1.0 equiv) was added dropwise. The reaction was slowly warmed to room temperature and stirred for another 2 h. After removal of the solvent *in vacuo*, the residue was diluted with EtOAc, washed with sat. $NaHCO_3$ (20 mL, ×1) and brine (20 mL, ×1), and concentrated *in vacuo*. Purification using silica gel column chromatography with hexanes:EtOAc as the eluent gave the product as light-yellow solid or oil.



1b

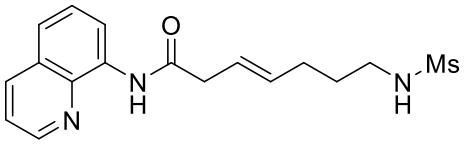
***tert*-butyl (*E*)-(7-oxo-7-(quinolin-8-ylamino)hept-4-en-1-yl)carbamate (1b):** The title compound was

prepared from intermediate **S10** (799 mg, 2 mmol), di-tert-butyl decarbonate (423 mg, 2 mmol) according to General Procedure B. Purification using silica gel column chromatography with 3:1 hexanes:EtOAc as the eluent gave the product as a light-yellow oil (236 mg, 32% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.82–8.73 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.58–7.48 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.88–5.71 (m, 2H), 4.64 (s, 1H), 3.31–3.25 (m, 2H), 3.26–3.16 (m, 2H), 2.26–2.16 (m, 2H), 1.75–1.66 (m, 2H), 1.44 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 156.1, 148.4, 138.7, 136.5, 136.1, 134.5, 128.1, 127.5, 123.3, 121.7, 121.7, 116.5, 79.3, 42.2, 40.3, 30.1, 29.7, 28.6; **HRMS** (ESI-TOF) Calcd for $C_{21}H_{28}N_3O_3^+$ [M+H] 370.2131, found 370.2126.



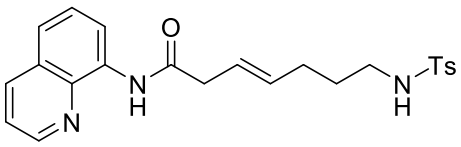
1bb

benzyl (*E*)-(7-oxo-7-(quinolin-8-ylamino)hept-4-en-1-yl)carbamate (1bb): The title compound was prepared from intermediate **S10** (799 mg, 2 mmol), benzyl carbonochloridate (341 mg, 2 mmol) and according to General Procedure B. Purification using silica gel column chromatography with 2:1 hexanes:EtOAc as the eluent gave the product as a yellow solid (468 mg, 58% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.77 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.55–7.49 (m, 2H), 7.42 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.36–7.29 (m, 5H), 5.79 (m, 2H), 5.10 (s, 2H), 4.90 (s, 1H), 3.29 (dd, *J* = 14.8, 6.3 Hz, 4H), 2.22 (q, *J* = 6.7 Hz, 2H), 1.74 (p, *J* = 7.2 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.9, 156.5, 148.4, 138.6, 136.8, 136.5, 135.9, 134.5, 128.7, 128.2, 128.2, 128.1, 127.5, 123.4, 121.7, 121.7, 116.5, 66.7, 42.2, 40.7, 30.0, 29.5; **HRMS** (ESI-TOF) Calcd for $C_{24}H_{26}N_3O_3^+$ [M+H] 404.1974, found 404.1968.



1bc

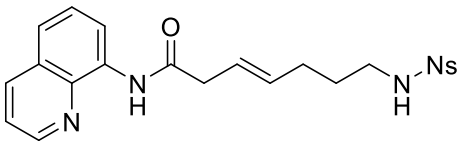
(*E*)-7-(methylsulfonamido)-*N*-(quinolin-8-yl)hept-3-enamide (1bc): The title compound was prepared from intermediate **S10** (500 mg, 1.2 mmol), methanesulfonyl chloride (137 mg, 1.2 mmol) according to General Procedure B. Purification using silica gel column chromatography with 1:1 hexanes:EtOAc as the eluent gave the product as yellow solid (211 mg, 49% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.57–7.48 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.83–5.76 (m, 2H), 4.49 (s, 1H), 3.32–3.27 (m, 2H), 3.23 (q, *J* = 6.8 Hz, 2H), 2.94 (s, 3H), 2.26 (q, *J* = 6.7 Hz, 2H), 1.80 (q, *J* = 7.1 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.9, 148.4, 138.6, 136.6, 135.2, 134.5, 128.1, 127.6, 124.0, 121.8, 121.8, 116.6, 42.9, 42.0, 40.6, 30.0, 29.8; **HRMS** (ESI-TOF) Calcd for $C_{17}H_{22}N_3O_3S^+$ [M+H] 348.1382, found 348.1381.



1bd

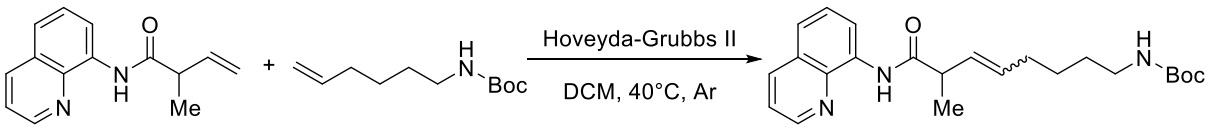
(*E*)-7-((4-methylphenyl)sulfonamido)-*N*-(quinolin-8-yl)hept-3-enamide (1bd): The title compound was prepared from intermediate **S10** (500 mg, 1.2 mmol), 4-methylbenzenesulfonyl chloride (229 mg, 1.2 mmol) according to General Procedure B. Purification using silica gel column chromatography with 1:1 hexanes:EtOAc as the eluent gave the product as a yellow solid (323 mg, 61% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.78–8.75 (m, 2H), 8.17 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.56–7.50 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.26–7.24 (m, 2H), 5.75–5.67 (m, 2H), 4.54 (t, *J* = 6.3 Hz, 1H), 3.26–3.23 (m, 2H), 3.05 (q, *J* = 6.7 Hz, 2H), 2.39 (s, 3H), 2.17 (q, *J* = 6.8 Hz, 2H), 1.70 (q, *J* = 7.0 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.8, 148.4, 143.5, 138.6, 137.2, 136.5, 135.3, 134.5, 129.8, 128.1, 127.6, 127.2, 123.8,

121.8, 121.8, 116.6, 42.8, 42.0, 29.9, 29.3, 21.6; **HRMS** (ESI-TOF) Calcd for $C_{23}H_{26}N_3O_3S^+$ [M+H] 424.1695, found 424.1694.



1be

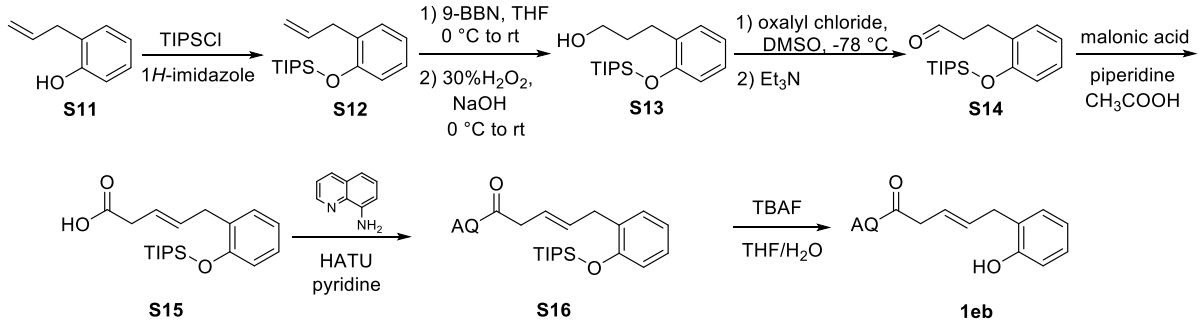
(*E*)-7-((4-nitrophenyl)sulfonamido)-*N*-(quinolin-8-yl)hept-3-enamide (1be): The title compound was prepared from intermediate **S10** (500 mg, 1.2 mmol), 4-nitrobenzenesulfonyl chloride (277 mg, 1.2 mmol) according to General Procedure B. Purification using silica gel column chromatography with 1:1 hexanes:EtOAc as the eluent gave the product as a yellow solid (302 mg, 53% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.74 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.71 (dd, *J* = 6.7, 2.3 Hz, 1H), 8.24–8.21 (m, 2H), 8.14 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.03–7.98 (m, 2H), 7.54–7.48 (m, 2H), 7.43 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.74–5.66 (m, 3H), 3.26 (d, *J* = 5.5 Hz, 1H), 3.09 (q, *J* = 6.6 Hz, 2H), 2.18 (q, *J* = 6.8 Hz, 2H), 1.72 (p, *J* = 6.9 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.2, 149.9, 148.4, 146.4, 138.5, 136.6, 135.2, 134.2, 128.3, 128.1, 127.4, 124.3, 123.9, 122.0, 121.8, 116.6, 43.0, 41.7, 30.1, 29.3; **HRMS** (ESI-TOF) Calcd for $C_{22}H_{23}N_4O_5S^+$ [M+H] 455.1389, found 455.1385.



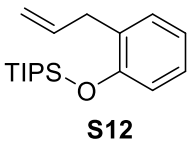
1e

36%, *E*:*Z* = 10:1

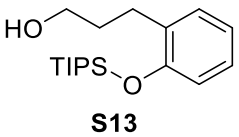
***tert*-butyl (7-methyl-8-oxo-8-(quinolin-8-ylamino)oct-5-en-1-yl)carbamate (1e)**: To a 50-mL Schlenk flask equipped with a magnetic stir bar were added 2-methyl-*N*-(quinolin-8-yl)but-3-enamide (170 mg, 0.75 mmol), *tert*-butyl hex-5-en-1-ylcarbamate (200 mg, 1 mmol), Hoveyda–Grubbs 2nd generation catalyst (50 mg, 0.08 mmol), and DCM (4 mL). The reaction was stirred at 40 ºC for 17 h. The dark brown solution was concentrated and purified by column chromatography (Hexanes:EtOAc = 10:1 to 5:1) to afford product as a yellow oil (106 mg, 36%, *E*/*Z* = 10:1). The ensuing analytical data correspond to the major product, the *E*-isomer. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.81–8.75 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.53 (t, *J* = 7.9 Hz, 1H), 7.49 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.46–7.43 (m, 1H), 5.84–5.76 (m, 1H), 5.73–5.66 (m, 1H), 4.48 (s, 1H), 3.30 (p, *J* = 7.2 Hz, 1H), 3.13 (d, *J* = 7.6 Hz, 2H), 2.19–2.12 (m, 2H), 1.56–1.48 (m, 4H), 1.42 (s, 9H), 1.41 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.31, 148.29, 138.76, 136.44, 134.74, 133.66, 132.91, 130.26, 128.09, 127.57, 121.72, 121.52, 116.39, 46.13, 40.61, 32.39, 29.73, 28.56, 27.46, 26.58, 17.45. **HRMS (ESI-TOF)** Calcd for $C_{23}H_{32}N_3O_3^+$ $[M+H]^+$ calc: 398.2444, found 398.2445.



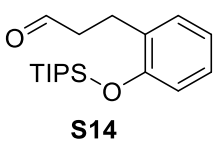
Scheme S3: Synthesis of substrates containing an oxygen nucleophile [O–H] for 5-exo-trig cyclization(**1eb**).



(2-allylphenoxy)triisopropylsilane (S12):[5] To a solution of 2-allylphenol (2.7 g, 20 mmol) in anhydrous DMF (15 mL) was added imidazole (4.1 g, 60 mmol) in one portion under N_2. After the reaction mixture was stirred for 15 min, TIPSCl (7.7 g, 40 mmol) was added. The reaction mixture was then stirred at room temperature for 10 h (at which point it had reached completion, as monitored by TLC). The reaction mixture was slowly poured into water (100 mL) and extracted with CH_2Cl_2 (3 × 50 mL). The combined organic layers were washed with water (3 × 50 mL) and the solvent was removed under reduced pressure. Purification using silica gel column chromatography with hexanes as the eluent gave the product as a colorless oil (5.7 g, 97%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.07 (td, *J* = 7.7, 1.9 Hz, 1H), 6.87 (td, *J* = 7.4, 1.2 Hz, 1H), 6.80 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.00 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.08–5.03 (m, 2H), 3.42 (dd, *J* = 6.6, 1.6 Hz, 2H), 1.36–1.28 (m, 3H), 1.12 (d, *J* = 7.5 Hz, 18H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 153.9, 137.3, 130.4, 130.2, 127.1, 120.8, 118.1, 115.5, 34.7, 18.2, 13.2.

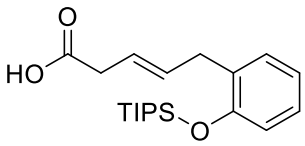


3-(2-((triisopropylsilyl)oxy)phenyl)propan-1-ol (S13):[6] To a stirring solution of **S12** (3.0 g, 10 mmol) in anhydrous THF (50 mL) at 0 °C was added 9-BBN (0.5 M solution in THF, 44.0 mL, 22 mmol) dropwise under a nitrogen atmosphere. The mixture was then stirred at room temperature for 6 h. The reaction was carefully terminated by the addition of H_2O (2 mL) at 0 °C. Next, 1 M NaOH solution (27 mL) and 30% H_2O_2 (18 mL) were added sequentially, and the reaction mixture was stirred for an additional 12 h at rt. The reaction mixture was then partitioned between brine (50 mL) and EtOAc (50 mL). The aqueous phase was extracted with EtOAc (40 mL). The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification using silica gel column chromatography with 5:1 hexanes:EtOAc as the eluent gave the product as a colorless oil (2.7 g, 84%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.05 (ddd, *J* = 8.0, 7.4, 1.8 Hz, 1H), 6.87 (td, *J* = 7.4, 1.2 Hz, 1H), 6.79 (dd, *J* = 8.1, 1.2 Hz, 1H), 3.65 (q, *J* = 6.1 Hz, 2H), 2.73 (dd, *J* = 8.3, 6.9 Hz, 2H), 1.89–1.85 (m, 2H), 1.45 (s, 1H), 1.35–1.29 (m, 3H), 1.12 (d, *J* = 7.5 Hz, 18H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.0, 131.9, 130.4, 127.0, 121.0, 118.2, 62.6, 33.2, 26.8, 18.2, 13.3.



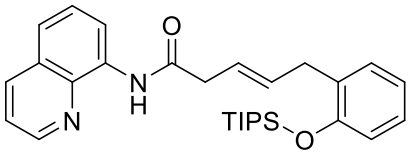
3-(2-((triisopropylsilyl)oxy)phenyl)propanal (S14): The title compound was prepared from oxalyl chloride (1.3 mL, 15.3 mmol), DMSO (1.5 mL, 21.4 mmol), intermediate **S13** (3.1 g, 10.2 mmol), and Et_3N (7.1 mL, 51 mmol) using a procedure similar to the one described above for the synthesis of intermediate **S3**. Purification using silica gel column chromatography with 20:1 hexanes:EtOAc as the eluent was performed quickly to afford the

product as a colorless oil (2.7 g, 86% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.82 (t, *J* = 1.6 Hz, 1H), 7.13 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.08 (td, *J* = 7.7, 1.8 Hz, 1H), 6.86 (td, *J* = 7.4, 1.2 Hz, 1H), 6.80 (dd, *J* = 8.2, 1.2 Hz, 1H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.75 (ddd, *J* = 8.8, 7.1, 1.6 Hz, 2H), 1.35–1.29 (m, 3H), 1.11 (d, *J* = 7.4 Hz, 18H); **^{13}C NMR** (150 MHz, CDCl3) δ 202.4, 154.1, 130.5, 130.3, 127.5, 121.0, 118.2, 44.2, 23.9, 18.2, 13.2.



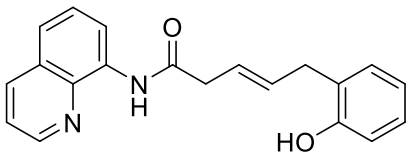
S15

(*E*)-5-(2-((triisopropylsilyl)oxy)phenyl)pent-3-enoic acid (S15): The title compound was prepared from intermediate **S14** (2.7 g, 8.8 mmol), malonic acid (1.0 g, 9.7 mmol), piperidine (10 μL) and acetic acid (6 μL) in the same manner as described above for the synthesis of the intermediate **S4**. Purification using silica gel column chromatography with 3:1 hexanes:EtOAc as the eluent gave the product as yellow solid (2.2 g, 72% yield). **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.14 (s, 1H), 7.13–7.08 (m, 2H), 6.86 (td, *J* = 7.4, 1.2 Hz, 1H), 6.79 (dd, *J* = 8.1, 1.1 Hz, 1H), 5.66 (dtt, *J* = 14.9, 6.7, 1.4 Hz, 1H), 5.51 (dtt, *J* = 15.4, 7.0, 1.5 Hz, 1H), 3.32–3.30 (m, 2H), 2.96 (dq, *J* = 6.9, 1.2 Hz, 2H), 1.34–1.27 (m, 3H), 1.07 (d, *J* = 7.5 Hz, 18H); **^{13}C NMR** (150 MHz, DMSO-d_6) δ 172.7, 153.1, 131.2, 130.0, 129.9, 127.2, 123.8, 120.9, 117.7, 37.5, 32.7, 17.9, 12.4.



S16

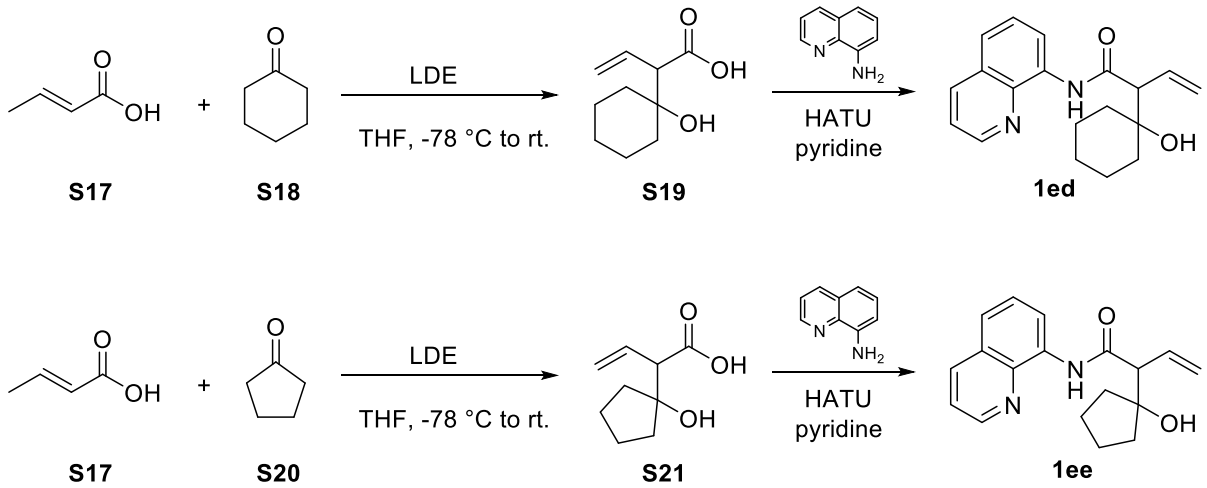
(*E*)-*N*-(quinolin-8-yl)-5-(2-((triisopropylsilyl)oxy)phenyl)pent-3-enamide (S16): The title compound was prepared from intermediate **S15** (2.1 g, 6.0 mmol), 8-aminoquinoline (782 mg, 5.4 mmol), pyridine (880 μL, 11 mmol), and HATU (2.5 g, 6.5 mmol) using a procedure similar to the one described above for the synthesis of the compound **1c**. Purification using silica gel column chromatography with 2:1 hexanes:EtOAc as the eluent gave the product as light-yellow solid (2.2 g, 76% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.77 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.75 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.56–7.48 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.28 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.08 (td, *J* = 7.7, 1.8 Hz, 1H), 6.87 (td, *J* = 7.5, 1.1 Hz, 1H), 6.81 (dd, *J* = 8.1, 1.1 Hz, 1H), 6.00 (dtt, *J* = 14.6, 6.6, 1.3 Hz, 1H), 5.86–5.78 (m, 1H), 3.54 (d, *J* = 6.7 Hz, 2H), 3.31 (dd, *J* = 7.2, 1.2 Hz, 2H), 1.31 (m, 3H), 1.10 (d, *J* = 7.5 Hz, 18H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 153.9, 148.3, 138.7, 136.4, 135.1, 134.6, 130.3, 130.3, 128.1, 127.5, 127.2, 123.6, 121.7, 121.6, 120.9, 118.1, 116.5, 42.3, 33.5, 18.2, 13.2.



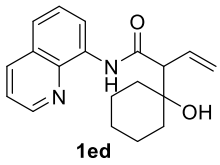
1eb

(*E*)-5-(2-hydroxyphenyl)-*N*-(quinolin-8-yl)pent-3-enamide (1eb): To a stirring solution of **S16** (500 mg, 1.1 mmol) in THF/H_2O (1:1, 5 mL) was added TBAF (412 mg in 1:1 THF/H_2O mixed solvent, 5 mL) under a nitrogen atmosphere at 0 °C. The mixture was then stirred at room temperature for 24 h, at which point the reaction has reached completion (as monitored by TLC). The reaction mixture was then partitioned between brine (20 mL) and EtOAc (20 mL). The aqueous phase was extracted with another portion of EtOAc (20 mL). The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification using silica gel column chromatography with 4:1 hexanes:EtOAc as the eluent gave the product as a yellow solid (264 mg, 79% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.83 (s, 1H), 8.86 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.80 (dd, *J* = 7.1, 1.9 Hz, 1H), 8.20 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.58–7.50 (m, 2H), 7.50 (dd, *J* = 8.3, 4.3 Hz, 1H), 7.20 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.13 (td, *J* = 7.7, 1.7 Hz, 1H), 6.90 (td, *J* = 7.4, 1.2 Hz, 1H), 6.82 (dd, *J* = 8.0, 1.2 Hz, 1H), 5.99 (dtt, *J* = 15.1, 6.2, 1.3

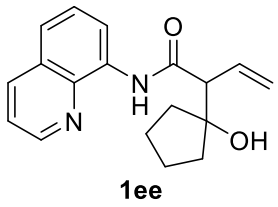
Hz, 1H), 5.84–5.78 (m, 1H), 3.52 (d, *J* = 6.5 Hz, 2H), 3.33 (dq, *J* = 7.2, 1.1 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.4, 153.7, 147.8, 138.0, 136.4, 134.1, 133.8, 130.1, 127.7, 127.4, 127.0, 125.7, 123.1, 121.4, 121.1, 120.6, 116.9, 115.9, 41.3, 33.7; **HRMS** (ESI-TOF) Calcd for $C_{20}H_{19}N_2O_2^+$ [M+H] 319.1447, found 319.1449.



Scheme S4: Synthesis of the substrates containing an oxygen nucleophile [O-H] for 5-endo-trig cyclization (**1ec, 1ed**).

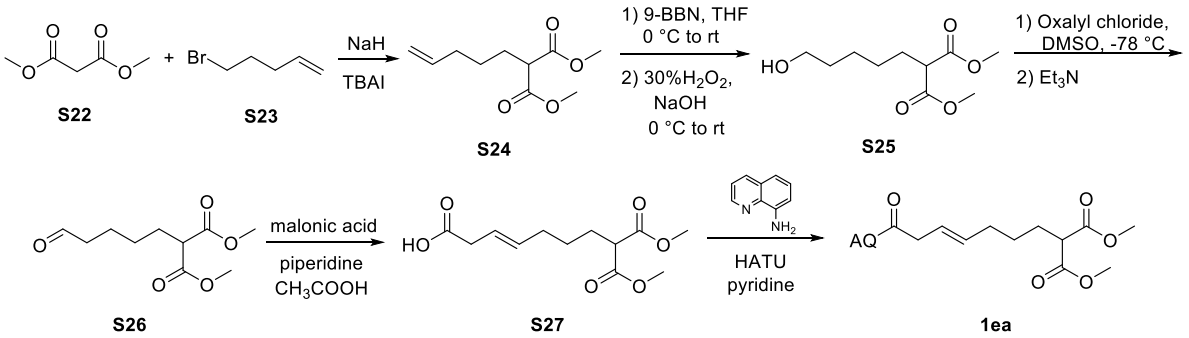


2-(1-hydroxycyclohexyl)-*N*-(quinolin-8-yl)but-3-enamide (1ed): Key intermediate **S19** was prepared from 2-isopropylbut-3-enoic acid (1.7 g, 20 mmol), cyclohexanone (2.0 g, 20 mmol), *n*-BuLi (17.6 mL, 44 mmol, 2.5 M in hexanes), and diethylamine (4.6 mL, 44 mmol) according to a literature procedure. [4]Purification using silica gel column chromatography with 10:1 hexanes:EtOAc as the eluent gave the product as a yellow oil (3.2 g, 86% yield). Next, title compound **1ec** was prepared from acid **S19** (3.1 g, 17 mmol), 8-aminoquinoline (2.2 g, 15 mmol), pyridine (2.7 mL, 34 mmol), and HATU (7.7 g, 20 mmol) using a procedure similar to the one described above for the synthesis of the compound **1c**. The crude product was purified by column chromatography with 7:1 hexanes:EtOAc as the eluent to afford the product as light-yellow solid (2.2 g, 43% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.13 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 5.3, 3.7 Hz, 1H), 8.17 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.57–7.51 (m, 2H), 7.46 (dd, *J* = 8.2, 4.2 Hz, 1H), 6.22 (ddd, *J* = 17.1, 10.2, 9.6 Hz, 1H), 5.43–5.34 (m, 2H), 4.20 (d, *J* = 0.9 Hz, 1H), 3.19 (d, *J* = 9.5 Hz, 1H), 1.79–1.63 (m, 4H), 1.57 (m, 2H), 1.51 (dq, *J* = 13.5, 4.3 Hz, 2H), 1.41–1.33 (m, 1H), 1.31–1.23 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.7, 148.5, 138.7, 136.5, 134.2, 133.6, 128.1, 127.4, 122.2, 121.8, 120.2, 117.1, 72.6, 61.9, 37.2, 35.1, 25.9, 22.2, 21.7; **HRMS** (ESI-TOF) Calcd for $C_{19}H_{23}N_2O_2^+$ [M+H] 311.1760, found 311.1760.

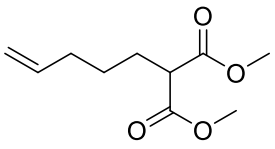


2-(1-hydroxycyclopentyl)-*N*-(quinolin-8-yl)but-3-enamide (1ee): Key intermediate **S21** was prepared from 2-isopropylbut-3-enoic acid (1.7 g, 20 mmol), cyclopentanone (2.0 g, 20 mmol), *n*-BuLi (17.6 mL, 44 mmol, 2.5 M in hexanes), and diethylamine (4.6 mL, 44 mmol) according to a literature procedure.[4] Next, title compound **1ed** was prepared from acid **S21** (2.6 g, 15 mmol), 8-aminoquinoline (2.0 g, 13.5 mmol), pyridine (2.4 mL, 30 mmol), and HATU (6.9 g, 18 mmol) using a procedure similar to the one described above for

synthesis of the compound **1ec**. The crude product was purified by column chromatography with 7:1 hexanes:EtOAc as the eluent to afford the product as light-yellow oil (1.5 g, 34% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.13 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 6.0, 3.0 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.56–7.53 (m, 2H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H), 6.24 (ddd, *J* = 17.1, 10.2, 9.2 Hz, 1H), 5.43 (ddd, *J* = 17.2, 1.5, 0.8 Hz, 1H), 5.38 (dd, *J* = 10.2, 1.5 Hz, 1H), 4.22 (s, 1H), 3.24 (d, *J* = 9.1 Hz, 1H), 1.90–1.85 (m, 2H), 1.80–1.72 (m, 2H), 1.66–1.61 (m, 4H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.8, 148.6, 138.7, 136.5, 134.3, 134.2, 128.1, 127.4, 122.2, 121.8, 119.9, 117.0, 82.9, 61.4, 39.8, 38.0, 24.2, 23.9; **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}N_2O_2^+$ [M+H] 297.1603, found 297.1604.

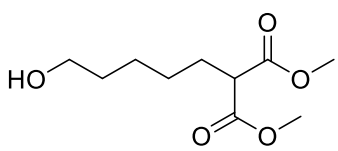


Scheme S5: Synthesis of the substrates containing a carbon nucleophile [C-H] for 5-exo-trig cyclization (**1ea**).



S24

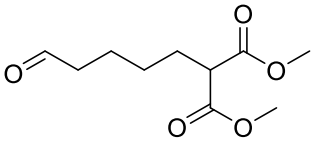
dimethyl 2-(pent-4-en-1-yl)malonate (S24): [7]Anhydrous NaH (720 mg, 18 mmol, 1.2 equiv) and anhydrous THF (60 mL) were introduced into a two-neck flask, and the suspension was cooled to 0 °C. Dimethyl malonate (2.7 mL, 16.8 mmol, 1.13 equiv) was then added dropwise over 5 min. The ice bath was removed, and the solution was stirred at room temperature for an additional 30 min. Tetrabutylammonium iodide (1.7 g, 4.5 mmol, 0.3 equiv) was added, followed by 5-bromopent-1-ene (1.7 mL, 15 mmol, 1.0 equiv), and the mixture was purged with N_2 and heated at reflux (80 °C) overnight. The solution was then allowed to cool to room temperature and quenched by addition of aq. sat. NH_4Cl solution. The aqueous layer was extracted with diethyl ether (3 × 20 mL), and the combined organic layers were eashed with brine (20 mL), dried over $MgSO_4$, concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (20:1 hexane:EtOAc) to afford **S22** as a colorless oil (1.8 g, 6.82 mmol, 59%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.77 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.01 (dq, *J* = 17.1, 1.7 Hz, 1H), 4.96 (ddt, *J* = 10.2, 2.1, 1.2 Hz, 1H), 3.73 (s, 6H), 3.36 (t, *J* = 7.6 Hz, 1H), 2.11–2.04 (m, 2H), 1.95–1.88 (m, 2H), 1.45–1.37 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 138.0, 115.2, 52.6, 51.7, 33.4, 28.4, 26.7.



S25

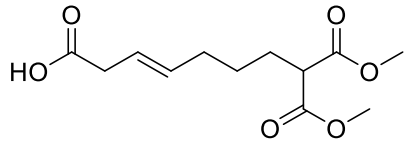
dimethyl 2-(5-hydroxypentyl)malonate (S25): The title compound was prepared from intermediate **S24** (1.8 g, 8.9 mmol), 9-BBN (0.5 M solution in THF, 37.4 mL, 18.7 mmol), 1 M NaOH solution (30 mL), and 30% H_2O_2 (24 mL) using a procedure similar to the one described above for the synthesis of compound **S13**. Purification using silica gel column chromatography with 2:1 hexanes:EtOAc as the eluent gave the product as a colorless oil (1.38 g, 71%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.74 (s, 6H), 3.63 (t, *J* = 6.6 Hz, 2H), 3.37 (t, *J*

= 7.5 Hz, 1H), 1.94–1.89 (m, 2H), 1.56 (m, 2H), 1.42–1.33 (m, 4H), 1.25 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 62.9, 52.6, 51.8, 32.5, 28.9, 27.2, 25.5.



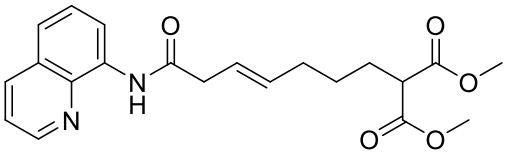
S26

dimethyl 2-(5-oxopentyl)malonate (S26): The title compound was prepared from oxalyl chloride (0.31 mL, 3.6 mmol), DMSO (0.36 mL, 5.0 mmol), intermediate **S25** (522 mg, 2.4 mmol), and Et_3N (1.7 mL, 12.0 mmol) using a procedure similar to the one described above for the synthesis of intermediate **S3**. Purification using silica gel column chromatography with 3:1 hexanes:EtOAc as the eluent was performed quickly to afford the product as a colorless oil (410 mg, 79% yield).**^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.74 (s, 6H), 3.63 (t, *J* = 6.6 Hz, 2H), 3.37 (t, *J* = 7.5 Hz, 1H), 1.94–1.89 (m, 2H), 1.56 (m, 2H), 1.42–1.33 (m, 4H), 1.25 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 62.9, 52.6, 51.8, 32.5, 28.9, 27.2, 25.5.



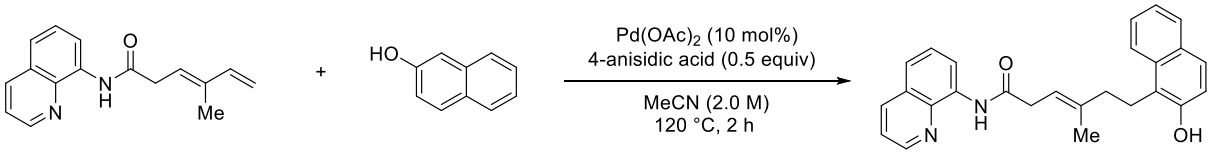
S27

(*E*)-9-methoxy-8-(methoxycarbonyl)-9-oxonon-3-enoic acid (S27): The title compound was prepared from intermediate **S26** (410 mg, 1.9 mmol), malonic acid (217 mg, 2.1 mmol), piperidine (10 μL) and acetic acid (6 μL) using a procedure similar to the one described above for the synthesis of intermediate **S4**. Purification using silica gel column chromatography with 1:1 hexanes:EtOAc as the eluent gave the product as a colorless oil (370 mg, 75% yield). **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.12 (s, 1H), 5.49–5.45 (m, 2H), 3.65 (s, 9H), 3.52 (t, *J* = 7.5 Hz, 1H), 2.96–2.92 (m, 2H), 2.02–1.96 (m, 2H), 1.75 (dd, *J* = 8.0, 2.5 Hz, 2H), 1.33–1.27 (m, 2H); **^{13}C NMR** (150 MHz, DMSO-d_6) δ 172.8, 169.5, 132.5, 123.3, 52.3, 50.7, 37.5, 31.4, 27.8, 26.2.



1ea

dimethyl (*E*)-2-(7-oxo-7-(quinolin-8-ylamino)hept-4-en-1-yl)malonate (1ea): The title compound was prepared from intermediate **S27** (350 mg, 1.4 mmol), 8-aminoquinoline (176 mg, 1.2 mmol), pyridine (220 μL, 2.7 mmol), and HATU (620 mg, 1 .6 mmol) using a procedure similar to the one described above for the synthesis of compound **1c**. Purification using silica gel column chromatography with 4:1 hexanes:EtOAc as the eluent gave the product as light-yellow oil (296 mg, 63% yield). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.56–7.47 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 5.84–5.72 (m, 2H), 3.71 (s, 6H), 3.39 (t, *J* = 7.5 Hz, 1H), 3.27 (d, *J* = 6.0 Hz, 1H), 2.23–2.17 (m, 2H), 2.02–1.94 (m, 2H), 1.57–1.49 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.0, 169.9, 148.4, 138.7, 136.4, 135.9, 134.6, 128.1, 127.5, 123.3, 121.7, 121.6, 116.5, 52.6, 51.7, 42.2, 32.4, 28.6, 27.1; **HRMS** (ESI-TOF) Calcd for $C_{21}H_{25}N_2O_5^+$ [M+H] 385.1763, found 385.1758.

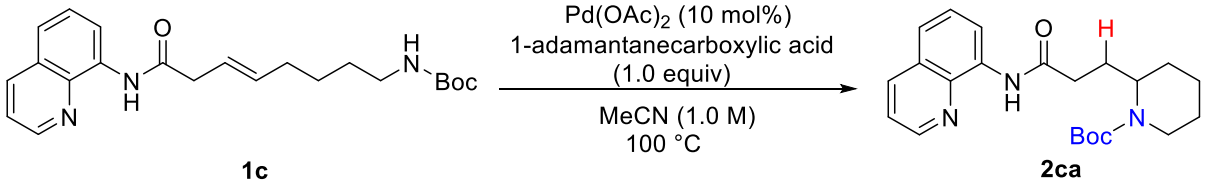


1ec

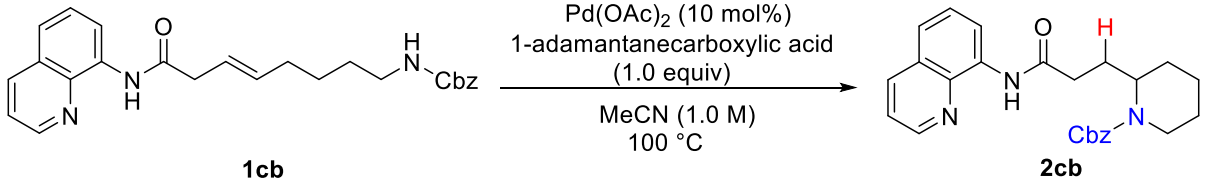
(*E*)-6-(3-hydroxynaphthalen-2-yl)-4-methyl-N-(quinolin-8-yl)hex-3-enamide (1ec): To a 1 dram (4 mL) vial equipped with a magnetic stir bar were added $Pd(OAc)_2$ (19.8 mg, 0.09 mmol), diene (227 mg, 0.9 mmol), *p*-methoxybenzoic acid (68.4 mg, 0.45 mmol), 2-naphthol (194 mg, 1.35 mmol), and MeCN (0.45 mL). The vial was sealed with an unpunctured TFE septum-covered screw cap and placed in a heating block that was pre-heated to 80 °C for 2 h. The reaction vial was cooled to room temperature, and the dark brown solution was directly purified by preparative TLC with 2:1 hexanes:EtOAc as the eluent to afford the desired product as a yellow solid (7.4 mg, 2% yield). Also observed in the crude reaction mixture were the unreacted starting material and the cyclized product **3c**.[16] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.98 (s, 1H), 9.18–8.70 (m, 2H), 8.20 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.95 (dd, *J* = 8.6, 1.0 Hz, 1H), 7.82 (s, 1H), 7.80–7.72 (m, 1H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.58–7.52 (m, 2H), 7.51–7.45 (m, 2H), 7.31 (ddd, *J* = 8.0, 6.8, 1.1 Hz, 1H), 7.14 (d, *J* = 8.8 Hz, 1H), 5.56 (td, *J* = 8.0, 1.6 Hz, 1H), 3.33 (dd, *J* = 8.1, 1.0 Hz, 2H), 3.32–3.26 (m, 2H), 2.58–2.46 (m, 2H), 1.92 (q, *J* = 0.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.17, 152.16, 148.42, 142.42, 138.55, 136.84, 134.34, 133.14, 129.37, 128.82, 128.20, 128.01, 127.70, 126.43, 122.86, 122.54, 122.15, 121.80, 119.00, 118.93, 117.41, 117.23, 38.16, 32.53, 24.92, 24.20. **HRMS (ESI-TOF)** Calcd for $C_{26}H_{25}N_2O_2^+$ $[M+H]^+$ 397.1916, found 397.1913.

General Procedure C for Alkene Intramolecular Hydrofuctionalization

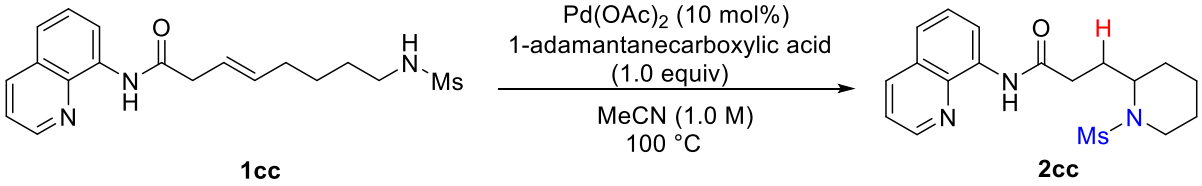
To an 8-mL reaction tube equipped with a Teflon-coated magnetic stir bar were added the alkene substrate (0.1 mmol), 1-adamantanecarboxylic acid (0.1 mmol), $Pd(OAc)_2$ (10 mol%), Acetonitrile (0.1 mL). The vial was sealed with an unpunctured TFE septum-covered screw cap and placed in a heating block that was pre-heated to 100 °C. After the reaction reached completion (as monitored by TLC), the dark black reaction mixture was allowed to cool to room temperature, filtered through a plug of silica gel, and washed with DCM to elute all organic materials. The filtrate was concentrated by vacuum, re-dissolved in DCM, and separated by preparative TLC.



***tert*-butyl 2-(3-oxo-3-(quinolin-8-ylamino)propyl)piperidine-1-carboxylate (2ca):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 35.1 mg (92%) of **2ca** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.82 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.55–7.46 (m, 2H), 7.44 (dd, *J* = 8.2, 4.1 Hz, 1H), 4.37 (s, 1H), 4.02 (s, 1H), 2.85 (s, 1H), 2.59–2.47 (m, 2H), 2.27 (s, 1H), 1.89 (d, *J* = 7.6 Hz, 1H), 1.69–1.58 (m, 5H), 1.40 (m, 10H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.5, 155.4, 148.2, 138.4, 136.4, 134.7, 128.0, 127.5, 121.7, 121.5, 116.5, 79.5, 50.2, 38.9, 34.9, 29.2, 28.5, 25.8, 25.7, 19.3; **HRMS** (ESI-TOF) Calcd for $C_{22}H_{30}N_3O_3^+$ [M+H] 384.2287, found 384.2282.

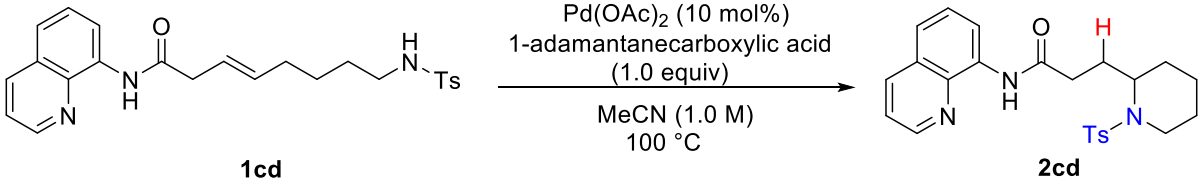


benzyl 2-(3-oxo-3-(quinolin-8-ylamino)propyl)piperidine-1-carboxylate (2cb): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 37.2 mg (89%) of **2cb** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.74 (d, *J* = 6.7 Hz, 1H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.53–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.26 (m, 5H), 5.05 (d, *J* = 11.6 Hz, 2H), 4.46 (s, 1H), 4.07 (s, 1H), 2.94 (s, 1H), 2.51 (m, 2H), 2.35 (s, 1H), 1.88 (s, 1H), 1.73–1.63 (m, 5H), 1.42 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.3, 155.8, 148.2, 138.4, 136.9, 136.4, 134.7, 128.5, 128.1, 127.9, 127.8, 127.5, 121.7, 121.5, 116.5, 67.1, 50.8, 39.3, 38.9, 36.6, 29.3, 28.0, 25.7, 19.2; **HRMS** (ESI-TOF) Calcd for $C_{25}H_{28}N_3O_3^+$ [M+H] 418.2131, found 418.2134.



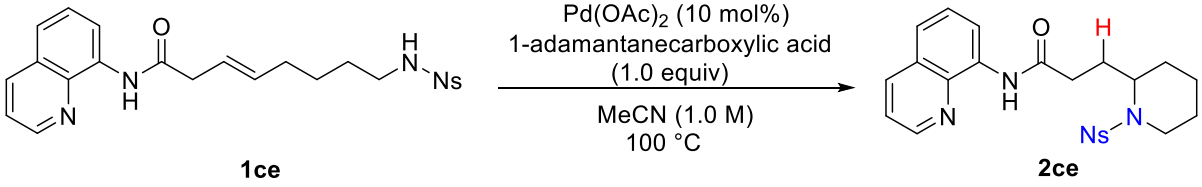
1cc 2cc

3-(1-(methylsulfonyl)piperidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2cc): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 29.7 mg (82%) of **2cc** as a light-yellow solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.83 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.54–7.48 (m, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.09 (dt, *J* = 10.1, 4.9 Hz, 1H), 3.76 (dq, *J* = 14.7, 1.9 Hz, 1H), 3.14 (ddd, *J* = 14.6, 13.3, 2.8 Hz, 1H), 2.91 (s, 3H), 2.69–2.65 (m, 2H), 2.38–2.31 (m, 1H), 1.93 (dtd, *J* = 14.1, 7.6, 5.0 Hz, 1H), 1.80–1.65 (m, 5H), 1.54–1.46 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.2, 148.3, 138.5, 136.4, 134.7, 128.1, 127.5, 121.8, 121.6, 116.5, 52.6, 41.0, 40.6, 34.8, 29.0, 25.4, 25.2, 18.8; **HRMS** (ESI-TOF) Calcd for $C_{18}H_{24}N_3O_3S^+$ [M+H] 362.1538, found 362.1533.



1cd 2cd

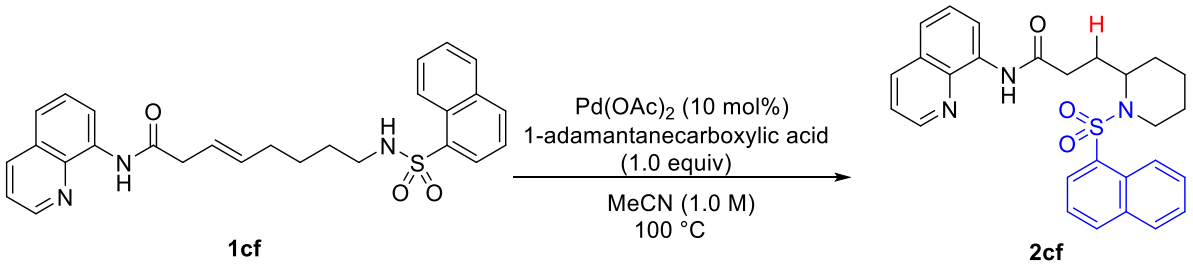
***N*-(quinolin-8-yl)-3-(1-tosylpiperidin-2-yl)propanamide (2cd):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 42.1 mg (97%) of **2cd** as a light-yellow solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.82 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.54–7.48 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.26 (d, *J* = 7.7 Hz, 2H), 4.14 (dt, *J* = 10.5, 5.0 Hz, 1H), 3.88–3.83 (m, 1H), 3.11 (ddd, *J* = 14.6, 13.3, 2.9 Hz, 1H), 2.71–2.61 (m, 2H), 2.36 (s, 3H), 2.33–2.25 (m, 1H), 1.84 (dddd, *J* = 14.1, 9.3, 6.6, 4.7 Hz, 1H), 1.58 (dddd, *J* = 16.9, 13.1, 8.8, 3.9 Hz, 1H), 1.50–1.36 (m, 4H), 1.12 (qt, *J* = 13.2, 4.3 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.4, 148.3, 143.0, 139.1, 138.5, 136.4, 134.7, 129.8, 128.1, 127.5, 127.1, 121.7, 121.5, 116.4, 52.8, 40.8, 34.8, 28.1, 25.4, 24.1, 21.6, 18.7; **HRMS** (ESI-TOF) Calcd for $C_{24}H_{28}N_3O_3S^+$ [M+H] 438.1851, found 438.1851.



1ce 2ce

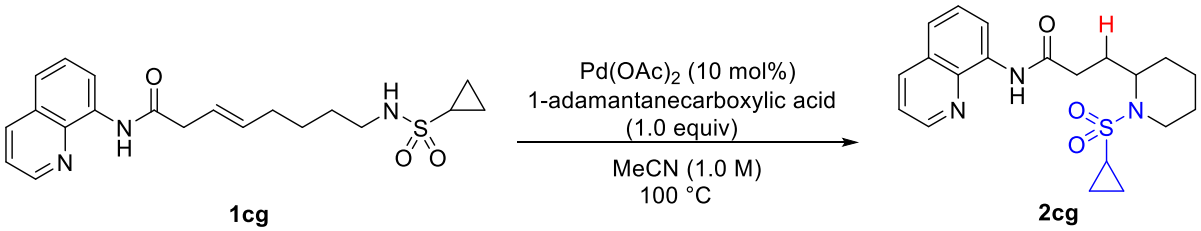
3-(1-((4-nitrophenyl)sulfonyl)piperidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2ce): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 15.0 mg (32%) of **2ce** as a light-yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.73 (dd, *J* = 7.3, 1.7 Hz, 1H), 8.32–8.26 (m, 2H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.06–8.01 (m, 2H), 7.55–7.50 (m, 2H), 7.47 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.21 (dt, *J* = 10.4, 5.1 Hz, 1H), 3.91–3.87 (m, 1H), 3.19 (ddd, *J* = 14.5, 13.4, 2.6 Hz, 1H), 2.64 (t, *J* = 7.4 Hz, 2H), 2.30 (ddd, *J* = 14.4, 7.2, 3.2 Hz, 1H), 1.93–1.88 (m, 1H), 1.59 (d, *J* = 4.1 Hz, 2H), 1.55–1.50 (m, 2H), 1.40 (tq, *J* = 12.0, 3.6 Hz, 1H), 1.16–1.09 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.8, 149.9, 148.4, 147.8, 138.4, 136.5, 134.6, 128.2, 128.1, 127.5, 124.6, 121.8, 121.7, 116.5, 53.4, 41.2, 34.4, 28.4, 25.2, 24.5, 18.5; **HRMS** (ESI-TOF) Calcd for $C_{23}H_{25}N_4O_5S^+$ [M+H] 469.1546, found 469.1546.



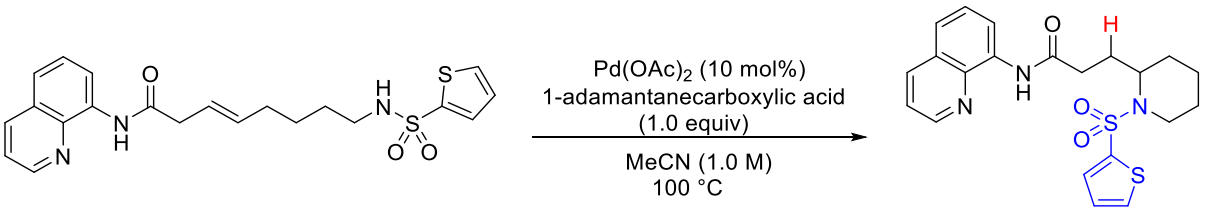
1cf **2cf**

3-(1-(naphthalen-1-ylsulfonyl)piperidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2cf): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 35.7 mg (75%) of **2cf** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.73 (dd, *J* = 7.3, 1.7 Hz, 1H), 8.32–8.26 (m, 2H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.06–8.01 (m, 2H), 7.55–7.50 (m, 2H), 7.47 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.21 (dt, *J* = 10.4, 5.1 Hz, 1H), 3.91–3.87 (m, 1H), 3.19 (ddd, *J* = 14.5, 13.4, 2.6 Hz, 1H), 2.64 (t, *J* = 7.4 Hz, 2H), 2.30 (ddd, *J* = 14.4, 7.2, 3.2 Hz, 1H), 1.93–1.88 (m, 1H), 1.59 (d, *J* = 4.1 Hz, 2H), 1.55–1.50 (m, 2H), 1.40 (tq, *J* = 12.0, 3.6 Hz, 1H), 1.16–1.09 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.3, 148.3, 138.8, 138.5, 136.4, 134.7, 134.7, 132.4, 129.6, 129.3, 128.6, 128.1, 128.0, 127.9, 127.5, 127.5, 122.6, 121.7, 121.5, 116.4, 53.0, 40.9, 34.7, 28.3, 25.5, 24.3, 18.6; **HRMS** (ESI-TOF) Calcd for $C_{27}H_{28}N_3O_3S^+$ [M+H] 474.1851, found 474.1855.



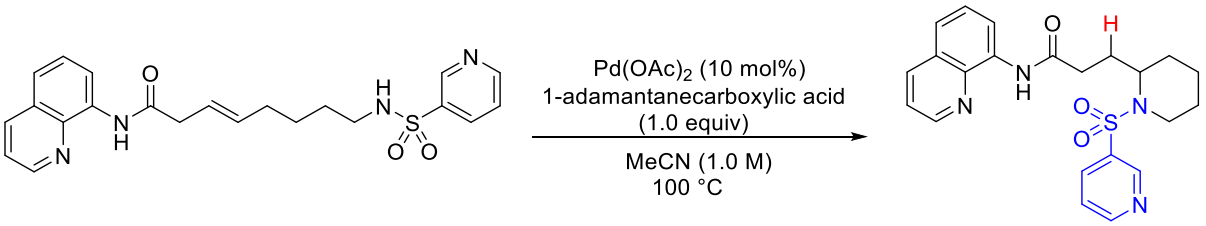
1cg **2cg**

3-(1-(cyclopropylsulfonyl)piperidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2cg): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 30.7 mg (80%) of **2cg** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.82 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.74 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.13 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.53–7.47 (m, 2H), 7.43 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.05 (dt, *J* = 10.4, 5.1 Hz, 1H), 3.75 (ddd, *J* = 14.8, 4.7, 1.9 Hz, 1H), 3.14 (ddd, *J* = 14.6, 13.0, 3.0 Hz, 1H), 2.67 (td, *J* = 8.9, 6.3 Hz, 2H), 2.40–2.32 (m, 2H), 1.94–1.88 (m, 1H), 1.86–1.80 (m, 1H), 1.69 (dd, *J* = 7.2, 3.3 Hz, 2H), 1.56 (dddd, *J* = 18.7, 9.8, 7.5, 3.8 Hz, 1H), 1.20–1.16 (m, 2H), 0.99–0.94 (m, 2H); **^{13}C NMR** (150 MHz, CDCl3) δ 171.3, 148.3, 138.4, 136.4, 134.7, 128.0, 127.4, 121.7, 121.5, 116.5, 52.9, 40.9, 34.8, 31.1, 29.2, 25.4, 25.4, 18.8, 5.7; **HRMS** (ESI-TOF) Calcd for $C_{20}H_{26}N_3O_3S^+$ [M+H] 388.1695, found 388.1699.



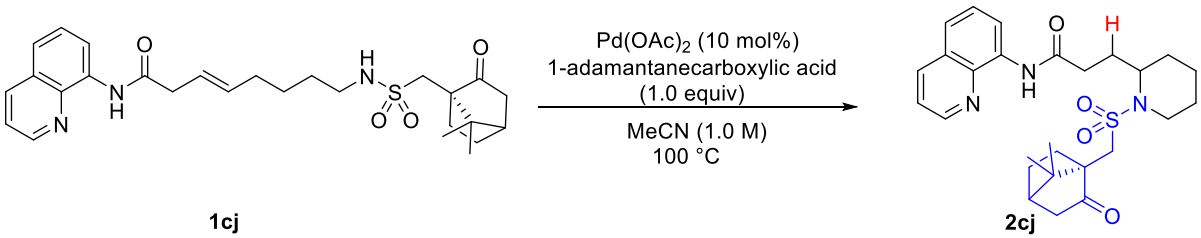
1ch **2ch**

***N*-(quinolin-8-yl)-3-(1-(thiophen-2-ylsulfonyl)piperidin-2-yl)propanamide (2ch):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 37.6 mg (88%) of **2ch** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.58 (dd, *J* = 3.7, 1.3 Hz, 1H), 7.54–7.48 (m, 3H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.05 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.19 (dt, *J* = 10.3, 5.0 Hz, 1H), 3.92–3.87 (m, 1H), 3.16 (ddd, *J* = 14.6, 13.2, 2.8 Hz, 1H), 2.73–2.63 (m, 2H), 2.32 (dddd, *J* = 14.2, 10.4, 9.1, 6.1 Hz, 1H), 1.88 (dddd, *J* = 14.0, 9.2, 6.6, 4.8 Hz, 1H), 1.63–1.46 (m, 5H), 1.26–1.22 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.3, 148.3, 142.9, 138.5, 136.4, 134.7, 131.5, 131.3, 128.0, 127.5, 127.5, 121.7, 121.5, 116.5, 53.3, 41.1, 34.8, 28.1, 25.5, 24.1, 18.6; **HRMS** (ESI-TOF) Calcd for $C_{21}H_{24}N_3O_3S_2^+$ [M+H] 430.1259, found 430.1253.



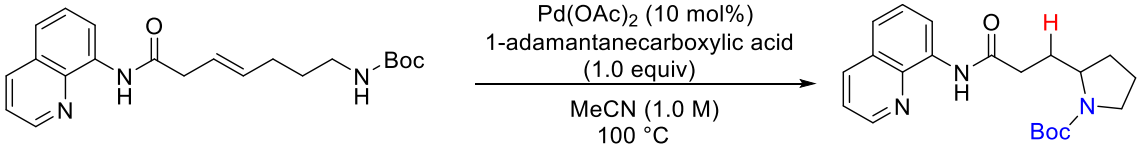
1ci **2ci**

3-(1-(pyridin-3-ylsulfonyl)piperidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2ci): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 28.6 mg (67%) of **2ci** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.84 (s, 1H), 9.09 (dd, *J* = 2.3, 0.8 Hz, 1H), 8.83 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.75 (dt, *J* = 6.0, 1.4 Hz, 2H), 8.17–8.12 (m, 2H), 7.55–7.49 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.41 (ddd, *J* = 8.0, 4.9, 0.9 Hz, 1H), 4.19 (dt, *J* = 10.4, 5.0 Hz, 1H), 3.86 (ddd, *J* = 14.6, 3.7, 2.0 Hz, 1H), 3.18 (ddd, *J* = 14.7, 13.5, 2.6 Hz, 1H), 2.68 (ddd, *J* = 7.9, 6.9, 2.0 Hz, 2H), 2.32 (dddd, *J* = 14.7, 10.4, 8.0, 6.8 Hz, 1H), 1.90 (dddd, *J* = 14.3, 8.3, 7.2, 4.9 Hz, 1H), 1.65–1.48 (m, 4H), 1.36 (tdd, *J* = 13.6, 5.5, 3.7 Hz, 1H), 1.10 (tdd, *J* = 13.1, 9.1, 4.6 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.0, 153.0, 148.3, 148.0, 138.6, 138.5, 136.4, 134.7, 134.6, 128.1, 127.5, 123.9, 121.8, 121.6, 116.5, 53.2, 41.0, 34.6, 28.3, 25.4, 24.3, 18.6; **HRMS** (ESI-TOF) Calcd for $C_{22}H_{25}N_4O_3S^+$ [M+H] 425.1647, found 425.1642.



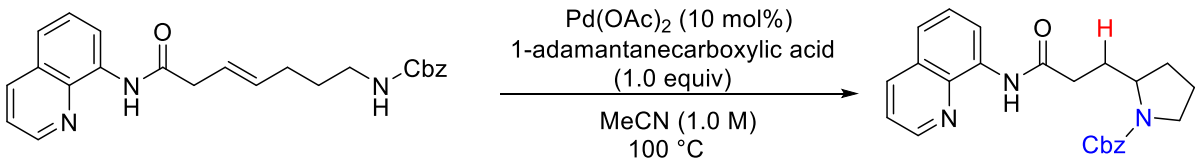
1cj **2cj**

3-(1-((((1*S*)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methyl)sulfonyl)piperidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2cj): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 35.1 mg (71%) of **2cj** as a colorless oil. The product was isolated as a 1:1 mixture of diastereomers. The ensuing analytical data corresponds to the mixture. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.83 (d, *J* = 3.2 Hz, 1H), 8.79 (dt, *J* = 4.2, 1.8 Hz, 1H), 8.74 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.14 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.53–7.47 (m, 2H), 7.43 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.12 (ddt, *J* = 11.9, 10.1, 4.5 Hz, 1H), 3.79 (td, *J* = 13.9, 4.4 Hz, 1H), 3.41 (dd, *J* = 14.5, 12.8 Hz, 1H), 3.15 (dddd, *J* = 14.4, 12.9, 10.4, 2.6 Hz, 1H), 2.85 (dd, *J* = 14.5, 7.2 Hz, 1H), 2.74–2.63 (m, 2H), 2.56 (dddd, *J* = 14.9, 11.4, 7.2, 4.0 Hz, 1H), 2.40–2.32 (m, 2H), 2.07 (td, *J* = 4.5, 1.6 Hz, 1H), 2.05–2.00 (m, 1H), 1.96–1.89 (m, 2H), 1.84–1.74 (m, 1H), 1.70 (ddt, *J* = 8.6, 5.9, 3.0 Hz, 3H), 1.63 (dddd, *J* = 15.9, 9.4, 4.9, 2.5 Hz, 2H), 1.60–1.49 (m, 1H), 1.40 (ddd, *J* = 13.1, 9.3, 4.0 Hz, 1H), 1.14 (d, *J* = 8.8 Hz, 3H), 0.87 (d, *J* = 15.4 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 215.5, 215.4, 171.4, 171.3, 148.2, 138.5, 138.5, 136.4, 136.3, 134.7, 134.7, 128.0, 127.5, 127.5, 121.7, 121.5, 116.5, 58.8, 52.7, 52.5, 50.4, 50.1, 47.8, 47.8, 43.1, 43.0, 42.7, 40.7, 40.6, 35.0, 34.9, 29.3, 29.1, 27.0, 27.0, 25.6, 25.6, 25.5, 25.5, 25.3, 25.2, 20.3, 20.2, 20.0, 19.9, 18.8, 18.8; **HRMS** (ESI-TOF) Calcd for $C_{27}H_{36}N_3O_4S^+$ [M+H] 498.2427, found 498.2438.



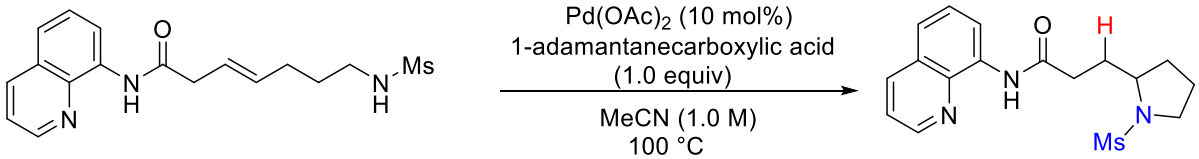
1b **2ba**

***tert*-butyl 2-(3-oxo-3-(quinolin-8-ylamino)propyl)pyrrolidine-1-carboxylate (2ba):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 33.5 mg (91%) of **2ba** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.78–8.74 (m, 1H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.50 (dd, *J* = 18.6, 7.9 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 1H), 3.93 (d, *J* = 45.2 Hz, 1H), 3.41 (m, 2H), 2.56 (m, 1H), 2.22–2.13 (m, 1H), 2.05–1.79 (m, 4H), 1.73 (m, 1H), 1.46 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ171.3, 154.9, 148.2, 138.5, 136.4, 134.8, 128.0, 127.5, 121.7, 121.5, 116.5, 79.2, 57.0, 38.8, 36.6, 30.7, 28.7, 28.6, 28.0; **HRMS** (ESI-TOF) Calcd for $C_{21}H_{28}N_3O_3^+$ [M+H] 370.2131, found 370.2130.



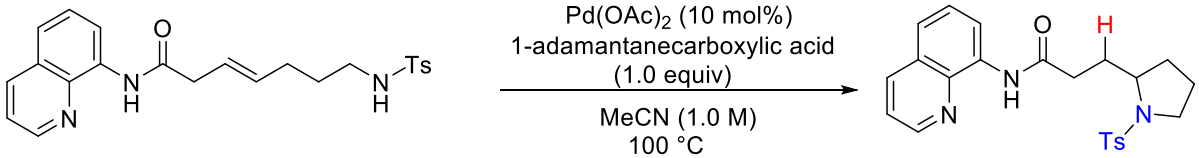
1bb **2bb**

benzyl 2-(3-oxo-3-(quinolin-8-ylamino)propyl)pyrrolidine-1-carboxylate (2bb): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 35.0 mg (87%) of **2bb** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.83–8.72 (m, 2H), 8.15 (t, *J* = 9.4 Hz, 1H), 7.55–7.43 (m, 3H), 7.33 (m, 3H), 7.30–7.17 (m, 2H), 5.18–5.03 (m, 2H), 4.10–4.00 (m, 1H), 3.57–3.41 (m, 2H), 2.70–2.61 (m, 1H), 2.53 (t, *J* = 8.0 Hz, 1H), 2.21 (dt, *J* = 14.7, 7.4 Hz, 1H), 2.02–1.92 (m, 3H), 1.87 (h, *J* = 4.9, 3.5 Hz, 1H), 1.76 (d, *J* = 15.5 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ171.6, 155.5, 148.2, 138.5, 137.1, 136.4, 134.8, 128.5, 128.1, 127.9, 127.9, 127.5, 121.7, 121.5, 116.6, 67.0, 57.6, 46.4, 35.4, 31.1, 30.5, 23.9; **HRMS** (ESI-TOF) Calcd for $C_{24}H_{26}N_3O_3^+$ [M+H] 404.1974, found 404.1982.



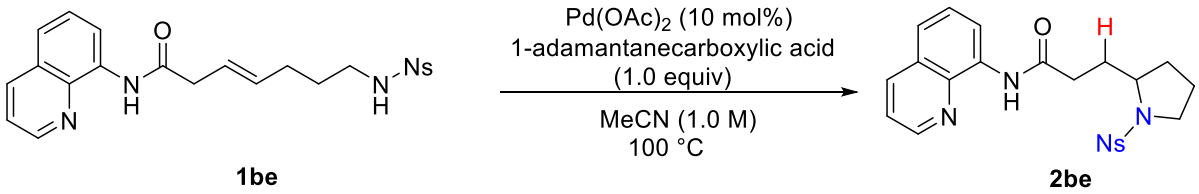
1bc **2bc**

3-(1-(methylsulfonyl)pyrrolidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2bc): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (1:1 hexanes:EtOAc) to afford 31.6 mg (91%) of **2bc** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.74 (dd, *J* = 7.4, 1.6 Hz, 1H), 8.14 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.54–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 3.89 (qd, *J* = 6.8, 3.4 Hz, 1H), 3.46–3.35 (m, 2H), 2.82 (s, 3H), 2.71 (t, *J* = 7.7 Hz, 2H), 2.12 (dq, *J* = 14.7, 7.4 Hz, 1H), 2.07–1.98 (m, 3H), 1.96–1.89 (m, 1H), 1.85–1.78 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.3, 148.3, 138.5, 136.4, 134.7, 128.1, 127.5, 121.8, 121.6, 116.5, 60.0, 48.9, 35.5, 34.6, 31.7, 31.6, 24.7; **HRMS** (ESI-TOF) Calcd for $C_{17}H_{22}N_3O_3S^+$ [M+H] 348.1382, found 348.1383.



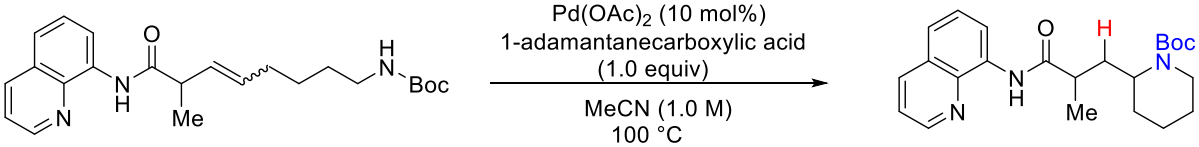
1bd **2bd**

***N*-(quinolin-8-yl)-3-(1-tosylpyrrolidin-2-yl)propanamide (2bd):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 37.8 mg (89%) of **2bd** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.77 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.17–8.14 (m, 1H), 7.73–7.71 (m, 2H), 7.55–7.49 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.26 (d, *J* = 1.4 Hz, 2H), 3.86–3.82 (m, 1H), 3.43 (ddd, *J* = 10.5, 7.5, 4.6 Hz, 1H), 3.25 (dt, *J* = 10.9, 7.4 Hz, 1H), 2.83–2.73 (m, 2H), 2.40 (s, 3H), 2.13 (ddt, *J* = 14.0, 8.4, 6.7 Hz, 1H), 2.06–2.00 (m, 1H), 1.88–1.80 (m, 1H), 1.63–1.48 (m, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.5, 148.3, 143.5, 138.5, 136.4, 134.9, 134.8, 129.8, 128.1, 127.7, 127.5, 121.7, 121.5, 116.5, 60.1, 49.0, 34.7, 31.7, 31.3, 24.2, 21.6; **HRMS** (ESI-TOF) Calcd for $C_{23}H_{26}N_3O_3S^+$ [M+H] 424.1695, found 424.1695.



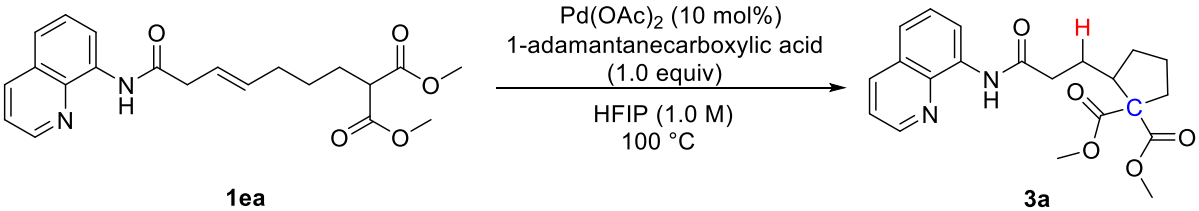
1be **2be**

3-(1-((4-nitrophenyl)sulfonyl)pyrrolidin-2-yl)-*N*-(quinolin-8-yl)propanamide (2be): The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 33.1 mg (73%) of **2be** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.82 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.77 (dd, *J* = 7.4, 1.6 Hz, 1H), 8.35–8.29 (m, 2H), 8.17 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.06–8.00 (m, 2H), 7.57–7.51 (m, 2H), 7.47 (dd, *J* = 8.2, 4.2 Hz, 1H), 3.89 (qd, *J* = 7.0, 3.5 Hz, 1H), 3.51 (ddd, *J* = 10.7, 7.6, 4.6 Hz, 1H), 3.27 (dt, *J* = 10.5, 7.4 Hz, 1H), 2.79 (ddd, *J* = 15.2, 8.2, 6.7 Hz, 1H), 2.72 (ddd, *J* = 15.3, 8.2, 6.6 Hz, 1H), 2.20 (ddt, *J* = 13.7, 8.2, 6.7 Hz, 1H), 2.06–2.01 (m, 1H), 1.96–1.89 (m, 1H), 1.70 (tt, *J* = 10.8, 3.8 Hz, 1H), 1.66–1.58 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.0, 150.2, 148.4, 143.8, 138.5, 136.5, 134.6, 128.8, 128.1, 127.5, 124.5, 121.8, 121.7, 116.6, 60.4, 49.1, 34.4, 31.4, 31.4, 24.2; **HRMS** (ESI-TOF) Calcd for $C_{22}H_{23}N_4O_5S^+$ [M+H] 455.1389, found 455.1395.



2e

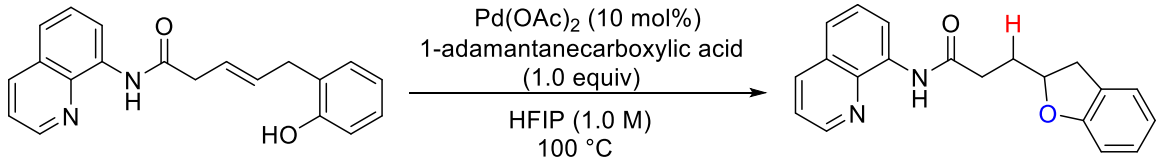
***tert*-butyl 2-(2-methyl-3-oxo-3-(quinolin-8-ylamino)propyl)piperidine-1-carboxylate (2e):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (3:1 hexanes:EtOAc) to afford 35.2 mg (88%) of **2e** as a colorless oil (1.5:1 dr, as determined by LC). The ensuing analytical data correspond to the diastereomeric mixture. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.87 (s, 1H), 9.04–8.64 (m, 3H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 2H), 7.62–7.36 (m, 4H), 4.42 (br, 1H), 4.06 (br, 1H), 2.88 (br, 1H), 2.66–2.54 (m, 1H), 2.11–1.85 (m, 2H), 1.77–1.55 (m, 6H), 1.46–1.35 (m, 3H), 1.52–1.16 (m, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.74, 154.76 (d, *J* = 11.8 Hz), 147.71, 138.04, 135.81, 134.28 (d, *J* = 16.1 Hz), 127.44, 126.93 (d, *J* = 2.8 Hz), 121.09, 120.87, 115.98, 78.83, 48.20, 38.22, 35.99, 33.72, 27.87, 27.79, 27.40, 25.19, 18.63. **HRMS** (ESI-TOF) Calcd for $C_{21}H_{31}N_3O_3^+$ [M+H] 384.2287, found 384.2286.



1ea **3a**

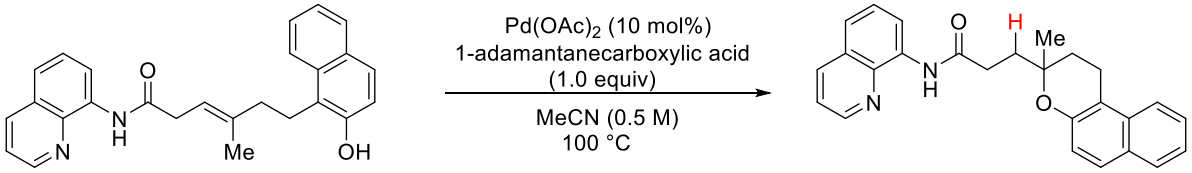
dimethyl 2-(3-oxo-3-(quinolin-8-ylamino)propyl)cyclopentane-1,1-dicarboxylate (3a): The reaction was carried out according to General Procedure C with HFIP instead of acetonitrile as solvent. The product was purified by preparative TLC (2:1 hexanes:EtOAc) to afford 30.0 mg (79%) of **3a** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.77 (dd, *J* = 7.4, 1.5 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.7 Hz, 1H),

7.54–7.48 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 3.75 (s, 3H), 3.72 (s, 3H), 2.67–2.56 (m, 3H), 2.46 (ddd, *J* = 13.8, 8.7, 7.2 Hz, 1H), 2.11–2.00 (m, 3H), 1.92–1.85 (m, 1H), 1.69 (dtd, *J* = 13.5, 9.8, 6.0 Hz, 1H), 1.62–1.56 (m, 1H), 1.50 (ddt, *J* = 12.5, 10.5, 9.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.1, 172.0, 171.5, 148.2, 138.5, 136.5, 134.7, 128.1, 127.6, 121.7, 121.5, 116.6, 63.5, 52.7, 52.4, 46.3, 37.4, 35.0, 31.1, 27.5, 23.1; **HRMS** (ESI-TOF) Calcd for $C_{21}H_{25}N_2O_5^+$ [M+H] 385.1763, found 385.1771.



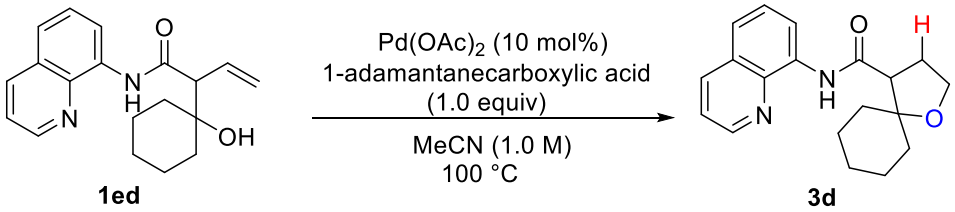
1eb **3b**

3-(2,3-dihydrobenzofuran-2-yl)-*N*-(quinolin-8-yl)propanamide (3b): The reaction was carried out according to General Procedure C with HFIP instead of acetonitrile as solvent. The product was purified by preparative TLC (3:1 hexanes:EtOAc) to afford 22.5 mg (71%) of **2eb** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.81 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.78 (dd, *J* = 7.5, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.56–7.49 (m, 2H), 7.46 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.16 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.10 (dddd, *J* = 8.8, 7.4, 1.5, 0.8 Hz, 1H), 6.83 (td, *J* = 7.4, 1.0 Hz, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 4.93 (tdd, *J* = 8.8, 7.5, 4.3 Hz, 1H), 3.37 (dd, *J* = 15.5, 9.0 Hz, 1H), 2.96 (dd, *J* = 15.5, 7.5 Hz, 1H), 2.86–2.76 (m, 2H), 2.30 (dddd, *J* = 14.1, 8.7, 7.1, 4.3 Hz, 1H), 2.21 (dtd, *J* = 14.3, 8.5, 5.9 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.1, 159.5, 148.3, 138.5, 136.5, 134.6, 128.1, 128.1, 127.5, 126.8, 125.1, 121.8, 121.6, 120.5, 116.6, 109.5, 82.3, 35.6, 34.0, 31.8; **HRMS** (ESI-TOF) Calcd for $C_{20}H_{19}N_2O_2^+$ [M+H] 319.1447, found 319.1449.

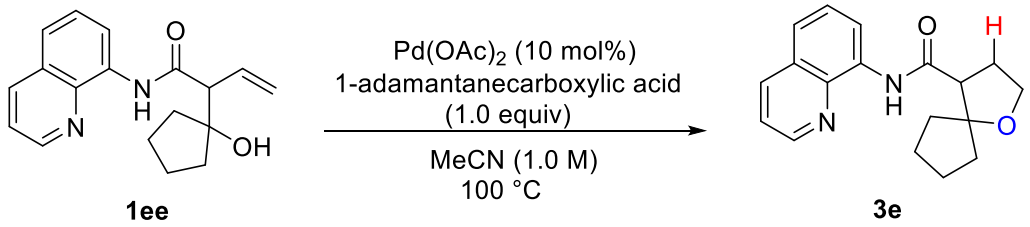


1ec **3c**

3-(3-methyl-2,3-dihydro-1H-benzo[f]chromen-3-yl)-N-(quinolin-8-yl)propanamide (3c): The reaction was carried out according to slightly modified version of General Procedure C. (*E*)-6-(3-hydroxynaphthalen-2-yl)-4-methyl-*N*-(quinolin-8-yl)hex-3-enamide (4.9 mg, 0.012 mmol), 1-adamantanecarboxylic acid (2.3 mg, 0.012 mmol) and 0.05 M $Pd(OAc)_2$ solution in MeCN (26 μL, 0.0012 mmol [Pd]) was added, and heated to 100 °C for 15 h. The product was purified by preparative TLC (3:1 hexanes:EtOAc) to afford 4.2 mg (86%) of **XX** as a yellow solid. Analytical data were in agreement with literature values.[16] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.91–8.54 (m, 2H), 8.15 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.55–7.40 (m, 4H), 7.33 (ddd, *J* = 8.0, 6.8, 1.2 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 1H), 3.23–2.97 (m, 2H), 2.92–2.74 (m, 2H), 2.41–2.14 (m, 2H), 2.12–1.97 (m, 2H), 1.40 (s, 3H).

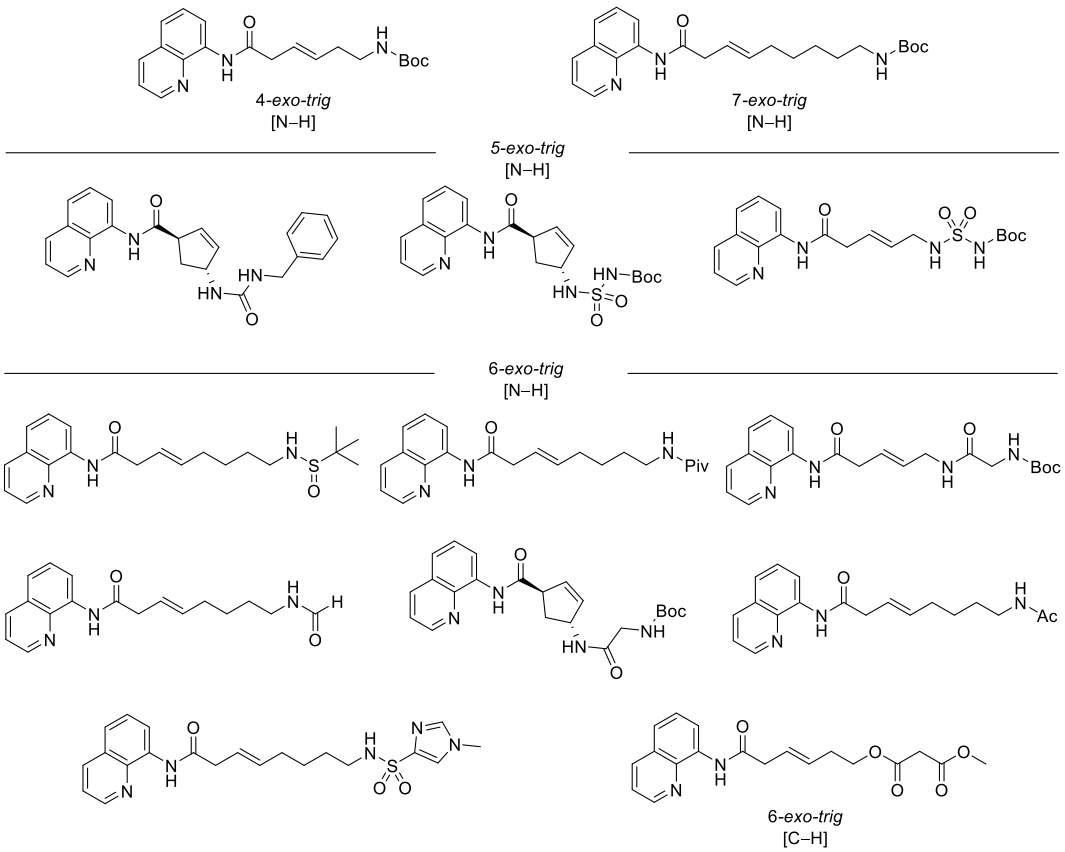


***N*-(quinolin-8-yl)-1-oxaspiro[4.5]decane-4-carboxamide (3d):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (3:1 hexanes:EtOAc) to afford 30.9 mg (99%) of **3c** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.85 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.80 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.19 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.58–7.52 (m, 2H), 7.49 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.18 (td, *J* = 8.6, 5.0 Hz, 1H), 3.97 (ddd, *J* = 8.6, 8.0, 7.1 Hz, 1H), 2.92 (dd, *J* = 8.5, 7.1 Hz, 1H), 2.60 (ddt, *J* = 12.6, 8.5, 7.1 Hz, 1H), 2.31 (dtd, *J* = 13.0, 8.2, 4.9 Hz, 1H), 1.86–1.80 (m, 2H), 1.80–1.68 (m, 2H), 1.62 (dddd, *J* = 15.1, 12.8, 8.3, 3.5 Hz, 3H), 1.56–1.51 (m, 1H), 1.43–1.37 (m, 1H), 1.20 (tdd, *J* = 15.7, 7.1, 3.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.8, 148.5, 138.6, 136.5, 134.6, 128.1, 127.5, 121.8, 121.7, 116.6, 83.8, 65.3, 56.9, 37.1, 31.9, 29.3, 25.6, 23.3, 22.5; **HRMS** (ESI-TOF) Calcd for $C_{19}H_{23}N_2O_2^+$ [M+H] 311.1760, found 311.1763.

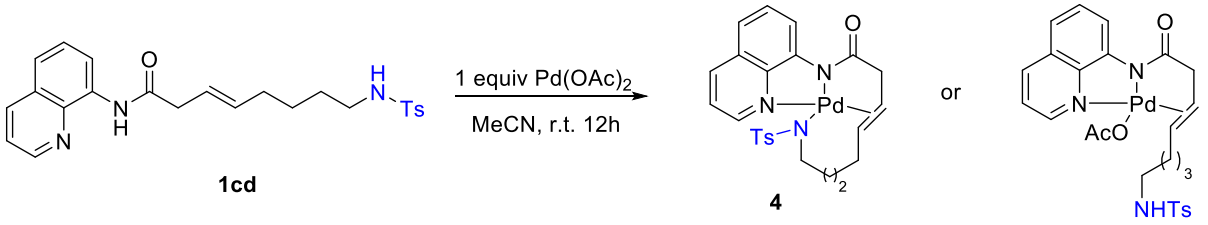


***N*-(quinolin-8-yl)-1-oxaspiro[4.4]nonane-4-carboxamide (3e):** The reaction was carried out according to General Procedure C. The product was purified by preparative TLC (3:1 hexanes:EtOAc) to afford 29.1 mg (99%) of **3d** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.83 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.77 (dd, *J* = 7.4, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.55–7.49 (m, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.18 (td, *J* = 8.7, 5.4 Hz, 1H), 3.94 (td, *J* = 8.6, 6.3 Hz, 1H), 3.07 (dd, *J* = 8.5, 5.7 Hz, 1H), 2.51 (dddd, *J* = 12.8, 8.7, 6.3, 5.7 Hz, 1H), 2.35 (dtd, *J* = 12.8, 8.5, 5.4 Hz, 1H), 1.98–1.92 (m, 1H), 1.87 (tdd, *J* = 9.0, 7.2, 3.4 Hz, 1H), 1.84–1.73 (m, 4H), 1.67–1.59 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.8, 148.5, 138.7, 136.4, 134.7, 128.1, 127.5, 121.7, 121.7, 116.7, 93.1, 65.2, 54.7, 38.3, 33.7, 30.0, 24.3, 24.0; **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}N_2O_2^+$ [M+H] 297.1603, found 297.1606.

Table S2. Representative unsuccessful substrates [a]



[a] Selected example of low-yielding (<10% yield) substrates in intramolecular hydrofunctionalization using General Procedure C



Procedure for Synthesis of Palladium Complex 4: Substrate **1cd** (43.8 mg, 0.1 mmol), $Pd(OAc)_2$ (22.4 mg, 0.1 mmol), and MeCN (1 mL) were added to a 1-dram vial. The reaction mixture was stirred at room temperature for 12 h under air. The reaction mixture was filtered through celite. The filtrate was concentrated in vacuo to give a yellow oil in 95% yield. The structure of the product was assigned based on NMR analysis of the crude reaction mixture. In the solid state, the NTs group is coordinated as the fourth ligand, but in the solution state, we were unable to determine if the NTs group or OAc is bound. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.79 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.39–8.35 (m, 2H), 7.66–7.62 (m, 2H), 7.53–7.47 (m, 2H), 7.42–7.39 (m, 1H), 7.17 (s, 2H), 6.37 (td, *J* = 8.0, 5.1 Hz, 1H), 5.90 (q, *J* = 7.7 Hz, 1H), 5.48 (t, *J* = 5.9 Hz, 1H), 3.51 (dd, *J* = 17.5, 7.6 Hz, 1H), 3.22–3.16 (m, 1H), 2.94–2.87 (m, 2H), 2.51 (dt, *J* = 14.6, 7.2 Hz, 1H), 2.37–2.36 (m, 1H), 2.34 (s, 3H), 2.04 (s, 3H), 1.78 (q, *J* = 7.5 Hz, 2H), 1.60 (dtd, *J* = 11.3, 6.5, 2.9 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 180.5, 178.2, 174.6, 146.5, 146.3, 146.0, 143.2, 140.4, 137.1, 130.1, 129.7, 127.1, 123.0, 121.0, 120.7, 117.4, 92.0, 42.7, 37.0, 30.7, 28.8, 25.5, 23.8, 21.5. **X-ray** (single-crystal) Yellow block crystals of X-ray diffraction quality were obtained by vapor diffusion of hexanes into a saturated solution of palladium complex in dichloromethane (CCDC 1995204).[17]

X-RAY CRYSTALLOGRAPHY

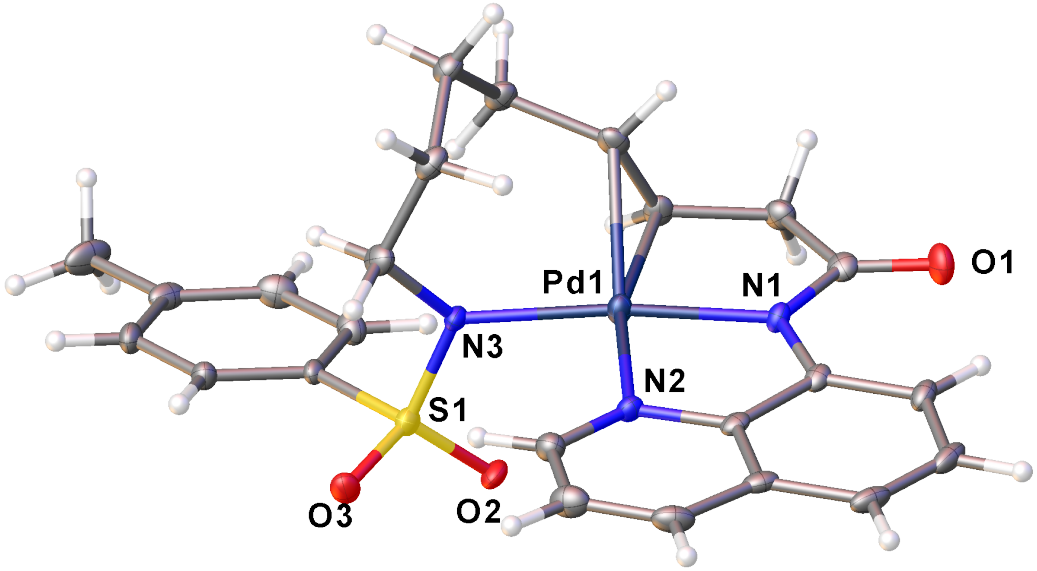


Table S3. Crystal data and structure refinement for complex **4**.

Identification code	X-1-260-2	
Empirical formula	C24 H25 N3 O3 Pd S	
Formula weight	541.93	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.2960(9) Å	α= 111.695(3)°.
	b = 11.0174(14) Å	β= 91.745(3)°.
	c = 12.5614(12) Å	γ = 93.375(4)°.
Volume	1063.2(2) $Å^3$	
Z	2	
Density (calculated)	1.693 Mg/m^3	
Absorption coefficient	1.004 mm^{-1}	
F(000)	552	
Crystal size	0.28 x 0.1 x 0.05 mm^3	
Theta range for data collection	1.748 to 27.492°.	
Index ranges	-10<=h<=10, -9<=k<=14, -16<=l<=16	
Reflections collected	11304	
Independent reflections	4882 [R(int) = 0.0238]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7048	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4882 / 0 / 290	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.0981	
R indices (all data)	R1 = 0.0449, wR2 = 0.1020	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.829 and -0.525 e.$Å^{-3}$	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Pd-1cd**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	2513(1)	3258(1)	7184(1)	14(1)
S(1)	5788(1)	4933(1)	7650(1)	16(1)
O(2)	5904(3)	4087(3)	8291(2)	22(1)
O(3)	6916(3)	4768(3)	6761(2)	22(1)
N(1)	1322(4)	1667(3)	7209(2)	15(1)
N(3)	3971(3)	4810(3)	7172(2)	15(1)
O(1)	-448(3)	810(3)	8168(2)	27(1)
N(2)	3312(4)	1919(3)	5695(2)	16(1)
C(9)	2573(4)	686(3)	5441(3)	16(1)
C(6)	1148(5)	-1789(4)	5027(3)	24(1)
C(7)	815(5)	-732(3)	6039(3)	20(1)
C(22)	7367(4)	8767(4)	9073(3)	22(1)
C(18)	6176(4)	6580(3)	8634(3)	15(1)
C(23)	7046(4)	7485(3)	8304(3)	18(1)
C(4)	2840(4)	-359(4)	4412(3)	19(1)
C(8)	1521(4)	508(3)	6258(3)	16(1)
C(14)	1021(5)	6007(4)	8057(3)	20(1)
C(16)	1916(5)	5358(4)	5987(3)	21(1)
C(2)	4518(5)	1159(4)	3887(3)	27(1)
C(1)	4260(4)	2145(4)	4949(3)	20(1)
C(17)	3671(5)	5526(4)	6403(3)	22(1)
C(5)	2115(5)	-1620(4)	4227(3)	24(1)
C(12)	1357(4)	4169(4)	8800(3)	18(1)
C(13)	665(4)	4644(4)	8040(3)	19(1)
C(20)	5933(5)	8244(4)	10485(3)	26(1)
C(10)	376(4)	1721(4)	8090(3)	19(1)
C(21)	6823(5)	9155(4)	10175(3)	23(1)
C(19)	5595(4)	6953(4)	9718(3)	21(1)
C(3)	3827(5)	-71(4)	3626(3)	25(1)
C(15)	811(5)	6138(4)	6890(3)	20(1)
C(11)	476(5)	3069(4)	9052(3)	21(1)
C(24)	7198(6)	10541(4)	11029(4)	36(1)

Table S5. Bond lengths [Å] and angles [°] for **Pd-1cd**.

Pd(1)-N(1)	1.972(3)
Pd(1)-N(3)	2.040(3)
Pd(1)-N(2)	2.065(3)
Pd(1)-C(12)	2.185(3)
Pd(1)-C(13)	2.236(4)
S(1)-O(2)	1.445(3)
S(1)-O(3)	1.445(3)
S(1)-N(3)	1.585(3)
S(1)-C(18)	1.781(3)
N(1)-C(8)	1.412(4)
N(1)-C(10)	1.361(5)
N(3)-C(17)	1.480(4)
O(1)-C(10)	1.217(5)
N(2)-C(9)	1.375(4)
N(2)-C(1)	1.324(5)
C(9)-C(4)	1.412(5)
C(9)-C(8)	1.427(5)
C(6)-H(6)	0.9500
C(6)-C(7)	1.419(5)
C(6)-C(5)	1.363(6)
C(7)-H(7)	0.9500
C(7)-C(8)	1.379(5)
C(22)-H(22)	0.9500
C(22)-C(23)	1.389(5)
C(22)-C(21)	1.388(6)
C(18)-C(23)	1.388(5)
C(18)-C(19)	1.380(5)
C(23)-H(23)	0.9500
C(4)-C(5)	1.414(5)
C(4)-C(3)	1.413(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(14)-C(13)	1.505(5)
C(14)-C(15)	1.531(5)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(16)-C(17)	1.509(5)

C(16)-C(15)	1.516(5)
C(2)-H(2)	0.9500
C(2)-C(1)	1.407(5)
C(2)-C(3)	1.357(6)
C(1)-H(1)	0.9500
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(5)-H(5)	0.9500
C(12)-H(12)	1.0000
C(12)-C(13)	1.373(5)
C(12)-C(11)	1.516(5)
C(13)-H(13)	1.0000
C(20)-H(20)	0.9500
C(20)-C(21)	1.387(6)
C(20)-C(19)	1.397(6)
C(10)-C(11)	1.525(5)
C(21)-C(24)	1.514(5)
C(19)-H(19)	0.9500
C(3)-H(3)	0.9500
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800

N(1)-Pd(1)-N(3)	173.73(12)
N(1)-Pd(1)-N(2)	81.49(12)
N(1)-Pd(1)-C(12)	82.26(13)
N(1)-Pd(1)-C(13)	96.28(13)
N(3)-Pd(1)-N(2)	95.61(12)
N(3)-Pd(1)-C(12)	100.39(13)
N(3)-Pd(1)-C(13)	89.10(13)
N(2)-Pd(1)-C(12)	163.65(13)
N(2)-Pd(1)-C(13)	148.56(13)
C(12)-Pd(1)-C(13)	36.17(14)
O(2)-S(1)-O(3)	116.66(16)

O(2)-S(1)-N(3)	108.11(15)
O(2)-S(1)-C(18)	107.77(16)
O(3)-S(1)-N(3)	111.89(16)
O(3)-S(1)-C(18)	105.70(16)
N(3)-S(1)-C(18)	106.11(16)
C(8)-N(1)-Pd(1)	115.2(2)
C(10)-N(1)-Pd(1)	120.9(2)
C(10)-N(1)-C(8)	123.9(3)
S(1)-N(3)-Pd(1)	117.34(16)
C(17)-N(3)-Pd(1)	123.8(2)
C(17)-N(3)-S(1)	115.1(2)
C(9)-N(2)-Pd(1)	111.8(2)
C(1)-N(2)-Pd(1)	128.2(3)
C(1)-N(2)-C(9)	119.6(3)
N(2)-C(9)-C(4)	121.3(3)
N(2)-C(9)-C(8)	117.3(3)
C(4)-C(9)-C(8)	121.4(3)
C(7)-C(6)-H(6)	118.9
C(5)-C(6)-H(6)	118.9
C(5)-C(6)-C(7)	122.1(4)
C(6)-C(7)-H(7)	120.0
C(8)-C(7)-C(6)	120.1(4)
C(8)-C(7)-H(7)	120.0
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(21)-C(22)-C(23)	120.5(3)
C(23)-C(18)-S(1)	119.9(3)
C(19)-C(18)-S(1)	119.7(3)
C(19)-C(18)-C(23)	120.3(3)
C(22)-C(23)-H(23)	120.0
C(18)-C(23)-C(22)	120.1(3)
C(18)-C(23)-H(23)	120.0
C(9)-C(4)-C(5)	118.7(3)
C(9)-C(4)-C(3)	117.3(3)
C(3)-C(4)-C(5)	124.0(4)
N(1)-C(8)-C(9)	114.1(3)
C(7)-C(8)-N(1)	127.8(3)
C(7)-C(8)-C(9)	118.2(3)

H(14A)-C(14)-H(14B)	107.5
C(13)-C(14)-H(14A)	108.5
C(13)-C(14)-H(14B)	108.5
C(13)-C(14)-C(15)	115.0(3)
C(15)-C(14)-H(14A)	108.5
C(15)-C(14)-H(14B)	108.5
H(16A)-C(16)-H(16B)	107.7
C(17)-C(16)-H(16A)	108.8
C(17)-C(16)-H(16B)	108.8
C(17)-C(16)-C(15)	113.9(3)
C(15)-C(16)-H(16A)	108.8
C(15)-C(16)-H(16B)	108.8
C(1)-C(2)-H(2)	120.2
C(3)-C(2)-H(2)	120.2
C(3)-C(2)-C(1)	119.7(4)
N(2)-C(1)-C(2)	121.7(4)
N(2)-C(1)-H(1)	119.1
C(2)-C(1)-H(1)	119.1
N(3)-C(17)-C(16)	111.7(3)
N(3)-C(17)-H(17A)	109.3
N(3)-C(17)-H(17B)	109.3
C(16)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	107.9
C(6)-C(5)-C(4)	119.5(3)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
Pd(1)-C(12)-H(12)	116.1
C(13)-C(12)-Pd(1)	73.9(2)
C(13)-C(12)-H(12)	116.1
C(13)-C(12)-C(11)	120.0(3)
C(11)-C(12)-Pd(1)	106.7(2)
C(11)-C(12)-H(12)	116.1
Pd(1)-C(13)-H(13)	113.7
C(14)-C(13)-Pd(1)	113.7(2)
C(14)-C(13)-H(13)	113.7
C(12)-C(13)-Pd(1)	69.9(2)
C(12)-C(13)-C(14)	124.5(3)

C(12)-C(13)-H(13)	113.7
C(21)-C(20)-H(20)	119.3
C(21)-C(20)-C(19)	121.4(4)
C(19)-C(20)-H(20)	119.3
N(1)-C(10)-C(11)	113.3(3)
O(1)-C(10)-N(1)	126.1(3)
O(1)-C(10)-C(11)	120.6(3)
C(22)-C(21)-C(24)	121.0(4)
C(20)-C(21)-C(22)	118.6(3)
C(20)-C(21)-C(24)	120.4(4)
C(18)-C(19)-C(20)	119.0(3)
C(18)-C(19)-H(19)	120.5
C(20)-C(19)-H(19)	120.5
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-C(4)	120.2(4)
C(2)-C(3)-H(3)	119.9
C(14)-C(15)-H(15A)	108.5
C(14)-C(15)-H(15B)	108.5
C(16)-C(15)-C(14)	115.3(3)
C(16)-C(15)-H(15A)	108.5
C(16)-C(15)-H(15B)	108.5
H(15A)-C(15)-H(15B)	107.5
C(12)-C(11)-C(10)	116.0(3)
C(12)-C(11)-H(11A)	108.3
C(12)-C(11)-H(11B)	108.3
C(10)-C(11)-H(11A)	108.3
C(10)-C(11)-H(11B)	108.3
H(11A)-C(11)-H(11B)	107.4
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Pd-1d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	16(1)	11(1)	14(1)	4(1)	3(1)	0(1)
S(1)	14(1)	10(1)	22(1)	6(1)	1(1)	0(1)
O(2)	20(1)	16(1)	35(2)	16(1)	-3(1)	1(1)
O(3)	21(1)	16(1)	27(1)	4(1)	9(1)	3(1)
N(1)	20(2)	12(1)	14(1)	6(1)	-1(1)	-1(1)
N(3)	14(1)	11(1)	20(1)	7(1)	-1(1)	0(1)
O(1)	30(2)	26(2)	28(2)	14(1)	7(1)	-5(1)
N(2)	17(1)	12(1)	17(1)	5(1)	2(1)	3(1)
C(9)	16(2)	15(2)	17(2)	7(1)	-4(1)	4(1)
C(6)	26(2)	12(2)	33(2)	7(2)	-13(2)	1(2)
C(7)	22(2)	15(2)	25(2)	11(2)	-6(1)	-2(1)
C(22)	18(2)	16(2)	34(2)	12(2)	-1(2)	-3(1)
C(18)	12(2)	11(2)	21(2)	7(1)	-2(1)	-2(1)
C(23)	17(2)	16(2)	21(2)	8(1)	4(1)	1(1)
C(4)	19(2)	18(2)	20(2)	5(1)	-3(1)	9(1)
C(8)	18(2)	14(2)	16(2)	7(1)	-5(1)	0(1)
C(14)	24(2)	18(2)	17(2)	5(1)	4(1)	6(1)
C(16)	31(2)	17(2)	17(2)	8(1)	0(2)	4(2)
C(2)	27(2)	35(2)	21(2)	13(2)	7(2)	10(2)
C(1)	19(2)	20(2)	22(2)	10(2)	4(1)	3(1)
C(17)	23(2)	24(2)	22(2)	14(2)	7(1)	5(2)
C(5)	25(2)	15(2)	25(2)	0(2)	-7(2)	8(2)
C(12)	22(2)	16(2)	15(2)	2(1)	6(1)	3(1)
C(13)	18(2)	20(2)	17(2)	3(1)	7(1)	4(1)
C(20)	26(2)	32(2)	16(2)	5(2)	1(2)	6(2)
C(10)	20(2)	22(2)	17(2)	11(2)	-2(1)	2(1)
C(21)	19(2)	16(2)	27(2)	1(2)	-9(2)	2(1)
C(19)	19(2)	25(2)	20(2)	11(2)	0(1)	-1(2)
C(3)	22(2)	29(2)	20(2)	2(2)	1(1)	11(2)
C(15)	24(2)	18(2)	20(2)	10(2)	2(1)	4(2)
C(11)	21(2)	24(2)	19(2)	9(2)	6(1)	4(2)
C(24)	37(2)	16(2)	39(2)	-5(2)	-14(2)	5(2)

Computational Details

All DFT calculations were carried out using the *Gaussian 16* program[8] on Pitt CRC and XSEDE[9] supercomputers. Geometries of all stationary points were fully optimized using the M06 functional[10] with the SDD[11] effective core potential basis set for Pd and the 6-31G(d) basis set[12] for other atoms. Vibrational frequency calculations at the same level of theory of the geometry optimization were performed to confirm if each structure is a local minimum or a transition state. Single-point energy calculations were carried out using the SDD basis set for Pd and 6-311+G(d,p) basis set for other atoms. Solvation energy corrections in acetonitrile solvent were calculated using the SMD solvation model[13] in the single-point energy calculations. The Gibbs free energies were calculated at the standard state (1 mol/L, 298K).[14]

Computed Energy Profiles

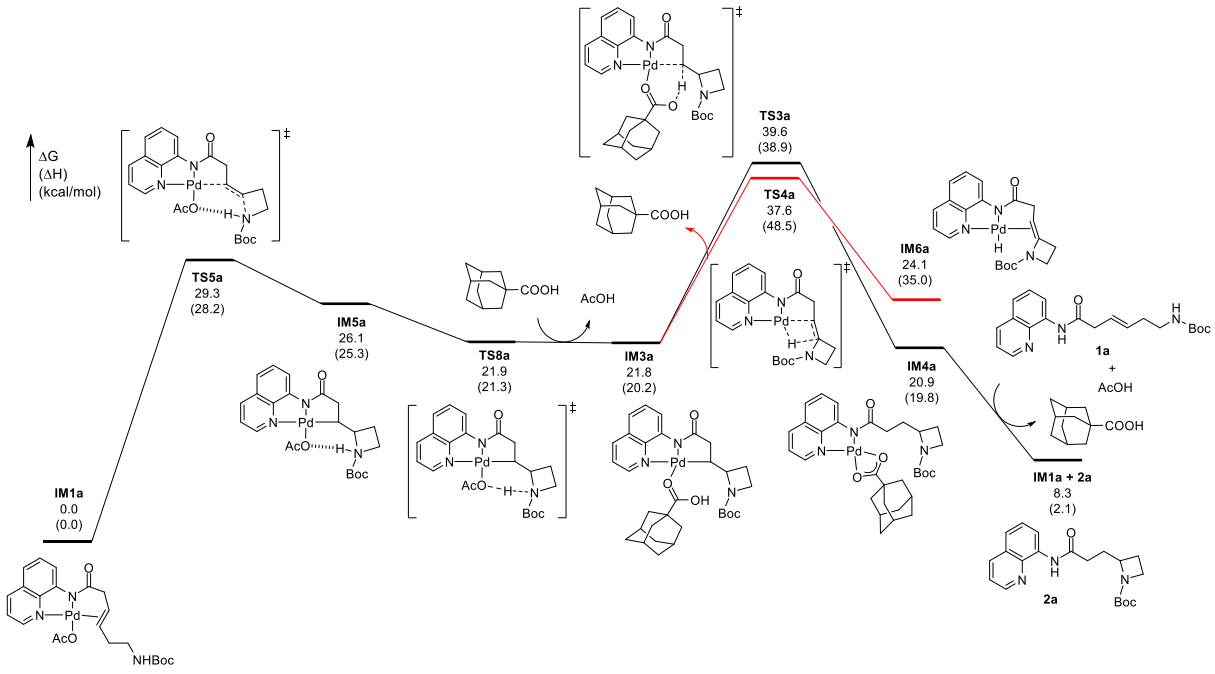


Figure S1. Computed energy profile (kcal/mol) for the 4-*exo-trig* cyclization of **1a**.

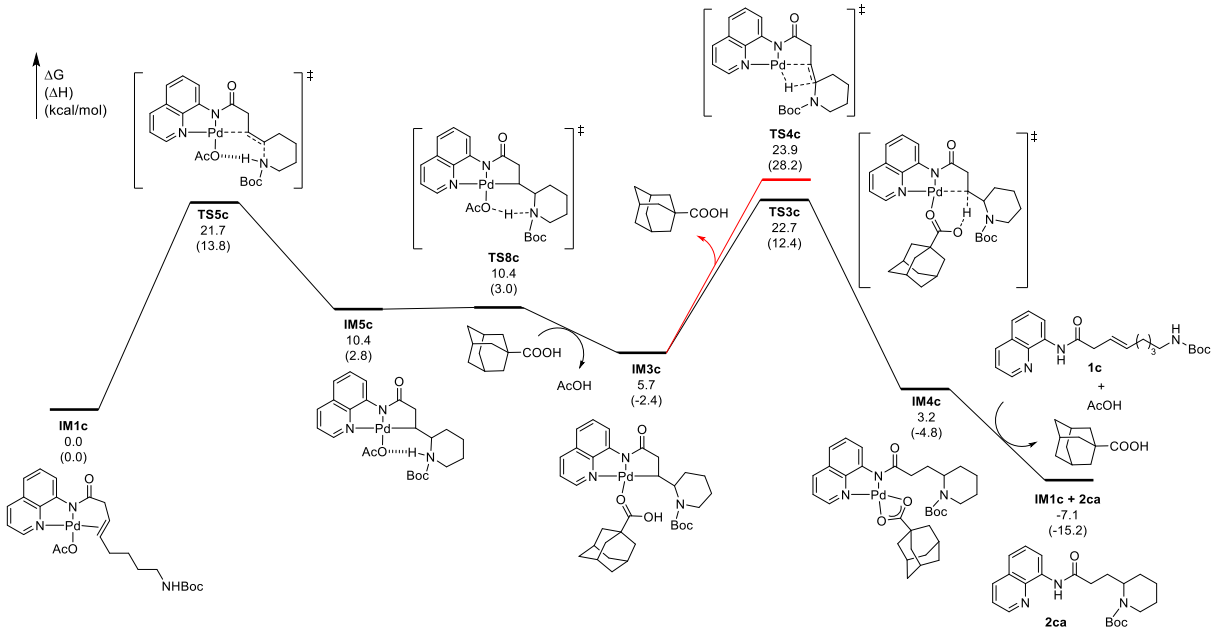


Figure S2. Computed energy profile (kcal/mol) for the 6-*exo-trig* cyclization of **1c**.

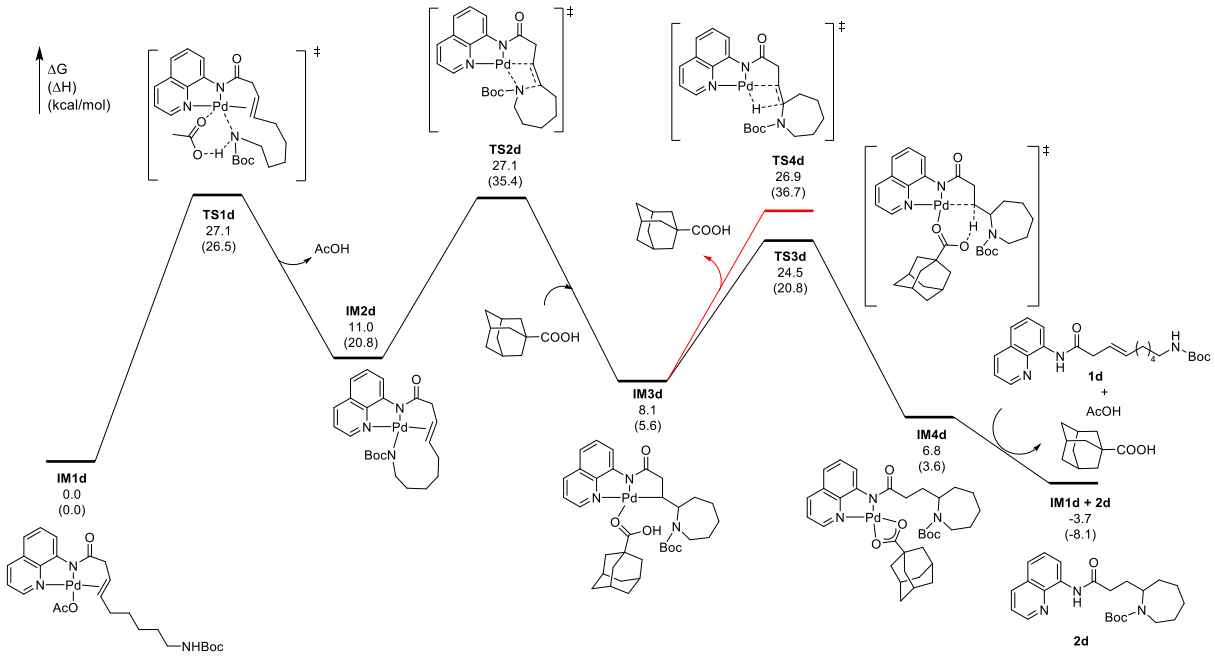


Figure S3. Computed energy profile (kcal/mol) for the 7-*exo-trig* cyclization of **1d**.

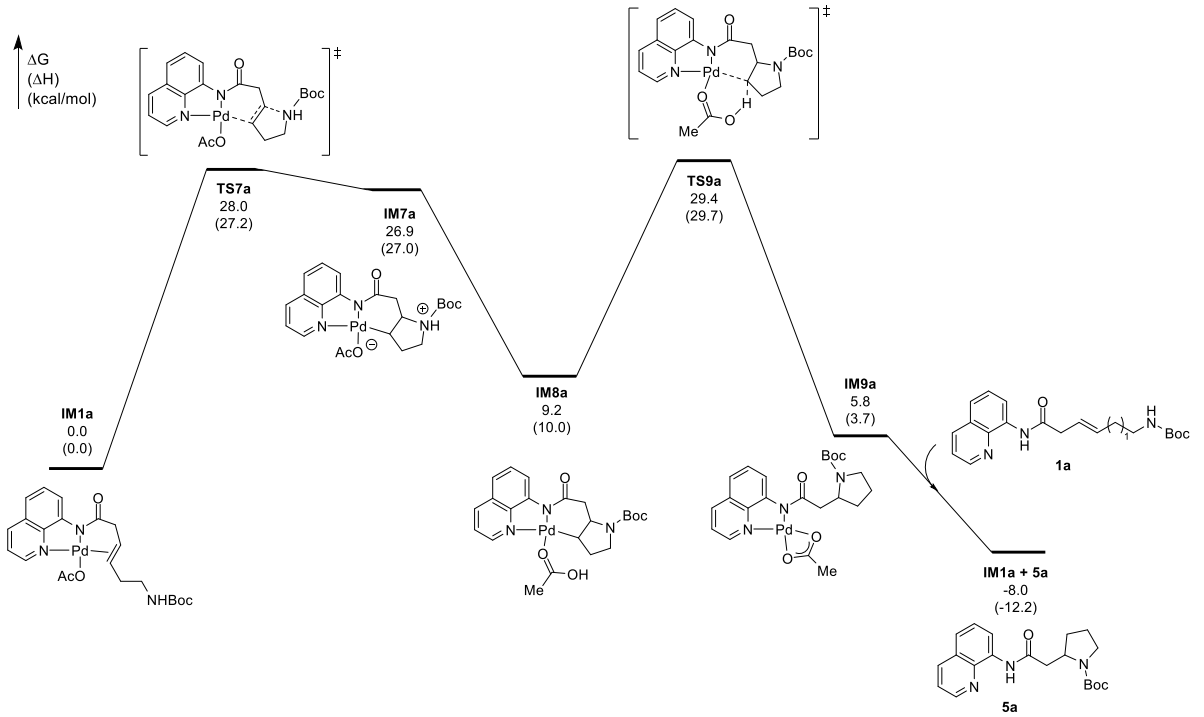


Figure S4. Computed energy profile (kcal/mol) for the 5-*endo-trig* cyclization of **1a**.

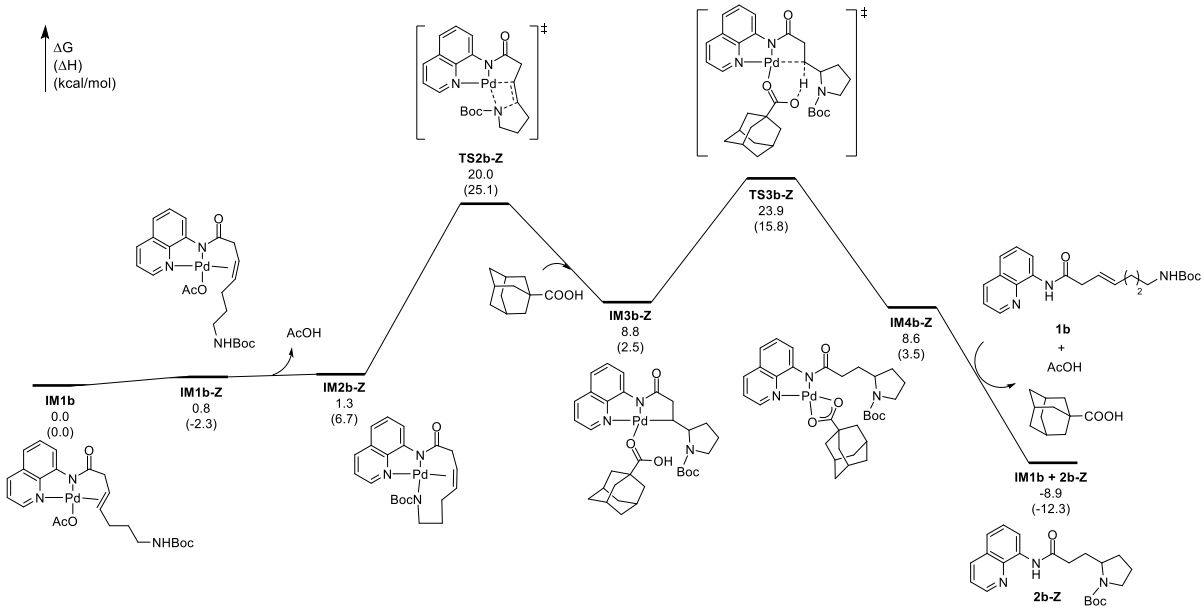


Figure S5. Computed energy profile (kcal/mol) for the 5-*exo-trig* cyclization for *Z*-isomer of **1b**.

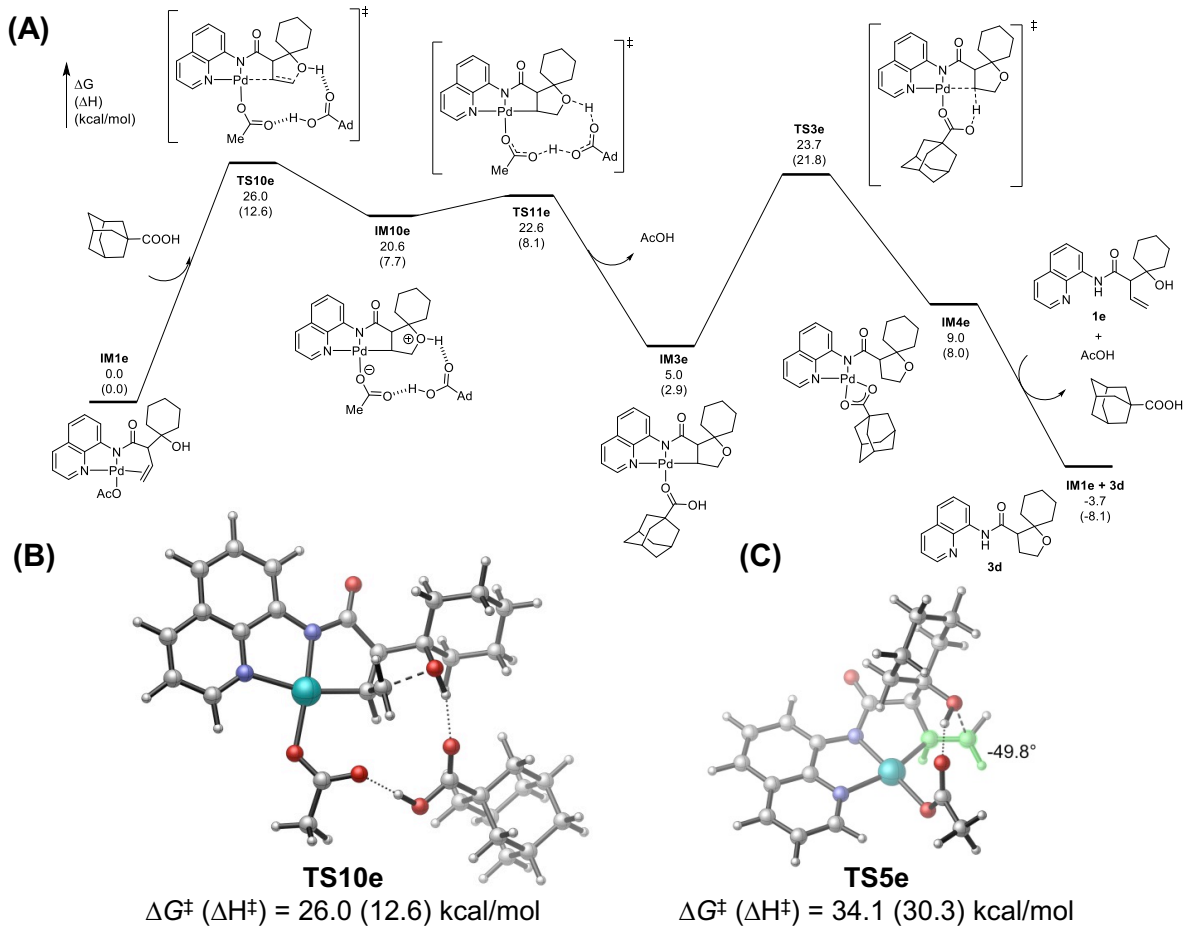


Figure S6. (A) Computed energy profile (kcal/mol) and optimized structures of (B) the *anti*-nucleopalladation transition state **TS10e** and (C) the *syn*-nucleopalladation transition state **TS5e** for the 5-*endo-trig* cyclization of **1e** to form oxaspiro compound **3d**. The nucleopalladation transition state with the deprotonated O-nucleophile is 4.6 kcal/mol higher in energy than **TS10e**. The *syn*-nucleopalladation transition state **TS5e** is disfavored because of the steric repulsions between the spiro center and the Pd and the geometrical constrain of the spiro center that is attached to the α-carbon of the amide. Due to these constrains, the oxygen nucleophile cannot be placed syn-periplanar with the Pd, leading to large distortion of this TS.

Correlation of the stability of the palladacycle intermediate 3 and ring strain energy of the N-heterocycle

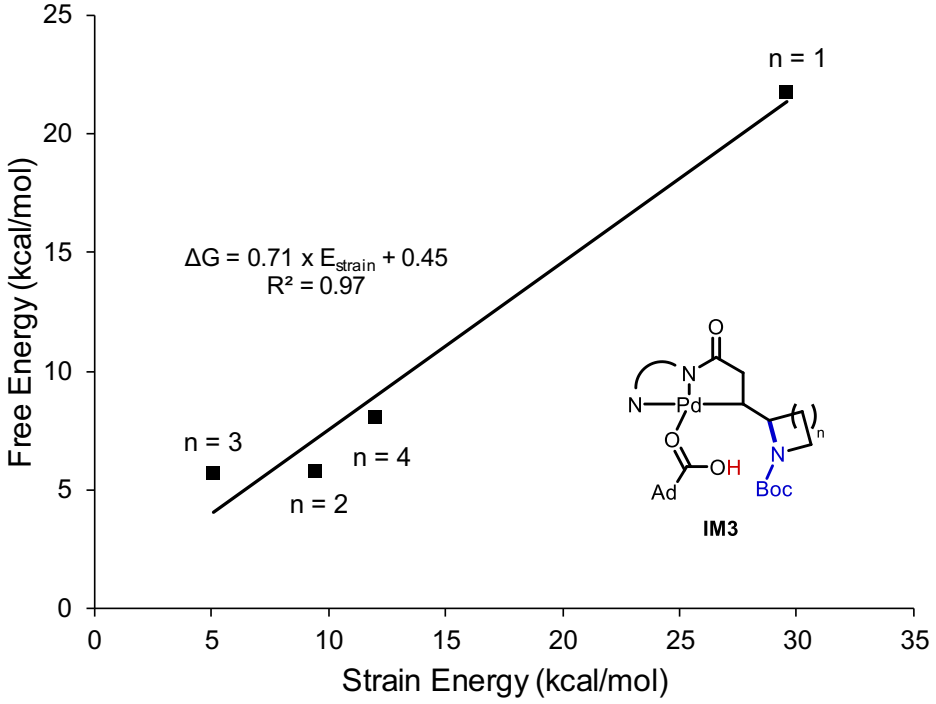
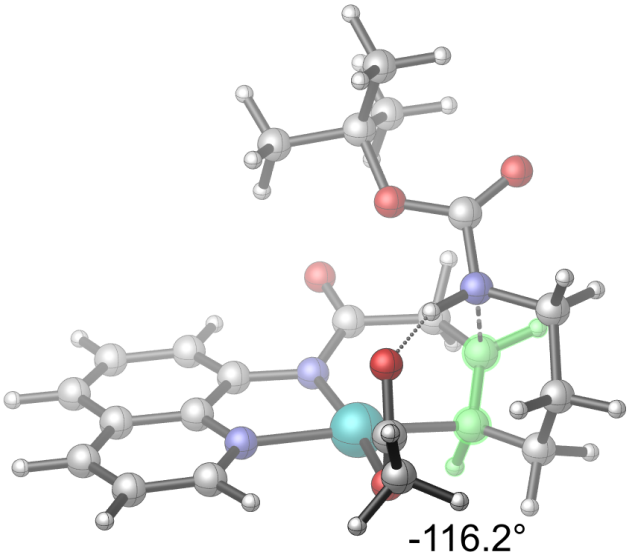


Figure S7. Correlation between Gibbs free energies of cyclic intermediates **IM3** relative to **IM1** and ring strain energies of the N-heterocycles.[15]

The ring strain energy of heterocycles were taken from ref. 15.



TS7b-*syn*

$\Delta G^{\ddagger}$ ($\Delta H^{\ddagger}$) = 33.4 (25.8) kcal/mol

Figure S8. Optimized transition state for the formation of *6-endo-trig* product via the *syn*-nucleopalladation, **TS7b-*syn***. The calculated energies are relative to **IM1b**. This transition state is 8.1 kcal/mol higher in energy than the anti-nucleopalladation TS giving 6-endo-trig product, **TS7b**. **TS7b-*syn*** is disfavored because the N-nucleophile and the Pd cannot achieve the syn-periplanar conformation.

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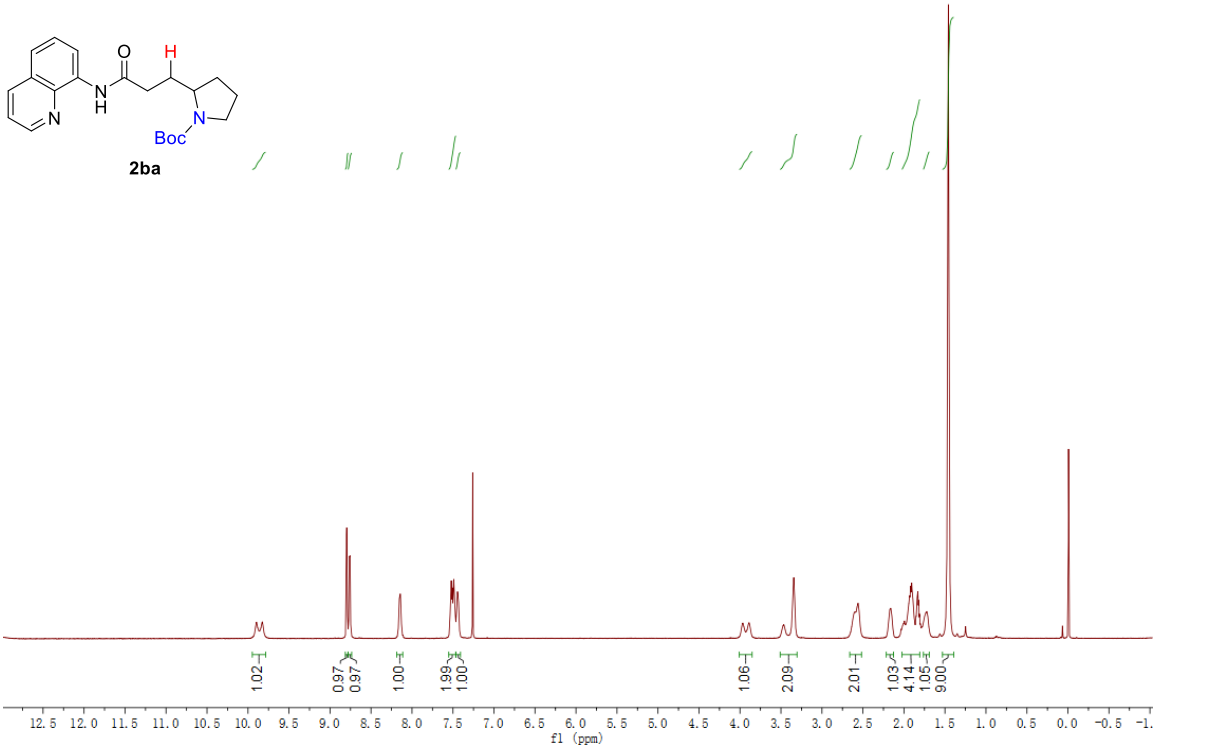
NMR Spectra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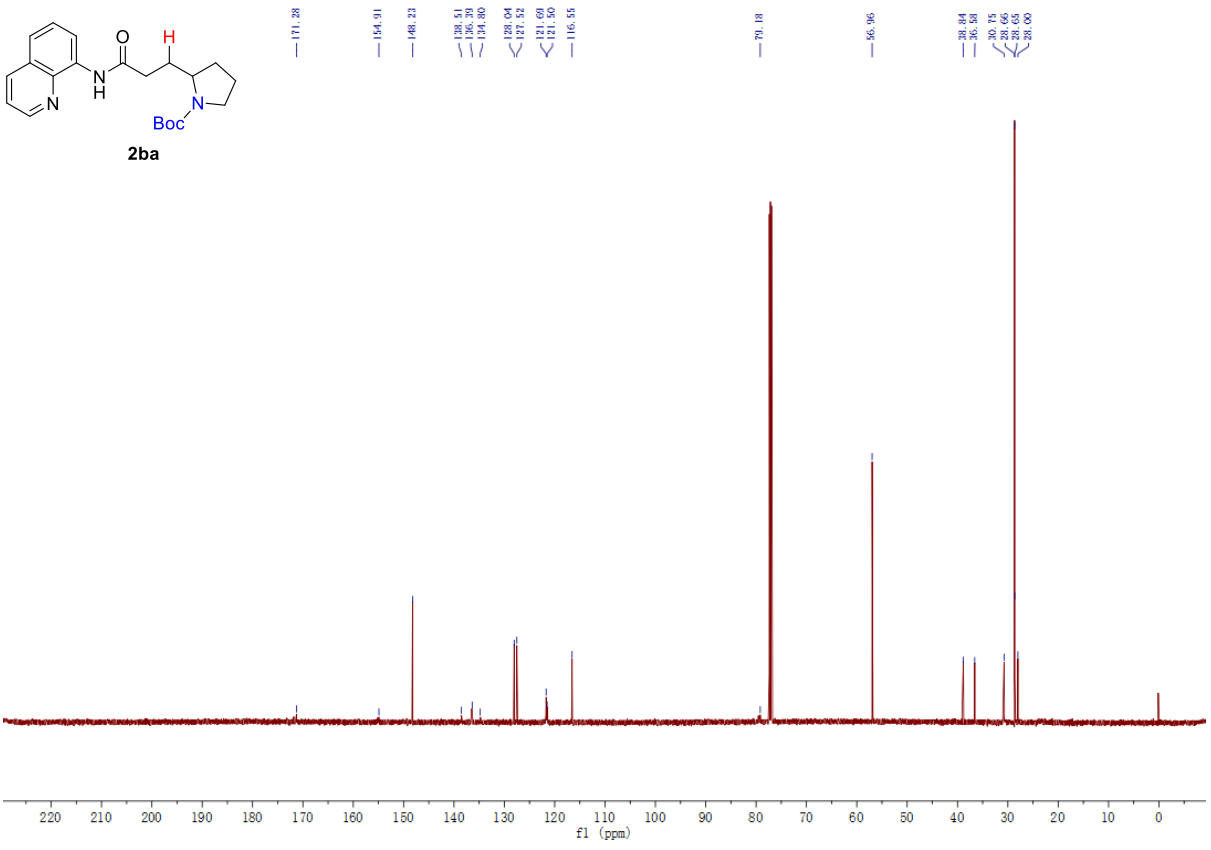
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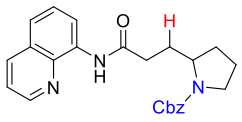
f1 (ppm)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H
N
Cbz

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1.04
2.04
1.07
0.91
1.09
3.12
1.02
1.11
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
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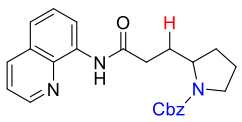
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127.90
127.52
121.70
121.47
116.56
66.99
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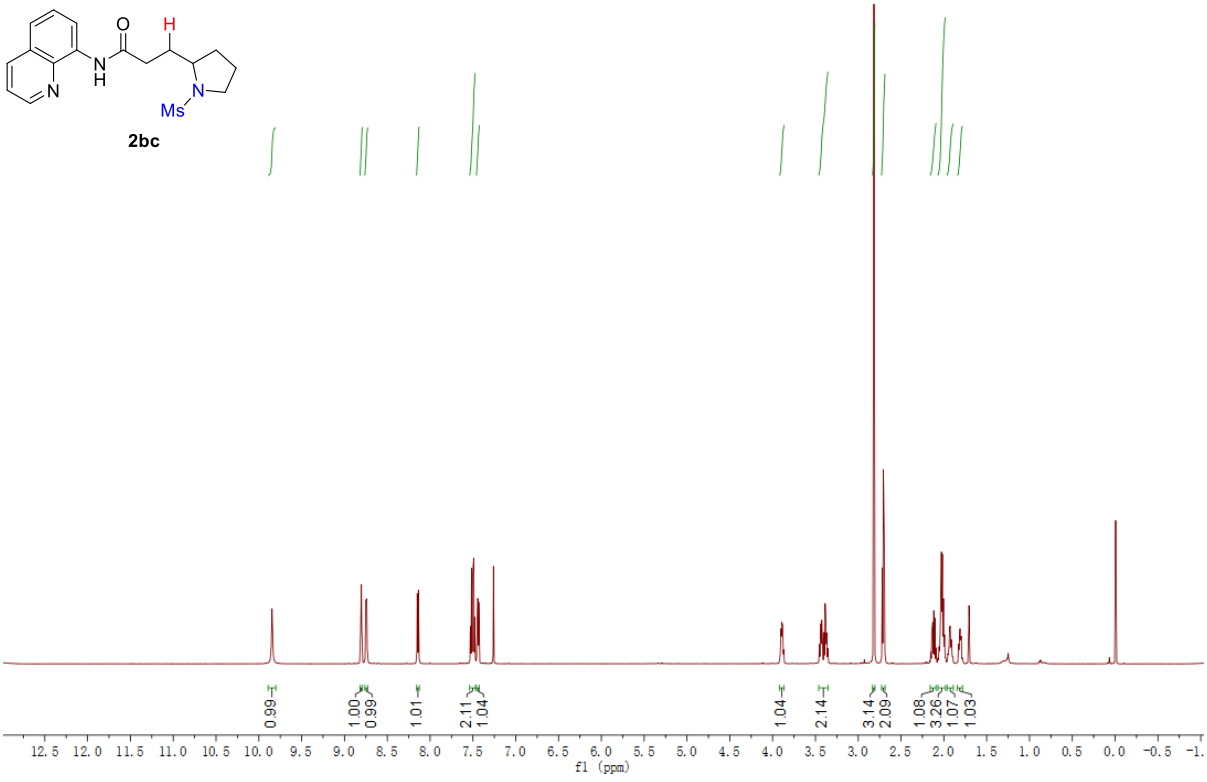
f1 (ppm)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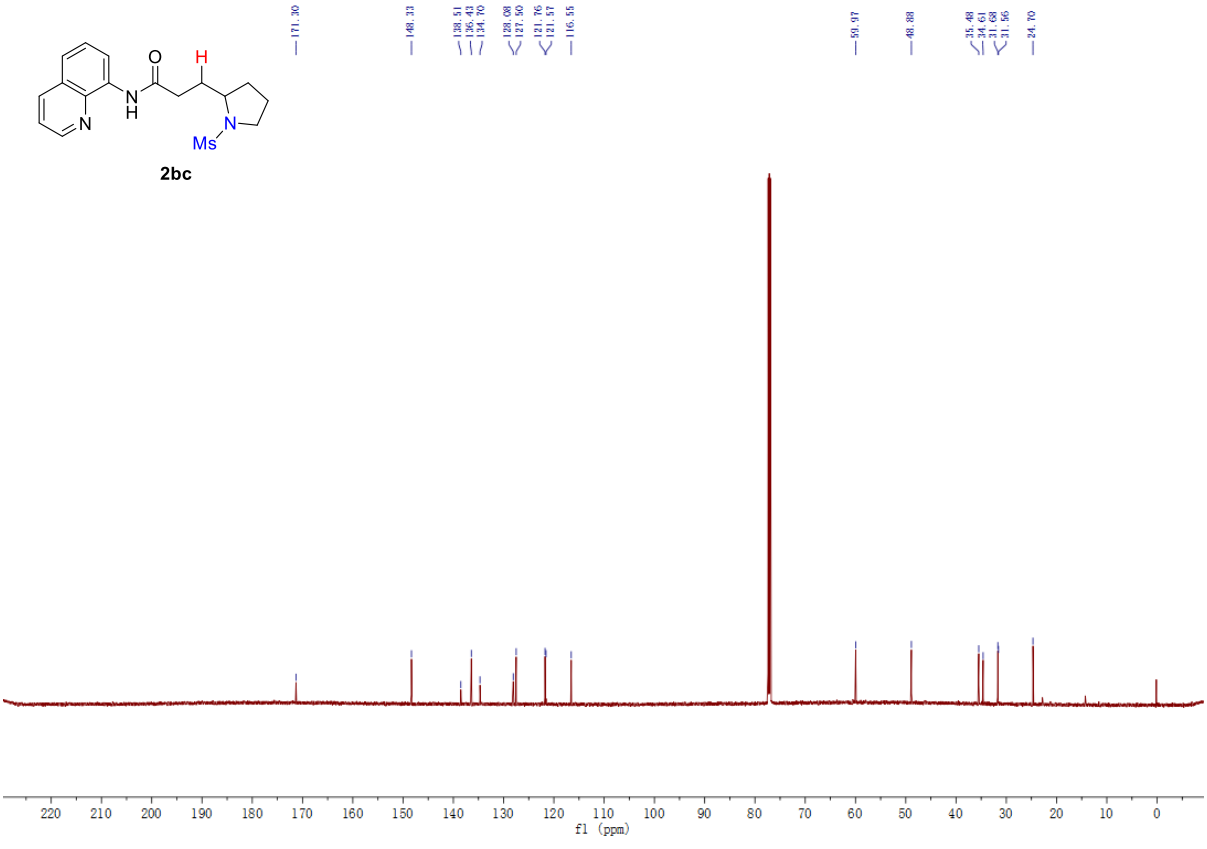
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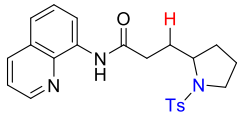

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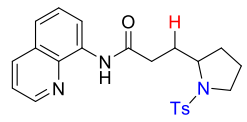

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60.09
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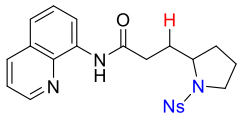

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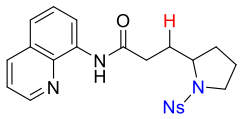

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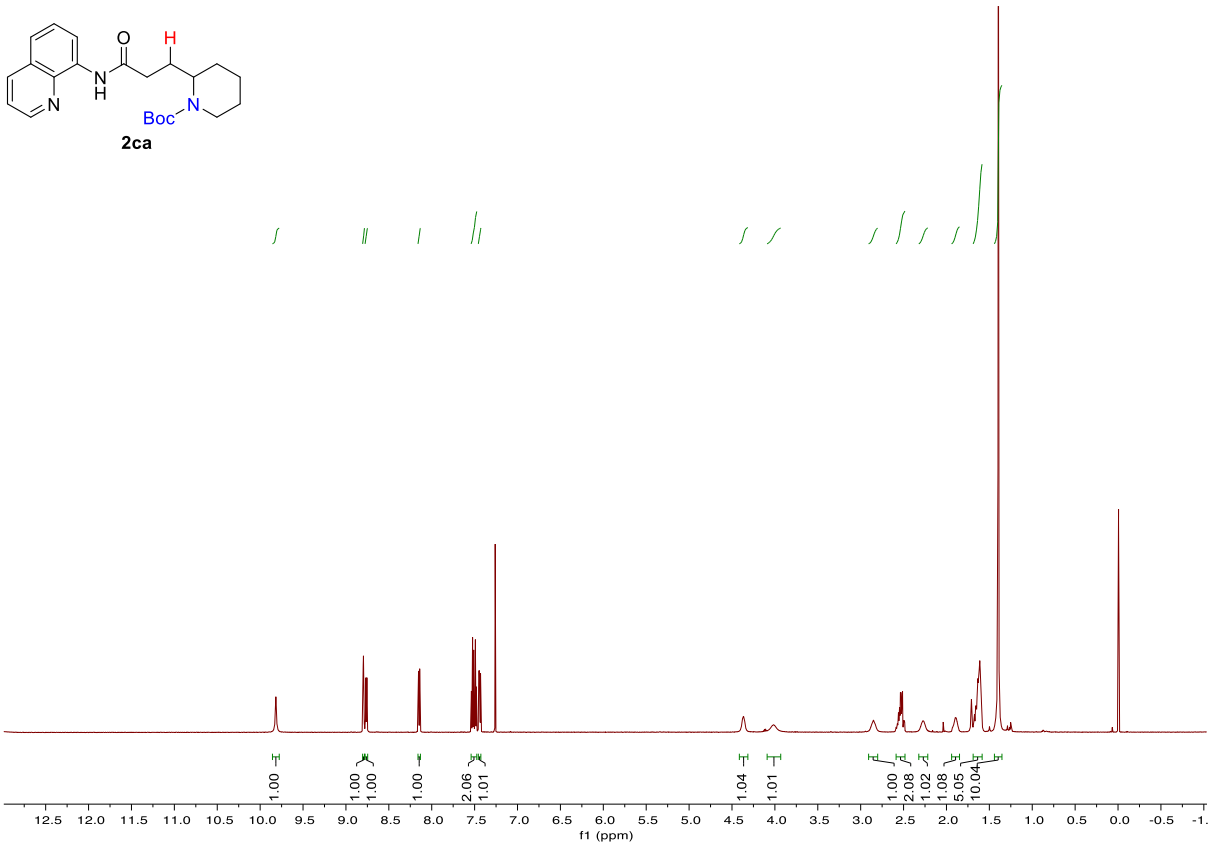
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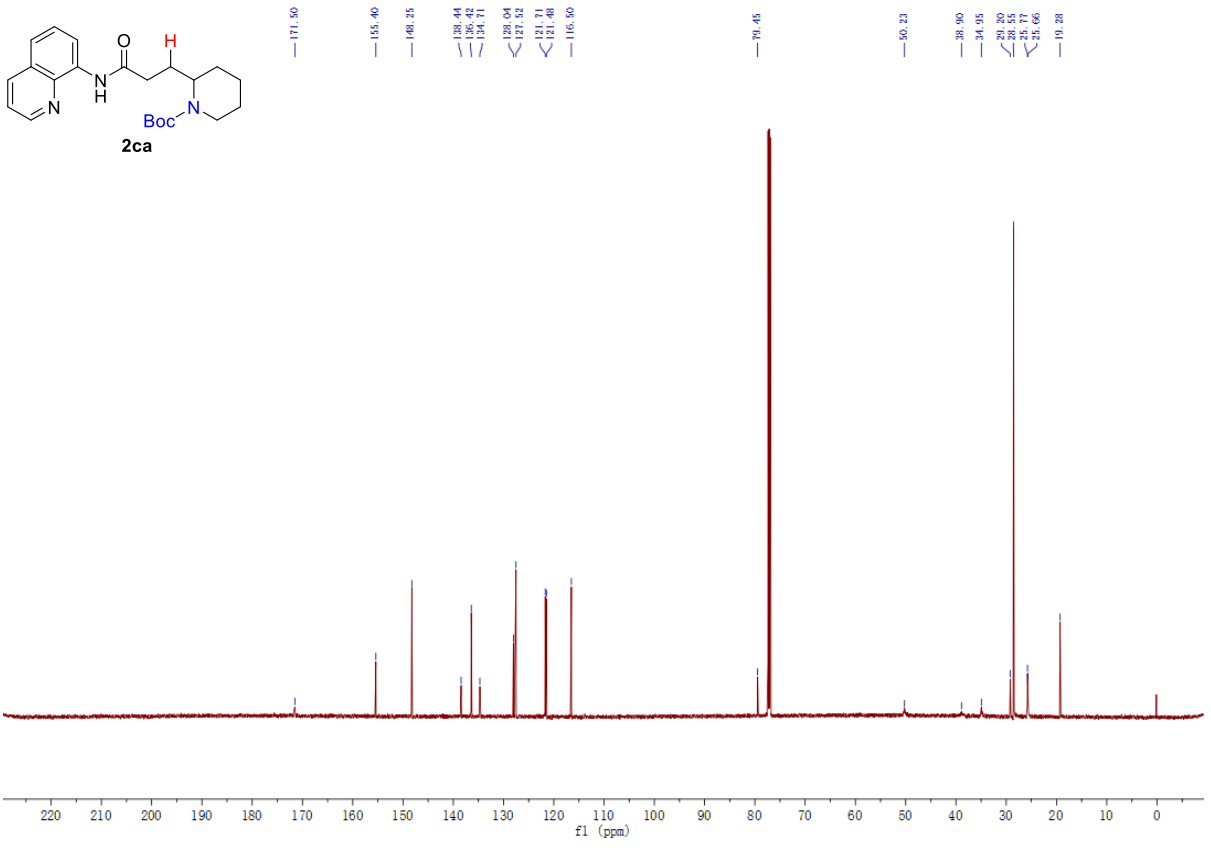
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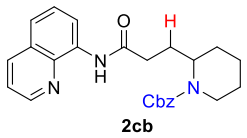
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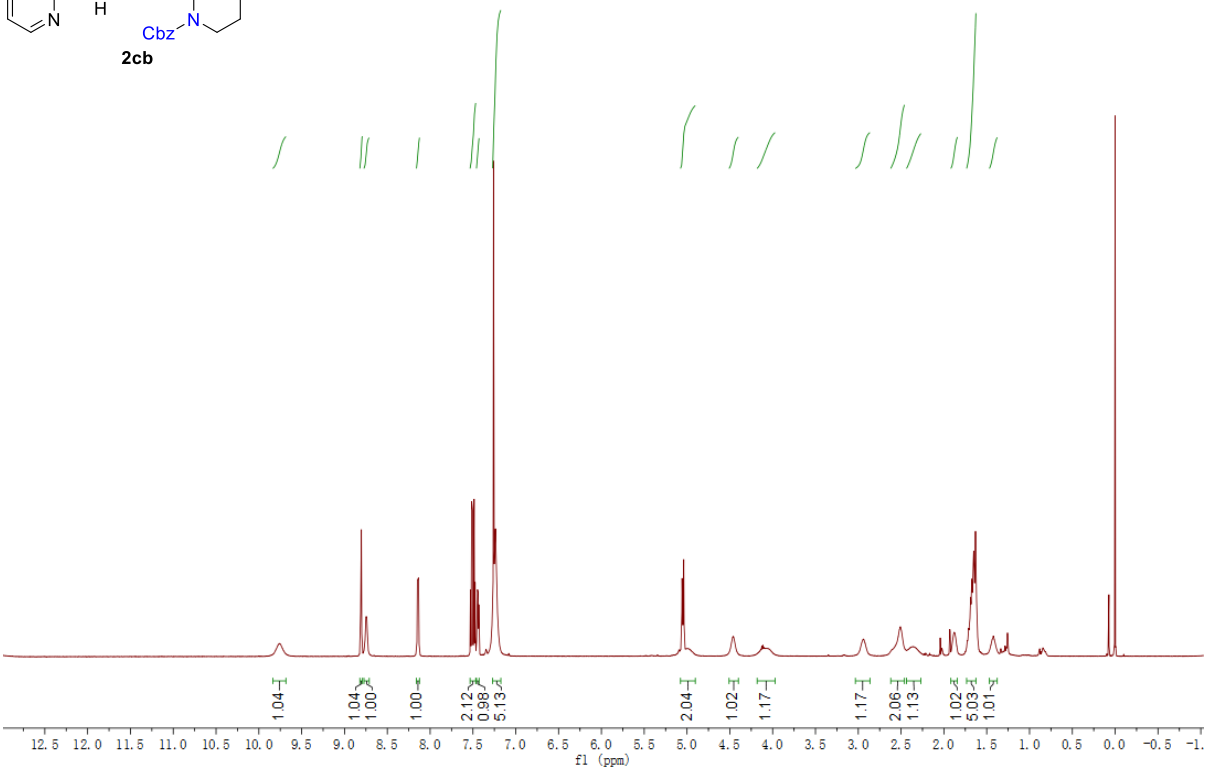
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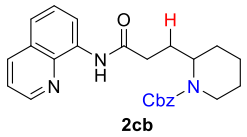
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Cbz
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2cb

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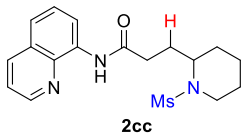
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1.06
3.04
2.04
1.04
1.06
5.04
1.00
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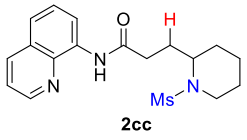
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2cc

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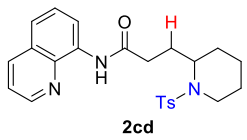
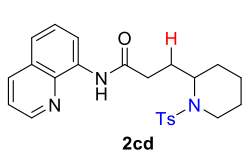
25.39
25.15
18.84
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
H
N
H
N
Ts
N

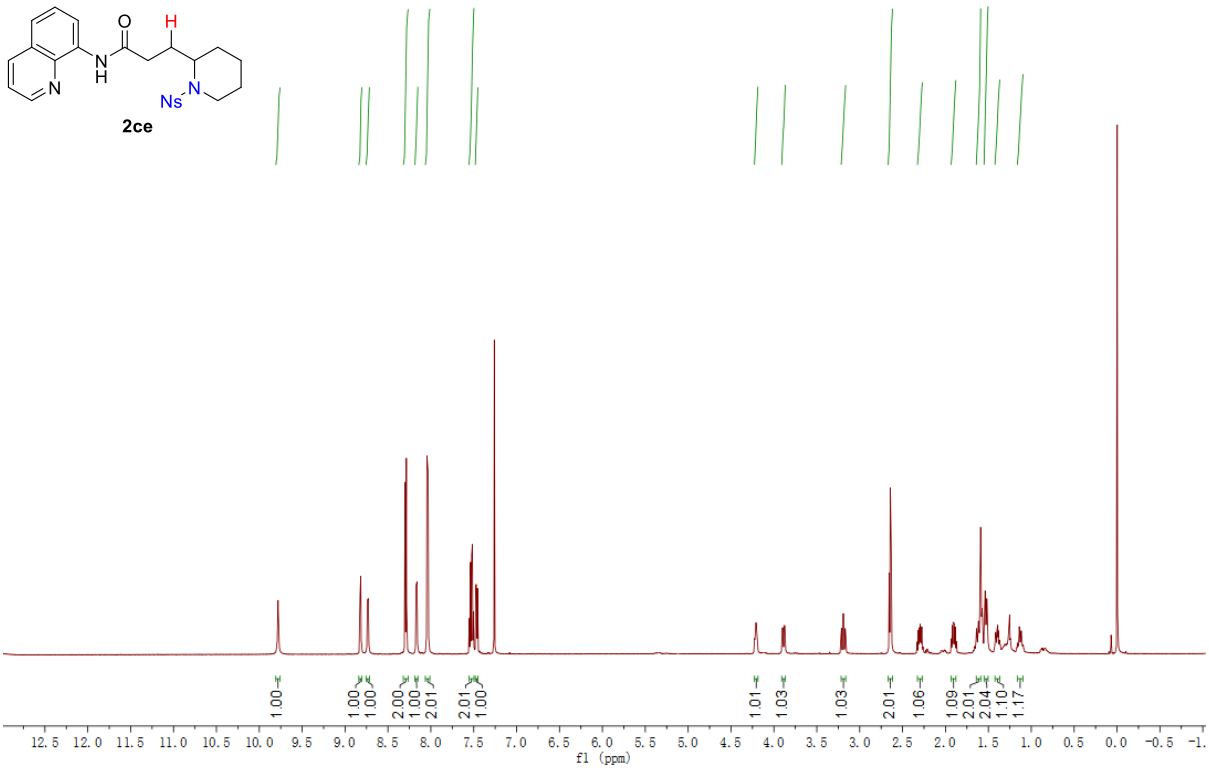
2cd

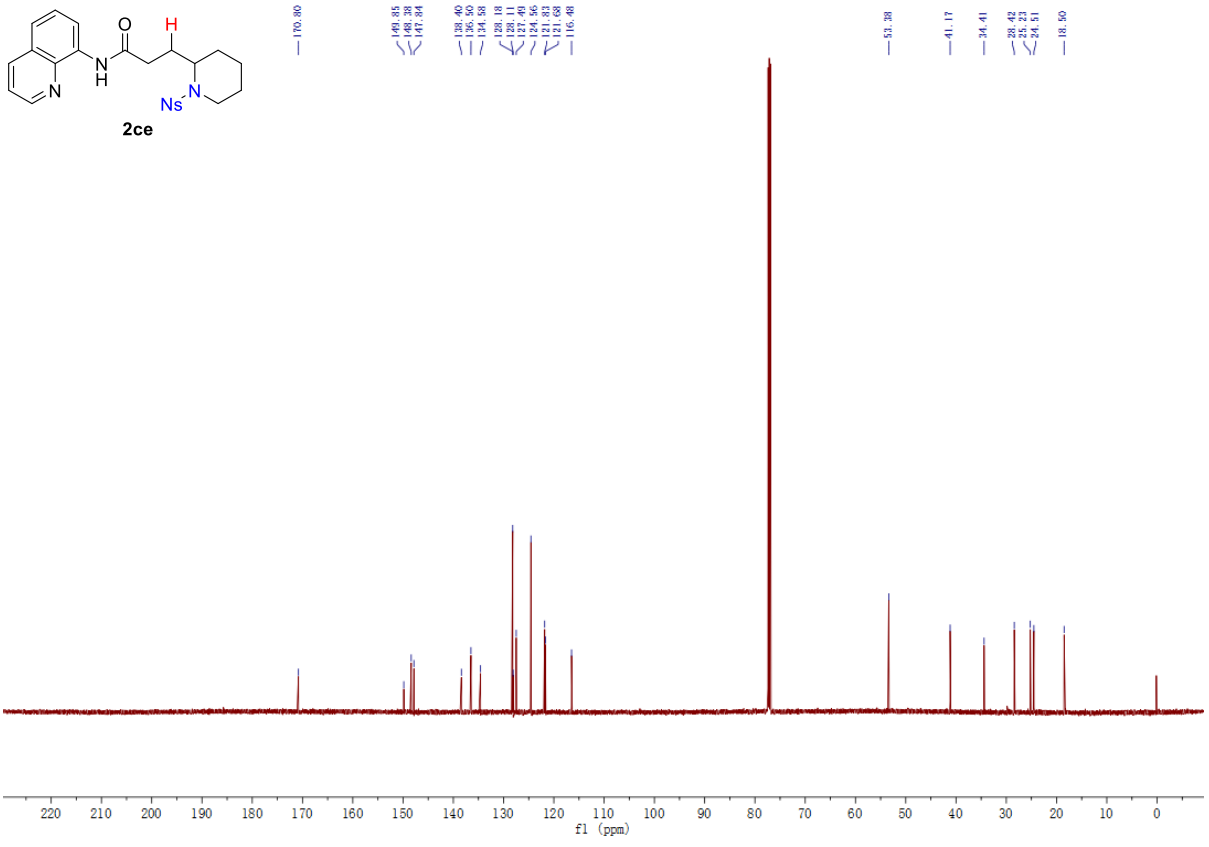
0.99
1.02
1.00
1.00
2.02
2.12
1.03
1.05
1.00
1.07
1.07
1.08
2.18
3.00
1.13
1.09
1.15
4.11
1.14
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

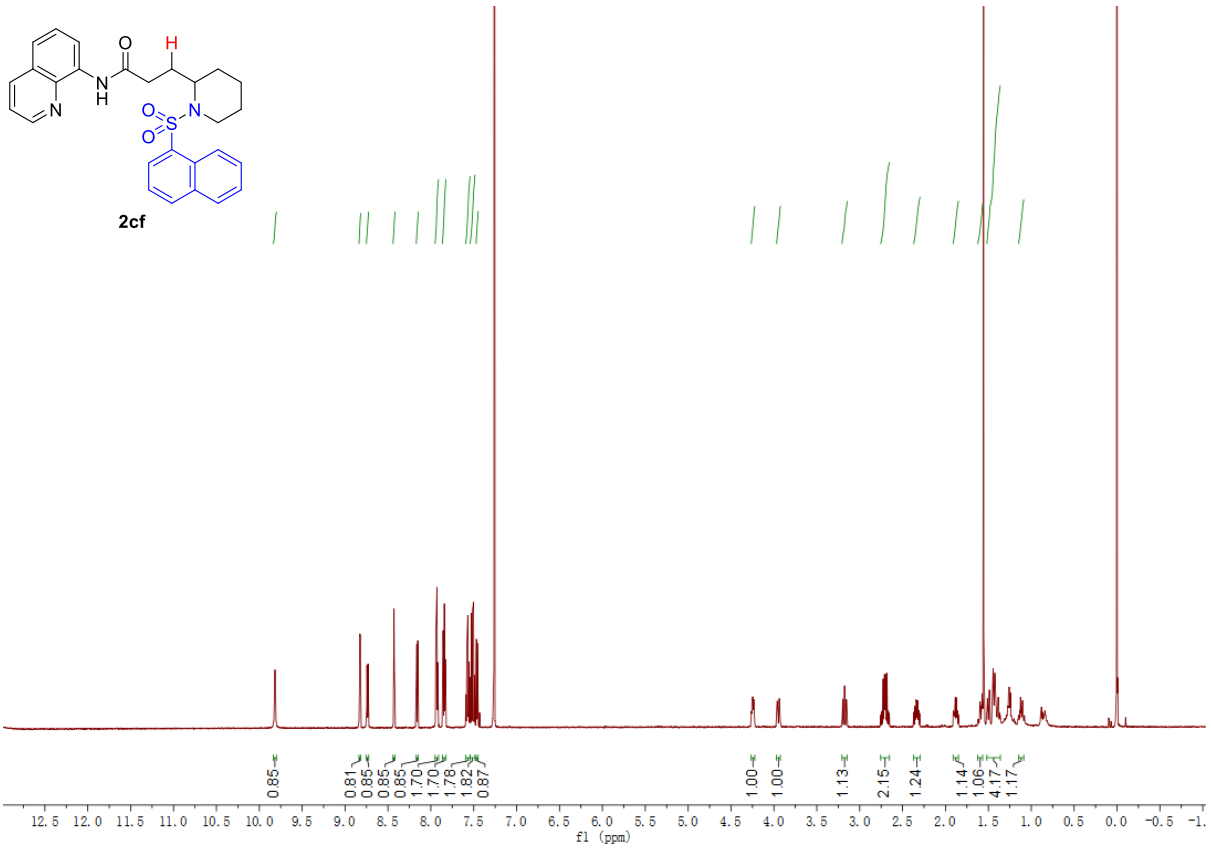

O
H
N
H
N
Ts
N

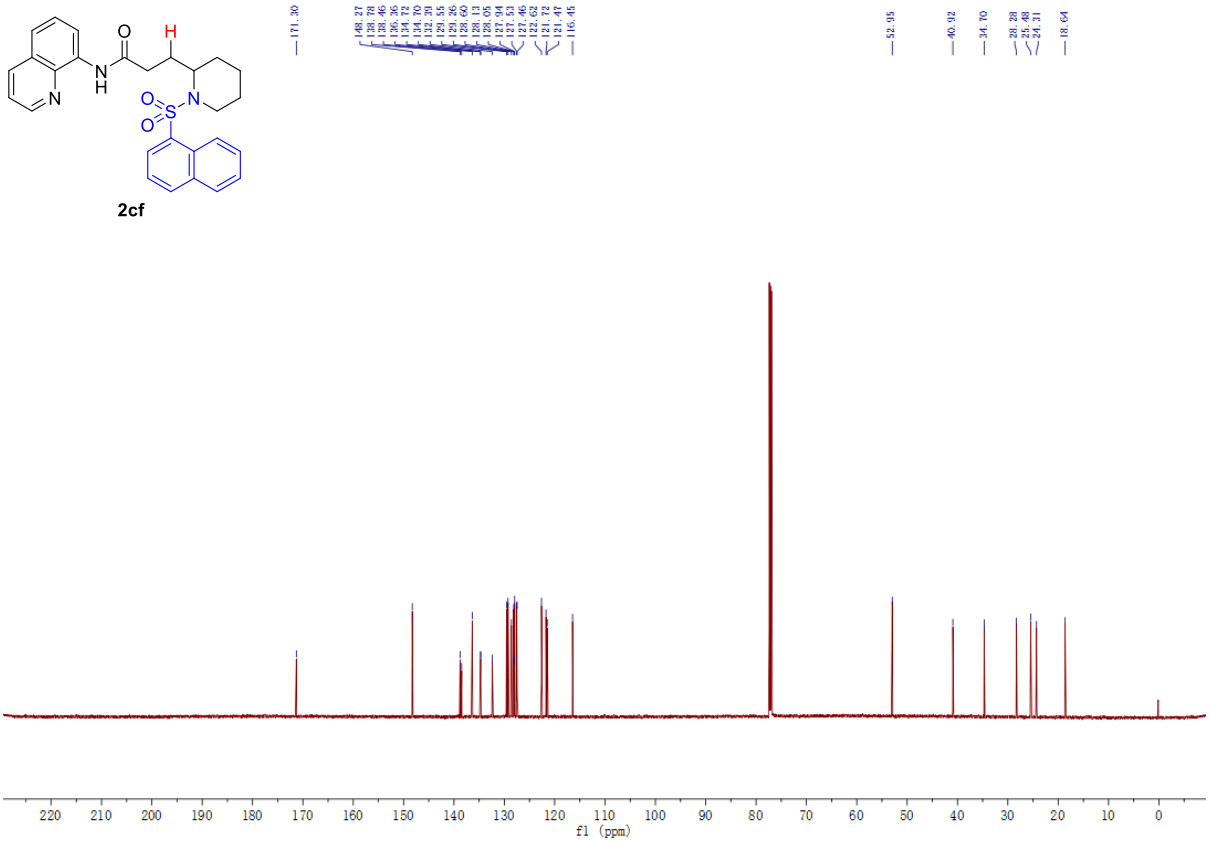
2cd

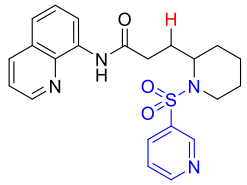
171.38
148.29
143.03
139.05
138.47
136.37
134.75
129.82
128.05
127.47
127.06
121.73
121.47
116.45
52.81
40.81
34.79
28.11
25.45
24.14
21.59
18.68
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


2ce
1.00
1.00
1.00
2.00
1.00
2.01
2.01
1.00
1.01
1.03
1.03
2.01
1.06
1.09
2.01
2.04
1.10
1.17
f1 (ppm)


2ce
170.80
149.85
148.38
147.84
138.40
135.50
134.58
128.18
128.11
127.40
124.56
121.83
121.68
116.48
53.38
41.17
34.41
28.42
25.23
24.51
18.50
f1 (ppm)

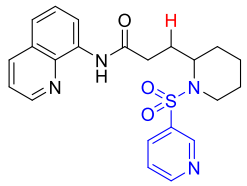

2cf
0.85
0.81
0.85
0.85
0.85
1.70
1.70
1.78
1.82
0.87
1.00
1.00
1.13
2.15
1.24
1.14
1.06
4.17
1.17
f1 (ppm)


2cf
171.30
148.27
138.78
138.46
135.36
134.72
134.70
132.39
129.55
129.35
128.60
128.13
128.05
127.94
127.53
127.46
122.62
121.72
121.47
116.45
52.95
40.92
34.70
28.28
25.48
24.31
18.64
f1 (ppm)



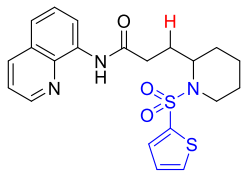
2cg

0.96
0.99
1.01
1.94
1.92
1.95
0.97
0.97
1.00
0.99
1.02
1.78
1.04
1.06
4.07
1.07
1.13
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)



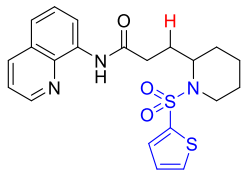
2cg

171.03
152.97
148.32
147.98
138.56
138.46
135.41
134.62
134.55
128.07
127.48
123.88
121.76
121.58
116.51
53.16
40.96
34.64
28.34
25.42
24.34
18.55
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



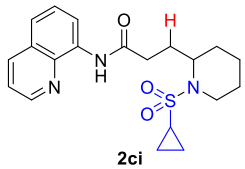
2ch

0.97
1.00
0.99
1.00
1.00
3.05
1.02
0.99
1.02
1.02
1.02
2.07
1.03
1.01
5.06
1.13
f1 (ppm)

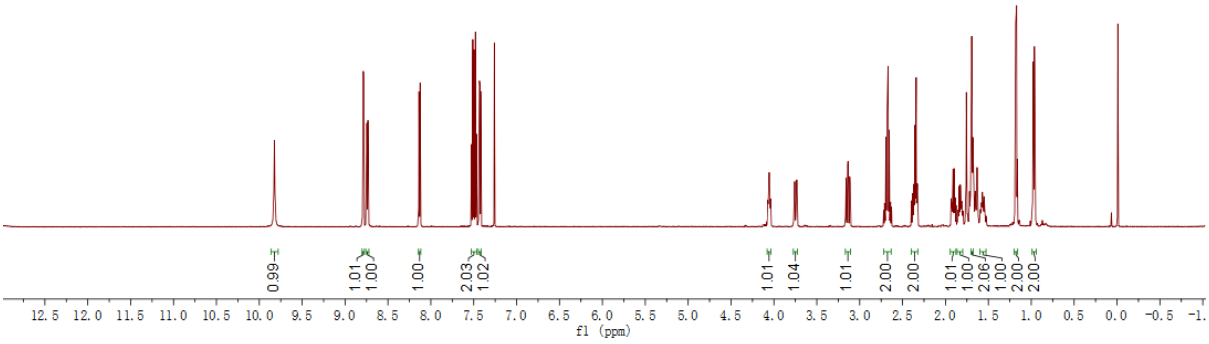


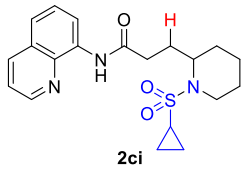
2ch

171.25
148.29
142.94
139.46
136.28
134.71
131.48
131.30
128.05
127.52
127.46
121.74
121.51
116.46
53.25
41.11
34.81
28.12
25.45
24.08
18.55
f1 (ppm)



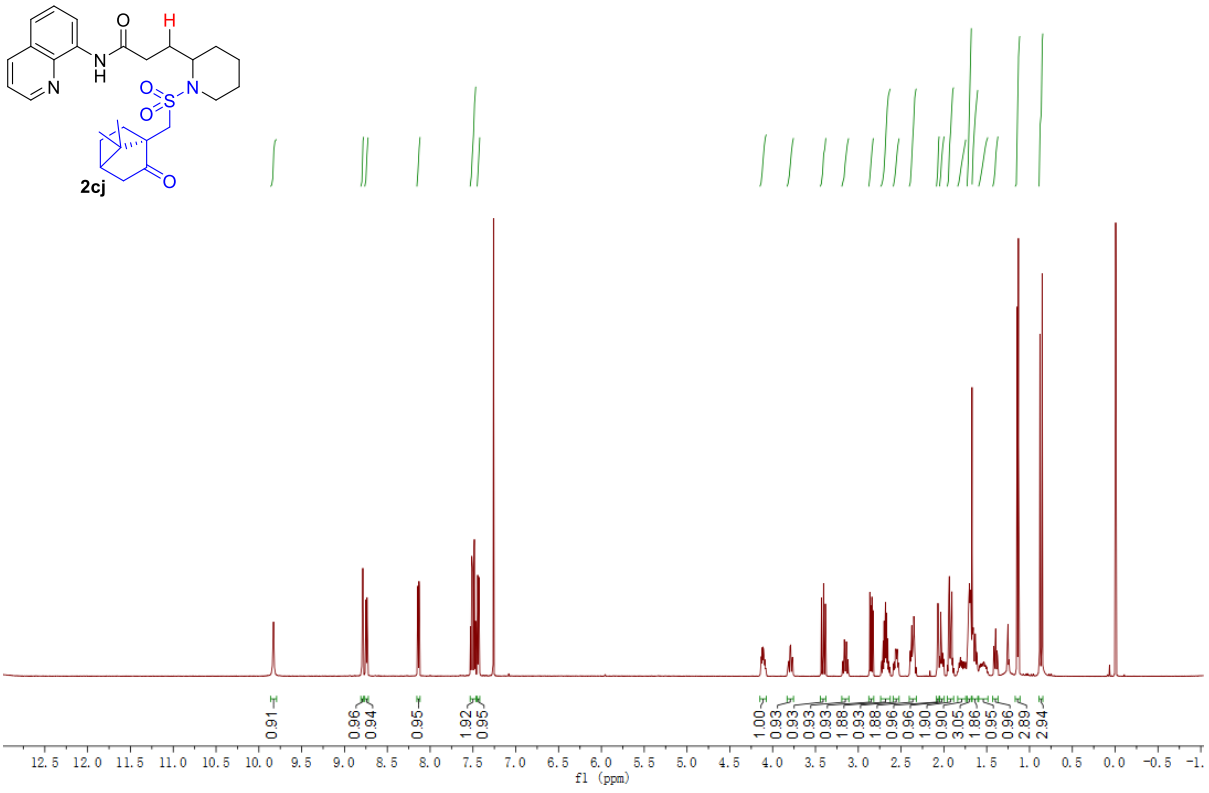
2ci

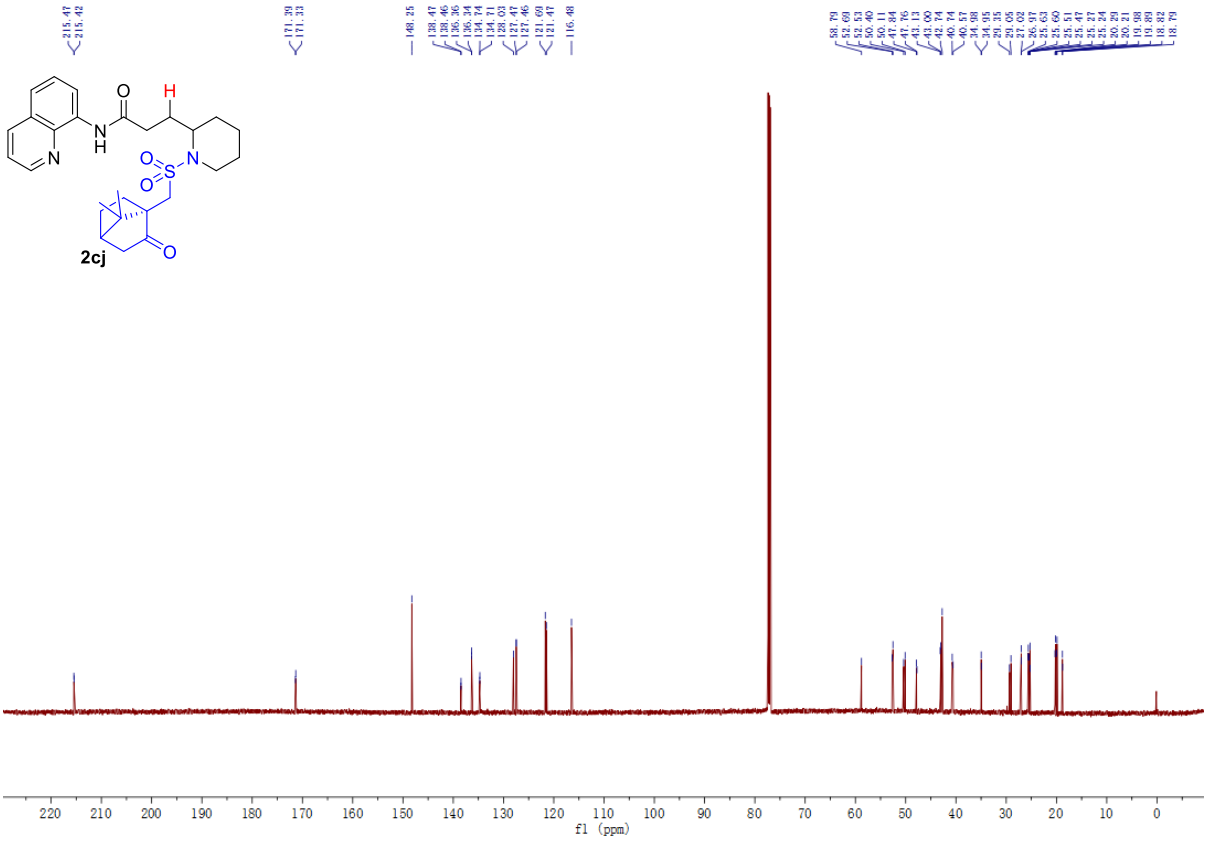

0.99
1.01
1.00
1.00
2.03
1.02
1.01
1.04
1.01
2.00
2.00
1.01
1.00
2.06
1.00
2.00
2.00
f1 (ppm)

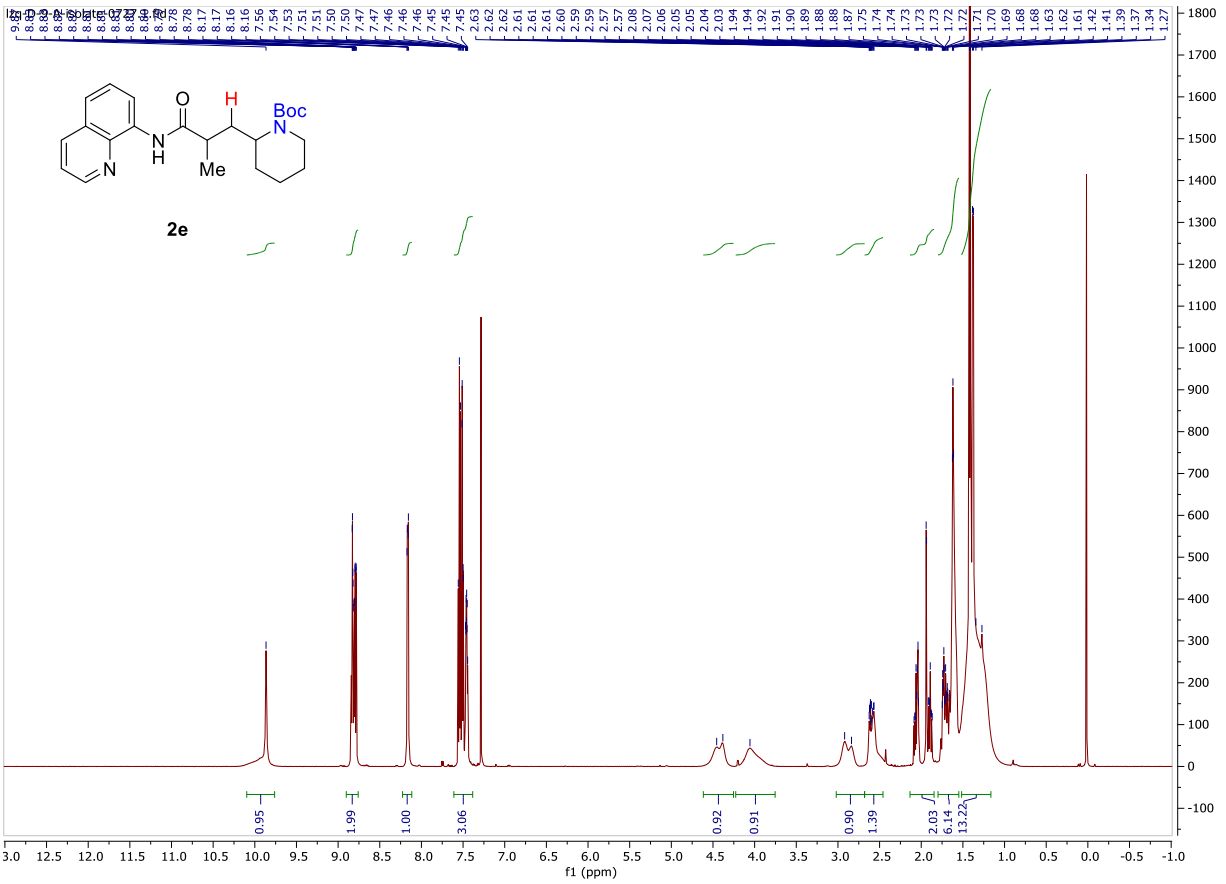


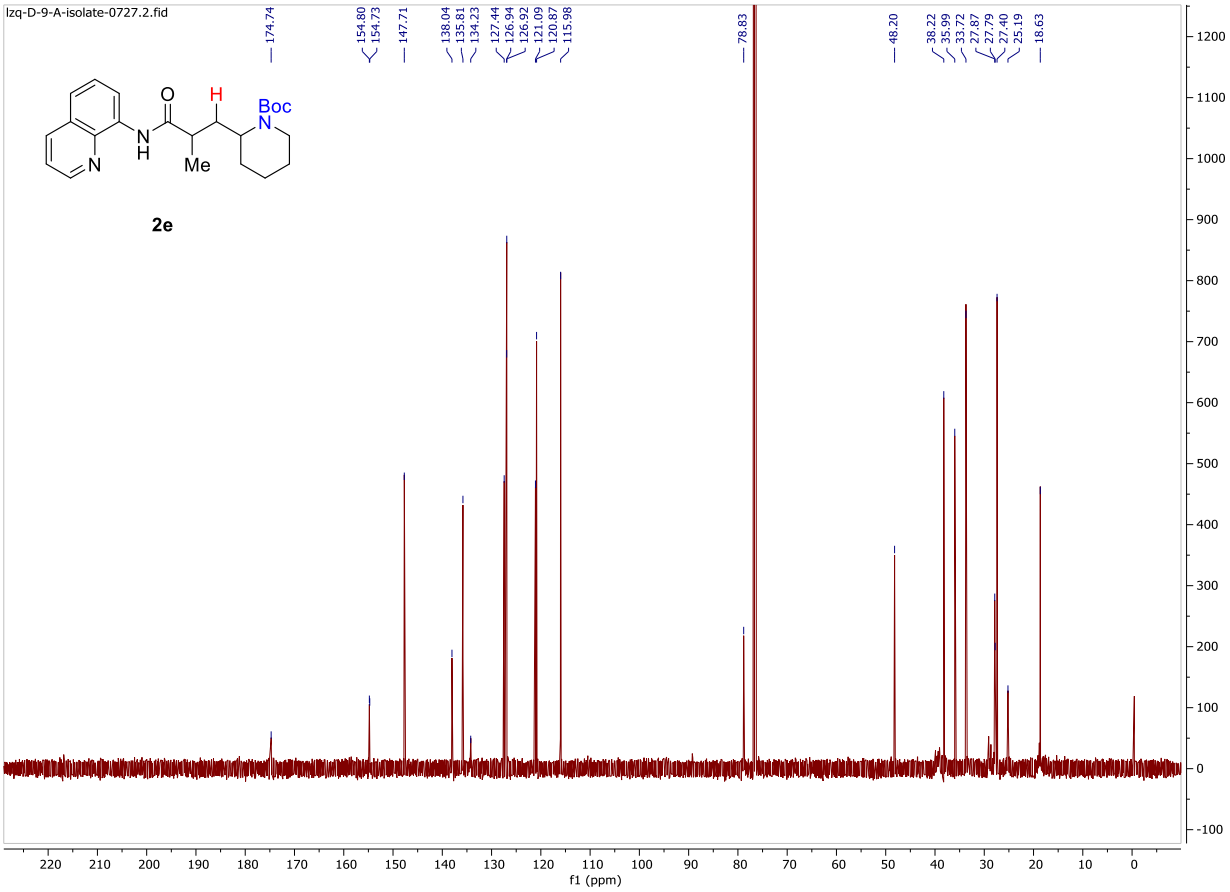
2ci

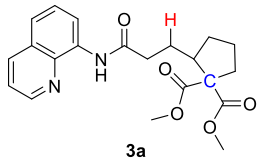
171.33
148.27
138.43
135.35
134.66
128.02
127.43
121.71
121.50
116.46
52.91
40.93
34.80
31.13
29.18
25.42
25.40
18.82
5.69
f1 (ppm)


2cj
0.91
0.96
0.94
0.95
1.92
0.95
1.00
0.93
0.93
0.93
1.88
0.93
1.88
0.96
0.96
1.90
0.90
3.05
1.86
0.95
0.96
2.89
2.94
f1 (ppm)

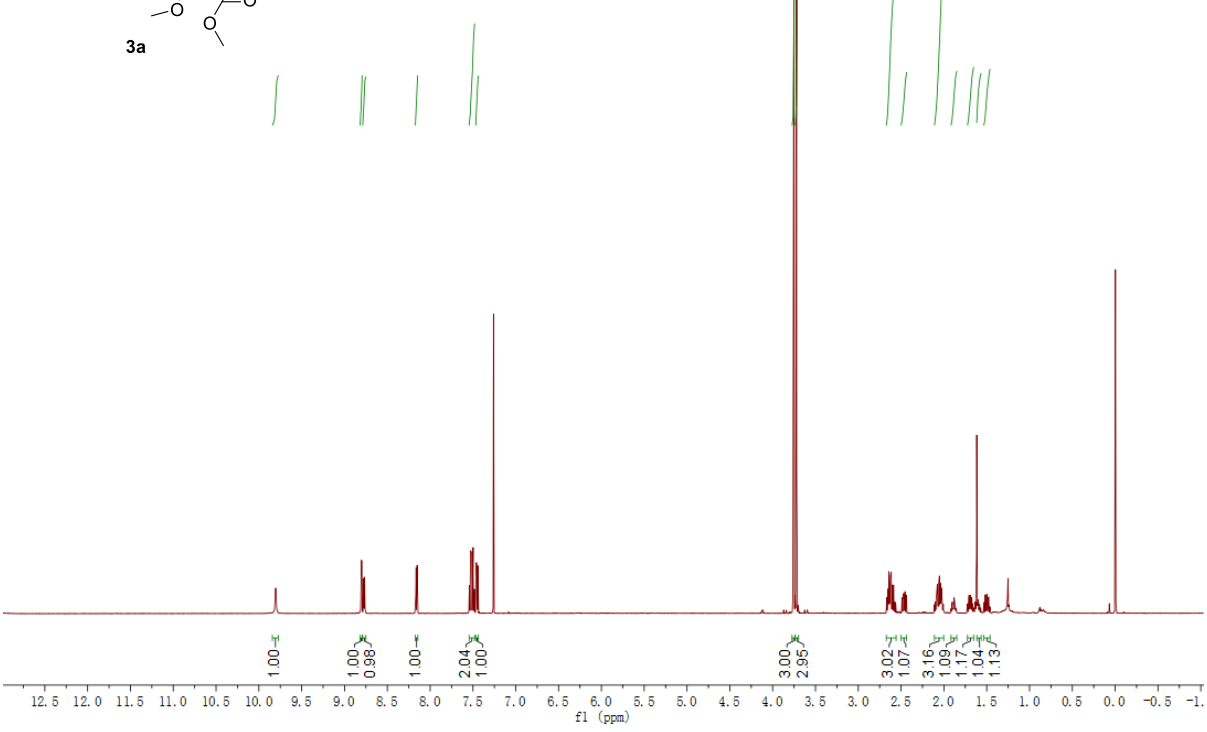

215.47
215.42
171.39
171.33
148.25
138.47
138.46
135.36
134.74
134.71
128.03
127.47
127.46
121.69
121.47
116.48
2cj
f1 (ppm)

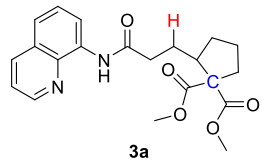

lzq-D-9-A-isolate-0727.1.fid
2e
f1 (ppm)


lzq-D-9-A-isolate-0727.2.fid
2e
f1 (ppm)



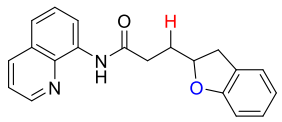
3a


1.00
1.00
0.98
1.00
2.04
1.00
3.00
2.95
3.02
1.07
3.16
1.09
1.17
1.04
1.13
f1 (ppm)



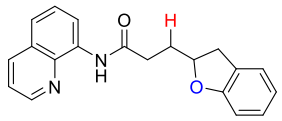
3a

173.09
171.95
171.47
148.23
138.49
135.50
134.69
128.08
127.58
121.72
121.56
116.58
63.53
52.66
52.37
46.31
37.38
34.97
31.13
27.51
25.07
f1 (ppm)



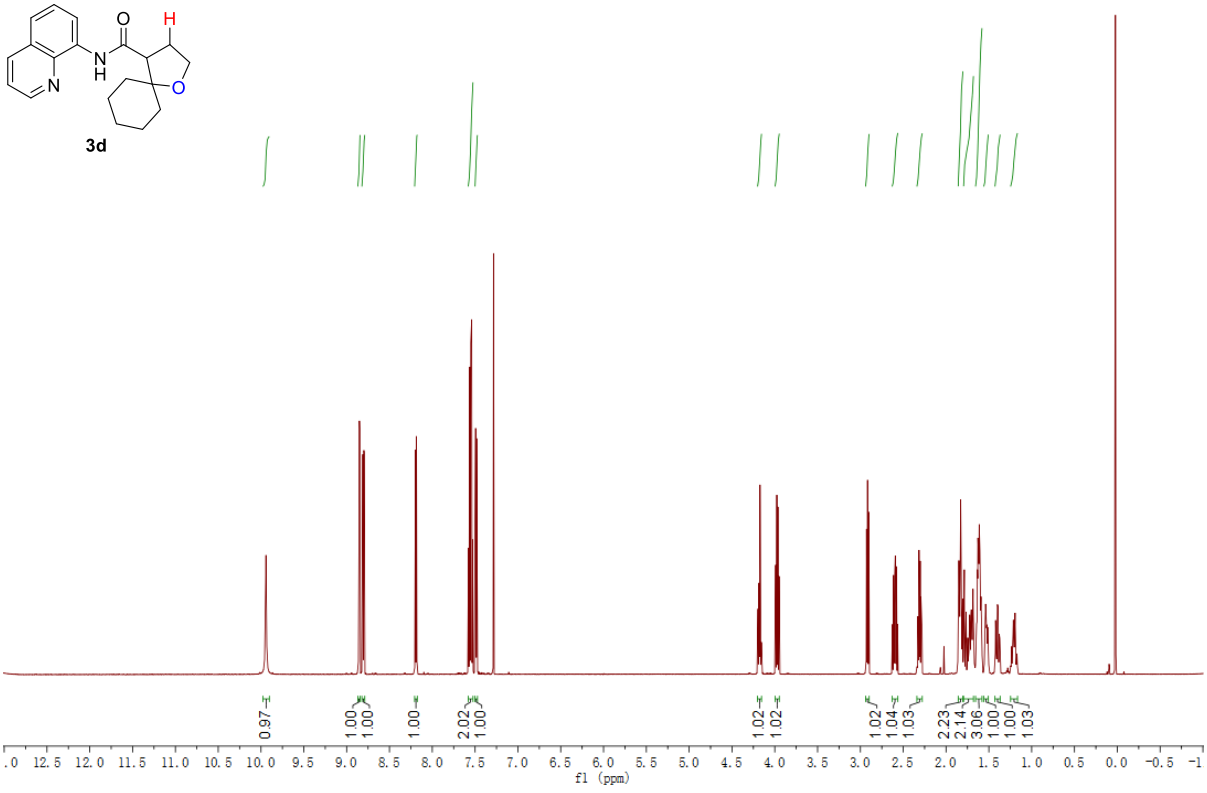
3b

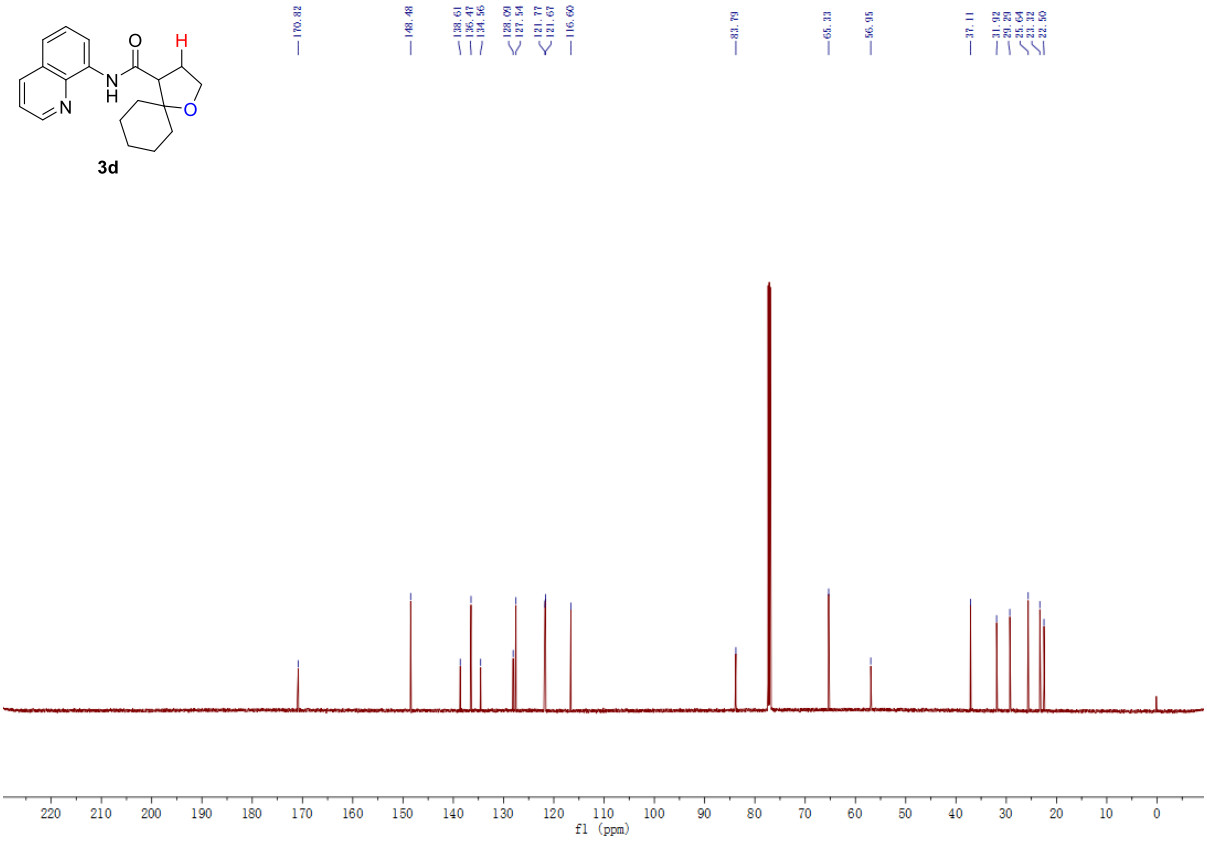
1.00
1.00
1.00
1.00
2.06
1.02
1.00
1.00
1.00
1.03
1.05
1.05
2.16
1.09
1.10
f1 (ppm)

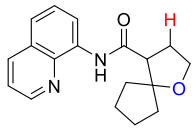


3b

171.06
159.50
148.30
138.47
135.49
134.63
128.14
128.08
127.54
126.82
125.14
121.75
121.62
120.45
116.58
109.52
82.28
35.60
34.63
31.79
f1 (ppm)

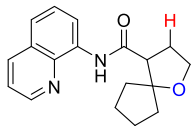

3d
0.97
1.00
1.00
1.00
2.02
1.00
1.02
1.02
1.02
1.04
1.03
2.23
2.14
3.06
1.00
1.00
1.03
f1 (ppm)


3d
170.82
148.48
138.61
135.47
134.96
128.09
127.54
121.77
121.67
116.60
83.79
65.33
56.95
37.11
31.92
29.29
25.64
23.32
22.50
f1 (ppm)



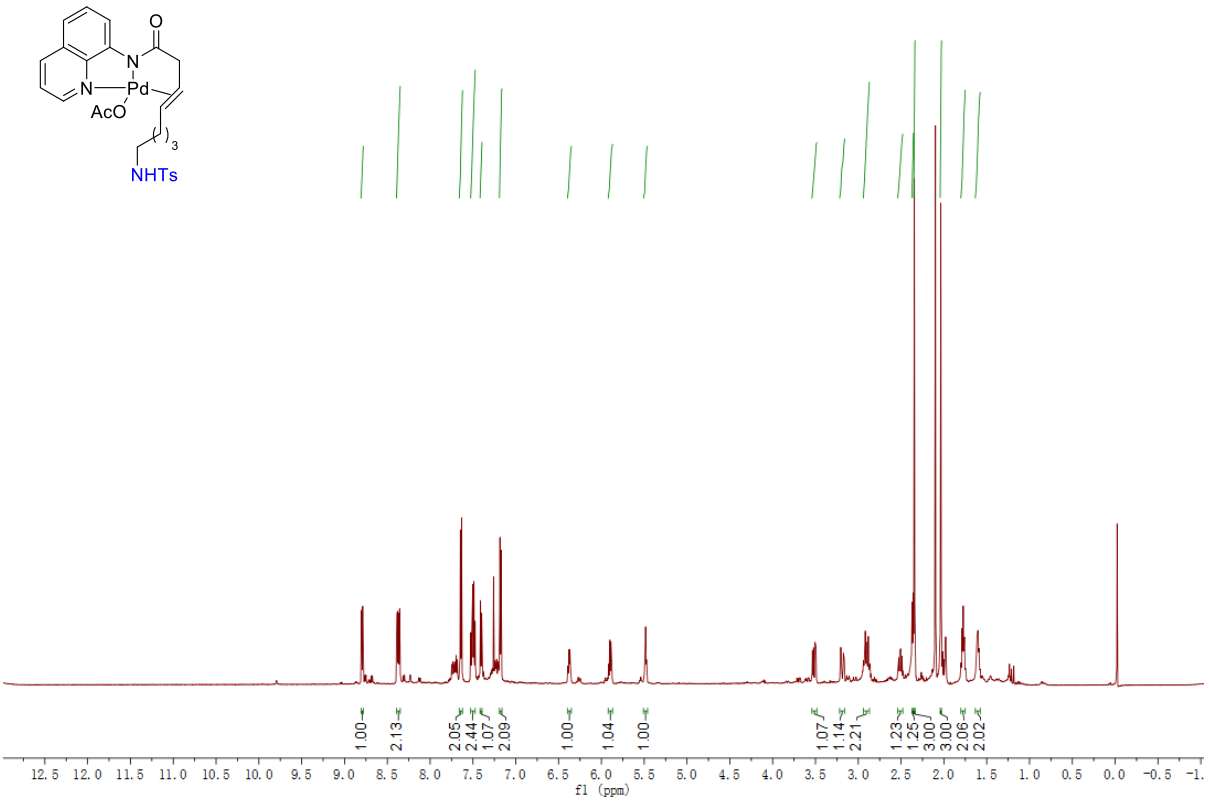
3e

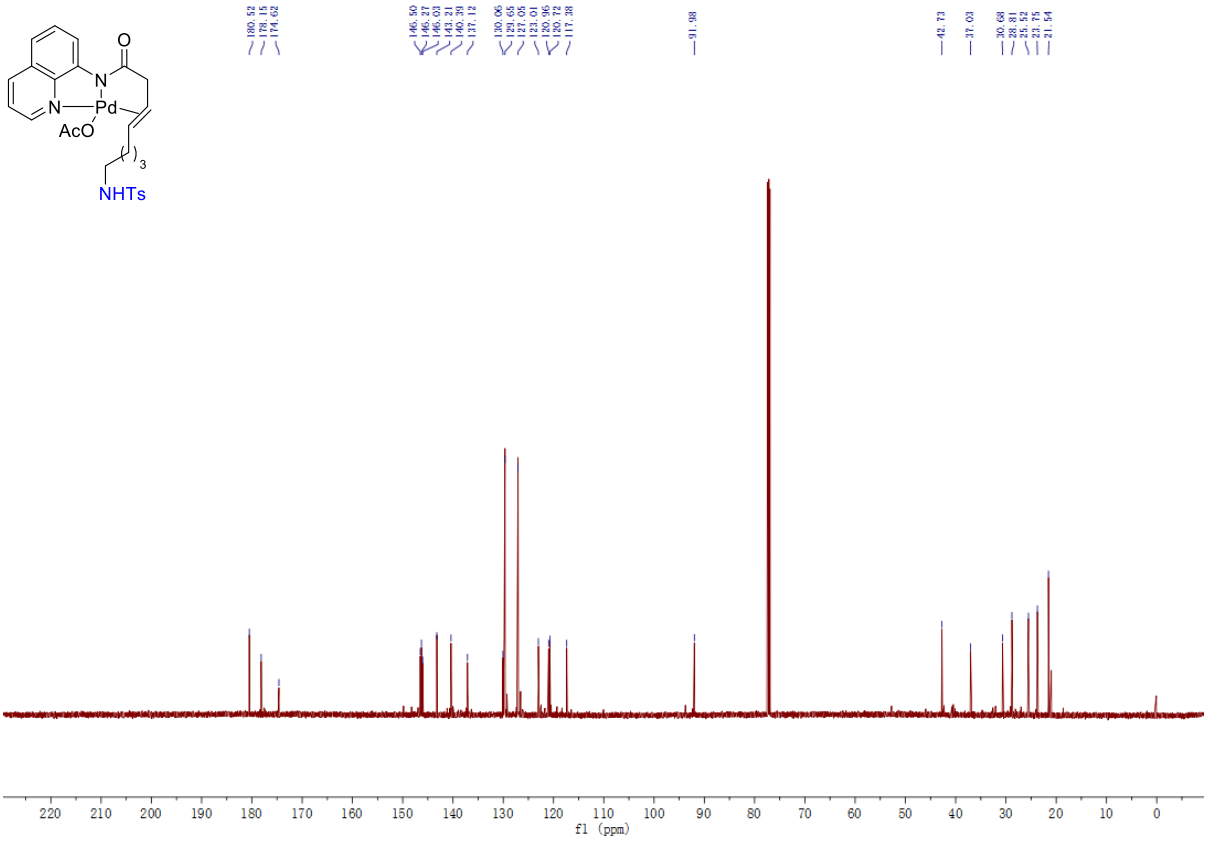
1.00
1.00
1.00
1.00
2.02
1.00
1.01
1.02
1.00
1.05
1.04
1.00
1.03
4.07
2.14
f1 (ppm)



3e

171.75
148.53
138.71
135.42
134.67
128.08
127.50
121.74
121.66
116.67
93.11
65.17
54.69
38.34
33.68
30.03
24.39
24.00
f1 (ppm)


O
N
N
Pd
AcO
3
NHTs
1.00
2.13
2.05
2.44
1.07
2.09
1.00
1.04
1.00
1.07
1.14
2.21
1.23
1.25
3.00
3.00
2.06
2.02
f1 (ppm)


O
N
N
Pd
AcO
3
NHTs
180.52
178.15
174.62
146.50
146.27
146.03
143.21
140.39
137.12
130.06
129.65
127.06
123.01
120.96
120.72
117.38
91.98
42.73
37.03
30.68
29.81
25.52
23.75
21.64
f1 (ppm)

Cartesian Coordinates

1a

M06 SCF energy (au)	-1166.341418
M06 enthalpy (au)	-1165.888822
M06 free energy (au)	-1165.976382
M06 SCF energy in solution (au)	-1166.696957
M06 enthalpy in solution (au)	-1166.244361
M06 free energy in solution (au)	-1166.331921

Cartesian coordinates

ATOM	X	Y	Z
C	0.26127200	0.88382400	2.05171500
O	0.79898900	1.85947800	2.54469100
N	-0.33370100	-0.11620500	2.77696700
C	-0.47153400	-0.21282600	4.16079800
C	-1.16891200	-1.37495600	4.62079400
C	0.00381200	0.70405800	5.07611100
C	-1.36155400	-1.56655000	6.01500000
C	-0.19929600	0.49345700	6.45587100
H	0.53171600	1.58148800	4.71922400
C	-2.26202300	-3.32275300	4.10200000
C	-2.05683400	-2.73142000	6.41004100
C	-0.86359900	-0.60968000	6.92888400
H	0.18701800	1.23414100	7.15405600
C	-2.50868100	-3.61195200	5.46077600
H	-2.22380700	-2.91236600	7.47231700
H	-1.01563300	-0.76463200	7.99667200
H	-3.04657800	-4.51654600	5.73512900
N	-1.62076300	-2.25292200	3.68928000
H	-2.61301500	-4.01000400	3.32921500
C	1.29870700	1.30998200	-0.18321100
H	1.56018200	2.32478800	0.12500600
C	1.99067300	0.70663800	-1.14797800
H	1.72819600	-0.31898400	-1.43206500
C	3.14795500	1.31302500	-1.87117000
H	2.97438600	1.30419800	-2.95878500
H	3.27405200	2.36447100	-1.57011200
C	4.44116200	0.54297700	-1.60423400
H	4.67048700	0.54822600	-0.53044600
H	4.31721100	-0.50518900	-1.90643800
N	5.58264000	1.06894400	-2.32040200
H	6.10179300	1.85003600	-1.94430100
C	5.78518900	0.76067600	-3.63302400
O	5.13278600	-0.05939200	-4.24972900
O	6.81348600	1.48916600	-4.11040200
C	7.25729300	1.32510700	-5.48713300
C	8.40528100	2.31434800	-5.59016200
H	8.83763800	2.28717600	-6.59859000
H	8.05575600	3.33495800	-5.38858900
H	9.19303500	2.06906100	-4.86657800
C	6.14423500	1.70361300	-6.45061400
H	5.30924000	0.99963700	-6.39042800
H	5.77595300	2.71362600	-6.22620000
H	6.53346300	1.70426400	-7.47771000
C	7.75717100	-0.09211100	-5.71400900
H	8.52872500	-0.34455000	-4.97450200

H	6.94224500	-0.81787700	-5.63832200
H	8.20609800	-0.16713300	-6.71362700
C	0.15211200	0.69092900	0.54694800
H	0.04915500	-0.37228300	0.28489700
H	-0.79364200	1.17553000	0.24669800
H	-0.75867800	-0.90251500	2.28955100

2a

M06 SCF energy (au)	-1166.347582
M06 enthalpy (au)	-1165.894223
M06 free energy (au)	-1165.971919
M06 SCF energy in solution (au)	-1166.694406
M06 enthalpy in solution (au)	-1166.241047
M06 free energy in solution (au)	-1166.318743

Cartesian coordinates

ATOM	X	Y	Z
C	0.00331300	1.07868000	1.15922500
O	-0.61319100	2.10367900	0.93116000
N	-0.08378000	0.37919200	2.34342000
C	-0.71182600	0.78843600	3.51581900
C	-0.28748200	0.12579200	4.71113700
C	-1.70299200	1.74720600	3.58581600
C	-0.88979900	0.46981700	5.95158100
C	-2.28224600	2.07903400	4.82810700
H	-2.02023800	2.24453400	2.67525700
C	1.07613300	-1.43372900	5.69851700
C	-0.43383500	-0.21861600	7.09798700
C	-1.89567200	1.46281600	5.99212000
H	-3.05693100	2.84408000	4.84982200
C	0.54635300	-1.17026300	6.97899100
H	-0.87337800	0.02019800	8.06691900
H	-2.34996300	1.72110300	6.94826800
H	0.91652900	-1.71631800	7.84366900
N	0.68329100	-0.81853400	4.60556300
H	1.85838400	-2.18663300	5.58028000
C	1.98569000	1.40040600	-0.37496200
H	1.49809600	2.33868800	-0.67524000
C	3.04987100	1.73103700	0.65856100
H	3.73479400	2.48827800	0.24496100
C	3.77896700	0.57752200	1.39341800
H	3.42366500	-0.42730800	1.13737500
H	4.86890500	0.59309800	1.30038000
C	3.22855300	1.13642400	2.72399700
H	2.58237600	0.47002700	3.31552400
H	3.98410600	1.57168800	3.39324600
N	2.50184600	2.13812700	1.94934200
H	2.47128500	0.98257200	-1.26924200
C	2.07994200	3.39332600	2.27687900
O	1.96491600	4.29013200	1.46576200
O	1.81193500	3.44243100	3.59205700
C	1.27542300	4.65772000	4.18957300
C	0.96763700	4.22177600	5.61179600
H	0.59135200	5.07341300	6.19365500
H	0.20336100	3.43139400	5.61579200
H	1.87101800	3.83626600	6.10193500
C	0.00066500	5.09263600	3.48519000
H	0.20202700	5.48410600	2.48484200
H	-0.67956400	4.23683000	3.39019300
H	-0.49717400	5.86781800	4.08396100

C	2.33879900	5.74257200	4.17058100
H	3.24814400	5.39722900	4.68062900
H	2.59071100	6.02431300	3.14285000
H	1.96915700	6.63337800	4.69641400
C	0.90560600	0.43945700	0.11931700
H	1.34234200	-0.50198900	0.48469200
H	0.25918500	0.17453400	-0.72897100
H	0.55839500	-0.39391300	2.49689200

1b

M06 SCF energy (au)	-1205.622845
M06 enthalpy (au)	-1205.140285
M06 free energy (au)	-1205.231109
M06 SCF energy in solution (au)	-1205.989755
M06 enthalpy in solution (au)	-1205.507195
M06 free energy in solution (au)	-1205.598019

Cartesian coordinates

ATOM	X	Y	Z
C	0.55119900	-0.37190400	1.52412200
O	1.30685000	0.56072000	1.73354600
N	-0.31001900	-0.89108100	2.45436100
C	-0.48351400	-0.49872000	3.78135700
C	-1.46077000	-1.24715600	4.51119600
C	0.19987700	0.52381000	4.40698400
C	-1.71272100	-0.92504300	5.87152000
C	-0.06583300	0.82561800	5.75895500
H	0.93725500	1.08738300	3.84614100
C	-3.01136600	-2.93620900	4.52131600
C	-2.68873800	-1.69697200	6.54094900
C	-0.99623300	0.12740000	6.48611300
H	0.48895100	1.63762200	6.22595500
C	-3.34056000	-2.70174400	5.87305900
H	-2.90935700	-1.47874200	7.58629600
H	-1.19561200	0.36789600	7.53000900
H	-4.09634000	-3.31195800	6.36221000
N	-2.11156700	-2.24449800	3.85952800
H	-3.51791900	-3.73158100	3.97038900
C	0.69983000	-0.14459300	-0.95676400
H	1.48784800	0.60217400	-0.82585300
C	-0.04520300	-0.14235400	-2.06177800
H	-0.84128400	-0.89007800	-2.16682400
C	0.13253500	0.79587900	-3.21233500
H	-0.78167100	1.39470400	-3.34881400
H	0.93713700	1.51106100	-2.98235400
C	1.70351300	-0.78014700	-4.46012400
H	1.58231000	-1.58953600	-3.72772900
H	1.89104300	-1.24168000	-5.43728000
N	2.88982100	-0.03613800	-4.08818500
H	3.14244400	0.06379600	-3.11470500
C	3.53921900	0.74716200	-4.99372500
O	3.25702300	0.80079200	-6.17556300
O	4.52888300	1.42220900	-4.37554900
C	5.38947800	2.32215200	-5.12876700
C	6.33375300	2.85384500	-4.06445900
H	7.04793200	3.55765000	-4.51087500
H	5.77496600	3.37642200	-3.27766600
H	6.89614900	2.03295700	-3.60170600
C	4.57313000	3.45641400	-5.72685000
H	3.88596600	3.08941100	-6.49475900

H	3.99416800	3.96114000	-4.94184400
H	5.24824100	4.19521500	-6.17945400
C	6.16287700	1.55114900	-6.18599700
H	6.70402000	0.71459100	-5.72416800
H	5.49561600	1.15870500	-6.95891500
H	6.90029500	2.21462000	-6.65774700
C	0.52220500	-1.09330200	0.18540300
H	1.36017900	-1.81128500	0.21513600
H	-0.39371400	-1.68858300	0.05989200
C	0.44331400	0.07386400	-4.52397500
H	0.55669100	0.80858700	-5.33347200
H	-0.40241500	-0.57604700	-4.80095300
H	-0.91707700	-1.66687300	2.19774500

2b

M06 SCF energy (au)	-1205.651814
M06 enthalpy (au)	-1205.167963
M06 free energy (au)	-1205.253318
M06 SCF energy in solution (au)	-1206.010724
M06 enthalpy in solution (au)	-1205.526873
M06 free energy in solution (au)	-1205.612228

Cartesian coordinates

ATOM	X	Y	Z
C	-1.02763000	0.53013800	0.95060300
O	-0.76057800	1.40949200	1.74950600
N	-2.02358900	-0.39831700	1.13269700
C	-2.90345100	-0.52911400	2.20433900
C	-3.83478400	-1.61096400	2.09484700
C	-2.93307300	0.28461500	3.31877800
C	-4.77547300	-1.83038100	3.13631500
C	-3.87601000	0.04763500	4.34064000
H	-2.22474700	1.10198100	3.39552100
C	-4.62552100	-3.38436400	0.87427200
C	-5.66920100	-2.91219600	2.97319200
C	-4.78119200	-0.98047300	4.26589100
H	-3.87445300	0.70632100	5.20755600
C	-5.59996300	-3.69175100	1.84706400
H	-6.40560300	-3.11092900	3.75246700
H	-5.50586400	-1.15612700	5.06040000
H	-6.27481900	-4.53093800	1.69467500
N	-3.77487000	-2.38885600	0.98386500
H	-4.55224300	-3.99178000	-0.03040200
C	0.87763300	1.30596300	-0.51986000
H	1.60703000	1.11534800	0.27838900
C	1.56007900	1.14779200	-1.87650800
H	1.68748400	0.07454400	-2.08717600
C	0.81816600	1.85497200	-3.01644700
H	1.01843200	1.34300600	-3.96849200
H	-0.26942700	1.86551700	-2.86719400
C	2.90988700	2.98025700	-2.77600100
H	3.45934900	2.75946700	-3.70579400
H	3.43292600	3.80480100	-2.27754500
N	2.87062700	1.80366500	-1.91659400
C	4.02100700	1.31370700	-1.38150100
O	5.10525100	1.85268400	-1.50574800
O	3.77496200	0.16733400	-0.71172700
C	4.82201400	-0.47600400	0.06567500
C	4.09459400	-1.65448300	0.69037000
H	4.78186500	-2.23523900	1.31885500

H	3.26160300	-1.30554500	1.31543700
H	3.69105700	-2.31585500	-0.08725400
C	5.32781200	0.46610000	1.14574200
H	5.85066500	1.32364300	0.71193100
H	4.48777500	0.83057100	1.75301200
H	6.01879100	-0.07196900	1.80853200
C	5.93709800	-0.95953500	-0.84653700
H	5.52735400	-1.60071500	-1.63844100
H	6.46242500	-0.11832600	-1.30784000
H	6.65605000	-1.55310700	-0.26562700
C	-0.29085600	0.35166600	-0.36368100
H	0.06129000	-0.69117600	-0.43636300
H	-1.01816000	0.47432600	-1.18432000
C	1.43542600	3.25243100	-3.03922800
H	1.01544700	3.86709500	-2.23042600
H	1.26515900	3.78449900	-3.98176800
H	0.53739100	2.34323300	-0.38200200
H	-2.17831500	-1.10540300	0.41614100

1c

M06 SCF energy (au)	-1244.899238
M06 enthalpy (au)	-1244.387066
M06 free energy (au)	-1244.483171
M06 SCF energy in solution (au)	-1245.279594
M06 enthalpy in solution (au)	-1244.767422
M06 free energy in solution (au)	-1244.863527

Cartesian coordinates

ATOM	X	Y	Z
C	-0.03744700	0.34613100	2.04423800
O	-0.00331600	1.56095900	2.12785500
N	-0.80523400	-0.45987400	2.84486400
C	-1.65187000	-0.08432100	3.88666800
C	-2.31125700	-1.16602200	4.55278000
C	-1.88463700	1.21257700	4.29716000
C	-3.19693700	-0.88687400	5.62774200
C	-2.76743700	1.46600800	5.36749200
H	-1.38226700	2.02630800	3.78596000
C	-2.65849500	-3.42614700	4.72457200
C	-3.82011200	-1.99357800	6.24660800
C	-3.41503900	0.45181400	6.02629000
H	-2.93125600	2.49936200	5.66858200
C	-3.55611500	-3.26336300	5.80089000
H	-4.50676800	-1.81790300	7.07531100
H	-4.09622100	0.65670600	6.85174000
H	-4.02121000	-4.13403800	6.25755700
N	-2.05660600	-2.42715400	4.11971500
H	-2.43353100	-4.42837200	4.35343700
C	0.96371300	0.31884800	-0.24519900
H	1.19398100	1.38313500	-0.15748600
C	0.81383600	-0.23641400	-1.44619200
H	0.57393700	-1.30458400	-1.51222400
C	0.98321500	0.47822900	-2.74735200
H	0.05137100	0.42136500	-3.33653500
H	1.16027700	1.54713400	-2.55337500
C	2.48772600	1.95077200	-5.02270200
H	1.64707700	2.50470200	-4.58726300
H	3.38051400	2.19084000	-4.42595300
N	2.67969700	2.46950400	-6.36077200
H	3.56847900	2.34989300	-6.82687800

C	1.60894400	2.78696900	-7.14364200
O	0.45828000	2.80847000	-6.75217000
O	2.03664400	3.08148700	-8.38763800
C	1.08993900	3.49258900	-9.41401800
C	1.98257500	3.72412800	-10.62099600
H	1.37996900	4.04520100	-11.48025600
H	2.72714400	4.50154600	-10.40758600
H	2.51271600	2.80230100	-10.89255100
C	0.40077200	4.78529700	-9.00896700
H	-0.24617100	4.63562400	-8.13962400
H	1.14774000	5.55359000	-8.76886700
H	-0.20928000	5.15303300	-9.84508300
C	0.09754700	2.37623100	-9.69591800
H	0.63085500	1.44751800	-9.93938900
H	-0.55383200	2.19677700	-8.83571700
H	-0.52385700	2.64784600	-10.55991700
C	0.82160800	-0.41683000	1.04822500
H	1.80954400	-0.52822700	1.52840800
H	0.44194000	-1.43494800	0.87888800
C	2.12226400	-0.11226800	-3.58048600
H	1.99237000	-1.20467100	-3.63746700
H	3.07476400	0.04914600	-3.04823200
C	2.21214500	0.45332600	-4.99135900
H	3.00729200	-0.06646300	-5.54883900
H	1.27251100	0.26656200	-5.53557800
H	-0.78289000	-1.46805700	2.70753800

2c

M06 SCF energy (au)	-1244.938225
M06 enthalpy (au)	-1244.423459
M06 free energy (au)	-1244.506548
M06 SCF energy in solution (au)	-1245.306451
M06 enthalpy in solution (au)	-1244.791685
M06 free energy in solution (au)	-1244.874774

Cartesian coordinates

ATOM	X	Y	Z
C	-1.99449000	1.85789200	-0.35525500
O	-2.35380600	2.95993100	0.02908500
N	-2.35255700	0.67903400	0.24615300
C	-3.16613000	0.48606600	1.36240600
C	-3.20051800	-0.85377400	1.86263600
C	-3.92574600	1.46265700	1.97325100
C	-4.00376300	-1.15413200	2.99478300
C	-4.71489800	1.14292900	3.09759600
H	-3.90270600	2.47410700	1.58175200
C	-2.47952500	-3.02202100	1.67524100
C	-3.99628500	-2.49272400	3.44700700
C	-4.76043200	-0.12962000	3.60836300
H	-5.29947600	1.93526200	3.56182100
C	-3.23716900	-3.42947800	2.79376400
H	-4.59984200	-2.76096800	4.31459400
H	-5.37141300	-0.36847200	4.47835100
H	-3.21154800	-4.46699500	3.11886200
N	-2.45479000	-1.78942400	1.22110500
H	-1.87037700	-3.75231400	1.13834100
C	0.30780900	2.25384200	-1.24666200
H	0.18075600	3.27598100	-0.85919700
C	1.07501100	1.43059000	-0.20400900
H	0.39726100	1.23053600	0.63444900

C	1.58589000	0.08632200	-0.72386400
H	1.88726300	-0.52064300	0.14388300
H	0.76275700	-0.45683600	-1.21252500
C	3.37859700	2.35573600	-0.49526400
H	4.12728500	2.89106400	0.09527600
H	3.14724200	2.99222200	-1.37016100
N	2.19603500	2.20082800	0.34448500
C	1.98706300	3.16232500	1.30715500
O	2.79629300	4.02629400	1.58835500
O	0.78999500	2.99233500	1.89315300
C	0.27065300	3.97262700	2.83874100
C	-1.07512800	3.38121700	3.21729000
H	-1.59054100	4.03994200	3.92874700
H	-1.69892200	3.26763300	2.32191400
H	-0.94971800	2.39479100	3.68416400
C	0.08069000	5.30088100	2.12656700
H	1.04021700	5.72809500	1.81734700
H	-0.55767500	5.15745800	1.24337200
H	-0.41932400	6.01223500	2.79762700
C	1.17077200	4.08012100	4.05791800
H	1.33677600	3.08549400	4.49316300
H	2.13856200	4.52230700	3.80746000
H	0.67754700	4.70357200	4.81623100
C	-1.08168700	1.69946500	-1.55428900
H	-1.03067100	0.65485000	-1.89443600
H	-1.53157500	2.28200100	-2.36883500
C	2.77891500	0.22581500	-1.66098700
H	2.48375700	0.75200600	-2.58409300
H	3.13275300	-0.76678200	-1.97168300
C	3.88655200	1.00354900	-0.96375100
H	4.24104300	0.43242300	-0.09103200
H	4.74845300	1.14905800	-1.62943600
H	0.88334600	2.33535500	-2.18029600
H	-1.94066100	-0.19113200	-0.08577900

1d

M06 SCF energy (au)	-1284.179769
M06 enthalpy (au)	-1283.637917
M06 free energy (au)	-1283.735865
M06 SCF energy in solution (au)	-1284.571969
M06 enthalpy in solution (au)	-1284.030117
M06 free energy in solution (au)	-1284.128065

Cartesian coordinates

ATOM	X	Y	Z
C	-0.01004200	0.57754100	1.57550200
O	-0.47697600	1.68001900	1.35037300
N	-0.59930300	-0.35647200	2.38862500
C	-1.78516900	-0.24241300	3.11244700
C	-2.13565400	-1.39171900	3.89012700
C	-2.60871600	0.86498200	3.12321400
C	-3.32808500	-1.37388800	4.66237100
C	-3.78729300	0.86048700	3.89795600
H	-2.33662600	1.73092800	2.53004500
C	-1.61507200	-3.52100300	4.56295500
C	-3.62329700	-2.53642800	5.40922200
C	-4.15135800	-0.22479000	4.65404400
H	-4.41672600	1.74876800	3.88641400
C	-2.77292400	-3.61148300	5.36403900
H	-4.53030700	-2.55964600	6.01410100

H	-5.06404300	-0.22016400	5.24928400
H	-2.97430700	-4.51939600	5.92797800
N	-1.30074800	-2.46128900	3.85287500
H	-0.92391900	-4.36511600	4.51221500
C	1.54984000	0.68776800	-0.37237800
H	1.33066200	1.75135300	-0.49047100
C	1.97715200	-0.02518200	-1.41263100
H	2.17270000	-1.09609100	-1.28027000
C	2.18857400	0.51455300	-2.78960000
H	1.98489000	1.59743000	-2.79854300
H	3.24598100	0.39657500	-3.08416100
C	0.90588400	0.18434800	-7.67935800
H	0.68100700	1.26007300	-7.71684200
H	1.96111900	0.06489600	-7.95829500
N	0.11689200	-0.47840800	-8.69675000
H	-0.84978200	-0.21882600	-8.83639700
C	0.51745400	-1.67394600	-9.21605700
O	1.59882200	-2.18535600	-8.99878200
O	-0.45769400	-2.16940200	-10.00413300
C	-0.26585600	-3.42900900	-10.70790700
C	-1.57739100	-3.60006500	-11.45472800
H	-1.56129400	-4.52957900	-12.03809300
H	-2.41958600	-3.64429800	-10.75240700
H	-1.74337300	-2.76041100	-12.14158700
C	-0.06924700	-4.56439300	-9.71638900
H	0.87267600	-4.45703800	-9.17062700
H	-0.89809900	-4.58619500	-8.99618400
H	-0.06039400	-5.52243600	-10.25350400
C	0.89069100	-3.31467100	-11.68735000
H	0.73496000	-2.46012000	-12.35921800
H	1.84267000	-3.18583400	-11.16409900
H	0.94364900	-4.22460700	-12.30025800
C	1.32430300	0.13348700	0.99719000
H	2.09461900	0.51415200	1.69061200
H	1.42207800	-0.96194300	0.99695200
C	0.67970300	-0.36083800	-6.27756700
H	-0.38660200	-0.26618500	-6.01190200
H	0.90722300	-1.43847400	-6.28381200
C	1.31471100	-0.18221300	-3.82961000
H	0.25530000	-0.06488000	-3.54865200
H	1.51397400	-1.26727900	-3.80904700
C	1.53547100	0.34509600	-5.23840800
H	1.32712000	1.42927000	-5.25942300
H	2.60044400	0.23866600	-5.50777900
H	-0.14829900	-1.25910400	2.52182800

2d

M06 SCF energy (au)	-1284.207114
M06 enthalpy (au)	-1283.662831
M06 free energy (au)	-1283.753666
M06 SCF energy in solution (au)	-1284.587341
M06 enthalpy in solution (au)	-1284.043058
M06 free energy in solution (au)	-1284.133893

Cartesian coordinates

ATOM	X	Y	Z
C	-0.52344000	0.29247300	2.19416100
O	-0.28020100	1.38441900	2.67816600
N	-0.59818700	-0.86857600	2.92278400
C	-0.45210500	-1.03457900	4.29833400

C	-0.60745100	-2.37750700	4.76901400
C	-0.17718900	-0.02478000	5.19841600
C	-0.47571400	-2.64984400	6.15697800
C	-0.05201000	-0.31846600	6.57210000
H	-0.05883400	0.98942900	4.83323100
C	-1.01925400	-4.57884700	4.27624800
C	-0.63789100	-3.99335900	6.56320400
C	-0.19495700	-1.59466900	7.05484500
H	0.16519200	0.49903300	7.25764700
C	-0.90889200	-4.96107900	5.63001500
H	-0.54354200	-4.24032200	7.62115000
H	-0.09554700	-1.81296600	8.11778100
H	-1.03821900	-6.00323200	5.91311800
N	-0.87682700	-3.34307700	3.85381700
H	-1.23457600	-5.33281100	3.51601200
C	-0.08409400	1.13418800	-0.13340000
H	0.99724100	1.01757500	0.01788100
C	-0.35924500	0.98036300	-1.62953600
H	-0.06518100	-0.04470100	-1.90008600
C	-1.83312600	1.12384300	-2.01912000
H	-1.91532200	1.09694300	-3.11774800
H	-2.33425300	0.20768500	-1.67230100
C	0.09849900	3.10095100	-3.01960900
H	-0.44413000	2.89753100	-3.96084400
H	1.00416800	3.64184700	-3.30030500
N	0.53994200	1.85084100	-2.40780500
C	1.79539300	1.34263900	-2.62021700
O	2.18060300	0.28664700	-2.14630000
O	2.53841100	2.14195500	-3.41130200
C	3.92284500	1.80256300	-3.71036100
C	4.37004300	2.96601300	-4.57937700
H	5.41437600	2.82732500	-4.88712200
H	3.74812700	3.03686600	-5.48083300
H	4.29279100	3.91272600	-4.02943100
C	3.99082500	0.50277600	-4.49529800
H	3.67246400	-0.34675100	-3.88487500
H	3.34924400	0.56382300	-5.38454100
H	5.02258000	0.33230000	-4.83146700
C	4.74803800	1.75031400	-2.43511700
H	4.63256100	2.68505200	-1.87027100
H	4.44858200	0.91238200	-1.79959500
H	5.80994400	1.63820400	-2.69257000
C	-0.81182300	0.10581800	0.71735400
H	-0.55163700	-0.91397000	0.39244600
H	-1.90419500	0.19639400	0.59522300
C	-0.76462300	3.99511700	-2.13372600
H	-0.36189000	4.00079900	-1.10898100
H	-0.65170300	5.02296100	-2.50907000
C	-2.59425500	2.32685500	-1.46912500
H	-2.42627500	2.40991000	-0.38353400
H	-3.67217600	2.14264600	-1.58912700
C	-2.24787000	3.64909100	-2.13690000
H	-2.59290400	3.62348400	-3.18525700
H	-2.81289400	4.45805400	-1.65101600
H	-0.33666000	2.14215400	0.22154100
H	-0.79460600	-1.74478900	2.44352400

5a

M06 SCF energy (au)	-1166.374000
M06 enthalpy (au)	-1165.919891

M06 free energy (au)	-1166.000770
M06 SCF energy in solution (au)	-1166.717892
M06 enthalpy in solution (au)	-1166.263783
M06 free energy in solution (au)	-1166.344662

Cartesian coordinates

ATOM	X	Y	Z
C	2.00638400	0.09874300	1.70608900
O	2.69771100	1.10136200	1.77883300
N	0.93591700	-0.15322600	2.52766200
C	0.44439900	0.63053400	3.56920800
C	-0.70070700	0.09942100	4.24359400
C	0.97482800	1.83902200	3.97492900
C	-1.27326500	0.82495600	5.32208500
C	0.38915800	2.54199700	5.04812600
H	1.84351000	2.23384100	3.45928900
C	-2.24347700	-1.58689100	4.43038700
C	-2.40103000	0.25176500	5.95122300
C	-0.70838100	2.05960400	5.71531000
H	0.83042900	3.49170000	5.34599700
C	-2.89042400	-0.95141600	5.51157700
H	-2.86716700	0.78026000	6.78339800
H	-1.15448300	2.60860200	6.54410900
H	-3.75652900	-1.41683600	5.97659100
N	-1.19347800	-1.09112400	3.81587800
H	-2.61591100	-2.54593600	4.06381200
C	3.43352900	-0.68980700	-0.21810200
H	4.29667000	-0.44729600	0.41486600
C	3.15861300	0.40879100	-1.24716600
H	2.46657000	1.16692000	-0.86560300
C	2.64164900	-0.35073400	-2.46658900
H	1.58740600	-0.63202800	-2.32672600
H	2.70764800	0.22432100	-3.39713900
C	3.51255900	-1.59994900	-2.48700800
H	3.03016700	-2.46636200	-2.95455400
H	4.46152500	-1.42330400	-3.01960600
N	3.75463100	-1.84202600	-1.06826600
C	4.40898600	-2.91552600	-0.55186000
O	4.64486200	-3.05483800	0.63651500
O	4.73969000	-3.78107700	-1.53134100
C	5.43416700	-5.02086800	-1.21455800
C	5.59511200	-5.67317500	-2.57691700
H	6.11808300	-6.63289000	-2.47652500
H	4.61560900	-5.85676600	-3.03665700
H	6.17660700	-5.02813900	-3.24780800
C	4.57817400	-5.89118900	-0.30889100
H	4.45371700	-5.43601300	0.67790700
H	3.58808600	-6.04638200	-0.75824900
H	5.05430000	-6.87366200	-0.18851800
C	6.79511900	-4.72256500	-0.60708200
H	7.36687800	-4.05730000	-1.26778500
H	6.69712200	-4.24952800	0.37417100
H	7.35966500	-5.65815500	-0.49531500
C	2.25147300	-0.99845300	0.69137500
H	2.45603100	-1.93987200	1.22300100
H	1.33758500	-1.16292200	0.09643900
H	4.09899400	0.91984700	-1.49665400
H	0.41085400	-1.01733000	2.40569200

AcOH

M06 SCF energy (au)	-228.954066
M06 enthalpy (au)	-228.886374
M06 free energy (au)	-228.919291
M06 SCF energy in solution (au)	-229.040586
M06 enthalpy in solution (au)	-228.972894
M06 free energy in solution (au)	-229.005811

Cartesian coordinates

ATOM	X	Y	Z
C	-0.17601100	-0.41767800	-0.00065500
O	1.02813400	-0.48275900	0.00000200
O	-0.83950700	0.75753500	0.00011600
H	-0.15401900	1.44871600	0.00043100
C	-1.12763000	-1.57335500	-0.00001600
H	-1.77768600	-1.52474000	0.88103800
H	-1.77789300	-1.52547300	-0.88095400
H	-0.56848600	-2.51082100	0.00031600

1-AdaCOOH

M06 SCF energy (au)	-578.896680
M06 enthalpy (au)	-578.627396
M06 free energy (au)	-578.673605
M06 SCF energy in solution (au)	-579.075351
M06 enthalpy in solution (au)	-578.806067
M06 free energy in solution (au)	-578.852276

Cartesian coordinates

ATOM	X	Y	Z
C	-0.32160000	-0.12471400	-0.00734900
H	0.78099500	-0.11169400	-0.00134200
H	-0.65917000	0.92245500	-0.00621000
C	-0.83364400	-0.83832800	1.25996700
C	-0.83553900	-0.85116700	-1.25260600
H	-0.46001800	-0.33467300	-2.14926500
C	-0.34073600	-2.29972800	-1.24388600
H	0.76088800	-2.32353100	-1.26310700
H	-0.69001500	-2.82218600	-2.14910500
C	-0.34420100	-2.29015700	1.25450100
H	-0.68893500	-2.79658300	2.16913900
H	0.75607300	-2.30627300	1.28753300
C	-0.85970900	-3.01143400	0.00845000
H	-0.50034200	-4.05164100	0.01884600
C	-2.39084800	-2.99533300	0.00651000
H	-2.77437900	-3.52955200	-0.87773600
H	-2.77538200	-3.52366400	0.89390000
C	-2.37543600	-0.82212700	1.24575200
H	-2.73637200	0.21710100	1.26189300
H	-2.75617600	-1.31342500	2.15657800
C	-2.36684500	-0.83582200	-1.25206600
H	-2.73513200	0.20252300	-1.27824500
H	-2.74880900	-1.33617500	-2.15648400
C	-2.88823700	-1.54761700	-0.00046800
H	-3.98894800	-1.53213700	0.00340200
C	-0.32188600	-0.13283300	2.49210100
O	0.36964200	-0.61844900	3.35620900
O	-0.72631300	1.15495300	2.54755700
H	-0.34693200	1.51234200	3.36986800

IM1a

M06 SCF energy (au)	-1522.084441

M06 enthalpy (au)	-1521.584160
M06 free energy (au)	-1521.677904
M06 SCF energy in solution (au)	-1522.495499
M06 enthalpy in solution (au)	-1521.995218
M06 free energy in solution (au)	-1522.088962

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.36871600	-2.26416500	1.75301000
C	-1.97212600	-3.90802400	-0.06666100
O	-1.96648400	-2.95860000	-0.84091900
O	-1.29126400	-3.97796000	1.04527300
C	-2.80032800	-5.14707900	-0.33016700
H	-3.24679400	-5.10058900	-1.32698900
H	-2.18701400	-6.05089700	-0.23534400
H	-3.59892900	-5.22134800	0.41865900
C	0.91840800	0.36398600	1.99775200
O	1.46587000	1.34080000	2.48451100
N	0.35194300	-0.66623900	2.70057200
C	0.18142100	-0.69175100	4.08329300
C	-0.61309000	-1.77123000	4.56254600
C	0.70068200	0.19789600	5.01261600
C	-0.84421400	-1.96548000	5.94518500
C	0.45631800	0.00843000	6.38761300
H	1.30359700	1.02892100	4.66357700
C	-1.83831800	-3.68389500	4.01014100
C	-1.61555200	-3.08903300	6.31860000
C	-0.28757700	-1.04557000	6.86182800
H	0.88573200	0.72189500	7.08920600
C	-2.10905100	-3.94397600	5.36466400
H	-1.80541000	-3.26713100	7.37718700
H	-0.45448100	-1.18866900	7.92845300
H	-2.69427900	-4.81893200	5.63426200
N	-1.13282300	-2.63597000	3.63736400
H	-2.17763300	-4.33516600	3.20521300
C	0.45877700	-1.17806600	-0.00122200
H	-0.30656400	-1.33294900	-0.76550000
C	1.32860200	-2.21672500	0.26521200
H	2.18381400	-2.01589800	0.92543700
C	1.41739700	-3.48152700	-0.53242100
H	0.43067500	-3.73066100	-0.94219500
H	2.06105700	-3.27391800	-1.40496800
C	2.04263700	-4.65200300	0.22787000
H	2.00110900	-5.55101600	-0.40317600
H	3.10080600	-4.45045500	0.42178800
N	1.41677100	-4.94176200	1.50246700
H	0.41062300	-5.09975000	1.49054900
C	1.86933900	-4.53163800	2.72534500
O	1.21531100	-4.63992100	3.74825000
O	3.11221200	-4.02115100	2.64212200
C	3.80787800	-3.53548900	3.82808900
C	5.13676500	-3.06535700	3.26191000
H	5.77277900	-2.67398800	4.06595500
H	5.66460200	-3.89334200	2.77174500
H	4.98142500	-2.26630600	2.52459700
C	4.02093000	-4.67102000	4.81452200
H	3.06992500	-5.02542200	5.22260500
H	4.53280200	-5.50961800	4.32396700
H	4.65389200	-4.32245900	5.64166700
C	3.05586700	-2.36694500	4.44160200

H	2.85425200	-1.59783000	3.68074500
H	2.10441500	-2.68419100	4.88142700
H	3.66810200	-1.90747700	5.22981800
C	0.71850400	0.22230900	0.49360000
H	-0.13281500	0.86971200	0.23987900
H	1.59225900	0.65961200	-0.00969800

TS5a

M06 SCF energy (au)	-1522.038078
M06 enthalpy (au)	-1521.539447
M06 free energy (au)	-1521.631395
M06 SCF energy in solution (au)	-1522.448962
M06 enthalpy in solution (au)	-1521.950331
M06 free energy in solution (au)	-1522.042279

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.65151500	-1.75516100	1.97419000
C	-1.21815600	-4.48302900	1.09152000
O	-1.57460200	-3.27038700	0.87615700
O	-0.23409600	-4.84442700	1.76034400
C	-2.12991800	-5.52206300	0.47652400
H	-2.44989200	-5.21486200	-0.52474900
H	-1.63790600	-6.49819400	0.44058100
H	-3.03685200	-5.61152700	1.08921300
C	1.00343900	0.59421800	2.41023800
O	1.65587900	1.46912800	2.96576300
N	0.12118700	-0.25672100	3.02408600
C	-0.28208100	-0.18395200	4.34649900
C	-1.24532500	-1.16743200	4.73837900
C	0.13380300	0.73373200	5.30564600
C	-1.74966700	-1.21828500	6.06250300
C	-0.37675800	0.67625300	6.61674400
H	0.85970900	1.48875400	5.02318800
C	-2.54882300	-2.99029800	4.09349300
C	-2.69362900	-2.22831200	6.35722500
C	-1.29138300	-0.27315300	7.00757300
H	-0.02386500	1.41132800	7.33879900
C	-3.09443400	-3.11000600	5.38470200
H	-3.09685000	-2.29143000	7.36818400
H	-1.67354300	-0.30973400	8.02683000
H	-3.82062900	-3.89218900	5.59048100
N	-1.66380300	-2.06245300	3.79020400
H	-2.83962000	-3.65784400	3.28271500
C	0.65650400	-1.05024200	0.47506600
H	-0.02511700	-1.11879000	-0.38478300
C	1.74774600	-1.97019100	0.32529800
H	2.75343500	-1.56182900	0.50156100
C	1.74108500	-3.14333600	-0.62836400
H	0.70906800	-3.46935800	-0.81335100
H	2.22663300	-2.93517900	-1.58928700
C	2.47038600	-4.07638700	0.32687900
H	2.15452900	-5.12339600	0.34278700
H	3.55987700	-4.00364100	0.24933900
N	2.04534700	-3.37239700	1.56058400
H	1.12493100	-3.73428200	1.90381900
C	3.00005900	-3.05185100	2.55724800
O	4.16935200	-2.89400500	2.29294200
O	2.38240300	-2.90097800	3.71320900
C	3.12202700	-2.44429000	4.90797300

C	2.05492600	-2.45774200	5.98492500
H	2.49848500	-2.16908800	6.94637000
H	1.25578200	-1.74570300	5.74725400
H	1.61894700	-3.45981800	6.08625400
C	3.64487800	-1.04014400	4.67001600
H	4.43668300	-1.02678000	3.91398500
H	2.83870600	-0.36338200	4.35313600
H	4.06121000	-0.65110100	5.60884300
C	4.22346100	-3.43722200	5.23564000
H	3.80965500	-4.44951900	5.33493400
H	5.00796200	-3.44398600	4.47341300
H	4.67505100	-3.16086200	6.19743800
C	1.04355100	0.36335200	0.90701800
H	0.32925700	1.08104100	0.47578400
H	2.03649800	0.66906300	0.54277900

IM5a

M06 SCF energy (au)	-1522.043576
M06 enthalpy (au)	-1521.543402
M06 free energy (au)	-1521.636014
M06 SCF energy in solution (au)	-1522.454997
M06 enthalpy in solution (au)	-1521.954823
M06 free energy in solution (au)	-1522.047435

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.68702600	-1.74521700	1.96874900
C	-1.12415600	-4.50017000	1.11823400
O	-1.59174500	-3.32879700	0.93123500
O	-0.03205000	-4.77614100	1.66021100
C	-2.01410700	-5.63265600	0.65717600
H	-2.65420300	-5.32039700	-0.17348000
H	-1.41577500	-6.50535000	0.37786200
H	-2.66647600	-5.93001000	1.48918100
C	1.05803300	0.52713600	2.42621000
O	1.78145300	1.34084600	2.99068800
N	0.10641800	-0.25594500	3.02640600
C	-0.29170900	-0.17313900	4.34760200
C	-1.28845700	-1.12392600	4.74795300
C	0.16035800	0.73126300	5.30471300
C	-1.78542400	-1.14988800	6.07669400
C	-0.34401100	0.69630400	6.61843100
H	0.91148100	1.45920500	5.01630000
C	-2.64990700	-2.90845800	4.12644900
C	-2.76109500	-2.12612500	6.38401500
C	-1.29002400	-0.21878600	7.01681300
H	0.03826000	1.42098400	7.33627800
C	-3.19507700	-3.00170400	5.42070600
H	-3.16045600	-2.16775900	7.39778000
H	-1.66856600	-0.23881300	8.03802600
H	-3.94594900	-3.75776300	5.63643100
N	-1.73862300	-2.01204100	3.80907900
H	-2.96363100	-3.57469300	3.32194500
C	0.64387500	-1.11712000	0.51100600
H	0.07903300	-1.11139600	-0.43345600
C	1.80330700	-2.04573600	0.32237900
H	2.77308800	-1.52118200	0.28969000
C	1.78555700	-3.16722200	-0.71748700
H	0.76428600	-3.53336000	-0.87934600
H	2.25953900	-2.94624900	-1.67776400

C	2.55612400	-4.04106500	0.26761900
H	2.24694700	-5.07866400	0.41305200
H	3.64326100	-3.94431900	0.18915400
N	2.08321500	-3.17111200	1.40343500
H	1.16316400	-3.57724300	1.74946300
C	3.02264300	-2.84125000	2.47224400
O	4.17897300	-2.62803900	2.22069600
O	2.37722700	-2.82047100	3.60633000
C	3.07995500	-2.47645300	4.87393900
C	1.96955600	-2.57880500	5.89884600
H	2.37841300	-2.39385000	6.90018600
H	1.19126000	-1.83266200	5.70074600
H	1.51610500	-3.57798000	5.88309600
C	3.62361200	-1.06486500	4.77912400
H	4.46370500	-0.99786200	4.08020400
H	2.84529200	-0.35556500	4.46441800
H	3.97833700	-0.75966000	5.77250700
C	4.15667700	-3.51395200	5.13078300
H	3.72685400	-4.52425400	5.13633200
H	4.95786300	-3.46615100	4.38658800
H	4.59575400	-3.32807600	6.11947100
C	1.06971200	0.29726900	0.92365200
H	0.35069400	1.02249500	0.51172500
H	2.05742300	0.59174700	0.53292000

TS8a

M06 SCF energy (au)	-1522.043109
M06 enthalpy (au)	-1521.548127
M06 free energy (au)	-1521.640874
M06 SCF energy in solution (au)	-1522.456242
M06 enthalpy in solution (au)	-1521.961260
M06 free energy in solution (au)	-1522.054007

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.44612000	-1.71912300	2.31197600
C	-0.60544900	-4.62633900	1.25597700
O	-1.08095900	-3.70211100	1.96749000
O	0.51272700	-4.62394200	0.66458600
C	-1.43766300	-5.87771600	1.12968200
H	-2.50326600	-5.65048000	1.22589800
H	-1.23436700	-6.38062800	0.17960400
H	-1.16168600	-6.56679700	1.93880700
C	0.36330200	0.99084500	1.65437000
O	0.67533400	2.17011100	1.73221200
N	-0.01979700	0.18315000	2.69991900
C	-0.24207400	0.59951900	4.00093100
C	-0.87006900	-0.36151400	4.86098600
C	0.07090700	1.84251800	4.54091700
C	-1.13523900	-0.06064800	6.22377900
C	-0.20768600	2.12988700	5.88950900
H	0.52973100	2.58473500	3.89669600
C	-1.78289100	-2.49453000	5.08180600
C	-1.73548400	-1.07428600	7.00504400
C	-0.79078300	1.21106700	6.73054100
H	0.05725900	3.11511600	6.27115400
C	-2.06204300	-2.28478500	6.44542600
H	-1.93955100	-0.87244900	8.05711500
H	-0.99322400	1.44251200	7.77557400
H	-2.53395800	-3.07200200	7.02851200

N	-1.20234300	-1.57971800	4.33168900
H	-2.03252500	-3.43131800	4.58076100
C	0.46737200	-1.27874500	0.52926600
H	-0.00851700	-1.85693400	-0.27741900
C	1.93296400	-1.59518800	0.59972600
H	2.48706300	-0.83793000	1.17465700
C	2.70762900	-2.01379400	-0.66588100
H	2.03110500	-2.41550600	-1.43045400
H	3.36893300	-1.26705100	-1.11381000
C	3.36070100	-3.11111600	0.16752400
H	3.39002300	-4.13110600	-0.22851100
H	4.32999200	-2.82434300	0.58902500
N	2.29633100	-2.95406500	1.22311100
H	1.41080300	-3.70079600	1.03726500
C	2.75583000	-2.92398600	2.60475700
O	3.66026700	-2.20992700	2.95015800
O	2.05713900	-3.78238500	3.30815800
C	2.26546900	-3.92250800	4.76521200
C	1.17302400	-4.90187200	5.14741500
H	1.22588500	-5.11890300	6.22174100
H	0.18631000	-4.47683000	4.92138500
H	1.28240100	-5.84277600	4.59314900
C	2.06110600	-2.58548100	5.45298200
H	2.87077800	-1.88157400	5.23841300
H	1.11057100	-2.13787300	5.13635700
H	2.01721600	-2.74805200	6.53831300
C	3.64427400	-4.50551800	5.00968500
H	3.76422400	-5.45495000	4.47172400
H	4.43360900	-3.81309500	4.69878400
H	3.76480800	-4.70515300	6.08244100
C	0.29050700	0.22972900	0.33666000
H	-0.70561100	0.43236400	-0.08423200
H	1.01536100	0.67350800	-0.36709600

IM3a

M06 SCF energy (au)	-1871.994271
M06 enthalpy (au)	-1871.292784
M06 free energy (au)	-1871.397283
M06 SCF energy in solution (au)	-1872.497689
M06 enthalpy in solution (au)	-1871.796202
M06 free energy in solution (au)	-1871.900701

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.69089500	-1.81792900	2.24503300
C	-1.23964300	-4.62719600	1.34340800
O	-1.51089100	-3.45170400	1.08343300
O	-0.19327100	-4.97988700	2.05785000
C	0.79374600	0.61432000	2.78873000
O	1.24097500	1.60600600	3.35045500
N	-0.05140400	-0.30855800	3.35746000
C	-0.53233500	-0.26090100	4.65570300
C	-1.46439800	-1.29087000	5.01449300
C	-0.19615300	0.67048000	5.63487900
C	-2.00906800	-1.36149500	6.32495600
C	-0.74074200	0.58458600	6.92913800
H	0.49077700	1.46831000	5.37544800
C	-2.68177100	-3.15545900	4.34082700
C	-2.92441800	-2.40353700	6.59360900
C	-1.62585900	-0.40352900	7.28804800

H	-0.44347500	1.33339400	7.66219800
C	-3.26651900	-3.29905500	5.61158800
H	-3.35425600	-2.47862600	7.59279500
H	-2.04166100	-0.46088700	8.29313800
H	-3.97242300	-4.10518300	5.79549900
N	-1.81889300	-2.20139300	4.05630900
H	-2.93320500	-3.83854700	3.52636300
C	0.63885600	-1.08619300	0.85584000
H	0.04773100	-0.98655300	-0.06893000
C	1.75967100	-2.07013000	0.57810100
H	2.72156500	-1.53474800	0.47490000
C	1.59395200	-3.09569100	-0.55871400
H	0.53220400	-3.30467400	-0.74853200
H	2.09565100	-2.87344000	-1.50503400
C	2.24198700	-4.14104200	0.35881500
H	1.77338700	-5.12930200	0.44262300
H	3.32041700	-4.27627400	0.19137300
N	1.97789300	-3.23575800	1.49312400
H	0.41200900	-4.19169900	2.16598400
C	2.76189600	-3.26664800	2.63578600
O	3.18299400	-4.31205200	3.08853100
O	2.92735500	-2.03918100	3.12701400
C	3.55574000	-1.84635400	4.44074800
C	3.56831200	-0.33919000	4.60731300
H	4.09284100	-0.07761200	5.53563100
H	4.09036300	0.13958700	3.76814000
H	2.55574000	0.07826400	4.65080700
C	4.97740700	-2.38464600	4.42739200
H	5.00027800	-3.47181000	4.31531500
H	5.54698000	-1.92833300	3.60660200
H	5.47104500	-2.11410000	5.37038100
C	2.69150100	-2.50014200	5.50467200
H	1.66049000	-2.12316600	5.43649300
H	2.68493400	-3.59057000	5.40405800
H	3.08055100	-2.24372300	6.49915900
C	1.10118400	0.29225400	1.34062400
H	0.62269900	1.08878300	0.75019100
H	2.18498000	0.44208300	1.20663000
C	-2.05887600	-5.77839400	0.82531200
C	-2.29939800	-6.82977200	1.92459700
C	-3.40436200	-5.28679500	0.27908000
C	-1.25900300	-6.43796600	-0.32233500
H	-2.85006200	-6.37020200	2.76286000
H	-1.33731600	-7.17862300	2.32557800
C	-3.09688400	-8.00228400	1.34822800
H	-3.23381200	-4.52546200	-0.49596000
H	-3.97242700	-4.79159300	1.08356900
C	-4.19679700	-6.46533500	-0.28943900
H	-0.28606300	-6.78466300	0.05949800
H	-1.06016700	-5.68881600	-1.10742300
C	-2.05693800	-7.61171100	-0.89510600
H	-3.26622900	-8.74266300	2.14435600
C	-4.43986000	-7.49972000	0.81256600
C	-2.30046600	-8.64463500	0.20863500
H	-5.16003900	-6.09740600	-0.67299900
C	-3.40050300	-7.10795100	-1.42854800
H	-1.47872500	-8.06920100	-1.71192000
H	-5.03011900	-7.05196800	1.62842600
H	-5.02730100	-8.34340800	0.41702100
H	-1.34016200	-9.02953100	0.58717700

H	-2.85432800	-9.50517300	-0.19857200
H	-3.96949100	-7.94539200	-1.86232900
H	-3.23824500	-6.37650800	-2.23631400

TS3a

M06 SCF energy (au)	-1871.960522
M06 enthalpy (au)	-1871.264145
M06 free energy (au)	-1871.370137
M06 SCF energy in solution (au)	-1872.462765
M06 enthalpy in solution (au)	-1871.766388
M06 free energy in solution (au)	-1871.872380

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.60767800	-1.64705000	2.69252600
C	-0.97598900	-3.68850600	0.75788600
O	-0.76623100	-3.61014700	2.01142700
O	-1.06551100	-2.67281400	0.02005200
C	0.04747700	1.19761000	2.77376900
O	0.28628100	2.31487100	3.20887200
N	-0.46074300	0.15661000	3.51091900
C	-0.80065400	0.21756800	4.85517500
C	-1.23551300	-1.01846600	5.41609400
C	-0.77369300	1.32897000	5.68861800
C	-1.63389700	-1.12588400	6.77186100
C	-1.17138700	1.21688900	7.03513700
H	-0.44116500	2.27772900	5.28267200
C	-1.63753500	-3.29182700	5.03733900
C	-2.04500700	-2.39972100	7.22351900
C	-1.59526900	0.02892400	7.58342200
H	-1.13767700	2.11133700	7.65539700
C	-2.04853500	-3.47584900	6.36919000
H	-2.35807400	-2.51314300	8.26157800
H	-1.89832200	-0.04059300	8.62705300
H	-2.36090300	-4.46270000	6.70049000
N	-1.25077000	-2.11119100	4.59091700
H	-1.61640400	-4.10679500	4.31414500
C	0.41736100	-0.64833400	0.98177900
H	0.27203000	-0.71810500	-0.11235500
C	1.81213000	-1.22478300	1.17136800
H	1.76830700	-2.31989300	1.02823900
C	2.69797600	-0.81718600	2.37011900
H	2.32645600	0.05795500	2.91394300
H	2.91577800	-1.61247300	3.08976200
C	3.81257000	-0.46980900	1.36440700
H	4.23796300	0.53938200	1.42450900
H	4.63418800	-1.19877700	1.31679200
N	2.83799300	-0.64521800	0.28486300
H	-0.56718900	-1.61033500	0.76786600
C	3.04340800	-1.07859400	-0.99245300
O	2.18966600	-1.65417000	-1.64362600
O	4.28478200	-0.76158700	-1.39523300
C	4.71692500	-1.04625900	-2.75797000
C	6.13390700	-0.50070100	-2.78228500
H	6.58106300	-0.65639600	-3.77244100
H	6.13769600	0.57436400	-2.56271200
H	6.75694000	-1.00825300	-2.03490900
C	3.84319100	-0.30023200	-3.75257600
H	2.81721200	-0.67990200	-3.74528200
H	3.82810000	0.77156200	-3.51438300

H	4.25671300	-0.41847500	-4.76316100
C	4.72039800	-2.54571700	-3.00528400
H	5.32239300	-3.05462600	-2.24058400
H	3.70555100	-2.95357900	-2.98872600
H	5.16965000	-2.75436700	-3.98561900
C	0.24804600	0.83169400	1.31776200
H	-0.63115600	1.22361300	0.78393700
H	1.10559500	1.40658700	0.93602200
C	-1.00766800	-5.06214400	0.12533200
C	-1.50856100	-6.14085600	1.09348500
C	-1.86481400	-5.07313900	-1.14771000
C	0.45679400	-5.37834000	-0.25965800
H	-2.54483000	-5.91486200	1.39584700
H	-0.89728400	-6.13013200	2.00802300
C	-1.43796400	-7.51490600	0.42200100
H	-1.51106300	-4.29042300	-1.83292700
H	-2.90815100	-4.82545400	-0.89193600
C	-1.79202800	-6.44918500	-1.81265400
H	1.08161600	-5.35921100	0.64897600
H	0.83259800	-4.59186400	-0.93407100
C	0.52887200	-6.75313800	-0.92738000
H	-1.80491200	-8.27932500	1.12417500
C	-2.30278200	-7.51640800	-0.84142700
C	0.01502900	-7.81920000	0.04448200
H	-2.41506000	-6.44437600	-2.71997100
C	-0.33898600	-6.75382800	-2.18873100
H	1.57488800	-6.96722000	-1.19545600
H	-3.35477000	-7.31722000	-0.57983000
H	-2.27215900	-8.50941400	-1.31835600
H	0.64408600	-7.84157600	0.94918600
H	0.08304400	-8.81612600	-0.42005200
H	-0.27498600	-7.73394600	-2.68843600
H	0.03187600	-6.00148000	-2.90275300

IM4a

M06 SCF energy (au)	-1872.004654
M06 enthalpy (au)	-1871.301891
M06 free energy (au)	-1871.407249
M06 SCF energy in solution (au)	-1872.499528
M06 enthalpy in solution (au)	-1871.796765
M06 free energy in solution (au)	-1871.902123

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.66162500	-2.34187400	2.64801800
C	1.18123000	-4.13250400	1.03385300
O	0.86747900	-4.37411700	2.25015000
O	1.18860400	-2.91435000	0.66544500
C	0.97727700	0.63024200	2.02411800
O	0.89325700	1.83721300	2.21731200
N	0.50709800	-0.32231300	2.90496600
C	-0.03263500	0.02992100	4.14164900
C	-0.25524300	-1.06206600	5.02448600
C	-0.36815400	1.29407500	4.62022900
C	-0.77345500	-0.90255300	6.33457200
C	-0.89106300	1.45411600	5.91838200
H	-0.21482400	2.15590900	3.98415400
C	-0.09830600	-3.38616800	5.29393100
C	-0.93423500	-2.07023300	7.11189800
C	-1.09506300	0.39818900	6.77503600

H	-1.13900500	2.46308200	6.24478200
C	-0.59856000	-3.30267200	6.60331500
H	-1.33036200	-1.97688200	8.12305600
H	-1.49783100	0.54250600	7.77624100
H	-0.71611500	-4.21099700	7.18797000
N	0.06014400	-2.30292000	4.55351000
H	0.17466300	-4.33268500	4.82896800
C	2.53031800	1.12568200	0.11213000
H	3.16609100	1.59128400	0.87610000
C	3.40892900	0.56523900	-0.99336800
H	4.12090700	1.34162500	-1.31084400
C	2.70002100	-0.14529900	-2.17086000
H	1.60531600	-0.11876500	-2.13356500
H	3.02866800	0.19585900	-3.15747700
C	3.34133900	-1.46799500	-1.70889400
H	2.64144000	-2.17918900	-1.24356700
H	3.96770500	-1.99743600	-2.43943600
N	4.09479900	-0.71371100	-0.71327600
H	1.92252900	1.93863900	-0.31128400
C	4.60355100	-1.24182100	0.42934500
O	4.77665700	-2.43710900	0.59825700
O	4.88754100	-0.26475400	1.31025300
C	5.28227600	-0.58470500	2.67401300
C	5.34497400	0.78413200	3.32964900
H	5.65712800	0.68936300	4.37776200
H	6.06279700	1.42983200	2.80805600
H	4.35853200	1.26787900	3.30203800
C	6.64748900	-1.25114500	2.67492400
H	6.60772500	-2.22761600	2.18221600
H	7.37727100	-0.61881700	2.15225500
H	6.99217300	-1.38802600	3.70895000
C	4.22359800	-1.43880900	3.35603400
H	3.23844700	-0.95105300	3.29588600
H	4.15195400	-2.43489100	2.90578600
H	4.47796400	-1.55056600	4.41919700
C	1.63878000	0.08982000	0.77669500
H	2.21782700	-0.80648300	1.03091200
H	0.85067700	-0.27046900	0.09536300
C	1.58061700	-5.23720700	0.10172900
C	3.12509000	-5.32466900	0.13929900
C	0.99463000	-6.58463500	0.54702000
C	1.12887500	-4.93409800	-1.33551100
H	3.44808200	-5.53301600	1.17294600
H	3.56882100	-4.35656600	-0.13862600
C	3.59493600	-6.43555800	-0.80137100
H	-0.10634800	-6.52875800	0.55065400
H	1.30597500	-6.80027400	1.57956600
C	1.46949900	-7.69271300	-0.39661200
H	1.53315400	-3.96361400	-1.65672800
H	0.02993600	-4.85001600	-1.36863000
C	1.60718500	-6.04457800	-2.27275200
H	4.69354100	-6.48725000	-0.76833200
C	2.99816300	-7.77397900	-0.35832600
C	3.13607600	-6.12037100	-2.22796100
H	1.03884500	-8.65164400	-0.06990200
C	1.01355800	-7.38263200	-1.82492900
H	1.27697400	-5.81642400	-3.29775600
H	3.33856900	-8.02062800	0.66026900
H	3.34862900	-8.58255400	-1.02010500
H	3.57158100	-5.16364500	-2.55984800

H	3.49555700	-6.89763600	-2.92151600
H	1.33554000	-8.18622600	-2.50669800
H	-0.08693000	-7.34248400	-1.87143100

TS4a

M06 SCF energy (au)	-1293.028796
M06 enthalpy (au)	-1292.603981
M06 free energy (au)	-1292.685299
M06 SCF energy in solution (au)	-1293.369802
M06 enthalpy in solution (au)	-1292.944987
M06 free energy in solution (au)	-1293.026305

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.00320400	-1.73223600	1.99812700
C	0.82357000	1.02293200	2.31201900
O	1.02073300	2.16080500	2.70585600
N	-0.04880300	0.10806400	2.84849800
C	-0.74621200	0.23178500	4.02917200
C	-1.32096400	-0.98906400	4.52093400
C	-0.92959400	1.38982000	4.77468300
C	-2.07487500	-0.99459500	5.72546500
C	-1.67207900	1.36449000	5.96883300
H	-0.48195200	2.31047700	4.41430400
C	-1.63901300	-3.27882000	4.24027500
C	-2.62277300	-2.22617100	6.14640900
C	-2.24481400	0.20908600	6.44496300
H	-1.79673100	2.29463200	6.52173500
C	-2.41326000	-3.36516300	5.41072700
H	-3.21103600	-2.25261000	7.06412400
H	-2.82683100	0.19936400	7.36568300
H	-2.82419500	-4.32460900	5.71474500
N	-1.11413000	-2.14634700	3.80941000
H	-1.43710400	-4.16266800	3.63672000
C	0.89126400	-0.73149000	0.46855100
H	0.10210100	-0.43311000	-0.22916100
C	1.40131300	-2.05637000	0.23828400
H	0.60851400	-3.01093800	1.05493400
C	2.81930100	-2.60092600	0.43500200
H	3.57741900	-1.85101100	0.18035600
H	3.04578500	-3.04088100	1.40899400
C	2.51496500	-3.57142900	-0.72495500
H	3.22813500	-3.60850400	-1.55490200
H	2.27566600	-4.59515100	-0.40107600
N	1.31478300	-2.77788100	-1.00343400
C	0.16990100	-3.11042400	-1.68329700
O	-0.88908300	-2.54386300	-1.50861700
O	0.43209700	-4.10941700	-2.53358900
C	-0.60277600	-4.59909900	-3.44473100
C	0.12520400	-5.67613000	-4.22842900
H	-0.55399400	-6.13145600	-4.96020400
H	0.98243800	-5.25179400	-4.76607100
H	0.49149300	-6.46333300	-3.55737500
C	-1.05559600	-3.48025800	-4.36692700
H	-1.58228200	-2.69488600	-3.81653600
H	-0.19240500	-3.03819100	-4.88176400
H	-1.73267200	-3.88898500	-5.12865400
C	-1.75256800	-5.19795800	-2.65315800
H	-1.37901800	-5.96346400	-1.96014200
H	-2.28814300	-4.43316700	-2.08310700

H	-2.45728400	-5.68006200	-3.34381700
C	1.62649700	0.40553800	1.14914200
H	1.88585700	1.20376900	0.43979900
H	2.57371500	0.04893700	1.58533000

IM6a

M06 SCF energy (au)	-1293.053568
M06 enthalpy (au)	-1292.626758
M06 free energy (au)	-1292.707934
M06 SCF energy in solution (au)	-1293.393389
M06 enthalpy in solution (au)	-1292.966579
M06 free energy in solution (au)	-1293.047755

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.09033200	-1.95279300	1.97307700
C	0.42687700	0.99478700	2.13440500
O	0.47820000	2.16180800	2.49523400
N	-0.17765900	-0.04753400	2.77549200
C	-0.78784900	0.02530900	4.01048700
C	-1.22929200	-1.22947400	4.53842700
C	-1.00705800	1.16399600	4.77887700
C	-1.87582900	-1.30688000	5.80081500
C	-1.64511200	1.07479800	6.02900400
H	-0.67023300	2.11941800	4.39077800
C	-1.41091200	-3.54126200	4.23828900
C	-2.28817800	-2.58129200	6.24595700
C	-2.07902700	-0.12384500	6.54425400
H	-1.79805000	1.99105200	6.59762600
C	-2.06190000	-3.69319000	5.47352300
H	-2.78844400	-2.66377200	7.21112100
H	-2.57700100	-0.18254500	7.51107900
H	-2.37111500	-4.68417100	5.79555400
N	-1.00966400	-2.36217100	3.79022700
H	-1.20703400	-4.39521000	3.59645000
C	0.48898300	-0.71334900	0.25602300
H	-0.45386400	-0.56867500	-0.27533500
C	1.17582300	-1.87911800	-0.00577400
H	-0.04744300	-3.48690500	1.50864800
C	2.58997600	-2.37436600	0.22932900
H	3.34233500	-1.76301000	-0.28513800
H	2.88660800	-2.52423200	1.27095200
C	2.16727300	-3.63408800	-0.55786300
H	2.78218900	-3.93086200	-1.41299300
H	1.95434500	-4.50615200	0.07632300
N	0.93897900	-2.92306000	-0.92424700
C	-0.24164400	-3.54979300	-1.27896500
O	-0.28187100	-4.71423600	-1.60598800
O	-1.25026600	-2.68267000	-1.19739200
C	-2.63979700	-3.13177500	-1.29606500
C	-3.41578400	-1.85816600	-1.01360500
H	-4.49435800	-2.05426100	-1.06455400
H	-3.17713000	-1.47630700	-0.01157600
H	-3.16918300	-1.08280700	-1.75062300
C	-2.92456900	-4.17778900	-0.23165200
H	-2.37462400	-5.10520800	-0.42076800
H	-2.64346800	-3.79431500	0.75979500
H	-3.99961800	-4.40248000	-0.22554800
C	-2.91602300	-3.63951000	-2.70006000
H	-2.65782700	-2.87163600	-3.44103000

H	-2.34237600	-4.54651400	-2.91396400
H	-3.98571400	-3.86593200	-2.80263900
C	1.12930700	0.50594000	0.86795400
H	1.15859700	1.33094300	0.14335200
H	2.17455100	0.29029000	1.14255300

IM1b

M06 SCF energy (au)	-1561.351667
M06 enthalpy (au)	-1560.821499
M06 free energy (au)	-1560.925109
M06 SCF energy in solution (au)	-1561.781987
M06 enthalpy in solution (au)	-1561.251819
M06 free energy in solution (au)	-1561.355429

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.84081000	-2.52665900	2.20021500
C	-1.82043800	-4.76899100	0.66194200
O	-2.14809500	-3.94865400	-0.18859800
O	-1.21989200	-4.49832200	1.78504800
C	-2.03444100	-6.25314500	0.45358000
H	-2.72161900	-6.42600200	-0.37917700
H	-1.06767200	-6.72048900	0.22001600
H	-2.41125100	-6.73271900	1.36364500
C	-0.25136700	0.35614100	2.01106500
O	-0.06725900	1.52083700	2.32428900
N	-0.59057500	-0.65874500	2.86796100
C	-0.94132200	-0.47200900	4.20299300
C	-1.54308400	-1.60267500	4.82685700
C	-0.78935800	0.67925900	4.96383300
C	-1.98009800	-1.56728600	6.17423700
C	-1.22436000	0.70959000	6.30374800
H	-0.34064400	1.55379700	4.50672600
C	-2.23917600	-3.82448400	4.58112300
C	-2.56507100	-2.74360200	6.69370600
C	-1.80680500	-0.37617500	6.91286300
H	-1.08659900	1.63124200	6.86688600
C	-2.69539600	-3.86479800	5.91002000
H	-2.91017000	-2.74527400	7.72778800
H	-2.13436000	-0.33879800	7.95071600
H	-3.14157500	-4.77782600	6.29517000
N	-1.69211300	-2.73659900	4.07342500
H	-2.30068000	-4.67800100	3.90654300
C	-0.17118000	-1.57274100	0.29948900
H	-0.86657000	-1.98798300	-0.43395900
C	0.85625300	-2.38433800	0.73922900
H	1.63638900	-1.92511800	1.36061400
C	1.21017100	-3.71244000	0.14733400
H	1.36119100	-4.45275900	0.94713400
H	0.37965400	-4.06745900	-0.48067700
C	2.90160800	-4.93989000	-1.28359600
H	2.09738800	-5.34201300	-1.91559000
H	3.78532800	-4.80330100	-1.91865300
N	3.22422500	-5.94151900	-0.28872600
H	2.51811600	-6.57563300	0.05729500
C	4.43310100	-5.93402900	0.34271900
O	5.33553800	-5.16638400	0.07013400
O	4.45527900	-6.89829200	1.28220600
C	5.64279700	-7.10298600	2.10069800
C	5.23147700	-8.24960900	3.00774100

H	6.05456000	-8.50760100	3.68629700
H	4.35722700	-7.97190200	3.61024100
H	4.97624000	-9.13804200	2.41627800
C	5.93966200	-5.85822700	2.92081800
H	6.23848100	-5.02213500	2.28183900
H	5.05374600	-5.56585600	3.50055500
H	6.75285500	-6.07104700	3.62771400
C	6.81866800	-7.51173100	1.22904600
H	6.55285800	-8.38536100	0.61918000
H	7.12547400	-6.69671200	0.56715500
H	7.66899900	-7.78804700	1.86692200
C	-0.19886600	-0.08697200	0.55415800
H	-1.08508900	0.35514600	0.07850900
H	0.66687500	0.40318100	0.08657400
C	2.48635700	-3.60121900	-0.68545800
H	3.31753100	-3.22279600	-0.07081100
H	2.33769200	-2.87621600	-1.50071600

TS1b

M06 SCF energy (au)	-1561.333243
M06 enthalpy (au)	-1560.807956
M06 free energy (au)	-1560.901400
M06 SCF energy in solution (au)	-1561.761133
M06 enthalpy in solution (au)	-1561.235846
M06 free energy in solution (au)	-1561.329290

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.50485000	-2.13299000	1.41811700
C	-4.71238700	-2.63867000	2.31710800
O	-4.19970700	-1.65326300	1.75693500
O	-4.42913400	-3.86645500	2.06241200
C	-5.70299300	-2.43027100	3.44200000
H	-5.15868800	-2.50348800	4.39555400
H	-6.15908100	-1.43740000	3.38504300
H	-6.47159800	-3.21042200	3.44294200
C	0.41140600	0.07747800	2.08297000
O	1.11798200	0.83292300	2.72757100
N	-0.53164600	-0.78144200	2.58793800
C	-0.82975000	-0.86146400	3.94785800
C	-1.48656400	-2.05115300	4.34729900
C	-0.53640300	0.08924100	4.91504600
C	-1.80569600	-2.28510800	5.70840900
C	-0.88704600	-0.13282900	6.25984800
H	-0.01327600	0.99348400	4.62718800
C	-2.28586300	-4.14011100	3.72073900
C	-2.40673100	-3.52077200	6.03256800
C	-1.50577500	-1.29019200	6.66430100
H	-0.64890900	0.63814400	6.99066100
C	-2.63027700	-4.44883500	5.05017800
H	-2.67284300	-3.72353400	7.07010200
H	-1.76885100	-1.46081100	7.70735000
H	-3.07665700	-5.41586800	5.26521700
N	-1.76165000	-2.97875000	3.37352300
H	-2.42989900	-4.87358600	2.93853500
C	-0.88515000	-0.41400100	0.06679400
H	-1.68125600	0.31765900	0.24223700
C	-1.16269200	-1.45256800	-0.78370900
H	-0.34474500	-2.11751900	-1.08885400
C	-2.40067700	-1.46701100	-1.61967700

H	-3.18707400	-0.88104300	-1.11761600
H	-2.14794300	-0.92816600	-2.54873600
C	-3.47584600	-3.55056000	-0.75718100
H	-4.29203300	-2.95201000	-0.33546100
H	-3.88336700	-4.53067300	-1.04259300
N	-2.54423600	-3.77094900	0.37131400
H	-3.30971100	-3.91874000	1.22791800
C	-1.58285200	-4.76566400	0.10845500
O	-1.34562000	-5.21936400	-0.98920000
O	-0.95927000	-5.11583900	1.23955500
C	0.33646100	-5.79380300	1.20423100
C	0.74290300	-5.81297600	2.66695000
H	1.71974500	-6.30039100	2.77878500
H	0.81349200	-4.79059800	3.06213600
H	0.01003300	-6.36887900	3.26680300
C	1.31692000	-4.96059100	0.39521300
H	1.05667600	-4.94830900	-0.66850800
H	1.33485200	-3.92805000	0.77652000
H	2.32677400	-5.37845400	0.49921000
C	0.18263300	-7.20550500	0.66697400
H	-0.57479200	-7.75076300	1.24521000
H	-0.11150800	-7.20316900	-0.38631200
H	1.13698700	-7.73959800	0.76836600
C	0.46787500	-0.04130800	0.57410700
H	0.79446200	0.91964900	0.15585000
H	1.21597100	-0.79836000	0.29241800
C	-2.90953800	-2.85069500	-1.96987300
H	-2.11532000	-3.45266300	-2.42962100
H	-3.71516900	-2.76375500	-2.71221200

IM2b

M06 SCF energy (au)	-1332.376095
M06 enthalpy (au)	-1331.915912
M06 free energy (au)	-1331.998348
M06 SCF energy in solution (au)	-1332.727513
M06 enthalpy in solution (au)	-1332.267330
M06 free energy in solution (au)	-1332.349766

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.42672600	-2.26267700	2.36483000
C	-0.33229900	0.71490600	2.07133600
O	-0.55333300	1.90584100	2.22033400
N	-0.90046000	-0.31931300	2.76712200
C	-1.77931300	-0.13951000	3.83032700
C	-2.20202400	-1.34135600	4.46783700
C	-2.26530800	1.06079400	4.33469600
C	-3.07296900	-1.32480400	5.58711500
C	-3.13417300	1.07145000	5.44315400
H	-1.95947400	1.98779400	3.86389800
C	-2.08315700	-3.67439400	4.50601100
C	-3.42208100	-2.56947000	6.15498800
C	-3.53828600	-0.08227800	6.07047600
H	-3.48967000	2.03425100	5.80715100
C	-2.93337500	-3.73764200	5.62311500
H	-4.08631300	-2.58475000	7.01935200
H	-4.20870800	-0.06050000	6.92844000
H	-3.19091400	-4.70666400	6.04300700
N	-1.73598200	-2.52406200	3.96104200
H	-1.66910100	-4.56487700	4.03313900

C	0.44527500	-1.19913400	0.61084800
H	-0.31760600	-1.30564600	-0.16690400
C	1.28220100	-2.26660600	0.86282400
H	2.14112200	-2.07951800	1.51704100
C	1.35316000	-3.51097200	0.01643800
H	1.83121600	-3.22126100	-0.93336800
H	2.02852000	-4.23714100	0.49147600
C	-0.43189900	-4.97792100	0.97497800
H	-1.51241500	-5.18238600	0.91614600
H	0.08928500	-5.94554700	0.99167500
N	-0.12450000	-4.28436500	2.20867300
C	0.81946100	-4.83482700	3.01241400
O	1.29561100	-5.95852800	2.92681600
O	1.15802900	-3.94236400	3.98929000
C	1.90925100	-4.35146400	5.15669700
C	1.89986600	-3.09485100	6.01241600
H	2.43600900	-3.26655300	6.95502400
H	2.38252900	-2.26359800	5.48178600
H	0.86688700	-2.79782900	6.24306500
C	3.33101700	-4.72733000	4.77200400
H	3.34324500	-5.62557700	4.14793600
H	3.80062100	-3.90312200	4.21754300
H	3.92677200	-4.91124100	5.67671300
C	1.19496200	-5.48344600	5.87969400
H	0.16203700	-5.18790200	6.11594100
H	1.17584500	-6.39293200	5.27167100
H	1.70805300	-5.70066900	6.82630000
C	0.70520600	0.20097400	1.08471800
H	0.75053100	0.89493300	0.23576500
H	1.68267500	0.25083800	1.58980900
C	0.01250000	-4.18232400	-0.25349200
H	0.09264100	-4.85669500	-1.11697400
H	-0.74393100	-3.42943500	-0.52441300

TS2b

M06 SCF energy (au)	-1332.347059
M06 enthalpy (au)	-1331.888738
M06 free energy (au)	-1331.970874
M06 SCF energy in solution (au)	-1332.697506
M06 enthalpy in solution (au)	-1332.239185
M06 free energy in solution (au)	-1332.321321

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.60798900	-2.31825900	2.46295000
C	-0.14065200	0.49862200	2.45464200
O	-0.15151600	1.69352800	2.70047200
N	-1.02876800	-0.43514700	2.93649700
C	-1.94791600	-0.24919300	3.95075300
C	-2.44300100	-1.45611700	4.54527500
C	-2.41220800	0.96145700	4.44792100
C	-3.39521900	-1.41362100	5.59702700
C	-3.35384300	0.98934200	5.49351600
H	-2.02778800	1.88035600	4.01706200
C	-2.38046400	-3.78749600	4.60371500
C	-3.83059400	-2.64912600	6.12724500
C	-3.85042200	-0.16016900	6.06255100
H	-3.69780200	1.95817300	5.85306600
C	-3.33216300	-3.83174000	5.63884800
H	-4.56564400	-2.64453900	6.93253500

H	-4.58434100	-0.12523200	6.86659100
H	-3.65192500	-4.79178800	6.03590000
N	-1.95727400	-2.65246300	4.08151900
H	-1.94249000	-4.69996900	4.19366200
C	0.50872200	-1.46377700	0.95034800
H	-0.16874100	-1.31718100	0.09862800
C	1.29944800	-2.65314700	0.88059700
H	2.19781700	-2.67995300	1.50189800
C	1.27928600	-3.49905900	-0.36217000
H	1.46130200	-2.85624300	-1.23577700
H	2.08345700	-4.24762400	-0.31699400
C	-0.20747500	-4.97813200	0.84940100
H	-1.25497900	-5.24449600	1.05684800
H	0.37342300	-5.91112500	0.81428300
N	0.33357200	-4.12539000	1.89512800
C	1.02639600	-4.73918900	2.91175700
O	1.07860700	-5.94066700	3.10329000
O	1.64895100	-3.80519800	3.66206500
C	2.18828700	-4.12135000	4.97471100
C	2.61550900	-2.75774800	5.49033300
H	3.03577400	-2.84532600	6.50053900
H	3.37821800	-2.31845200	4.83400000
H	1.75499700	-2.07492100	5.52339100
C	3.38234700	-5.05222000	4.84814300
H	3.08050800	-6.03152300	4.46495100
H	4.12989100	-4.62024600	4.16945000
H	3.85323800	-5.18387100	5.83181600
C	1.09632800	-4.70071100	5.85890700
H	0.23498000	-4.01749000	5.88745900
H	0.76692200	-5.68098100	5.49885100
H	1.47420300	-4.81432500	6.88369100
C	0.95455100	-0.16391500	1.60588500
H	1.31484800	0.56994800	0.87073200
H	1.79532000	-0.36250800	2.29242500
C	-0.06610700	-4.21143200	-0.45935500
H	-0.10914500	-4.88235100	-1.32590800
H	-0.87792800	-3.47771400	-0.57315000

IM3b

M06 SCF energy (au)	-1911.306481
M06 enthalpy (au)	-1910.573552
M06 free energy (au)	-1910.679331
M06 SCF energy in solution (au)	-1911.819825
M06 enthalpy in solution (au)	-1911.086896
M06 free energy in solution (au)	-1911.192675

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.58169000	-1.71884400	2.84505200
C	-2.25822200	-4.47332400	1.61985000
O	-1.80975800	-3.85353300	2.58415300
O	-2.73938600	-3.84818400	0.55989800
C	-1.05593700	1.10407800	2.36560200
O	-0.73633400	2.27173500	2.53498400
N	-1.26962200	0.17477300	3.35549500
C	-1.20835300	0.42822800	4.71706400
C	-1.48746300	-0.68614700	5.57220000
C	-0.90996500	1.64509500	5.32212800
C	-1.44262900	-0.55598300	6.98615800
C	-0.88282700	1.76327900	6.72373400

H	-0.69657700	2.49878900	4.68885900
C	-2.01498600	-2.94935700	5.72945500
C	-1.69781900	-1.71569400	7.75183900
C	-1.13734000	0.69871700	7.55546400
H	-0.64442500	2.73576700	7.15254800
C	-1.98162700	-2.90879000	7.13511800
H	-1.66281200	-1.64355500	8.83928500
H	-1.10306700	0.79969100	8.63947600
H	-2.17944000	-3.81224800	7.70667300
N	-1.77749600	-1.88776100	4.98518300
H	-2.23233000	-3.87352300	5.19143000
C	-1.15989300	-1.00830800	0.93302200
H	-1.84564100	-1.39153800	0.15319500
C	0.26317100	-1.40504800	0.53231700
H	0.97336700	-0.92771300	1.22209400
C	0.58948500	-1.07089400	-0.93249600
H	0.14100500	-0.12833500	-1.26727100
H	1.67929400	-0.98327000	-1.05404600
C	0.45578600	-3.45435600	-0.79665700
H	-0.25801400	-4.28620700	-0.85483500
H	1.44919100	-3.86197100	-1.03814500
N	0.48027400	-2.86477500	0.54436500
H	-2.60792900	-2.88532900	0.72233300
C	1.04478800	-3.58830000	1.55154300
O	1.30132200	-4.78003900	1.44979800
O	1.27361000	-2.82823100	2.63455200
C	1.93867500	-3.36900100	3.81235500
C	1.89153500	-2.20603800	4.78926600
H	2.46785400	-2.44932300	5.69146600
H	2.31520200	-1.30098300	4.33518700
H	0.85626600	-1.98862100	5.08418800
C	3.37542100	-3.71817700	3.46155200
H	3.41412500	-4.51602500	2.71274200
H	3.89974700	-2.83515400	3.07278800
H	3.90315000	-4.05903300	4.36252700
C	1.18422100	-4.56083500	4.38058200
H	0.10859200	-4.33999700	4.42521700
H	1.33333200	-5.45951600	3.77468200
H	1.53998500	-4.75802300	5.40155700
C	-1.33835300	0.51019700	1.00103800
H	-2.38608300	0.76619700	0.77857300
H	-0.73367700	1.05668700	0.26041900
C	0.07776600	-2.28639300	-1.69850600
H	0.50950900	-2.38002500	-2.70127500
H	-1.01425500	-2.23319200	-1.81886800
C	-2.32009400	-5.97266400	1.55730300
C	-1.69973000	-6.58444900	2.81840600
C	-3.79310200	-6.41848100	1.43707900
C	-1.54027100	-6.47458200	0.32184400
H	-2.23050000	-6.21517000	3.71131600
H	-0.65484000	-6.25030000	2.90099200
C	-1.77613300	-8.11015600	2.74707000
H	-4.24492900	-5.97462900	0.53740700
H	-4.36310200	-6.04957800	2.30616500
C	-3.85886100	-7.94648800	1.37062700
H	-0.49134100	-6.14507700	0.40079100
H	-1.96912000	-6.03146600	-0.59058700
C	-1.61908300	-8.00142200	0.25550400
H	-1.33137500	-8.53316700	3.66031500
C	-3.24004900	-8.54457000	2.63679200

C	-1.00017300	-8.59890700	1.52127800
H	-4.91298500	-8.25247100	1.29037300
C	-3.08295600	-8.43574300	0.14452800
H	-1.06136900	-8.34500900	-0.62858700
H	-3.80193900	-8.21433400	3.52562400
H	-3.30763200	-9.64360900	2.60382800
H	0.05691600	-8.29970100	1.60031600
H	-1.02582700	-9.69920000	1.47117000
H	-3.14699100	-9.53324700	0.07413300
H	-3.53146800	-8.02730900	-0.77540300

TS3b

M06 SCF energy (au)	-1911.279436
M06 enthalpy (au)	-1910.552502
M06 free energy (au)	-1910.656183
M06 SCF energy in solution (au)	-1911.790164
M06 enthalpy in solution (au)	-1911.063230
M06 free energy in solution (au)	-1911.166911

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.28826300	-1.96418800	2.58045200
C	-1.26019400	-4.52440800	1.30188600
O	-1.27454200	-4.03755600	2.47555400
O	-1.31430800	-3.79804700	0.27281100
C	-1.10998900	0.88000500	1.93924900
O	-1.02382100	2.09361700	2.05764300
N	-1.28779700	-0.01058600	2.96401500
C	-1.49368000	0.32505200	4.29294500
C	-1.77112100	-0.78039200	5.14748500
C	-1.46957400	1.59175500	4.86363600
C	-2.00245000	-0.61439600	6.53562000
C	-1.71026000	1.75248400	6.24192700
H	-1.26564800	2.44667900	4.22846800
C	-2.02183900	-3.10103200	5.30200600
C	-2.24194700	-1.78342900	7.29194300
C	-1.96969000	0.68960900	7.07586700
H	-1.68311200	2.76072300	6.65260400
C	-2.25287200	-3.01692300	6.68634700
H	-2.41697100	-1.68913400	8.36381700
H	-2.14550700	0.83163700	8.14109600
H	-2.43588100	-3.92597100	7.25321300
N	-1.78879100	-2.02402300	4.57484000
H	-2.01090100	-4.05093900	4.76686600
C	-0.53363900	-1.24138800	0.56750300
H	-0.76860400	-1.59658400	-0.45334500
C	0.99908200	-1.29534900	0.69534100
H	1.31915800	-0.73508800	1.58312000
C	1.69945500	-0.80795500	-0.57953600
H	1.22175800	0.07110800	-1.02894800
H	2.73623900	-0.53504900	-0.33680200
C	1.87968000	-3.21120900	-0.52829900
H	1.26268400	-4.08099800	-0.78900200
H	2.92494100	-3.54780200	-0.48803200
N	1.50099400	-2.67062600	0.77886100
H	-1.12969800	-2.49648900	0.71946900
C	1.87905000	-3.34801100	1.89636800
O	2.32860000	-4.48277400	1.86221200
O	1.70195900	-2.60817900	3.00859600
C	2.17124100	-3.09213800	4.30072500

C	1.75349800	-1.98112400	5.24982900
H	2.14641300	-2.17846300	6.25576800
H	2.14024200	-1.01275400	4.90652700
H	0.65987800	-1.91116600	5.31212000
C	3.68557900	-3.22241100	4.27578400
H	4.00384400	-3.98320300	3.55616800
H	4.14835800	-2.26194700	4.01214200
H	4.04561100	-3.51201100	5.27227200
C	1.49214400	-4.39855900	4.68247000
H	0.41482700	-4.34088500	4.47488200
H	1.90369400	-5.24477100	4.12485500
H	1.63337900	-4.57901100	5.75751800
C	-1.10342000	0.18065300	0.59707500
H	-2.15160500	0.15188300	0.26085200
H	-0.57786500	0.83129000	-0.11723800
C	1.67508100	-2.03767600	-1.48680800
H	2.44217700	-2.00363100	-2.26842100
H	0.70470000	-2.12406000	-1.99548200
C	-1.20038600	-6.02983400	1.15294100
C	-0.73439200	-6.70948000	2.44672200
C	-2.61660300	-6.52668100	0.79778800
C	-0.23623200	-6.41213600	0.01693200
H	-1.40273000	-6.43181900	3.27734200
H	0.27159600	-6.33902600	2.70274900
C	-0.72166900	-8.22861100	2.26294600
H	-2.95741600	-6.02967900	-0.12395300
H	-3.31686100	-6.24350200	1.60179800
C	-2.59969300	-8.04641200	0.61741000
H	0.77402900	-6.04740500	0.26800400
H	-0.54952300	-5.91250900	-0.91212500
C	-0.22539100	-7.93120400	-0.16747600
H	-0.38921300	-8.70210000	3.19951500
C	-2.13325000	-8.71090600	1.91574300
C	0.23800700	-8.59877900	1.12946000
H	-3.61546800	-8.38976700	0.36766800
C	-1.63672500	-8.41287900	-0.51545300
H	0.46557500	-8.18858800	-0.98474400
H	-2.82883500	-8.46817700	2.73575600
H	-2.14139100	-9.80686500	1.80072400
H	1.25949000	-8.26986100	1.37791200
H	0.26977600	-9.69311900	1.00242300
H	-1.63669100	-9.50403700	-0.66978000
H	-1.97161900	-7.95349900	-1.45947200

IM4b

M06 SCF energy (au)	-1911.318373
M06 enthalpy (au)	-1910.584835
M06 free energy (au)	-1910.689604
M06 SCF energy in solution (au)	-1911.821873
M06 enthalpy in solution (au)	-1911.088335
M06 free energy in solution (au)	-1911.193104

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.34783900	-1.71851600	2.99227000
C	-0.75345800	-3.46159200	1.35354400
O	-0.94651000	-3.73670500	2.58799300
O	-0.96063500	-2.26120300	0.98804600
C	-1.52283600	1.21592800	2.18170300
O	-1.25696900	2.39980200	2.35312800

N	-1.59536000	0.29510700	3.21306800
C	-1.61862900	0.69455600	4.54535900
C	-1.63639800	-0.37091300	5.48796100
C	-1.66114100	1.98540100	5.06935900
C	-1.72365200	-0.16367000	6.88809100
C	-1.75034300	2.19313200	6.45901300
H	-1.61921000	2.83026200	4.39376100
C	-1.56111600	-2.69794600	5.76434900
C	-1.73498600	-1.31203200	7.71000500
C	-1.78584100	1.16097400	7.36776800
H	-1.78811000	3.22114600	6.81680600
C	-1.65581600	-2.56947900	7.15956200
H	-1.80389700	-1.18326800	8.79020100
H	-1.85069000	1.34304700	8.43923400
H	-1.66014600	-3.46278800	7.77823600
N	-1.55709300	-1.63443500	4.97984100
H	-1.48228500	-3.66411800	5.26720500
C	-1.49115000	1.61140600	-0.32072900
H	-1.79638300	2.64532100	-0.10691000
C	0.01157200	1.61251100	-0.59948800
H	0.53409400	2.07619800	0.24538400
C	0.33793100	2.28423300	-1.93341500
H	-0.29797400	3.15739700	-2.12770400
H	1.38467800	2.62039200	-1.93534900
C	0.66844200	-0.08097900	-2.22657000
H	0.09646200	-0.98813200	-2.46514300
H	1.72120900	-0.29197400	-2.46247100
N	0.55383300	0.25845600	-0.80716800
H	-2.02471100	1.29525400	-1.23110600
C	1.31563100	-0.43576200	0.08127700
O	1.97815300	-1.41581700	-0.22515700
O	1.24543600	0.10500100	1.31586300
C	2.30305000	-0.13261500	2.28905200
C	1.91592000	0.77606700	3.44310600
H	2.68544400	0.73748000	4.22530100
H	1.80872600	1.81414300	3.10273800
H	0.95772400	0.46208700	3.87662500
C	3.63737400	0.29957800	1.70090400
H	3.92134200	-0.32993700	0.85101800
H	3.58551400	1.34633800	1.37105200
H	4.42071500	0.22245100	2.46661100
C	2.33138100	-1.58239300	2.74408300
H	1.32710300	-1.90463400	3.06102300
H	2.68059400	-2.24709900	1.94896500
H	3.00503600	-1.67732500	3.60753400
C	-1.90770800	0.69800600	0.81585200
H	-1.51988100	-0.30789600	0.63892200
H	-3.00524200	0.59265900	0.83186100
C	0.14627000	1.15979000	-2.95123000
H	0.67685700	1.33884600	-3.89330900
H	-0.91777100	1.04391000	-3.19828700
C	-0.23495700	-4.48998500	0.39551100
C	-0.92377600	-5.84616700	0.61155100
C	-0.42318100	-4.03171200	-1.05660800
C	1.27946700	-4.64241100	0.67300700
H	-2.00777300	-5.74464600	0.43635900
H	-0.79426100	-6.16526500	1.65648000
C	-0.32722900	-6.88123500	-0.34611500
H	0.07091500	-3.05821400	-1.19150600
H	-1.49611300	-3.88745000	-1.26444800

C	0.17050800	-5.07419100	-2.00598800
H	1.42975100	-4.94033100	1.72354300
H	1.76534000	-3.66631600	0.52013800
C	1.87047100	-5.68549100	-0.27681500
H	-0.83167900	-7.84738100	-0.19085000
C	-0.52842100	-6.41973900	-1.79254000
C	1.17086100	-7.03051200	-0.06522700
H	0.02253100	-4.74067900	-3.04461900
C	1.66813700	-5.22068100	-1.72156700
H	2.94633100	-5.78846000	-0.06781100
H	-1.60434400	-6.32639000	-2.01335400
H	-0.12140400	-7.17258000	-2.48690500
H	1.32876800	-7.38124000	0.96765700
H	1.60449600	-7.79146300	-0.73419300
H	2.11658200	-5.94721900	-2.41863400
H	2.17588900	-4.25577600	-1.87841600

TS4b

M06 SCF energy (au)	-1332.335192
M06 enthalpy (au)	-1331.879746
M06 free energy (au)	-1331.962282
M06 SCF energy in solution (au)	-1332.686935
M06 enthalpy in solution (au)	-1332.231489
M06 free energy in solution (au)	-1332.314025

Cartesian coordinates

ATOM	X	Y	Z
Pd	-2.68753000	-1.36427100	0.47447700
C	-1.73214600	0.55903000	-1.47857100
O	-1.57768400	1.27100900	-2.45781300
N	-2.86644800	-0.13866800	-1.14221100
C	-3.98428000	-0.30684800	-1.92666200
C	-4.87919500	-1.34332400	-1.49227500
C	-4.31501200	0.40402600	-3.07483500
C	-6.07606000	-1.60771000	-2.21133700
C	-5.50031900	0.12433100	-3.77748000
H	-3.63154600	1.17451600	-3.41673500
C	-5.35293500	-3.03679400	0.03477300
C	-6.91558200	-2.63450600	-1.72711400
C	-6.37701700	-0.85138200	-3.36563300
H	-5.72394400	0.70727900	-4.67010200
C	-6.56371500	-3.34761300	-0.60929500
H	-7.84253400	-2.84926700	-2.25975900
H	-7.29754700	-1.05784100	-3.91032000
H	-7.19200000	-4.14453500	-0.21914600
N	-4.54445300	-2.07925900	-0.38119100
H	-5.02959700	-3.59004300	0.91536800
C	-1.10922100	-0.15110100	0.87238900
H	-1.53331200	0.66666900	1.46836200
C	-0.77753200	-1.31488600	1.66646700
H	-1.98338300	-2.21721700	1.74590800
C	-0.60743500	-1.13855100	3.17578500
H	-1.08020500	-1.96697300	3.72099700
H	-1.05504800	-0.20246000	3.52647900
C	1.26677500	-2.35900600	2.39056500
H	1.14621700	-3.34102700	2.87433200
H	2.28863100	-2.30212600	2.00142900
N	0.29983100	-2.20245800	1.29646700
C	0.30743000	-2.98457500	0.16866700
O	-0.51314400	-2.91233200	-0.72527800

O	1.35137900	-3.82646300	0.21444900
C	1.61324200	-4.74534000	-0.89291200
C	2.86688600	-5.46812600	-0.43221200
H	3.17357700	-6.20429500	-1.18591100
H	2.68605500	-5.99386800	0.51388100
H	3.69132100	-4.75923800	-0.28372800
C	0.46136200	-5.72387600	-1.04533000
H	-0.44974100	-5.22214700	-1.38360600
H	0.25957900	-6.22482800	-0.08913800
H	0.73369500	-6.49288300	-1.78055600
C	1.88714900	-3.96830700	-2.16914600
H	2.68398700	-3.23125200	-2.00277300
H	0.99261600	-3.45079500	-2.52717100
H	2.22581900	-4.66215700	-2.95000500
C	-0.58997800	0.28647300	-0.47856800
H	0.02552900	1.19323900	-0.39863700
H	0.03564800	-0.49431900	-0.93083200
C	0.90621200	-1.21833600	3.33071700
H	1.37328900	-0.28418000	2.98719400
H	1.22880900	-1.40360000	4.36094400

IM1c

M06 SCF energy (au)	-1600.631807
M06 enthalpy (au)	-1600.071959
M06 free energy (au)	-1600.178806
M06 SCF energy in solution (au)	-1601.073935
M06 enthalpy in solution (au)	-1600.514087
M06 free energy in solution (au)	-1600.620934

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.24819000	-2.65633800	2.43271300
C	-2.11023500	-5.26045200	1.52808500
O	-2.63200900	-4.67831700	0.58303300
O	-1.41944900	-4.69679600	2.47729700
C	-2.16746600	-6.76718400	1.65904900
H	-2.92795000	-7.17850600	0.98959600
H	-1.18841200	-7.18283500	1.38463600
H	-2.36719800	-7.06955300	2.69294400
C	-1.05439900	0.16585100	1.59386300
O	-0.99098200	1.38346100	1.64072800
N	-1.16725400	-0.67194800	2.67298900
C	-1.39406400	-0.23996900	3.97770000
C	-1.77363500	-1.26604200	4.89041000
C	-1.31190200	1.05756700	4.46483800
C	-2.06337400	-0.98677300	6.24901400
C	-1.60043800	1.33063000	5.81676400
H	-1.03204300	1.85499100	3.78603100
C	-2.19797100	-3.54866600	5.19209300
C	-2.43088200	-2.07767600	7.06791800
C	-1.96784600	0.34694100	6.70359600
H	-1.52377800	2.36127900	6.15948800
C	-2.49826400	-3.34884800	6.55076700
H	-2.65896100	-1.89200300	8.11766600
H	-2.18361700	0.57252200	7.74688100
H	-2.77735600	-4.19878400	7.16781200
N	-1.85538400	-2.54481900	4.40761400
H	-2.22073200	-4.52907400	4.71668400
C	-0.92089600	-2.06716400	0.30916700
H	-1.63823000	-2.69341400	-0.22682100

C	0.23969400	-2.66622900	0.75893700
H	1.02363900	-2.01288700	1.16412700
C	0.68770300	-4.04139100	0.37236700
H	1.07138900	-4.58602800	1.24845800
H	-0.16745100	-4.61046500	-0.01967400
C	3.36309000	-5.24264000	-2.20003200
H	4.22616800	-4.69254200	-1.80529400
H	3.70780300	-6.25354100	-2.45771200
N	2.96519400	-4.56078800	-3.41375500
H	2.26816200	-4.97917800	-4.01555700
C	3.20762100	-3.22924500	-3.59431200
O	3.91391600	-2.55373000	-2.87136500
O	2.55088600	-2.80447700	-4.69088000
C	2.57341900	-1.39567100	-5.06081400
C	1.70226000	-1.36073200	-6.30436100
H	1.63426000	-0.33496700	-6.68854100
H	2.12508500	-1.99954200	-7.09009400
H	0.68877900	-1.71556400	-6.07780700
C	3.98932700	-0.95484200	-5.39308400
H	4.63092500	-0.97413600	-4.50757800
H	4.42014400	-1.61339000	-6.15891000
H	3.96927400	0.06704800	-5.79532600
C	1.95167700	-0.55787600	-3.95452900
H	0.94687500	-0.93354700	-3.71550600
H	2.56494800	-0.57619100	-3.04833500
H	1.85292300	0.48258600	-4.29165400
C	-1.09688300	-0.57072100	0.26073500
H	-2.07167800	-0.32432600	-0.18209700
H	-0.34448900	-0.11419400	-0.39846400
C	1.77854800	-3.94139200	-0.69433700
H	2.63326500	-3.35708600	-0.31705600
H	1.38573000	-3.37694000	-1.55578100
C	2.25695300	-5.31034300	-1.15387800
H	2.62667100	-5.88446500	-0.28880600
H	1.40168000	-5.88040500	-1.55545100

TS5c

M06 SCF energy (au)	-1600.615656
M06 enthalpy (au)	-1600.057035
M06 free energy (au)	-1600.151291
M06 SCF energy in solution (au)	-1601.050787
M06 enthalpy in solution (au)	-1600.492166
M06 free energy in solution (au)	-1600.586422

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.14741000	-1.85164000	2.61916300
C	-1.01520400	-4.76184900	2.07215500
O	-1.77078400	-3.73044600	1.95581200
O	0.17642800	-4.75651000	2.42016300
C	-1.67819700	-6.06361700	1.67692000
H	-2.71755400	-6.10055800	2.02027600
H	-1.69935900	-6.12694200	0.57904700
H	-1.11386700	-6.91821700	2.06139000
C	-0.39892200	0.96960700	2.46104300
O	-0.20638800	2.13971400	2.76820600
N	-0.79855700	-0.02309300	3.31646200
C	-1.00863700	0.13978200	4.67872700
C	-1.42854600	-1.03832800	5.37138200
C	-0.81507600	1.29518700	5.42838000

C	-1.63015400	-1.03851200	6.77487500
C	-1.01738900	1.28440200	6.82169100
H	-0.50000600	2.19901700	4.91915200
C	-1.98680300	-3.29817100	5.21834500
C	-2.03570900	-2.25394900	7.37102100
C	-1.41318100	0.15501300	7.49794800
H	-0.84991100	2.20915800	7.37210700
C	-2.21643800	-3.37758700	6.60386400
H	-2.20022000	-2.28112100	8.44842500
H	-1.56562500	0.16067600	8.57638800
H	-2.52836900	-4.32196200	7.04241100
N	-1.60772100	-2.17892000	4.63502600
H	-2.11786700	-4.15968400	4.56492900
C	-0.61870100	-0.95140800	0.76088500
H	-1.67121700	-1.02812500	0.43935900
C	0.20278100	-1.75673800	-0.07584300
H	1.08819100	-1.28858300	-0.52442800
C	-0.41862800	-2.86423400	-0.86709600
H	-1.10713000	-3.42526000	-0.21636400
H	-1.06225000	-2.35416200	-1.60484100
C	2.38499200	-3.66322500	0.09939400
H	3.12676700	-4.24835500	0.66383300
H	2.93993500	-2.99103000	-0.56904800
N	1.62546900	-2.81941500	1.04140400
H	1.07593200	-3.39239600	1.71563400
C	2.43615100	-1.85191000	1.68339100
O	3.25964200	-1.20296900	1.07647900
O	2.13813800	-1.78497700	2.97103700
C	2.95637200	-0.98176200	3.89951100
C	2.30469700	-1.25713000	5.24152100
H	2.87645500	-0.76345700	6.03783800
H	1.27870200	-0.86913500	5.26374600
H	2.27618200	-2.33551800	5.44346500
C	2.89295700	0.49440000	3.55470700
H	3.34557200	0.70213800	2.58012800
H	1.86135800	0.86909500	3.56108700
H	3.44959700	1.05488300	4.31817300
C	4.37936600	-1.51489200	3.87755600
H	4.38779200	-2.59301600	4.08626500
H	4.86598800	-1.33078600	2.91444400
H	4.96316800	-1.01328100	4.66021600
C	-0.14074100	0.46325600	1.05457500
H	-0.56898500	1.19850700	0.35650500
H	0.95156700	0.53190400	0.91185600
C	0.53732800	-3.79125000	-1.60495000
H	1.14653000	-3.20336000	-2.31226100
H	-0.05472800	-4.48789500	-2.21446600
C	1.46075000	-4.57146500	-0.68284900
H	0.88165100	-5.18667800	0.02362500
H	2.07819900	-5.26335000	-1.27208300

IM5c

M06 SCF energy (au)	-1600.635164
M06 enthalpy (au)	-1600.074295
M06 free energy (au)	-1600.168950
M06 SCF energy in solution (au)	-1601.070507
M06 enthalpy in solution (au)	-1600.509638
M06 free energy in solution (au)	-1600.604293

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.13915800	-1.83785800	2.64204500
C	-0.82151400	-4.74931500	2.13966700
O	-1.66824200	-3.80164800	2.06563100
O	0.42123600	-4.61795800	2.21374400
C	-1.39298400	-6.14657000	2.05605500
H	-2.41866100	-6.18470300	2.43654400
H	-1.41771100	-6.45089600	0.99987800
H	-0.75457700	-6.85618800	2.59141100
C	-0.30528900	0.95569900	2.50651500
O	-0.06563400	2.12040900	2.80802300
N	-0.78049100	-0.01153300	3.35142600
C	-1.03048100	0.16880400	4.70386200
C	-1.52599500	-0.98270500	5.40045800
C	-0.81970500	1.32777700	5.44537800
C	-1.79381500	-0.93916000	6.79380700
C	-1.08606400	1.35571100	6.82711400
H	-0.45061100	2.20944700	4.93338200
C	-2.17830000	-3.21485900	5.27368200
C	-2.28208000	-2.12062700	7.39735400
C	-1.56287400	0.25894300	7.50455500
H	-0.90650700	2.28486500	7.36664300
C	-2.47820800	-3.25350300	6.64825800
H	-2.49907400	-2.11229300	8.46594700
H	-1.76877600	0.29366800	8.57373000
H	-2.85528700	-4.17125400	7.09286300
N	-1.72106400	-2.13064300	4.68223300
H	-2.31652000	-4.08577000	4.63158600
C	-0.52918400	-1.00565800	0.84547900
H	-1.48860200	-0.93904600	0.30927400
C	0.38542000	-1.83935100	-0.03291300
H	1.00308400	-1.20681600	-0.69837100
C	-0.38401800	-2.85564300	-0.86647700
H	-1.03080800	-3.44230500	-0.19591000
H	-1.05846200	-2.27694700	-1.51267200
C	2.32688000	-3.48544900	-0.03699000
H	3.01511000	-3.97745700	0.66269800
H	2.90556900	-2.82473200	-0.69480800
N	1.44752400	-2.59253000	0.79901500
H	0.94452800	-3.22576100	1.49991900
C	2.34712700	-1.67082300	1.54163200
O	3.13552000	-0.98658100	0.94656900
O	2.13649300	-1.82029300	2.81541200
C	2.96937900	-1.12819300	3.83835800
C	2.28949600	-1.53356100	5.13046300
H	2.86520800	-1.15011700	5.98242000
H	1.27453400	-1.11793300	5.18100500
H	2.22415100	-2.62612700	5.20878100
C	2.93352500	0.37409600	3.64343700
H	3.41101000	0.68114600	2.70761200
H	1.90871600	0.76553800	3.66899800
H	3.48236200	0.83683600	4.47454200
C	4.37268300	-1.69610700	3.74044200
H	4.35549800	-2.78897500	3.84402500
H	4.85058000	-1.42937300	2.79098000
H	4.98343600	-1.28685400	4.55525400
C	-0.00917900	0.41228100	1.12148300
H	-0.38841800	1.14167100	0.38879100
H	1.08727900	0.47355600	1.02066800
C	0.50218600	-3.76412100	-1.70467400

H	1.04308700	-3.16568100	-2.45703000
H	-0.11223000	-4.48560800	-2.25881200
C	1.50456900	-4.48544600	-0.81825600
H	0.99172400	-5.15360600	-0.11096500
H	2.19339100	-5.10239500	-1.41065600

TS8c

M06 SCF energy (au)	-1600.631235
M06 enthalpy (au)	-1600.075339
M06 free energy (au)	-1600.170256
M06 SCF energy in solution (au)	-1601.065265
M06 enthalpy in solution (au)	-1600.509369
M06 free energy in solution (au)	-1600.604286

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.02892400	-1.77151900	2.70049700
C	-0.61288600	-4.73515900	2.17952600
O	-1.45647200	-3.80632100	2.23101400
O	0.61263500	-4.60772100	1.86969600
C	-1.07688300	-6.12429900	2.52877500
H	-2.16629500	-6.19895000	2.46817500
H	-0.60196700	-6.86661000	1.87947100
H	-0.76753700	-6.34794500	3.55848100
C	-0.31779500	1.05127800	2.47797100
O	-0.15153000	2.23582900	2.73854800
N	-0.78382700	0.09502100	3.34764800
C	-1.09993500	0.31968100	4.67925600
C	-1.55847000	-0.82366300	5.41241800
C	-0.99431300	1.52464300	5.36776200
C	-1.90072900	-0.72560900	6.78745500
C	-1.33345800	1.60656700	6.73096400
H	-0.65194600	2.39995700	4.82736600
C	-2.08058400	-3.09288800	5.37358500
C	-2.34959800	-1.90217000	7.42911500
C	-1.78023600	0.51881600	7.44291900
H	-1.23765000	2.57161700	7.22712800
C	-2.44459800	-3.08116300	6.73291000
H	-2.62043400	-1.85280900	8.48424500
H	-2.04400900	0.59524800	8.49708500
H	-2.79248100	-3.99549200	7.20750800
N	-1.65464600	-2.01516900	4.74716900
H	-2.14242600	-4.00043100	4.77087700
C	-0.47119800	-0.95983800	0.88710300
H	-1.45862000	-0.88010700	0.40422700
C	0.39936100	-1.77973500	-0.05296100
H	0.97596900	-1.10329700	-0.71549900
C	-0.41666600	-2.73190800	-0.91839300
H	-0.99030300	-3.40559500	-0.26248400
H	-1.15655900	-2.12357600	-1.45652800
C	2.34734100	-3.32388400	-0.31398200
H	3.09964700	-3.86370300	0.27730000
H	2.86617200	-2.56889800	-0.92177300
N	1.47074700	-2.60044500	0.66331200
H	0.95917600	-3.48635100	1.34978200
C	2.34859800	-1.77145000	1.49849300
O	3.12593700	-0.98798300	1.01658600
O	2.16014500	-2.08570700	2.75453600
C	2.94470800	-1.46250000	3.84463800
C	2.32848900	-2.09542300	5.07712200

H	2.82974900	-1.71912200	5.97785800
H	1.25993900	-1.84876400	5.13892800
H	2.43166300	-3.18760700	5.04553000
C	2.75277400	0.04140800	3.85143300
H	3.16028600	0.51340300	2.95169600
H	1.69060600	0.29951900	3.94689000
H	3.27892800	0.45468500	4.72214000
C	4.39832200	-1.86535500	3.67930900
H	4.49152500	-2.95791000	3.62124300
H	4.84078200	-1.41760500	2.78302800
H	4.96795300	-1.52207700	4.55258600
C	0.06411600	0.45464300	1.13913200
H	-0.24321500	1.16078300	0.35142300
H	1.16548500	0.47789500	1.11613500
C	0.43539000	-3.51810100	-1.90360800
H	0.89010000	-2.82113900	-2.62749900
H	-0.18825800	-4.21121200	-2.48356000
C	1.53504300	-4.27136700	-1.17213900
H	1.10319900	-5.05500000	-0.53336700
H	2.21542800	-4.76699600	-1.87776600

IM3c

M06 SCF energy (au)	-1950.589407
M06 enthalpy (au)	-1949.826320
M06 free energy (au)	-1949.933556
M06 SCF energy in solution (au)	-1951.114099
M06 enthalpy in solution (au)	-1950.351012
M06 free energy in solution (au)	-1950.458248

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.19757400	-3.89618400	2.01312800
C	-1.71319700	-5.35105800	-0.13823300
O	-0.62442800	-5.28006000	0.43270000
O	-2.72783000	-4.57718300	0.20884500
C	0.03548000	-1.32912200	3.35242500
O	0.38486200	-0.43880800	4.11338200
N	0.29634200	-2.67225400	3.50175500
C	0.95327300	-3.25688100	4.57058600
C	1.05747500	-4.68657600	4.53438200
C	1.50764300	-2.59570000	5.66178700
C	1.72506300	-5.39603800	5.56905200
C	2.15421100	-3.31320500	6.68433000
H	1.43117500	-1.51470100	5.70323700
C	0.60029500	-6.66029500	3.38657400
C	1.81033900	-6.80062000	5.44161200
C	2.27473900	-4.68241200	6.65568900
H	2.57528600	-2.75352000	7.51851000
C	1.25457300	-7.43696400	4.35974200
H	2.32522200	-7.36655100	6.21853600
H	2.78724900	-5.22705100	7.44762500
H	1.30906500	-8.51658600	4.24370900
N	0.50932200	-5.34772200	3.46810400
H	0.14298400	-7.12148900	2.50916000
C	-0.49838300	-2.10791200	1.00810100
H	-1.34228600	-2.16359200	0.30215900
C	0.79933000	-1.83024900	0.23155000
H	1.65465800	-2.06910300	0.87347400
C	0.98293600	-0.37837000	-0.23423200
H	0.92482200	0.29863800	0.62756700

H	2.00743000	-0.28871700	-0.63015000
C	0.01675000	-2.38595000	-2.07613100
H	-1.03829800	-2.58334600	-1.80666300
H	0.27576200	-3.06855700	-2.89068300
N	0.88912500	-2.70441500	-0.95301900
H	-2.40127600	-4.00140200	0.94417700
C	1.59876700	-3.87377300	-0.99678600
O	1.57406900	-4.65579000	-1.93651900
O	2.33462500	-4.03330400	0.11680900
C	3.27953700	-5.12891500	0.26269300
C	3.79348100	-4.93118200	1.67986000
H	4.56446500	-5.67773400	1.91114600
H	4.22954300	-3.93076400	1.79623200
H	2.97474200	-5.03439300	2.40639500
C	4.40232900	-4.96264500	-0.74761700
H	4.02372000	-5.05414700	-1.77111700
H	4.88097900	-3.98151700	-0.62962000
H	5.16463100	-5.73673800	-0.58589200
C	2.59911600	-6.48268900	0.13469300
H	1.68783600	-6.50980700	0.74700200
H	2.32869700	-6.70006200	-0.90263200
H	3.28416200	-7.26305300	0.49479100
C	-0.81229900	-1.10169500	2.11352900
H	-1.85788400	-1.24076700	2.43260600
H	-0.72835800	-0.04855200	1.80760900
C	-0.00117600	0.01127700	-1.32675800
H	0.16196600	1.05195000	-1.63861000
H	-1.03498500	-0.04268900	-0.94553700
C	0.16629300	-0.93494000	-2.50777400
H	-0.56239700	-0.71926900	-3.30181700
H	1.16947000	-0.79636000	-2.94180800
C	-1.96650300	-6.28454200	-1.28501200
C	-0.85949800	-7.34527300	-1.35169100
C	-3.34283400	-6.96194600	-1.17137400
C	-1.91810900	-5.44692000	-2.58573000
H	-0.84550300	-7.92729600	-0.41440800
H	0.11361400	-6.84064600	-1.43664400
C	-1.09468200	-8.26285100	-2.55202500
H	-4.13433500	-6.19995500	-1.12185700
H	-3.39442700	-7.54407600	-0.23634700
C	-3.56044400	-7.87784200	-2.37876500
H	-0.92997000	-4.96567300	-2.65854300
H	-2.68457500	-4.65603500	-2.54739500
C	-2.15096400	-6.36449800	-3.78835700
H	-0.30140700	-9.02473900	-2.57966700
C	-2.46064800	-8.94172200	-2.42434600
C	-1.05065200	-7.42760300	-3.83461800
H	-4.54402000	-8.36226000	-2.28425200
C	-3.51736500	-7.04294200	-3.66180300
H	-2.12009100	-5.75681300	-4.70524800
H	-2.49356300	-9.55941300	-1.51207600
H	-2.62855100	-9.61879000	-3.27701800
H	-0.06548500	-6.94523900	-3.93523600
H	-1.19081700	-8.07595500	-4.71422800
H	-3.69936500	-7.68801400	-4.53601800
H	-4.31806800	-6.28597200	-3.64790400

TS3c

M06 SCF energy (au)	-1950.564045
M06 enthalpy (au)	-1949.806268

M06 free energy (au)	-1949.910024
M06 SCF energy in solution (au)	-1951.085250
M06 enthalpy in solution (au)	-1950.327473
M06 free energy in solution (au)	-1950.431229

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.23427300	-3.66543400	1.98700400
C	-1.48041400	-4.80200000	-0.31416200
O	-0.77695200	-5.18071400	0.67272700
O	-1.83113100	-3.59842100	-0.46674800
C	0.28559000	-1.03877100	3.15713200
O	0.72304700	-0.15799100	3.88331300
N	0.39393500	-2.38695000	3.38155000
C	0.93830100	-2.97824800	4.50962900
C	0.84694400	-4.40024000	4.53705600
C	1.53637300	-2.34802300	5.59389700
C	1.35367700	-5.16112000	5.62003200
C	2.03202300	-3.10872700	6.67043500
H	1.61084100	-1.26605400	5.59235000
C	0.14433000	-6.32609400	3.40961000
C	1.22697300	-6.56572200	5.53419600
C	1.95494400	-4.48194900	6.70209200
H	2.49501500	-2.57938700	7.50190800
C	0.62825700	-7.14772000	4.44271500
H	1.61251900	-7.17875100	6.34905700
H	2.35018000	-5.05478200	7.53960900
H	0.52166200	-8.22625600	4.36155200
N	0.25708900	-5.01167900	3.46280200
H	-0.33199900	-6.73003300	2.51576600
C	-0.27578500	-1.76348800	0.76054200
H	-0.94489600	-1.41673700	-0.04726400
C	1.15463300	-1.77792900	0.18344600
H	1.84622800	-2.14955400	0.94540700
C	1.65904600	-0.39758100	-0.25696700
H	1.58589800	0.31114100	0.57921000
H	2.73254600	-0.50174300	-0.48146200
C	0.59488900	-2.26848800	-2.20276400
H	-0.50026500	-2.25812900	-2.07212900
H	0.81906600	-3.02766200	-2.95767200
N	1.23500000	-2.69657300	-0.96067800
H	-1.08698900	-2.86909800	0.42764800
C	1.81887000	-3.93399200	-0.91798600
O	1.79788600	-4.73183900	-1.84175500
O	2.42440200	-4.14902500	0.26509400
C	3.20496600	-5.35544900	0.50054500
C	3.61972700	-5.20051300	1.95477500
H	4.27640900	-6.02874600	2.25121600
H	4.15905300	-4.25631100	2.10448100
H	2.73899200	-5.20009100	2.61150100
C	4.42574200	-5.35229100	-0.40455300
H	4.13314400	-5.41432600	-1.45764900
H	5.01561200	-4.43914300	-0.24938100
H	5.06293400	-6.21503100	-0.16746100
C	2.36572500	-6.61092300	0.31880800
H	1.38953200	-6.49329900	0.80870600
H	2.19259300	-6.82702700	-0.73946400
H	2.88906700	-7.46312500	0.77495000
C	-0.50700200	-0.76383800	1.89623200
H	-1.57113500	-0.79283900	2.17857800

H	-0.30634900	0.26872800	1.57792800
C	0.94686000	0.11842000	-1.49996500
H	1.35991300	1.09202200	-1.79686500
H	-0.12226200	0.29041400	-1.28791000
C	1.09387500	-0.89545700	-2.62791200
H	0.54723000	-0.57371600	-3.52528900
H	2.15707700	-0.97320900	-2.90672500
C	-1.91583800	-5.82915300	-1.33618800
C	-1.21425100	-7.17638500	-1.12750200
C	-3.44044300	-6.02310800	-1.21392900
C	-1.58991800	-5.31127700	-2.74998900
H	-1.41621200	-7.55039700	-0.11058300
H	-0.12520300	-7.03152600	-1.20759200
C	-1.69792100	-8.18484700	-2.17174800
H	-3.94398200	-5.05398600	-1.35058200
H	-3.68637200	-6.38004800	-0.19938500
C	-3.91746700	-7.03274500	-2.26066700
H	-0.50158700	-5.15301800	-2.83240500
H	-2.07902700	-4.33738300	-2.90231400
C	-2.07092500	-6.32091100	-3.79423700
H	-1.18943400	-9.14710000	-2.00604100
C	-3.21156700	-8.37307900	-2.03817300
C	-1.36825600	-7.66242100	-3.57246800
H	-5.00602500	-7.16460100	-2.16219100
C	-3.58481000	-6.50933900	-3.66107700
H	-1.83218700	-5.93890100	-4.79858500
H	-3.45744500	-8.76881700	-1.03911000
H	-3.56753200	-9.11236700	-2.77376300
H	-0.27906100	-7.53938600	-3.68200000
H	-1.69219800	-8.39028900	-4.33402300
H	-3.94645100	-7.21917600	-4.42256100
H	-4.10243300	-5.55307400	-3.83971200

IM4c

M06 SCF energy (au)	-1950.603365
M06 enthalpy (au)	-1949.839912
M06 free energy (au)	-1949.947225
M06 SCF energy in solution (au)	-1951.118409
M06 enthalpy in solution (au)	-1950.354956
M06 free energy in solution (au)	-1950.462269

Cartesian coordinates

ATOM	X	Y	Z
Pd	-2.24272000	-1.29821100	0.46025500
C	-2.10091400	-0.92296100	2.89378800
O	-1.14936800	-0.56922500	2.12873300
O	-3.08075600	-1.54755100	2.35598000
C	-0.17635100	-0.18142300	-1.48809700
O	0.13842300	0.38702500	-2.52780300
N	-1.35904800	-0.87804800	-1.33158700
C	-2.17963700	-1.16588600	-2.41989300
C	-3.39712400	-1.82454400	-2.09240700
C	-1.95280200	-0.92479800	-3.77395600
C	-4.33690000	-2.24465500	-3.06769500
C	-2.88281100	-1.34425800	-4.74441700
H	-1.05265100	-0.40370100	-4.07310700
C	-4.74132400	-2.63076200	-0.34802600
C	-5.50574700	-2.88649100	-2.60314200
C	-4.05320400	-1.99245600	-4.42571600
H	-2.65442100	-1.13626700	-5.78882700

C	-5.71166500	-3.08104500	-1.25778700
H	-6.24441200	-3.22184000	-3.33118400
H	-4.76210400	-2.30461200	-5.19085900
H	-6.60709400	-3.57001800	-0.88387100
N	-3.63806400	-2.03548900	-0.76671800
H	-4.84910500	-2.74347700	0.73016900
C	1.77333900	0.92505300	-0.33020400
H	2.57007700	0.71811300	0.39930500
C	1.11615000	2.27589500	-0.04451100
H	0.35328200	2.43971700	-0.81190600
C	2.11991800	3.43022000	-0.10149400
H	1.55807000	4.37804300	-0.11685700
H	2.67605300	3.37174700	-1.04831700
C	1.27367500	2.32039900	2.44249400
H	0.61593600	2.41756600	3.31040700
H	1.79785400	1.35149200	2.52864000
N	0.42834200	2.30397700	1.25722600
C	-0.92571800	2.38079100	1.42195000
O	-1.47935600	2.57541500	2.49379900
O	-1.56859300	2.21020400	0.24991800
C	-2.94075600	2.65382900	0.06628500
C	-3.18432400	2.36336000	-1.40546000
H	-4.19140600	2.69010000	-1.69607100
H	-3.09054200	1.28694100	-1.60508300
H	-2.44928700	2.88671000	-2.03071000
C	-3.91187900	1.86359600	0.92842100
H	-3.78323800	2.08798800	1.99100400
H	-3.76863900	0.78256500	0.77681700
H	-4.94109100	2.11360100	0.63402300
C	-3.03129200	4.14599700	0.34332100
H	-2.31321500	4.69418000	-0.28146500
H	-2.82747700	4.36484400	1.39709900
H	-4.03962100	4.50759300	0.10163000
C	0.78760900	-0.22928000	-0.32188100
H	1.32858000	-1.18511700	-0.41934300
H	0.27103400	-0.27825800	0.64020100
C	3.07006800	3.44211300	1.09059200
H	3.71865100	2.55124200	1.07040100
H	3.74051000	4.31083700	1.03201500
C	2.27393000	3.46650100	2.38880200
H	1.71895200	4.41602200	2.45905400
H	2.93827800	3.41518500	3.26300400
H	2.25271200	0.99258000	-1.31649800
C	-2.11524900	-0.59064100	4.35544000
C	-2.48150100	-1.83457900	5.18367300
C	-3.19252200	0.49607500	4.57884600
C	-0.75875000	-0.04165200	4.81275800
H	-3.45009200	-2.23195300	4.84544400
H	-1.73049600	-2.62488400	5.01754700
C	-2.53922200	-1.46402500	6.66777800
H	-2.93170400	1.38133700	3.97845700
H	-4.16759700	0.12126700	4.22873300
C	-3.25351700	0.85751500	6.06395100
H	0.02905200	-0.79038500	4.62923600
H	-0.51411800	0.84489800	4.21048200
C	-0.82248300	0.31928300	6.29805500
H	-2.79470000	-2.36134700	7.25224300
C	-3.60651500	-0.38705900	6.88259400
C	-1.17751800	-0.92530500	7.11585700
H	-4.02356600	1.63022600	6.21150300

C	-1.89085000	1.39597800	6.50852500
H	0.15819000	0.70438800	6.61718100
H	-4.59556900	-0.76958600	6.58231100
H	-3.67114400	-0.13040100	7.95242300
H	-0.40294000	-1.69831200	6.98355000
H	-1.20586800	-0.67837200	8.18953200
H	-1.92841700	1.69076200	7.56986400
H	-1.63597300	2.29603300	5.92594800

TS4c

M06 SCF energy (au)	-1371.618848
M06 enthalpy (au)	-1371.133180
M06 free energy (au)	-1371.217006
M06 SCF energy in solution (au)	-1371.981952
M06 enthalpy in solution (au)	-1371.496284
M06 free energy in solution (au)	-1371.580110

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.24215200	-3.90467200	2.39854400
C	0.91068800	-1.29571000	3.50149900
O	1.18963900	-0.34640800	4.21611400
N	0.50514900	-2.54232400	3.90163300
C	0.47843400	-3.02428200	5.19034100
C	0.29939300	-4.44597000	5.29532800
C	0.61708100	-2.29324600	6.36380800
C	0.24678300	-5.07233200	6.56905500
C	0.56865200	-2.93049400	7.61674700
H	0.76815600	-1.22108200	6.28735100
C	0.02382000	-6.49028500	4.21064800
C	0.05922300	-6.47164900	6.60049200
C	0.38230100	-4.28733900	7.73584300
H	0.67738400	-2.32138600	8.51320700
C	-0.05552100	-7.18211000	5.43223800
H	0.00959000	-6.97285300	7.56763400
H	0.33744100	-4.77272500	8.71002400
H	-0.19917600	-8.25968200	5.43150100
N	0.19352800	-5.18231200	4.13984000
H	-0.04900800	-7.01721100	3.26036000
C	0.17110000	-2.23132700	1.25349200
H	-0.88129300	-1.92720100	1.19869900
C	0.51995000	-3.27814600	0.32043400
H	0.26519100	-4.72355100	0.96078900
C	1.93567000	-3.39233100	-0.21465200
H	2.66861500	-3.28727300	0.59613900
H	2.06996300	-4.39921200	-0.63719800
C	-0.32944800	-2.32888000	-1.71772600
H	-0.47517100	-1.39094200	-1.16285500
H	-1.13074000	-2.40720500	-2.45441700
N	-0.45403400	-3.43656300	-0.75393000
C	-0.75083200	-4.70411500	-1.22537400
O	-0.43292700	-5.73847400	-0.66814000
O	-1.45922200	-4.63068100	-2.36063400
C	-1.88457500	-5.84430500	-3.05466400
C	-2.61576800	-5.29160700	-4.26571500
H	-2.99700700	-6.11506800	-4.88269500
H	-3.46376800	-4.66857200	-3.95486000
H	-1.94233200	-4.68044100	-4.88021500
C	-2.83454500	-6.64594500	-2.18163900
H	-2.32467700	-7.05779000	-1.30617900

H	-3.66543800	-6.01246400	-1.84448300
H	-3.25471000	-7.47411300	-2.76796900
C	-0.67286600	-6.65079000	-3.49074400
H	0.01861200	-6.01698300	-4.06302300
H	-0.14106600	-7.07539300	-2.63458000
H	-0.99810300	-7.47121800	-4.14416200
C	1.06349500	-1.23541400	1.96495600
H	0.86023100	-0.20695900	1.63348100
H	2.12661400	-1.42879100	1.75444100
C	2.14828600	-2.32473400	-1.29452300
H	3.13720800	-2.45083900	-1.75557500
H	2.14806000	-1.32983500	-0.81898000
C	1.05264200	-2.36638700	-2.35783300
H	1.16653300	-1.53086400	-3.06259500
H	1.13513200	-3.29520200	-2.94782800

IM1d

M06 SCF energy (au)	-1639.926977
M06 enthalpy (au)	-1639.336758
M06 free energy (au)	-1639.438431
M06 SCF energy in solution (au)	-1640.375994
M06 enthalpy in solution (au)	-1639.785775
M06 free energy in solution (au)	-1639.887448

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.08348100	-3.40166500	2.25437800
C	-1.68160400	-5.90086600	0.93212400
O	-2.35405700	-5.21539400	0.17292800
O	-0.93202700	-5.42734500	1.89334600
C	-1.61036300	-7.40567000	0.79516800
H	-2.58177900	-7.79358300	0.47133200
H	-0.88078300	-7.65529500	0.01242800
H	-1.29431000	-7.88562400	1.72918700
C	-1.39394900	-0.50378300	1.93053400
O	-1.54178900	0.67911400	2.18916800
N	-1.32746400	-1.51857500	2.85010700
C	-1.60006100	-1.37749500	4.21001200
C	-1.79648400	-2.60251900	4.90974100
C	-1.71890900	-0.19542400	4.92676400
C	-2.10093000	-2.62973100	6.29245800
C	-2.02335000	-0.22693800	6.30241800
H	-1.58489500	0.74765600	4.40871700
C	-1.85898800	-4.94147800	4.77254400
C	-2.27215800	-3.89848800	6.89116400
C	-2.21065300	-1.40429400	6.98647200
H	-2.10747300	0.72091300	6.83150700
C	-2.15162900	-5.04459800	6.14367300
H	-2.49991800	-3.94975100	7.95601100
H	-2.43913900	-1.41274100	8.05115800
H	-2.27334300	-6.03126300	6.58494600
N	-1.68860100	-3.76680300	4.19412900
H	-1.75065200	-5.82175800	4.13690400
C	-0.84192800	-2.40796700	0.28183200
H	-1.40115700	-3.06989400	-0.38418700
C	0.42260100	-2.79564800	0.67630100
H	1.02880700	-2.06522200	1.22812600
C	1.15876800	-4.00196800	0.18496200
H	0.43924600	-4.72287000	-0.22857300
H	1.79337100	-3.68620200	-0.66079100

C	2.37282400	-6.67784400	3.51797000
H	2.86077400	-7.34122200	4.24074000
H	2.52697100	-5.64723600	3.87450100
N	0.95791200	-6.98494500	3.55864200
H	0.29500600	-6.43523300	3.00702000
C	0.47327300	-8.03367500	4.26841700
O	1.13535900	-8.84441000	4.88634500
O	-0.88666400	-8.02783000	4.19278800
C	-1.66273300	-9.14024100	4.71582400
C	-3.09229600	-8.73141000	4.40067600
H	-3.79135000	-9.51271000	4.72548200
H	-3.35612100	-7.79900400	4.91953800
H	-3.22482100	-8.57232900	3.32234700
C	-1.47199400	-9.27562500	6.21829300
H	-0.45333100	-9.58632200	6.46452400
H	-1.67510900	-8.31722800	6.71646900
H	-2.18022900	-10.01706300	6.61229300
C	-1.30114200	-10.42002600	3.97991100
H	-1.43281100	-10.28821200	2.89717600
H	-0.26526100	-10.71109900	4.17968600
H	-1.96306400	-11.23359000	4.30563700
C	-1.35316300	-1.00351800	0.48981300
H	-2.38551300	-0.92824000	0.12103100
H	-0.76987600	-0.28287300	-0.10056900
C	2.99865000	-6.85576500	2.13732400
H	4.03927900	-6.49701100	2.18954900
H	3.04669600	-7.92946100	1.90322200
C	2.02209400	-4.65425800	1.26753300
H	1.51424900	-4.52443700	2.23545500
H	2.98493500	-4.12448700	1.35938500
C	2.25341600	-6.13722000	1.01705700
H	1.27045900	-6.61534400	0.88018500
H	2.79338200	-6.27600800	0.06715600

TS1d

M06 SCF energy (au)	-1639.872475
M06 enthalpy (au)	-1639.287275
M06 free energy (au)	-1639.387529
M06 SCF energy in solution (au)	-1640.328767
M06 enthalpy in solution (au)	-1639.743567
M06 free energy in solution (au)	-1639.843821

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.51046900	-2.14558900	1.20463200
C	-5.37768600	-4.23931800	2.18676500
O	-5.25847200	-3.02201700	2.35322400
O	-4.50249600	-4.99478200	1.60553300
C	-6.59309300	-4.97973300	2.70699500
H	-6.28869300	-5.66793500	3.50681900
H	-7.33811300	-4.27978300	3.09614000
H	-7.03158700	-5.59662800	1.91384100
C	0.96652700	-0.54975300	1.64917200
O	1.91953500	-0.06020700	2.22914700
N	-0.21897000	-0.93677700	2.22410400
C	-0.43607900	-0.86871000	3.60079900
C	-1.34547600	-1.82618200	4.10227600
C	0.15621400	0.01740000	4.48674300
C	-1.62671300	-1.91010100	5.48711300
C	-0.14741500	-0.04761500	5.85968800

H	0.87231500	0.74190400	4.11674300
C	-2.69151600	-3.66399500	3.63480900
C	-2.50491300	-2.93137700	5.91259400
C	-1.01572000	-0.98588600	6.36283500
H	0.32869800	0.66500600	6.53084500
C	-3.01930500	-3.80828100	4.99656900
H	-2.75066700	-3.01162000	6.97152600
H	-1.24371600	-1.03527900	7.42667900
H	-3.69019600	-4.61433900	5.28288700
N	-1.91132100	-2.69361000	3.19770800
H	-3.07655000	-4.37509900	2.91172400
C	-0.48138300	-0.70374000	-0.31033700
H	-0.94380900	0.27167700	-0.12294600
C	-1.14123300	-1.55268000	-1.15078300
H	-0.65249000	-2.48762600	-1.44699700
N	-2.69666200	-3.78883400	0.33732300
H	-3.50018600	-4.25879100	1.07668400
C	-1.61858500	-4.68901900	0.16314600
O	-1.07704200	-4.93302700	-0.89481300
O	-1.28188100	-5.19917000	1.35113600
C	-0.00419700	-5.87830200	1.55250000
C	0.00672700	-6.12550200	3.05093000
H	0.91192200	-6.67683000	3.33558500
H	-0.00870600	-5.17473600	3.60170600
H	-0.87020600	-6.71460800	3.34905800
C	1.13437300	-4.95005000	1.16173100
H	1.15587400	-4.76968400	0.08118800
H	1.03486400	-3.98834600	1.68910100
H	2.09180000	-5.39968600	1.45622800
C	0.01827100	-7.19001400	0.78813000
H	-0.84885300	-7.80334100	1.06509600
H	0.00179400	-7.02274400	-0.29275300
H	0.92854800	-7.74763100	1.04625300
C	0.93131400	-0.81918600	0.15945900
H	1.56905400	-0.08336500	-0.34904600
H	1.34404600	-1.81751500	-0.05179400
C	-2.28908900	-1.06268600	-1.99942800
H	-1.83657600	-0.34264400	-2.70262600
H	-2.66297000	-1.87264900	-2.63349100
C	-4.24552800	-1.22432500	-0.31268900
H	-5.17384500	-0.69160200	-0.06265500
H	-3.71807300	-1.30225500	0.65150700
C	-3.46304300	-0.37205200	-1.30659000
H	-4.14227500	-0.03912600	-2.10678300
H	-3.12134500	0.54946800	-0.80868400
C	-4.61836400	-2.62205600	-0.79230200
H	-5.38226600	-3.00579100	-0.10626200
H	-5.09143500	-2.56042300	-1.78723500
C	-3.50551800	-3.66177000	-0.89525400
H	-2.84129700	-3.51001200	-1.74758900
H	-3.97716700	-4.64436100	-1.05562500

IM2d

M06 SCF energy (au)	-1410.925484
M06 enthalpy (au)	-1410.405841
M06 free energy (au)	-1410.493261
M06 SCF energy in solution (au)	-1411.299324
M06 enthalpy in solution (au)	-1410.779681
M06 free energy in solution (au)	-1410.867101

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.22083000	-2.31056600	2.61124100
C	1.09137700	-0.51776500	3.21769600
O	1.83089500	0.27722400	3.77436900
N	-0.19010800	-0.84220400	3.58388700
C	-0.79778400	-0.37267800	4.74261600
C	-2.01354600	-1.02677000	5.09278400
C	-0.34094500	0.63592400	5.58286600
C	-2.73122100	-0.67561900	6.26542900
C	-1.06300900	0.98567900	6.73953700
H	0.58774800	1.13833300	5.33890400
C	-3.57253200	-2.68079200	4.55551000
C	-3.91447600	-1.39286300	6.54424700
C	-2.23236000	0.35564700	7.09027200
H	-0.67000000	1.78198200	7.36976900
C	-4.33345900	-2.39026300	5.70034700
H	-4.48212600	-1.14277900	7.44065900
H	-2.78236500	0.63209700	7.98862100
H	-5.23543200	-2.96376900	5.89608700
N	-2.46327200	-2.02236500	4.26339800
H	-3.85991100	-3.48350900	3.88009600
C	0.35612700	-1.69405500	1.14243600
H	-0.10556700	-0.85776800	0.60452400
C	0.00181800	-2.96473000	0.75675600
H	0.55572900	-3.81305300	1.17377700
C	-0.83635300	-3.21338000	-0.46506300
H	-1.69360200	-2.52368300	-0.45180300
H	-0.23029400	-2.88385100	-1.32596400
C	-3.59140900	-3.75764800	1.19202100
H	-3.58437600	-2.75329300	0.73862000
H	-4.48738400	-3.79721800	1.83903800
N	-2.37757100	-3.89307100	1.98014600
C	-2.26251500	-4.98797000	2.75677700
O	-3.11642000	-5.84791800	2.94850000
O	-1.01766700	-5.01732000	3.32641000
C	-0.73398600	-5.83300000	4.48616600
C	0.67080300	-5.39111700	4.86426500
H	1.01952800	-5.92874700	5.75578500
H	1.37036900	-5.59138100	4.04148400
H	0.68579900	-4.31154600	5.07440500
C	-0.75524100	-7.30829500	4.11897400
H	-1.76238200	-7.62245800	3.82932700
H	-0.07245400	-7.49658700	3.27954700
H	-0.41996100	-7.91169900	4.97393100
C	-1.70238900	-5.51332900	5.61573800
H	-1.66635900	-4.43978400	5.85619500
H	-2.72846100	-5.78803400	5.34768000
H	-1.41609600	-6.07116700	6.51764100
C	1.52148400	-1.33942000	2.01412900
H	2.27653200	-0.77493100	1.45143400
H	2.00799900	-2.25507700	2.38707400
C	-3.74778500	-4.82611000	0.10965000
H	-4.77989900	-4.77568000	-0.27049600
H	-3.65173200	-5.80439000	0.60050400
C	-1.30448400	-4.65502900	-0.71388200
H	-1.10011000	-5.27965900	0.16741000
H	-0.70940000	-5.08118200	-1.53423600
C	-2.78903700	-4.74842300	-1.07481400
H	-3.05132300	-3.88954700	-1.71691100

H	-2.95686400	-5.64028600	-1.69634900

TS2d

M06 SCF energy (au)	-1410.902764
M06 enthalpy (au)	-1410.384817
M06 free energy (au)	-1410.469821
M06 SCF energy in solution (au)	-1411.273519
M06 enthalpy in solution (au)	-1410.756465
M06 free energy in solution (au)	-1410.841469

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.58325100	-2.02632400	2.79357900
C	0.79960100	-0.58201800	3.42307200
O	1.63837500	0.13389700	3.94518400
N	-0.53496900	-0.63524400	3.74670600
C	-1.14278600	-0.06093700	4.84703000
C	-2.42547000	-0.60571500	5.17944500
C	-0.63300300	0.95087500	5.64894100
C	-3.15976900	-0.11337900	6.28935200
C	-1.37273400	1.43216900	6.74539900
H	0.34753000	1.35328800	5.41559000
C	-4.07557200	-2.18637200	4.69756600
C	-4.41062200	-0.71488500	6.55613100
C	-2.61082000	0.92877800	7.06940700
H	-0.94317100	2.23102900	7.34824400
C	-4.86904400	-1.74458900	5.77231200
H	-4.99839400	-0.35164600	7.39965200
H	-3.17580400	1.31226900	7.91802500
H	-5.82311200	-2.22749000	5.96768500
N	-2.91164600	-1.63362500	4.40969500
H	-4.38149800	-3.02641500	4.06967900
C	-0.02162000	-1.95497700	1.42513900
H	-0.25178900	-1.16288600	0.69966200
C	-0.35260000	-3.26557700	0.97957800
H	0.05536900	-4.10779200	1.54431800
C	-0.63008200	-3.51512500	-0.46460200
H	-1.16416600	-2.64963100	-0.88913000
H	0.37622800	-3.46526600	-0.91980600
C	-3.43660700	-3.35953900	0.82565800
H	-3.19005800	-2.43433500	0.27991000
H	-4.31452600	-3.12648600	1.44979100
N	-2.29490600	-3.67937500	1.67593500
C	-2.50272900	-4.67743000	2.59766700
O	-3.58993600	-5.13954300	2.90916400
O	-1.32329500	-5.08811500	3.11552700
C	-1.26476000	-5.85724700	4.34840800
C	0.22496900	-5.88837800	4.64483800
H	0.42123200	-6.46003600	5.56092200
H	0.77356100	-6.35876400	3.81828800
H	0.60783700	-4.86736400	4.78126200
C	-1.79931700	-7.26048800	4.11742200
H	-2.86676500	-7.23962700	3.87843800
H	-1.25979800	-7.74030900	3.28995600
H	-1.64786700	-7.86750500	5.02040600
C	-2.00252600	-5.13280500	5.46289000
H	-1.65221100	-4.09263800	5.53491100
H	-3.08470000	-5.13293200	5.29725000
H	-1.79716700	-5.63041400	6.42012600
C	1.14588800	-1.61779600	2.34494500

H	2.01667600	-1.25329200	1.78132500
H	1.47561900	-2.52428800	2.87976400
C	-3.77610600	-4.47987300	-0.14991400
H	-4.76619900	-4.27627700	-0.58473000
H	-3.88408700	-5.41095200	0.42499800
C	-1.31090300	-4.82900700	-0.85907100
H	-1.22585600	-5.55542500	-0.03475700
H	-0.75981700	-5.26329800	-1.70493800
C	-2.77328600	-4.67509200	-1.27974800
H	-2.84245100	-3.82868900	-1.98482600
H	-3.07128000	-5.56416100	-1.85486800

IM3d

M06 SCF energy (au)	-1989.863855
M06 enthalpy (au)	-1989.071549
M06 free energy (au)	-1989.182618
M06 SCF energy in solution (au)	-1990.402307
M06 enthalpy in solution (au)	-1989.610001
M06 free energy in solution (au)	-1989.721070

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.26054700	-2.28081000	2.83371900
C	-3.23457100	-3.84056600	1.28988700
O	-3.74041700	-2.63623700	1.09243600
O	-2.26347400	-4.03014300	2.02400400
C	0.20028200	0.20434700	2.52085900
O	0.84330400	1.21868500	2.74833900
N	-0.38852600	-0.60852600	3.46159100
C	-0.41747000	-0.38149300	4.82647000
C	-1.16104300	-1.33090400	5.60303100
C	0.19081400	0.67198100	5.50060500
C	-1.25974600	-1.19816500	7.01459100
C	0.07695100	0.79337200	6.89717600
H	0.75518400	1.39598100	4.92335300
C	-2.44388300	-3.27201500	5.63146400
C	-1.99626700	-2.18306800	7.70962700
C	-0.62638600	-0.11175500	7.65570900
H	0.57107600	1.63390100	7.38289300
C	-2.58495300	-3.21989600	7.03003200
H	-2.08381200	-2.10373400	8.79365700
H	-0.70172400	-0.01341000	8.73796100
H	-3.15176900	-3.99102500	7.54604700
N	-1.76897500	-2.36851100	4.94960600
H	-2.89375400	-4.07853500	5.04979400
C	-0.33058100	-1.80254400	1.06244500
H	-0.96944400	-2.07818300	0.20220700
C	0.96141300	-2.62323300	0.99874000
H	1.53398900	-2.46241600	1.92373500
C	1.86607400	-2.22356700	-0.17788500
H	1.25763700	-2.02681900	-1.07857600
H	2.32210600	-1.25922800	0.08300000
C	0.33267300	-4.70331900	-0.29054600
H	-0.11455400	-3.94091200	-0.94807000
H	-0.44051100	-5.46074300	-0.11015400
N	0.66879900	-4.06208900	0.97151800
H	-3.17031900	-1.99912800	1.60421600
C	0.68490200	-4.74635600	2.15262100
O	0.96003400	-4.24738100	3.23197500
O	0.35957600	-6.04408700	1.97022600

C	0.21699700	-6.92923100	3.11629200
C	-0.25479300	-8.22661900	2.47995300
H	-0.36584800	-9.00487400	3.24597400
H	-1.22578800	-8.08756600	1.98407200
H	0.46901500	-8.57512400	1.73209600
C	-0.83582100	-6.40429500	4.08211500
H	-0.49419000	-5.49809200	4.59228300
H	-1.76262700	-6.17041200	3.53953300
H	-1.05516800	-7.17678400	4.83232300
C	1.56416700	-7.13223300	3.79020800
H	2.30372400	-7.48729700	3.05995800
H	1.92510900	-6.20179000	4.23785300
H	1.47153100	-7.89185200	4.57834700
C	-0.11187400	-0.29194900	1.11737900
H	-1.04292800	0.21758500	0.82072000
H	0.66327100	0.07879000	0.43052300
C	1.54772300	-5.33490900	-0.95932500
H	2.03329600	-5.98806200	-0.21783100
H	1.21152300	-5.98866300	-1.77887100
C	2.97040800	-3.22728700	-0.51684100
H	3.35682100	-3.68125100	0.41075200
H	3.81429800	-2.68092500	-0.96215900
C	2.54425600	-4.31703800	-1.50030600
H	2.10922400	-3.82559000	-2.38800500
H	3.43605200	-4.85146800	-1.85993400
C	-3.90361500	-4.93912900	0.51446200
C	-3.34440000	-6.30436900	0.92974600
C	-5.42953700	-4.92514300	0.72493700
C	-3.60889400	-4.69879500	-0.98470900
H	-3.54395500	-6.47230100	2.00141700
H	-2.24883300	-6.30975500	0.81492200
C	-3.98696600	-7.40844100	0.08995200
H	-5.83787300	-3.94515700	0.43824300
H	-5.65660700	-5.07265700	1.79359900
C	-6.06955100	-6.03726100	-0.11136000
H	-2.51793100	-4.67799200	-1.14454700
H	-4.00226200	-3.71583600	-1.28407700
C	-4.25072500	-5.81067100	-1.81665100
H	-3.57344900	-8.38049600	0.39995000
C	-5.50227500	-7.39554200	0.30983900
C	-3.67938100	-7.16514200	-1.39013500
H	-7.15767400	-6.02182200	0.05099400
C	-5.76570900	-5.79824800	-1.59316500
H	-4.03014600	-5.63070300	-2.87952300
H	-5.73219100	-7.59123900	1.36957600
H	-5.97721000	-8.19861600	-0.27561300
H	-2.59003500	-7.18715800	-1.55799900
H	-4.11635600	-7.96824200	-2.00432400
H	-6.24225900	-6.58030100	-2.20505000
H	-6.18840700	-4.83383100	-1.91698300

TS3d

M06 SCF energy (au)	-1989.838610
M06 enthalpy (au)	-1989.051703
M06 free energy (au)	-1989.160774
M06 SCF energy in solution (au)	-1990.372701
M06 enthalpy in solution (au)	-1989.585794
M06 free energy in solution (au)	-1989.694865

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.38765200	-2.47065900	2.64657200
C	-2.57187000	-4.47674400	0.98728700
O	-2.27940300	-3.62233200	0.10556500
O	-2.30763700	-4.30618000	2.21585900
C	-0.06007900	0.11918800	2.37493400
O	0.52643800	1.15728400	2.64707000
N	-0.56505000	-0.77329000	3.28274600
C	-0.51054100	-0.63782500	4.66128200
C	-1.15068200	-1.68244500	5.38859000
C	0.07836200	0.38898700	5.38884700
C	-1.18835700	-1.69189500	6.80524200
C	0.03607400	0.37540300	6.79641400
H	0.56663800	1.19498100	4.85252200
C	-2.33688500	-3.69293600	5.26574200
C	-1.84046900	-2.78091000	7.42494600
C	-0.57579100	-0.63082800	7.50693300
H	0.51114600	1.19643800	7.33146000
C	-2.40944100	-3.77592700	6.66753200
H	-1.88218400	-2.81782100	8.51373800
H	-0.59420400	-0.62913800	8.59582100
H	-2.91338400	-4.62203600	7.12755500
N	-1.73363100	-2.68602900	4.66368000
H	-2.76583300	-4.45320300	4.61300100
C	-0.38644500	-1.82283800	0.72835900
H	-0.67185600	-1.94053300	-0.33488400
C	0.98558600	-2.50081100	0.88669800
H	1.41161400	-2.21704400	1.85769600
C	1.97224900	-2.05251600	-0.19961500
H	1.46104200	-1.98923100	-1.17667900
H	2.27201600	-1.02311400	0.04265900
C	0.75759900	-4.73303400	-0.28772000
H	0.27354200	-4.09576400	-1.04224300
H	0.07652100	-5.57666100	-0.11874300
N	0.86639400	-3.96037500	0.94498000
H	-1.50923200	-2.68623000	0.71733900
C	1.00679400	-4.56104100	2.16695100
O	1.21273900	-3.95997300	3.20944500
O	0.87771600	-5.89878100	2.06787600
C	1.01729000	-6.73433400	3.25263400
C	0.75774900	-8.13106300	2.71270600
H	0.90037300	-8.87417000	3.50775100
H	-0.26941200	-8.22213000	2.33469200
H	1.45108300	-8.36073200	1.89307400
C	-0.02573400	-6.36708200	4.29801400
H	0.21011900	-5.41468400	4.78238500
H	-1.01368500	-6.27977400	3.82317500
H	-0.07280900	-7.15740900	5.06008100
C	2.43600900	-6.63678000	3.78945300
H	3.15761200	-6.88884800	2.99991900
H	2.65160300	-5.63082400	4.16126800
H	2.56834500	-7.35218300	4.61231200
C	-0.36094400	-0.30980200	0.95345900
H	-1.34688700	0.10766500	0.69624800
H	0.36020700	0.18639600	0.28802200
C	2.11352800	-5.22689600	-0.77678700
H	2.59387700	-5.76798300	0.05400900
H	1.95928200	-5.96492100	-1.57863700
C	3.21685400	-2.93087400	-0.33837200
H	3.53847800	-3.27947700	0.65761100

H	4.04074500	-2.31410000	-0.72478000
C	3.03168900	-4.11981000	-1.28207200
H	2.64076600	-3.73757700	-2.24097900
H	4.01482200	-4.55655700	-1.51195400
C	-3.27649800	-5.75710200	0.58654200
C	-4.72079300	-5.71284400	1.12492300
C	-3.31556300	-5.92720400	-0.93698000
C	-2.55859500	-6.96376800	1.21352400
H	-5.24609300	-4.84280700	0.69739300
H	-4.69935500	-5.57696600	2.21748100
C	-5.45033700	-7.00773600	0.75774200
H	-2.28728000	-5.93933100	-1.33337300
H	-3.81560000	-5.05968200	-1.39237500
C	-4.04521700	-7.22201800	-1.30123600
H	-2.52924400	-6.84257800	2.30753500
H	-1.50975900	-6.98968900	0.86873700
C	-3.28302100	-8.25829600	0.84222400
H	-6.47931600	-6.96259200	1.14607500
C	-5.47828800	-7.16539500	-0.76486100
C	-4.71694800	-8.20114500	1.37745700
H	-4.06458500	-7.32887000	-2.39647200
C	-3.31255600	-8.41415200	-0.68013200
H	-2.75121100	-9.11068100	1.29439300
H	-6.01990700	-6.32228500	-1.22297400
H	-6.02181000	-8.08412400	-1.03809000
H	-4.70734900	-8.11148400	2.47585100
H	-5.24800200	-9.13568700	1.13532500
H	-3.81699800	-9.35476300	-0.95383200
H	-2.28492400	-8.47293100	-1.07398100

IM4d

M06 SCF energy (au)	-1989.879895
M06 enthalpy (au)	-1989.086534
M06 free energy (au)	-1989.196464
M06 SCF energy in solution (au)	-1990.406570
M06 enthalpy in solution (au)	-1989.613209
M06 free energy in solution (au)	-1989.723139

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.80025200	-2.10843200	2.57954700
C	-0.52782400	-3.66409000	0.67781900
O	-0.44528600	-2.41049400	0.48985700
O	-0.76347100	-4.06436500	1.87060600
C	-0.28177000	0.89411500	2.40890300
O	0.16735200	1.93463000	2.87672600
N	-0.74712500	-0.15248700	3.18210700
C	-0.91617700	-0.00714900	4.55589900
C	-1.18412100	-1.21263300	5.26095500
C	-0.88968100	1.16013300	5.31799200
C	-1.42416100	-1.25673500	6.65807600
C	-1.13649900	1.12065600	6.70308100
H	-0.66279900	2.10173000	4.83483800
C	-1.40263700	-3.54041900	5.07819900
C	-1.66477100	-2.52463100	7.23146200
C	-1.40031600	-0.04690900	7.38131200
H	-1.10938100	2.06190400	7.25035700
C	-1.65425400	-3.65890500	6.45489900
H	-1.85468900	-2.58803600	8.30293800
H	-1.58137900	-0.05748300	8.45484300

H	-1.83273400	-4.64227600	6.88140400
N	-1.18464900	-2.36029700	4.52447700
H	-1.37247400	-4.40034400	4.40983900
C	0.57987400	1.53490000	0.12022600
H	0.55373300	2.59063800	0.42536700
C	2.01451400	1.03690500	0.28147900
H	2.30277800	1.15332500	1.33298000
C	2.97304500	1.87779500	-0.56776600
H	2.50490100	2.11196600	-1.53969000
H	3.07779300	2.84609900	-0.05643400
C	2.20592500	-0.84783600	-1.39085900
H	1.63599100	-0.13572600	-2.00605500
H	1.68859600	-1.81395800	-1.45192200
N	2.14301500	-0.39704200	-0.00647600
H	0.30239400	1.50399800	-0.94613400
C	2.38658500	-1.34295100	0.94381400
O	2.69267000	-2.49795700	0.68855400
O	2.23009000	-0.85927400	2.19453500
C	3.01568300	-1.40898000	3.28966400
C	2.69120300	-0.47426300	4.44219400
H	3.29053700	-0.73884500	5.32338400
H	2.90297900	0.56745500	4.16741400
H	1.62820800	-0.53838600	4.71053700
C	4.48999300	-1.31345000	2.92738500
H	4.73162400	-1.95106900	2.06888800
H	4.75155800	-0.27289400	2.68611900
H	5.10763200	-1.63187700	3.77747000
C	2.60176800	-2.83430600	3.62146300
H	1.51975200	-2.88063000	3.81366200
H	2.83395000	-3.52116100	2.80251900
H	3.12599400	-3.16058400	4.53116900
C	-0.44293600	0.74105700	0.91343300
H	-0.43625800	-0.30547100	0.59876300
H	-1.45427400	1.11586800	0.68513300
C	3.63974400	-0.98347000	-1.88983400
H	4.16992600	-1.63966500	-1.18381400
H	3.63226500	-1.51001000	-2.85673500
C	4.34682900	1.25679200	-0.81913600
H	4.68157000	0.70693800	0.07778800
H	5.07803500	2.06340200	-0.97310400
C	4.38440500	0.33781300	-2.04100700
H	3.97028000	0.89503200	-2.89937000
H	5.43138700	0.12137500	-2.30086100
C	-0.33058900	-4.65070200	-0.43604400
C	-1.25096100	-5.86912000	-0.25650600
C	-0.60505300	-4.00320800	-1.80029000
C	1.14026000	-5.12553400	-0.38542300
H	-2.30449900	-5.54375500	-0.26621300
H	-1.06660900	-6.32959300	0.72503000
C	-0.99704300	-6.87916600	-1.37870300
H	0.03475500	-3.11797500	-1.92765400
H	-1.64736600	-3.64638800	-1.83799100
C	-0.34640200	-5.01659600	-2.91661500
H	1.33849900	-5.57753000	0.60030500
H	1.81181300	-4.25944100	-0.47650000
C	1.38932300	-6.13784200	-1.50420300
H	-1.66577800	-7.74296800	-1.24243100
C	-1.27160000	-6.22273700	-2.73445700
C	0.46152700	-7.34252100	-1.32651500
H	-0.54590100	-4.54015700	-3.88871700

C	1.11343500	-5.47549500	-2.85705000
H	2.43878800	-6.46665000	-1.46005600
H	-2.32468200	-5.90303200	-2.79447300
H	-1.10928200	-6.95079500	-3.54561200
H	0.66686900	-7.83811400	-0.36393000
H	0.64870500	-8.08580300	-2.11845500
H	1.32024900	-6.18419000	-3.67530400
H	1.78622300	-4.61302300	-2.99714900

TS4d

M06 SCF energy (au)	-1410.896720
M06 enthalpy (au)	-1410.380862
M06 free energy (au)	-1410.468360
M06 SCF energy in solution (au)	-1411.270193
M06 enthalpy in solution (au)	-1410.754335
M06 free energy in solution (au)	-1410.841833

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.74922400	-2.51133300	2.64382200
C	-0.08604900	0.29296200	3.09696100
O	0.12050200	1.39309700	3.58165100
N	-0.67714100	-0.78065300	3.72108900
C	-1.01862600	-0.86501500	5.05247900
C	-1.35066900	-2.18594600	5.50950900
C	-1.05994000	0.17446700	5.97449600
C	-1.72973500	-2.40656000	6.86127800
C	-1.43126400	-0.06293300	7.30991000
H	-0.79388700	1.17123300	5.63794700
C	-1.58593900	-4.45001400	5.01343500
C	-2.05233700	-3.72730700	7.24194800
C	-1.76805200	-1.31743000	7.75977700
H	-1.45476500	0.78040300	7.99885900
C	-1.98574800	-4.74820300	6.32767900
H	-2.35171100	-3.91773900	8.27299300
H	-2.06255500	-1.49225100	8.79381400
H	-2.22741700	-5.77313500	6.59773000
N	-1.28192800	-3.22755300	4.61594100
H	-1.50684100	-5.23398200	4.26155200
C	-0.42278700	-1.22429800	1.09969000
H	-1.40928800	-0.92532900	0.72979500
C	0.03412600	-2.47922300	0.55227100
H	-0.42342500	-3.64044000	1.45279800
C	1.51993600	-2.76380900	0.44476900
H	1.87496700	-2.15939300	-0.40681900
H	2.02671400	-2.37973900	1.34086300
C	-1.25541800	-4.27465600	-0.68883800
H	-1.81583500	-4.33124300	-1.62300100
H	-1.98089600	-4.39140600	0.12982600
N	-0.72315900	-2.91915800	-0.60936500
C	-0.59794300	-2.09272400	-1.70928300
O	-0.05689500	-1.00284600	-1.66696300
O	-1.13217200	-2.64987100	-2.80599500
C	-1.09138800	-1.95012300	-4.08856700
C	-1.78090800	-2.93121200	-5.02072500
H	-1.81604700	-2.52133100	-6.03800000
H	-1.23939800	-3.88532600	-5.04915000
H	-2.80882700	-3.12462100	-4.68875800
C	0.34890800	-1.73228600	-4.52063100
H	0.86058200	-1.01968400	-3.86770900

H	0.89607200	-2.68488400	-4.50963200
H	0.36585700	-1.34417300	-5.54778200
C	-1.87758900	-0.65298200	-4.00909300
H	-2.89354800	-0.84675200	-3.64035800
H	-1.39186700	0.07165400	-3.34991300
H	-1.95905200	-0.21595500	-5.01330300
C	0.37662700	-0.08103800	1.67588700
H	0.30442000	0.80255900	1.02734700
H	1.44634600	-0.32689400	1.74713600
C	-0.19773900	-5.39140700	-0.62666100
H	-0.21366700	-5.86131700	0.36914600
H	-0.49158300	-6.18033000	-1.33354300
C	1.91034800	-4.22230000	0.24388700
H	1.71198700	-4.78157400	1.17424300
H	3.00024400	-4.25156900	0.10212800
C	1.23490400	-4.95218800	-0.91928600
H	1.26871500	-4.33316500	-1.83212900
H	1.82409600	-5.85243700	-1.14529300

TS7a

M06 SCF energy (au)	-1522.030325
M06 enthalpy (au)	-1521.530322
M06 free energy (au)	-1521.622848
M06 SCF energy in solution (au)	-1522.451826
M06 enthalpy in solution (au)	-1521.951823
M06 free energy in solution (au)	-1522.044349

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.87890600	-2.96539900	2.39999100
C	-2.41254400	-4.92221500	0.95547500
O	-2.42392700	-4.11259000	0.02141600
O	-1.73054200	-4.81930700	2.04773400
C	-3.26096500	-6.17758500	0.89448800
H	-2.69430100	-7.04880200	1.24179100
H	-4.12138500	-6.06404500	1.56684600
H	-3.63128600	-6.34465900	-0.12128800
C	0.09439000	-0.10430500	1.90166100
O	0.30803000	1.08357700	2.11327100
N	-0.34160300	-1.02634900	2.80531800
C	-0.74106300	-0.62421400	4.08808000
C	-1.63733500	-1.50333200	4.77519200
C	-0.36013600	0.53518200	4.75252900
C	-2.13560800	-1.19283200	6.06814400
C	-0.84878500	0.83091100	6.03984200
H	0.31030600	1.22591700	4.25712600
C	-2.83478000	-3.50677700	4.72638100
C	-3.02443600	-2.11706800	6.66216900
C	-1.72227200	0.00091100	6.69775600
H	-0.51658500	1.75207500	6.51670700
C	-3.37840800	-3.26675300	6.00122600
H	-3.41946400	-1.89883700	7.65481400
H	-2.09816200	0.23866900	7.69222500
H	-4.05910600	-3.99051900	6.44247600
N	-2.00770800	-2.65915300	4.14876300
H	-3.05900600	-4.40854600	4.15554000
C	-0.07777700	-1.96688300	0.09429900
H	-1.14636600	-2.08897600	-0.12378300
C	0.49810500	-3.07326100	0.86554300
H	1.46528400	-2.78078500	1.30300200

C	0.65162400	-4.30034200	-0.02693800
H	1.68955600	-4.65563900	0.00964300
H	0.00998100	-5.13793700	0.26246300
C	0.28470500	-3.86264000	-1.44838900
H	0.88476800	-4.32966900	-2.23619400
H	-0.78123600	-4.04386300	-1.62304400
N	0.44702000	-2.36847200	-1.52503400
H	-0.21292100	-1.93151300	-2.17183000
C	1.74728400	-1.81870000	-1.84291100
O	1.84108500	-0.80348300	-2.48232600
O	2.67777000	-2.56125300	-1.29274500
C	4.10247200	-2.15876800	-1.31346100
C	4.76293800	-3.29128800	-0.55255600
H	5.84263000	-3.11138500	-0.48070000
H	4.35407800	-3.36429900	0.46365600
H	4.60318800	-4.24968200	-1.06259300
C	4.25857300	-0.84209800	-0.57799600
H	3.75661800	-0.01968300	-1.09825900
H	3.86009100	-0.92112400	0.44268900
H	5.32634300	-0.59923300	-0.50304500
C	4.59018500	-2.09571300	-2.74767800
H	4.39546100	-3.04525300	-3.26282800
H	4.11434900	-1.28161300	-3.30303800
H	5.67491200	-1.92813500	-2.74808300
C	0.35756400	-0.57867300	0.45919100
H	-0.09860800	0.18146800	-0.18797100
H	1.44616400	-0.48076800	0.32287900

IM7a

M06 SCF energy (au)	-1522.030362
M06 enthalpy (au)	-1522.030362
M06 free energy (au)	-1522.030362
M06 SCF energy in solution (au)	-1522.453355
M06 enthalpy in solution (au)	-1521.952256
M06 free energy in solution (au)	-1522.046072

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.86555200	-2.97089800	2.40171800
C	-2.40834500	-4.92221500	0.95841800
O	-2.42521300	-4.10873900	0.02712900
O	-1.71820700	-4.82606300	2.04532600
C	-3.26163100	-6.17465000	0.89806900
H	-2.69721100	-7.04860700	1.24213400
H	-4.11926400	-6.05875300	1.57363100
H	-3.63654700	-6.33885100	-0.11653900
C	0.11376700	-0.10264200	1.90466200
O	0.33109200	1.08488700	2.12003300
N	-0.33015300	-1.02542400	2.80256600
C	-0.73117700	-0.62385000	4.08530800
C	-1.62942900	-1.50171700	4.77281600
C	-0.34944500	0.53511600	4.75059400
C	-2.12921100	-1.18830500	6.06476400
C	-0.83918200	0.83293000	6.03690900
H	0.32264000	1.22456900	4.25586200
C	-2.82861300	-3.50385800	4.72741700
C	-3.02004000	-2.11011600	6.65959600
C	-1.71541100	0.00538500	6.69403200
H	-0.50581600	1.75393100	6.51336900
C	-3.37451300	-3.26071300	6.00073400

H	-3.41590000	-1.88910200	7.65131900
H	-2.09285800	0.24464100	7.68758600
H	-4.05670400	-3.98279400	6.44251400
N	-1.99961600	-2.65875000	4.14906800
H	-3.05275000	-4.40694600	4.15854400
C	-0.06109900	-1.94660800	0.07297000
H	-1.14078100	-2.04446100	-0.10242100
C	0.49570400	-3.06445000	0.86352400
H	1.46752900	-2.78004100	1.29723300
C	0.64712700	-4.28546400	-0.04093400
H	1.68664000	-4.63768900	-0.02321000
H	0.01112800	-5.12707700	0.24930600
C	0.25833900	-3.83222300	-1.44910700
H	0.84446800	-4.27910000	-2.25865800
H	-0.81188600	-4.00324800	-1.60796200
N	0.42634300	-2.33082700	-1.49305800
H	-0.22893000	-1.88638800	-2.14104300
C	1.73748800	-1.79238600	-1.83230100
O	1.82733100	-0.79369500	-2.49545500
O	2.66250300	-2.53152600	-1.27603000
C	4.09249300	-2.13958000	-1.30526500
C	4.74353300	-3.26628300	-0.52843200
H	5.82389600	-3.09137400	-0.45491200
H	4.32997900	-3.32398100	0.48687600
H	4.58029500	-4.23005100	-1.02707000
C	4.25610600	-0.81371700	-0.58886600
H	3.75603100	0.00391400	-1.11863400
H	3.86121500	-0.87670900	0.43427600
H	5.32513400	-0.57437900	-0.52163600
C	4.57615600	-2.10034700	-2.74130000
H	4.37356900	-3.05548800	-3.24280800
H	4.10531100	-1.29035500	-3.30695900
H	5.66203500	-1.94074200	-2.74643100
C	0.38808700	-0.56657800	0.46087000
H	-0.04995600	0.20787300	-0.18230100
H	1.47974900	-0.48119500	0.33979500

IM8a

M06 SCF energy (au)	-1522.063982
M06 enthalpy (au)	-1521.563138
M06 free energy (au)	-1521.658161
M06 SCF energy in solution (au)	-1522.480169
M06 enthalpy in solution (au)	-1521.979325
M06 free energy in solution (au)	-1522.074348

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.84904500	-3.12973200	2.50482400
C	-2.78856300	-5.12986900	1.57989500
O	-3.42291500	-4.05677400	1.14883800
O	-1.73374800	-5.07951600	2.21172300
C	-3.43929500	-6.41235400	1.19837100
H	-3.06600600	-7.22480800	1.82536000
H	-4.52864800	-6.33458400	1.26232400
H	-3.18301400	-6.62814700	0.15252800
C	1.00205000	-0.67952000	2.26472300
O	1.66442500	0.20719700	2.78766200
N	-0.12925600	-1.24031000	2.83521500
C	-0.71512000	-0.63766100	3.95513000
C	-1.67500800	-1.39734600	4.69777000

C	-0.49774900	0.67034000	4.38771000
C	-2.34698100	-0.85318700	5.82985900
C	-1.17815900	1.20516300	5.49451200
H	0.22848300	1.28031500	3.86657100
C	-2.78937600	-3.43028600	4.95556000
C	-3.25942300	-1.68715800	6.51195700
C	-2.08431800	0.47352400	6.22277500
H	-0.96312800	2.23475200	5.77719600
C	-3.48249200	-2.97358100	6.08857700
H	-3.78010400	-1.28764200	7.38261400
H	-2.59771500	0.88960200	7.08844400
H	-4.17561200	-3.63347000	6.60411600
N	-1.93484900	-2.67440000	4.29334300
H	-2.92834600	-4.44503400	4.57948500
C	0.49052000	-2.05018500	0.13749200
H	-0.46699300	-1.51477900	-0.00169500
C	0.28192100	-3.37290800	0.84299200
H	1.25022700	-3.71534200	1.25587400
C	-0.13682400	-4.31846200	-0.27161300
H	-0.04986400	-5.38035400	-0.01018500
H	-1.17459400	-4.12226100	-0.59164600
C	0.81459900	-3.91054500	-1.39951200
H	1.77894100	-4.43563600	-1.31168900
H	0.41845500	-4.10898500	-2.40148800
N	0.98334300	-2.47223500	-1.18682200
C	1.16859700	-1.55823600	-2.17821300
O	1.04814900	-0.35549500	-2.02411100
O	1.50739300	-2.17156200	-3.33278800
C	1.78247500	-1.38670800	-4.52685000
C	2.12337800	-2.45052400	-5.55657500
H	2.36101200	-1.98145500	-6.52004100
H	2.99109400	-3.03845000	-5.23145700
H	1.27706600	-3.13422300	-5.70206100
C	2.97566600	-0.47363900	-4.29620700
H	2.74783900	0.29791500	-3.55519700
H	3.83757900	-1.05818000	-3.94785500
H	3.25316300	0.01228500	-5.24145800
C	0.54356700	-0.61630300	-4.95439900
H	-0.30826100	-1.30080200	-5.06567200
H	0.28516900	0.15682100	-4.22527300
H	0.72580300	-0.14005900	-5.92738500
C	1.44879200	-1.16526300	0.89760700
H	1.67441900	-0.26004700	0.32218900
H	2.40750000	-1.69346800	1.02795800
H	-2.87648200	-3.26572300	1.39814600

TS9a

M06 SCF energy (au)	-1522.033488
M06 enthalpy (au)	-1521.537471
M06 free energy (au)	-1521.631748
M06 SCF energy in solution (au)	-1522.443869
M06 enthalpy in solution (au)	-1521.947852
M06 free energy in solution (au)	-1522.042129

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.87993200	-3.13511400	2.64177400
C	-2.17977200	-5.49145200	1.81796700
O	-2.28421000	-4.79531000	0.76624400
O	-1.46109900	-5.14642900	2.80285100

C	-2.95244100	-6.77174500	1.90353700
H	-2.63262100	-7.36948100	2.76039300
H	-4.01822200	-6.53468800	2.00653400
H	-2.83558400	-7.33939900	0.97502200
C	0.01193500	-0.31597900	1.70228600
O	0.07449700	0.90517100	1.76966000
N	-0.56822000	-1.10661600	2.67568100
C	-1.04097400	-0.53035700	3.86549100
C	-1.49117500	-1.44234500	4.86450500
C	-1.11087500	0.82229700	4.19899000
C	-1.94992500	-1.01775900	6.14062900
C	-1.57783000	1.24234900	5.45910000
H	-0.79157600	1.55761000	3.47460100
C	-1.84602600	-3.68965000	5.42763000
C	-2.34775800	-2.01482500	7.05629900
C	-1.98742100	0.36136600	6.42859200
H	-1.60572500	2.31284600	5.65723200
C	-2.29324300	-3.34333000	6.71186000
H	-2.69914100	-1.70856300	8.04172800
H	-2.34066400	0.69824100	7.40197900
H	-2.59272000	-4.12561900	7.40420800
N	-1.46839400	-2.77076300	4.55581900
H	-1.79756300	-4.72217900	5.08603100
C	-0.01211800	-2.13514500	-0.18354500
H	-1.03515600	-1.83364500	-0.46378700
C	0.00567800	-3.42196900	0.63122100
H	0.91448000	-3.42146300	1.26195400
C	0.27028700	-4.54489300	-0.39670500
H	0.67469600	-5.45064300	0.07264700
H	-0.64097800	-4.82026400	-0.94257400
C	1.23899000	-3.86402300	-1.35222000
H	2.26946400	-3.87642600	-0.95798700
H	1.25320100	-4.30975600	-2.35133000
N	0.71615300	-2.50660100	-1.40814200
C	0.65338800	-1.71102300	-2.51147600
O	0.05858400	-0.64864400	-2.53801800
O	1.33531000	-2.25940600	-3.53785000
C	1.40303100	-1.57342400	-4.82096900
C	2.24463800	-2.51790600	-5.66199700
H	2.37773400	-2.10733600	-6.67113400
H	3.23465700	-2.65982000	-5.21025300
H	1.75878900	-3.49845500	-5.74715900
C	2.10586300	-0.23451300	-4.66669900
H	1.51454300	0.45764800	-4.06037100
H	3.08670700	-0.37436300	-4.19299400
H	2.26703100	0.21051100	-5.65791500
C	0.01315500	-1.42904200	-5.41908100
H	-0.48016500	-2.40894400	-5.47189700
H	-0.60680500	-0.75097500	-4.82566600
H	0.09375900	-1.03369800	-6.44072400
C	0.68579000	-0.98381900	0.51961300
H	0.84982900	-0.17556200	-0.20030100
H	1.67919300	-1.33471400	0.85047100
H	-1.29167300	-3.94722700	0.85804200

IM9a

M06 SCF energy (au)	-1522.091558
M06 enthalpy (au)	-1521.589601
M06 free energy (au)	-1521.679900
M06 SCF energy in solution (au)	-1522.491326

M06 enthalpy in solution (au)	-1521.989369
M06 free energy in solution (au)	-1522.079668

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.05267400	-1.68284700	2.06382700
C	-1.91372600	-3.37417900	0.51806500
O	-0.66634300	-3.15231700	0.60322700
O	-2.68407600	-2.79048200	1.35076700
C	-2.45422800	-4.24934200	-0.55562900
H	-3.50022900	-4.50509500	-0.36390500
H	-2.37924800	-3.69970400	-1.50310400
H	-1.84609700	-5.15520200	-0.64878500
C	1.79844600	-0.65980600	1.81026200
O	2.87346800	-0.23519000	2.22602300
N	0.66311200	-0.73884000	2.58980600
C	0.55165400	-0.04407000	3.79147800
C	-0.78190800	0.08899800	4.27159500
C	1.55215000	0.56799000	4.54171300
C	-1.10803600	0.83130200	5.43373700
C	1.22935500	1.29560400	5.70470700
H	2.58064800	0.48108300	4.21469900
C	-3.03039300	-0.44617600	3.89270600
C	-2.47294300	0.90815500	5.78794900
C	-0.06088300	1.44163500	6.15681800
H	2.04558800	1.75592400	6.25959200
C	-3.43018500	0.28242600	5.02502900
H	-2.75390500	1.47201500	6.67745600
H	-0.29005400	2.00918900	7.05731100
H	-4.48459700	0.33082000	5.28330400
N	-1.75858600	-0.52841400	3.54440600
H	-3.73922600	-0.98310500	3.26298000
C	1.18078600	0.18836900	-0.50027600
H	1.11100600	-0.17308700	-1.53507900
C	2.08311700	1.42119900	-0.39249600
H	3.12258900	1.15294200	-0.17247700
C	1.45126800	2.26866800	0.71248700
H	1.80980300	1.93443800	1.69380300
H	1.69727500	3.33293900	0.62108400
C	-0.04811400	2.01943000	0.56573100
H	-0.57048100	1.98093500	1.53254100
H	-0.53996300	2.79301100	-0.04228600
N	-0.12789600	0.72785200	-0.11764200
C	-1.28270400	0.20211900	-0.60434500
O	-1.35185200	-0.80399400	-1.29278000
O	-2.33257300	0.95949900	-0.21265100
C	-3.65089800	0.77343400	-0.79657200
C	-4.46445500	1.87496200	-0.13789000
H	-5.49691300	1.85848200	-0.51007300
H	-4.48424200	1.73865800	0.95165000
H	-4.03054700	2.85943100	-0.35409000
C	-4.22426100	-0.58561500	-0.43754500
H	-3.68335500	-1.39457600	-0.93575900
H	-4.16333900	-0.75377300	0.64539500
H	-5.28094400	-0.62597300	-0.73661800
C	-3.58744100	0.98752300	-2.30031100
H	-3.15471500	1.97106700	-2.52768200
H	-2.98439800	0.21317500	-2.78488500
H	-4.60177300	0.95640900	-2.72026700
C	1.63676100	-1.01199300	0.35094800

H	2.62668100	-1.31728000	-0.01378800
H	0.94142400	-1.83925300	0.18315000
H	2.06254900	1.96741700	-1.34627000

1e

M06 SCF energy (au)	-996.519590
M06 enthalpy (au)	-996.118335
M06 free energy (au)	-996.187432
M06 SCF energy in solution (au)	-996.817273
M06 enthalpy in solution (au)	-996.416018
M06 free energy in solution (au)	-996.485115

Cartesian coordinates

ATOM	X	Y	Z
C	0.14560200	3.04512700	-0.96857900
O	-0.12442400	3.57912400	0.10523600
N	-0.43897900	3.41752400	-2.13966900
C	-1.40914000	4.39741900	-2.35504500
C	-1.90204100	4.46446600	-3.69715000
C	-1.90043900	5.26725600	-1.40350200
C	-2.88646100	5.43221500	-4.03097100
C	-2.87919400	6.21981700	-1.75697600
H	-1.52933800	5.20699300	-0.38677600
C	-1.84730900	3.63839300	-5.83474500
C	-3.33566700	5.45192100	-5.37051400
C	-3.36825900	6.31249700	-3.03508700
H	-3.24737700	6.89360100	-0.98524400
C	-2.82111100	4.55936800	-6.27568700
H	-4.09046000	6.18195300	-5.66435200
H	-4.12430200	7.05138900	-3.29925700
H	-3.14759900	4.55047400	-7.31307300
N	-1.40029000	3.58469800	-4.60068100
H	-1.42458300	2.91793300	-6.53821600
C	1.14623200	1.05921700	-2.27639300
H	2.10004000	0.81540900	-2.74914600
C	0.04187500	0.48564600	-2.75518000
H	0.08107400	-0.20024600	-3.59878600
C	1.24133100	1.97907900	-1.08764600
H	2.16921800	2.57037000	-1.18990800
H	-0.94604200	0.67790600	-2.33372700
C	1.44943300	1.21476300	0.26178600
C	0.18760100	0.45993700	0.69986100
C	2.61238000	0.23114100	0.12683500
C	0.42364500	-0.30884200	1.99596700
H	-0.10301900	-0.24462000	-0.09667600
H	-0.64274100	1.17049500	0.82393400
C	2.85842100	-0.52723200	1.42581500
H	2.38451500	-0.49031800	-0.67405900
H	3.51167600	0.79044900	-0.17602100
C	1.59978000	-1.26887300	1.86171000
H	-0.48936900	-0.85215100	2.27847400
H	0.63151900	0.41057300	2.80203800
H	3.69488400	-1.22838200	1.29409200
H	3.15598600	0.18699800	2.20694500
H	1.77331500	-1.80083500	2.80811200
H	1.35429600	-2.03919700	1.10903800
O	1.85018200	2.14419400	1.24602700
H	1.15014000	2.82369900	1.26359100
H	-0.20349500	2.90055000	-2.98619600

3d

M06 SCF energy (au)	-996.545614
M06 enthalpy (au)	-996.142768
M06 free energy (au)	-996.210819
M06 SCF energy in solution (au)	-996.835662
M06 enthalpy in solution (au)	-996.432816
M06 free energy in solution (au)	-996.500867

Cartesian coordinates

ATOM	X	Y	Z
C	-0.42977000	1.91159800	-0.54324300
O	-1.09750600	2.19506000	0.43659200
N	-0.58317800	2.50745800	-1.77202800
C	-1.27834000	3.67917100	-2.06597500
C	-0.87884900	4.33353400	-3.27390300
C	-2.28210700	4.22356200	-1.29241900
C	-1.53408100	5.53084100	-3.66690200
C	-2.91451800	5.41757000	-1.69792200
H	-2.56746900	3.72807600	-0.37067800
C	0.50498800	4.37354500	-5.10206700
C	-1.09783500	6.13346800	-4.86780400
C	-2.56297600	6.06325300	-2.85636700
H	-3.70343300	5.82535800	-1.06818800
C	-0.08136000	5.56086300	-5.58882100
H	-1.57874400	7.05291100	-5.20302400
H	-3.05963800	6.98305900	-3.16392100
H	0.27648800	6.00326700	-6.51566300
N	0.12963300	3.77653000	-3.99309200
H	1.31932800	3.90373500	-5.65762300
C	0.54077700	-0.09938100	0.63552700
H	0.88435500	-1.09532700	0.32729100
C	1.49763300	0.47940400	1.65977700
H	1.86311600	-0.24260300	2.39908200
C	0.68590500	0.88465800	-0.52598000
H	0.68823000	0.35970900	-1.49306700
H	1.02604800	1.32297400	2.19446000
C	2.10597800	1.52668300	-0.29920200
C	3.05703900	1.15396400	-1.43229100
C	2.10013300	3.04731200	-0.10066100
C	4.46469400	1.68852100	-1.20174600
H	2.65184800	1.57126600	-2.37225700
H	3.06218700	0.05766900	-1.53658900
C	3.50838700	3.57551700	0.14911800
H	1.69101600	3.53088000	-1.00434900
H	1.42916700	3.31078200	0.73049700
C	4.44451900	3.19870300	-0.99357900
H	5.11153500	1.42046000	-2.04911300
H	4.88592000	1.19962700	-0.31038800
H	3.47688400	4.66627800	0.27970600
H	3.88763100	3.15030400	1.09029300
H	5.45961500	3.57406800	-0.80107200
H	4.09850100	3.68839600	-1.92108600
O	2.60062300	0.90909400	0.89174100
H	-0.49124500	-0.16877800	0.99479600
H	0.08225100	2.26760800	-2.50531800

IM1e

M06 SCF energy (au)	-1352.250507
M06 enthalpy (au)	-1351.801547
M06 free energy (au)	-1351.885483

M06 SCF energy in solution (au)	-1352.612957
M06 enthalpy in solution (au)	-1352.163997
M06 free energy in solution (au)	-1352.247933

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.11838300	2.30984900	-3.76468200
C	-0.05551000	0.10683400	-5.57209600
O	-0.27373300	-0.56167300	-4.57040600
O	0.27466000	1.37217700	-5.57426000
C	-0.15202100	-0.47075300	-6.96705900
H	-0.30921300	-1.55148500	-6.91726300
H	-0.99365000	-0.00905400	-7.49954600
H	0.75404200	-0.24691700	-7.54131700
C	0.16264400	3.10550800	-0.89442600
O	-0.28367200	3.52791100	0.16916500
N	-0.31700700	3.42991300	-2.13110400
C	-1.34067300	4.35976300	-2.33681700
C	-1.85185400	4.40769800	-3.66321200
C	-1.87646100	5.24742100	-1.41303800
C	-2.86155300	5.32523100	-4.04597400
C	-2.88076000	6.15892900	-1.79496600
H	-1.51867400	5.22746700	-0.39082700
C	-1.75477400	3.50569100	-5.82089000
C	-3.29506500	5.28793300	-5.38960500
C	-3.37419600	6.21354500	-3.07581200
H	-3.27135000	6.83746800	-1.03842000
C	-2.74887900	4.38981600	-6.27372200
H	-4.07037700	5.98377100	-5.71040500
H	-4.15213600	6.92161900	-3.35720900
H	-3.06955400	4.34674200	-7.31111500
N	-1.33458800	3.52403600	-4.57012400
H	-1.27750500	2.76622600	-6.46452400
C	1.15186200	1.18947400	-2.10503600
H	0.43364600	0.38234900	-1.93273400
C	1.93990200	1.15562900	-3.22942000
H	1.89880800	0.30872400	-3.90793500
C	1.36370500	2.16003000	-0.98037300
H	2.22386000	2.80032000	-1.24425700
H	2.77389900	1.85170800	-3.34175600
C	1.64610000	1.43902800	0.36842800
C	2.58962300	0.24891300	0.19742300
C	2.25627000	2.40098200	1.39944400
C	4.01662000	0.65301300	-0.15199800
H	2.18061400	-0.45738300	-0.53918700
H	2.58363000	-0.28425100	1.16151200
C	3.69275400	2.81063000	1.08887000
H	1.61029800	3.28116300	1.51048700
H	2.23348000	1.86146100	2.36058700
C	4.59016900	1.59367100	0.90149800
H	4.04275500	1.14709800	-1.13879800
H	4.64145900	-0.24573900	-0.24861700
H	3.72565700	3.43253200	0.17785700
H	4.07372400	3.45014000	1.89758600
H	4.66510000	1.05188600	1.85961900
H	5.61104200	1.90082500	0.63354400
O	0.43283700	0.89638600	0.85121100
H	-0.13595700	1.65914000	1.05536000

TS10e

M06 SCF energy (au)	-1931.145290
M06 enthalpy (au)	-1930.426202
M06 free energy (au)	-1930.531850
M06 SCF energy in solution (au)	-1931.669118
M06 enthalpy in solution (au)	-1930.950030
M06 free energy in solution (au)	-1931.055678

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.64023500	1.87463500	-3.85594800
C	-1.36484800	-0.54678100	-5.46734500
O	-1.30473900	-1.27884600	-4.45893000
O	-1.27797200	0.72556100	-5.46775800
C	-1.57198800	-1.19350700	-6.81864000
H	-2.53745600	-1.71342600	-6.82697000
H	-1.54041500	-0.46643000	-7.63433700
H	-0.79831200	-1.95622200	-6.97428200
C	0.93679300	2.64056000	-1.51259500
O	1.51247500	3.32710700	-0.67694800
N	0.03805300	3.10063300	-2.43849900
C	-0.30118700	4.44015000	-2.62006500
C	-1.05805200	4.73123400	-3.79963300
C	0.01741600	5.49990900	-1.78067400
C	-1.47007100	6.05505800	-4.10048800
C	-0.39867300	6.80968900	-2.08741100
H	0.59897700	5.30089700	-0.88797200
C	-2.05310000	3.90747600	-5.74549900
C	-2.20663200	6.25072200	-5.29092300
C	-1.12721600	7.10052400	-3.21518800
H	-0.12770800	7.60980000	-1.40007000
C	-2.49837000	5.19064900	-6.11264200
H	-2.53495900	7.25931000	-5.54340500
H	-1.44326500	8.11772500	-3.44288200
H	-3.06130800	5.32277400	-7.03312200
N	-1.36900500	3.69528500	-4.63965600
H	-2.25057900	3.02657100	-6.35654500
C	0.29978800	0.47570600	-2.67125400
H	0.71696200	-0.33673700	-3.27360700
C	-0.85515200	0.09466100	-1.93221700
H	-1.47321200	-0.73145700	-2.28014400
C	1.25378100	1.14947800	-1.70408000
H	2.27272000	1.15627600	-2.12208000
H	-1.33754000	0.82683800	-1.28336500
C	1.27701200	0.23291600	-0.41887600
C	2.52921800	-0.64154000	-0.43734000
C	1.13640700	0.95613000	0.91281700
C	2.61788000	-1.58955900	0.75282400
H	3.39518800	0.04038200	-0.42580900
H	2.57247800	-1.19298000	-1.39244200
C	1.22354100	0.00295700	2.10017700
H	1.92326500	1.72033000	0.96516300
H	0.18446200	1.50798800	0.92406800
C	2.50713200	-0.81811400	2.06250400
H	3.56294000	-2.15001200	0.70683400
H	1.81221700	-2.34022600	0.69367200
H	1.16489000	0.57929100	3.03383100
H	0.35604300	-0.67455400	2.09195600
H	2.55229700	-1.50526700	2.91888100
H	3.37399200	-0.14130400	2.15530300
O	0.10213900	-0.65163400	-0.49667700

H	0.35293500	-1.49146100	-0.95398900
C	0.81334400	-3.47540700	-3.08797800
O	0.25600900	-3.37571300	-4.27474300
O	0.50478900	-2.77178100	-2.13438100
H	-0.41677000	-2.62183500	-4.30340200
C	1.88719400	-4.53970700	-3.02549800
C	2.44584600	-4.66267500	-1.60443900
C	1.31673800	-5.90067100	-3.46879600
C	3.03444100	-4.15057300	-3.98110500
H	1.63118500	-4.90896600	-0.90498300
H	2.85053600	-3.68917000	-1.28369100
C	3.53998600	-5.73069400	-1.55927600
H	0.90492400	-5.81450800	-4.48457600
H	0.48399900	-6.18463000	-2.80423500
C	2.41613300	-6.96404100	-3.42227500
H	3.44086800	-3.16812300	-3.68429100
H	2.64266200	-4.04459300	-5.00332400
C	4.13303300	-5.21498100	-3.93383000
H	3.92610000	-5.80876000	-0.53153100
C	2.95897500	-7.07828400	-1.99554400
C	4.67504300	-5.33321700	-2.50713800
H	1.99441900	-7.93040400	-3.73816100
C	3.55060400	-6.56268500	-4.36953000
H	4.94486300	-4.92331100	-4.61750300
H	2.15388700	-7.38353400	-1.30773900
H	3.73586800	-7.85818100	-1.94795600
H	5.11579700	-4.37464600	-2.18849200
H	5.47958900	-6.08512800	-2.47092500
H	4.33844800	-7.33287200	-4.36204500
H	3.17448600	-6.49609200	-5.40301500

IM10e

M06 SCF energy (au)	-1931.152432
M06 enthalpy (au)	-1930.432125
M06 free energy (au)	-1930.538674
M06 SCF energy in solution (au)	-1931.678176
M06 enthalpy in solution (au)	-1930.957869
M06 free energy in solution (au)	-1931.064418

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.61213000	1.90528600	-3.86112500
C	-1.32897900	-0.60801100	-5.36152000
O	-1.30671600	-1.29802400	-4.31566100
O	-1.23789500	0.65667100	-5.41894600
C	-1.49506500	-1.32687300	-6.68259100
H	-2.46912800	-1.83061500	-6.70177700
H	-1.41886300	-0.64597700	-7.53446300
H	-0.73036200	-2.11012800	-6.76579500
C	0.92897300	2.70370000	-1.51182600
O	1.47959000	3.37335500	-0.64211000
N	0.06105900	3.16065200	-2.46053900
C	-0.28802300	4.49517200	-2.64652500
C	-1.05774400	4.77672800	-3.82339200
C	0.03246800	5.55963500	-1.81352700
C	-1.47861100	6.09943300	-4.11992100
C	-0.39149800	6.86670000	-2.11936900
H	0.62060500	5.36395900	-0.92407900
C	-2.07151800	3.95108000	-5.75387500
C	-2.23057500	6.29319200	-5.30123800

C	-1.13229200	7.14942700	-3.24103700
H	-0.11809700	7.67058700	-1.43717700
C	-2.52836700	5.23166200	-6.11787600
H	-2.56565000	7.30082400	-5.54910400
H	-1.45636500	8.16417300	-3.46921200
H	-3.10380800	5.36024900	-7.03130300
N	-1.37172900	3.73785900	-4.65862400
H	-2.27543400	3.07150800	-6.36501100
C	0.25511400	0.53132200	-2.65979600
H	0.71274300	-0.28262400	-3.23738800
C	-0.75730100	-0.01427700	-1.72329200
H	-1.38017000	-0.81868600	-2.11656900
C	1.24947400	1.21486000	-1.71634100
H	2.25478000	1.21554200	-2.16626500
H	-1.34520500	0.73967000	-1.18742800
C	1.30692000	0.32117200	-0.44715100
C	2.54640300	-0.55893000	-0.43273900
C	1.05607600	0.97598000	0.89675700
C	2.59171000	-1.54148100	0.73210300
H	3.40050900	0.13398000	-0.36139400
H	2.64125800	-1.07426900	-1.40264800
C	1.10294100	-0.01581200	2.05464000
H	1.81916200	1.75788100	1.01160100
H	0.09622900	1.51188700	0.87053300
C	2.40156900	-0.81345500	2.05735200
H	3.54918100	-2.08102200	0.71474200
H	1.80931200	-2.30927800	0.60837900
H	0.98474500	0.52936700	3.00074700
H	0.24926300	-0.70791300	1.98450900
H	2.41493400	-1.52656100	2.89285400
H	3.25009900	-0.12616600	2.21558500
O	0.10568100	-0.62898400	-0.63125300
H	0.40682800	-1.49290500	-1.04974800
C	0.86116400	-3.47666400	-2.98902000
O	0.24936200	-3.34656900	-4.13583700
O	0.63040500	-2.78316500	-2.00019300
H	-0.42160000	-2.57451900	-4.15107000
C	1.91249900	-4.56475500	-2.98631300
C	2.50162800	-4.75015100	-1.58408100
C	1.31018400	-5.89832900	-3.46773200
C	3.04459200	-4.15634500	-3.95329400
H	1.69916400	-5.01185300	-0.87596000
H	2.92845800	-3.79596100	-1.23503600
C	3.57895200	-5.83599600	-1.60518500
H	0.87724900	-5.76700400	-4.46961400
H	0.48789900	-6.19488700	-2.79575700
C	2.39297800	-6.97935900	-3.48687500
H	3.47339700	-3.19242100	-3.62872900
H	2.63102800	-4.00541100	-4.96129200
C	4.12611400	-5.23888300	-3.97170000
H	3.98697600	-5.95935300	-0.59046200
C	2.96614700	-7.15673800	-2.07870400
C	4.69837000	-5.41969500	-2.56354600
H	1.94832300	-7.92607500	-3.82933000
C	3.51204500	-6.55968500	-4.44449100
H	4.92662000	-4.93344400	-4.66254400
H	2.17216900	-7.47585500	-1.38430400
H	3.73114300	-7.94960800	-2.07892800
H	5.16173300	-4.48085400	-2.21926600
H	5.49132200	-6.18446600	-2.57464000

H	4.28723800	-7.34151900	-4.48444200
H	3.11393900	-6.44797600	-5.46569600

TS11e

M06 SCF energy (au)	-1931.147371
M06 enthalpy (au)	-1930.432806
M06 free energy (au)	-1930.536813
M06 SCF energy in solution (au)	-1931.671658
M06 enthalpy in solution (au)	-1930.957093
M06 free energy in solution (au)	-1931.061100

Cartesian coordinates

ATOM	X	Y	Z
Pd	-0.52275500	1.96851200	-3.87991100
C	-0.77606700	-0.58976800	-5.44266500
O	-1.10013400	-1.19997500	-4.35552600
O	-0.80504100	0.65017200	-5.54450000
C	-0.37869800	-1.43074600	-6.62023600
H	-1.24146500	-2.01843400	-6.95684600
H	-0.01288700	-0.80974300	-7.44087000
H	0.39191900	-2.14873500	-6.31190500
C	0.80821600	2.78761300	-1.41679400
O	1.25712200	3.47552000	-0.50671300
N	-0.04887300	3.21064500	-2.39803400
C	-0.48124200	4.52332600	-2.56879200
C	-1.17452300	4.79788400	-3.79353400
C	-0.30735300	5.57219900	-1.67485500
C	-1.66648700	6.09948700	-4.07572300
C	-0.80149300	6.85745200	-1.96690200
H	0.22303700	5.38279000	-0.74871400
C	-1.96790200	3.98783700	-5.83000700
C	-2.33378300	6.29050100	-5.30685600
C	-1.46984400	7.13374900	-3.13455400
H	-0.64321500	7.64895700	-1.23573100
C	-2.48667200	5.24682000	-6.18438200
H	-2.72071800	7.28186700	-5.54421200
H	-1.84901100	8.13149400	-3.35213600
H	-2.99446000	5.37335200	-7.13724700
N	-1.34419700	3.77543600	-4.68893100
H	-2.05903600	3.12554700	-6.49094500
C	0.33450200	0.62381600	-2.64427100
H	0.87310500	-0.15592600	-3.20225800
C	-0.66731900	-0.00718900	-1.73419400
H	-1.26524600	-0.81664800	-2.15404700
C	1.24800700	1.33501800	-1.64385700
H	2.26839900	1.41827700	-2.04931000
H	-1.30420400	0.71140000	-1.20396800
C	1.30269300	0.39654900	-0.40436500
C	2.61129700	-0.37610400	-0.34192300
C	0.93456500	0.98968100	0.94315000
C	2.66939400	-1.39324000	0.79159500
H	3.39625300	0.38426900	-0.19559200
H	2.80562500	-0.85193900	-1.31527600
C	0.98971400	-0.03747300	2.06946500
H	1.63319600	1.81720200	1.12861400
H	-0.05955300	1.45628600	0.88252600
C	2.34434700	-0.73358400	2.12621600
H	3.66724500	-1.85303300	0.81435400
H	1.96192300	-2.21299900	0.58844600
H	0.77221400	0.46175600	3.02353400

H	0.19889300	-0.78937900	1.92186800
H	2.36242300	-1.47522800	2.93664200
H	3.12472400	0.01019200	2.36232400
O	0.19784300	-0.61858400	-0.69150100
H	0.56099800	-1.49240900	-1.18870900
C	0.99052900	-3.33742300	-2.89584200
O	0.25579200	-3.15742000	-3.91103400
O	1.01138200	-2.64375000	-1.84717500
H	-0.54604800	-2.13098200	-4.13839900
C	1.93483100	-4.53147000	-2.97455800
C	2.82177100	-4.64943000	-1.73066900
C	1.10187900	-5.81963900	-3.11978800
C	2.83279400	-4.38869300	-4.21798500
H	2.18938200	-4.73802100	-0.83363000
H	3.40984800	-3.72508300	-1.60633000
C	3.74790700	-5.86173200	-1.85443100
H	0.45292100	-5.73388300	-4.00368000
H	0.44305600	-5.93090200	-2.24214900
C	2.02656400	-7.03238700	-3.24176100
H	3.42728800	-3.46226600	-4.13796400
H	2.20093300	-4.29291500	-5.11351000
C	3.75984600	-5.59960300	-4.34127400
H	4.37681600	-5.93134100	-0.95344600
C	2.90624400	-7.13351200	-1.99290600
C	4.63679100	-5.70288000	-3.09082600
H	1.41689600	-7.94377000	-3.34149300
C	2.91601600	-6.87029000	-4.47769100
H	4.39561000	-5.47974400	-5.23222500
H	2.27777600	-7.26965000	-1.09785600
H	3.56242800	-8.01620800	-2.06308300
H	5.26300200	-4.80114100	-2.99273700
H	5.32111100	-6.56223100	-3.17897900
H	3.57227900	-7.74870800	-4.58836700
H	2.29447900	-6.81541500	-5.38603300

IM3e

M06 SCF energy (au)	-1702.192724
M06 enthalpy (au)	-1701.541316
M06 free energy (au)	-1701.635176
M06 SCF energy in solution (au)	-1702.644031
M06 enthalpy in solution (au)	-1701.992623
M06 free energy in solution (au)	-1702.086483

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.61101400	2.82200100	-4.02549000
C	-0.11639800	0.86780600	-6.12066100
O	-1.14195300	0.66631000	-5.30822900
O	0.74884000	1.71277900	-5.88625000
C	1.29037600	3.23181900	-1.22753700
O	1.31115700	3.66010000	-0.07994100
N	0.49516500	3.70560500	-2.24630200
C	-0.43527300	4.72678000	-2.12940000
C	-1.21112900	5.00935400	-3.30286400
C	-0.68330900	5.49139100	-0.99368600
C	-2.19053900	6.04007300	-3.29753400
C	-1.65880300	6.50436000	-1.00354400
H	-0.10665700	5.28710900	-0.09880100
C	-1.67089500	4.50545200	-5.52913000
C	-2.90695400	6.26494200	-4.49387300

C	-2.40579000	6.78925000	-2.12110900
H	-1.81580200	7.07635400	-0.09007700
C	-2.65327200	5.50782900	-5.61001000
H	-3.66167900	7.05162500	-4.51184700
H	-3.15631500	7.57861400	-2.12107000
H	-3.19032700	5.66666400	-6.54177500
N	-0.98399900	4.26423200	-4.42938400
H	-1.43427300	3.88232300	-6.39372200
C	2.12447200	1.76967600	-3.16903400
H	3.01388400	2.16549400	-3.68023200
C	2.04168400	0.24381300	-3.25500700
H	2.81392900	-0.18759300	-3.90760900
C	2.14612500	2.06144000	-1.66543800
H	3.17274200	2.26760800	-1.32086100
H	1.06290100	-0.11197800	-3.63565500
C	1.72609300	0.71673000	-1.02715700
C	2.38430000	0.47452100	0.32130600
C	0.20614100	0.55120900	-0.91162100
C	1.99905100	-0.87212800	0.92400100
H	2.08503400	1.30064600	0.98646200
H	3.47469200	0.54250300	0.19008400
C	-0.16402100	-0.81435300	-0.34602900
H	-0.17992300	1.34333400	-0.24971600
H	-0.26846800	0.71057400	-1.89304200
C	0.48533900	-1.02569000	1.01706600
H	2.46026600	-0.98360800	1.91570200
H	2.40776900	-1.67553900	0.29152100
H	-1.25711900	-0.90821600	-0.27354000
H	0.18037600	-1.59599300	-1.04196400
H	0.22211700	-2.01339100	1.42241100
H	0.08646800	-0.27777100	1.72427300
O	2.25823700	-0.24294000	-1.94753000
H	-1.02625700	1.26983400	-4.52963100
C	-0.06836700	-0.04990200	-7.30786600
C	0.93362500	0.46548100	-8.34808200
C	0.40542700	-1.43126000	-6.79383000
C	-1.45479500	-0.20975700	-7.95707400
H	1.92023600	0.59292000	-7.87948400
H	0.62084300	1.46150100	-8.70050600
C	1.01620600	-0.51625100	-9.51855200
H	-0.29547900	-1.80354000	-6.03088400
H	1.39057600	-1.32215300	-6.31086600
C	0.49164800	-2.40863200	-7.96846300
H	-1.81400600	0.77258500	-8.30687000
H	-2.17815900	-0.57262700	-7.21300500
C	-1.36075100	-1.18903900	-9.12981800
H	1.73411300	-0.13114400	-10.25774300
C	1.48672200	-1.87970900	-9.00435100
C	-0.36412400	-0.66110600	-10.16450900
H	0.82939800	-3.38519200	-7.59071400
C	-0.88952900	-2.55188700	-8.61377400
H	-2.35577600	-1.29046000	-9.58833300
H	2.48924200	-1.79034900	-8.55660700
H	1.57036600	-2.59080800	-9.84126000
H	-0.70330200	0.31155900	-10.55598900
H	-0.31026900	-1.35105400	-11.02137700
H	-0.84198400	-3.27263800	-9.44516300
H	-1.61077400	-2.95082200	-7.88280100

TS3e

M06 SCF energy (au)	-1702.162035
M06 enthalpy (au)	-1701.516149
M06 free energy (au)	-1701.610373
M06 SCF energy in solution (au)	-1702.608344
M06 enthalpy in solution (au)	-1701.962458
M06 free energy in solution (au)	-1702.056682

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.35556500	2.35444500	-3.88702700
C	0.96838800	0.74487600	-6.15475700
O	2.13679000	1.04451000	-5.79243300
O	-0.06467200	1.12839500	-5.51926400
C	1.54832000	3.35929100	-1.43094500
O	1.72422400	4.00276000	-0.40391500
N	0.53878100	3.56911400	-2.32945600
C	-0.51817400	4.45230800	-2.14648200
C	-1.58613800	4.30011800	-3.07667300
C	-0.64641300	5.43301600	-1.17188900
C	-2.74540700	5.11325500	-3.02551600
C	-1.80014600	6.24013300	-1.12519000
H	0.15017300	5.55963700	-0.44774500
C	-2.40466600	3.11239500	-4.91831600
C	-3.74415900	4.87202900	-3.99509900
C	-2.83415300	6.10201200	-2.02101200
H	-1.86299000	6.99959100	-0.34737500
C	-3.58065900	3.88246300	-4.93438300
H	-4.64660500	5.48343600	-3.98325800
H	-3.71766400	6.73671100	-1.97227200
H	-4.33961500	3.68271600	-5.68615700
N	-1.45545100	3.32138200	-4.02497400
H	-2.21894000	2.31306800	-5.63573600
C	2.36254500	1.56724200	-3.20648900
H	3.31570800	1.84572900	-3.68314900
C	2.34457500	0.04908500	-2.94819500
H	3.06193300	-0.49322900	-3.57685000
C	2.42480500	2.18049300	-1.78087400
H	3.45898800	2.49979000	-1.58373600
H	1.34300900	-0.38024500	-3.14445900
C	2.16733200	0.96110800	-0.85349100
C	2.94448300	1.05147400	0.45024900
C	0.67968000	0.72188000	-0.56923300
C	2.72407800	-0.16821500	1.33882000
H	2.62810400	1.97259900	0.96463800
H	4.01179100	1.16555100	0.20842500
C	0.47350500	-0.52174000	0.28732700
H	0.28205500	1.60317400	-0.03906900
H	0.11343100	0.64722200	-1.51111600
C	1.24100200	-0.40518200	1.59925200
H	3.26753300	-0.04145100	2.28583900
H	3.15250800	-1.05281900	0.84276400
H	-0.59879400	-0.67231500	0.47650100
H	0.82783300	-1.40377800	-0.26934200
H	1.09696400	-1.30605900	2.21278300
H	0.83344600	0.44054600	2.18007400
O	2.71446300	-0.12519900	-1.60294400
H	1.97356900	1.62371400	-4.51325200
C	0.78031600	-0.17333200	-7.34291300
C	1.80595700	0.13862600	-8.44303500
C	1.02583800	-1.60971000	-6.82868900

C	-0.63636400	-0.09185300	-7.92405700
H	2.81973300	0.09304000	-8.02103500
H	1.65633000	1.16923800	-8.80496000
C	1.65293300	-0.85629700	-9.59534400
H	0.30538500	-1.83713700	-6.02492300
H	2.03539300	-1.67078800	-6.39169700
C	0.87423900	-2.60457600	-7.98175400
H	-0.83463800	0.93586500	-8.27156300
H	-1.37259200	-0.31028100	-7.13625200
C	-0.78357700	-1.08436700	-9.08017500
H	2.39031000	-0.61837600	-10.37698700
C	1.89535500	-2.27594100	-9.07448900
C	0.23839000	-0.75878100	-10.17244000
H	1.04969000	-3.62286800	-7.60248000
C	-0.53983400	-2.50432500	-8.56041400
H	-1.80216600	-1.01136700	-9.49113000
H	2.91839200	-2.36231000	-8.67482200
H	1.80896500	-3.00121400	-9.89944600
H	0.06037600	0.25470500	-10.56727500
H	0.12452000	-1.45760300	-11.01673200
H	-0.66388700	-3.23244900	-9.37799700
H	-1.28403800	-2.75739500	-7.78807400

IM4e

M06 SCF energy (au)	-1702.194930
M06 enthalpy (au)	-1701.542663
M06 free energy (au)	-1701.638190
M06 SCF energy in solution (au)	-1702.636738
M06 enthalpy in solution (au)	-1701.984471
M06 free energy in solution (au)	-1702.079998

Cartesian coordinates

ATOM	X	Y	Z
Pd	0.02062500	2.12690100	-4.05684200
C	0.99457400	0.15813400	-5.18462700
O	1.10275600	0.29591300	-3.92663600
O	0.36158100	1.06602600	-5.82543500
C	0.22922800	2.56779300	-1.04175400
O	-0.20143800	2.94830900	0.04278700
N	-0.25038900	3.03705900	-2.25055200
C	-1.12071900	4.12600800	-2.31837900
C	-1.52606100	4.48052500	-3.63389400
C	-1.60104400	4.92792700	-1.28559400
C	-2.35858300	5.59387000	-3.91360900
C	-2.42953100	6.03341000	-1.56032700
H	-1.33246200	4.69087400	-0.26466800
C	-1.38166500	3.93077100	-5.90980900
C	-2.67833400	5.83797000	-5.26672600
C	-2.81218500	6.38021800	-2.83443500
H	-2.77554700	6.62926000	-0.71701200
C	-2.19604200	5.01907100	-6.26035500
H	-3.31589800	6.68794900	-5.50978100
H	-3.45501100	7.23773500	-3.02633300
H	-2.43318000	5.19258400	-7.30642900
N	-1.07043500	3.68997300	-4.64781400
H	-0.97587800	3.23942300	-6.64728200
C	0.72806000	0.16665200	-0.65809600
H	1.29003100	-0.65543900	-1.12099300
C	0.97171800	0.22705500	0.84028100
H	1.05682300	-0.76536200	1.30410400

C	1.30672800	1.51211700	-1.12522400
H	1.68563300	1.44386900	-2.14795600
H	0.16381600	0.78125400	1.34346100
C	2.50556800	1.68961100	-0.15985500
C	3.75768800	1.09302800	-0.81965800
C	2.80055600	3.12216300	0.27985000
C	4.96557400	1.13865200	0.10585300
H	3.97593700	1.67225500	-1.73411700
H	3.54329700	0.06129500	-1.13983800
C	4.02343100	3.19298000	1.18868600
H	2.97100700	3.73315100	-0.62563200
H	1.91883600	3.52717700	0.78821400
C	5.25289900	2.57236500	0.53631000
H	5.84108500	0.69775700	-0.39234200
H	4.75555900	0.52222100	0.99314100
H	4.21930500	4.23829100	1.46775800
H	3.79435400	2.65315500	2.12025500
H	6.11274100	2.60712400	1.22102200
H	5.53399700	3.16664200	-0.35141100
O	2.20079200	0.90584500	1.00131400
H	-0.32996400	0.04062500	-0.92408600
C	1.55293800	-1.03668200	-5.90156900
C	2.27551900	-0.59336800	-7.18585800
C	2.52321500	-1.82053600	-5.00868800
C	0.37208400	-1.95394000	-6.29000100
H	3.10822300	0.08077000	-6.92600100
H	1.58238400	-0.02032400	-7.81893900
C	2.80021600	-1.82085600	-7.93344700
H	2.01089300	-2.12720700	-4.08430200
H	3.35672800	-1.16759000	-4.70436500
C	3.04702900	-3.04417700	-5.76429300
H	-0.33765800	-1.39053000	-6.91542400
H	-0.16603900	-2.26237800	-5.37847900
C	0.89783900	-3.18010800	-7.03974500
H	3.31981500	-1.49080100	-8.84586300
C	3.77154600	-2.59128100	-7.03509500
C	1.62430300	-2.72694200	-8.30932700
H	3.74472900	-3.59557200	-5.11622600
C	1.87125700	-3.94950700	-6.14276600
H	0.04853200	-3.82672900	-7.30821000
H	4.63141400	-1.95381200	-6.77334000
H	4.17125200	-3.46520200	-7.57402600
H	0.92818200	-2.18843200	-8.97242400
H	1.98769700	-3.60434900	-8.86781200
H	2.23785300	-4.84582300	-6.66822300
H	1.35437800	-4.29788500	-5.23416400