Total Synthesis of (+)-Shearilicine

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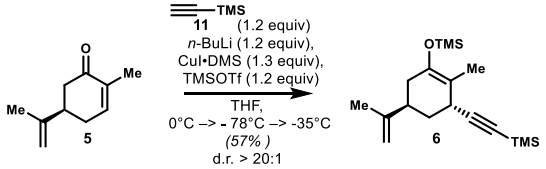
General Experimental

General Experimental Procedures: All reactions were carried out under an inert nitrogen atmosphere with dry solvents under anhydrous conditions unless otherwise stated. All reactions were capped with a rubber septum or Teflon-coated silicon microwave cap unless otherwise stated. Stainless steel cannula or syringes were used to transfer solvent, and air-and moisture-sensitive liquid reagents. Reactions were monitored by thin-layer chromatography (TLC) and carried out on 0.25 mm Merck silica gel plates (60F-254) using UV light as the visualizing agent and potassium permanganate or an acidic solution of *p*-anisaldehyde as developing agents. Flash column chromatography employed SiliaFlash®P60 (40–60 μm, 230–400 mesh) silica gel purchased from SiliCycle Inc.

Materials: All reaction solvents were purified using a Seca solvent purification system by Glass Contour, with the exception of *tert*-butanol and H_2O. *Tert*-butanol was purchased from Fischer Scientific and used as received. Deionized water was taken from the tap and used as is. $Sc(OTf)_3$, *n*-BuLi (2.7 M in Hex), MeLi (1.6 M in THF), CsF, $Zn(TMP)_2$, $Pd(OAc)_2$, 2-(Di-*tert*-butylphosphino)-1-phenylindole, $K_2OsO_4 \cdot 2H_2O$ and $(DHQ)_2PHAL$ were purchased from Sigma-Aldrich. CuI, $Mo(CO)_6$ and $CuSO_4$ were purchased from Strem Inc. The molarity of MeLi solutions and *n*-BuLi solutions was determined by titration with *N*-benzylbenzamide. All other reagents were used as received without further purification, unless otherwise stated.

Instrumentation: All new compounds were characterized by means of ^{1}H-NMR, ^{13}C-NMR, FT-IR (thin film), HR-MS and polarimetry. Copies of the ^{1}H-and ^{13}C-NMR spectra can be found at the end of each experimental procedure. NMR spectra were recorded using a Varian 400 MHz NMR spectrometer, Varian 500 MHz NMR spectrometer, or Varian 600 MHz NMR spectrometer. All ^{1}H-NMR data are reported in δ units, parts per million (ppm), and were calibrated relative to the signals for residual chloroform (7.26 ppm) in deuterochloroform ($CDCl_3$) or for residual dichloromethane (5.33 ppm) in dichloromethane-d_2 (CD_2Cl_2). All ^{13}C-NMR data were reported in ppm relative to $CDCl_3$ (77.16 ppm) or CD_2Cl_2 (54.24 ppm), and were obtained with ^{1}H decoupling unless otherwise stated. The following abbreviations or combinations thereof were used to explain the multiplicities: s= singlet, d= doublet, t= triplet, q= quartet, br= broad, m= multiplet, and a= apparent. All IR spectra were taken on an FT-IR/Raman Thermo Nicolet 6700. High resolution mass spectra (HR-MS) were recorded on a Bruker microTOF mass spectrometer using ESI-TOF (electrospray ionization-time of flight). All optical rotations were taken on a Rudolph Research Analytical Autopol VI Automatic Polarimeter.

Synthesis of Silyl Enol Ether 6:



A flame-dried, three-necked, 1 L round-bottomed flask was equipped with a magnetic stir bar, fitted with two dropping funnels, sealed with a rubber septum, evacuated and backfilled with nitrogen three times and placed under a nitrogen atmosphere. **11** (11.7 g, 119.8 mmol, 1.2 equiv) was added to the reaction flask in a single portion via syringe and dissolved in anhydrous THF (150 mL, 0.80 M). The reaction apparatus was cooled to 0 °C by transferring to an ice-water bath. After stirring at this temperature for 10 minutes, *n*-BuLi (2.7 M solution in hexanes, 45.0 mL 119.8 mmol, 1.2 equiv) was added dropwise via the dropping funnel over the course of 10 minutes. The resulting solution was left to stir at 0 °C for 20 minutes, after which CuI·DMS (35.4 g, 129.8 mmol, 1.3 equiv) was added to the flask as a solid in a single portion. This reaction mixture was stirred at 0 °C for an additional 1 hour, after which it was cooled to –78 °C by transferring the reaction apparatus to a dry ice-acetone bath.

After stirring at –78 °C for 10 minutes, freshly distilled trimethylsilyl trifluoromethanesulfonate (22 mL, 119.8 mmol, 1.2 equiv) was added to the flask dropwise via the second dropping funnel over the course of 10 minutes. Following this, the reaction mixture was allowed to stir for 5 minutes at –78 °C before a solution of (*R*)–carvone (**5**) (15.0 g, 99.9 mmol, 1.0 equiv) in anhydrous THF (109 mL, 1.1 M) was added to the flask by cannula over a span of 20 minutes. Once the addition was completed, the reaction was allowed to stir for 5 minutes at –78 °C, after which the reaction apparatus was transferred to a dry ice-acetonitrile bath to warm the reaction mixture to –35 °C.

After stirring at –35 °C for 3 hours, the reaction was quenched by pouring into sat. aq. NH_4Cl (500 mL). The layers were separated and the aqueous layer was extracted with Et_2O (3 × 500 mL). The combined organic layers were rinsed with sat. aq. $NaHCO_3$ (3 × 500 mL), washed with brine (500 mL) and concentrated under reduced pressure by rotary evaporation to provide a mixture of crude yellow liquid and bright yellow solids. The mixture was filtered through a silica plug with hexane as the washing solvent to afford a crude yellow liquid. Purification by flash column chromatography on silica gel (0% to 2% Et_2O in pentane) afforded **6** (18.2 g, 57%, d.r. >20:1) as a colorless clear liquid.

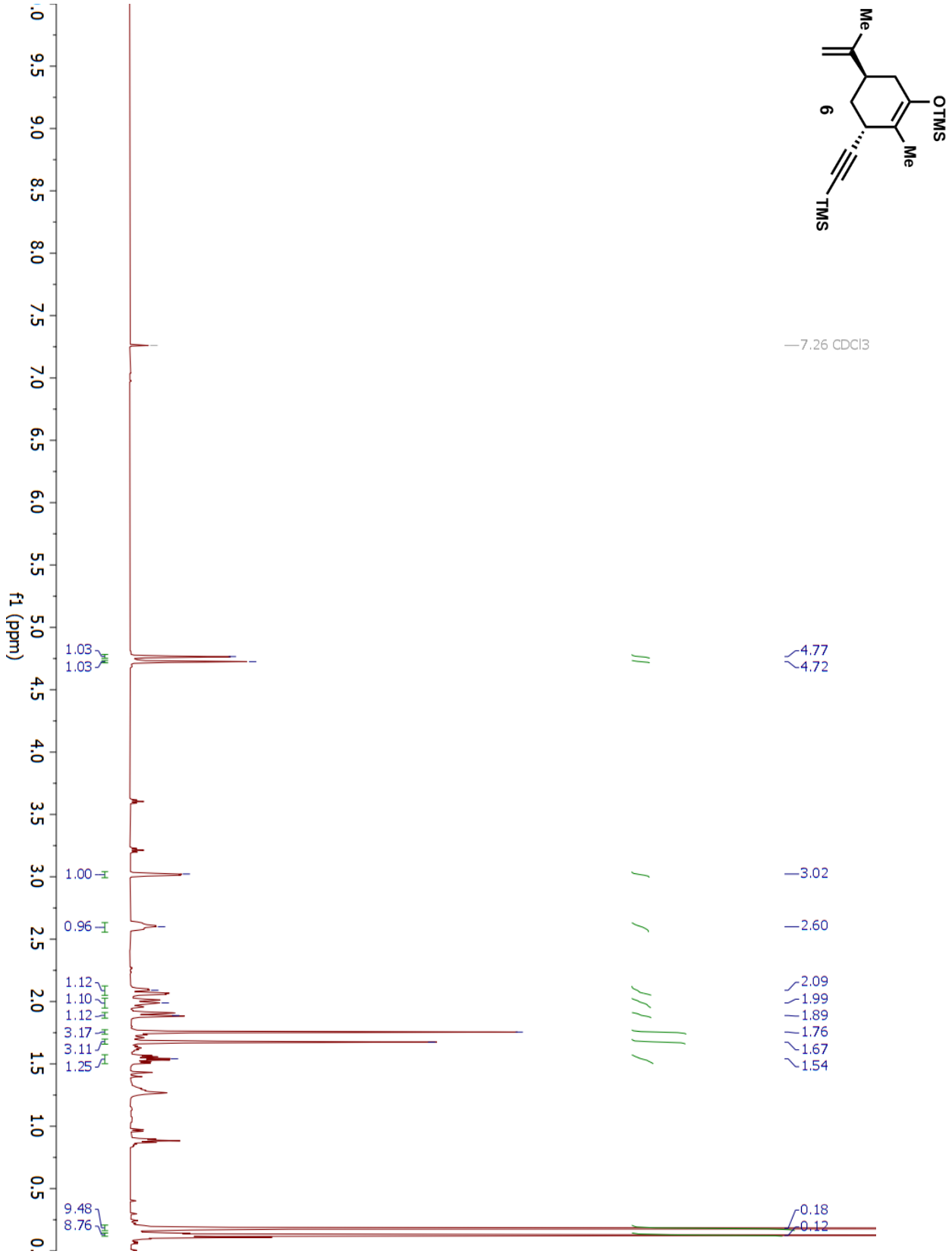
R_f: 0.85 (2% Et_2O/98% hexanes)

^{1}H NMR (500 MHz, $CDCl_3$): δ 4.77 (s, 1H), 4.72 (s, 1H), 3.02 (d, *J* = 4.8 Hz, 1H), 2.60 (td, *J* = 10.7, 4.1 Hz, 1H), 2.08 (dd, *J* =16.5, 5.1 Hz, 1H), 2.02–1.95 (m, 1H), 1.89 (add, *J* = 12.4, 1.6 Hz, 1H), 1.74 (s, 3H), 1.67 (s, 3H), 1.53 (atd, *J* = 12.8, 5.4 Hz, 1H), 0.18 (s, 9H), 0.12 (s, 9H)

^{13}C NMR (125 MHz, $CDCl_3$): δ 148.8, 144.1, 111.7, 109.9, 109.1, 84.4, 38.4, 35.7, 34.1, 33.3, 21.1, 15.1, 0.8, 0.3

IR (cm^{-1}): 2163, 1688, 1447, 1184, 1065, 927, 833, 757, 697, 637

Optical Rotation: $[\alpha]_D^{20}$ = +139.43° (*c* 0.18, $CHCl_3$)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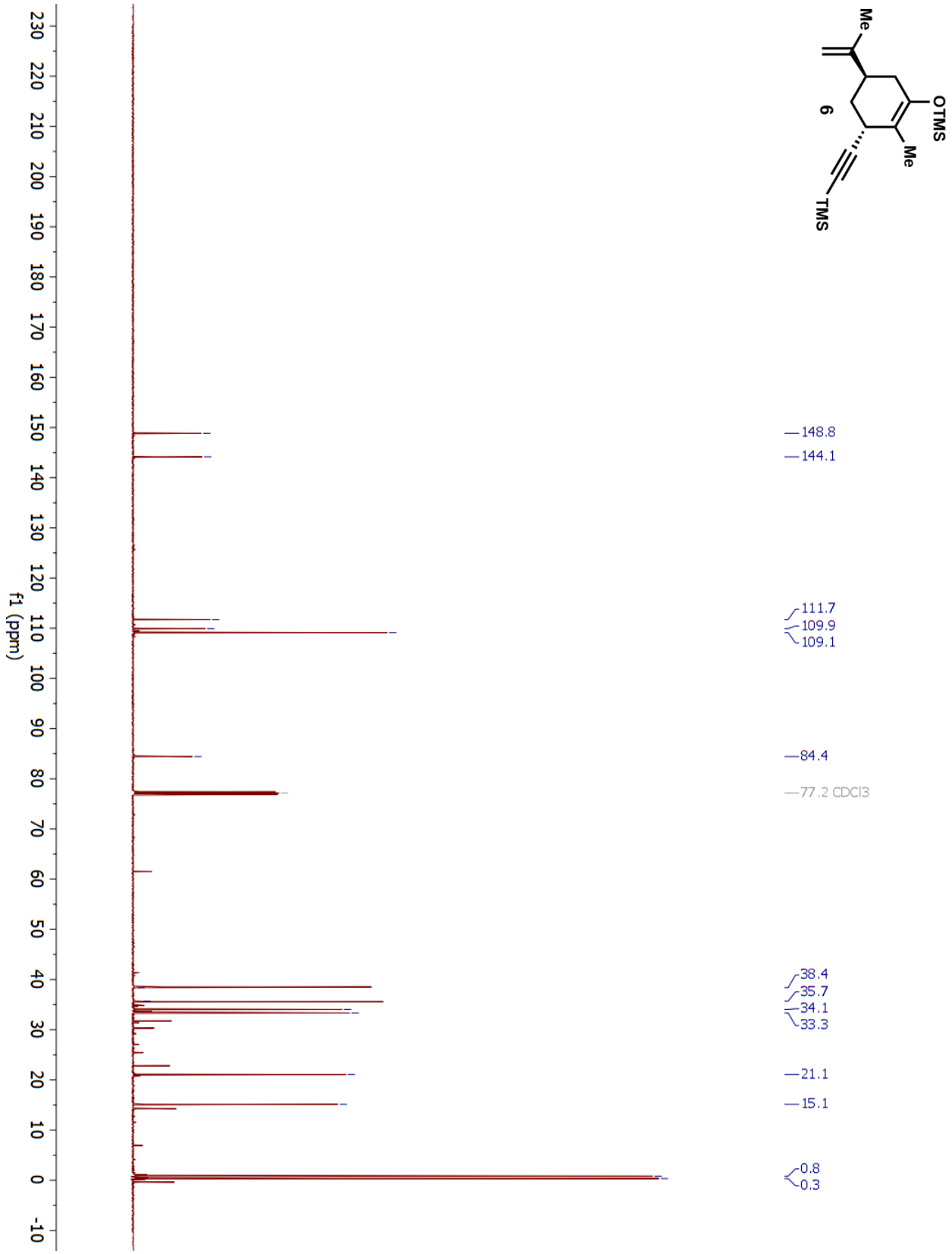
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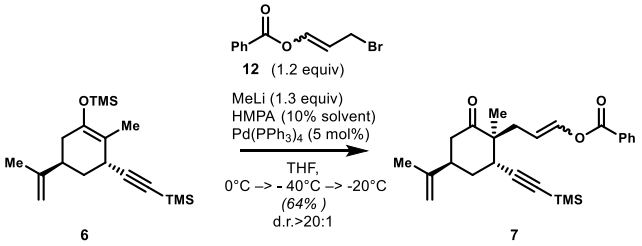
f1 (ppm)

Synthesis of Ketone 7:



A flame-dried, 1 L round-bottomed flask was equipped with a magnetic stir bar, sealed with a rubber septum, and was charged with **12**[1] (20.4 g, 84.3 mmol, 1.2 equiv), which was prepared according to reported procedures. The flask was then evacuated and backfilled with nitrogen three times and placed under a nitrogen atmosphere. **12** was dissolved in anhydrous THF (350 mL, 0.24 M) and cooled to 0 °C by transferring the reaction apparatus to an ice-water bath. $Pd(PPh_3)_4$ (4.06 g, 3.51 mmol, 5 mol%) was added to the mixture in a single portion and the solution was left to stir at 0 °C for 1 hour while the other flask was being prepared.

An additional flame-dried 2 L round-bottomed flask was equipped with a magnetic stir bar, fitted with a dropping funnel, and charged with **6** (22.5 g, 70.2 mmol, 1.0 equiv), after which the reaction apparatus was evacuated and backfilled with nitrogen three times and placed under a nitrogen atmosphere. **6** was dissolved in anhydrous THF (350 mL, 0.2 M) and the resulting solution was cooled to 0 °C by transferring the reaction apparatus to an ice-water bath. After stirring at this temperature for 15 minutes, MeLi (1.6 M solution in Et_2O, 58.0 mL, 91.3 mmol, 1.3 equiv) was added dropwise via the dropping funnel over the course of 10 minutes. The resulting solution was left to stir at 0 °C for 30 minutes, after which the dropping funnel was replaced with a rubber septum and HMPA (35.0 mL, 2.4 M) was added to the reaction as a single portion via syringe. The resulting solution was cooled to –40 °C by transferring the reaction apparatus to an acetonitrile-dry ice bath. The solution containing **12** and $Pd(PPh_3)_4$ in the first reaction flask was slowly cannulated into the flask containing **6** in a dropwise fashion over 30 minutes, after which the resulting solution was left to stir for 4 hours, during which the mixture was gradually warmed to –20 °C.

After stirring for 4 hours, the reaction was warmed to room temperature and quenched by pouring into sat. aq. NH_4Cl (800 mL). The layers were separated and the aqueous layer was extracted with Et_2O (3 × 800 mL). The combined organic layers were washed with brine (500 mL), dried over anhydrous $NaSO_4$, and concentrated under reduced pressure by rotary evaporation to provide a dark brown oil. Purification by flash column chromatography on silica gel (0 to 4% Et_2O in hexanes) afforded pale yellow viscous oil **7** (18.4 g, 64%, d.r.>20:1) as an inseparable mixture of *E* and *Z* isomers (5:1).

Rf: 0.26 (10% Et_2O in hexanes)

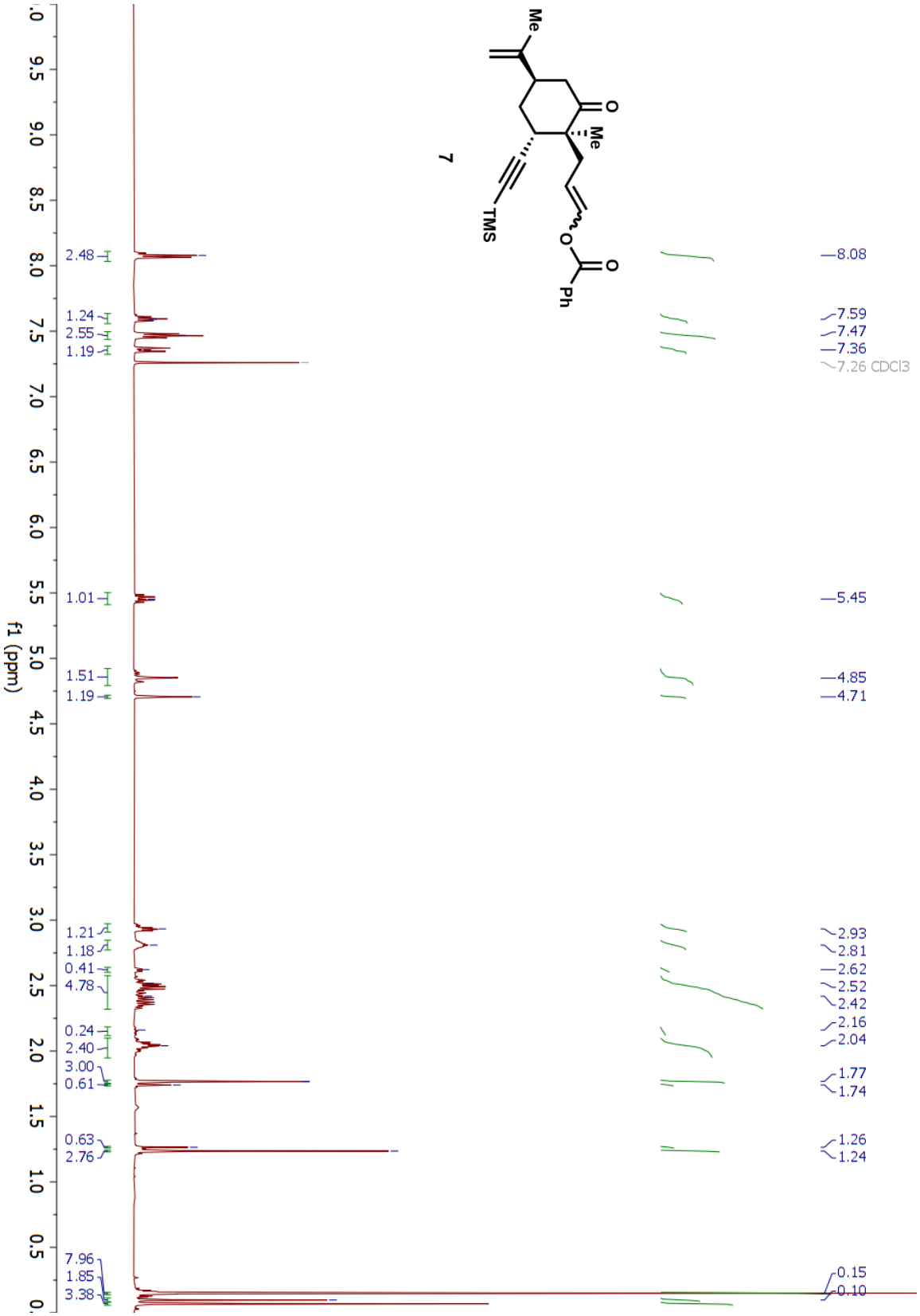
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10–8.06 (m, 2.4H), 7.63–7.57 (m, 1.2H), 7.46 (at, *J* = 9.5 Hz, 2.4H), 7.38–7.34 (m, 1.2H), 5.48–5.43 (m, 1H), 4.85 (m, 1.4H), 4.71 (ov, 1.2H), 2.97–2.92 (m, 1.2H), 2.84–2.77 (m, 1.2H), 2.62 (m, 0.4H), 2.57–2.32 (m, 4.8 H), 2.10–1.95 (m, 2.4H), 1.77 (s, 3H), 1.74 (s, 0.6H), 1.26 (s, 0.6H), 1.24 (s, 3H), 0.15 (s, 9H), 0.10 (s, 1.8 H)

^{13}C NMR (125 MHz, $CDCl_3$): δ 212.6, 212.5, 163.7, 163.5, 147.1, 146.9, 137.9, 136.8, 133.8, 133.7, 130.1, 129.2, 128.8, 128.7, 111.3, 110.7, 109.8, 108.6, 106.2, 106.0, 89.2, 89.0, 51.0, 50.9, 42.6, 42.6, 41.2, 41.0, 38.0, 36.8, 34.9, 32.2, 31.1, 30.6, 21.5, 21.3, 20.6, 20.5, 1.2, 0.2, 0.1

IR (cm^{-1}): 2957, 1730, 1713, 1263, 1258, 1128, 843, 760, 752

ESI-HRMS (m/z): $[M+H]^+$ calc'd for $C_{25}H_{33}O_3Si^+$: 409.2194; found: 409.2188

Optical Rotation: $[\alpha]_D^{20} = -13.88°$ (*c* 1.2, $CHCl_3$)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0.24
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0.63
2.76
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7.59
7.47
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7.26 CDCl3
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4.71
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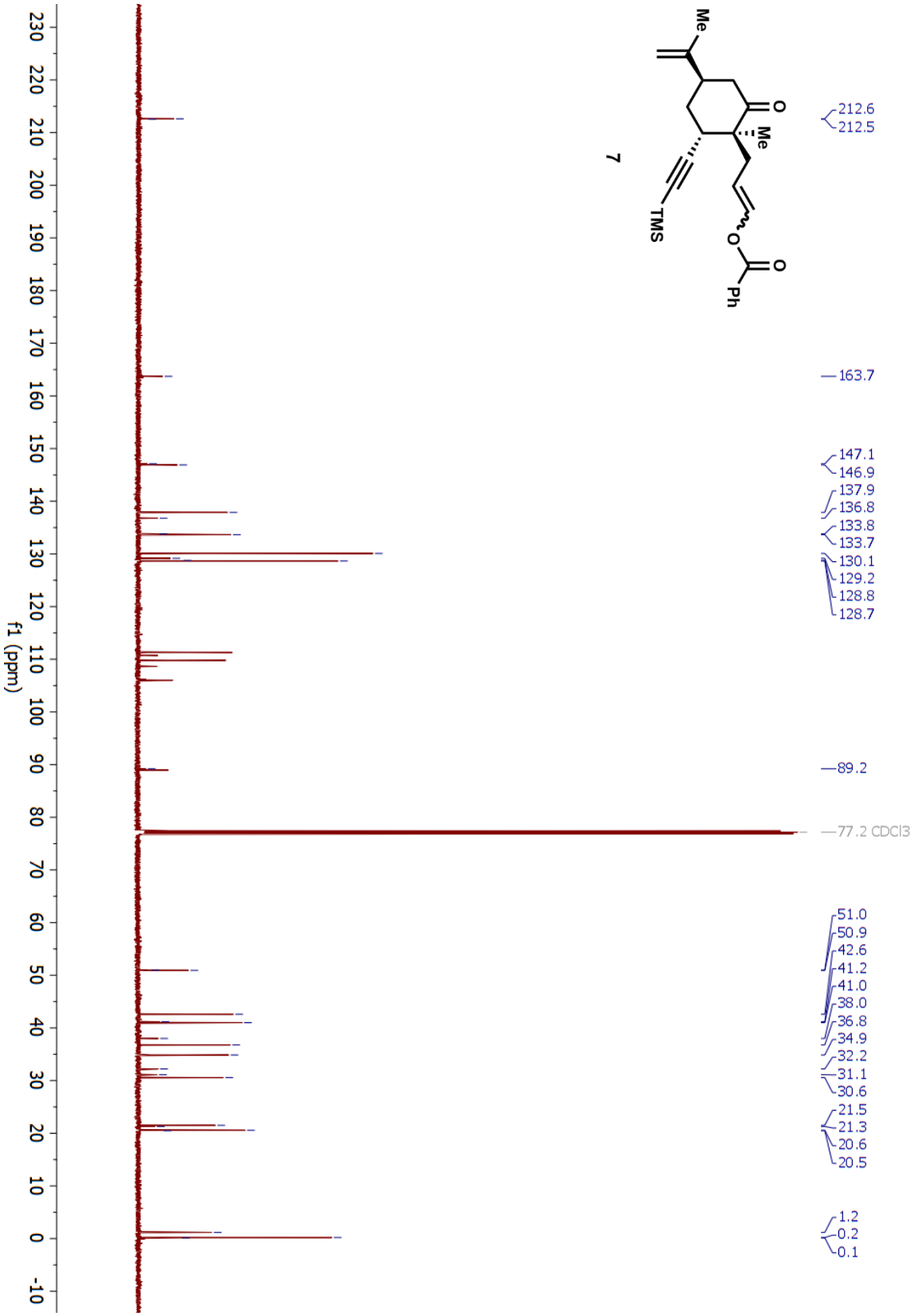
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40
30
20
10
0
-10
Me
O
Me
TMS
O
O
Ph
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212.6
212.5
163.7
147.1
146.9
137.9
136.8
133.8
133.7
130.1
129.2
128.8
128.7
89.2
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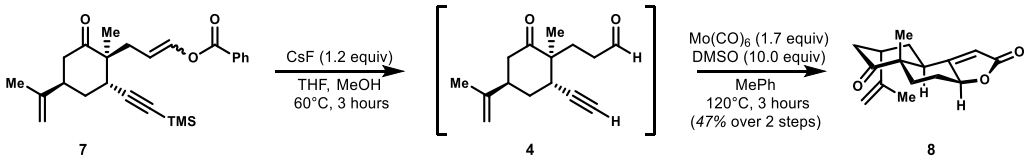
0.1

Synthesis of Butenolide 8:



7 4 8

A 1L round-bottomed flask was equipped with a magnetic stir bar, fitted with a reflux condenser and charged with **7** (21.6 g, 52.8 mmol, 1.0 equiv), after which the reaction flask was placed under a nitrogen atmosphere. **7** was dissolved in a 1:1 mixture of methanol and THF (520 mL, 0.1 M). CsF (9.6 g, 63.4 mmol, 1.2 equiv) was added to the solution as a solid in a single portion. The resulting solution was heated to 60 °C by transferring the reaction apparatus to a preheated oil bath. The reaction mixture was stirred at this temperature for 3 hours.

After the starting material was fully consumed, the reaction apparatus was allowed to cool to room temperature and quenched by pouring into $NaHCO_3$ (500 mL). The layers were separated and the aqueous layer was extracted with DCM (3 × 500 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated by rotary evaporation under reduced pressure. The crude material (**4**) was afforded as a yellow, viscous oil and was directly subjected to the subsequent reaction conditions without further purification.

A flame-dried 1L round-bottomed flask was equipped with a magnetic stir bar and charged with crude **4** and $Mo(CO)_6$ (23.7 g, 89.8 mmol, 1.7 equiv). The reaction flask was evacuated and placed under a carbon monoxide atmosphere. Toluene (350 mL, 0.15 M) and DMSO (37.5 mL, 528 mmol, 10.0 equiv) were sequentially added to the reaction flask. The resulting solution was sparged with carbon monoxide for 20 minutes. Following this, the reaction apparatus was fitted with a reflux condenser, sealed with a rubber septum and placed under a carbon monoxide atmosphere. The reaction apparatus was transferred to an oil bath and was heated to 120 °C. The reaction was allowed to stir for 3 hours at this temperature after which the reaction apparatus was transferred out of the oil bath and allowed to cool to room temperature.

The reaction mixture was quenched by pouring into sat. aq. $NaHCO_3$ (350 mL). The layers were separated and the aqueous layer was extracted with EtOAc (3 × 350 mL). The combined organic layers were washed with brine (500 mL), dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure by rotary evaporation to provide a crude orange solid. Purification by flash column chromatography on silica gel (0 to 30% EtOAc in hexanes) afforded **8** (6.46 g, 47% over two steps) as a yellow granular solid.

R_f: 0.32 (5% Et_2O in DCM)

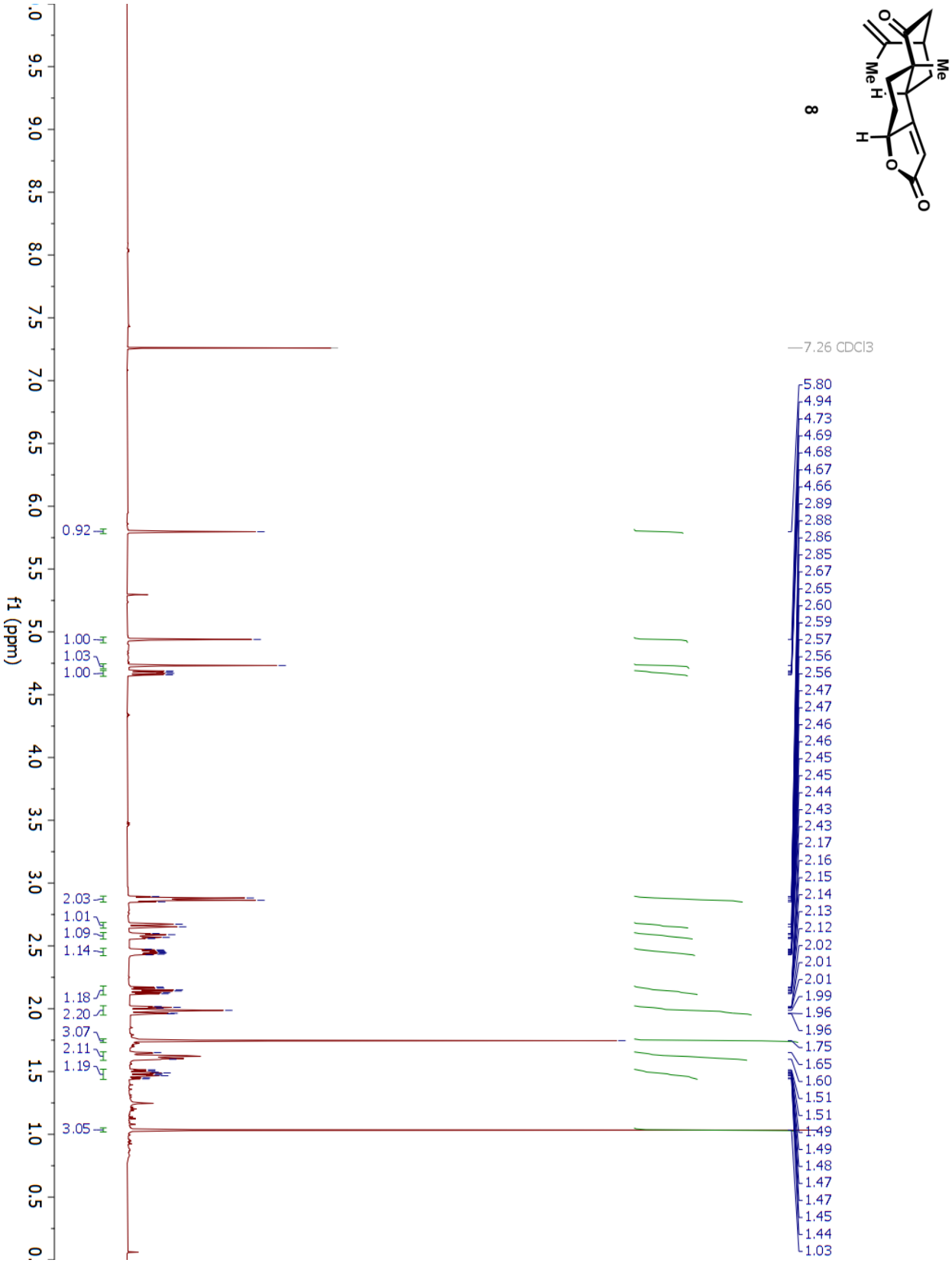
^{1}H NMR (600 MHz, $CDCl_3$): δ 5.80 (s, 1H), 4.94 (s, 1H), 4.73 (s, 1H), 4.67 (dd, *J* = 10.7, 7.2 Hz, 1H), 2.89–2.85 (m, 2H), 2.66 (d, *J* = 12.7 Hz, 1H), 2.58 (dd, *J* = 17.9, 4.9 Hz, 1H), 2.47–2.43 (m, 1H), 2.14 (atd, *J* = 13.6, 5.0 Hz, 1H), 1.99 (at, *J* = 14.5 Hz, 2H), 1.75 (s, 3H), 1.65–1.60 (m, 1H), 1.51–1.44 (m, 1H), 1.03 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$): δ 212.5, 173.0, 171.6, 146.4, 113.9, 113.6, 81.1, 51.0, 40.9, 40.5, 40.4, 29.3, 29.1, 24.4, 22.4, 17.1

IR (cm^{-1}): 2952, 1747, 1704, 1644, 1451, 1378, 1349, 1308, 1255, 1175, 1134, 1083, 1070, 1041, 1012, 937, 908, 852, 819, 728, 548, 509

ESI-HRMS (m/z): $[M+H]^+$ calc'd for $C_{16}H_{21}O_3^+$: 261.1548; found: 261.1491

Optical Rotation: $[\alpha]_D^{20}$ = +160.25 ° (*c* 0.2, $CHCl_3$)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4.66
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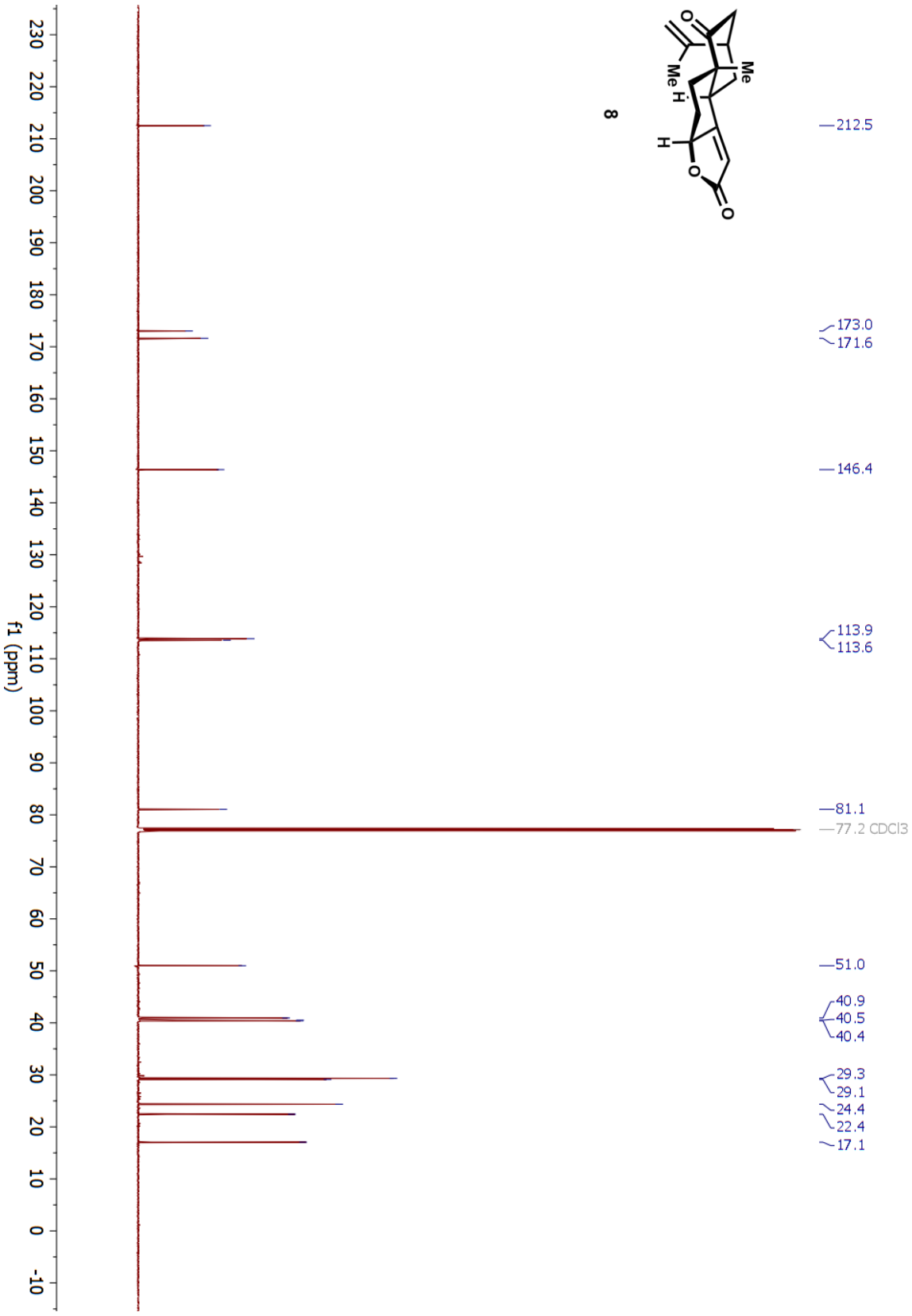
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O
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113.9
113.6
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40.5
40.4
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29.1
24.4
22.4
17.1
f1 (ppm)
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220
210
200
190
180
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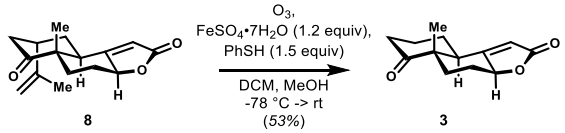


8 (878 mg, 3.373 mmol, 1.0 equiv) was transferred to an open 250 mL round-bottomed flask and dissolved in 3:1 mixture of MeOH and DCM (85.0 mL, 0.04M). This solution was cooled to –78 °C by transferring the reaction flask to a dry ice-acetone bath. The mixture was stirred for 10 minutes, before ozone was bubbled through the solution until full consumption of the starting material was observed by TLC (ca. 5 minutes of bubbling). (Note: a 50% EtOAc/50% Hexane mobile phase was used to visualize the progression of the reaction.) Bubbling of ozone was ceased and nitrogen was bubbled through the solution for 2 minutes. Following this, PhSH (0.52 mL, 5.059 mmol, 1.5 equiv) was added to the reaction mixture dropwise at -78 °C, followed by the immediate addition of $FeSO_4 \cdot 7H_2O$ (1.13 g, 4.065 mmol, 1.2 equiv) as a solid in a single portion.

The mixture was stirred at –78 °C for 15 minutes, after which the cooling bath was removed and the reaction was warmed to room temperature. The reaction was left to stir at ambient temperature overnight, after which the mixture was poured into H_2O (100 mL). The layers were separated and the aqueous layer was extracted with DCM (3 × 100 mL). The organic layers were combined and concentrated under reduced pressure by rotary evaporation to provide a crude orange solid. Purification by flash column chromatography on silica gel (0 to 2% Et_2O in DCM) afforded **3** (394 mg, 53%) as a white granular solid.

R_f: 0.21 (5% Et_2O in DCM)

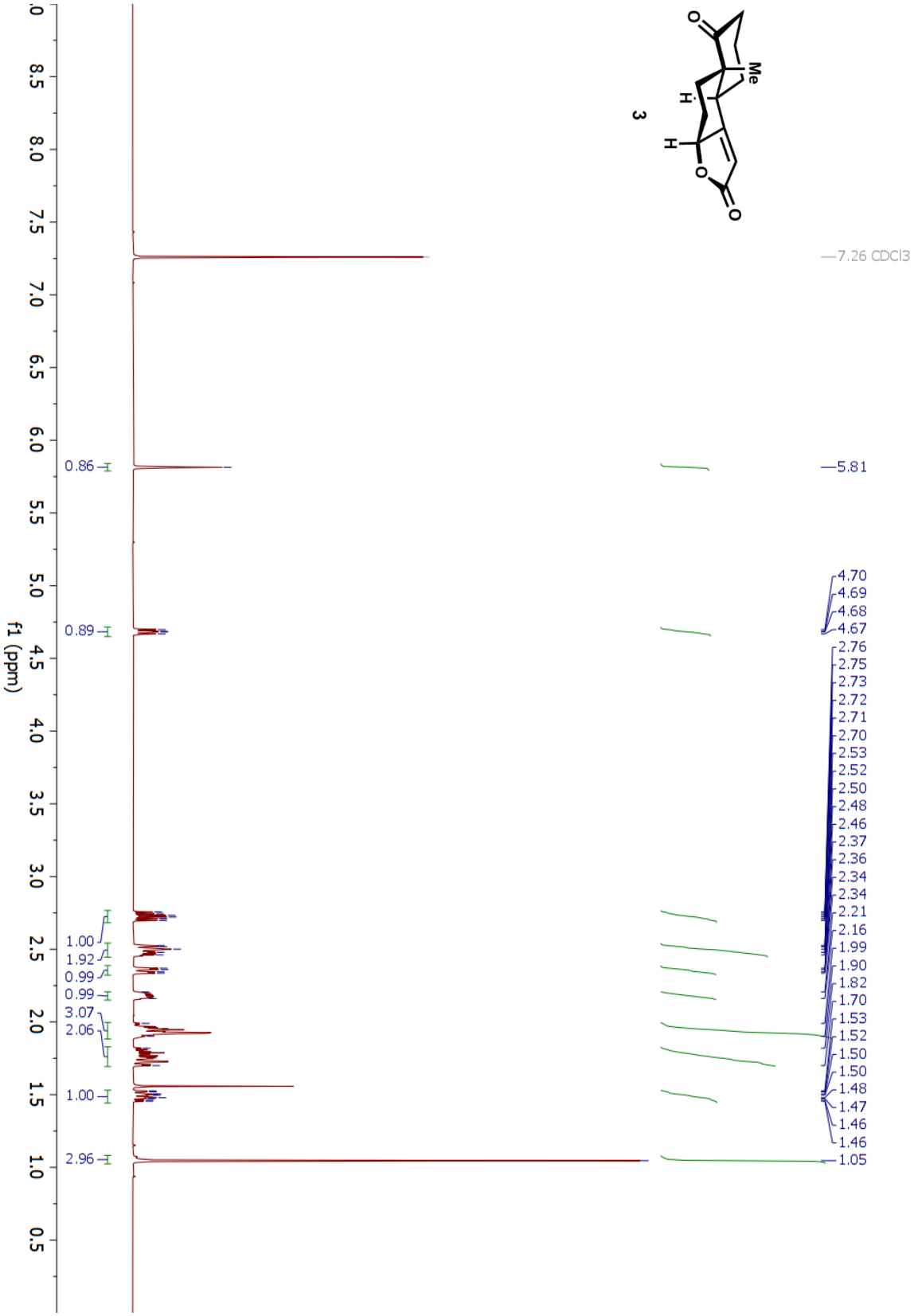
^{1}H NMR (600 MHz, $CDCl_3$): δ 5.81 (s, 1H), 4.68 (dd, *J* = 10.9, 7.2 Hz, 1H), 2.73 (atd, *J* = 14.5, 7.1 Hz, 1H), 2.53–2.46 (m, 2H), 2.35 (dd, *J* = 14.9, 5.1 Hz, 1H), 2.21–2.16 (m, 1H), 1.99–1.89 (m, 3H), 1.82–1.76 (m, 1H), 1.73 (atd, *J* = 14.7, 3.7 Hz, 1H), 1.49 (aqd, *J* = 14.9, 4.1 Hz, 1H), 1.05 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$): δ 212.5, 173.0, 171.3, 114.2, 81.0, 51.1, 47.0, 36.8, 29.3, 29.2, 25.3, 22.3, 16.9

IR (cm^{-1}): 2951, 1750, 1707, 1645, 1447, 1349, 1310, 1264, 1173, 1092, 1028, 941, 918, 891

ESI-HRMS (m/z): $[M+H]^+$ calc'd for $C_{13}H_{17}O_3^+$: 221.2681; found: 221.1178

Optical Rotation: $[\alpha]_D^{20}$ = +90.4 ° (*c* 0.2, $CHCl_3$)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1.52
1.50
1.50
1.48
1.47
1.46
1.46
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0.99
0.99
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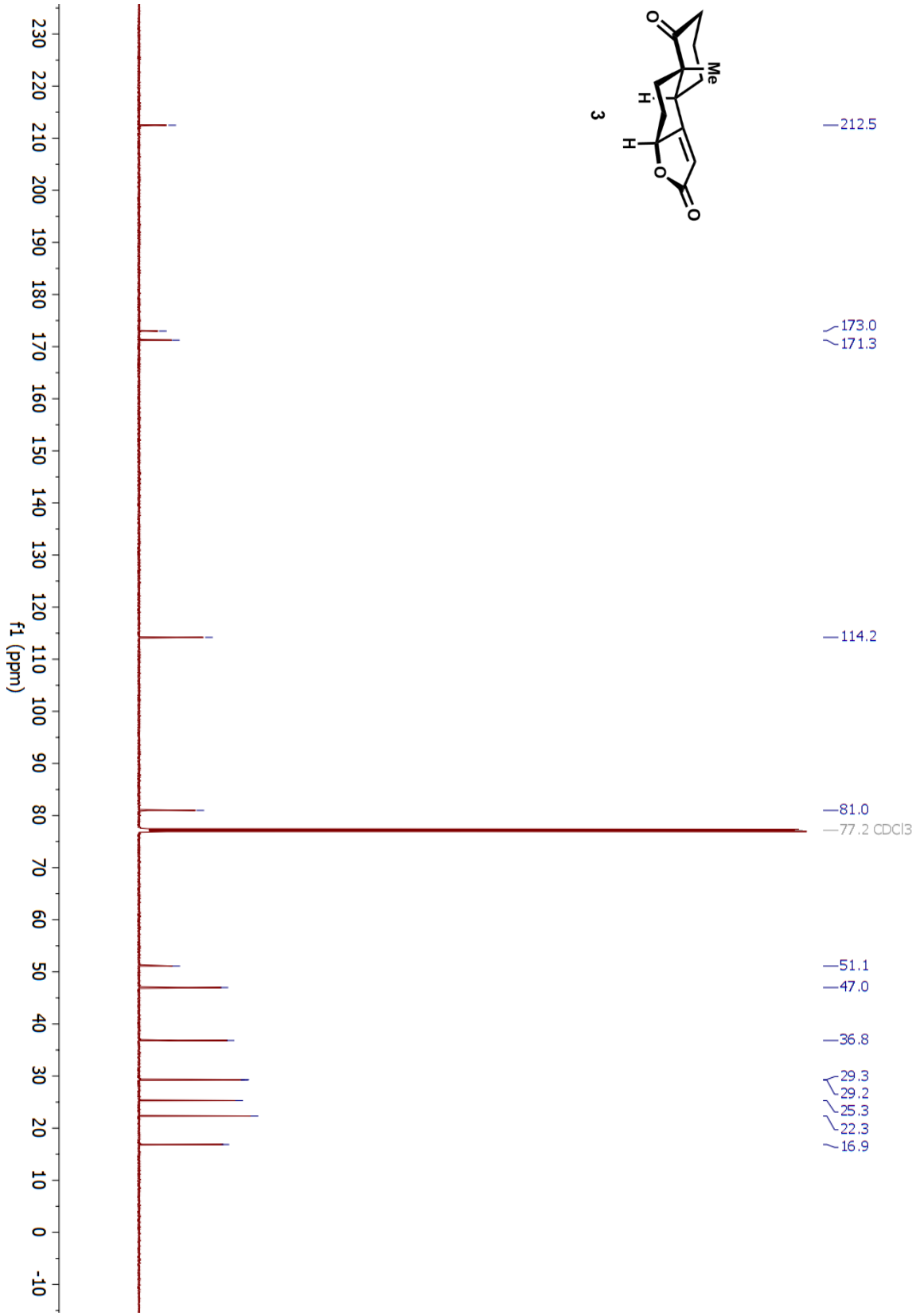
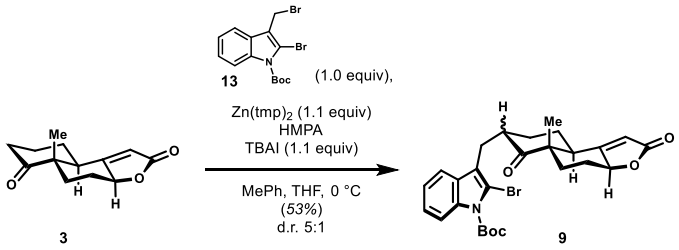
2.06
1.00
2.96
f1 (ppm)


3
Me
H
H
O
O
O
f1 (ppm)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
212.5
173.0
171.3
114.2
81.0
77.2 CDCl3
51.1
47.0
36.8
29.3
29.2
25.3
22.3
16.9

Synthesis of Indole 9:



A flame-dried, 25 mL round-bottomed flask equipped with a magnetic stir bar was charged with **3** (303 mg, 1.376 mmol, 1.0 equiv), sealed with a rubber septum, evacuated and backfilled with nitrogen three times, and placed under a nitrogen atmosphere. **3** was dissolved in anhydrous toluene (7.0 mL, 0.2 M) and HMPA (1.4 mL, 0.98 M) and the resulting solution was cooled to 0 °C by transferring the reaction apparatus to an ice-water bath. After stirring for 5 minutes, a solution of $Zn(TMP)_2$ (0.5 M in toluene, 3.0 mL 1.51 mmol, 1.1 equiv) was added to the reaction flask in a dropwise fashion over 5 minutes. The resulting enolate was stirred at 0 °C for 1 hour while another flask was prepared.

A flame-dried, 50 mL round-bottomed flask equipped with a magnetic stir bar was charged with **13**[2] (535 mg, 1.375 mmol, 1.0 equiv), sealed with a rubber septum, evacuated and backfilled with nitrogen three times, and placed under an atmosphere of nitrogen. The solid was dissolved in anhydrous THF (7.0 mL, 0.2 M) and HMPA (0.7 mL, 2.0M). The resulting solution was cooled to 0 °C by transferring the reaction apparatus to an ice-water bath and was left to stir at that temperature for 5 minutes, after which TBAI (559 mg, 1.513 mmol, 1.1 equiv) was added to the reaction flask as a solid in a single portion. The first reaction flask containing the enolate solution of **3** was removed from the cooling bath and its contents were slowly cannulated into the flask containing the solution of **13** in a dropwise fashion over 15 minutes. Upon addition of the enolate solution, the colorless reaction mixture became dark orange in color. The resulting reaction mixture was allowed to stir at 0 °C for 1 hour.

After this time, the reaction was quenched by pouring into sat. aq. $NaHCO_3$ (100 mL). The layers were separated and the aqueous layer was extracted with Et_2O (3 × 100 mL). The combined organic layers were washed with brine (500 mL), dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure by rotary evaporation to provide a crude orange foam. Purification by flash column chromatography on silica gel (0 to 40% Et_2O in hexanes) afforded **9** (383 mg, 53%, d.r. 5:1) as a white foam. Additionally, **3** was recovered (34 mg, 11%).

R_f: 0.51 (5% Et_2O in DCM)

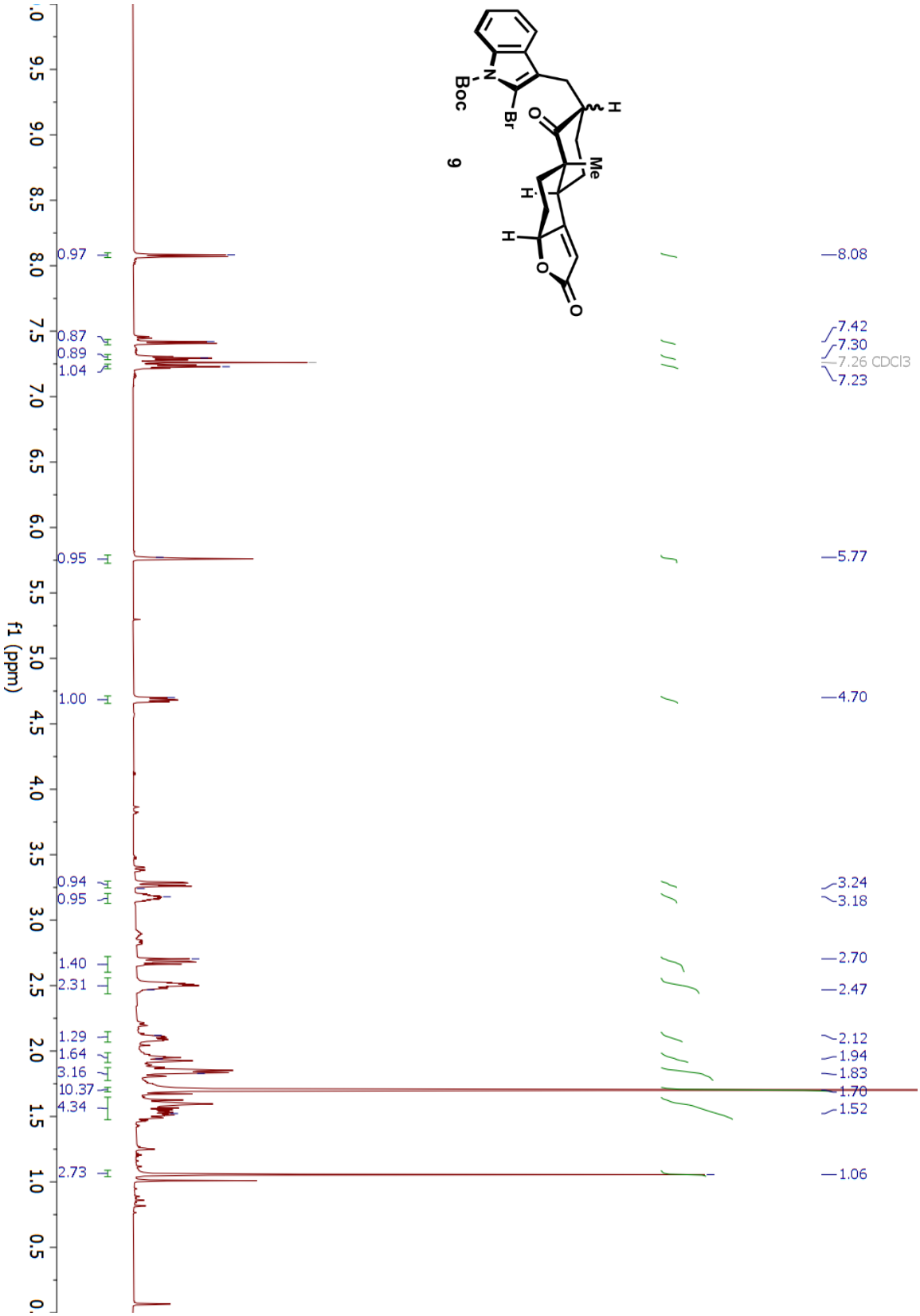
^{1}H NMR for **9-major isomer**(600 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.4 Hz, 1H), 7.41 (d, *J* = 7.4 Hz, 1H), 7.29 (at, *J* = 7.9 Hz, 1H), 7.23 (at, *J* = 7.4 Hz, 1H), 5.76 (s, 1H), 4.68 (dd, *J* = 10.4, 7.9 Hz, 1H), 3.27 (dd, *J* = 14.6, 4.0 Hz, 1H), 3.20–3.15 (m, 1H), 2.68 (dd, *J* = 14.6, 9.8 Hz, 1H), 2.52–2.48 (m, 2H), 2.12–2.08 (m, 1H), 1.88–1.80 (m, 3H), 1.70 (s, 9H), 1.36–1.49 (m, 3H), 1.06 (s, 3H)

^{13}C NMR for **9-major isomer** (151 MHz, $CDCl_3$): δ 212.9, 172.9, 171.0, 149.2, 136.6, 128.9, 124.8, 123.1, 121.1, 118.2, 115.6, 114.1, 109.9, 85.2, 80.9, 51.3, 47.9, 44.6, 32.3, 29.6, 29.2 28.4, 25.1, 22.5, 17.0

IR (cm^{-1}): 2943,1746, 1708, 1646, 1448, 1394, 1370, 1351, 1313, 1254, 1210, 1155, 1101, 1016, 974, 912, 843, 732

ESI-HRMS (m/z): $[M+H]^+$ calc'd for $C_{27}H_{31}BrNO_5^+$: 528.1386; found: 528.1385

Optical Rotation: $[\alpha]_D^{20}$ = +53.4 ° (*c* 0.9, $CHCl_3$)


f1 (ppm)
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Boc
N
Br
O
H
Me
H
H
O
O
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0.87
0.89
1.04
0.95
1.00
0.94
0.95
1.40
2.31
1.29
1.64
3.16
10.37
4.34
2.73
8.08
7.42
7.30
7.26 CDCl3
7.23
5.77
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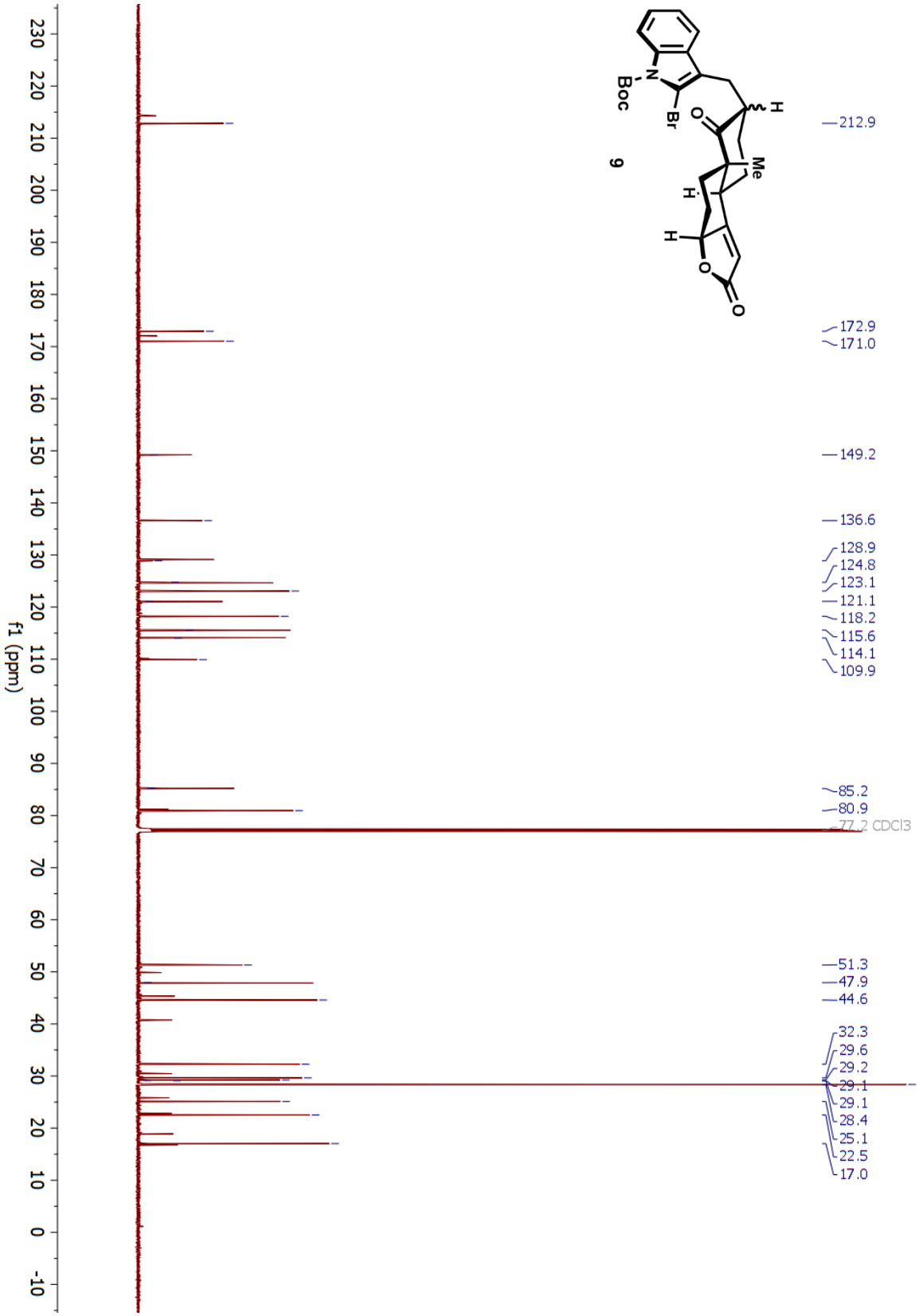
2.70
2.47
2.12
1.94
1.83
1.70
1.52
1.06


f1 (ppm)
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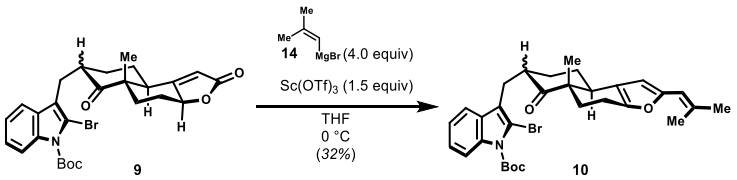
Boc
Br
O
H
Me
H
H
O
O
9
212.9
172.9
171.0
149.2
136.6
128.9
124.8
123.1
121.1
118.2
115.6
114.1
109.9
85.2
80.9
77.2 CDCl3
51.3
47.9
44.6
32.3
29.6
29.2
29.1
29.1
28.4
25.1
22.5
17.0

Synthesis of Indole 10:



A flame-dried 10 mL microwave vial was equipped with a magnetic stir bar and charged with **9** (100 mg, 0.189 mmol, 1.0 equiv), after which the apparatus was sealed with a rubber septum, evacuated and backfilled with nitrogen three times, and placed under a nitrogen atmosphere. The compound was then dissolved in anhydrous THF (1.9 mL 0.10 M), and the resulting solution was cooled to 0 °C by transferring the reaction apparatus to an ice-water bath. After 10 minutes of stirring, $Sc(OTf)_3$ (140 mg, 0.284 mmol, 1.5 equiv) was added to the flask in a single portion as a solid. The mixture was left to stir for 15 minutes at 0 °C. A solution of **14** (0.5 M in THF, 1.5 mL, 0.757 mmol, 4.0 equiv) was syringed into the reaction vial over the course of 5 minutes. After full consumption of the starting material was observed by TLC, the reaction was left stirring for another 15 minutes.

The reaction mixture was diluted with DCM and quenched by pouring sat. aq. NH_4Cl (5 mL) to the flask. The layers were separated and the aqueous layer was extracted with DCM (3 × 5 mL). The combined organic layers were washed with brine (15 mL) and dried over anhydrous Na_2SO_4. The solution was then filtered and concentrated by rotary evaporation under reduced pressure to afford an orange solid.

The orange solid was transferred to another 10 mL microwave vial redissolved in DCM (1.9 mL, 0.10 M) at room temperature, after which *p*TsOH·H_2O (18 mg, 0.095 mmol, 0.5 equiv) was added to the reaction mixture as a solid in a single portion. The reaction was left to stir at room temperature for 1 hour, before it was quenched by pouring into sat. aq. $NaHCO_3$ (5 mL). The layers were separated and the aqueous layer was extracted with DCM (3 × 5 mL). The combined organic layers were washed with brine (15 mL), dried over anhydrous sodium sulfate, filtered, concentrated by rotary evaporation under reduced pressure to afford crude **10** as an orange foam. Purification by flash chromatography (0 to 2% Et_2O in hexanes) afforded **10** in the form of a white solid (34 mg, 32%) as an inconsequential mixture of 3:1 diastereomers.

10 – major diastereomer:

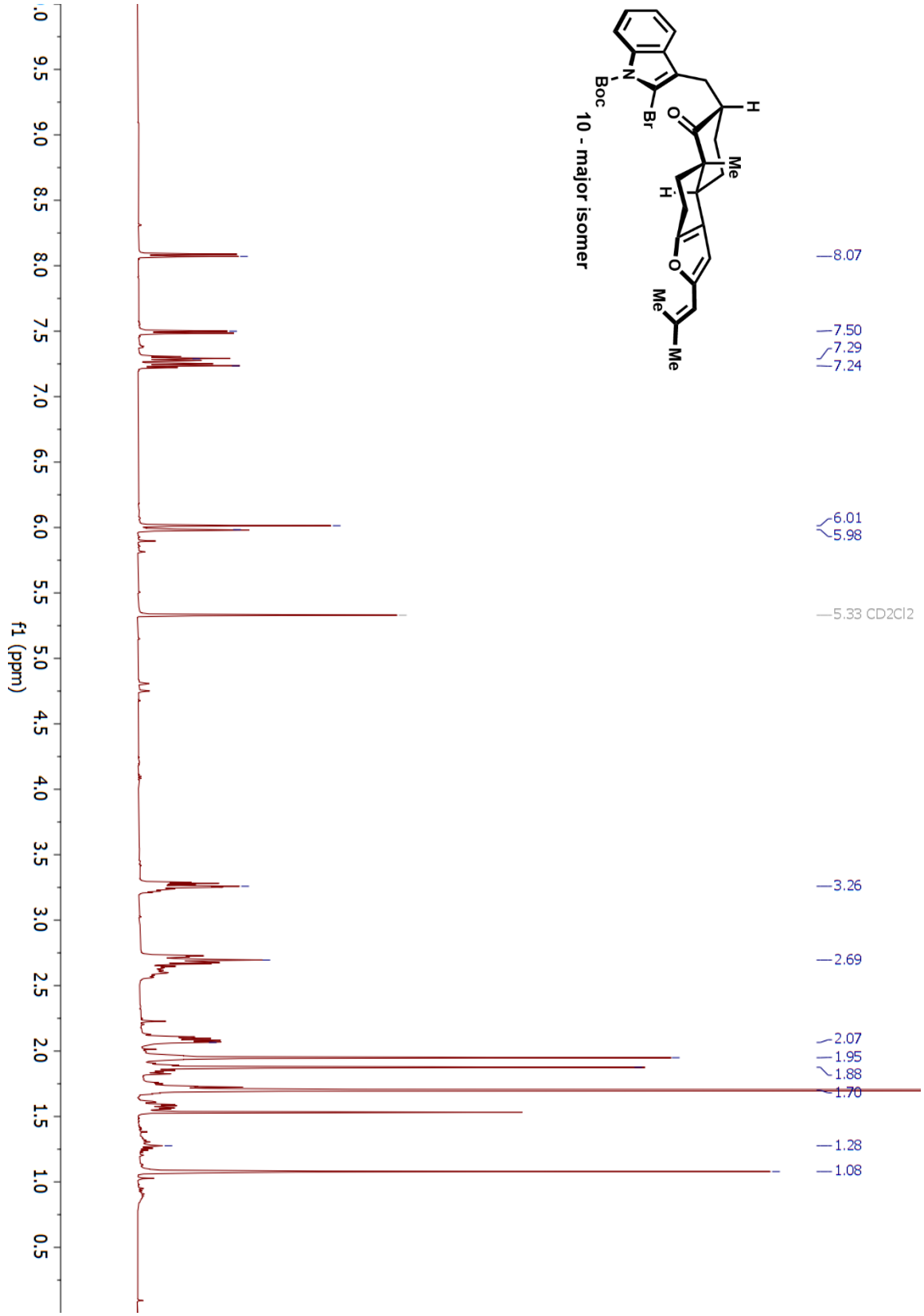
R_f: 0.39 (20% Et_2O in hexanes)

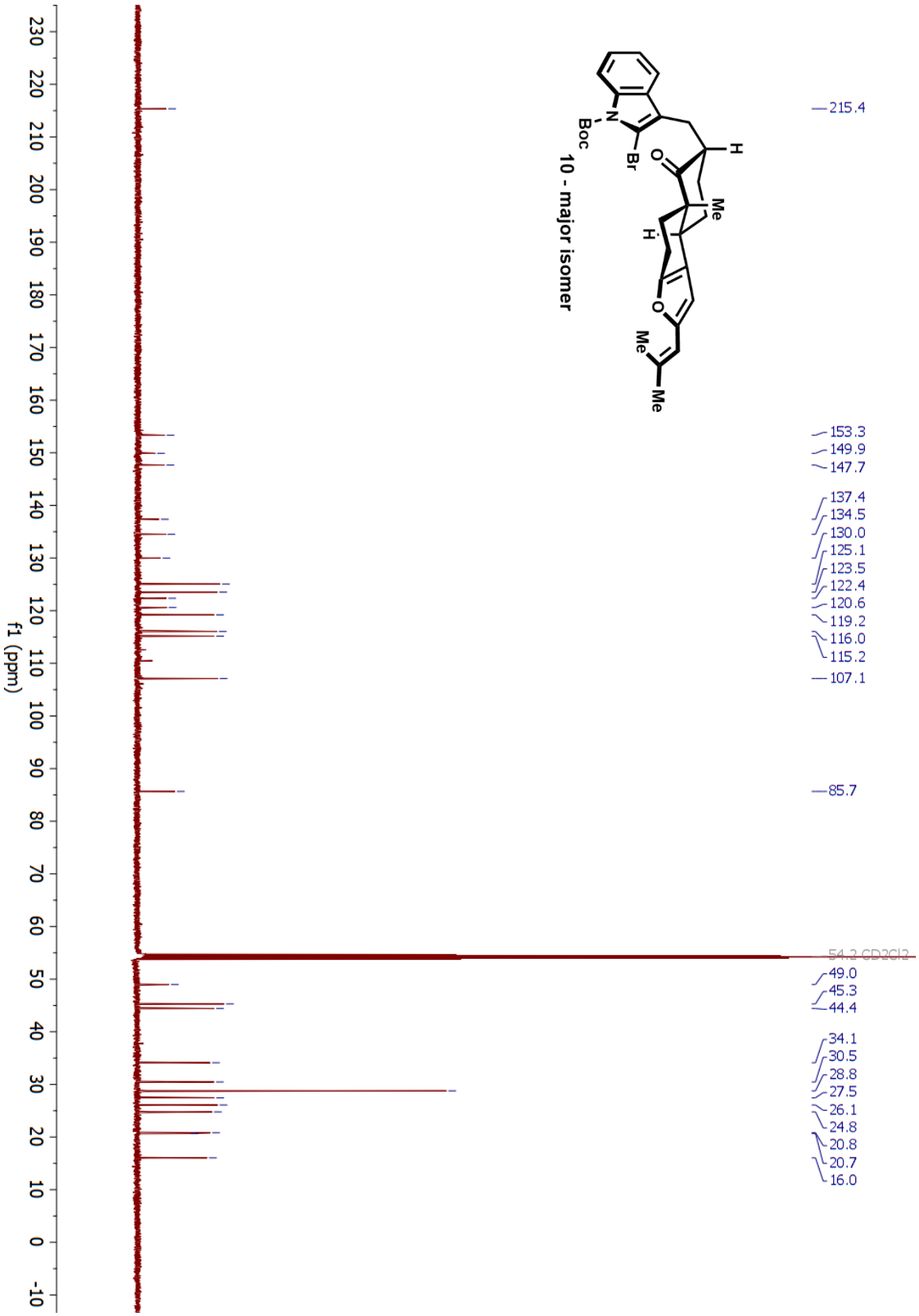
^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.07 (d, *J* = 9.0 Hz, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.24 (t, *J* = 7.9 Hz, 1H), 6.01 (s, 1H), 5.98 (s, 1H), 3.30–3.20 (m, 2H), 2.74–2.55 (m, 4H), 2.11–2.05 (m, 2H), 1.99–1.92 (m, 4H), 1.91–1.81 (m, 4H), 1.74–1.67 (m, 10H), 1.62–1.55 (m, 1H), 1.08 (s, 3H)

^{13}C NMR (125 MHz, CD_2Cl_2): δ 215.4, 153.3, 149.9, 147.7, 137.4, 134.5, 130.0, 125.1, 123.5, 122.4, 120.6, 119.2, 116.0, 115.2, 107.1, 85.7, 49.0, 45.3, 44.4, 34.1, 30.5, 28.8, 27.5, 26.1, 24.8, 20.8, 20.7, 16.0

IR (cm^{-1}): 1744, 1444, 1369, 1307, 1164, 1108

Optical Rotation: $[\alpha]_D^{25} = -7.4\ °$ (*c* 0.3, $CHCl_3$)


10 - major isomer
Boc
N
Br
O
H
Me
H
O
Me
Me
8.07
7.50
7.29
7.24
6.01
5.98
5.33 CD2Cl2
3.26
2.69
2.07
1.95
1.88
1.70
1.28
1.08
f1 (ppm)


10 - major isomer
f1 (ppm)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
215.4
153.3
149.9
147.7
137.4
134.5
130.0
125.1
123.5
122.4
120.6
119.2
116.0
115.2
107.1
85.7
54.2 CD2Cl2
49.0
45.3
44.4
34.1
30.5
28.8
27.5
26.1
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20.8
20.7
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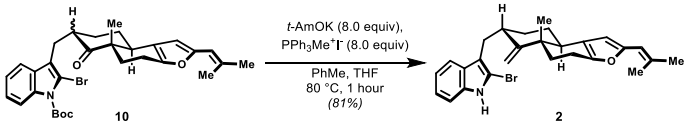
N
Boc
Br
O
H
Me
H
O
Me
Me

Synthesis of Olefin 2:



A flame-dried 10 mL microwave reaction vial equipped with a stir bar was charged with methyltriphenylphosphonium iodide (771 mg, 1.906 mmol, 8.0 equiv), sealed with a PTFE crimp cap, evacuated and backfilled with nitrogen three times, and placed under a nitrogen atmosphere. The vial was transferred to an oil bath preheated to 80 °C, and heated at that temperature for 5 minutes. Potassium tert-pentoxide (1.7 M in toluene, 1.1 mL, 8.0 equiv) was added to the solids in a single portion via syringe. Following this, toluene (0.27 mL) was syringed into the vial, and the resulting mixture was left to stir vigorously for 15 minutes.

Another flame-dried 10 mL microwave reaction vial was charged with **10** (135 mg, 0.238 mmol, 1.0 equiv). The vial was sealed with a rubber septum, evacuated and backfilled with nitrogen three times, and placed under a nitrogen atmosphere. **10** was dissolved in anhydrous toluene (0.32 mL, 0.75M) and the resulting solution was syringed into the solution of ylide at 80 °C. The transfer was quantitated by rinsing with toluene (2 × 0.32 mL).

After stirring at 80 °C for 1 hour, the reaction vial was removed from the oil bath and allowed to cool to the room temperature. The reaction mixture was diluted with DCM (30 mL) and quenched by pouring into sat. aq. NH_4Cl (50 mL). The layers were separated and the aqueous layer was extracted with DCM (3 × 50 mL). The combined organic layers were washed with brine (50 mL), dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure by rotary evaporation to provide a crude orange foam. Purification by flash column chromatography on silica gel (0 to 2% Et_2O in hexanes) afforded **2** (90 mg, 81%) as a white foam.

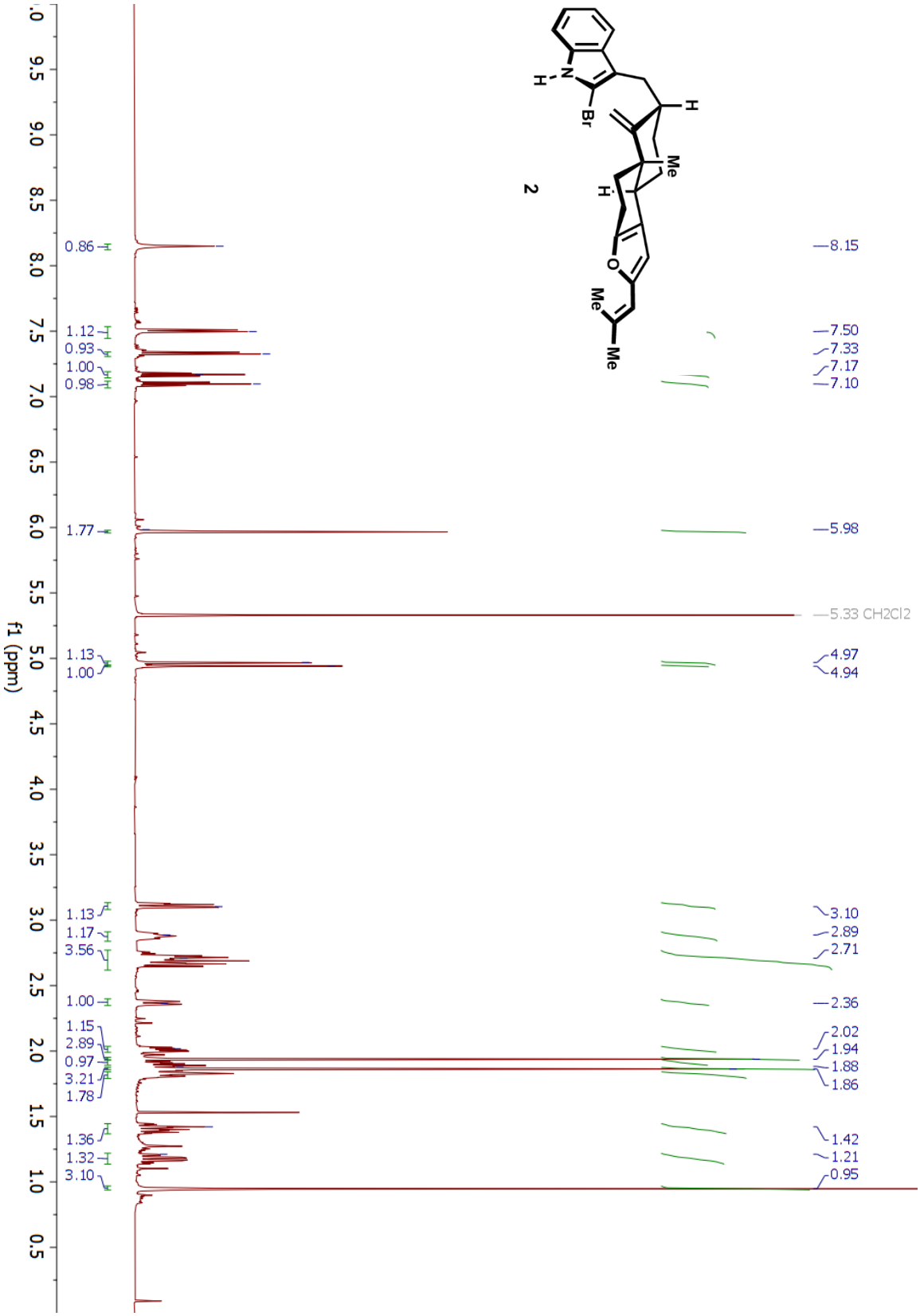
R_f: 0.36 (20% Et_2O in hexanes)

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.15 (bs, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.17 (t, *J* = 8.1 Hz, 1H), 7.10 (t, *J* = 6.9 Hz, 1H), 5.96 (ov, 1H), 5.96 (ov, 1H), 4.97 (s, 1H), 4.94 (s, 1H), 3.10 (dd, *J* = 13.2, 2.9 Hz, 1H), 2.87 (at, *J* = 10.1 Hz, 1H), 2.75–2.64 (m, 3H), 2.36 (d, *J* = 12.2 Hz, 1H), 2.02–1.98 (m, 1H), 1.93 (s, 3H), 1.91–1.79 (m, 6H), 1.40 (dddd, *J* = 10.9, 16.7, 13.3, 3.6 Hz, 1H), 1.21–1.12 (m, 1H), 0.94 (s, 3H)

^{13}C NMR (600 MHz, CD_2Cl_2): δ 160.7, 152.9, 147.8, 137.0, 133.9, 128.9, 122.9, 122.2, 120.7, 118.1, 115.5, 115.3, 111.2, 109.5, 107.1, 103.0, 44.5, 40.7, 38.8, 34.5, 34.2, 29.4, 27.4, 25.9, 21.6, 20.6, 17.1

IR (cm^{-1}): 3397, 2924, 2439, 1371, 1213, 737

Optical Rotation: $[\alpha]_D^{20}$ = –58.0° (*c* 0.12, $CHCl_3$)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1.15
2.89
0.97
3.21
1.78
1.36
1.32
3.10
8.15
7.50
7.33
7.17
7.10
5.98
5.33 CH2Cl2
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4.94
3.10
2.89
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2.02
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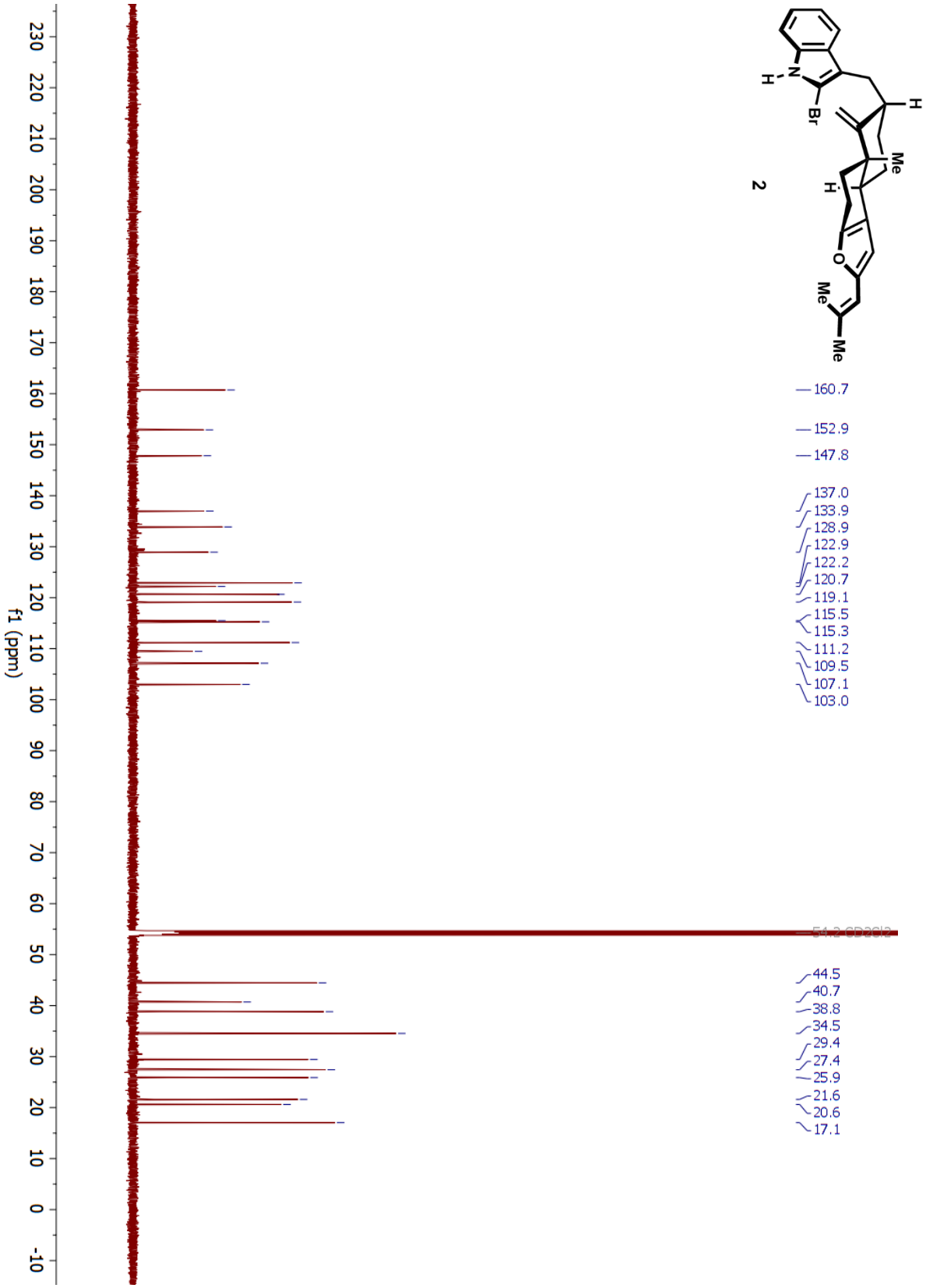
2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H
Br
H
Me
H
O
Me
Me
2
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152.9
147.8
137.0
133.9
128.9
122.9
122.2
120.7
119.1
115.5
115.3
111.2
109.5
107.1
103.0
44.5
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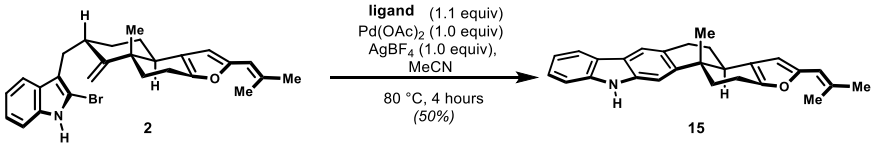
29.4
27.4
25.9
21.6
20.6
17.1

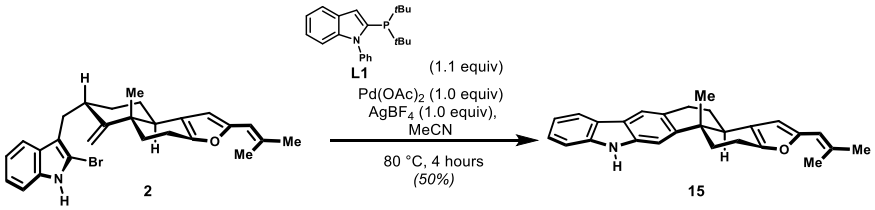
General Experimental Procedure for Ligand Optimization to Access Carbazole 15:



A flame-dried, 5 mL microwave reaction vial equipped with a magnetic stir bar was charged with **2** (5.0 mg, 0.011 mmol, 1.0 equiv), $Pd(OAc)_2$ (2.4 mg, 0.011 mmol, 1.0 equiv), and the ligand (0.012mmol, 1.1 equiv), sealed with a PTFE crimp cap, evacuated and backfilled with nitrogen three times, and placed under an argon atmosphere. The contents of the reaction flask were dissolved in anhydrous acetonitrile (0.27 mL, 0.04 M). Following this, a solution of $AgBF_4$ (2.1 mg, 0.011 mmol 1.0 equiv) in anhydrous acetonitrile (0.014 mL, 0.78M) was syringed into the reaction vial. The resulting solution was warmed to 80 °C by transferring the reaction apparatus to a preheated oil bath, after which the reaction mixture was allowed to stir at 80 °C for 4 hours.

After this time, the reaction flask was removed from the oil bath and allowed to cool. The reaction mixture was diluted with EtOAc (3 mL) and filtered through a pad of Celite®. The resulting filtrate was concentrated under reduced pressure by rotary evaporation. The crude mixture was purified by thin layer chromatography silica gel.

Synthesis of Carbazole 15:



A flame-dried, 20 mL microwave reaction vial equipped with a magnetic stir bar was charged with **2** (72 mg, 0.155 mmol, 1.0 equiv), $Pd(OAc)_2$ (35 mg, 0.155 mmol, 1 equiv), and **L1** (58 mg, 0.171 mmol, 1.1 equiv), sealed with a PTFE crimp cap, evacuated and backfilled with nitrogen three times, and placed under an argon atmosphere. The contents of the reaction flask were dissolved in anhydrous acetonitrile (3.9 mL, 0.04 M). Following this, a solution of $AgBF_4$ (30mg, 0.155 mmol 1.0 equiv) in anhydrous acetonitrile (0.2 mL, 0.78M) was syringed into the reaction vial. The resulting solution was warmed to 80 °C by transferring the reaction apparatus to a preheated oil bath, after which the reaction mixture was allowed to stir at 80 °C for 4 hours.

After this time, the reaction flask was removed from the oil bath and allowed to cool. The reaction mixture was filtered through a pad of Celite® and the resulting filtrate was concentrated under reduced pressure by rotary evaporation to provide a crude red solid. Purification by flash column chromatography on silica gel (0 to 2% Et_2O in hexanes) afforded **15** (30 mg, 50%) as a yellow foam.

R_f: 0.35 (20% Et_2O in hexanes)

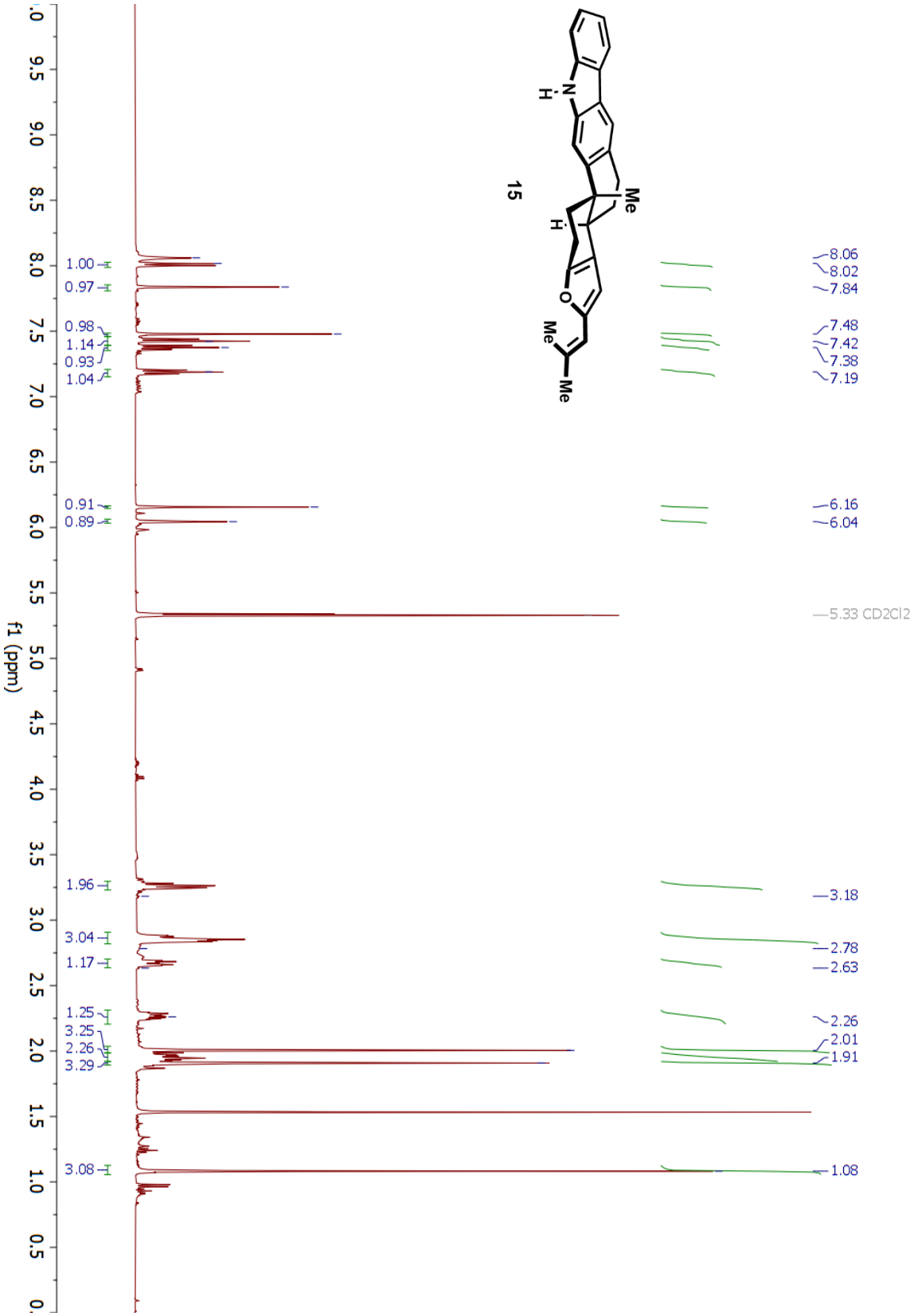
^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.06 (bs, 1H), 8.00 (d, *J* = 6.6 Hz, 1H), 7.84 (s, 1H), 7.48 (s, 1H), 7.43 (d, *J* = 8.3 Hz, 1H), 7.38 (at, *J* = 6.9 Hz, 1H), 7.19 (at, *J* = 7.5 Hz, 1H), 6.16 (s, 1H), 6.04 (s, 1H), 3.31–3.22 (m, 2H), 2.89–2.82 (m, 3H), 2.69–2.65 (m, 1H), 2.30–2.24 (m, 1H), 2.01 (s, 3H), 1.99–1.92 (m, 2H), 1.91 (s, 3H), 1.08 (s, 3H)

^{13}C NMR (150 MHz, CD_2Cl_2): δ 153.0, 148.2, 146.2, 140.9, 139.2, 134.1, 127.9, 126.2, 123.8, 122.3, 122.2, 121.3, 120.7, 119.9, 115.3, 111.3, 107.4, 106.7, 40.1, 38.3, 34.7, 29.5, 27.5, 22.9, 22.1, 21.7, 20.7

IR (cm^{-1}): 3394, 2922, 2856, 1441, 1366, 1206, 746

ESI-HRMS (m/z): $[M]^+$ calc'd for $C_{27}H_{28}NO^+$:381.2087; found: 381.2083

Optical Rotation: $[\alpha]_D^{20}$ = –29.7° (*c* 0.23, $CHCl_3$)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Me
Me
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N
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H
O
f1 (ppm)
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0.91
0.89
1.96
3.04
1.17
1.25
3.25
2.26
3.29
3.08
8.06
8.02
7.84
7.48
7.42
7.38
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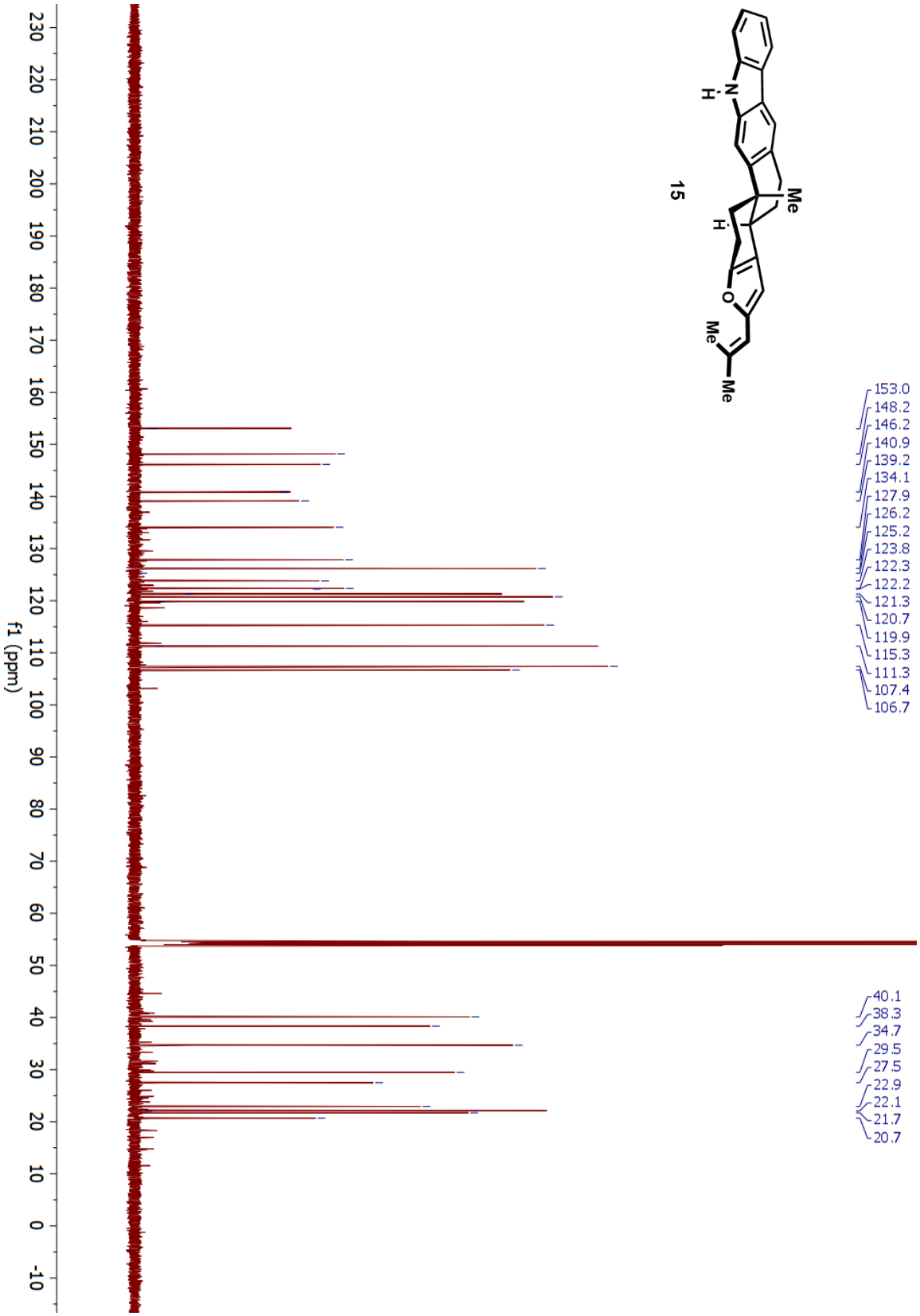
1.91
1.08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107.4
106.7
40.1
38.3
34.7
29.5
27.5
22.9
22.1
21.7
20.7
f1 (ppm)
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220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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0
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15
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H
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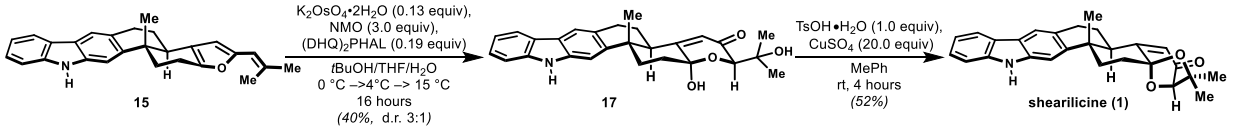
H
O
Me
Me

Synthesis of Shearilicine (1):



A 10 mL microwave reaction vial equipped with a magnetic stir bar was charged with **15** (25 mg 0.066 mmol, 1.0 equiv)**,** $(DHQ)_2PHAL$ (10 mg, 0.012 mmol, 0.19 equiv), and *N*-methylmorpholine *N*-oxide (NMO) (23 mg, 0.197 mmol, 3.0 equiv), after which the mixture was dissolved in a 1:1:1 mixture of *tert*-butanol, THF, and H_2O (2.82 mL, 0.023 M). The resulting solution was cooled to 0 °C by transferring the reaction apparatus to an ice-water bath. After 10 minutes of stirring, $K_2OsO_4 \cdot 2H_2O$ (3 mg, 0.008 mmol, 0.13 equiv) was added to the vial in a single portion. The reaction vial was sealed with a rubber septum and moved to a 4 °C water bath. The reaction mixture was left to stir overnight in this water bath, which gradually warmed up to 15 °C.

After this time, Na_2SO_3 (132 mg, 1.048 mmol, 16.0 equiv) was added to the vial as a solid in a single portion. The mixture was left to stir for 30 minutes, after which it was poured into sat. aq. $NaHCO_3$ (3 mL) and the layers were separated. The aqueous layer was extracted with EtOAc (3 × 3 mL). The combined organic layers were washed with brine (3 mL), dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure by rotary evaporation to provide a crude brown solid. Thin layer chromatography silica gel (EtOAc/hexanes = 4/1) afforded **17** as a white solid (10 mg, 40%, d.r. 3:1).

The purified diol **17** (10 mg, 0.023 mmol, 1.0 equiv) was transferred to a flame-dried 10 mL microwave reaction vial, evacuated and backfilled with nitrogen three times, and placed under a nitrogen atmosphere, after which the compound was dissolved in anhydrous toluene (1.2 mL, 0.02 M). $CuSO_4$ (74 mg, 0.464 mmol, 20.0 equiv) and *p*$TsOH \cdot H_2O$ (4 mg, 0.023, 1.0 equiv) were added to the vial in single portions as solids. The resulting mixture was left to stir at room temperature for 2 hours, before the mixture was diluted with EtOAc (1 mL), filtered through a pad of silica gel, and quenched by pouring the filtrate into sat. aq. $NaHCO_3$ (1 mL). The layers were separated and the aqueous layer was extracted with EtOAc (3 × 1 mL). The combined organic layers were washed with brine (1 mL), dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure by rotary evaporation. The crude residue was purified by thin layer chromatography silica gel (Et_2O/DCM/hexanes = 20%/20%/60%) to afford shearilicine **1** as a white solid (5 mg, 52%).

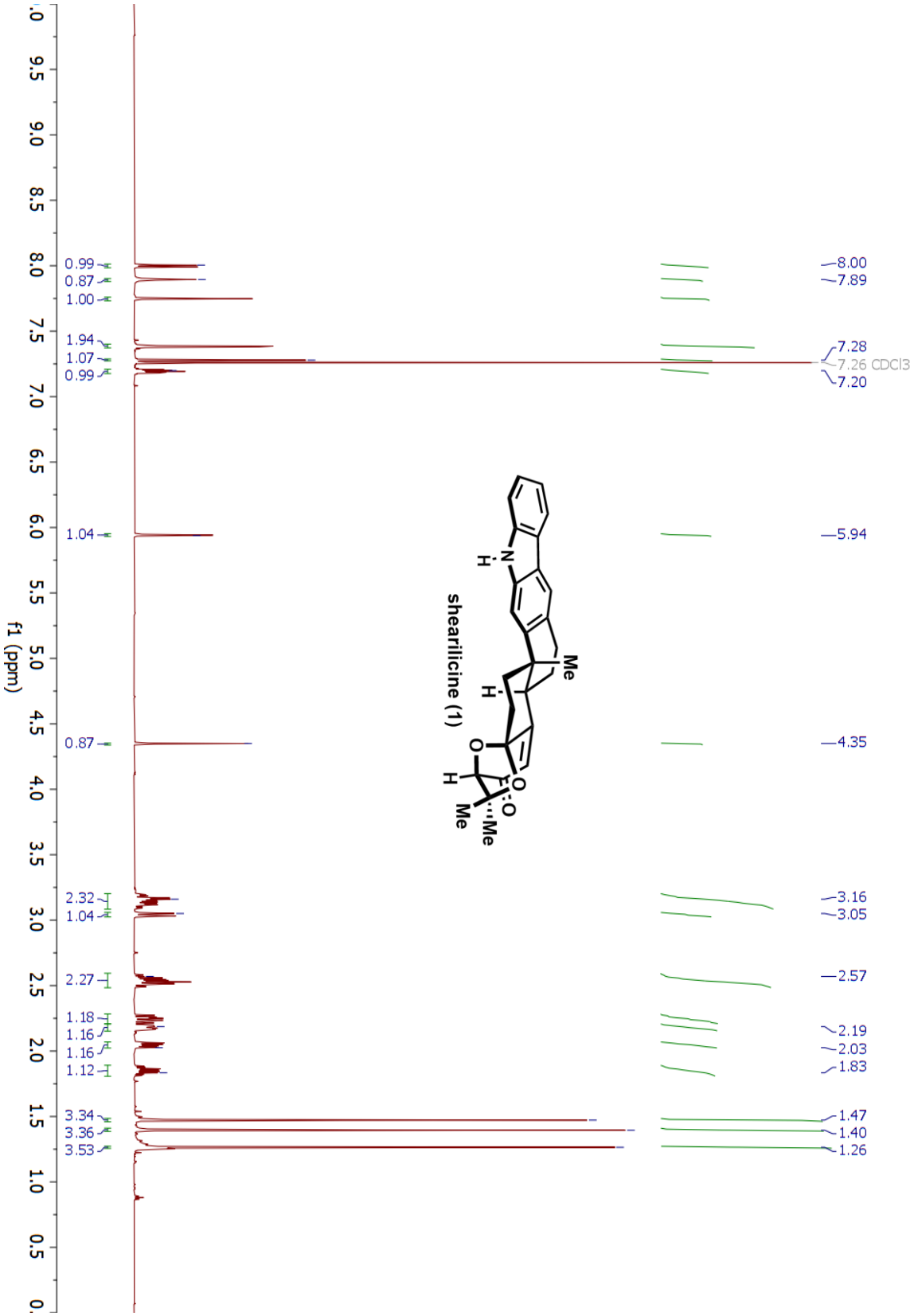
^{1}H NMR (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.6 Hz, 1H), 7.91 (br s, 1H), 7.75 (s, 1H), 7.38 (ov, 1H),7.38 (ov, 1H), 7.27 (s, 1H), 7.19 (m, 1H), 5.93 (br s, 1H), 4.35 (d, *J* = 1.1 Hz, 1H), 3.15 (m, 2H), 3.04 (dt, *J* = 12.1, 2.6 Hz, 1H), 2.53 (m, 2H), 2.25 (ddd, *J* = 13.9, 11.3, 9.6 Hz, 1H), 2.18 (m, 1H), 2.04 (br dd, *J* = 13.9, 7.4 Hz, 1H), 1.85 (qd, *J* = 12.4, 6.1 Hz, 1H), 1.47 (s, 3H), 1.39 (s, 3H), 1.26 (s, 3H)

^{13}C NMR (150 MHz, $CDCl_3$): 196.3, 170.9, 147.5, 140.4, 139.0, 125.9, 125.1, 123.1, 122.1, 120.4, 120.4, 119.9, 119.5, 110.6, 108.2, 104.1, 88.3, 78.4, 43.5, 36.1, 34.8, 30.7, 29.8, 29.1, 28.4, 23.4, 19.8

IR (cm^{-1}): 3417, 2940, 2870, 1689, 1463, 1428, 1064, 760

ESI-HRMS (m/z): $[M+H]^+$ calc'd for $C_{27}H_{27}NO_3^+$:414.2064; found: 414.2055

Optical Rotation: $[\alpha]_D^{20}$ = +212.0° (*c* 0.04, $CHCl_3$)


f1 (ppm)
shearilicine (1)
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0.87
1.00
1.94
1.07
0.99
1.04
0.87
2.32
1.04
2.27
1.18
1.16
1.16
1.12
3.34
3.36
3.53
8.00
7.89
7.28
7.26 CDCl3
7.20
5.94
4.35
3.16
3.05
2.57
2.19
2.03
1.83
1.47
1.40
1.26

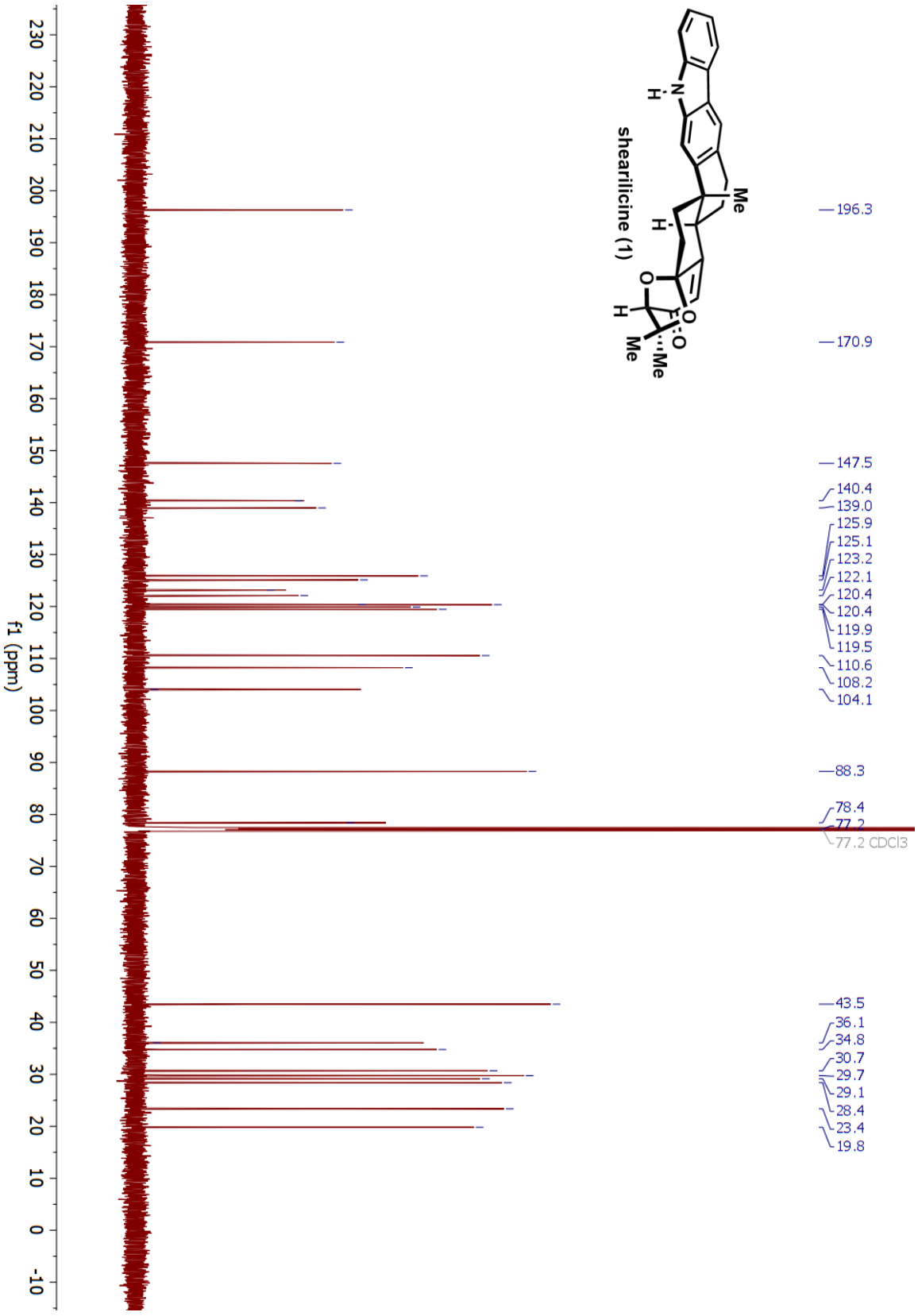
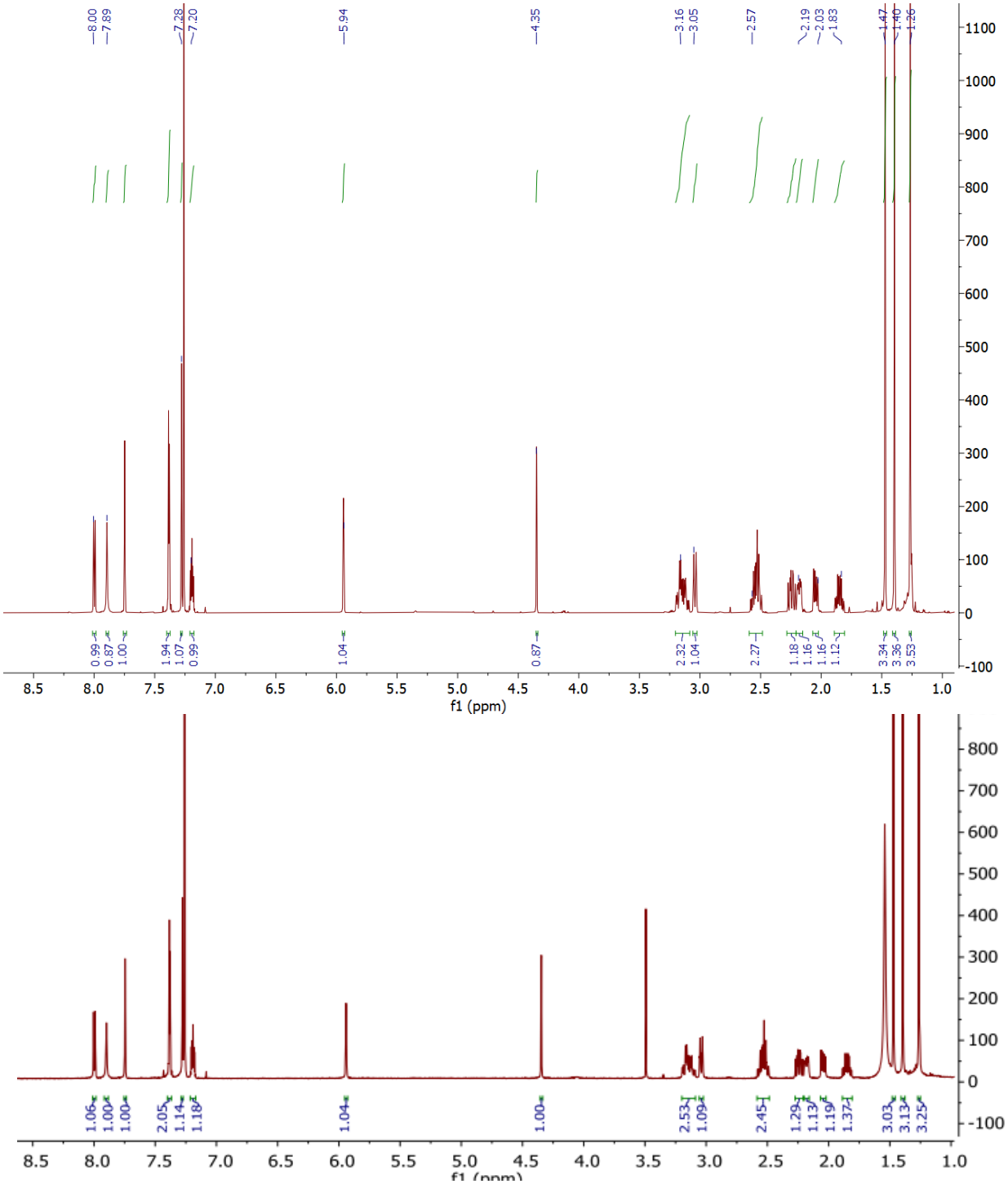

shearilicine (1)
196.3
170.9
147.5
140.4
139.0
125.9
125.1
123.2
122.1
120.4
120.4
119.9
119.5
110.6
108.2
104.1
88.3
78.4
77.2
77.2 CDCl3
43.5
36.1
34.8
30.7
29.7
29.1
28.4
23.4
19.8
f1 (ppm)

Table S1. Comparison of Synthetic and Natural ^{1}H NMR for Shearilicine (**1**)

	Proksch's isolation report (ppm)		**This report (ppm)**		**Difference**
^{1}H NMR ($CDCl_3$)	8.00	(d, *J* = 7.7 Hz, 1 H)	8.00	(d, *J* = 7.6 Hz, 1H)	0.00
	7.90	(s, 1H)	7.91	(br s, 1H)	0.01
	7.75	(s, 1H)	7.75	(s, 1H)	0.00
	7.38	(ov, 1H)	7.38	(ov, 1H)	0.00
	7.38	(ov, 1H)	7.38	(ov, 1H)	0.00
	7.28	(s, 1H)	7.27	(s, 1H)	0.01
	7.19	(m, 1H)	7.19	(m, 1H)	0.00
	5.94	(br s, 1H)	5.93	(br s, 1H)	0.00
	4.35	(d, *J* = 1.2 Hz, 1H)	4.35	(d, *J* = 1.1 Hz, 1H)	0.00
	3.14	(m, 2H)	3.15	(m, 2H)	0.01
	3.04	(dt, *J* = 12.0, 2.6 Hz, 1H)	3.04	(dt, *J* = 12.1, 2.6 Hz, 1H)	0.00
	2.53	(m, 2H)	2.53	(m, 2H)	0.00
	2.24	(ddd, *J* = 14.0, 11.9, 9.2 Hz, 1H)	2.25	(ddd, *J* = 13.9, 11.3, 9.6 Hz, 1H)	0.01
	2.18	(m, 1H)	2.18	(m, 1H)	0.00
	2.04	(br dd, *J* = 14.0, 6.3 Hz, 1H)	2.04	(br dd, *J* = 13.9, 7.4 Hz, 1H)	0.00
	1.85	(qd, *J* = 12.0, 6.1 Hz, 1H)	1.85	(qd, *J* = 12.4, 6.1 Hz, 1H)	0.00
	1.47	(s, 3H)	1.47	(s, 3H)	0.00
	1.39	(s, 3H)	1.39	(s, 3H)	0.00
	1.26	(s, 3H)	1.26	(s, 3H)	0.00



Top: synthetic ^{1}H NMR;
Bottom: isolated ^{1}H NMR (Ariantari, N. P.; Ancheeva, E.; Wang, C.; Mandi, A.; Knedel, T. O.; Kurtan, T.; Chaidir, C.; Muller, W. E. G.; Kassack, M. U.; Janiak, C.; Daletos, G.; Proksch, P. Indole Diterpenoids from an Endophytic Penicillium sp. *J. Nat. Prod.* **2019**, *82*, 1412–1423.)

Table S2. Comparison of Synthetic and Natural ^{13}C NMR for Shearilicine (**1**)

Note: The isolation report extracted ^{13}C chemical shifts from HMBC and HSQC spectra, which might be the cause for discrepancies.

	Proksch's isolation report (ppm)	**This report (ppm)**	**Difference**
^{13}C NMR ($CDCl_3$)	197.5	196.3	–1.2
	171.0	170.9	–0.1
	147.6	147.5	–0.1
	140.1	140.4	0.3
	139.8	139.0	–0.8
	125.8	125.9	0.1
	125.6	125.1	–0.5
	123.1	123.2	0.1
	122.2	122.1	–0.1
	120.4	120.4	0.0
	120.2	120.4	0.2
	119.7	119.9	0.2
	119.1	119.5	0.4
	110.7	110.6	–0.1
	107.8	108.2	0.4
	103.9	104.1	0.2
	88.1	88.3	0.2
	78.7	78.4	–0.3
	43.3	43.5	0.2
	35.9	36.1	0.2
	34.5	34.8	0.3
	30.8	30.7	–0.1
	29.5	29.7	0.2
	28.7	29.1	0.4
	27.7	28.4	0.7
	22.8	23.4	0.6
	19.9	19.8	–0.1

Computational Details

Density functional theory calculations were performed with Gaussian 16 program.[3] The molecular structure optimizations were carried out using the hybrid density functional method based on Becke's three-parameter exchange function and the Lee-Yang-Parr nonlocal correlation functional (rB3LYP)[4], the LANL2DZ basis set for Pd,[5] and the 6-31G* basis set for H, C, N, O, and P[6] with an empirical dispersion correction. The vibrational frequencies were computed at the same level to check whether each optimized structure is at an energy minimum on the potential energy surfaces (no imaginary frequency) or a transition state (one imaginary frequency) and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298.15 K. The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.[7] Single point energies were calculated at the rωb97xd[8] level using the SDD basis set for Pd,[9] and the 6-311+G**[10] basis set for H, C, N, O, and P in acetonitrile solvent (cpcm model).

	E(rB3LYP/LANL2DZ and 6-31G*) (A.U.)	**E(rωb97xd/SDD and 6-311+G**) (A.U.)**
CP1A	-5126.671897	-5130.267602
TS1A	-5126.656024	-5130.249201
CP2A	-5126.679841	-5130.281765
CP3A	-2783.746228	-2784.572751
CP4A	-2783.745552	-2784.571844
TS2A (= TS-L1 in Figure 3)	-2783.705254	-2784.5258
CP5A	-2783.764065	-2784.593939
TS3A	-2783.756111	-2784.588231
CP6A	-2783.77168	-2784.595221
AgOAc	-374.26547	-375.514993

AgBr	-2717.2197	-2721.250902
CP3B	-2568.72745	-2569.564738
TS2B (= TS-L2 in Figure 3)	-2568.670108	-2569.512624
CP5B	-2568.716587	-2569.562324
TS3B	-2568.709488	-2569.557892
CP6B	-2568.723257	-2569.562587

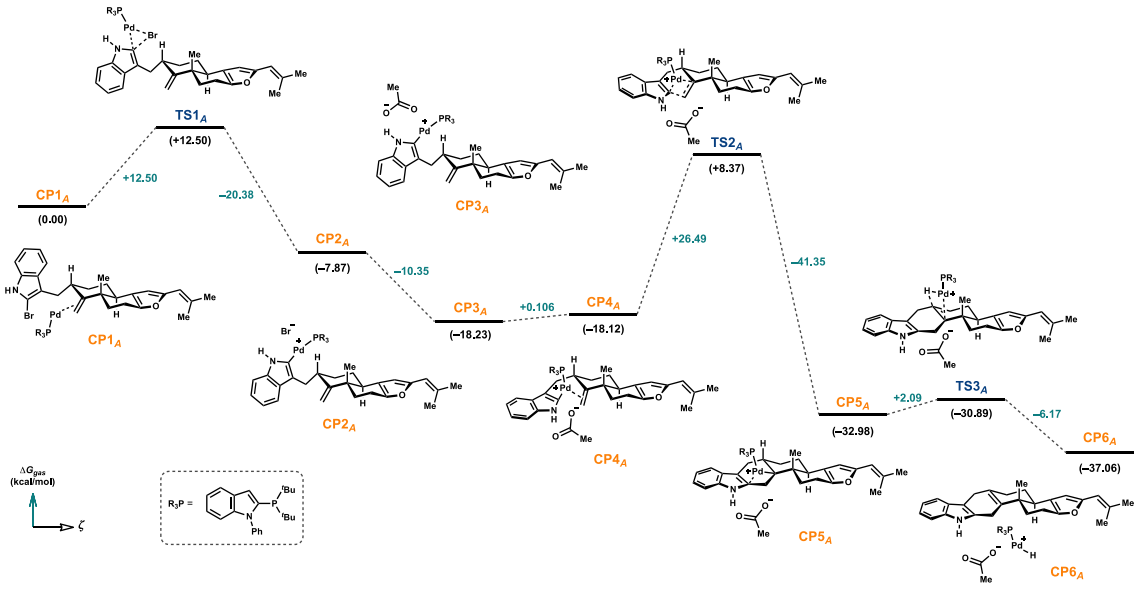


Figure S1. Gibbs free-energy profile for the reaction process of Pd-mediated Heck cyclization.

The computation was performed at the rωb97xd/SDD(Pd)/6-311+G**(C, H, C, N, O, and P)//rB3LYP/LANL2DZ(Pd)/6-31G*(H, C, N, O, and P) level of theory in MeCN solvent (cpcm model).

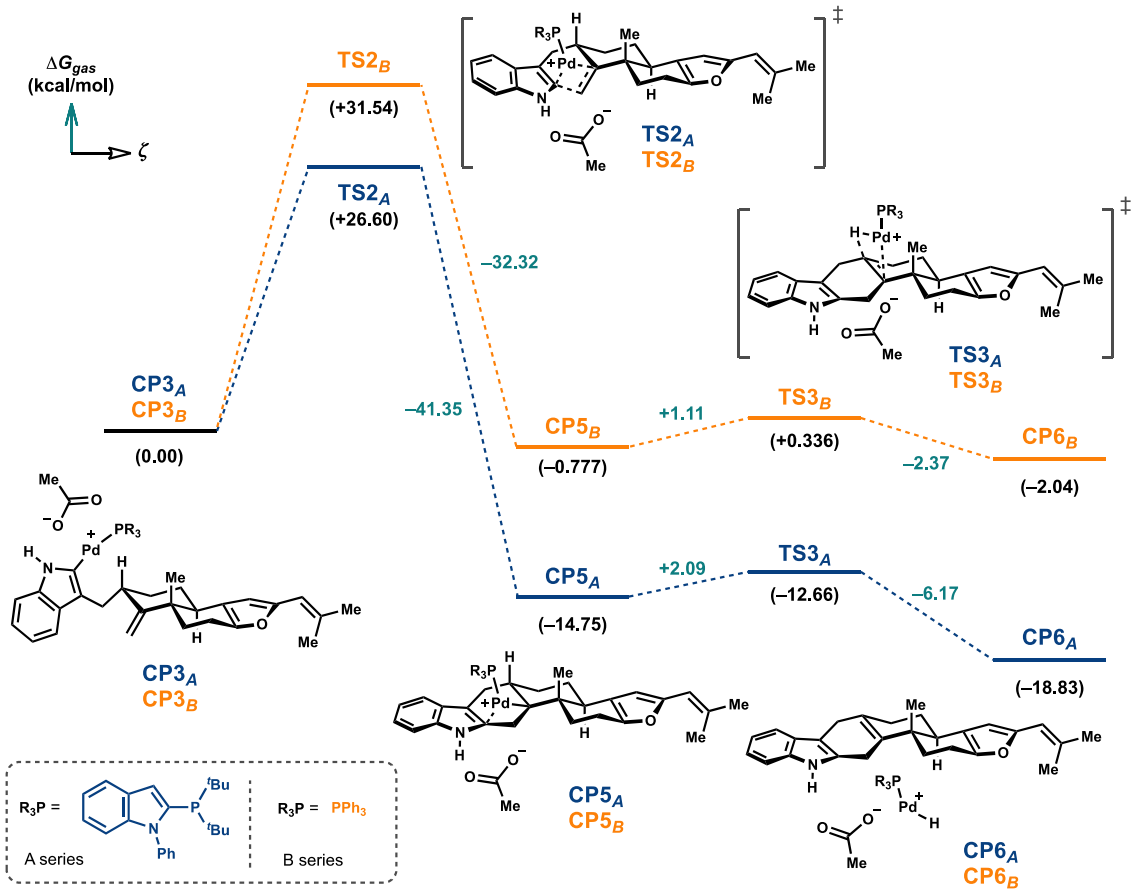
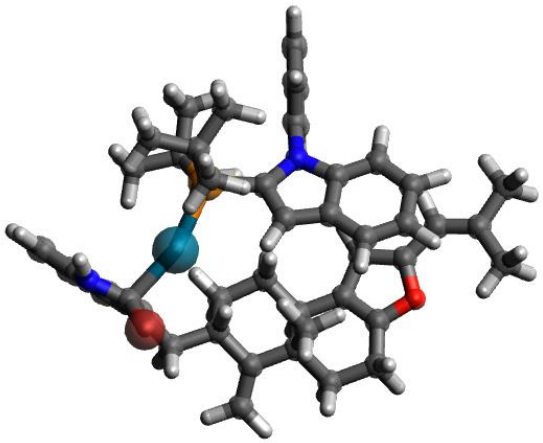


Figure S2. Comparison of Gibbs Free-Energies for the Reaction Process of the Migratory Insertion and *syn* *β*-hydride Elimination Using CataCXium Ligand and PPh_3.

The computation was performed at the rωb97xd/SDD(Pd)/6-311+G**(C, H, C, N, O, and P)//rB3LYP/LANL2DZ(Pd)/6-31G*(H, C, N, O, and P) level of theory in MeCN solvent (cpcm model).

CP1A



Zero-point correction= 0.962251 (Hartree/Particle)
Thermal correction to Energy= 1.017590
Thermal correction to Enthalpy= 1.018534
Thermal correction to Gibbs Free Energy= 0.870800
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Sum of electronic and thermal Energies= -5125.654307
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Sum of electronic and thermal Free Energies= -5125.801097

Cartesian Coordinates

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C	0.88435200	-5.19421400	0.80481400
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H	0.24766600	-6.07193700	0.78844600
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H	-0.73450800	-0.78062800	0.64697300
H	-1.03323200	-0.79498500	2.37918000
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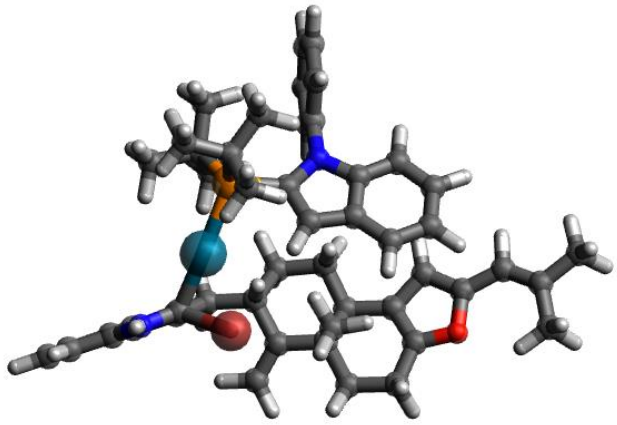
TS1A



Zero-point correction= 0.962000 (Hartree/Particle)
Thermal correction to Energy= 1.016640
Thermal correction to Enthalpy= 1.017585
Thermal correction to Gibbs Free Energy= 0.872325
Sum of electronic and zero-point Energies= -5125.694024
Sum of electronic and thermal Energies= -5125.639383
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Sum of electronic and thermal Free Energies= -5125.783699

Cartesian Coordinates

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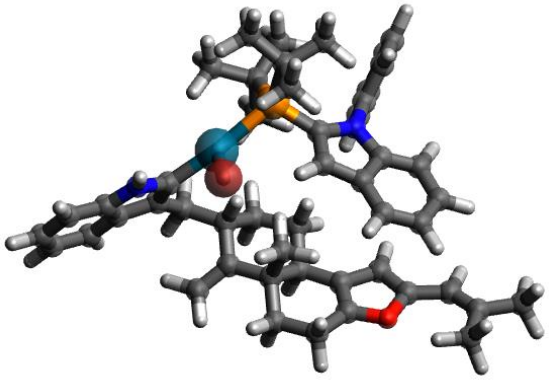
C	6.76253600	-2.90679000	0.07686200
C	6.46813400	-3.36834600	2.45682300
H	6.90064100	-3.70820800	3.39344500
C	7.27163200	-3.33696000	1.29783000
H	8.30820000	-3.65576800	1.35893100
H	4.52960800	-2.98722100	3.31727100
H	7.38303300	-2.87857100	-0.81442400
C	0.07661800	-3.16708000	0.91977500
C	0.75164600	-4.31939400	0.97846200
H	1.80018500	-4.36037800	1.25182800
H	0.29833800	-5.27133700	0.72744500
Pd	2.61787800	0.14663300	-0.87113000
P	1.70921300	2.32596600	-0.67861600
C	-0.15087200	-1.07104800	2.31234900
H	-0.14184800	-1.61834300	3.26669800
H	0.30089100	-0.09171700	2.50185300
C	-2.19801000	-2.27453900	1.53422000
H	-2.11631600	-2.85717700	2.46634700
C	-1.58920700	-0.90401400	1.83143000
H	-1.62247000	-0.26911300	0.93957100
H	-2.18828200	-0.39855000	2.60045300
C	-1.41539400	-2.39319400	-0.91892500
H	-0.92337100	-3.03326500	-1.65713400
H	-2.43978200	-2.19925900	-1.24105700
H	-0.88969900	-1.44092800	-0.91069200
C	-2.06625800	-4.46762400	0.32621600
H	-1.48709800	-5.10259800	-0.35149400
H	-2.06332600	-4.95935300	1.30662600
C	-3.64063600	-2.22237900	1.12365600
C	-3.52055600	-4.39730400	-0.20804300

H	-3.52064400	-4.33104500	-1.30565100
H	-4.05020600	-5.32699500	0.03893400
C	-4.19991300	-3.20603700	0.36369400
C	-4.65540700	-1.23033800	1.29854100
H	-4.56827500	-0.28280800	1.81069700
C	-5.76923600	-1.66777700	0.62135500
O	-5.49327700	-2.89266500	0.04579800
C	2.46542000	3.04027700	0.91713800
C	1.89936700	3.53076700	-2.14336800
C	-2.10541500	1.21765400	-1.29082800
C	-2.38522900	2.29084800	-0.40836700
C	-3.69198800	2.63854600	-0.04331200
C	-4.72593200	1.89603200	-0.60023600
C	-4.47249500	0.83626800	-1.49751700
C	-3.17623400	0.49464500	-1.84965800
C	-0.68058400	1.11821600	-1.36396400
H	-3.88475700	3.45533800	0.64435800
H	-5.75329500	2.13204900	-0.33825100
H	-5.30946700	0.27096400	-1.89446700
H	-2.98429300	-0.32590100	-2.53320300
H	-0.10758600	0.39882600	-1.93098200
C	-0.11665500	2.10819500	-0.57519900
N	-1.17675700	2.84923600	-0.00252900
C	-1.16831600	3.86809400	0.99642400
C	-1.22157500	3.50828700	2.34599300
C	-1.22931700	5.21362500	0.62774100
C	-1.25468900	4.49722800	3.32818000
H	-1.24471900	2.45596100	2.61008100
C	-1.26861200	6.20121700	1.61277300
H	-1.23837400	5.47506600	-0.42326200
C	-1.26704600	5.84505200	2.96262300
H	-1.27959600	4.21513200	4.37646100
H	-1.30249200	7.24759500	1.32446100
H	-1.29148600	6.61517500	3.72788200
C	3.99153200	2.80720800	0.83475100
H	4.47634400	3.43079600	0.08191600
H	4.43534100	3.05403900	1.80760400
H	4.22180300	1.75905800	0.61056500
C	2.21003000	4.52048200	1.22849600
H	2.70223800	4.77596000	2.17596800

H	2.63088300	5.17428600	0.45913900
H	1.15243200	4.75227900	1.33358000
C	1.94687400	2.14576500	2.05582000
H	0.86732300	2.21630200	2.17989700
H	2.20372900	1.09892400	1.86546300
H	2.41679100	2.44740400	3.00035500
C	3.35990400	3.99709800	-2.24695300
H	3.63558300	4.68485700	-1.44313100
H	4.05305400	3.14895100	-2.23430600
H	3.49961000	4.52933400	-3.19625600
C	0.95519700	4.73770800	-2.07048400
H	1.11208400	5.38045800	-2.94668900
H	-0.08932500	4.41317500	-2.07951500
H	1.12184700	5.34407800	-1.17698200
C	-7.04048400	-1.01364200	0.43080500
H	-7.08810400	-0.07092600	0.97415600
C	-8.12095000	-1.35956200	-0.30156700
C	-9.32667800	-0.45541600	-0.33187600
H	-9.55502300	-0.13689800	-1.35923000
H	-10.22171000	-0.97906900	0.03393300
H	-9.18547000	0.44182300	0.27903700
C	-8.25284800	-2.61315000	-1.12499900
H	-8.48340900	-2.35893100	-2.16959100
H	-7.35501900	-3.22802600	-1.10617600
H	-9.09689700	-3.21865400	-0.76406500
C	1.56502500	2.71305700	-3.40558200
H	0.53250100	2.35368800	-3.39058700
H	1.69014000	3.34954200	-4.29097500
H	2.22554800	1.84531200	-3.50238500
C	3.37692700	-1.72569800	-0.53017800
Br	1.95489800	-2.10675400	-2.10304400

CP2A



Zero-point correction= 0.962776 (Hartree/Particle)
Thermal correction to Energy= 1.017888
Thermal correction to Enthalpy= 1.018832
Thermal correction to Gibbs Free Energy= 0.872415
Sum of electronic and zero-point Energies= -5125.717064
Sum of electronic and thermal Energies= -5125.661952
Sum of electronic and thermal Enthalpies= -5125.661008
Sum of electronic and thermal Free Energies= -5125.807426

Cartesian Coordinates

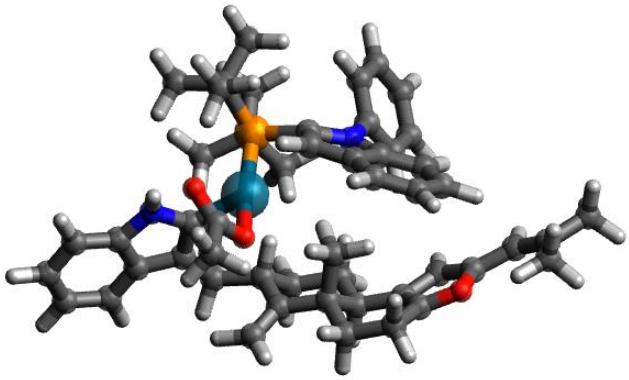
Atom	X	Y	Z
C	-0.35269800	-3.09537500	0.49051500
C	1.37608800	-1.64333200	1.70820000
H	1.26150700	-0.90019000	0.89670300
C	2.81286700	-1.47752700	2.22659600
H	2.85334200	-0.55260100	2.82047100
H	3.04892000	-2.28142200	2.93350800
C	5.69586100	-1.95791600	-0.15633300
C	5.08190500	-2.17759100	1.11297600
C	3.83994600	-1.45095000	1.12878700
N	4.87436900	-1.10041300	-0.85456000
H	4.98044800	-0.80572400	-1.81327600
C	5.72476000	-3.01836900	2.03995400
C	6.91615400	-2.54299800	-0.50441800
C	6.93076900	-3.61232500	1.69060000
H	7.43268600	-4.26668500	2.39784000
C	7.52123000	-3.37569700	0.43138700
H	8.46554400	-3.85390000	0.18698800
H	5.28340900	-3.20054500	3.01640500
H	7.37151600	-2.36066000	-1.47393100

C	1.04208100	-3.01073600	1.11814100
C	1.88615900	-4.04491800	1.17074400
H	2.88509900	-3.95882900	1.58144300
H	1.62519900	-5.02137100	0.77858000
Pd	2.46496300	0.64722700	-0.50961800
P	0.94853700	2.60065700	-0.48269900
C	0.32486200	-1.27585600	2.77275400
H	0.37102700	-2.01186000	3.58801200
H	0.56298100	-0.30268200	3.21524300
C	-1.39382100	-2.64361900	1.57448900
H	-1.27698600	-3.35967700	2.40446900
C	-1.08060600	-1.26681500	2.16819400
H	-1.15868300	-0.49076800	1.39523800
H	-1.82506100	-1.02528100	2.93843900
C	-0.36704500	-2.18488000	-0.75345100
H	0.35981600	-2.54458300	-1.48818600
H	-1.35587500	-2.15036900	-1.21364500
H	-0.09630800	-1.15977300	-0.51554100
C	-0.74432800	-4.52572200	0.04607700
H	0.01088400	-4.91967700	-0.64153100
H	-0.75266100	-5.18175500	0.92528300
C	-2.78443800	-2.78541800	1.02814300
C	-2.12619400	-4.59532500	-0.65237800
H	-2.03573300	-4.30784900	-1.70966700
H	-2.49125000	-5.63072700	-0.64943600
C	-3.07206500	-3.68627100	0.04588700
C	-4.01477200	-2.12069500	1.32919700
H	-4.17753500	-1.32452900	2.04195100
C	-4.97460400	-2.65250500	0.50044800
O	-4.39533000	-3.62156700	-0.29357200
C	1.44804200	3.26311100	1.23058600
C	1.01865500	3.94761500	-1.81867200
C	-2.43326100	0.68597600	-1.43462100
C	-3.00771500	1.57418500	-0.49165500
C	-4.37464000	1.55671400	-0.18555300
C	-5.16140800	0.62826400	-0.85377200
C	-4.61053000	-0.26526900	-1.79820000
C	-3.25804000	-0.24332700	-2.09623000
C	-1.03189900	0.96017900	-1.45075600
H	-4.79693100	2.24015700	0.54374300

H	-6.22322500	0.57201100	-0.63595500
H	-5.26002300	-0.99071800	-2.27671100
H	-2.83332900	-0.93475800	-2.81777600
H	-0.28127300	0.46705300	-2.05189100
C	-0.76664500	1.97939700	-0.55187100
N	-1.99674600	2.38057200	0.02242700
C	-2.27114400	3.28928700	1.08695900
C	-2.35072200	2.80761400	2.39735200
C	-2.56696300	4.62648400	0.81413600
C	-2.65315300	3.68032800	3.44172300
H	-2.18236200	1.75120700	2.58129400
C	-2.87275000	5.49703800	1.86116500
H	-2.55139300	4.97412700	-0.21136900
C	-2.90359200	5.02844600	3.17583800
H	-2.70032200	3.30643800	4.46010700
H	-3.09071000	6.53924000	1.64798900
H	-3.13753700	5.70826200	3.98969400
C	2.99330700	3.33221200	1.25524700
H	3.39654400	4.11124500	0.60778700
H	3.31966400	3.54340700	2.28105500
H	3.45754300	2.38019700	0.95596400
C	0.88999400	4.62210500	1.66809900
H	1.25966800	4.85177200	2.67605800
H	1.22641200	5.42668900	1.00799000
H	-0.19761400	4.63750700	1.70272600
C	1.04330000	2.16018400	2.22166300
H	-0.03078100	1.98558300	2.24187500
H	1.53146300	1.21233200	1.96853100
H	1.36506200	2.43656800	3.23332300
C	2.38496100	4.64936100	-1.77283400
H	2.49408700	5.29024900	-0.89348900
H	3.20867900	3.92758200	-1.78890500
H	2.48594600	5.28888000	-2.65813900
C	-0.11964700	4.96884400	-1.69282300
H	-0.02820100	5.71347600	-2.49405000
H	-1.09006800	4.47745400	-1.80701000
H	-0.10880400	5.50005400	-0.73806500
C	-6.37182400	-2.31720300	0.37628900
H	-6.68240500	-1.60510500	1.13931800
C	-7.30400500	-2.71014500	-0.51771300

C	-8.71184500	-2.18116700	-0.41527300
H	-9.00299800	-1.65410900	-1.33534800
H	-9.43368900	-3.00099700	-0.28927700
H	-8.83340300	-1.49134100	0.42595500
C	-7.07053100	-3.66436000	-1.65890700
H	-7.38686600	-3.20574700	-2.60681200
H	-6.02984000	-3.97072000	-1.74733800
H	-7.68628100	-4.56721100	-1.53590200
C	0.88552700	3.22161300	-3.17069000
H	-0.08048800	2.71750000	-3.26117400
H	0.95651400	3.96304400	-3.97663600
H	1.66886300	2.47286500	-3.31166800
C	3.77465300	-0.76874000	-0.08478800
Br	2.35135200	-0.23820100	-2.80263100

CP3A



Zero-point correction= 1.015883 (Hartree/Particle)
Thermal correction to Energy= 1.073435
Thermal correction to Enthalpy= 1.074380
Thermal correction to Gibbs Free Energy= 0.924951
Sum of electronic and zero-point Energies= -2782.730345
Sum of electronic and thermal Energies= -2782.672792
Sum of electronic and thermal Enthalpies= -2782.671848
Sum of electronic and thermal Free Energies= -2782.821276

Cartesian Coordinates

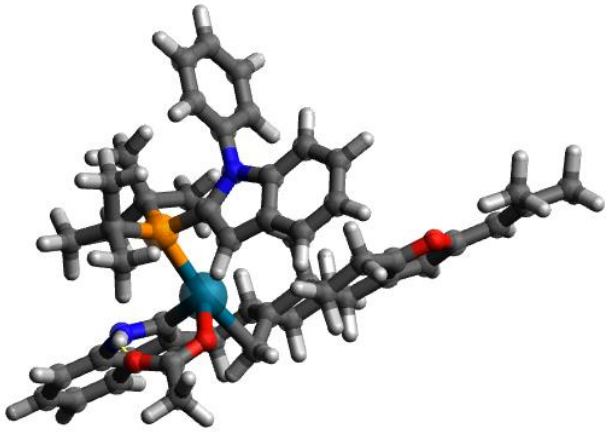
Atom	X	Y	Z
C	-0.93743300	2.72012800	-0.75851400
C	0.98856100	1.61422900	-2.03138100
H	0.83122300	0.73517300	-1.39385700
C	2.47166000	1.57837900	-2.42524300

H	2.57461000	0.81816900	-3.21645300
H	2.74808600	2.52433400	-2.90965500
C	5.46895300	1.18473900	-0.18009600
C	4.85081900	1.65645300	-1.37226400
C	3.45183200	1.28396300	-1.32045900
C	3.28824900	0.60150700	-0.13128000
N	4.49984400	0.50543200	0.54133900
H	4.49910700	0.37128100	1.55017800
C	5.63050600	2.35000700	-2.31125600
C	6.81694900	1.41233100	0.09941900
C	6.97646200	2.57741100	-2.03724000
H	7.58640300	3.11910300	-2.75537900
C	7.56299700	2.11820400	-0.84257700
H	8.61470900	2.31430300	-0.65259100
H	5.18953100	2.71059700	-3.23718600
H	7.26783100	1.05069000	1.01977000
C	0.51649600	2.82358100	-1.23418200
C	1.30642000	3.86870400	-0.97906200
H	2.34769900	3.88328700	-1.28126900
H	0.96337900	4.73490000	-0.42453800
Pd	1.69179500	-0.02562900	0.84694300
P	1.46665800	-2.20613300	0.21882000
C	0.07782100	1.43867900	-3.26351000
H	0.17908300	2.31956600	-3.91303300
H	0.41034900	0.57337500	-3.84980200
C	-1.85994100	2.44304900	-1.99947900
H	-1.78619300	3.33869800	-2.63559800
C	-1.38483700	1.26441500	-2.85176400
H	-1.50136600	0.32960400	-2.28872700
H	-2.02458000	1.17309700	-3.73920100
C	-1.02796200	1.58340700	0.27969500
H	-0.35916500	1.80352100	1.11399900
H	-2.03830100	1.46291200	0.66695400
H	-0.74160600	0.61753700	-0.14108000
C	-1.46231100	4.01073400	-0.08519100
H	-0.79934100	4.29186000	0.73868600
H	-1.43328700	4.82863500	-0.81519300
C	-3.27063700	2.29242900	-1.50208800
C	-2.90334600	3.86917400	0.47829900
H	-2.87694400	3.44785100	1.49278800

H	-3.36546800	4.86097200	0.57072500
C	-3.69730600	2.96418900	-0.39435900
C	-4.32608400	1.38808400	-1.84650400
H	-4.35243500	0.69147600	-2.67381100
C	-5.32731400	1.55919300	-0.91565500
O	-4.94341100	2.53632700	-0.02360100
C	1.53691200	-2.75694100	-1.60065500
C	2.43403800	-3.39848600	1.34594300
C	-1.52003000	-0.73664800	2.41688900
C	-2.31603100	-1.24803500	1.36612100
C	-3.67697000	-0.94331400	1.25485200
C	-4.21162800	-0.06737100	2.19195200
C	-3.42629000	0.47017500	3.23343100
C	-2.08697500	0.13275300	3.36337600
C	-0.19216900	-1.22550800	2.20770100
H	-4.29370700	-1.33885200	0.45816900
H	-5.25500200	0.21537500	2.10431500
H	-3.88038200	1.15903800	3.93925900
H	-1.47611100	0.54775900	4.15922500
H	0.65252600	-1.02743300	2.85297700
C	-0.18627000	-2.01665500	1.04610500
N	-1.49105300	-2.02592300	0.53826500
C	-2.02730100	-2.87863000	-0.46226000
C	-2.84317800	-2.33725400	-1.46252500
C	-1.77330200	-4.25062900	-0.42212500
C	-3.38599900	-3.17580200	-2.43348500
H	-3.02165600	-1.26762600	-1.48836300
C	-2.30573800	-5.07961800	-1.41038000
H	-1.16800100	-4.65725100	0.38097700
C	-3.11185800	-4.54595300	-2.41696600
H	-4.01138500	-2.75395900	-3.21458700
H	-2.10000200	-6.14559100	-1.38360800
H	-3.52915400	-5.19435600	-3.18120000
C	2.89067100	-2.21626900	-2.12144400
H	3.75246800	-2.67130300	-1.63357700
H	2.95278100	-2.45267400	-3.19049100
H	2.97366100	-1.13623000	-1.99517900
C	1.45581600	-4.26848500	-1.85797900
H	1.46188700	-4.42877200	-2.94335500
H	2.31081700	-4.80915300	-1.44615100

H	0.53501600	-4.70537300	-1.46813900
C	0.42324100	-2.04810200	-2.38789000
H	-0.51995900	-2.58448800	-2.33358500
H	0.26510500	-1.02575600	-2.04551700
H	0.71890900	-1.99923900	-3.44208500
C	3.85492400	-3.57634000	0.78038700
H	3.87151100	-4.12558100	-0.16313800
H	4.35098100	-2.61039600	0.63870200
H	4.44443000	-4.15291300	1.50265100
C	1.71179200	-4.74953600	1.48380400
H	2.27914900	-5.38668800	2.17344900
H	0.71163500	-4.61297700	1.90873400
H	1.61857600	-5.28607300	0.53829400
C	-6.58061900	0.86084900	-0.76696800
H	-6.73611900	0.13706900	-1.56610400
C	-7.53902700	0.94677900	0.18146500
C	-8.75716900	0.06302400	0.09795800
H	-8.85257300	-0.56205800	0.99738500
H	-9.67610200	0.66387600	0.04180000
H	-8.72988200	-0.59753200	-0.77425400
C	-7.52141600	1.88186000	1.36210900
H	-7.62375900	1.31467700	2.29876700
H	-6.61602100	2.48341600	1.41418400
H	-8.38635500	2.55941100	1.32162400
C	2.80846500	2.86404200	3.82605100
H	3.46970300	3.55890500	3.29441900
H	1.85011600	3.36854400	3.97552700
H	3.26450700	2.61404400	4.78637400
C	2.63856400	1.61426100	2.97435800
O	3.34071500	0.60573900	3.19187600
O	1.76124500	1.72383000	2.03269600
C	2.57250900	-2.77783600	2.75174300
H	1.62422000	-2.79806400	3.29318900
H	3.28049200	-3.39132200	3.32195200
H	2.94890200	-1.75011800	2.73368100

CP4A



Zero-point correction= 1.015749 (Hartree/Particle)
Thermal correction to Energy= 1.073333
Thermal correction to Enthalpy= 1.074277
Thermal correction to Gibbs Free Energy= 0.924213
Sum of electronic and zero-point Energies= -2782.729803
Sum of electronic and thermal Energies= -2782.672220
Sum of electronic and thermal Enthalpies= -2782.671275
Sum of electronic and thermal Free Energies= -2782.821339

Cartesian Coordinates

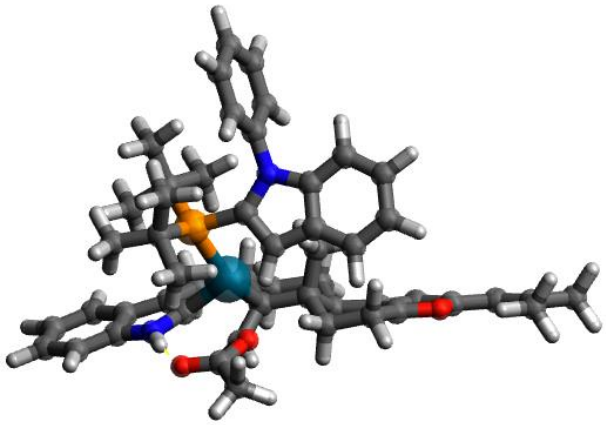
Atom	X	Y	Z
C	1.63544000	-1.71844600	-0.02222400
C	-0.25457900	-2.79297000	-1.41566600
H	-0.23124000	-1.93448200	-2.09421800
C	-1.66244600	-3.40608600	-1.49756100
H	-1.83188500	-3.65633200	-2.55442300
H	-1.64537700	-4.37806400	-0.97807100
C	-5.01170600	-2.14125100	-0.36722700
C	-4.21547200	-3.00775800	-1.16779400
C	-2.82964300	-2.61702800	-0.98118000
C	-2.86611700	-1.54695900	-0.12166000
N	-4.16500800	-1.21855700	0.23914600
H	-4.29065700	-0.86378100	1.20315000
C	-4.84109600	-4.01357700	-1.91880800
C	-6.39825600	-2.27211400	-0.29119700
C	-6.22627100	-4.14139200	-1.84975300
H	-6.72308300	-4.91723800	-2.42611100
C	-6.99548100	-3.28409000	-1.04106900
H	-8.07374400	-3.41166400	-1.00156800
H	-4.25581900	-4.68703600	-2.53995300

H	-6.98832500	-1.60808500	0.33401800
C	0.21715800	-2.31592000	-0.04358300
C	-0.44389100	-2.63817300	1.11365100
H	-1.34317400	-3.24289800	1.09732800
H	-0.02751000	-2.44477500	2.09389700
Pd	-1.43496400	-0.53064400	0.72537200
P	-2.08216100	1.55963700	-0.16208600
C	0.76150900	-3.82762000	-1.96517300
H	0.68303600	-4.73969300	-1.35694100
H	0.46624800	-4.10174700	-2.98525900
C	2.58276400	-2.86878500	-0.52908400
H	2.39689900	-3.72429900	0.14016300
C	2.20978800	-3.33513700	-1.93859500
H	2.35944800	-2.52250800	-2.65974500
H	2.87962100	-4.14753400	-2.24562600
C	1.73252600	-0.47735900	-0.93403800
H	1.15176000	0.34096700	-0.50537800
H	2.77037400	-0.15158900	-1.03472500
H	1.35249100	-0.66370700	-1.93842200
C	2.10164200	-1.32241500	1.40180200
H	1.39243000	-0.62188300	1.85003100
H	2.11291200	-2.21889800	2.03197300
C	4.01643700	-2.44715600	-0.36652700
C	3.51155100	-0.69497800	1.42503500
H	3.47755300	0.35338500	1.10244700
H	3.89049700	-0.67808900	2.45392300
C	4.39080300	-1.49327800	0.53413100
C	5.22091500	-2.87400500	-1.01375300
H	5.32393300	-3.62242800	-1.78735700
C	6.25354600	-2.14819200	-0.46567400
O	5.74135900	-1.29279300	0.48823700
C	-2.24239500	1.61158200	-2.05971700
C	-3.37240200	2.69324900	0.67119200
C	1.22962600	2.13208100	2.03941900
C	1.66809500	2.83726600	0.89305000
C	2.94631300	3.39878000	0.80722000
C	3.78903100	3.22712800	1.90037100
C	3.37142500	2.52710900	3.05254000
C	2.09920900	1.97934600	3.13351800
C	-0.11353700	1.71316500	1.77961600

H	3.26582000	3.94429000	-0.07395900
H	4.79150100	3.64315700	1.86583300
H	4.06080200	2.41522700	3.88389300
H	1.77442100	1.43818800	4.01714500
H	-0.74042600	1.14091800	2.45803400
C	-0.47876200	2.17476400	0.51139800
N	0.62172700	2.85940800	-0.03278300
C	0.70290100	3.70469000	-1.18067800
C	1.50083100	3.31953900	-2.26095300
C	0.08236400	4.95567200	-1.17419500
C	1.63142700	4.16685800	-3.36104100
H	2.00940000	2.36141200	-2.22890500
C	0.21132900	5.79731200	-2.27904400
H	-0.49532400	5.25714900	-0.30901300
C	0.97889600	5.40115800	-3.37608500
H	2.24255100	3.86159500	-4.20492200
H	-0.28118500	6.76499400	-2.27784200
H	1.07831000	6.05770900	-4.23517500
C	-3.44306700	0.72343900	-2.46283500
H	-4.39619700	1.07455100	-2.07085400
H	-3.50763900	0.74216400	-3.55801500
H	-3.30203500	-0.31097400	-2.15028300
C	-2.43032300	3.00495600	-2.67828700
H	-2.44951300	2.89540800	-3.76979200
H	-3.38120600	3.45567300	-2.38346100
H	-1.62467000	3.69404900	-2.43023300
C	-0.99039400	0.93536300	-2.63348300
H	-0.07902100	1.49403600	-2.43267600
H	-0.88436100	-0.06872500	-2.22110700
H	-1.10206900	0.85162300	-3.72145600
C	-4.77246400	2.40594200	0.10224300
H	-4.88803800	2.76174500	-0.92464700
H	-5.01041800	1.33915200	0.13666300
H	-5.50943900	2.93578400	0.71745700
C	-3.00519200	4.17526200	0.48862500
H	-3.78669900	4.78878600	0.95416100
H	-2.06289700	4.40270400	0.99630500
H	-2.92225000	4.47779300	-0.55655300
C	7.66673000	-2.18827700	-0.75605900
H	7.89735400	-2.92365900	-1.52548700

C	8.69965900	-1.48606900	-0.24371700
C	10.09904800	-1.74215400	-0.74197400
H	10.54185300	-0.82639600	-1.15928900
H	10.75774200	-2.05574400	0.08052700
H	10.12789800	-2.51674800	-1.51452000
C	8.59737900	-0.42757000	0.82220400
H	9.00903000	0.52266800	0.45264000
H	7.57574700	-0.25703400	1.15586000
H	9.20730500	-0.70694800	1.69330000
C	-2.98132900	-1.04233200	5.08637300
H	-2.40584600	-1.94472500	5.32036000
H	-2.52205800	-0.21591400	5.64109100
H	-4.01603500	-1.17061800	5.41092800
C	-2.90568900	-0.75694400	3.58495600
O	-3.98355700	-0.67197500	2.94581300
O	-1.72753900	-0.60773000	3.11537600
C	-3.39183900	2.38405100	2.17696200
H	-2.42450300	2.58100800	2.64464900
H	-4.12606900	3.05078600	2.64734300
H	-3.68255900	1.35233200	2.38307800

TS2A



Zero-point correction= 1.012937 (Hartree/Particle)
Thermal correction to Energy= 1.070410
Thermal correction to Enthalpy= 1.071355
Thermal correction to Gibbs Free Energy= 0.920389
Sum of electronic and zero-point Energies= -2782.692318
Sum of electronic and thermal Energies= -2782.634844
Sum of electronic and thermal Enthalpies= -2782.633900
Sum of electronic and thermal Free Energies= -2782.784866

Cartesian Coordinates

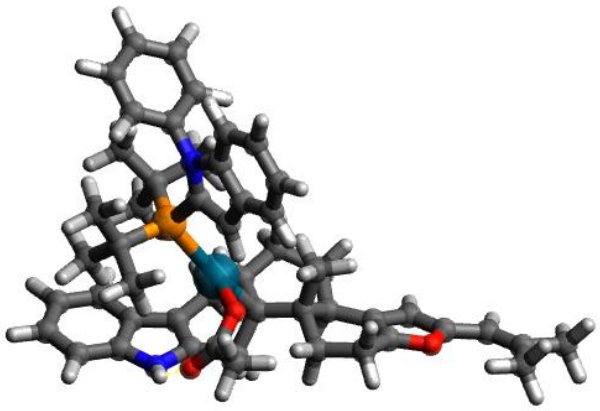
Atom	X	Y	Z
C	1.95077100	-1.46290300	-0.32027200
C	0.24924100	-2.44840500	-2.00701800
H	0.18993600	-1.47227400	-2.50147400
C	-1.10086300	-3.17479200	-2.26004500
H	-1.47679100	-2.84684200	-3.23926300
H	-0.90241400	-4.25227500	-2.38054500
C	-3.87947500	-3.44196700	0.25464900
C	-3.41260200	-3.67505200	-1.08285900
C	-2.14245300	-3.02219800	-1.19739100
C	-1.91121400	-2.42529900	0.03854300
N	-2.94138500	-2.68035000	0.91189500
H	-2.87355900	-2.38537200	1.91687900
C	-4.20267600	-4.43944500	-1.96219200
C	-5.10694500	-3.94683600	0.70121100
C	-5.41766200	-4.93756100	-1.51371200
H	-6.03944000	-5.52575900	-2.18272600
C	-5.86370000	-4.69104400	-0.19586200
H	-6.82071200	-5.09430500	0.12349000
H	-3.86656200	-4.63085500	-2.97806400
H	-5.44766000	-3.76306400	1.71566200
C	0.60620500	-2.18357800	-0.54079600
C	0.02862500	-3.05659600	0.42608100
H	-0.27903000	-4.06315500	0.16591700
H	0.25571800	-2.90338700	1.47587200
Pd	-0.89488000	-0.73279200	0.26945800
P	-2.47597800	1.11147600	0.20775800
C	1.38807000	-3.23047100	-2.70287100
H	1.41494400	-4.24683000	-2.28439600
H	1.15274300	-3.33466500	-3.76974900
C	3.03193400	-2.38044600	-1.01180000
H	2.92303900	-3.37163400	-0.54223000
C	2.75685000	-2.57713900	-2.50519400
H	2.81210900	-1.61655900	-3.03179400
H	3.53526000	-3.21503700	-2.94114600
C	1.94184400	-0.05465500	-0.96249700
H	1.37324700	0.64728000	-0.34655600
H	2.95835600	0.33617900	-1.05181200

H	1.50224900	-0.05090100	-1.96158200
C	2.33627800	-1.34780400	1.17726900
H	1.53899500	-0.87834800	1.75692400
H	2.45196400	-2.36063300	1.58186000
C	4.40589500	-1.85870200	-0.69436100
C	3.66331800	-0.59089000	1.39576400
H	3.51646100	0.49251500	1.28800700
H	4.01400500	-0.75332800	2.42296400
C	4.65046900	-1.08503600	0.40281100
C	5.66601000	-2.01209500	-1.35824400
H	5.87058800	-2.56373100	-2.26547500
C	6.59860100	-1.31903300	-0.62119300
O	5.97134800	-0.74317100	0.46453100
C	-3.11452600	1.23304700	-1.57973300
C	-3.78406500	1.65809400	1.47598800
C	1.01138600	2.66133600	1.47958600
C	0.75912800	3.62644100	0.47362300
C	1.66057300	4.65714900	0.18635500
C	2.84101900	4.69065100	0.92005200
C	3.11664000	3.73401300	1.92085200
C	2.21062600	2.72373100	2.21135300
C	-0.10925000	1.77312900	1.49151400
H	1.44719000	5.39660900	-0.57805200
H	3.56696400	5.47324300	0.71961500
H	4.05029600	3.79608900	2.47179500
H	2.41350400	1.99342400	2.98891800
H	-0.23664900	0.91307000	2.14445500
C	-1.01893500	2.19961200	0.52262800
N	-0.48105900	3.34470800	-0.09907900
C	-1.07592500	4.26315300	-1.01535900
C	-0.62352300	4.30935500	-2.33678700
C	-2.02845600	5.18207200	-0.56949900
C	-1.17258300	5.23167200	-3.22709300
H	0.15403400	3.62282900	-2.65477400
C	-2.58003900	6.09904000	-1.46398200
H	-2.33055800	5.16999700	0.46974500
C	-2.16064800	6.11870500	-2.79556000
H	-0.82816500	5.25613600	-4.25651800
H	-3.33086300	6.80272500	-1.11732600
H	-2.59217200	6.83205300	-3.49128500

C	-4.00861600	-0.00558200	-1.81643700
H	-4.94940000	0.04011400	-1.26699800
H	-4.25509600	-0.05012900	-2.88503500
H	-3.49816900	-0.93329900	-1.55205700
C	-3.90847900	2.49218400	-1.95414200
H	-4.20578900	2.41998600	-3.00836400
H	-4.82645900	2.57797100	-1.36604200
H	-3.33505800	3.40943800	-1.83402700
C	-1.88406900	1.07474900	-2.49203800
H	-1.15993200	1.87805000	-2.36481500
H	-1.37917500	0.12438800	-2.29142800
H	-2.21305000	1.07652900	-3.53873600
C	-5.09746700	0.90395000	1.20891800
H	-5.61140100	1.26496900	0.31392000
H	-4.93147900	-0.17393600	1.11073600
H	-5.77066100	1.06041600	2.06058100
C	-4.01613400	3.17466400	1.47900400
H	-4.80611600	3.41618700	2.20196600
H	-3.10921800	3.69688100	1.79811900
H	-4.32001900	3.56569700	0.50568900
C	8.01480900	-1.15388300	-0.84484800
H	8.34254900	-1.67653400	-1.74233900
C	8.95306100	-0.48172300	-0.14458900
C	10.38371800	-0.48122900	-0.61935400
H	10.73502100	0.54330100	-0.80852100
H	11.05219700	-0.89963600	0.14671000
H	10.51490800	-1.06098000	-1.53827800
C	8.71087700	0.30212900	1.11783500
H	9.01765500	1.34874000	0.97836700
H	7.67037400	0.28547900	1.43586100
H	9.33244200	-0.09291500	1.93419300
C	-0.96414400	-1.09255800	5.15217600
H	0.10038500	-1.24557100	5.35251700
H	-1.18898900	-0.03662300	5.35210100
H	-1.57067900	-1.70554800	5.82310000
C	-1.28906400	-1.39029300	3.68614500
O	-2.41236000	-1.91318600	3.44554200
O	-0.41790600	-1.03725000	2.83226100
C	-3.26056400	1.23669500	2.86029600
H	-2.29268300	1.69412800	3.08442100

H	-3.97481200	1.58126700	3.61950200
H	-3.16297600	0.15294900	2.95015100

CP5A



Zero-point correction= 1.014970 (Hartree/Particle)
Thermal correction to Energy= 1.072450
Thermal correction to Enthalpy= 1.073394
Thermal correction to Gibbs Free Energy= 0.922628
Sum of electronic and zero-point Energies= -2782.749094
Sum of electronic and thermal Energies= -2782.691614
Sum of electronic and thermal Enthalpies= -2782.690670
Sum of electronic and thermal Free Energies= -2782.841436

Cartesian Coordinates

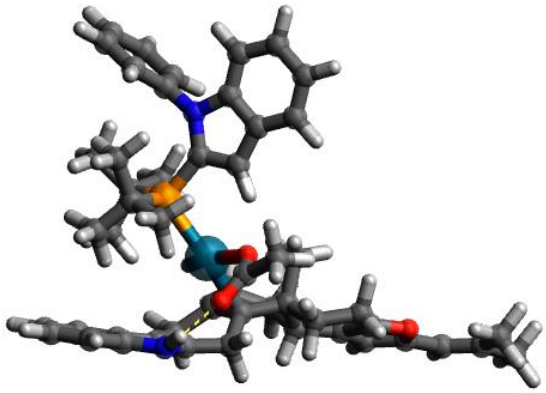
Atom	X	Y	Z
C	-2.89052500	0.33739600	0.00479000
C	-1.29260200	1.72454300	-1.47685500
H	-0.17897900	1.32057500	-1.50184200
C	-1.04456000	3.23238600	-1.78820000
H	-0.45679900	3.31170800	-2.70929100
H	-2.02429900	3.68754700	-2.00047600
C	1.08828200	4.69543400	0.94788900
C	0.85862900	4.61980000	-0.46329300
C	-0.35787300	3.86794300	-0.62816700
C	-0.79167600	3.53098200	0.62947500
N	0.04087000	4.05271300	1.59441500
H	0.12399400	3.55737000	2.48291600
C	1.79353000	5.19891200	-1.33545500
C	2.21540400	5.32517600	1.47833900
C	2.92392700	5.81263700	-0.80465500

H	3.65617100	6.25757200	-1.47281900
C	3.13310200	5.87561500	0.58712400
H	4.02394400	6.36355000	0.97202700
H	1.64119000	5.16056400	-2.41110000
H	2.37531100	5.37006600	2.55176900
C	-1.79804400	1.41562100	-0.08899000
C	-1.94475900	2.61625700	0.85628200
H	-2.89738200	3.13859800	0.65465300
H	-1.97205100	2.28384000	1.89216800
Pd	0.15513000	0.73861000	0.20533400
P	2.49766500	0.04217500	-0.11425100
C	-1.95146000	0.96532900	-2.65123700
H	-1.77834600	1.54768600	-3.56272900
H	-1.42154200	0.02233000	-2.80323000
C	-3.97070800	0.78436600	-1.04104500
H	-4.15624700	1.85210100	-0.84503200
C	-3.46194200	0.66665300	-2.48820500
H	-3.66091400	-0.34604000	-2.85419400
H	-4.04984200	1.34121300	-3.12044600
C	-2.34289600	-1.07630800	-0.29857400
H	-1.77965200	-1.43893500	0.56493100
H	-3.16186700	-1.77269400	-0.50370300
H	-1.66833200	-1.10114700	-1.15596000
C	-3.53901200	0.29634100	1.41331100
H	-2.75891600	0.09113900	2.14978600
H	-3.97197600	1.27455300	1.64640900
C	-5.25661400	0.03725600	-0.82249800
C	-4.66383600	-0.75245900	1.53411700
H	-4.24781900	-1.76670500	1.61482400
H	-5.23524200	-0.57993100	2.45480600
C	-5.53078700	-0.62919800	0.33548500
C	-6.39283600	-0.16504100	-1.67247700
H	-6.54104600	0.21431200	-2.67428000
C	-7.28677900	-0.94363300	-0.97486100
O	-6.75433500	-1.23306200	0.26464200
C	2.98708500	0.41012100	-1.92091700
C	3.74892900	0.79662700	1.10202700
C	1.95495100	-3.60439200	1.46316700
C	3.12685100	-3.91251900	0.72934000
C	3.72542000	-5.17731100	0.77428400

C	3.13958400	-6.12830200	1.60114900
C	1.98348200	-5.83675300	2.35740900
C	1.38606500	-4.58612300	2.29408600
C	1.61084300	-2.25547900	1.13858800
H	4.61353700	-5.40110500	0.19263600
H	3.58240200	-7.11804500	1.66789500
H	1.55746100	-6.60717400	2.99353000
H	0.49197200	-4.36394300	2.87002600
H	0.79928200	-1.67896200	1.56163700
C	2.54487800	-1.75895500	0.24580100
N	3.50131400	-2.78393900	0.00787700
C	4.49091600	-2.90944700	-1.01381800
C	4.11509800	-3.34966400	-2.28668900
C	5.84025700	-2.70865300	-0.71597300
C	5.07745400	-3.50630800	-3.28265800
H	3.07098100	-3.57062800	-2.48039600
C	6.80280100	-2.87160200	-1.71330900
H	6.12422700	-2.41963100	0.28811700
C	6.42205200	-3.25521200	-3.00022100
H	4.77903300	-3.83207800	-4.27465300
H	7.84993900	-2.69986200	-1.48258400
H	7.17212300	-3.37428500	-3.77647100
C	2.61263900	1.87255000	-2.24500100
H	3.27463200	2.59560500	-1.76927400
H	2.68758500	2.01777400	-3.33044800
H	1.59660500	2.12358000	-1.93945700
C	4.46705600	0.22497700	-2.29035100
H	4.59591200	0.45069200	-3.35708300
H	5.10591000	0.91604800	-1.73427300
H	4.82697600	-0.78601400	-2.12230200
C	2.09899300	-0.50504900	-2.78487300
H	2.29892800	-1.56172700	-2.60665200
H	1.03595000	-0.32798400	-2.58799100
H	2.28582500	-0.29776100	-3.84594000
C	4.00199300	2.26815900	0.73956800
H	4.63374000	2.37650300	-0.14612100
H	3.07238200	2.81843500	0.57564900
H	4.52277200	2.75524400	1.57296900
C	5.07215200	0.02535600	1.17464200
H	5.74316000	0.52925900	1.88251400

H	4.90875400	-0.99314400	1.53773500
H	5.58252300	-0.02752300	0.21054600
C	-8.58640500	-1.43391900	-1.36748000
H	-8.84796900	-1.11349300	-2.37490500
C	-9.48625800	-2.19393800	-0.70799600
C	-10.78689500	-2.56172900	-1.37520400
H	-10.89866900	-3.65333000	-1.44318500
H	-11.64453400	-2.19991600	-0.79020900
H	-10.86532700	-2.14810100	-2.38537100
C	-9.32094300	-2.73766700	0.68614000
H	-9.38455600	-3.83523500	0.67453400
H	-8.37737200	-2.45063400	1.14579600
H	-10.14317000	-2.39006700	1.32786900
C	-0.42793000	-0.22215600	4.49386400
H	-1.33428900	-0.82808300	4.39202800
H	0.41492100	-0.91560800	4.59583700
H	-0.49311900	0.40243500	5.38661800
C	-0.21989800	0.63775900	3.24949400
O	-0.01483200	1.85668200	3.36632000
O	-0.27044900	-0.03906000	2.15171300
C	3.07016100	0.74877100	2.48275800
H	2.76292800	-0.26736500	2.74950200
H	3.78524800	1.09536200	3.24008200
H	2.19083300	1.39403800	2.52281300

TS3A



Zero-point correction= 1.011693 (Hartree/Particle)
Thermal correction to Energy= 1.068961
Thermal correction to Enthalpy= 1.069905
Thermal correction to Gibbs Free Energy= 0.920252

Sum of electronic and zero-point Energies= -2782.744418
Sum of electronic and thermal Energies= -2782.687151
Sum of electronic and thermal Enthalpies= -2782.686207
Sum of electronic and thermal Free Energies= -2782.835859

Cartesian Coordinates

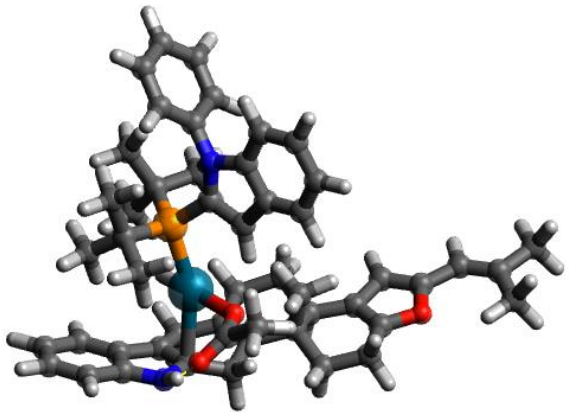
Atom	X	Y	Z
C	-2.91725300	0.48434200	0.01216200
C	-1.35838800	1.85050000	-1.44281100
H	0.14009000	1.20265200	-1.43048100
C	-0.86311400	3.26686900	-1.78858800
H	-0.20249300	3.22339600	-2.66128900
H	-1.75645900	3.82776800	-2.11396700
C	1.26609600	4.67544700	0.97440500
C	1.05628100	4.58784000	-0.43933000
C	-0.18945900	3.88936900	-0.61319100
C	-0.65882300	3.59274000	0.64047700
N	0.18159400	4.08977800	1.61279500
H	0.23401000	3.58702400	2.50259700
C	2.03057300	5.10948100	-1.30493600
C	2.41087300	5.26475400	1.51370400
C	3.17735300	5.68338700	-0.76443300
H	3.93945000	6.08467300	-1.42685800
C	3.36524900	5.76173300	0.62970300
H	4.26966300	6.21799300	1.02185900
H	1.89466400	5.06012200	-2.38236600
H	2.55458700	5.32061500	2.58887500
C	-1.84309100	1.57910600	-0.12808200
C	-1.85061100	2.73247300	0.88235500
H	-2.78094400	3.31387300	0.75495000
H	-1.84505200	2.35712900	1.90333200
Pd	0.21084200	0.78579000	0.09624100
P	2.44752700	-0.00074700	-0.22028200
C	-1.91805500	1.06099600	-2.63015200
H	-1.77015300	1.66546500	-3.53117600
H	-1.32666700	0.15648600	-2.78410900
C	-3.97960900	0.85709600	-1.07823000
H	-4.18316400	1.93219500	-0.94862300
C	-3.41529200	0.66019200	-2.49330000
H	-3.52873200	-0.39087200	-2.77712500

H	-4.02087700	1.23765900	-3.19999600
C	-2.34989100	-0.93589000	-0.21352700
H	-1.77162600	-1.23758000	0.66285600
H	-3.16094100	-1.65425900	-0.36781300
H	-1.68559900	-0.99819400	-1.07760900
C	-3.58476200	0.50987800	1.41019000
H	-2.81718700	0.33748600	2.16839600
H	-4.01737500	1.49969100	1.59131100
C	-5.25823600	0.10236100	-0.85073400
C	-4.71026200	-0.53468400	1.56444100
H	-4.29136500	-1.53957100	1.71614900
H	-5.30396700	-0.31099500	2.45958300
C	-5.55050500	-0.49337800	0.34102200
C	-6.37125500	-0.16950400	-1.71160700
H	-6.50107800	0.14383300	-2.73846400
C	-7.27078400	-0.91583400	-0.98642300
O	-6.76377600	-1.11852900	0.28066700
C	2.97694600	0.25196300	-2.03713700
C	3.71212700	0.77737200	0.96884900
C	1.78247800	-3.53079200	1.56432600
C	2.94377400	-3.91954500	0.85315500
C	3.50291300	-5.19719300	0.97769700
C	2.88821500	-6.07563200	1.86178000
C	1.74221000	-5.70182300	2.59719700
C	1.18364100	-4.43996400	2.45472000
C	1.48010400	-2.19465100	1.15783300
H	4.38325100	-5.48475700	0.41259300
H	3.30024400	-7.07246700	1.99094700
H	1.29347800	-6.41730500	3.28010900
H	0.29764700	-4.15367100	3.01459800
H	0.69208600	-1.56723100	1.55241900
C	2.42825200	-1.78236600	0.23773100
N	3.35247000	-2.85003900	0.06348800
C	4.34823100	-3.06996500	-0.93578200
C	3.97246500	-3.55751600	-2.19106700
C	5.70075300	-2.91425900	-0.62432100
C	4.94213900	-3.80519200	-3.16122000
H	2.92288200	-3.74324500	-2.39161100
C	6.67016200	-3.16932100	-1.59517200
H	5.98143900	-2.58698900	0.36905900

C	6.29207000	-3.59930400	-2.86821900
H	4.64472700	-4.16726600	-4.14084600
H	7.72031200	-3.03258700	-1.35497100
H	7.04775400	-3.78974300	-3.62452900
C	2.67876800	1.70378400	-2.46739400
H	3.31262400	2.43712900	-1.96967000
H	2.85827500	1.78350000	-3.54722400
H	1.64354500	1.98524100	-2.27384400
C	4.46019900	-0.01407400	-2.34597400
H	4.62212000	0.11467700	-3.42376400
H	5.10902900	0.70092700	-1.83394400
H	4.78092300	-1.01773200	-2.08406400
C	2.07867800	-0.67764900	-2.87338500
H	2.22508400	-1.72847500	-2.62359600
H	1.02040900	-0.43922200	-2.72439600
H	2.31138800	-0.54578000	-3.93733200
C	4.04472000	2.20862600	0.52085200
H	4.69318800	2.23050200	-0.35883300
H	3.14685800	2.79371100	0.31086800
H	4.57768600	2.71832700	1.33201900
C	4.99359800	-0.05440000	1.10724900
H	5.67835200	0.45975200	1.79393900
H	4.77581800	-1.03955400	1.52893200
H	5.51424400	-0.19017700	0.15709100
C	-8.55413100	-1.44921200	-1.37640500
H	-8.79668800	-1.19604100	-2.40744200
C	-9.45845200	-2.18028200	-0.69083800
C	-10.73828700	-2.60810900	-1.36247000
H	-10.83349000	-3.70337400	-1.36502100
H	-11.61393000	-2.22384700	-0.82003500
H	-10.79921200	-2.25882300	-2.39782100
C	-9.31809300	-2.63384800	0.73783200
H	-9.37005500	-3.73064200	0.79359500
H	-8.38799100	-2.30755900	1.19873500
H	-10.15782500	-2.25655500	1.33882700
C	-0.40046500	-0.16822000	4.45274500
H	-1.33041200	-0.73357600	4.32815500
H	0.41472200	-0.89912500	4.51056300
H	-0.43646800	0.40991300	5.37797000
C	-0.17175400	0.74489600	3.24913400

O	0.04708000	1.95557600	3.43259400
O	-0.22570400	0.12667600	2.12096500
C	3.01895800	0.84999500	2.34001600
H	2.66054500	-0.13044100	2.66773800
H	3.74345100	1.21126600	3.08111000
H	2.17080700	1.53601800	2.32990000

CP6A



Zero-point correction= 1.012299 (Hartree/Particle)
Thermal correction to Energy= 1.070193
Thermal correction to Enthalpy= 1.071138
Thermal correction to Gibbs Free Energy= 0.917415
Sum of electronic and zero-point Energies= -2782.759381
Sum of electronic and thermal Energies= -2782.701486
Sum of electronic and thermal Enthalpies= -2782.700542
Sum of electronic and thermal Free Energies= -2782.854265

Cartesian Coordinates

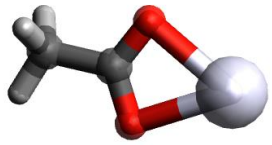
Atom	X	Y	Z
C	-3.14892400	1.52997000	0.06594500
C	-1.60331000	2.76607300	-1.48179300
H	1.29095300	1.72225400	-1.30351000
C	-0.48725300	3.75331300	-1.79109000
H	0.04548900	3.43880000	-2.69717300
H	-0.92653400	4.73608600	-2.03552900
C	2.10901800	4.42054400	0.85179600
C	1.78378100	4.44034600	-0.53667100
C	0.45725100	3.88577600	-0.64175000
C	0.03997600	3.58312100	0.65153600
N	1.01573900	3.96148200	1.56601700

H	1.12371900	3.43154500	2.45513500
C	2.73920000	4.87210600	-1.46798700
C	3.38376500	4.77098700	1.30716500
C	3.99810800	5.24681500	-1.01034200
H	4.75038700	5.58465000	-1.71736100
C	4.31663100	5.18722700	0.36200400
H	5.31178600	5.47543400	0.68900500
H	2.50339100	4.90105800	-2.52867000
H	3.62976100	4.72208800	2.36343200
C	-2.02980300	2.53085400	-0.22385700
C	-1.36789200	3.19704900	0.97889100
H	-1.93699300	4.09251700	1.27891700
H	-1.37244100	2.52213400	1.83700500
Pd	0.91594100	1.30134600	0.10687900
P	2.37237000	-0.37291300	-0.50845300
C	-2.18376000	2.10254800	-2.71142300
H	-2.64044900	2.88304600	-3.34130200
H	-1.35709200	1.69565800	-3.31148100
C	-4.04382800	1.40436900	-1.20457800
H	-4.41835700	2.42093200	-1.40924800
C	-3.21281300	1.00416100	-2.42099500
H	-2.71383500	0.04696800	-2.23467600
H	-3.85689200	0.85611800	-3.29556700
C	-2.49217100	0.18261000	0.45605100
H	-1.93957200	0.28124500	1.39402500
H	-3.23700500	-0.61173100	0.56220900
H	-1.76466000	-0.13008900	-0.29808800
C	-4.06591400	2.01031500	1.22620100
H	-3.47481100	2.22253700	2.12110400
H	-4.54245000	2.95255200	0.92597100
C	-5.22873900	0.52970900	-0.91297800
C	-5.16353900	0.98621400	1.60072600
H	-4.74533500	0.19631600	2.24118300
H	-5.94571100	1.47809200	2.19340700
C	-5.71758900	0.39970400	0.35339500
C	-6.07657400	-0.26764500	-1.74635600
H	-6.00272600	-0.41201600	-2.81551000
C	-7.02764800	-0.83686700	-0.93034500
O	-6.80573400	-0.42707500	0.36841300
C	2.43262900	-0.64795000	-2.39765600

C	4.03680800	0.20206300	0.20678700
C	1.06625200	-3.20230700	2.01671400
C	2.03309700	-3.99422300	1.35246900
C	2.28691200	-5.32169700	1.71738000
C	1.57263300	-5.83123800	2.79522600
C	0.62233800	-5.05014600	3.48810400
C	0.36083000	-3.74206700	3.10709900
C	1.04419300	-1.93662700	1.35201300
H	3.01550800	-5.92354800	1.18460000
H	1.75125000	-6.85468000	3.11257100
H	0.08793300	-5.48557200	4.32727100
H	-0.37570200	-3.14144300	3.63265100
H	0.46831800	-1.06723800	1.64057600
C	1.96853500	-1.95661800	0.32664600
N	2.60645100	-3.23510400	0.33423100
C	3.29383900	-3.92641500	-0.71378000
C	2.55507000	-4.52449500	-1.74035500
C	4.67644800	-4.11014000	-0.65494800
C	3.20680000	-5.22479900	-2.75311700
H	1.47396100	-4.43977900	-1.72969900
C	5.32701900	-4.81687700	-1.66806100
H	5.23394200	-3.69616200	0.17555400
C	4.59688000	-5.36001900	-2.72585100
H	2.62966200	-5.67236900	-3.55672300
H	6.40461800	-4.94433000	-1.62652200
H	5.10633200	-5.90303500	-3.51633600
C	2.36259900	0.68190600	-3.17884800
H	3.10881600	1.41165400	-2.85979000
H	2.53944800	0.46045300	-4.23890700
H	1.37646800	1.14528200	-3.09820500
C	3.69434200	-1.38581000	-2.88072100
H	3.56789400	-1.64781200	-3.93833000
H	4.57596800	-0.74224100	-2.80681000
H	3.89449400	-2.30495200	-2.33858500
C	1.15438800	-1.43731500	-2.73503900
H	1.14417000	-2.42732100	-2.28057900
H	0.26476800	-0.89655200	-2.39288900
H	1.08245100	-1.56002300	-3.82285700
C	4.52885900	1.43092300	-0.57505500
H	4.87503900	1.16962400	-1.57968200

H	3.75645000	2.20082900	-0.65439600
H	5.37610500	1.87507300	-0.03924200
C	5.10831500	-0.89467800	0.22484900
H	6.03830400	-0.47419800	0.62779500
H	4.80380600	-1.71512800	0.87880200
H	5.32654900	-1.29884300	-0.76510800
C	-8.11697700	-1.72323000	-1.26274900
H	-8.14417000	-1.94151200	-2.32942000
C	-9.06388500	-2.29809100	-0.49112000
C	-10.09739600	-3.19750200	-1.11972700
H	-10.06226800	-4.20461300	-0.67992400
H	-11.11287500	-2.81719600	-0.93779700
H	-9.95917100	-3.29373800	-2.20114500
C	-9.20288300	-2.12782000	0.99829500
H	-9.14265500	-3.10500600	1.49875100
H	-8.44443200	-1.47370700	1.42375100
H	-10.19414800	-1.71940000	1.24236600
C	0.50469400	0.06190500	4.38964700
H	-0.54218200	-0.25975200	4.40301600
H	1.11014100	-0.82066000	4.15057100
H	0.79289800	0.44297200	5.37108300
C	0.71140200	1.11977400	3.30956300
O	1.30992700	2.17482400	3.60165700
O	0.23042100	0.80949100	2.15612200
C	3.75095000	0.61966500	1.66300500
H	3.29069800	-0.19228000	2.23464700
H	4.70113300	0.87849600	2.14678300
H	3.09277800	1.48893100	1.72210900

AgOAc



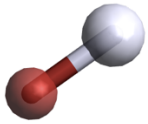
Zero-point correction= 0.050503 (Hartree/Particle)
Thermal correction to Energy= 0.056745
Thermal correction to Enthalpy= 0.057689
Thermal correction to Gibbs Free Energy= 0.017233
Sum of electronic and zero-point Energies= -374.214968
Sum of electronic and thermal Energies= -374.208725
Sum of electronic and thermal Enthalpies= -374.207781

Sum of electronic and thermal Free Energies= -374.248238

Cartesian Coordinates

Atom	X	Y	Z
C	-1.51872900	0.00951800	-0.00021800
O	-0.92288100	1.12905700	-0.00011600
O	-0.92359400	-1.11289100	-0.00005100
C	-3.04086000	-0.00357300	-0.00002900
H	-3.39697100	-0.54743100	-0.88050700
H	-3.39665600	-0.54394700	0.88274700
H	-3.44058800	1.01099000	-0.00184200
Ag	1.11411800	-0.00180000	0.00005100

AgBr

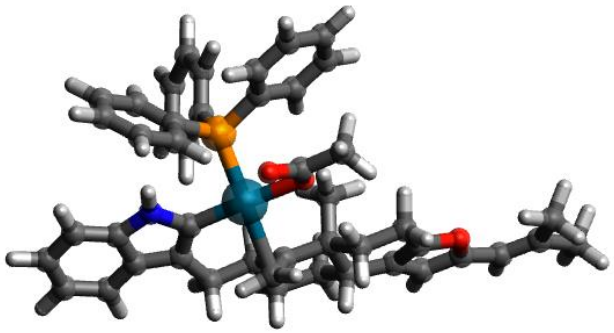


Zero-point correction= 0.000528 (Hartree/Particle)
Thermal correction to Energy= 0.003401
Thermal correction to Enthalpy= 0.004345
Thermal correction to Gibbs Free Energy= -0.024905
Sum of electronic and zero-point Energies= -2717.219172
Sum of electronic and thermal Energies= -2717.216299
Sum of electronic and thermal Enthalpies= -2717.215355
Sum of electronic and thermal Free Energies= -2717.244605

Cartesian Coordinates

Atom	X	Y	Z
Br	0.00000000	0.00000000	-1.40985700
Ag	0.00000000	0.00000000	1.04989300

CP3B



Zero-point correction= 0.841371 (Hartree/Particle)
Thermal correction to Energy= 0.890795
Thermal correction to Enthalpy= 0.891739
Thermal correction to Gibbs Free Energy= 0.755718
Sum of electronic and zero-point Energies= -2567.886079
Sum of electronic and thermal Energies= -2567.836655
Sum of electronic and thermal Enthalpies= -2567.835711
Sum of electronic and thermal Free Energies= -2567.971732

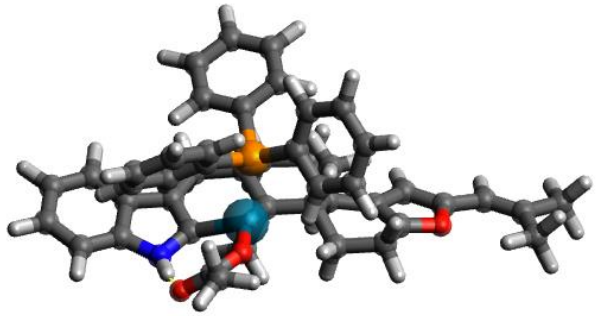
Cartesian Coordinates

Atom	X	Y	Z
C	-2.41101900	-0.97835600	-0.60479100
C	-0.65884600	-2.75778800	0.09351200
H	-0.40713300	-2.19751500	1.00253200
C	0.56689800	-3.60212000	-0.28420800
H	0.66355500	-4.37675500	0.48895500
H	0.33739000	-4.15619000	-1.20879800
C	4.17251000	-2.61402000	-0.53441200
C	3.15643900	-3.58911900	-0.33822000
C	1.88763200	-2.90300500	-0.40920500
C	2.15210700	-1.56395700	-0.64379900
N	3.53478100	-1.40397000	-0.70123100
H	3.99395100	-0.54414600	-0.95643800
C	3.53484600	-4.92553200	-0.12821600
C	5.53188400	-2.93371600	-0.52550100
C	4.88756500	-5.25066400	-0.11535400
H	5.19043800	-6.28146400	0.04732000
C	5.87639100	-4.26568500	-0.31249800
H	6.92471200	-4.55057700	-0.29735100
H	2.78290200	-5.69669500	0.01915200
H	6.28896500	-2.16841500	-0.67573100
C	-1.11830800	-1.73755300	-0.95220000

C	-0.50634300	-1.62370900	-2.16947800
H	0.30538500	-2.28211200	-2.45700000
H	-0.90192500	-0.97774200	-2.94395500
Pd	0.89284000	-0.03680000	-0.93651300
P	2.13760300	1.32543200	0.44724700
C	-1.81574300	-3.72007200	0.45924000
H	-1.99537200	-4.38644000	-0.39663700
H	-1.48324700	-4.35590100	1.28820200
C	-3.50860600	-2.07219800	-0.33016300
H	-3.54665300	-2.69565700	-1.23884900
C	-3.11623600	-3.00501000	0.81399600
H	-3.01147100	-2.43971500	1.74793400
H	-3.91032300	-3.74260900	0.98200500
C	-2.18349300	-0.08321100	0.63891300
H	-1.62793900	0.80657600	0.33825100
H	-3.14035900	0.22487300	1.06909000
H	-1.62037500	-0.59217700	1.42418700
C	-2.92376900	-0.10098500	-1.77692200
H	-2.14037600	0.59315000	-2.07897300
H	-3.15884300	-0.75527200	-2.62612800
C	-4.84860900	-1.41178300	-0.16295600
C	-4.18766800	0.70853100	-1.41693500
H	-3.91871400	1.58349100	-0.80795000
H	-4.64841200	1.10162100	-2.33220400
C	-5.12092000	-0.18021900	-0.68122600
C	-6.05016500	-1.84034000	0.48847900
H	-6.21999500	-2.76971600	1.01440500
C	-6.97834900	-0.83771600	0.32573100
O	-6.40432100	0.19009000	-0.39421400
C	0.13201400	2.45237500	-2.20744200
O	-0.40191500	1.59711600	-1.39197400
O	1.27025500	2.35725700	-2.68825600
C	-8.34511900	-0.76310700	0.78337400
H	-8.63277800	-1.65812300	1.33316700
C	-9.27931400	0.20105600	0.64170500
C	-9.08707600	1.50864500	-0.07936600
H	-9.27700700	2.34932100	0.60339400
H	-8.08877600	1.62082900	-0.49761000
H	-9.82008600	1.60378600	-0.89330800
C	-10.65132300	0.00673200	1.23501600

H	-10.88508100	0.80422900	1.95489000
H	-11.42672200	0.05683300	0.45716700
H	-10.74731600	-0.95453100	1.74931000
C	1.40254800	2.98930400	0.61447200
C	0.15576600	3.09883100	1.24908200
C	2.01898900	4.13432500	0.10086600
C	-0.45356900	4.34241000	1.38671200
H	-0.33430600	2.21053300	1.63354900
C	1.40213900	5.37973300	0.23656900
H	2.97328300	4.05740700	-0.40663200
C	0.16981500	5.48707200	0.88054500
H	-1.41791400	4.41799400	1.88054000
H	1.88790000	6.26443700	-0.16440500
H	-0.30767500	6.45720300	0.98461300
C	3.86463300	1.59421000	-0.09023600
C	4.94672200	1.43288000	0.78574700
C	4.09643600	1.88312800	-1.44745300
C	6.25195800	1.56301500	0.31059400
H	4.77264800	1.18737200	1.82726500
C	5.40624500	2.01965600	-1.90881200
H	3.24837300	1.99024600	-2.11950200
C	6.48386300	1.85566200	-1.03489400
H	7.08715300	1.42788300	0.99169300
H	5.58222800	2.24307700	-2.95699000
H	7.50174100	1.94946700	-1.40249800
C	2.25123600	0.74888700	2.18133300
C	2.46340300	1.67489200	3.21634000
C	2.17056000	-0.61686700	2.48448600
C	2.59294400	1.23722800	4.53324700
H	2.52234100	2.73468400	2.99140000
C	2.30206600	-1.04840200	3.80474900
H	2.00844700	-1.33659300	1.68958300
C	2.51149600	-0.12535800	4.82989200
H	2.75454500	1.96067800	5.32724300
H	2.23994100	-2.10949600	4.02804200
H	2.60964800	-0.46436300	5.85730800
C	-0.75529800	3.64856300	-2.51769600
H	-1.76134900	3.31863100	-2.79669900
H	-0.84918200	4.26148600	-1.61477800
H	-0.32253900	4.24995300	-3.31939700

TS2B



Zero-point correction= 0.838839 (Hartree/Particle)
Thermal correction to Energy= 0.887837
Thermal correction to Enthalpy= 0.888781
Thermal correction to Gibbs Free Energy= 0.753873
Sum of electronic and zero-point Energies= -2567.831269
Sum of electronic and thermal Energies= -2567.782271
Sum of electronic and thermal Enthalpies= -2567.781327
Sum of electronic and thermal Free Energies= -2567.916235

Cartesian Coordinates

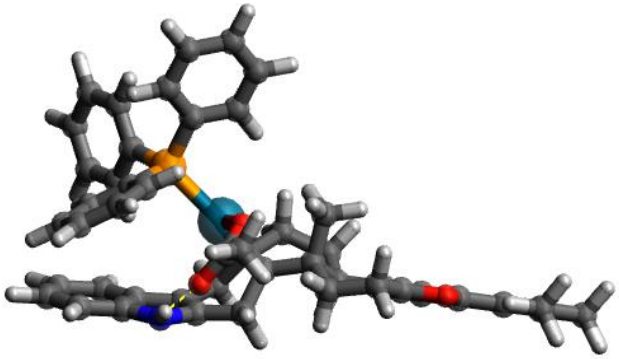
Atom	X	Y	Z
C	-2.07350200	-0.80367800	-0.31957400
C	-0.35259000	-2.23415800	0.99294700
H	-0.23123000	-1.45446100	1.75005900
C	0.95623300	-3.06692600	0.97182400
H	1.33680400	-3.11553900	1.99936700
H	0.69587400	-4.10691200	0.71155100
C	3.95004200	-2.56876600	-1.24468800
C	3.40236000	-3.06689700	-0.02237700
C	2.03486600	-2.61836300	0.03580700
C	1.84942700	-1.86238100	-1.10790800
N	2.95290600	-1.88388100	-1.92601300
H	3.13811200	-1.10682000	-2.60174000
C	4.22554900	-3.80893700	0.84255100
C	5.29437600	-2.74738300	-1.58086300
C	5.55936400	-3.99991200	0.50017400
H	6.20871500	-4.56371500	1.16423700
C	6.09000800	-3.46807200	-0.69345000
H	7.13847400	-3.62875700	-0.92810600
H	3.82911400	-4.21402800	1.77015700
H	5.69555600	-2.33822700	-2.50312900

C	-0.70846000	-1.53362900	-0.32079600
C	-0.22522800	-2.14179400	-1.54146100
H	0.10560500	-3.17251900	-1.54897100
H	-0.62198900	-1.82772200	-2.50143000
Pd	0.75164400	-0.16708900	-1.02743600
P	1.32382800	1.44629600	0.74851500
C	-1.50799600	-3.16021000	1.44662300
H	-1.52532300	-4.03364500	0.77879600
H	-1.28207100	-3.53968500	2.45086900
C	-3.14391500	-1.90032800	0.02583100
H	-2.99618100	-2.71408000	-0.70320000
C	-2.88848800	-2.50244300	1.41172200
H	-2.97825100	-1.72903700	2.18314400
H	-3.65602800	-3.25343200	1.63484100
C	-2.10574400	0.32325300	0.73144500
H	-1.56862400	1.20324100	0.36786500
H	-3.13486200	0.62108800	0.94732800
H	-1.64808600	0.02246900	1.67143600
C	-2.43294200	-0.19391200	-1.70120600
H	-1.63420200	0.48309700	-2.03130200
H	-2.50380200	-0.99445700	-2.44597900
C	-4.52619900	-1.34263600	-0.16930900
C	-3.77551500	0.56755300	-1.69456800
H	-3.66068300	1.55256500	-1.21978600
H	-4.09843100	0.75816100	-2.72554200
C	-4.76864600	-0.25841300	-0.96102700
C	-5.80114500	-1.74901600	0.34236700
H	-6.01115300	-2.57650900	1.00584300
C	-6.73851700	-0.88257000	-0.17086800
O	-6.10126500	0.04083600	-0.97417000
C	2.82987000	1.32984000	-2.97039200
O	1.75600200	1.32496600	-2.26138600
O	3.46429700	0.33112300	-3.36041400
C	-8.16815800	-0.84802400	0.02552300
H	-8.50081800	-1.64624300	0.68735900
C	-9.11275300	-0.01638900	-0.46271700
C	-8.86579300	1.14431300	-1.38913700
H	-9.22235800	2.07746000	-0.92997700
H	-7.81633200	1.26559100	-1.64974800
H	-9.44413200	1.01851600	-2.31558000

C	-10.55700500	-0.21951400	-0.08205600
H	-10.96232700	0.67482200	0.41239400
H	-11.17810600	-0.38714500	-0.97350200
H	-10.69162200	-1.07139100	0.59155200
C	0.60764500	3.12610400	0.77258800
C	0.12313700	3.61406000	-0.45198200
C	0.56481600	3.94758300	1.90846700
C	-0.41165900	4.89952300	-0.53010800
H	0.20902100	2.99232800	-1.33911200
C	0.01996400	5.22946300	1.82623800
H	0.95814300	3.58756500	2.85366000
C	-0.47268800	5.70489800	0.60920000
H	-0.78059400	5.27219400	-1.48144100
H	-0.01481400	5.85811900	2.71158400
H	-0.89702200	6.70306000	0.54818500
C	3.12576500	1.72845500	0.52976700
C	3.93909300	0.64080700	0.17672000
C	3.69978300	3.00101800	0.64427400
C	5.30179800	0.81751300	-0.05011400
H	3.50687900	-0.34346500	0.06088600
C	5.06546800	3.17629600	0.41362400
H	3.08402000	3.85652900	0.89898800
C	5.86801400	2.08823200	0.06510200
H	5.90606300	-0.03982700	-0.33084800
H	5.50003500	4.16839100	0.50072200
H	6.92817100	2.23228400	-0.12296300
C	1.16271100	0.76411700	2.44260900
C	0.04996700	1.04559200	3.25173100
C	2.06923800	-0.22289500	2.86450500
C	-0.15076300	0.35787700	4.44902200
H	-0.66725100	1.79843300	2.94438800
C	1.86345400	-0.91006400	4.05995900
H	2.93263100	-0.46542800	2.25630600
C	0.75155200	-0.62641400	4.85526000
H	-1.01644100	0.59215300	5.06226500
H	2.57673500	-1.66943000	4.36791200
H	0.59150200	-1.16473500	5.78490500
C	3.35998100	2.71974900	-3.29929400
H	2.53972500	3.40795300	-3.52280200
H	3.88328600	3.10129300	-2.41435300

H 4.06196500 2.67819400 -4.13479200

CP5B



Zero-point correction= 0.839511 (Hartree/Particle)
Thermal correction to Energy= 0.889003
Thermal correction to Enthalpy= 0.889947
Thermal correction to Gibbs Free Energy= 0.752065
Sum of electronic and zero-point Energies= -2567.877076
Sum of electronic and thermal Energies= -2567.827583
Sum of electronic and thermal Enthalpies= -2567.826639
Sum of electronic and thermal Free Energies= -2567.964521

Cartesian Coordinates

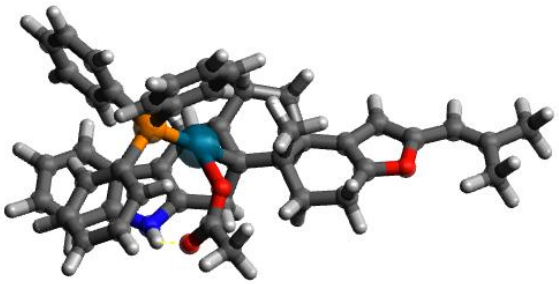
Atom	X	Y	Z
C	2.55907700	-0.26061600	0.08786200
C	0.78538000	-1.63533500	-1.20475000
H	-0.21934200	-1.06878800	-1.50458000
C	0.24751700	-3.10066800	-1.12498000
H	-0.22492700	-3.35759200	-2.07912700
H	1.11992900	-3.76242400	-1.01235400
C	-2.53295300	-3.06119000	1.39608500
C	-2.09632000	-3.55696300	0.12474900
C	-0.70760700	-3.19849500	0.01473300
C	-0.36956200	-2.55040000	1.17693700
N	-1.44416200	-2.48966200	2.03721900
H	-1.49331000	-1.71222600	2.69835300
C	-3.02296200	-4.20522000	-0.70852600
C	-3.86082200	-3.17340000	1.81123300
C	-4.34672600	-4.31050400	-0.29302600
H	-5.07314800	-4.80379800	-0.93310300
C	-4.76314300	-3.79266200	0.94969000
H	-5.80417000	-3.88751200	1.24531700

H	-2.71181900	-4.60868200	-1.66905600
H	-4.17826200	-2.77473800	2.76965300
C	1.23375900	-1.03774900	0.10804600
C	0.95623100	-1.89244600	1.35582800
H	1.74727300	-2.65474200	1.47352800
H	0.96105300	-1.27405400	2.25126100
Pd	-0.49401800	0.09984900	-0.09911000
P	-2.59580200	1.14316400	-0.53687900
C	1.70577400	-1.39329800	-2.42067400
H	1.46026900	-2.14121000	-3.18246300
H	1.45380900	-0.42925900	-2.86698000
C	3.56709100	-1.22514700	-0.62616200
H	3.45021200	-2.20161500	-0.13026900
C	3.22390300	-1.42470300	-2.11384100
H	3.71631100	-0.64311100	-2.70206000
H	3.65586400	-2.37511700	-2.44637100
C	2.43365300	1.09387300	-0.64784600
H	1.89456700	1.80037100	-0.01090700
H	3.42250200	1.50374300	-0.87569900
H	1.88667100	1.01912200	-1.58920600
C	3.06754900	0.03665300	1.52262800
H	2.30981600	0.62418300	2.04822400
H	3.19767900	-0.90390300	2.06730700
C	4.98012400	-0.75896100	-0.41415600
C	4.41775000	0.78316200	1.54636100
H	4.28210400	1.84679700	1.30463500
H	4.84305800	0.74976100	2.55728300
C	5.31930400	0.12817500	0.56499300
C	6.19738300	-1.06975000	-1.10386800
H	6.32556600	-1.74098700	-1.94201700
C	7.20089400	-0.34942800	-0.49873400
O	6.65943700	0.39271300	0.53067000
C	8.61160500	-0.29895300	-0.80022000
H	8.86537200	-0.94540000	-1.63908000
C	9.61865700	0.39493300	-0.22866700
C	11.02186100	0.25169200	-0.76030500
H	11.41832900	1.22280300	-1.08966100
H	11.70358900	-0.11000800	0.02270600
H	11.07557000	-0.44196600	-1.60506500
C	9.48273000	1.33889900	0.93625000

H	9.83727100	2.34087800	0.65494100
H	8.46035300	1.42255600	1.29925200
H	10.12314900	1.00959400	1.76702400
C	-0.22651100	2.24594600	3.73410000
H	-0.03866800	3.20740800	3.25171700
H	-1.09732500	2.31548900	4.39251800
H	0.63574000	1.98562100	4.35905000
C	-0.45712800	1.13209300	2.71432100
O	-0.89133500	0.04010600	3.11129100
O	-0.14190600	1.45237400	1.50332500
C	-2.43133600	2.91120000	-0.96628400
C	-1.19040500	3.36276000	-1.43439500
C	-3.49120400	3.82239500	-0.83950400
C	-1.01485600	4.70057800	-1.78929500
H	-0.36225300	2.66253800	-1.49996200
C	-3.31393300	5.15897600	-1.19374000
H	-4.44711700	3.48556600	-0.44998300
C	-2.07655300	5.59859800	-1.67161000
H	-0.04783900	5.04235000	-2.14710400
H	-4.13868600	5.85875800	-1.09232300
H	-1.93925700	6.64161500	-1.94270000
C	-3.64469800	0.40546000	-1.84473700
C	-4.41136900	1.15734400	-2.74438600
C	-3.67083400	-0.99558800	-1.92228600
C	-5.19730100	0.51456400	-3.70175800
H	-4.38972100	2.24103500	-2.70448200
C	-4.47410100	-1.63406900	-2.86569900
H	-3.07363800	-1.58991200	-1.23788600
C	-5.23551200	-0.87984600	-3.76058100
H	-5.78289500	1.10547200	-4.40069800
H	-4.49820600	-2.71869400	-2.89351700
H	-5.85393700	-1.37597800	-4.50343300
C	-3.65883600	1.14614600	0.95586400
C	-4.62141200	0.15147200	1.16576200
C	-3.40626500	2.08409700	1.96912100
C	-5.32537600	0.10148700	2.36946000
H	-4.81984700	-0.59160700	0.40178200
C	-4.11376000	2.03065700	3.16740900
H	-2.64851800	2.84609100	1.82161900
C	-5.07531600	1.03851800	3.37197700

H	-6.06951000	-0.67567900	2.51940800
H	-3.90946100	2.76166900	3.94475000
H	-5.62339600	0.99542900	4.30891500

TS3B



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Sum of electronic and thermal Energies= -2567.824038
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Cartesian Coordinates

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H	-0.51713600	-0.75578600	-1.51713600
C	0.05850000	-2.97506500	-1.32756500
H	-0.48864900	-3.01161500	-2.27577100
H	0.84229000	-3.74928300	-1.39294600
C	-2.64005300	-3.13419000	1.27299400
C	-2.24549800	-3.50321100	-0.05305100
C	-0.85294900	-3.16084300	-0.16248300
C	-0.47218600	-2.64460800	1.04972900
N	-1.52439200	-2.65207600	1.94062000
H	-1.54648100	-1.92364700	2.65819900
C	-3.20645200	-4.04005600	-0.92557500
C	-3.95882300	-3.26664000	1.71003300
C	-4.52242300	-4.16076900	-0.48975900
H	-5.27513600	-4.56729600	-1.15972500
C	-4.89614800	-3.77255800	0.81235900

H	-5.93105900	-3.88009400	1.12485900
H	-2.92780500	-4.34694400	-1.93091400
H	-4.24280200	-2.96882600	2.71456500
C	1.24704200	-1.18105100	0.07312200
C	0.87015600	-2.04127800	1.28813000
H	1.62789800	-2.83392500	1.41876200
H	0.86072300	-1.44669800	2.19941400
Pd	-0.51467600	0.07827700	-0.14274400
P	-2.51269600	1.21297000	-0.50825700
C	1.63557700	-1.25861600	-2.44804800
H	1.38742400	-1.96331100	-3.24836600
H	1.32741100	-0.27848000	-2.81449500
C	3.56228700	-1.23522400	-0.71547700
H	3.46492100	-2.26716100	-0.34190900
C	3.17249800	-1.24543500	-2.20297400
H	3.59962500	-0.36271300	-2.68977000
H	3.63376300	-2.11534100	-2.68281000
C	2.41363100	1.05121700	-0.44162800
H	1.84769400	1.66576800	0.26321700
H	3.39685500	1.50400700	-0.60212100
H	1.88520200	1.07316800	-1.39673600
C	3.08727000	-0.24958900	1.58142700
H	2.33980400	0.27423300	2.18362400
H	3.22038900	-1.24773000	2.01169100
C	4.97442900	-0.78035800	-0.48054400
C	4.43834900	0.49103100	1.67407900
H	4.29579400	1.57635200	1.57462000
H	4.88260500	0.32977100	2.66428500
C	5.32480000	-0.02458200	0.59980100
C	6.18005100	-0.98400600	-1.22782700
H	6.29763800	-1.53900300	-2.14849000
C	7.18872800	-0.33645000	-0.55300200
O	6.66124200	0.25858700	0.57457600
C	8.59249700	-0.23021400	-0.87190300
H	8.83481300	-0.75683200	-1.79381600
C	9.60484500	0.39294600	-0.23228800
C	10.99810300	0.33762200	-0.80489900
H	11.37927400	1.34837800	-1.00927100
H	11.69870800	-0.11734100	-0.09018800
H	11.04061600	-0.23670800	-1.73548300

C	9.48444200	1.17208700	1.05027400
H	9.82108500	2.20750100	0.89731200
H	8.46960900	1.19236600	1.44233700
H	10.14717500	0.74469600	1.81631800
C	-0.24557100	1.95283100	3.88686000
H	0.07864500	2.90384200	3.45909500
H	-1.16516700	2.09572400	4.46325500
H	0.51766600	1.58725400	4.58306500
C	-0.49329400	0.89629200	2.81022100
O	-0.94879000	-0.20494200	3.16100700
O	-0.18026400	1.26656300	1.61606300
C	-2.27343100	2.99683900	-0.81118300
C	-1.01373200	3.43271200	-1.24212700
C	-3.30107700	3.93501000	-0.62764800
C	-0.78788700	4.78417700	-1.50413600
H	-0.21246200	2.70783500	-1.35224600
C	-3.07301500	5.28509900	-0.88957600
H	-4.27107000	3.60827300	-0.26558300
C	-1.81724800	5.71040400	-1.33067100
H	0.19324300	5.11379400	-1.83369800
H	-3.87262600	6.00593500	-0.74433700
H	-1.64041700	6.76363200	-1.52968300
C	-3.58072800	0.60402700	-1.86510000
C	-4.34362200	1.44554700	-2.68456300
C	-3.64713900	-0.78450100	-2.05186400
C	-5.16464700	0.90176200	-3.67353800
H	-4.29141600	2.52169800	-2.56045000
C	-4.48675400	-1.32459000	-3.02412500
H	-3.05158000	-1.44313300	-1.42868600
C	-5.24341800	-0.48192800	-3.84087200
H	-5.74540300	1.56173400	-4.31201100
H	-4.54378500	-2.40272000	-3.13657800
H	-5.88961100	-0.90100400	-4.60715500
C	-3.57675200	1.13509600	0.97966600
C	-4.52135300	0.11273200	1.13228400
C	-3.34968100	2.02768900	2.03843800
C	-5.23540800	-0.00724300	2.32434900
H	-4.69883500	-0.59845200	0.33369100
C	-4.06789400	1.90380500	3.22524800
H	-2.60218200	2.80662500	1.93751800

C	-5.01276600	0.88611600	3.37211200
H	-5.96326000	-0.80641000	2.42948200
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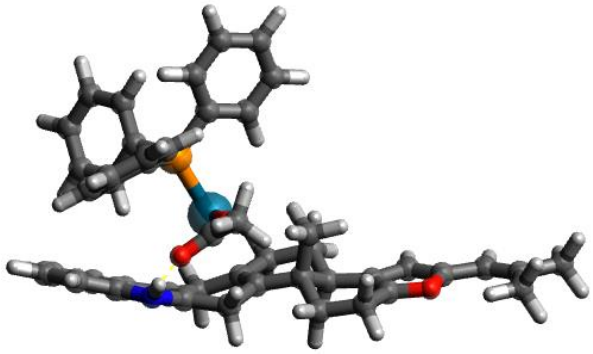
CP6B



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Sum of electronic and thermal Free Energies= -2567.972942

Cartesian Coordinates

Atom	X	Y	Z
C	2.69526800	-1.13043900	0.22176500
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C	-0.18686300	-3.00570400	-1.71986700
H	-0.66881400	-2.65511400	-2.64062100
H	0.25270500	-3.98760400	-1.96975800
C	-3.02013900	-3.04342000	0.74842900
C	-2.60004700	-3.29331200	-0.59641000
C	-1.17742900	-3.08978500	-0.60922500
C	-0.80374200	-2.78133600	0.67776200
N	-1.90102400	-2.78150500	1.51796700
H	-1.90406700	-2.13925200	2.33214800
C	-3.56221800	-3.61832900	-1.56663600
C	-4.37021900	-3.05939400	1.10803800
C	-4.90478500	-3.64566600	-1.20118900

H	-5.65918600	-3.89716400	-1.94192000
C	-5.30524400	-3.35627600	0.11925800
H	-6.36146400	-3.37849300	0.37258600
H	-3.26355600	-3.83440800	-2.58950000
H	-4.67378500	-2.84618600	2.12856200
C	1.36908700	-1.85578200	-0.07997400
C	0.60256900	-2.48406900	1.08611200
H	1.11524300	-3.40870600	1.39854600
H	0.61299900	-1.81728800	1.94918900
Pd	-0.69469100	-0.07408200	-0.21774000
P	-2.35336500	1.42950600	-0.35320300
C	1.74195700	-1.60739100	-2.58186100
H	2.01537000	-2.51293700	-3.14608100
H	1.06733700	-1.04556000	-3.23906000
C	3.64556400	-1.33988500	-1.00016600
H	3.73093600	-2.43127600	-1.13449900
C	3.00813400	-0.79992600	-2.27828700
H	2.77672400	0.26400600	-2.16406700
H	3.70544400	-0.87909000	-3.11999700
C	2.43673700	0.37012500	0.48670900
H	1.84628300	0.50480100	1.39472300
H	3.37564400	0.92461100	0.57369600
H	1.85836400	0.81823300	-0.32736500
C	3.39640800	-1.74579900	1.46645900
H	2.73076700	-1.71206800	2.33265500
H	3.60893200	-2.80331100	1.26376300
C	5.01427800	-0.80916600	-0.68686900
C	4.71653600	-1.03210500	1.84099900
H	4.50576300	-0.10916200	2.40000700
H	5.30401000	-1.66975600	2.51405000
C	5.46598800	-0.72286900	0.59674700
C	6.08687000	-0.34540500	-1.51419500
H	6.10242900	-0.26988700	-2.59278600
C	7.12413700	-0.00172400	-0.67749200
O	6.74072300	-0.23209300	0.62793300
C	8.43232700	0.51841800	-0.99551000
H	8.56664600	0.63473400	-2.06997900
C	9.46758500	0.86794900	-0.20270100
C	10.73908400	1.39200400	-0.81981900
H	10.96926000	2.40110600	-0.44894700

H	11.59720500	0.76069700	-0.54804400
H	10.68156300	1.43581600	-1.91183700
C	9.48749300	0.78584400	1.30045900
H	9.68521200	1.77789300	1.73128800
H	8.55717100	0.40614500	1.71806400
H	10.31077800	0.13775900	1.63370100
C	-0.31100700	1.05902000	4.14666900
H	-0.26187600	2.09821800	3.80979800
H	-0.94864300	0.97357700	5.02886600
H	0.70790200	0.75517200	4.41745400
C	-0.82095200	0.15041400	3.02782700
O	-1.61316100	-0.76339600	3.32146600
O	-0.31759500	0.41331700	1.87308400
C	-1.75093100	3.13574100	-0.57268600
C	-0.47144500	3.33195900	-1.10907900
C	-2.54006800	4.24969100	-0.24379300
C	0.00952900	4.62319900	-1.32489200
H	0.14017400	2.46575900	-1.34315800
C	-2.05495900	5.53876500	-0.45936500
H	-3.52330000	4.10721600	0.19325100
C	-0.78124600	5.72674200	-1.00131600
H	1.00403400	4.76604500	-1.73722100
H	-2.66928500	6.39604800	-0.19971200
H	-0.40407100	6.73233400	-1.16381400
C	-3.58108800	1.13460100	-1.67505100
C	-4.27318300	2.17968900	-2.30081000
C	-3.87435900	-0.19318100	-2.01461200
C	-5.25058000	1.89519500	-3.25462100
H	-4.04391200	3.21140200	-2.05826500
C	-4.86601800	-0.47180500	-2.95355300
H	-3.33221900	-1.00679300	-1.54517600
C	-5.55260100	0.57101600	-3.57783200
H	-5.77552700	2.71013600	-3.74504400
H	-5.09288600	-1.50612300	-3.18942700
H	-6.31798200	0.35370600	-4.31761500
C	-3.32813400	1.42149900	1.18858400
C	-4.34758400	0.47359200	1.34919900
C	-2.97609200	2.24934500	2.26350400
C	-5.01324000	0.36720600	2.56829400
H	-4.61465100	-0.19256100	0.53666300

C	-3.65012200	2.14076000	3.47771500
H	-2.16572100	2.96176400	2.15797700
C	-4.66850200	1.19946400	3.63331800
H	-5.79769500	-0.37481000	2.68426200
H	-3.36825600	2.78305800	4.30686100
H	-5.18418400	1.10868600	4.58484300

Computational Methods for Attractive Dispersion

To study the origin of the dispersion interactions between the ligands and the substrate, separate dispersion calculations were performed for groups that were informed to experience such interactions via the NCI analysis. For the CataCXium ligand, dispersive effects were evaluated between the *tert*-butyl group of CatCXium and the indole of the substrate as well as the indole of CatCXium and the methyl group of *trans*-decalin in the substrate. As for PPh_3, calculations were performed for the interactions of the Ph groups with the indole of the substrate and the methyl of the *trans*-decalin. The geometries for each of these dispersion calculations were taken from the optimized transition state structures. To isolate the structures of interest to dispersion, per Peng Liu's method, C-C, C-N and C-P bonds were cleaved and atoms that were not of interest were deleted. Hydrogen atoms were added to dangling carbon atoms at a distance of 1.07Å in the same direction as the cleaved bonds (Figure S3).

Calculations of the dispersive interaction energies were based on density functional theory (DFT) calculations using the Gaussian 16 suite of programs (revision A3). Single point energy calculations were performed using the M06 functional[11] and the 6-311+G(d,p) basis set[10] with Grimme's D3(BJ) dispersion correction.[12] The total calculated dispersion energy for the CataCXium ligand was 3.9 kcal/mol and for PPh_3 it was 1.8 kcal/mol (Figure S4). The higher attractive dispersion interactions help account for the effectiveness of the CataCXium ligand for the Heck cyclization.

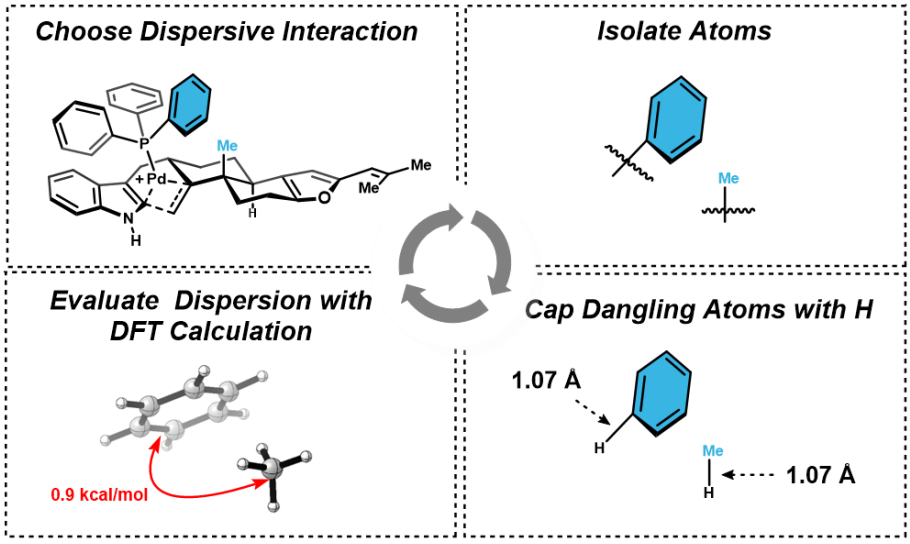

Figure S3. Method to Evaluate Attractive Dispersion Interactions

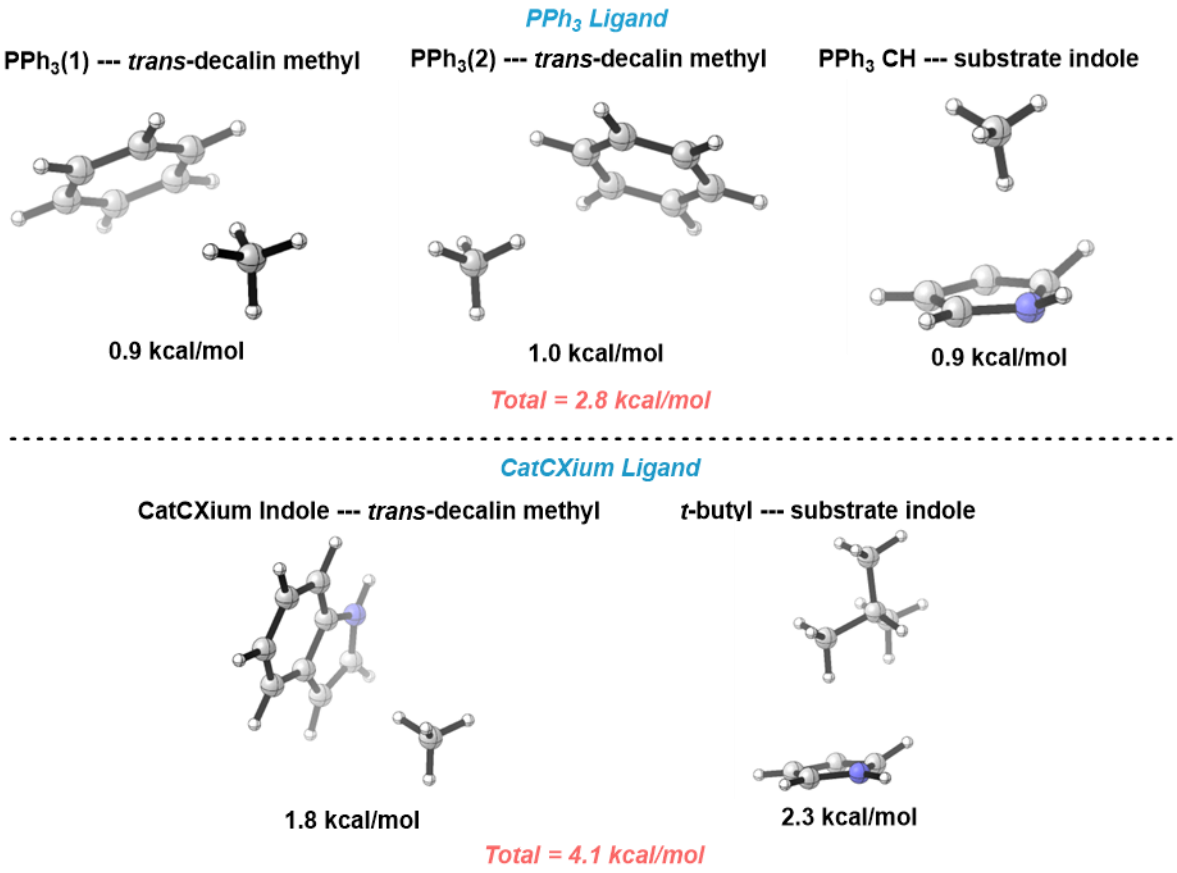

Figure S4. Evaluation of Attractive Dispersion Interactions via DFT Calculations Using Grimme's D3(BJ) Dispersion Correction.

Determining Anion-Ligand/Substrate Interactions

To evaluate the interactions between the acetate anion and the substate and ligand, bond distances were analyzed for possible stabilizing interactions (< 3 Å). CatCXium was found to have more associative interactions with the ligand and substrate than PPh_3 (Table S3 and Table S4). With the acetate anion interacting to a greater extent with the ligand of CatCXium, the distance between the acetate and Pd becomes greater (2.62Å compared to 2.18Å for PPh_3), which can then allow for a more efficient migratory insertion step of the transition state.

Table S3. Associated Distances between the CatCXium Ligand, Substrate and the Coordinating Acetate Anion.

Acetate O	Neighboring H	Distance (Å)
O 114	H 12 (^{t}Bu C-H)	2.25
O 114	H 119 (substrate indole N-H)	1.66
O 115	H 64 (ligand indole C-H)	2.07
O 115	H 24 (vicinal C-H)	2.40
O 115	H 40 (substrate C-H)	2.24
O 115	Pd	2.62

Table S4. Associated Distances between the PPh_3 Ligand, Substrate and the Coordinating Acetate Anion.

Acetate O	Neighboring H	Distance (Å)
O 53	H 12 (substrate indole N-H)	1.66
O 52	H 69 (Ph C-H)	2.45
O 52	H 24 (vicinal C-H)	3.96
O 52	Pd	2.18

CatCXium Indole --- trans-decalin methyl

C	2.32590	2.25920	-1.04280
H	1.90930	1.39830	-0.51310
H	1.48780	2.83750	-1.43930
H	2.89350	1.88140	-1.89530
C	-0.01620	-0.05360	0.79330
C	-0.28420	-0.85670	-0.34260
C	-1.48140	-0.75800	-1.05980
C	-2.40600	0.18460	-0.62460
C	-2.15590	1.00120	0.49940
C	-0.97270	0.88670	1.21550
C	1.28450	-0.41960	1.26140
H	-1.67760	-1.38920	-1.91990
H	-3.34410	0.29320	-1.16130
H	-2.90480	1.72480	0.80700
H	-0.78190	1.50440	2.08800
H	1.79960	0.00820	2.11810
C	1.78320	-1.42610	0.43290
N	0.81090	-1.69490	-0.55170
H	0.76200	-2.42880	-1.22920
H	2.79640	-1.72950	0.59510
H	2.92060	2.85700	-0.38400

t-butyl --- substrate indole

C	2.42290	-1.48710	-0.33670
C	2.30030	-0.24070	-1.03850
C	1.79860	0.71620	-0.09760
C	1.62940	0.02030	1.09590
N	2.00900	-1.29370	0.96080
H	2.03740	-1.92890	1.79580
C	-2.46090	-0.23610	0.28690
C	-1.46460	-0.61720	-0.83190
H	-1.45570	-1.68670	-1.04470
H	-1.77030	-0.10260	-1.75180
H	-0.44650	-0.30300	-0.59550
C	-3.85930	-0.72850	-0.11040
H	-4.14070	-0.25840	-1.06160
H	-3.87420	-1.81040	-0.26930
H	-4.62410	-0.47710	0.62210
C	-2.43690	1.29950	0.40020
H	-3.07380	1.67220	1.20100
H	-1.41710	1.65350	0.58160
H	-2.78980	1.73270	-0.54400
H	-2.05360	-0.61250	1.20200
H	0.86850	0.25000	1.81230
H	2.55470	-0.19740	-1.97730

H	2.74670	-2.29170	-0.77930
H	1.76380	1.78260	-0.17810

PPh3(1) --- trans-decalin methyl

C	-0.62840	1.14810	-0.34850
C	-1.02410	0.01570	-1.12510
C	-1.04430	-1.11550	-0.23370
C	-0.63390	-0.62210	0.99190
N	-0.45660	0.74000	0.96740
H	0.18740	1.21190	1.64360
C	2.61680	-0.18580	-0.24320
H	1.58970	-0.16520	0.05600
H	0.01420	-1.20590	1.61160
H	-1.45900	-2.08600	-0.40970
H	-1.19370	0.13090	-2.07700
H	-0.48430	2.02380	-0.74910
H	2.97780	0.81590	-0.34860
H	3.14220	-0.65070	0.43210
H	2.70560	-0.69730	-1.17880

PPh3(2) --- trans-decalin methyl

C	3.37370	-0.00080	-0.58970
H	3.44580	-0.61600	0.31110
H	4.01880	0.87110	-0.45560
H	2.34940	0.35820	-0.66280
C	0.02980	-1.00530	0.68080
C	0.32980	0.35350	0.86980
C	-1.11890	-1.34520	-0.05340
C	-0.49580	1.34460	0.33800
H	1.21430	0.64090	1.42720
C	-1.93960	-0.35190	-0.58580
H	-1.37050	-2.38580	-0.22060
C	-1.63030	0.99640	-0.39660
H	-0.24790	2.39030	0.49750
H	-2.82330	-0.63630	-1.15020
H	-2.26940	1.76870	-0.81450
H	0.72250	-1.77790	0.94180
H	3.66880	-0.56080	-1.45230

PPh3 CH --- substrate indole

C	-3.70650	0.00290	-0.57200
H	-2.71220	-0.31490	-0.24730
H	-3.76390	-0.12260	-1.65610
H	-3.79850	1.06600	-0.36030
C	-0.15500	0.41070	0.99040
C	0.09290	-0.95640	0.78540

C	0.64830	1.36220	0.34520
C	1.11940	-1.36070	-0.06740
H	-0.49820	-1.68750	1.33030
C	1.66790	0.95170	-0.51420
H	0.47910	2.42050	0.51570
C	1.90160	-0.40880	-0.72500
H	1.30850	-2.41970	-0.21800
H	2.28260	1.69450	-1.01480
H	2.69570	-0.72560	-1.39520
H	-0.94050	0.65290	1.67540
H	-4.46390	-0.57400	-0.08370

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