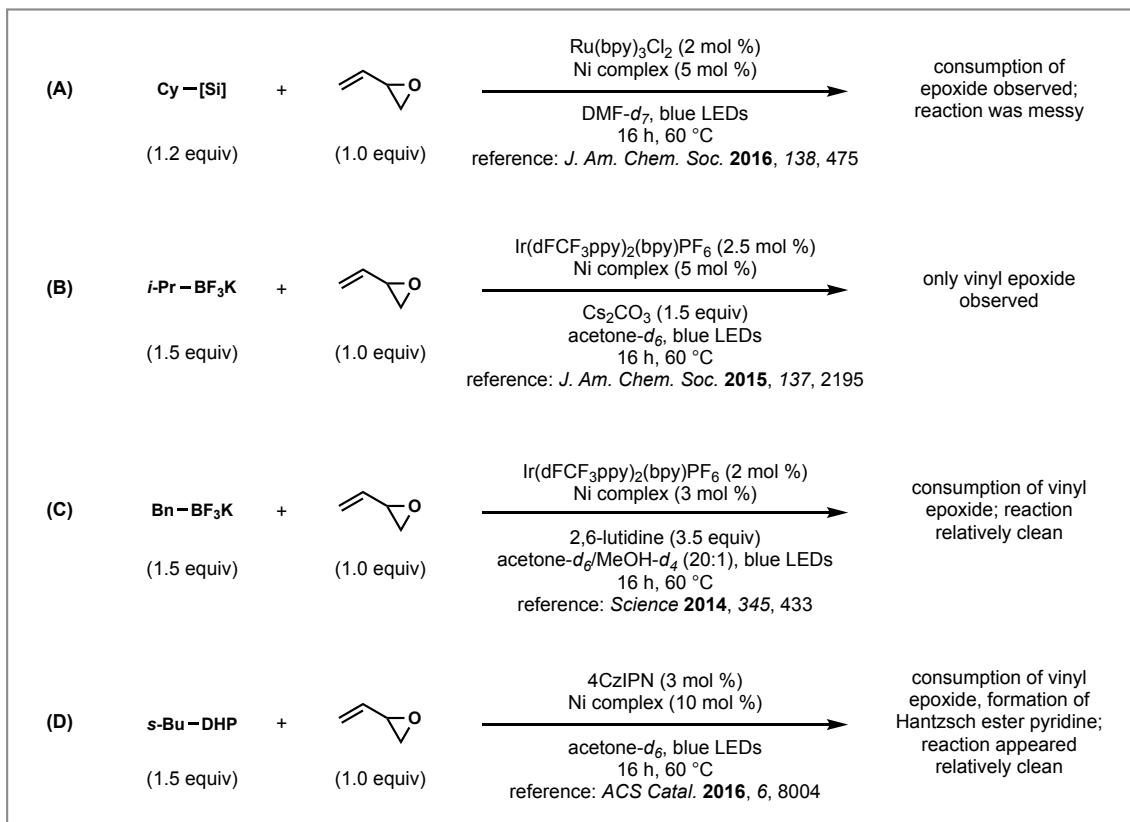# Table of Contents

General Considerations

NMR Spectra (^{1}H, ^{13}C, ^{19}F) were performed at 298 K. ^{1}H NMR spectra were referenced to residual non-deuterated chloroform (δ 7.26) in CDCl$_3$, residual DMSO-d_5 (δ 2.50 ppm) in DMSO-d_6, acetone-d_5 (δ 2.09 ppm) in acetone-d_6, and residual MeCN-d_2 (δ 1.94 ppm) in MeCN-d_3. ^{13}C NMR spectra were referenced to CDCl$_3$ (δ 77.2 ppm) and DMSO-d_6 (δ 39.5 ppm). Data is presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant J (Hz), and integration.

Reactions were monitored by HPLC, GC/MS, ^{1}H NMR, and/or by TLC on silica gel plates (60 Å porosity, 250 μm thickness). TLC analysis was performed using hexanes/EtOAc as the eluent and visualized using UV light. Silica plugs utilized flash silica gel (60 Å porosity, 32–63 μm). Flash chromatography was accomplished using an automated system (visualizing at 254 nm, monitoring at 280 nm) with silica cartridges (60 Å porosity, 20–40 μm). Solvents were purified by use of drying cartridges through a solvent delivery system. Melting points (°C) are uncorrected.

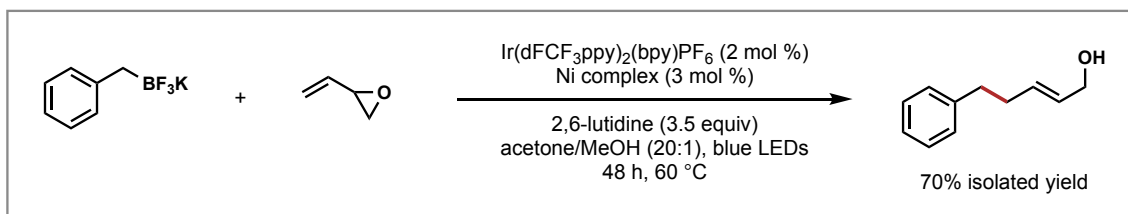Deuterated NMR solvents were either used as purchased (CDCl$_3$ and DMSO-d_6). Na$_2$SO$_4$, MgSO$_4$, acetone, *tert*-butanol, MeOH, and acetonitrile were used as purchased. 3,4-Epoxy-1-butene, 1,2-epoxy-3,4-cyclohexene, 3-bromo-1-propene, and 3-bromo-3,3-difluoro-1-propene were purchased from commercial suppliers and used without further purification. Solvent for reactions were degassed thoroughly with N$_2$.

Initial Benchtop Reagent Screen

To a 1 dram vial was added photocatalyst, [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$, and radical precursor. The vial was capped, purged and evacuated three times. Under an inert atmosphere, 1.0 mL of dry, degassed solvent was added to the reaction vials via syringe. The vinyl epoxide (0.10 mmol) was weighed in a tared syringe and added to the reaction mixtures under inert atmosphere. After 16 h, the reactions were quenched by addition of EtOAc (5 mL) and washed with brine (2 x 5 mL). Crude reaction mixtures were monitored by ^{1}H NMR.
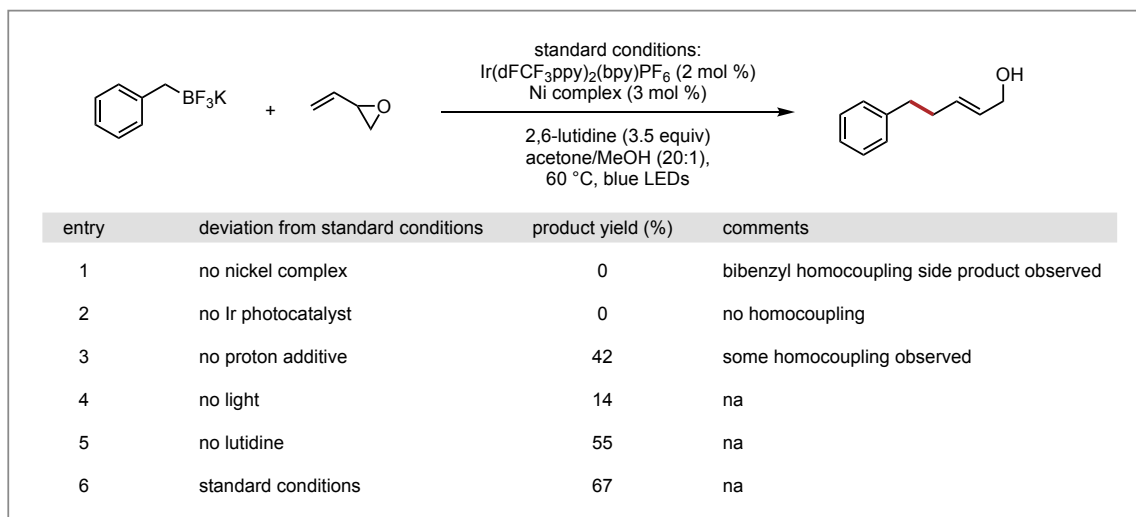
(A) Cy−[Si] (1.2 equiv) + [vinyl epoxide] (1.0 equiv)

Ru(bpy)$_3$Cl$_2$ (2 mol %)
Ni complex (5 mol %)
DMF-d_7, blue LEDs
16 h, 60 °C
reference: *J. Am. Chem. Soc.* **2016**, *138*, 475

consumption of epoxide observed; reaction was messy

(B) *i*-Pr−BF$_3$K (1.5 equiv) + [vinyl epoxide] (1.0 equiv)

Ir(dFCF$_3$ppy)$_2$(bpy)PF$_6$ (2.5 mol %)
Ni complex (5 mol %)
Cs$_2$CO$_3$ (1.5 equiv)
acetone-d_6, blue LEDs
16 h, 60 °C
reference: *J. Am. Chem. Soc.* **2015**, *137*, 2195

only vinyl epoxide observed

(C) Bn−BF$_3$K (1.5 equiv) + [vinyl epoxide] (1.0 equiv)

Ir(dFCF$_3$ppy)$_2$(bpy)PF$_6$ (2 mol %)
Ni complex (3 mol %)
2,6-lutidine (3.5 equiv)
acetone-d_6/MeOH-d_4 (20:1), blue LEDs
16 h, 60 °C
reference: *Science* **2014**, *345*, 433

consumption of vinyl epoxide; reaction relatively clean

(D) *s*-Bu−DHP (1.5 equiv) + [vinyl epoxide] (1.0 equiv)

4CzIPN (3 mol %)
Ni complex (10 mol %)
acetone-d_6, blue LEDs
16 h, 60 °C
reference: *ACS Catal.* **2016**, *6*, 8004

consumption of vinyl epoxide, formation of Hantzsch ester pyridine; reaction appeared relatively clean

Reaction **C** on 0.50 mmol scale with isolated yield:

[benzyl BF$_3$K] + [vinyl epoxide]

Ir(dFCF$_3$ppy)$_2$(bpy)PF$_6$ (2 mol %)
Ni complex (3 mol %)
2,6-lutidine (3.5 equiv)
acetone/MeOH (20:1), blue LEDs
48 h, 60 °C

[product with OH]

70% isolated yield

Control Reaction Studies

To a 2.0 mL dram vial was added photocatalyst, [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$, and alkytrifluoroborate (1.5 equiv). The vial was capped, purged and evacuated three times. Under an inert atmosphere, 1.5 mL (0.1 M) of dry, degassed solvent was added to the reaction vials via syringe. The vinyl epoxide (0.15 mmol) was weighed in a tared syringe and added to the reaction mixtures under an inert atmosphere. After stirring for 16 h at 60 ºC under blue LED irradiation, the reactions were quenched by addition of EtOAc (5 mL) and washed with brine (2 x 5 mL). Crude reaction mixtures were monitored by ^{1}H NMR. Yield was calculated using 2,4,6-trimethoxybenzene as an internal standard. Notably, secondary alkylsilicates and -trifluoroborates failed to afford any product, but benzyltrifluoroborate were suitable precursors. In further studies it was demonstrated that secondary alkyl motifs could be included in the scope using 4'-alkyl'-1,4'-dihydropyridines.

entry	deviation from standard conditions	product yield (%)	comments
1	no nickel complex	0	bibenzyl homocoupling side product observed
2	no Ir photocatalyst	0	no homocoupling
3	no proton additive	42	some homocoupling observed
4	no light	14	na
5	no lutidine	55	na
6	standard conditions	67	na

Further Benchtop Optimization

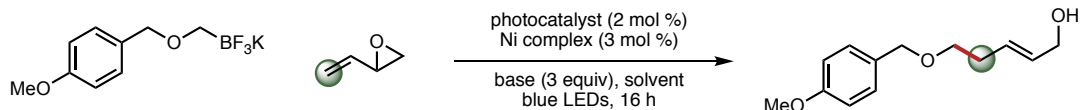| entry	deviation from standard conditions	product/IS
1	no deviation	2.40
2	4CzIPN (2 mol %)	1.73
3	0.2 M instead of 0.1 M	1.89
4	1.0 equiv trifluoroborates	1.08
5	2.0 equiv trifluoroborates	1.79
6	reaction run at room temperature	1.75
7	20 vol % of MeOH	1.67
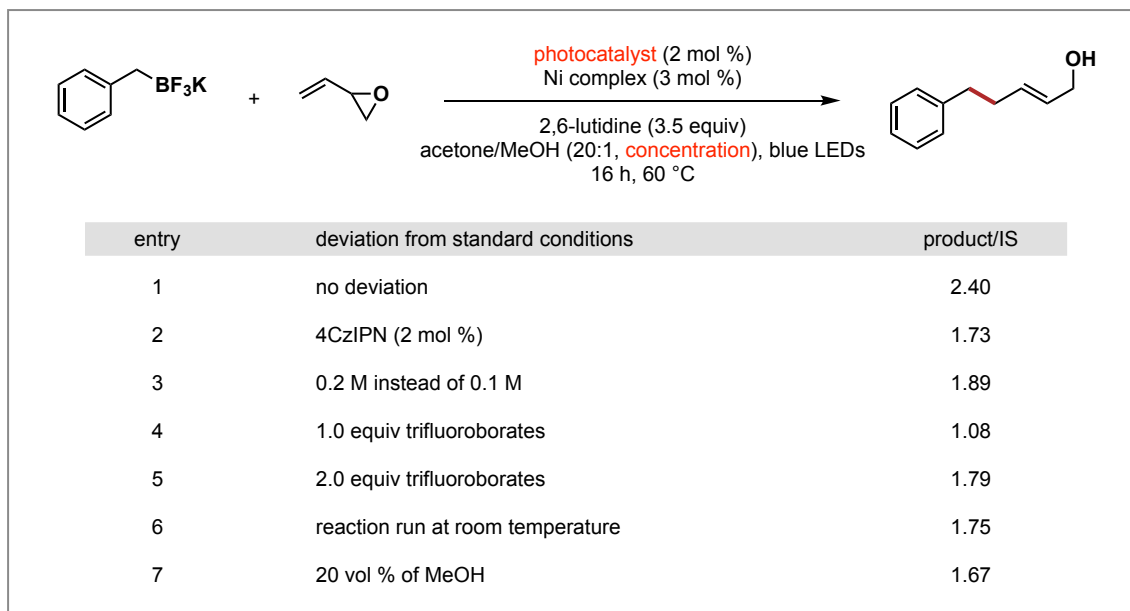
Optimization Studies in High Throughput Center

High Throughput Experimentation was performed at the Penn/Merck Center for High Throughput Experimentation at the University of Pennsylvania. The screens were analyzed by UPLC with addition of an internal standard. The areas for the internal standard (IS) and product (P) from each of the screens are shown in the tables below. The ratios calculated are pertinent only to that specific screen; the ratios from one screen should not be quantitatively compared to those from a different screen.

Procedure for high-throughput reactions: To a 96 well plate reactor containing 1 mL reaction vials equipped with Teflon-coated magnetic stir bar in a glovebox was added sequentially: (1) solution of [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$ (0.03 equiv) dissolved in THF, (2) solutions of photocatalysts (0.02 equiv) in THF, (3) slurries of inorganic bases (3.0 equiv), and (4) stock solution containing alkyltrifluoroborate (1.50 equiv) and internal standard (0.10 equiv) to each vial. The THF was then removed *via* Genevac and solutions of (1) vinyl epoxide in reaction solvents THF, toluene, dioxane, MeCN (0.1 M), (2) protic sources MeOH, trifluoroethanol, *tert*-butanol (0.01 M), and (3) basic amines (lutidine, DIPA, 3.00 equiv) were added to each vial. The vials were sealed and stirred over blue LED lights at rt (~23 °C). After 24 h, the reactions were opened to air and diluted with 500 μL of MeCN. After stirring for 15 min, 25 μL aliquots were then taken from the reaction vials and dosed

into a 96 well UPLC block. These aliquots were further diluted by the addition of 700 μL of MeCN. The reactions were then analyzed by UPLC.

	1	2	3	4	5	6	7	8	9	10	11	12		
A														THF
B														toluene
C													4CzIPN	dioxane
D	lutidine	DIPA	K$_2$HPO$_4$	Cs$_2$CO$_3$	lutidine	DIPA	K$_2$HPO$_4$	Cs$_2$CO$_3$	lutidine	DIPA	K$_2$HPO$_4$	Cs$_2$CO$_3$		MeCN
E														THF
F														toluene
G													Ir cat.	dioxane
H														MeCN
	MeOH				trifluoroethanol				*tert*-butanol					

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.3094	0.1915	0.212	0.1913	0.3346	0.234	0.2206	0.1915	0.333	0.1484	0.2164	0.1985
B	0.499	0.2845	0	0	0	0.3978	0.407	0	0.5474	0.1862	0	0.3812
C	0.3536	0.2543	0.217	0.2491	0.3696	0.2272	0.25	0	0	0.222	0.2249	0.2151
D	0.3572	0.2166	0.2136	0.1786	0.3499	0.2192	0.2193	0	0.3707	0	0.1985	0.2114
E	0.2883	0.1366	0.0933	0.0993	0.2737	0.1274	0.1165	0	0.2172	0	0.1099	0.1295
F	0.4684	0.3178	0	0.3149	0.5068	0.3359	0.3539	0	0.4783	0	0	0.3299
G	0.2599	0.1701	0.1373	0.1403	0.2846	0.1775	0.1471	0	0.299	0.1773	0.1682	0.1404
H	0.2327	0.1662	0.1357	0.1369	0.2568	0.1338	0.1201	0	0.2877	0.1605	0.1161	0.1307

Figure 1. Calculated product/internal standard ratios by peak area.
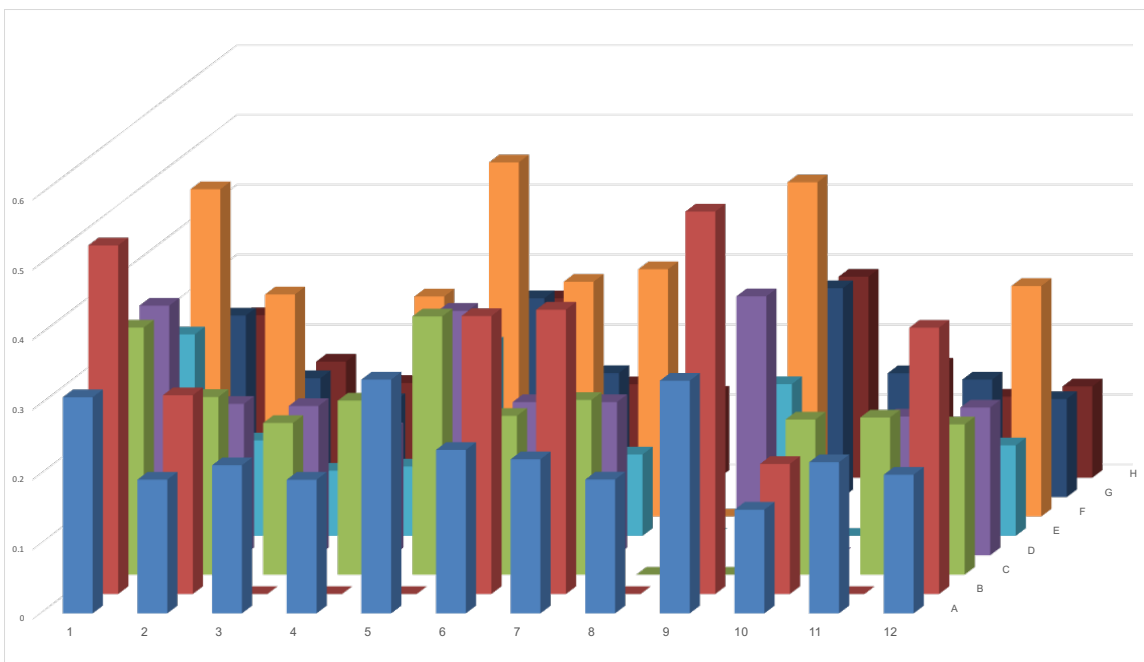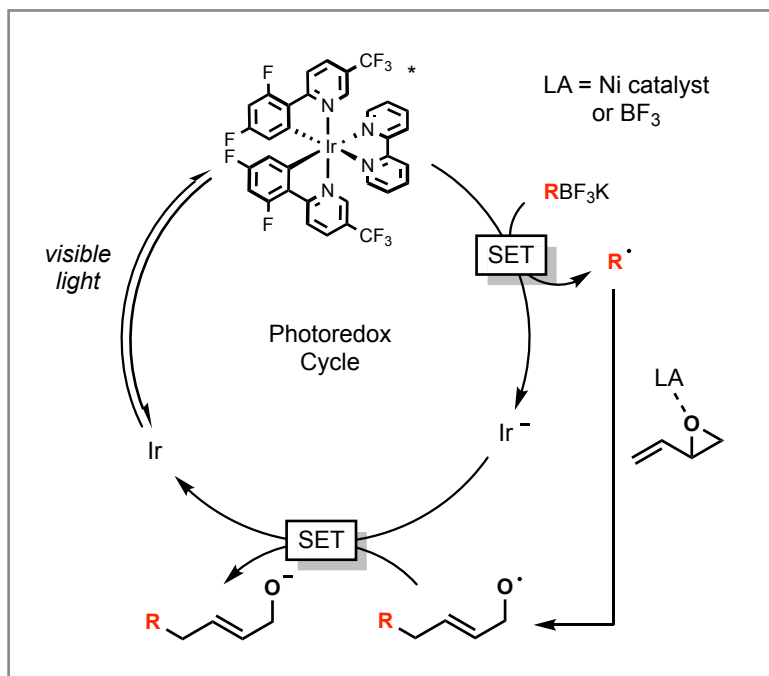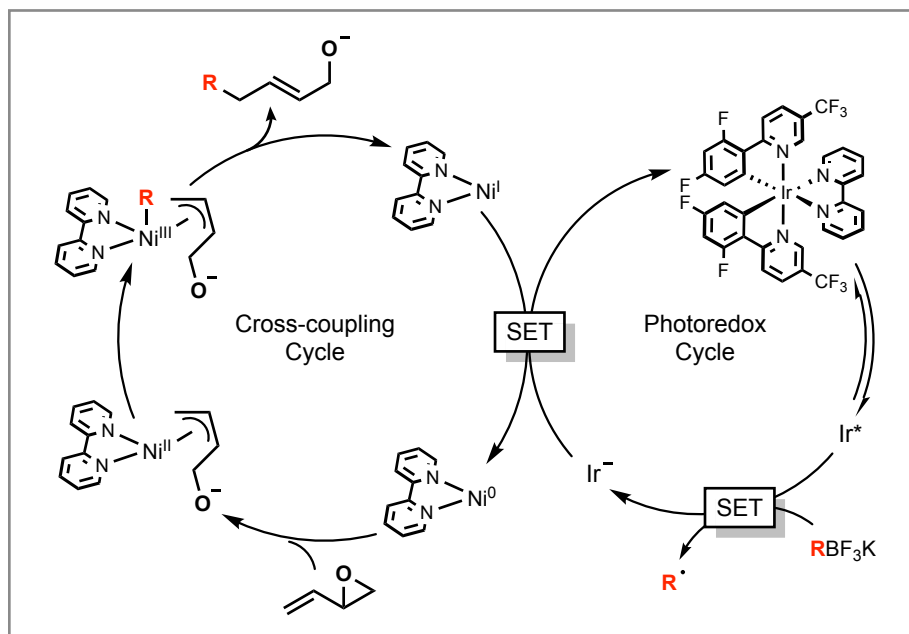
Figure 2. Product over internal standard (Y-axis).

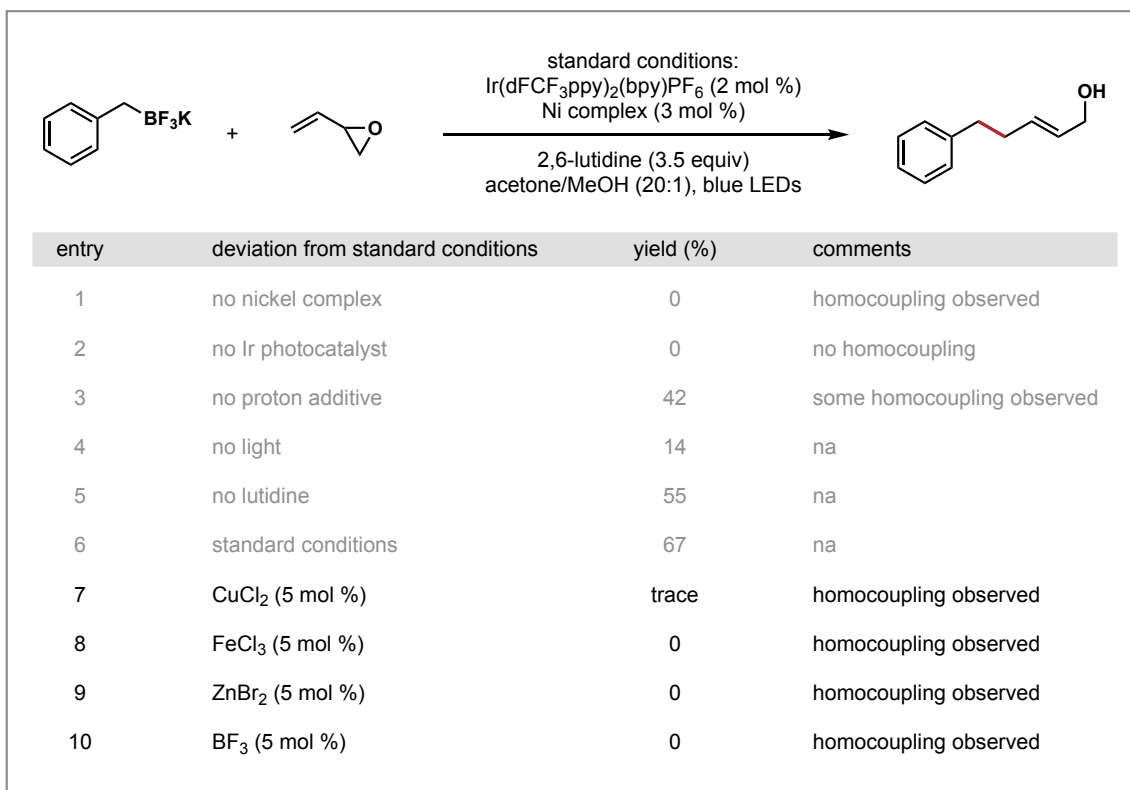## Ruling out Lewis Acid Activation of the Vinyl Epoxide

Potential *Lewis Acid catalyzed* mechanistic pathway:

Alternative *dual catalytic* mechanistic pathway:

Control studies with various Lewis Acids:

standard conditions:
Ir(dFCF$_3$ppy)$_2$(bpy)PF$_6$ (2 mol %)
Ni complex (3 mol %)

2,6-lutidine (3.5 equiv)
acetone/MeOH (20:1), blue LEDs

entry	deviation from standard conditions	yield (%)	comments
1	no nickel complex	0	homocoupling observed
2	no Ir photocatalyst	0	no homocoupling
3	no proton additive	42	some homocoupling observed
4	no light	14	na
5	no lutidine	55	na
6	standard conditions	67	na
7	CuCl$_2$ (5 mol %)	trace	homocoupling observed
8	FeCl$_3$ (5 mol %)	0	homocoupling observed
9	ZnBr$_2$ (5 mol %)	0	homocoupling observed
10	BF$_3$ (5 mol %)	0	homocoupling observed

General Procedure: Alkylation of Vinyl Epoxides with Alkyltrifluoroborates (Procedure A)

To an 8.0 mL reaction vial, Ir[dFCF$_3$ppy]$_2$(bpy)PF$_6$ (10.1 mg, 0.01 mmol, 2 mol %), [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$ (7.1 mg, 0.015 mmol, 3 mol %), and alkyltrifluoroborate (0.75 mmol, 1.5 equiv) were added. The vial was capped, purged, and evacuated three times. Under N$_2$, dry degassed solvent (5 mL) was added. Subsequently, vinyl epoxide (0.50 mmol, 1.0 equiv) and lutidine (202 μL, 1.75 mmol, 3.5 equiv) were added in succession. The reactions were stirred blue LED strips (see pictures below) for 16 h. The reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography. All reported E/Z ratios were determined by crude ^{1}H NMR.

## General Procedure: Alkylation of Vinyl Epoxides with α-Alkoxytrifluoroborates (Procedure B)

To an 8.0 mL reaction vial, Ir[dFCF$_3$ppy]$_2$(bpy)PF$_6$ (10.1 mg, 0.01 mmol, 2 mol %), [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$ (7.1 mg, 0.015 mmol, 3 mol %), and alkyltrifluoroborate (0.75 mmol, 1.5 equiv) were added. The vial was capped, purged, and evacuated three times. Under N$_2$, 5 mL of degassed MeCN/*t*-BuOH (10:1) was added. Subsequently, vinyl epoxide (0.50 mmol, 1.0 equiv) and lutidine (202 μL, 1.75 mmol, 3.5 equiv) were added in succession. Under a fan, the reactions were stirred blue LED strips (see pictures above) for 16–48 h. The reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography. All reported E/Z ratios were determined by crude ^{1}H NMR.

Figure 2. Reaction set up with blue LED strips.[1]

Compound Characterization
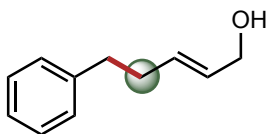
(*E*)-5-Phenylpent-2-en-1-ol[2] (**1a**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO₃ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 30% EtOAc/hexanes over 20 min).
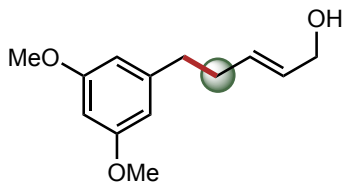
Physical state: 70% yield, *E/Z* = 95:5, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 7.31 (d, *J* = 7.6 Hz, 2H), 7.20 (d, *J* = 7.5 Hz, 3H), 5.72 (m, 2H), 4.10 (m, 2H), 2.73 (t, *J* = 7.9 Hz, 2H), 2.39 (m, 2H), 1.28 (d, *J* = 5.4 Hz, 1H).

¹³C NMR (126 MHz, CDCl₃) δ 141.8, 132.4, 129.8, 128.6, 128.5, 126.0, 63.9, 35.7, 34.1.

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[1] For details on photoreactor setup, see: Lin, K.; Wiles, R. J.; Kelly, C. B.; Davies, G. H. M.; Molander, G. A. *ACS Catal.* **2017**, *7*, 5129–6323.

[2] Zimmer, L. E.; Charette, A. B. *J. Am. Chem. Soc.* **2009**, *131*, 15624–15626.

(*E*)-5-(3,5-Dimethoxyphenyl)pent-2-en-1-ol (**1b**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 45% EtOAc/hexanes over 20 min).

Physical state: 55% yield, *E/Z* = 77:23, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 6.42 – 6.13 (m, 3H), 5.82 – 5.48 (m, 2H), 4.09 (m, 2H), 3.78 (s, 6H), 2.65 (t, *J* = 8.8 Hz, 2H), 2.42 – 2.30 (m, 2H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 160.9, 144.3, 144.0, 132.4, 131.8, 129.8, 129.4, 106.8, 106.7, 98.0, 97.9, 63.9, 58.6, 55.4, 36.2, 36.0, 33.9, 29.2 (inseparable mixture of E/Z isomers; two overlapping peaks).

HRMS (ES+) m/z calc. for C$_{13}$H$_{18}$O$_3$ [M$^+$] 222.1256, found 222.1271.

FT-IR (cm^{-1}, neat, ATR) 3368, 2999, 2924, 2854, 1595, 1461, 1429, 1349, 1293, 1148.
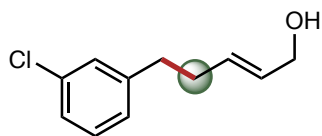
(*E*)-5-(3-Chlorophenyl)pent-2-en-1-ol (**1c**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 30% EtOAc/hexanes over 20 min).
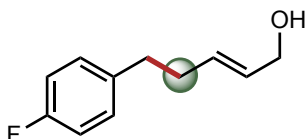
Physical state: 87% yield, *E/Z* = 90:10, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 7.34 (d, *J* = 7.6 Hz, 1H), 7.21 – 7.13 (m, 3H), 5.83 – 5.64 (m, 2H), 4.09 (m, 2H), 2.85 – 2.80 (m, 2H), 2.38 (d, *J* = 7.7 Hz, 2H).

13C NMR (126 MHz, CDCl₃) δ 139.4, 132.0, 130.5, 130.0, 129.6, 127.6, 126.9, 100.1, 63.8, 33.4, 32.4.

HRMS (ES+) m/z calc. for $C_{11}H_{13}ClO$ [M⁺] 196.0655, found 196.0684.

FT-IR (cm⁻¹, neat, ATR) 3325, 3066, 3017, 2928, 2861, 1670, 1572, 1474, 1051.

(*E*)-5-(4-Fluorophenyl)pent-2-en-1-ol (**1d**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO₃ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 45% EtOAc/hexanes over 20 min).

**Physical state:** 95% yield, *E/Z* = 90:10, clear oil.

1H NMR (500 MHz, CDCl₃) δ 7.13 (t, *J* = 6.8 Hz, 2H), 6.97 (t, *J* = 8.5 Hz, 2H), 5.77 – 5.61 (m, 2H), 4.15 – 4.07 (m, 2H), 2.69 (t, *J* = 7.9 Hz, 2H), 2.39 – 2.33 (m, 2H), 1.27 (s, 1H).

13C NMR (126 MHz, CDCl₃) δ 161.4 (d, *J* = 243.4 Hz), 137.4 (d, *J* = 3.2 Hz), 132.0, 129.8 (d, *J* = 8.8 Hz), 129.7, 115.0 (d, *J* = 21.0 Hz), 63.7, 34.7, 34.1.

19F NMR (471 MHz, C6D6) δ -117.4 (minor), -117.7 (major).

HRMS (ES+) m/z calc. for $C_{11}H_{13}FO$ [M⁺] 180.0950, found 180.0946.

FT-IR (cm⁻¹, neat, ATR) 3331, 2927, 2860, 1601, 1508, 1454, 1416, 1219, 1157, 999.
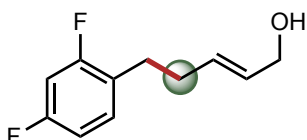
(*E*)-5-(2,4-Difluorophenyl)pent-2-en-1-ol (**1e**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO₃ (15 mL) and extracted with EtOAc (3 x 15 mL).

The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 25% EtOAc/hexanes over 20 min).

**Physical state:** 88% yield, *E/Z* = 88:12, yellow oil.

¹H NMR (500 MHz, CDCl₃) δ 7.13 (d, *J* = 6.7 Hz, 2H), 6.96 (d, *J* = 8.4 Hz, 2H), 5.69 (m, 2H), 4.09 (m, 2H), 2.69 (t, *J* = 8.0 Hz, 2H), 2.53 (m, 1H), 2.36 (m, 2H).

¹³C NMR (126 MHz, CDCl₃) δ 161.5 (dd, *J* = 246.2, 12.1 Hz), 161.1 (dd, *J* = 247.3, 11.7 Hz), 131.7, 131.2 (dd, *J* = 9.5, 2.6 Hz), 130.2, 124.4 (dd, *J* = 16.2, 3.8 Hz), 111.0 (dd, *J* = 20.9, 3.8 Hz), 103.7 (dd, *J* = 25.4, 0.7 Hz), 63.8, 32.8, 28.3.

¹⁹F NMR (471 MHz, C₆D₆) δ -113.31 (d, *J* = 7.0 Hz), -114.36 (d, *J* = 7.0 Hz) (minor *Z* isomer); -113.66 (d, *J* = 7.0 Hz), -114.49 (d, *J* = 6.8 Hz) (major *E* isomer).

HRMS (ES+) m/z calc. for $C_{11}H_{12}F_2O$ [M⁺] 198.0856, found 198.0877.

FT-IR (cm⁻¹, neat, ATR) 3341, 2932, 2864, 1618, 1601, 1504, 1456, 1427, 1375, 1272, 1136.
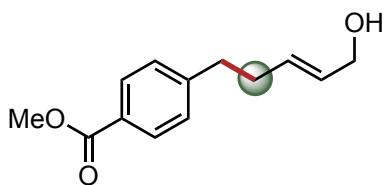
Methyl (*E*)-4-(5-Hydroxypent-3-en-1-yl)benzoate (**1f**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO₃ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 95% yield, *E/Z* = >20:1, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 7.88 (d, *J* = 8.1 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 5.67 – 5.53 (m, 2H), 4.01 (m, 2H), 3.83 (s, 3H), 2.72 – 2.66 (m, 2H), 2.32 (m, 2H).

¹³C NMR (126 MHz, CDCl₃) δ 167.3, 147.3, 131.7, 130.2, 129.8, 128.6, 128.1, 63.7, 52.1, 35.7, 33.7.

HRMS (ES+) m/z calc. for $C_{13}H_{16}O_3$ [M⁺] 220.1099, found 220.1099.

FT-IR (cm⁻¹, neat, ATR) 3418, 2950, 2858, 1717, 1610, 1435, 1415, 1310, 1276, 1107, 968.

(*E*)-5-(o-Tolyl)pent-2-en-1-ol (**1g**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 35% EtOAc/hexanes over 20 min).
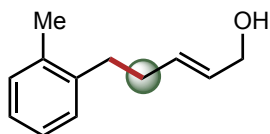
Physical state: 62% yield, *E/Z* = 85:15, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 7.19 – 7.09 (m, 4H), 5.87 – 5.56 (m, 2H), 4.10 (m, 2H), 2.76 – 2.64 (m, 2H), 2.39 – 2.28 (m, 5H), 1.27 (t, *J* = 5.7 Hz, 1H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 140.0, 136.0, 132.6, 130.3, 129.6, 128.9, 126.2, 126.1, 63.9, 33.0, 32.9, 19.5.

HRMS (ES+) m/z calc. for C$_{12}$H$_{16}$O [M$^+$] 176.1201, found 176.1214.

FT-IR (cm^{-1}, neat, ATR) 3326, 3016, 2926, 2865, 1670, 1604, 1492, 1458, 1379, 1218, 998.

(*E*)-5-(Cyclopentyloxy)pent-2-en-1-ol (**1h**)

Prepared according to General Procedure B. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 45% EtOAc/hexanes over 20 min).
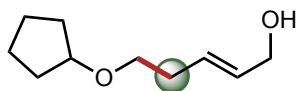
Physical state: 73% yield, *E/Z* = 88:12, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.88 (m, 1H), 5.62 (m, 1H), 4.09 (m, 2H), 3.90 (s (broad), 1H), 3.41 (d, *J* = 6.9 Hz, 2H), 2.38 (t, *J* = 6.8 Hz, 2H), 1.69 (m, 7H), 1.53 – 1.49 (m, 2H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 131.1, 130.5, 81.9, 67.2, 57.6, 32.2, 28.4, 23.6.

HRMS (ES+) m/z calc. for C$_{10}$H$_{18}$O$_2$ [M$^+$] 170.1307, found 170.1329.

FT-IR (cm^{-1}, neat, ATR) 3378, 3018, 2955, 2869, 1723, 1655, 1348, 1091, 10001, 703.

(*E*)-5-((4-Methoxybenzyl)oxy)pent-2-en-1-ol (**1i**)

Prepared according to General Procedure B. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 45% EtOAc/hexanes over 20 min).
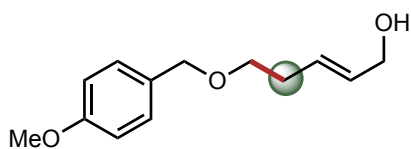
Physical state: 64% yield, *E/Z* = 81:19, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 7.25 (s, 2H), 6.88 (d, *J* = 8.1 Hz, 2H), 5.82 (m, 1H), 5.61 (m, 1H), 4.45 (s, 2H), 4.11 (m, 2H), 3.80 (s, 3H), 3.47 (t, *J* = 6.3 Hz, 2H), 2.40 (m, 2H), 2.05 (s, 1H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 159.5, 131.0, 130.0, 129.5, 129.4, 114.0, 73.0, 68.8, 57.9, 55.4, 28.2.

HRMS (ES+) m/z calc. for C$_{13}$H$_{18}$O$_3$ [M$^+$] 222.1256, found 222.1254.

FT-IR (cm^{-1}, neat, ATR) 3401, 3013, 2859, 1612, 1586, 1512, 1464, 1442, 1422, 1361, 1174, 1088, 1033.

(*E*)-5-(((1*R*,5*S*)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)methoxy)pent-2-en-1-ol (**1j**)

Prepared according to General Procedure B. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 50% EtOAc/hexanes over 20 min).
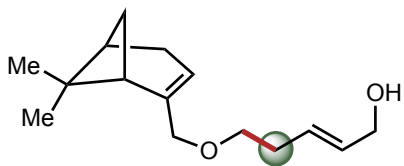
Physical state: 60% yield, *E/Z* = 84:16, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 5.94 – 5.54 (m, 2H), 5.49 (s, 1H), 4.13 (m, 2H), 3.85 (s, 2H), 3.41 (t, *J* = 6.3 Hz, 2H), 2.42 – 2.38 (m, 2H), 2.34 – 2.23 (m, 2H), 2.23 – 2.14 (m, 2H), 2.11 (d, *J* = 6.1 Hz, 1H), 1.30 (m, 4H), 1.17 (d, *J* = 8.4 Hz, 1H), 0.84 (d, *J* = 4.0 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 154.4, 131.1, 131.0, 130.8, 129.9, 73.6, 72.9, 63.9, 61.3, 60.0, 57.4, 33.7, 28.7, 27.7, 27.5.

HRMS (ES+) m/z calc. for $C_{15}H_{24}O_2$ [M⁺] 236.1776, found 236.1777.

FT-IR (cm⁻¹, neat, ATR) 3392, 2985, 2913, 1725, 1655, 1468, 1431, 1382, 1365, 1084, 1040.
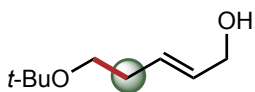
(*E*)-5-(*tert*-Butoxy)pent-2-en-1-ol (**1k**)

Prepared according to General Procedure B. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR. After 16 h, the reaction mixture was quenched with saturated NaHCO₃ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 62% yield, *E/Z* = 53:47, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 5.96 – 5.54 (m, 2H), 4.08 (m, 2H), 3.43 – 3.34 (m, 2H), 2.31 (m, 2H), 1.18 (s, 9H).

¹³C NMR (126 MHz, CDCl₃) δ 130.8, 130.7, 130.5, 129.7, 73.3, 72.7, 63.7, 61.1, 59.8, 57.2, 33.5, 28.5, 27.5, 27.3 (inseparable mixture of two diastereomers).

HRMS (ES+) m/z calc. for $C_9H_{18}O_2$ [M - CH₃] 143.1078, found 143.1078.

FT-IR (cm⁻¹, neat, ATR) 3386, 2973, 2932, 1391, 1195, 1078, 1019, 945.
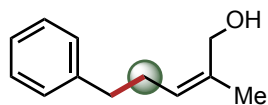
(*Z*)-2-Methyl-5-phenylpent-2-en-1-ol (**2f**)

Prepared according to General Procedure B. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR. After 16 h, the reaction mixture was quenched with saturated NaHCO₃ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The

crude mixture was purified by silica gel column chromatography (0 to 35% EtOAc/hexanes over 20 min).

Physical state: 49% yield, *E/Z* = 94:6, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 7.29 (t, *J* = 7.7 Hz, 2H), 7.21 (d, *J* = 7.4 Hz, 3H), 5.48 (t, *J* = 7.5 Hz, 1H), 4.00 (m, 2H), 2.69 (t, *J* = 7.9 Hz, 2H), 2.38 (m, 2H), 1.63 (s, 3H), 1.36 (s, 1H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 142.1, 135.6, 128.6, 128.4, 126.0, 125.4, 69.0, 35.9, 29.7, 13.8.

HRMS (ES+) m/z calc. for C$_{12}$H$_{16}$O [M$^+$] 176.1201, found 176.1201.

FT-IR (cm^{-1}, neat, ATR) 3370, 3062, 3027, 2922, 2858, 1672, 1603, 1496, 1453, 1259, 1003, 851, 748, 699.
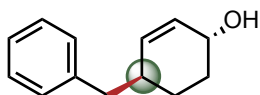
(1R,4S)-4-benzylcyclohex-2-en-1-ol (**2m**)

Prepared according to General Procedure B. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min). Characterization data agreed with reported literature values.[1]

Physical state: 46% yield, *E/Z* = 90:10, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 7.29 (m, 2H), 7.22 – 7.15 (m, 3H), 5.73 – 5.65 (m, 2H), 4.20 – 4.23 (m, 1H), 2.64 (dd, J = 13.3, 7.1 Hz, 1H), 2.52 (dd, J = 13.3, 8.1 Hz, 1H), 2.37 – 2.42 (m, 1H), 2.03 – 2.06 (m, 1H), 1.82 – 1.75 (m, 1H), 1.46 – 1.38 (m, 2H), 1.30 – 1.25 (m, 1H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 140.3, 133.8, 130.8, 129.2, 128.4, 126.1, 67.1, 42.3, 37.5, 31.8, 26.8.

HRMS (ES+) m/z calc. for C$_{13}$H$_{16}$O [M$^+$] 188.1201, found 188.1209.

FT-IR (cm^{-1}, neat, ATR) 3395, 3027, 2925, 1671, 1495, 1454, 1058, 701.

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[1] Narasaka, K.; Kusama, H.; Hayashi, Y. *Tetrahedron* **1992**, *48*, 2059–2068.

GENERAL PROCEDURE: ALKYLATION OF VINYL EPOXIDES WITH 1,4-DIHYDROPYRIDINES (PROCEDURE C)

To an 8.0 mL reaction vial, 4CzIPN (7.8 mg, 0.01 mmol, 2 mol %), [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$ (7.1 mg, 0.015 mmol, 3 mol %), and 1,4-dihydropyridine (0.75 mmol, 1.5 equiv) were added. The vial was capped, purged, and evacuated three times. Under N$_2$, dry degassed acetone (5 mL, 0.1 M) and vinyl epoxide (0.5 mmol, 1.0 equiv) were added. Under a fan, the reactions were stirred in the presence of blue LED strips (see pictures below) for 16 h. The reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography. All reported E/Z ratios were determined by crude ^{1}H NMR.
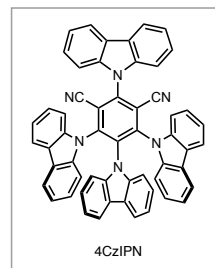

Figure 2. Reaction set up with blue LED strips.[1]

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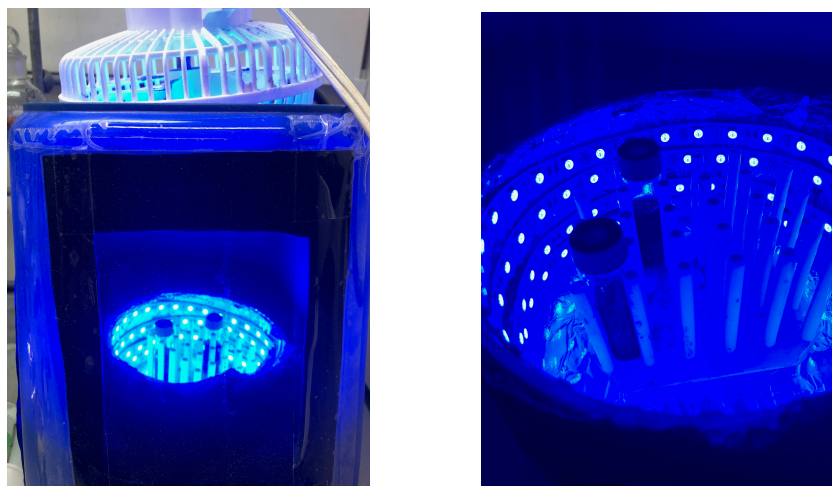
[1] For details on photoreactor setup, see: Lin, K.; Wiles, R. J.; Kelly, C. B.; Davies, G. H. M.; Molander, G. A. *ACS Catal.* **2017**, *7*, 5129–6323.

Compound Characterization
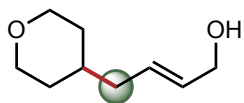
(*E*)-4-(Tetrahydro-2H-pyran-4-yl)but-2-en-1-ol (**2a**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 91% yield, *E/Z* = >20:1, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.73 – 5.61 (m, 2H), 4.14 – 4.05 (m, 2H), 3.94 (m, 2H), 3.35 (t, *J* = 11.7 Hz, 2H), 2.00 (d, *J* = 5.7 Hz, 2H), 1.65 – 1.51 (m, 4H), 1.39 – 1.34 (m, 1H), 1.28 (d, *J* = 12.5 Hz, 1H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 130.9, 130.6, 68.2, 63.8, 39.7, 35.2, 33.0.

HRMS (ES+) m/z calc. for C$_9$H$_{16}$O$_2$ [M$^+$] 156.1150, found 156.1158.

FT-IR (cm^{-1}, neat, ATR) 3403, 2916, 2843, 1724, 1444, 1233, 1134, 1090, 1013, 981, 850.
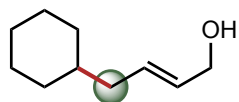
(*E*)-4-Cyclohexylbut-2-en-1-ol (**2b**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min). Spectra are in agreement with reported literature values.[2]

Physical state: 87% yield, *E/Z* = 94:6, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.70 – 5.67 (m, 2H), 4.10 (m, 2H), 2.18 – 1.88 (m, 7H), 1.78 – 1.61 (m, 3H), 1.34 – 1.14 (m, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 131.7, 130.4, 64.0, 39.4, 39.1, 33.7, 25.4, 25.2.

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[2] Guzman-Martinez, A.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2010**, *132*, 10634–10637

(E)-4-(Cyclohex-3-en-1-yl)but-2-en-1-ol (**2c**)

Prepared according to General Procedure C. The reaction was stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with KMnO$_4$ as a stain. After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 62% yield, *E/Z* = 86:14, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.72 – 5.63 (m, 4H), 4.10 (m, 2H), 2.13 – 1.96 (m, 6H), 1.74 – 1.64 (m, 2H), 1.23 (t, *J* = 5.8 Hz, 2H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 131.7, 130.4, 127.1, 126.5, 63.9, 39.4, 33.7, 31.7, 28.6, 25.2.

HRMS (ES+) m/z calc. for C$_{10}$H$_{16}$O [M$^+$] 152.1201, found 152.1221.

FT-IR (cm^{-1}, neat, ATR) 3342, 3021, 2912, 1729, 1563, 1438, 971.
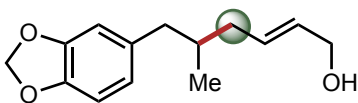
(*E*)-6-(Benzo[d][1,3]dioxol-5-yl)-5-methylhex-2-en-1-ol (**2d**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 85% yield, *E/Z* = 90:10, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 6.73 (d, *J* = 7.7 Hz, 1H), 6.65 (s, 1H), 6.59 (d, *J* = 7.9 Hz, 1H), 5.93 (s, 2H), 5.75 – 5.51 (m, 2H), 4.19 – 4.01 (m, 2H), 2.56 (dd, *J* = 13.5, 6.4 Hz, 1H), 2.32 (dd, *J* = 13.5, 7.9 Hz, 1H), 2.10 (dd, *J* = 12.4, 6.8 Hz, 1H), 1.91 (dt, *J* = 14.0, 6.6 Hz, 1H), 1.82 – 1.70 (m, 1H), 0.87 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 147.6, 145.7, 135.2, 131.6, 130.7, 122.1, 109.6, 108.1, 100.9, 63.9, 43.0, 39.3, 35.4, 19.4.

HRMS (ES+) m/z calc. for C$_{14}$H$_{18}$O$_3$ [M$^+$] 234.1256, found 234.1258.

FT-IR (cm^{-1}, neat, ATR) 3356, 2912, 1729, 1503, 1489, 1441, 1377, 1247, 1189, 1098, 936, 809.
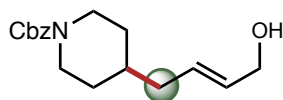
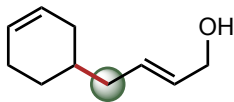Benzyl (E)-4-(4-hydroxybut-2-en-1-yl)piperidine-1-carboxylate (**2e**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 60% EtOAc/hexanes over 20 min).

Physical state: 68% yield, *E/Z* = 91:9, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) 7.39 – 7.31 (m, 5H), 5.69 – 5.61 (m, 2H), 5.13 – 5.10 (m, 2H), 4.17 (m, 2H), 4.10 (m, 2H), 2.80 – 2.70 (m, 2H), 2.01 (m, 2H), 1.67 (d, *J* = 13.0 Hz, 2H), 1.48 (m, 1H), 1.17 – 1.08 (m, 2H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 155.4, 137.1, 131.1, 130.4, 128.6, 128.1, 128.0, 128.0, 67.1, 63.7, 44.3, 39.3, 36.2.

HRMS (ES+) m/z calc. for C$_{17}$H$_{23}$NO$_3$ [M$^+$] 289.1678, found 289.1689.

FT-IR (cm^{-1}, neat, ATR) 3433, 2910, 1694, 1433, 1238, 1178, 1011, 969.
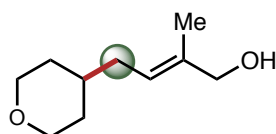
(*E*)-2-Methyl-4-(tetrahydro-2H-pyran-4-yl)but-2-en-1-ol (**2g**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 49% yield, *E/Z* = 82:18, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.36 – 5.25 (m, 1H), 4.13 (m, 2H), 3.94 (dd, *J* = 11.6, 4.5 Hz, 2H), 3.35 (t, *J* = 11.6 Hz, 2H), 2.00 (d, *J* = 6.9 Hz, 2H), 1.81 (s, 3H), 1.52 – 1.46 (m, 1H), 1.35 – 1.08 (m, 4H).

^{13}C NMR (126 MHz, CDCl$_3$) 135.7, 126.2, 123.8, 68.2, 61.7, 35.9, 34.9, 33.1, 21.5.

HRMS (ES+) m/z calc. for C$_{10}$H$_{18}$O$_2$ [M$^+$] 170.1307, found 170.1315.

FT-IR (cm^{-1}, neat, ATR) 3391, 2917, 2845, 1729, 1444, 1386, 1297, 1266, 1233, 1180, 1090, 982,
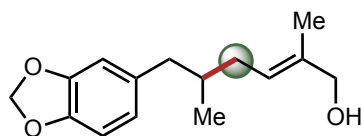
(E)-6-(Benzo[d][1,3]dioxol-5-yl)-2,5-dimethylhex-2-en-1-ol (**2h**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40 EtOAc/hexanes over 20 min).

Physical state: 85% yield, *E/Z* = 90:10, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 6.73 (d, *J* = 7.7 Hz, 1H), 6.65 (s, 1H), 6.60 (d, *J* = 7.9 Hz, 1H), 5.93 (s, 2H), 5.50 – 5.40 (m, 1H), 4.03 (m, 2H), 2.59 – 2.55 (m, 1H), 2.33 (dd, *J* = 13.5, 8.0 Hz, 1H), 2.09 – 2.03 (m, 1H), 1.92 (d, *J* = 7.2 Hz, 1H), 1.76 (dt, *J* = 14.0, 6.9 Hz, 1H), 1.65 (s, 3H), 0.87 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 147.5, 145.7, 135.9, 135.3, 124.9, 122.0, 109.6, 108.1, 100.8, 69.2, 43.1, 35.9, 34.6, 19.5, 14.0.

HRMS (ES+) m/z calc. for C$_{15}$H$_{20}$O$_3$ [M$^+$] 248.1412, found 248.1405.

FT-IR (cm^{-1}, neat, ATR) 3418, 2948, 2937, 1382, 1255, 1212, 1167, 1068, 999, 918, 512.
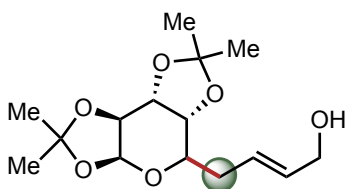
(E)-4-((3a*S*,5*R*,5a*R*,8a*R*,8b*S*)-2,2,7,7-Tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)but-2-en-1-ol (**2i**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (brown after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 60% EtOAc/hexanes over 20 min).

Physical state: 76% yield, *E/Z* = >20:1, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 5.85 – 5.68 (m, 2H), 5.21 (d, *J* = 2.5 Hz, 1H), 4.50 (d, *J* = 5.4 Hz, 1H), 4.21 (d, *J* = 2.4 Hz, 1H), 4.11 (m, 2H), 3.92 (dd, *J* = 9.6, 5.4 Hz, 1H), 3.23 (ddd, *J* = 10.2, 7.6, 3.5 Hz, 1H), 2.52 – 2.48 (m, 1H), 2.26 (dt, *J* = 14.1, 6.8 Hz, 1H), 1.52 (s, 3H), 1.44 (s, 3H), 1.38 (s, 3H), 1.35 (s, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 132.0, 128.2, 110.9, 108.9, 97.0, 76.1, 74.5, 73.0, 72.9, 63.8, 34.5, 28.2, 28.2, 26.1, 25.9.

HRMS (ES+) m/z calc. for C₁₅H₂₄O₆ [M⁺] 300.1573, found 300.1586.

FT-IR (cm⁻¹, neat, ATR) 3443, 2987, 2936, 1727, 1383, 1371, 1238, 1220, 1164, 1143, 1090, 1065, 860, 515.
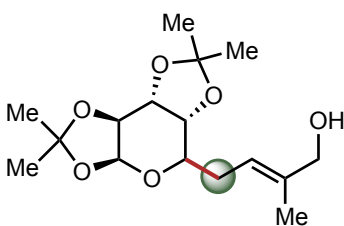
(*E*)-2-Methyl-4-((3a*S*,5*R*,5a*R*,8a*R*,8b*S*)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)but-2-en-1-ol (**2j**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 76% yield, *E/Z* = 89:11, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 5.53 (d, *J* = 5.1 Hz, 1H), 5.47 (t, *J* = 7.1 Hz, 1H), 4.58 (dd, *J* = 7.9, 2.4 Hz, 1H), 4.29 (dd, *J* = 5.1, 2.3 Hz, 1H), 4.14 (m, 1H), 4.02 (m, 2H), 3.75 (t, *J* = 7.1 Hz, 1H), 2.43 – 2.34 (m, 2H), 1.70 (s, 3H), 1.51 (s, 3H), 1.47 (s, 3H), 1.35 (s, 3H), 1.33 (s, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 137.7, 121.3, 109.2, 108.5, 96.7, 72.4, 71.0, 70.7, 68.9, 67.6, 28.8, 26.2, 26.2, 25.1, 24.6, 14.0.

HRMS (ES+) m/z calc. for C₁₆H₂₆O₆ [M⁺] 314.1729, found 314.1706.

FT-IR (cm⁻¹, neat, ATR) 3426, 2986, 2936, 1725, 1382, 1255, 1212, 1167, 1068, 999, 918, 513.
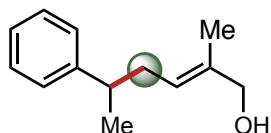
(*E*)-2-Methyl-5-phenylhex-2-en-1-ol (**2k**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark blue after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 45% EtOAc/hexanes over 20 min).

Physical state: 85% yield, *E/Z* = 90:10, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 7.29 (t, *J* = 7.6 Hz, 2H), 7.22 – 7.16 (m, 3H), 5.38 (t, *J* = 7.3 Hz, 1H), 4.03 – 3.89 (m, 2H), 2.78 (q, *J* = 7.1 Hz, 1H), 2.32 (q, *J* = 6.9 Hz, 2H), 1.61 (s, 3H), 1.27 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 147.3, 136.0, 128.4, 127.1, 126.1, 124.7, 69.1, 40.2, 36.5, 21.7, 13.9.

HRMS (ES+) m/z calc. for $C_{13}H_{18}O$ [M⁺] 190.1358, found 190.1350.

FT-IR (cm⁻¹, neat, ATR) 3339, 3061, 3027, 2960, 2926, 2871, 1723, 1602, 1493, 1452, 1376, 1271, 1224, 1075, 1010.
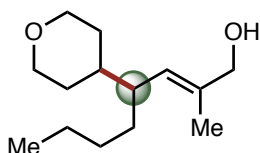
(*E*)-2-Methyl-4-(tetrahydro-2H-pyran-4-yl)oct-2-en-1-ol (**2l**)

Prepared according to General Procedure C. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with *para*-anisaldehyde as a stain (dark purple after heating). After 16 h, the reaction mixture was concentrated on Celite and purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 49% yield, *E/Z* = 84:16, clear oil.

¹H NMR (500 MHz, CDCl₃) δ 5.16 (d, *J* = 10.4 Hz, 1H), 4.06 – 4.02 (m, 2H), 3.99 – 3.94 (m, 2H), 3.35 (dd, *J* = 19.6, 10.4 Hz, 2H), 2.16 – 2.09 (m, 1H), 1.83 (d, *J* = 7.3 Hz, 1H), 1.66 (s, 3H), 1.49 – 1.42 (m, 2H), 1.32 (d, *J* = 7.0 Hz, 2H), 1.28 – 1.23 (m, 4H), 1.16 – 1.11 (m, 2H), 0.89 – 0.87 (m, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 135.81, 129.05, 69.19, 68.57, 42.79, 39.93, 31.90, 31.29, 30.25, 29.67, 23.08, 14.24.

HRMS (ES+) m/z calc. for C$_{14}$H$_{26}$O$_2$ [M$^+$] 226.1933, found 226.1943.

FT-IR (cm^{-1}, neat, ATR) 3388, 2930, 2856, 1729, 1457, 1378, 1239, 1092, 1015, 860.

General Procedure: Alkylation of Allyl Bromides with 1,4-Dihydropyridines (Procedure D)

To a 8.0 mL reaction vial, 4CzIPN (3.9 mg, 0.005 mmol, 2 mol %), [Ni(dtbbpy)(H$_2$O)$_4$]Cl$_2$ (3.6 mg, 0.008 mmol, 3 mol %), and 1,4-dihydropyridine (0.25 mmol, 1.0 equiv) were added. The vial was capped, purged, and evacuated three times. Under N$_2$, dry degassed acetone (2.5 mL, 0.1 M) and allyl bromide (0.50 mmol, 2.0 equiv) were added. The reactions were stirred blue LED strips (see pictures below) for 16 h. The reaction mixture was quenched with saturated NaHCO$_3$ (10 mL) and extracted with EtOAc (3 x 10 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography. All reported E/Z ratios were determined by crude ^{1}H NMR.

Figure 2. Reaction set up with blue LED strips.[1]

[1] For details on photoreactor setup, see: Lin, K.; Wiles, R. J.; Kelly, C. B.; Davies, G. H. M.; Molander, G. A. *ACS Catal.* **2017**, *7*, 5129–6323.

Compound Characterization
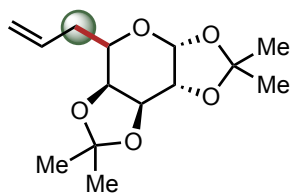
(3aR,5R,5aS,8aS,8bR)-5-Allyl-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran (**4a**)

Prepared according to General Procedure D. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with $KMnO_4$. The crude mixture was purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 70% yield, *dr* = >20:1, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.90 (ddt, *J* = 17.1, 10.2, 6.9 Hz, 1H), 5.22 (d, *J* = 2.5 Hz, 1H), 5.18 – 5.05 (m, 2H), 4.50 (d, *J* = 5.4 Hz, 1H), 4.21 (d, *J* = 2.4 Hz, 1H), 3.94 (dd, *J* = 9.6, 5.4 Hz, 1H), 3.29 – 3.20 (m, 1H), 2.56 – 2.45 (m, 1H), 2.27 (dt, *J* = 14.6, 7.2 Hz, 1H), 1.52 (s, 3H), 1.45 (s, 3H), 1.38 (s, 3H), 1.35 (s, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 134.0, 117.6, 110.9, 108.8, 97.0, 76.0, 74.4, 72.9, 72.8, 36.0, 28.2, 28.2, 26.1, 25.9.

HRMS (ES+) m/z calc. for $C_{14}H_{22}O_5$ [M$^+$] 270.1467, found 270.1480.

FT-IR (cm^{-1}, neat, ATR) 2987, 2937, 1382, 1370, 1282, 1236, 1218, 1165, 1122, 1062, 1040, 859.
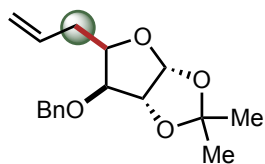
(3aR,5R,6S,6aR)-5-Allyl-6-(benzyloxy)-2,2-dimethyltetrahydrofuro[2,3-d][1,3]dioxole (**4b**)

Prepared according to General Procedure D. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with potassium permanganate. The crude mixture was purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

Physical state: 57% yield, *dr* = 80:20, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.91 (d, *J* = 3.7 Hz, 1H), 5.91 – 5.65 (m, 4H), 5.57 (d, *J* = 10.2 Hz, 1H), 5.04 (td, *J* = 9.9, 6.1 Hz, 2H), 4.63 (dd, = 14.4, 3.3 Hz, 2H), 4.37 (m, 1H),

3.74 – 3.66 (m, 1H), 3.59 (m, 1H), 2.88 – 2.75 (m, 1H), 2.18 (m, 2H), 1.46 (d, *J* = 7.1 Hz, 3H), 1.33 (s, 3H) (mixtures of diastereomers).

^{13}C NMR (126 MHz, CDCl$_3$) δ 135.8, 135.8, 131.9, 130.3, 128.6, 128.0, 126.9, 124.1, 124.0, 116.9, 113.0, 112.4, 106.6, 91.1, 90.4, 85.9, 85.4, 84.9, 84.7, 77.9, 77.7, 76.9, 49.0, 49.0, 40.3, 40.1, 36.3, 36.0, 27.5, 27.0, 26.9 (mixtures of diastereomers).

HRMS (ES+) m/z calc. for C$_{17}$H$_{22}$O$_4$ [M$^+$] 290.1518, found 290.1514.

FT-IR (cm^{-1}, neat, ATR) 2981, 2937, 1641, 1456, 1373, 1216, 1164, 1079, 1024, 912, 752.
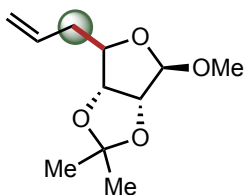
(3a*R*,4*R*,6*R*,6a*R*)-4-Allyl-6-methoxy-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxole (**4c**)

Prepared according to General Procedure D. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with KMnO$_4$. The crude mixture was purified by silica gel column chromatography (0 to 35% EtOAc/hexanes over 20 min).

Physical state: 94% yield, *dr* = >20:1, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 5.81 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.18 – 5.08 (m, 2H), 4.96 (s, 1H), 4.61 (d, *J* = 6.0 Hz, 1H), 4.57 (d, *J* = 6.0 Hz, 1H), 4.23 (t, *J* = 7.8 Hz, 1H), 3.34 (s, 3H), 2.42 (dt, *J* = 14.0, 6.8 Hz, 1H), 2.32 – 2.26 (m, 1H), 1.48 (s, 3H), 1.31 (s, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 134.5, 117.7, 112.4, 109.6, 86.6, 85.7, 83.6, 55.0, 39.6, 26.6, 25.2.

HRMS (ES+) m/z calc. for C$_{11}$H$_{18}$O$_4$ [M$^+$] 214.1205, found 214.1220.

FT-IR (cm^{-1}, neat, ATR) 2988, 2938, 2834, 1643, 1442, 1373, 1272, 1241, 1211, 1107, 1093, 870.
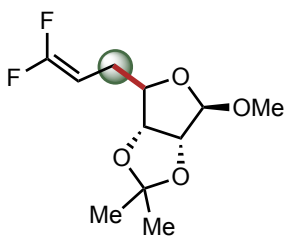
(3a*R*,4*R*,6*R*,6a*R*)-4-(3,3-Difluoroallyl)-6-methoxy-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxole (**4d**)

Prepared according to General Procedure D. The reactions were stirred under a fan near blue LED strips. The reaction progression was monitored *via* crude proton NMR and TLC with KMnO$_4$. The crude mixture was purified by silica gel column chromatography (0 to 25% EtOAc/hexanes over 20 min).

Physical state: 94% yield, *dr* = >20:1, clear oil.

^{1}H NMR (500 MHz, CDCl$_3$) δ 4.96 (s, 1H), 4.61 (d, *J* = 5.9 Hz, 1H), 4.52 (d, *J* = 5.9 Hz, 1H), 4.30 – 4.06 (m, 2H), 3.34 (s, 3H), 2.26 (m, 2H), 1.47 (s, 3H), 1.32 (s, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 157.0 (dd, *J* = 286.9 Hz), 112.6, 109.7, 86.5, 85.6, 83.6, 74.7 (dd, *J* = 24.2, 20.4 Hz), 55.1, 28.4, 26.6, 25.16.

^{19}F NMR (471 MHz, C$_6$D$_6$) δ -87.07 (d, *J* = 44.3 Hz), -89.46 (d, J = 43.5 Hz).

HRMS (ES+) m/z calc. for C$_{11}$H$_{16}$F$_2$O$_4$ [M$^+$] 250.1017, found 250.1029.

FT-IR (cm^{-1}, neat, ATR) 2991, 2939, 1747, 1374, 1345, 1308, 1275, 1260, 1211, 1185, 1107, 1093, 869.
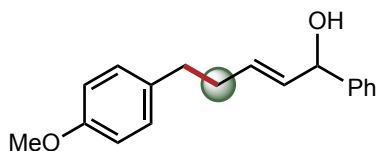
5-(4-methoxyphenyl)-1-phenylpent-2-en-1-ol (**5a**)

Prepared according to General Procedure A. To maintain the reaction temperature at 60 °C, the blue LED bay was covered with aluminum foil, and the temperature was periodically checked with a digital temperature sensor. After 16 h, the reaction mixture was quenched with saturated NaHCO$_3$ (15 mL) and extracted with EtOAc (3 x 15 mL). The organic extracts were combined and concentrated on Celite. The crude mixture was purified by silica gel column chromatography (0 to 40% EtOAc/hexanes over 20 min).

^{1}H NMR (500 MHz, CDCl$_3$): *δ* (Major isomer) δ 7.35 – 7.33 (m, 3H), 7.31 – 7.23 (m, 2H), 7.08 (d, J = 8.4 Hz, 2H), 6.82 (d, J = 8.3 Hz, 2H), 5.82 – 5.73 (m, 1H), 5.71 – 5.64 (m, 1H), 5.16 (d, J = 6.7 Hz, 1H), 3.79 (s, 3H), 2.69 – 2.66 (m, 2H), 2.40 – 2.32 (m, 2H), 1.88 (br, OH).

^{13}C NMR (125 MHz, CDCl$_3$): *δ* (Major isomer) 158.0, 143.39, 133.9, 133.1, 131.8, 129.5, 128.6, 127.7, 126.3, 113.9, 75.2, 55.4, 34.7, 34.3. (Minor isomer) 158.1, 133.7, 133.0, 131.1, 129.7, 127.5, 126.0, 114.0, 69.7, 34.9, 30.0.

FT-IR (cm^{-1}, neat, ATR) 3402, 1611, 1511, 1244, 700.

HRMS (EI) m/z: Calcd for C$_{18}$H$_{20}$O$_2$ [M] 268.1463. Found, 268.1479.

Computational Studies

Details about computational methods.

All optimizations of intermediates and transition state structures were carried out in the gas phase without constraints using spin-unrestricted broken symmetry (hybrid) DFT using UB3LYP[i]/6-31G(d) method with the "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian09.[ii] Frequency calculations were performed at the same level to determine vibrational frequencies, obtain thermal corrections to enthalpy ($H_{correction}$) and free energy ($G_{correction}$) at 298K, and to determine whether the optimized structures were transition states (if there existed only a single imaginary frequency) or intermediates (if no imaginary frequencies were found). Exhaustive conformational searches were performed for all structures to elucidate the lowest energy profiles, To refine the energies, we performed single point energy calculations on optimized geometries using implicit solvent (water; ε = 78.3553) with SMD[iii] as the solvation model in combination with the UM06 functional[iv] and the 6-311+G(d,p) basis set. For comparison, we also computed single point energies using D3 dispersion correction of Grimme et al.with UB3LYP (i.e., UB3LYP-D3)[v] and the UM06 functionals in combination the 6-311+G(d,p) basis set in solvent (water) using the SMD solvation model. Finally, for comparison, we also performed open-shell domain-based local pair natural orbital Coupled-Cluster calculations using single and double excitations with perturbative triple excitations (DLPNO-CCSD(T)) with def2-TZVPP basis set[vi] and def2-TZVPP/C auxiliary basis set[vii] were performed on the lowest energy pathways using ORCA software[viii] with the "NormalPNO" and "SlowConv" keywords. The total free energies using this method was computed as followed: $G = E^{DLPNO\text{-}CCSD(T))} + G_{thermal\ corrections}^{UB3LYP} + \Delta G_{solvation}^{UB3LYP\text{-}D3}$ where $\Delta G_{solvation}^{UB3LYP} = E^{UB3LYP\text{-}D3/6\text{-}311+G(d,p)\text{-}SMD(water)} - E^{UB3LYP\text{-}D3/6\text{-}311+G(d,p)\text{-}gas}$ This method provides accurate energies (within 3 kJ mol^{-1}) with the computational cost comparable to DFT calculations[ix] and has been used to study organometallic reaction mechanisms[x]. All structural figures were generated using CYLview[xi] (in manuscript) and GaussView 5[iv] (supporting information)

B''-TS$_B$-MeOH
19.5 (18.6) [18.0]

B''-TS$_L$-MeOH
17.6 (15.6) [14.9]

B''-H-TS$_B$-MeO⁻
19.2 (18.2) [17.5]

B''-H-TS$_L$-MeO⁻
16.6 (14.9) [14.3]

B''-MeOH
1.3 (1.1) [5.2]

B''-H-OMe
0.0 (0.0) [0.0]
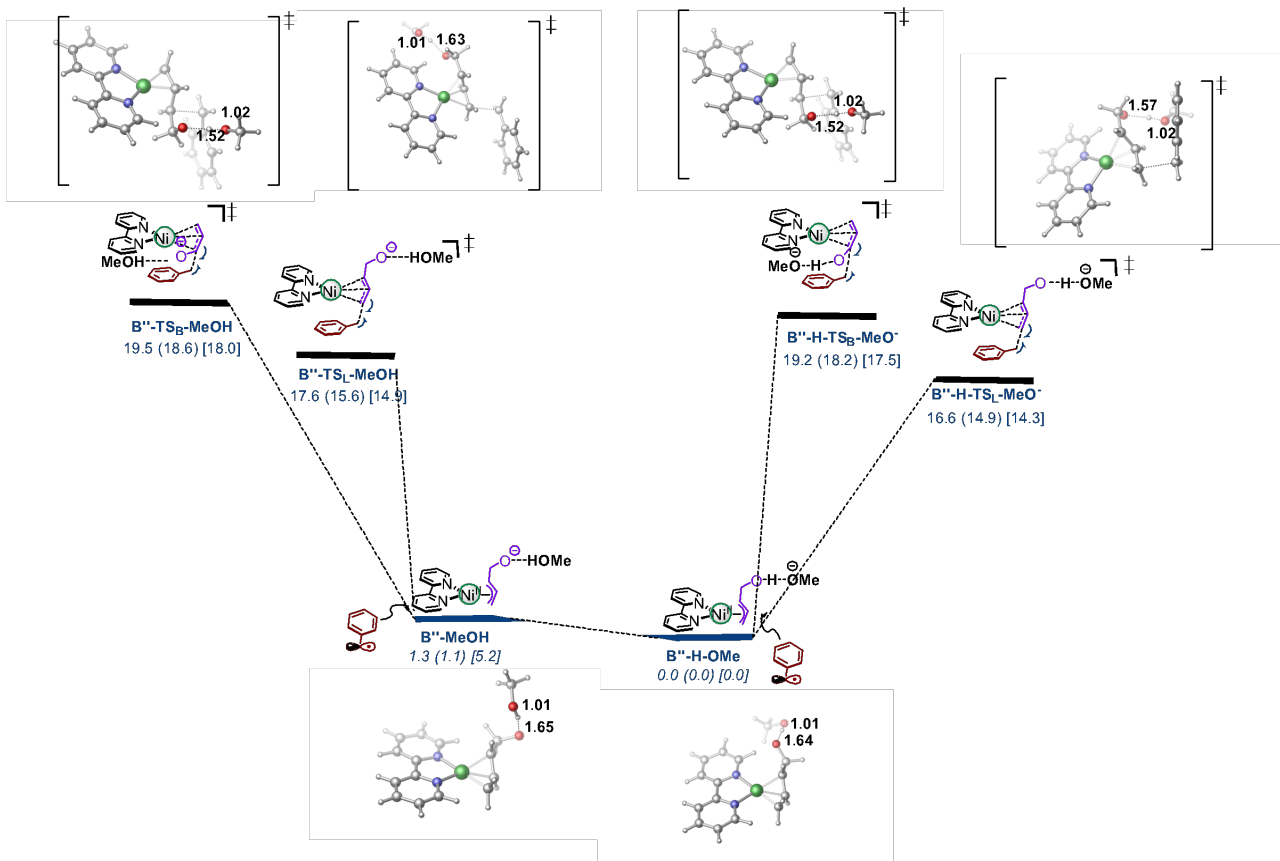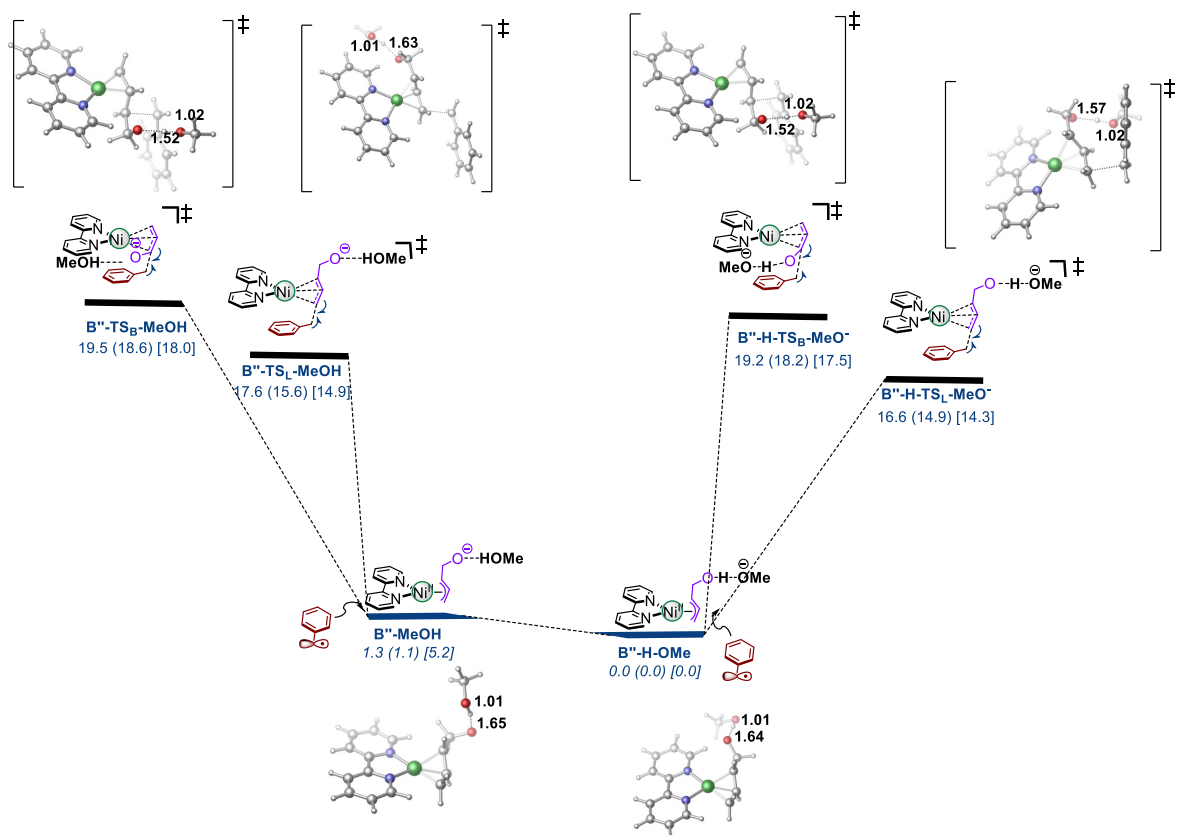
Figure SC1. Protonated outer-sphere transition states leading to the branched and linear products computed at the UM06/6-311+G(d,p)-SMD(water)//UB3LYP/6-31G(d)-gas, UB3LYP-D3/6-311+G(d,p)-SMD(water)//UB3LYP/6-31G(d)-gas (parenthesis) and DLPNO-CCSD(T)/def2-TZVPP-SMD(water)//UB3LYP/6-31G(d)-gas (brackets) levels.
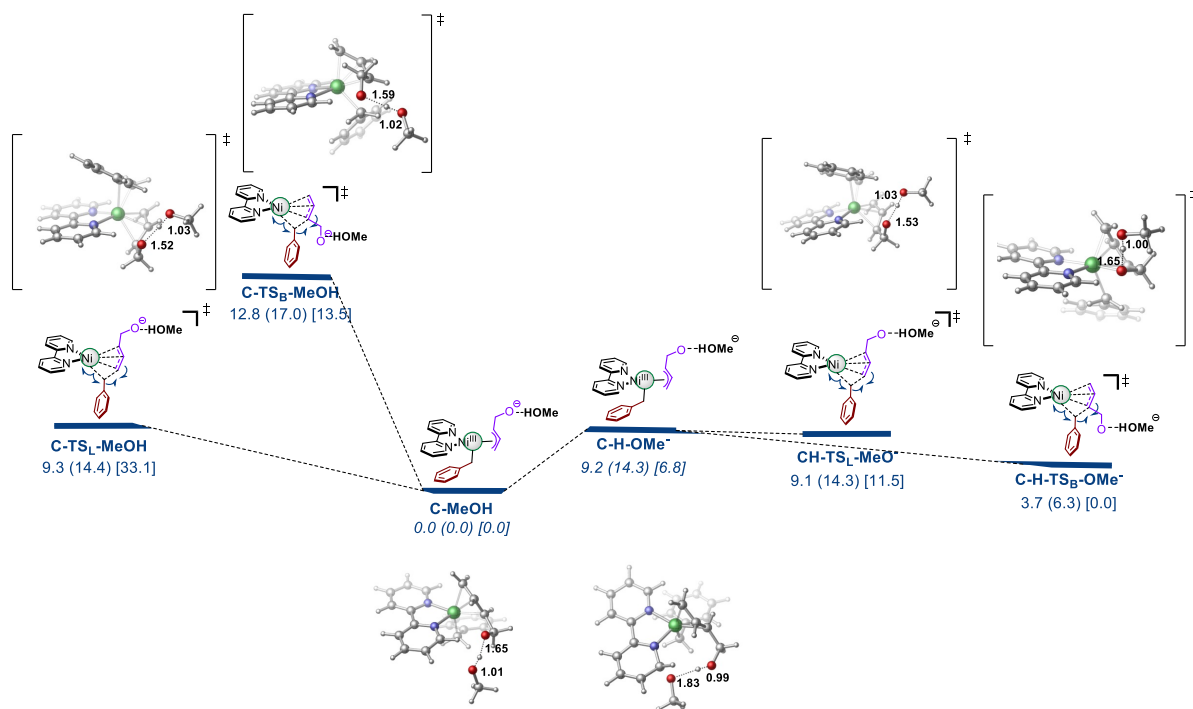
Figure SC2. Protonated inner sphere transition states leading to the branched and linear products computed at the UM06/6-311+G(d,p)-SMD(water)//UB3LYP/6-31G(d)-gas, UB3LYP-D3/6-311+G(d,p)-SMD(water)//UB3LYP/6-31G(d)-gas (parenthesis) and DLPNO-CCSD(T)/def2-TZVPP-SMD(water)//UB3LYP/6-31G(d)-gas (brackets) levels.
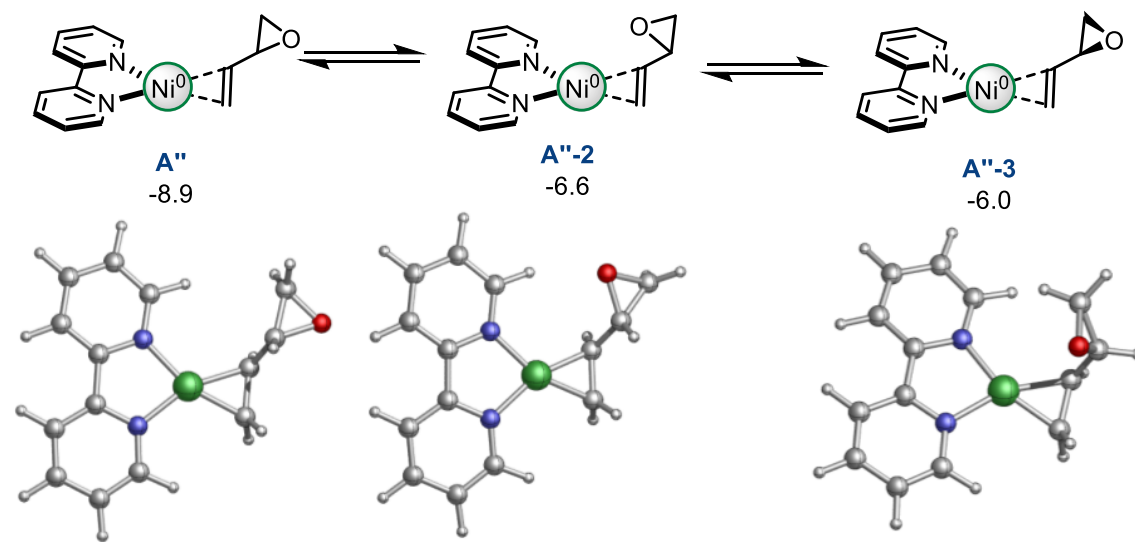
Figure SC3. Conformers of **A''** with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.
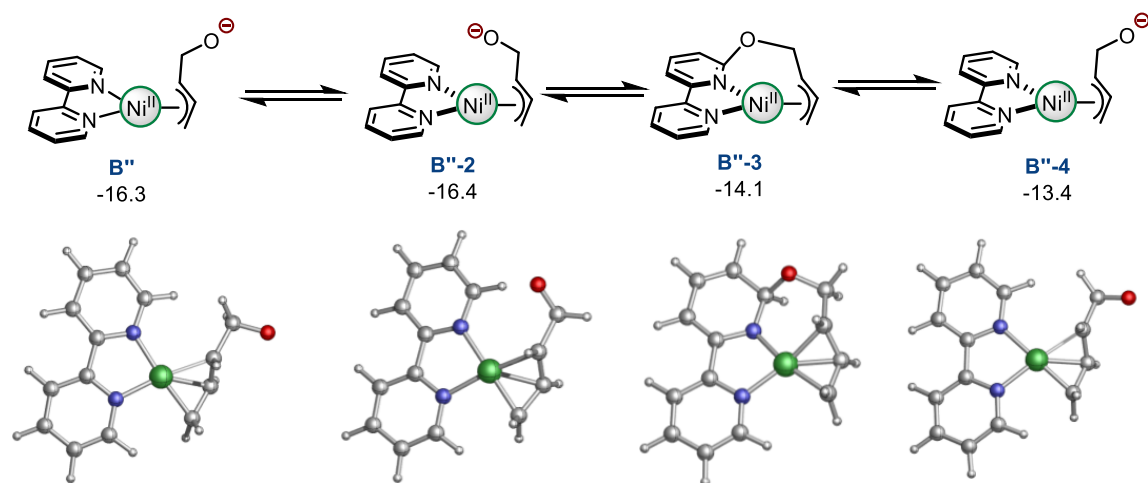
Figure SC4. Conformers of B'' with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

B''-C-TS
-15.6

B''-C-TS-2
-14.4

B''-C-TS-3
-11.8

2.80 Å

2.80 Å

4.24 Å

B''-C-TS-4
-15.6

B''-C-TS-5
-6.0

B''-C-TS-6
-0.7

3.0 Å

2.62 Å

4.00 Å
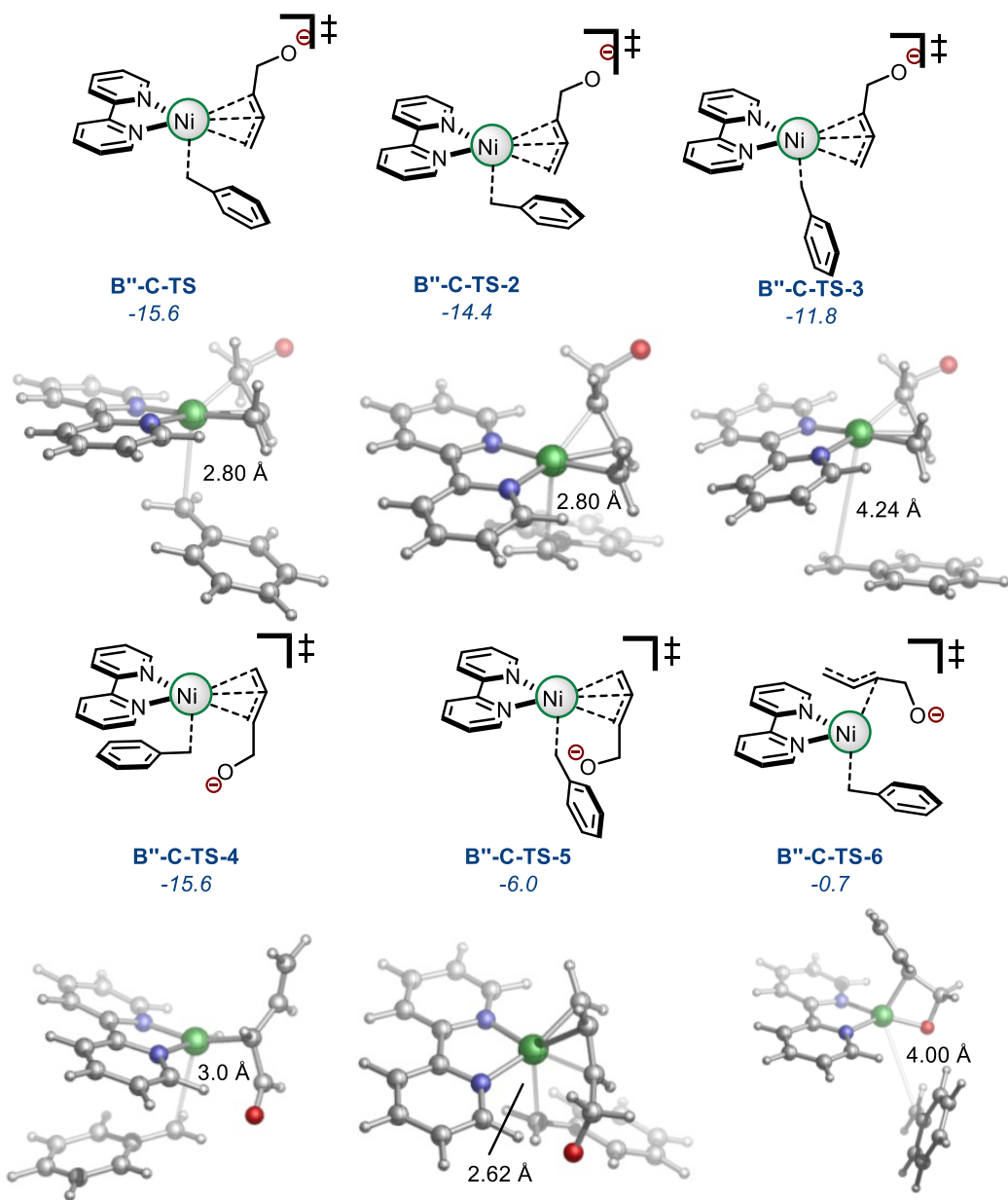
Figure SC5. Conformers of B''-C-TS. Free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

C
-16.0

C-2
-9.2

C-3
-9.3

C-4
-8.1

C-5
-8.0

C-6
-8.0

C-7
-9.6

C-8
0.1
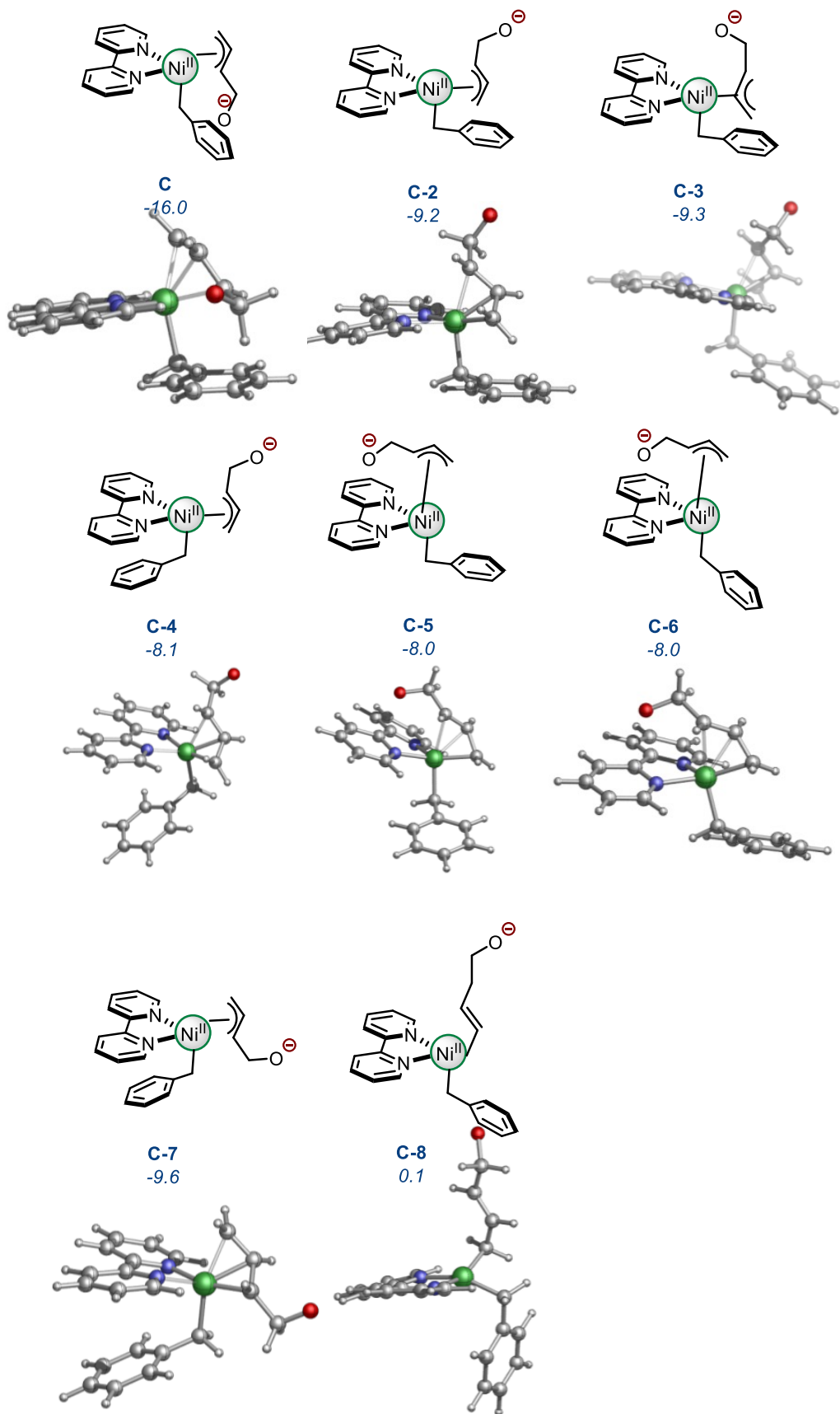
Figure SC6. Conformers of C. Free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

B'
-18.0

B'-2
-17.7

B'-3
-16.9

B'-4
-13.9
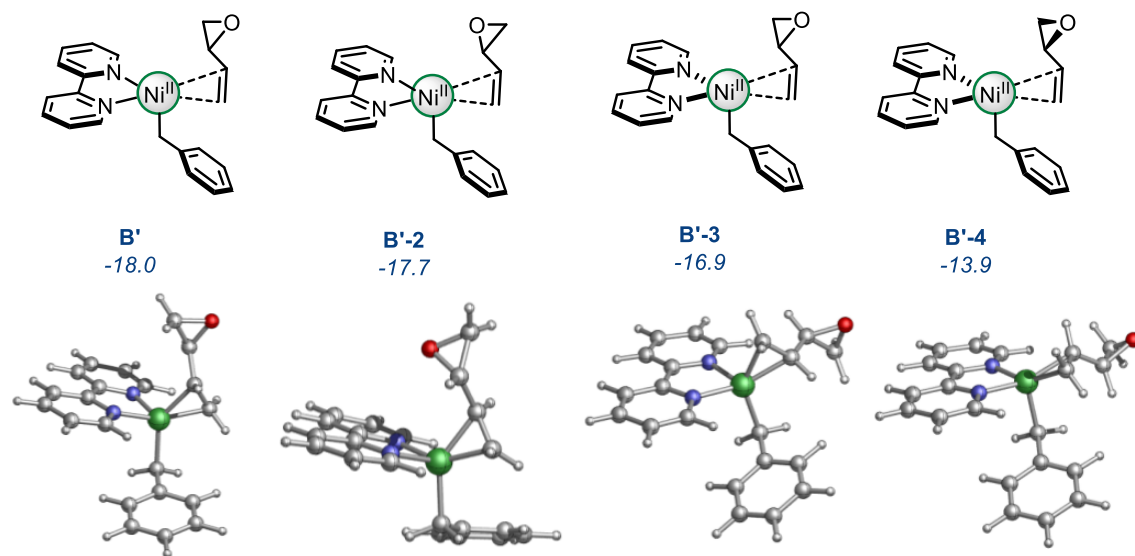
Figure SC7. Conformers of B'. Free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.
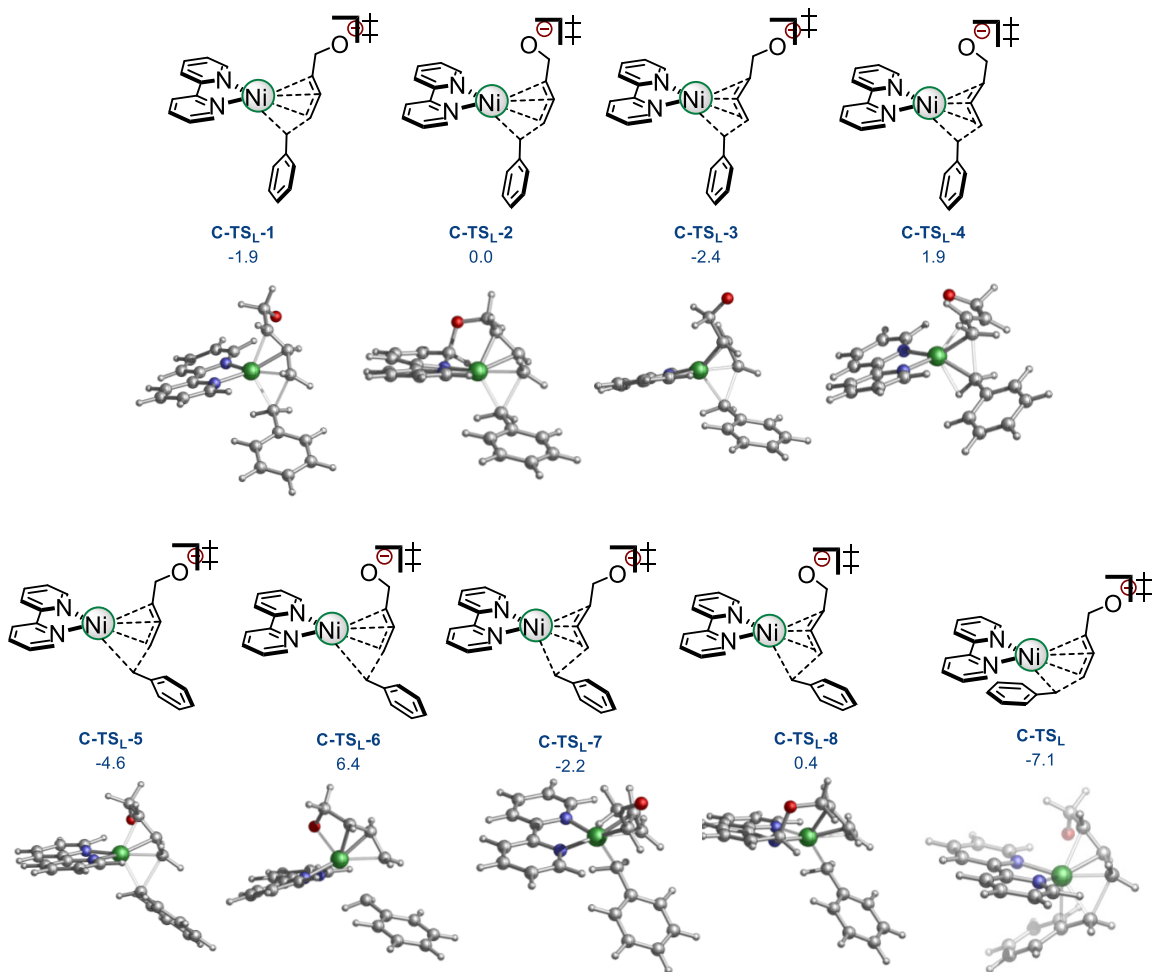
Figure SC8. Conformers of C-TS$_L$ with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

C-TS_B-1
-1.1

C-TS_B-2
-1.5

C-TS_B-3
1.3

C-TS_B-4
0.2

C-TS_B-5
1.6
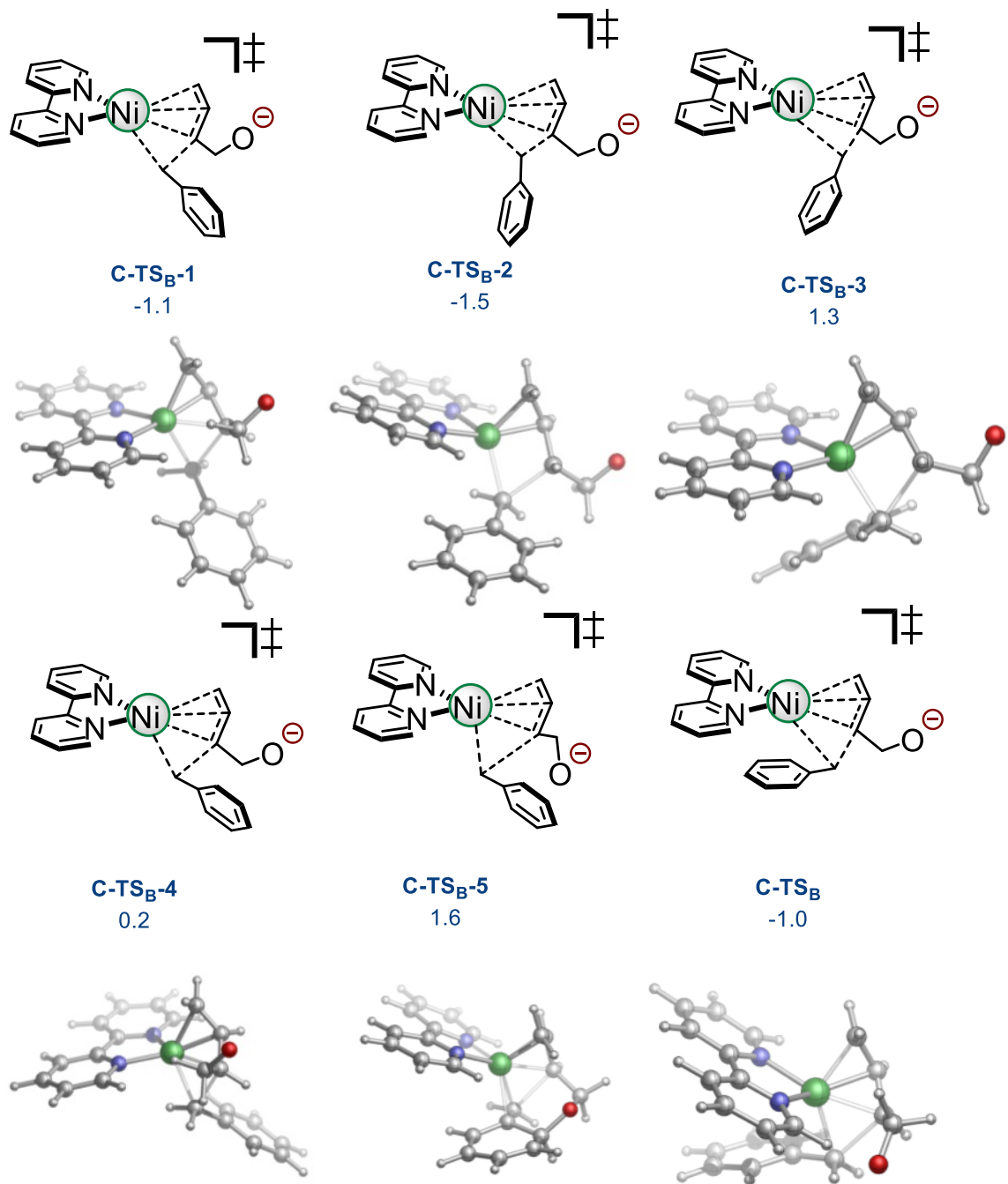
C-TS_B
-1.0

Figure SC9. Conformers of C-TS$_B$ with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

B''-TS_L
-2.0

B''-TS_L-2
0.9

B''-TS_L-3
-0.2
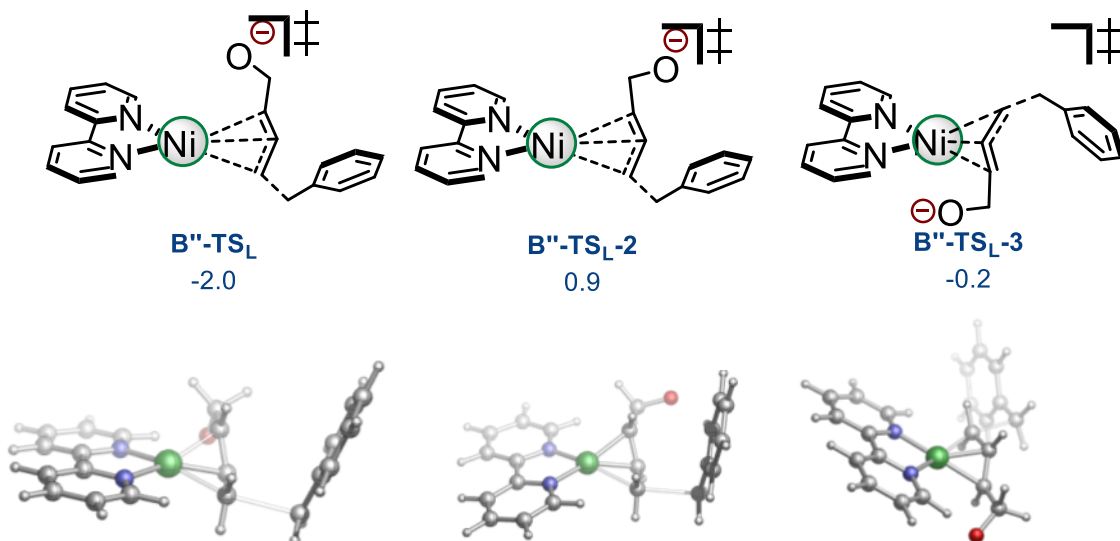
Figure S10. Conformers of C-TS$_B$ with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

B''-TS_B
3.0

B''-TS_B-2
4.2
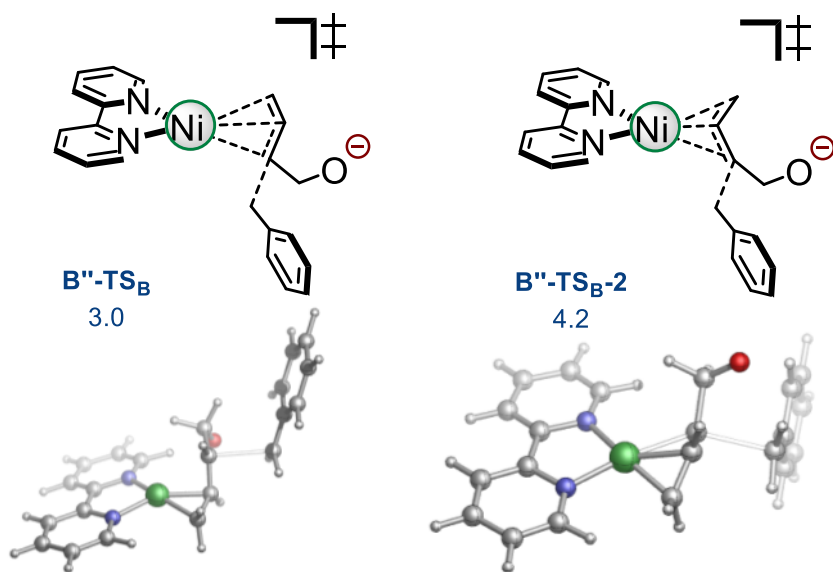
Figure SC11. Conformers of C-TS$_B$ with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas level.

B''-TS_B
3.0 (-1.6) [-1.9]

C-TS_B
-1.0 (-4.5) [-9.0]

1.95 Å
2.37 Å

2.09 Å
2.15 Å
2.07 Å

B''-TS_L
-2.0 (-7.6) [-7.1]

C-TS_L
-7.1 (-9.5) [-13.9]

2.0 Å
2.35 Å

2.26 Å
2.07 Å
2.07 Å
2.15 Å
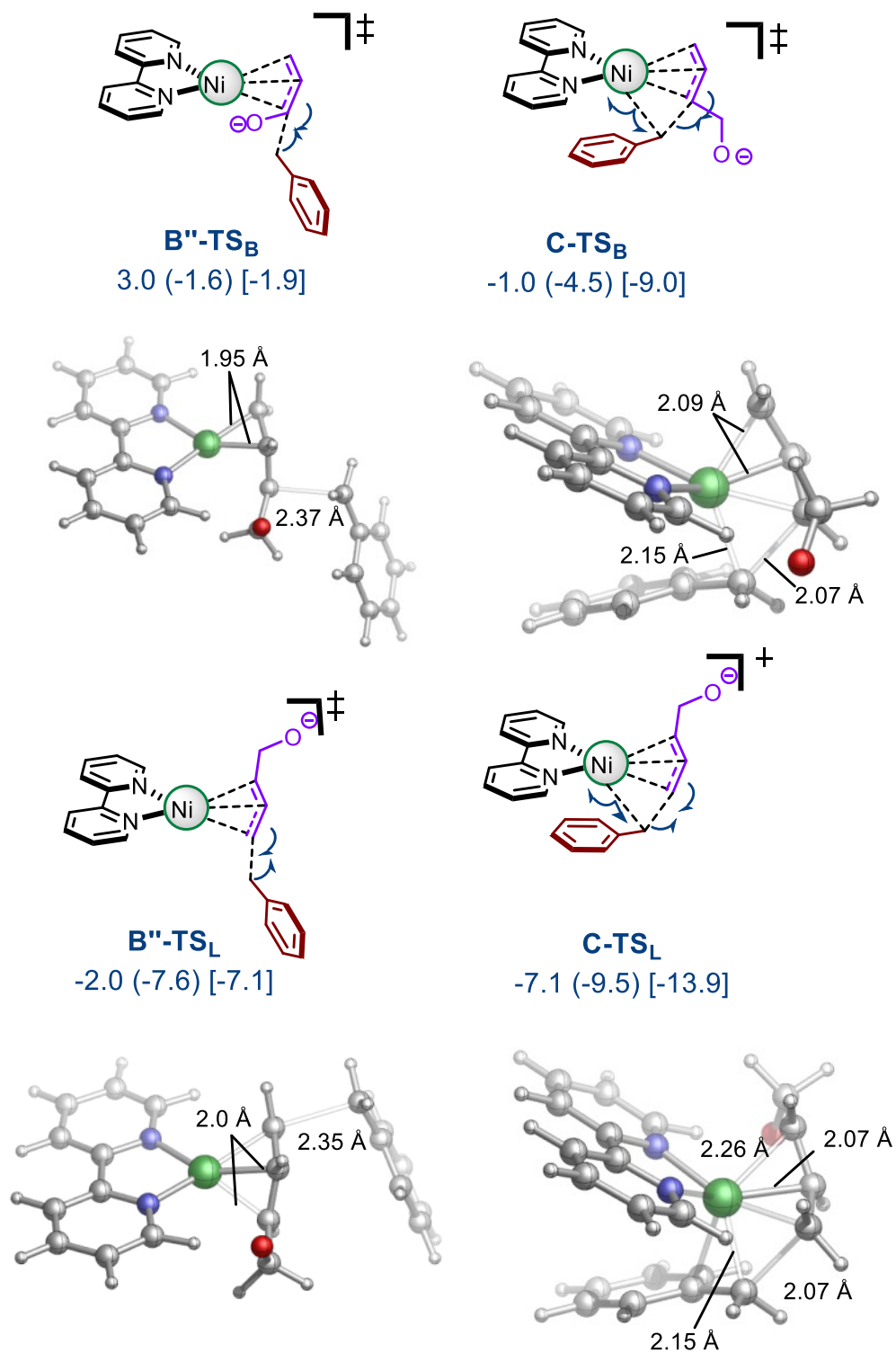
Figure SC12. Conformers of inner and outer sphere reductive elimination transition states with relative free energies computed at the UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas, UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas, (parenthesis) and DLPNO-CCSD(T)/def2-TZVPP (brackets) levels.

Coordinates and energies
A'
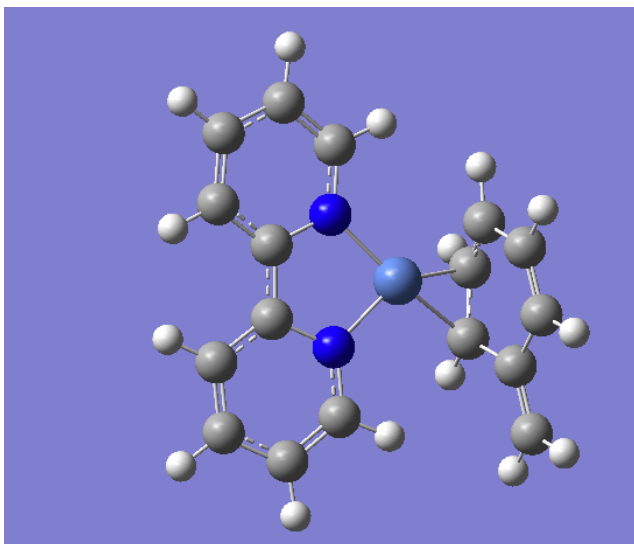
UB3LYP/6-31g(d)-gas
Zero-point correction=   0.276831 (Hartree/Particle)
 Thermal correction to Energy=   0.293478
 Thermal correction to Enthalpy=   0.294422
 Thermal correction to Gibbs Free Energy=   0.231429
 Sum of electronic and zero-point Energies=   -2274.226213
 Sum of electronic and thermal Energies=   -2274.209566
 Sum of electronic and thermal Enthalpies=   -2274.208622
 Sum of electronic and thermal Free Energies=   -2274.271616
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.1583862
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.8877466
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2272.472168063574

ΔG_{solv} = -0.0056383

 A-TS

A-TS
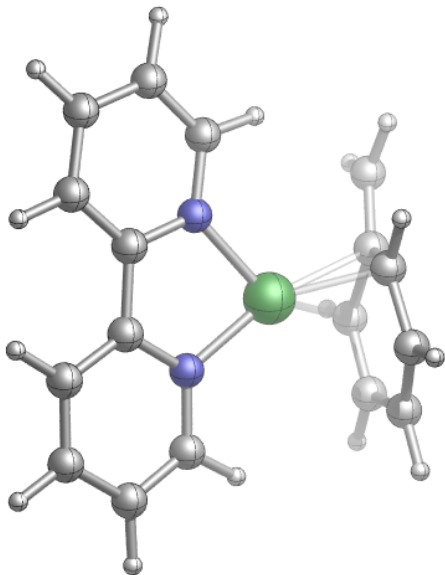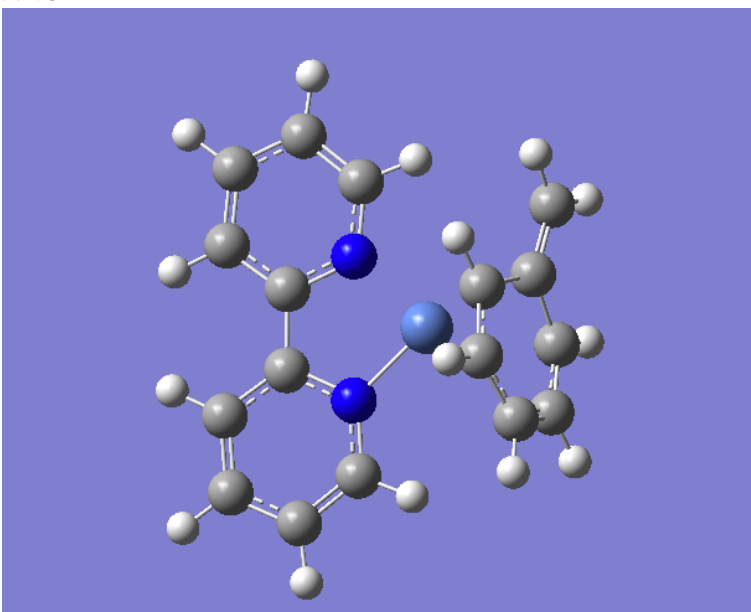
UB3LYP/6-31g(d)-gas
Imaginary frequency = -95.44 cm^{-1}
Zero-point correction=   0.274198 (Hartree/Particle)
 Thermal correction to Energy=   0.290971
 Thermal correction to Enthalpy=   0.291915
 Thermal correction to Gibbs Free Energy=   0.228224
 Sum of electronic and zero-point Energies=   -2274.210476
 Sum of electronic and thermal Energies=   -2274.193704
 Sum of electronic and thermal Enthalpies=   -2274.192759
 Sum of electronic and thermal Free Energies=   -2274.256450
 C   -1.45189 2.03439 0.64615
 C   0.67761 2.42732 -0.32566

C	0.31175	3.71701	-0.72049
C	-0.99473	4.17848	-0.41376
C	-1.87174	3.33392	0.27313
C	-2.2916	1.05112	1.32798
C	-2.38662	-1.16384	2.17232
C	-3.72767	-1.01974	2.537
C	-4.36744	0.22467	2.29653
C	-3.64418	1.25765	1.69363
H	1.6601	2.01724	-0.53888
H	1.02148	4.34238	-1.25216
H	-1.31177	5.17443	-0.71029
H	-2.87341	3.67357	0.51576
H	-1.84616	-2.08938	2.34594
H	-4.25663	-1.84703	2.99874
H	-5.40687	0.37283	2.57569
H	-4.12059	2.21311	1.50003
N	-0.17001	1.59816	0.34673
N	-1.67275	-0.16146	1.58786
Ni	0.25102	-0.1573	1.13903
C	1.92498	-0.99434	2.11151
C	1.26732	-2.10154	2.73545
C	1.02457	-3.29735	2.05169
C	1.48479	-3.41983	0.69751
C	2.15816	-2.38884	0.06614
C	2.4592	-1.1257	0.74295
H	2.28952	-0.17869	2.73528
H	0.96138	-1.99748	3.77551
H	0.52125	-4.12749	2.53988
H	1.30811	-4.35011	0.16002
H	2.5192	-2.51546	-0.95312
C	3.20819	-0.11799	0.12261
H	3.59594	-0.25122	-0.88413
H	3.50334	0.78007	0.66057

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.1527528
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.8833272
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2272.466173902212
ΔG_{solv} = -0.014615

B

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.114993 (Hartree/Particle)
 Thermal correction to Energy=   0.120659
 Thermal correction to Enthalpy=   0.121603
 Thermal correction to Gibbs Free Energy=   0.085325
 Sum of electronic and zero-point Energies=   -270.800147
 Sum of electronic and thermal Energies=   -270.794481
 Sum of electronic and thermal Enthalpies=   -270.793537
 Sum of electronic and thermal Free Energies=   -270.829815
C   2.74508 -1.15846 -0.78885
 C   3.96616 -0.54991 -0.48172
 C   4.44401 -0.53276 0.84965
 C   3.67794 -1.13642 1.87431
 C   2.45538 -1.74784 1.57891
 C   1.94812 -1.77888 0.23416
 H   2.38205 -1.16936 -1.81497
 H   4.55387 -0.08618 -1.27094
 H   5.39393 -0.05861 1.08397
 H   4.04368 -1.12389 2.89872
 H   1.8698 -2.21095 2.37103
 C   0.70797 -2.39894 -0.07206
 H   0.10525 -2.86798 0.70199
 H   0.32508 -2.42294 -1.08953
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2274.1761005
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2274.9135258
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas

HF = -2272.490424211042
ΔG$_{solv}$ = -0.0122301
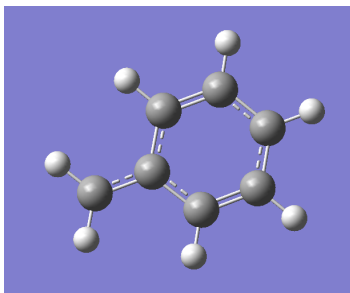
Ni-Bn-radical

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.114993 (Hartree/Particle)
 Thermal correction to Energy=   0.120659
 Thermal correction to Enthalpy=   0.121603
 Thermal correction to Gibbs Free Energy=   0.085325
 Sum of electronic and zero-point Energies=   -270.800147
 Sum of electronic and thermal Energies=   -270.794481
 Sum of electronic and thermal Enthalpies=   -270.793537
 Sum of electronic and thermal Free Energies=   -270.829815
C   2.74508 -1.15846 -0.78885
C   3.96616 -0.54991 -0.48172
C   4.44401 -0.53276 0.84965
C   3.67794 -1.13642 1.87431
C   2.45538 -1.74784 1.57891
C   1.94812 -1.77888 0.23416
H   2.38205 -1.16936 -1.81497
H   4.55387 -0.08618 -1.27094
H   5.39393 -0.05861 1.08397
H   4.04368 -1.12389 2.89872
H   1.8698 -2.21095 2.37103
C   0.70797 -2.39894 -0.07206
H   0.10525 -2.86798 0.70199
H   0.32508 -2.42294 -1.08953

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -270.75733

UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-270.9952919
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -270.397554147875
ΔG$_{solv}$ = -0.000751

Ni-VE-By-substrate
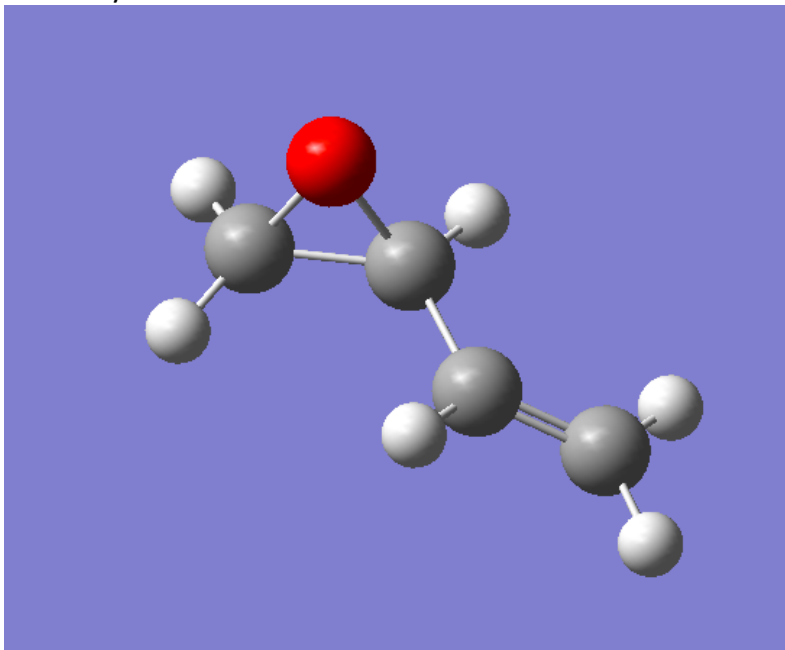
UB3LYP/6-31g(d)-gas
Zero-point correction=   0.090843 (Hartree/Particle)
 Thermal correction to Energy=   0.095976
 Thermal correction to Enthalpy=   0.096921
 Thermal correction to Gibbs Free Energy=   0.062850
 Sum of electronic and zero-point Energies=   -231.095575
 Sum of electronic and thermal Energies=   -231.090442
 Sum of electronic and thermal Enthalpies=   -231.089498
 Sum of electronic and thermal Free Energies=   -231.123568
C   1.63349 0.0152   1.78963
 H   2.27435 0.84994 1.49639
 C   1.2083 -0.94134 0.74956
 H   1.78433 -0.3319   2.68677
 H   1.04247 -1.86397 1.01291
 C   1.89387 -0.84922 -0.62634
 C   1.76105 -1.99599 -1.58584
 H   2.85325 -0.30568 -0.56929
 H   1.17447 -2.88181 -1.28537
 H   2.62542 -2.2722 -2.21482
 O   1.04532 -0.70447 -1.85607

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-231.0961417
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-231.2679346
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas

HF = -230.802082513855
ΔG$_{solv}$ = -0.0054462

B′

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.370239 (Hartree/Particle)
 Thermal correction to Energy=   0.393161
 Thermal correction to Enthalpy=   0.394106
 Thermal correction to Gibbs Free Energy=   0.313482
 Sum of electronic and zero-point Energies=   -2505.361098
 Sum of electronic and thermal Energies=   -2505.338175
 Sum of electronic and thermal Enthalpies=   -2505.337231
 Sum of electronic and thermal Free Energies=   -2505.417854
C   -1.08408 1.75012 0.69367
C   1.20805 1.4324   0.92934
C   1.31986 2.51277 1.79753
C   0.17173 3.23828 2.11524
C   -1.04231 2.84826 1.55937
C   -2.32473 1.25743 0.05758
C   -3.19768 -0.16329 -1.55011
C   -4.50409 0.21548 -1.25762
C   -4.71089 1.15569 -0.24603
C   -3.60965 1.68102 0.4217
H   2.06897 0.82662 0.67327
H   2.28763 2.77115 2.21412
H   0.21964 4.09302 2.7832

H	-1.94679	3.40226	1.78355
H	-2.98412	-0.89679	-2.32327
H	-5.33434	-0.21716	-1.80642
H	-5.71495	1.47037	0.0227
H	-3.75112	2.39786	1.22303
N	0.04077	1.05826	0.37497
N	-2.13	0.34052	-0.91687
Ni	-0.11549	-0.3651	-0.978
C	1.8752	-3.05474	0.46009
C	3.08711	-3.34317	1.08223
C	3.41955	-2.74473	2.30161
C	2.51274	-1.86055	2.8886
C	1.30057	-1.57219	2.26112
C	0.94589	-2.15456	1.02571
H	1.62974	-3.54356	-0.4801
H	3.77497	-4.04587	0.61733
H	4.36351	-2.97313	2.78918
H	2.74479	-1.39979	3.84657
H	0.59517	-0.89906	2.7439
C	-0.33231	-1.82424	0.35176
H	-1.06937	-1.46494	1.08141
H	-0.74897	-2.69932	-0.15538
C	0.13302	-1.60994	-2.47576
H	-0.70148	-1.50203	-3.17391
H	0.41179	-2.64307	-2.28903
C	1.14787	-0.61584	-2.46573
H	2.17897	-0.84164	-2.19988
C	0.69765	0.72139	-2.57881
H	-0.14932	0.91912	-3.23509
C	1.65112	1.8969	-2.44166
H	2.43771	1.65923	-1.6992
H	1.11032	2.80091	-2.10134
O	1.54377	1.15542	-3.7495

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3023645
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2104688
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.329788687910
ΔG_{solv} = -0.0193036

B'-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -319.59 cm^{-1}
Zero-point correction=   0.368655 (Hartree/Particle)
 Thermal correction to Energy=   0.391384
 Thermal correction to Enthalpy=   0.392328
 Thermal correction to Gibbs Free Energy=   0.313674
 Sum of electronic and zero-point Energies=   -2505.324378
 Sum of electronic and thermal Energies=   -2505.301649
 Sum of electronic and thermal Enthalpies=   -2505.300704
 Sum of electronic and thermal Free Energies=   -2505.379358
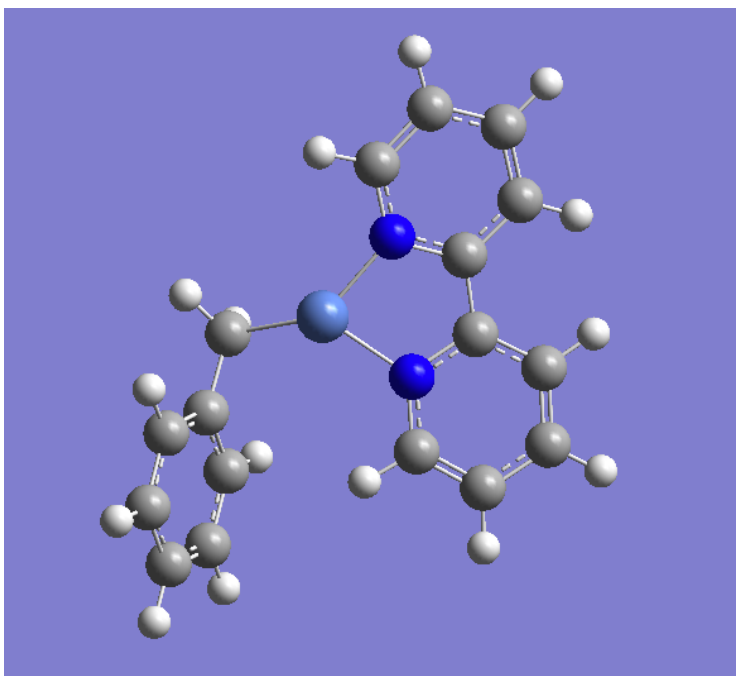C   -1.08408   1.75012   0.69367
 C   1.20805   1.4324   0.92934
 C   1.31986   2.51277   1.79753
 C   0.17173   3.23828   2.11524
 C   -1.04231   2.84826   1.55937

```
C          -2.32473  1.25743  0.05758
C          -3.19768 -0.16329 -1.55011
C          -4.50409  0.21548 -1.25762
C          -4.71089  1.15569 -0.24603
C          -3.60965  1.68102  0.4217
H           2.06897  0.82662  0.67327
H           2.28763  2.77115  2.21412
H           0.21964  4.09302  2.7832
H          -1.94679  3.40226  1.78355
H          -2.98412 -0.89679 -2.32327
H          -5.33434 -0.21716 -1.80642
H          -5.71495  1.47037  0.0227
H          -3.75112  2.39786  1.22303
N           0.04077  1.05826  0.37497
N          -2.13     0.34052 -0.91687
Ni         -0.11549 -0.3651  -0.978
C           1.8752  -3.05474  0.46009
C           3.08711 -3.34317  1.08223
C           3.41955 -2.74473  2.30161
C           2.51274 -1.86055  2.8886
C           1.30057 -1.57219  2.26112
C           0.94589 -2.15456  1.02571
H           1.62974 -3.54356 -0.4801
H           3.77497 -4.04587  0.61733
H           4.36351 -2.97313  2.78918
H           2.74479 -1.39979  3.84657
H           0.59517 -0.89906  2.7439
C          -0.33231 -1.82424  0.35176
H          -1.06937 -1.46494  1.08141
H          -0.74897 -2.69932 -0.15538
C           0.13302 -1.60994 -2.47576
H          -0.70148 -1.50203 -3.17391
H           0.41179 -2.64307 -2.28903
C           1.14787 -0.61584 -2.46573
H           2.17897 -0.84164 -2.19988
C           0.69765  0.72139 -2.57881
H          -0.14932  0.91912 -3.23509
C           1.65112  1.8969  -2.44166
H           2.43771  1.65923 -1.6992
H           1.11032  2.80091 -2.10134
O           1.8641   1.36807 -3.99328
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = - 2505.2857689
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2003958

DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.279192796534
ΔG_{solv} = -0.0390393

A''

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.252481 (Hartree/Particle)
 Thermal correction to Energy=   0.268299
 Thermal correction to Enthalpy=   0.269244
 Thermal correction to Gibbs Free Energy=   0.207211
 Sum of electronic and zero-point Energies=   -2234.523418
 Sum of electronic and thermal Energies=   -2234.507600
 Sum of electronic and thermal Enthalpies=   -2234.506656
 Sum of electronic and thermal Free Energies=   -2234.568688
C   -2.09139 2.31433 0.86226
C   -0.60045 2.29548 2.65039
C   -1.34907 3.2387 3.34487
C   -2.51948 3.72874 2.76326
C   -2.89366 3.25707 1.50751
C   -2.36718 1.74219 -0.47025
C   -1.59   0.23902 -2.07149
C   -2.62395 0.56782 -2.94186
C   -3.56447 1.51936 -2.54539
C   -3.42795 2.11877 -1.29569
H   0.30859 1.87258 3.06297
H   -1.01858 3.57672 4.32156
H   -3.13207 4.46249 3.27829
H   -3.80343 3.61582 1.03871
H   -0.81183 -0.46833 -2.33986
H   -2.68287 0.08483 -3.91175

```
H          -4.38439  1.79863 -3.20026
H          -4.13605  2.87402 -0.97226
N          -0.94936  1.83577  1.43434
N          -1.46337  0.79615 -0.85248
Ni         -0.13439  0.41052  0.46111
C           1.16771 -0.16166  2.17333
H           1.78899  0.70341  1.93011
C           0.53731 -0.90572  1.06587
H           1.44649 -0.66908  2.95621
H           0.37552 -1.85849  1.18485
C           0.99399 -0.57334 -0.36681
C           0.6564  -1.5233  -1.47899
H           1.97313 -0.06313 -0.37557
H           0.75491 -1.18219 -2.52445
H          -0.19424 -2.2159  -1.35341
O           1.79401 -2.7243  -1.61709
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5095924
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
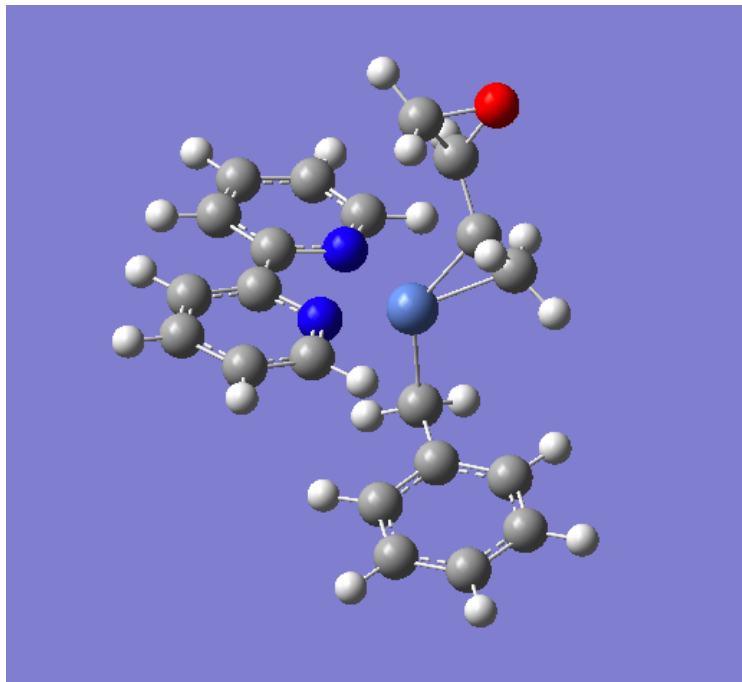HF=-2235.1741033
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.882939502140
ΔG_{solv} = -0.0206952

A''-TS

A''-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -329.39 cm^{-1}
Zero-point correction=   0.251353 (Hartree/Particle)
 Thermal correction to Energy=   0.266957
 Thermal correction to Enthalpy=   0.267901
 Thermal correction to Gibbs Free Energy=   0.207241
 Sum of electronic and zero-point Energies=   -2234.525252
 Sum of electronic and thermal Energies=   -2234.509648
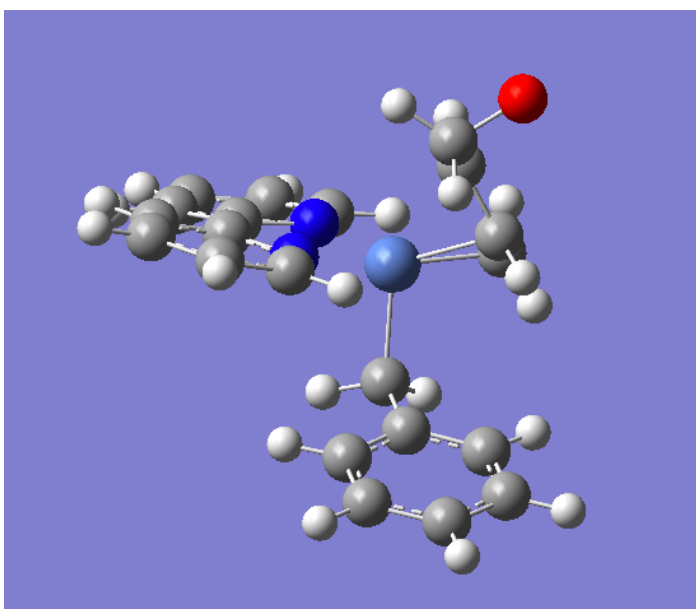 Sum of electronic and thermal Enthalpies=   -2234.508704
 Sum of electronic and thermal Free Energies=   -2234.569364

C	-2.21805	2.2067	1.01322
C	-0.8602	2.24573	2.90975
C	-1.85308	2.85778	3.66243
C	-3.08162	3.13915	3.06051
C	-3.26027	2.80848	1.72103
C	-2.26557	1.84905	-0.4142
C	-1.02128	0.94125	-2.16952
C	-2.06512	1.16928	-3.06505
C	-3.2467	1.7485	-2.60533
C	-3.34417	2.10529	-1.26234
H	0.10485	2.00186	3.33588
H	-1.66162	3.10734	4.70086
H	-3.88259	3.61019	3.62197
H	-4.20318	3.01742	1.2281
H	-0.03147	0.56791	-2.4532
H	-1.93935	0.90042	-4.1089
H	-4.07648	1.9356	-3.28106
H	-4.2424	2.58264	-0.88617
N	-1.02411	1.91274	1.61144
N	-1.12845	1.24983	-0.86255

```
Ni          0.12817  0.87645  0.57706
C           1.17951 -0.03141  1.83021
H           2.04927  0.49458  2.23892
C           1.36142 -0.67741  0.53589
H           0.659   -0.60703  2.5993
H           0.86863 -1.61779  0.2884
C           2.28411 -0.14783 -0.37521
C           2.61845 -0.66706 -1.7188
H           2.77675  0.79031 -0.12996
H           3.04322  0.11678 -2.38177
H           1.76236 -1.1248  -2.25478
O           3.35321 -1.31789 -0.75022
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5046845
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2235.1763672
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.854547783025
ΔG_{solv} = -0.039931

B''

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.251237 (Hartree/Particle)
 Thermal correction to Energy=   0.267198
 Thermal correction to Enthalpy=   0.268142
 Thermal correction to Gibbs Free Energy=   0.207218
 Sum of electronic and zero-point Energies=   -2234.499830
 Sum of electronic and thermal Energies=   -2234.483869
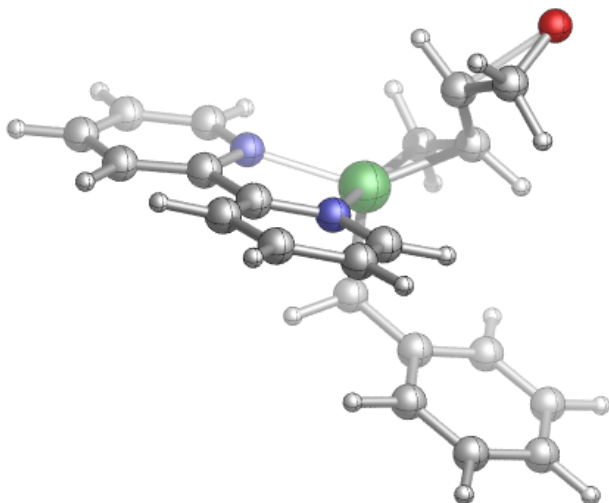 Sum of electronic and thermal Enthalpies=   -2234.482924
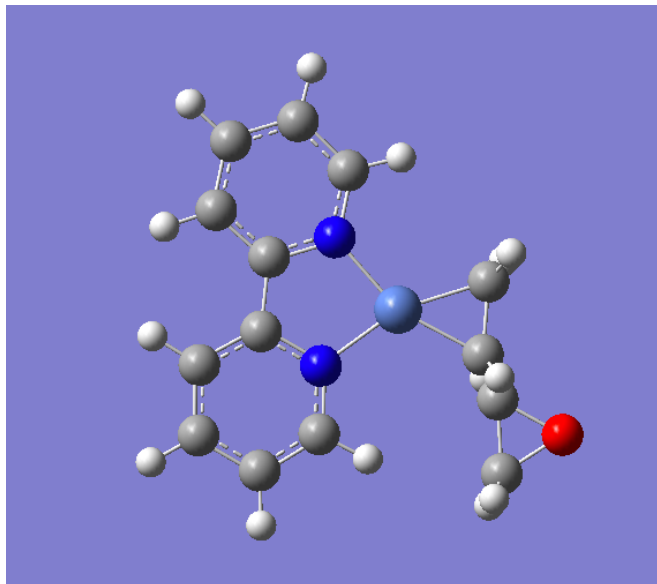
Sum of electronic and thermal Free Energies=   -2234.543848

C	-2.09139	2.31433	0.86226
C	-0.60045	2.29548	2.65039
C	-1.34907	3.2387	3.34487
C	-2.51948	3.72874	2.76326
C	-2.89366	3.25707	1.50751
C	-2.36718	1.74219	-0.47025
C	-1.59	0.23902	-2.07149
C	-2.62395	0.56782	-2.94186
C	-3.56447	1.51936	-2.54539
C	-3.42795	2.11877	-1.29569
H	0.30859	1.87258	3.06297
H	-1.01858	3.57672	4.32156
H	-3.13207	4.46249	3.27829
H	-3.80343	3.61582	1.03871
H	-0.81183	-0.46833	-2.33986
H	-2.68287	0.08483	-3.91175
H	-4.38439	1.79863	-3.20026
H	-4.13605	2.87402	-0.97226
N	-0.94936	1.83577	1.43434
N	-1.46337	0.79615	-0.85248
Ni	-0.13439	0.41052	0.46111
C	0.64814	-1.55952	1.45703
H	1.1168	-1.12328	2.34221
C	0.81569	-0.87001	0.16319
H	0.59959	-2.53195	1.44665
H	0.81451	-1.40784	-0.64849
C	1.84279	0.27536	0.09394
C	2.30199	0.76325	-1.24936
H	2.57003	0.22277	0.92308
H	2.83311	1.72887	-1.31668
H	1.66266	0.58597	-2.13189
O	3.57617	-0.13594	-1.81814

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5213308
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = - 2235.1929384
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.8431

ΔG_{solv} = -0.0624885

B''-C-TS

B''-C-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -118.30 cm^{-1}
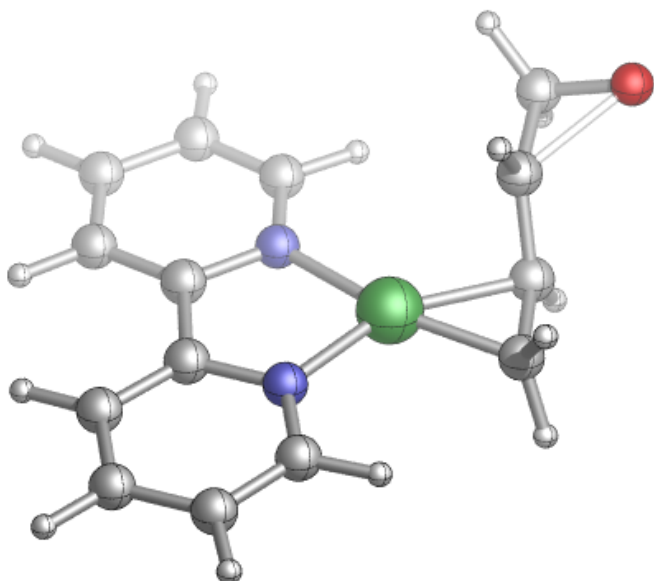Zero-point correction=   0.366489 (Hartree/Particle)
 Thermal correction to Energy=   0.389629
 Thermal correction to Enthalpy=   0.390573
 Thermal correction to Gibbs Free Energy=   0.309400
 Sum of electronic and zero-point Energies=   -2505.299540
 Sum of electronic and thermal Energies=   -2505.276400

Sum of electronic and thermal Enthalpies=   -2505.275456
Sum of electronic and thermal Free Energies=   -2505.356629

```
C        -1.6496   1.2818   1.34746
C         0.6055   1.81183  1.79102
C         0.26003  2.60437  2.89104
C        -1.10348  2.7151   3.24415
C        -2.05844  2.04413  2.46607
C        -2.5476   0.57738  0.44555
C        -2.6721  -0.94304 -1.35147
C        -4.07159 -0.88506 -1.37573
C        -4.72984 -0.05014 -0.44806
C        -3.95693  0.68734  0.46427
H         1.64164  1.68806  1.49557
H         1.03494  3.11664  3.45248
H        -1.4086   3.30577  4.10355
H        -3.11074  2.10083  2.72524
H        -2.13205 -1.57032 -2.04963
H        -4.62223 -1.47773 -2.09914
H        -5.81371  0.02789 -0.44136
H        -4.43693  1.3528   1.17458
N        -0.31562  1.15801  1.01642
N        -1.90476 -0.2391  -0.46238
Ni        0.01751 -0.13324 -0.34789
C         1.56911 -3.00405  1.49008
C         2.95027 -3.02211  1.61029
C         3.61524 -2.01623  2.32751
C         2.87324 -0.98619  2.92492
C         1.49182 -0.95578  2.80895
C         0.79031 -1.96584  2.08432
H         1.05923 -3.78806  0.93559
H         3.52074 -3.82184  1.14543
H         4.69728 -2.03556  2.41998
H         3.38443 -0.20695  3.48482
H         0.92196 -0.15344  3.27132
C        -0.61159 -1.94001  1.96292
H        -1.19995 -1.14607  2.41279
H        -1.14303 -2.71192  1.41599
C         1.9537  -0.27448 -0.22614
H         2.40663  0.58352 -0.72956
H         2.41666 -0.52918  0.72549
C         1.43789 -1.33452 -1.01819
H         1.41227 -2.35578 -0.63945
C         0.64903 -0.99034 -2.12941
H         0.9012  -0.06924 -2.66265
C         0.05869 -2.0586  -3.03744
H        -0.83786 -1.65833 -3.56619
```

H   -0.2854 -2.91871 -2.41372
O   1.1063 -2.31999 -3.85428
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2944336
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.2038158
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.253379015522
ΔG_{solv} = -0.0613693

C

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.368972 (Hartree/Particle)
 Thermal correction to Energy=   0.391340
 Thermal correction to Enthalpy=   0.392284
 Thermal correction to Gibbs Free Energy=   0.316297
 Sum of electronic and zero-point Energies=   -2505.338240
 Sum of electronic and thermal Energies=   -2505.315872
 Sum of electronic and thermal Enthalpies=   -2505.314928
 Sum of electronic and thermal Free Energies=   -2505.390915
C   -1.52959 -0.2832   2.37299
 C   0.66317   0.22089   2.98422
 C   0.26326   0.6746   4.23412
 C   -1.09331   0.63081   4.5604
 C   -1.99563   0.15047   3.61794
 C   -2.38927 -0.76001   1.2763
 C   -2.42354 -1.34748 -0.98999
 C   -3.81004 -1.52569 -0.93487
 C   -4.48983 -1.33293   0.26276
 C   -3.76889 -0.93058   1.38643
 H   1.70519   0.22769   2.68906
 H   1.00324   1.05034   4.93263

H	-1.44332	0.97224	5.52985
H	-3.05566	0.12324	3.8418
H	-1.82853	-1.35462	-1.94374
H	-4.33707	-1.81067	-1.84006
H	-5.56482	-1.47727	0.32793
H	-4.27553	-0.7549	2.3289
N	-0.20238	-0.25756	2.06901
N	-1.72559	-0.99121	0.10966
Ni	0.23847	-0.93697	0.33881
C	1.67633	1.50578	-2.73846
C	2.84579	2.028	-3.27364
C	3.62099	2.94076	-2.54419
C	3.21083	3.33156	-1.26172
C	2.04348	2.81837	-0.71381
C	1.24056	1.89302	-1.43653
H	1.06449	0.78834	-3.28509
H	3.1614	1.72688	-4.26954
H	4.53515	3.34542	-2.97039
H	3.80754	4.04302	-0.69574
H	1.72245	3.13122	0.27806
C	0.03438	1.35819	-0.9123
H	-0.40418	1.79883	-0.02053
H	-0.58769	0.76477	-1.57417
C	2.01628	-1.61358	0.74633
H	2.78574	-0.88668	0.47812
H	2.16834	-2.07883	1.72067
C	1.43097	-2.39603	-0.29719
H	1.03997	-3.39597	-0.10548
C	1.05503	-1.69432	-1.44099
H	1.63983	-0.81184	-1.69559
C	0.15883	-2.14958	-2.5765
H	-0.45509	-3.01103	-2.18333
H	0.81979	-2.6249	-3.34577
O	-0.57159	-1.09859	-3.03637

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3019133
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2165871
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.305941489868
ΔG_{solv} = -0.0344223

P_L

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.372785 (Hartree/Particle)
 Thermal correction to Energy=   0.395870
 Thermal correction to Enthalpy=   0.396814
 Thermal correction to Gibbs Free Energy=   0.313731
 Sum of electronic and zero-point Energies=   -2505.410880
 Sum of electronic and thermal Energies=   -2505.387795
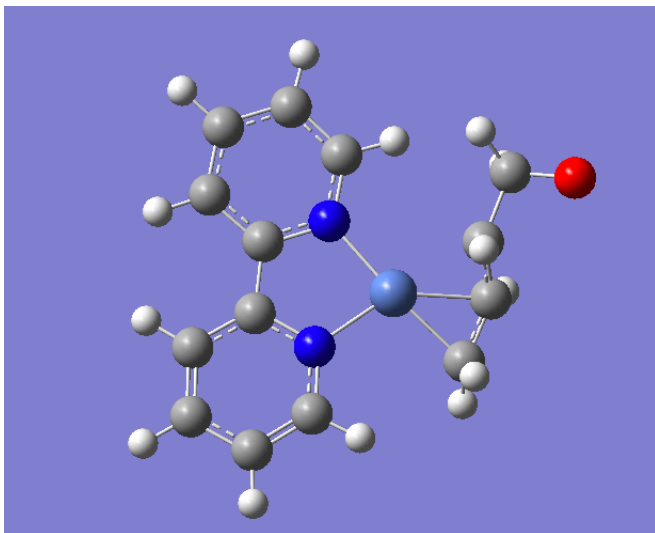 Sum of electronic and thermal Enthalpies=   -2505.386851
 Sum of electronic and thermal Free Energies=   -2505.469934
C   -3.28798   0.69913   0.35567
 C   -1.16957   0.00449   1.11144
 C   -1.61602 -0.10808   2.40753
 C   -2.96357   0.20076   2.70018
 C   -3.78778   0.60128   1.66201
 C   -4.06488   1.09337 -0.80647
 C   -3.94302   1.43252 -3.12511
 C   -5.27897   1.79434 -3.19524
 C   -6.03125   1.80196 -2.00734
 C   -5.42591   1.4509   -0.81182
 H   -0.14174 -0.22577   0.84886
 H   -0.93096 -0.43071   3.18486
 H   -3.34539   0.12329   3.71305
 H   -4.82893   0.83974   1.85454
 H   -3.29515   1.39766 -3.99607
 H   -5.72353   2.06298 -4.14756
 H   -7.08123   2.08033 -2.02368
 H   -5.99583   1.45223   0.11118
 N   -1.95981   0.405   0.07329
 N   -3.34871   1.09122 -1.96925
 Ni   -1.47546   0.57395 -1.72361

```
C          4.32524  0.11979   2.60261
C          4.98306 -0.41393   3.7086
C          5.16384 -1.79537   3.81703
C          4.67972 -2.62793   2.80987
C          4.01826 -2.0875    1.70303
C          3.82921 -0.7057    1.58072
H          4.19279  1.19742   2.52527
H          5.35865  0.24816   4.48476
H          5.67891 -2.21542   4.67684
H          4.81574 -3.70424   2.87985
H          3.65257 -2.75756   0.93098
C          3.10101 -0.0677    0.408
H          2.15091  0.35661   0.76544
H          3.68554  0.79635   0.06206
C          2.81071 -0.9796   -0.79727
H          2.1725  -1.82074  -0.49802
H          3.76114 -1.41612  -1.14112
C          2.16186 -0.2407   -1.93665
H          2.68558  0.65354  -2.28362
C          1.03111 -0.59687  -2.56021
H          0.50009 -1.49888  -2.24204
C          0.40375  0.14923  -3.71332
H          0.37852 -0.51522  -4.59707
H          1.05237  1.00112  -3.98582
O         -0.8974   0.58068  -3.41635
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3541091
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
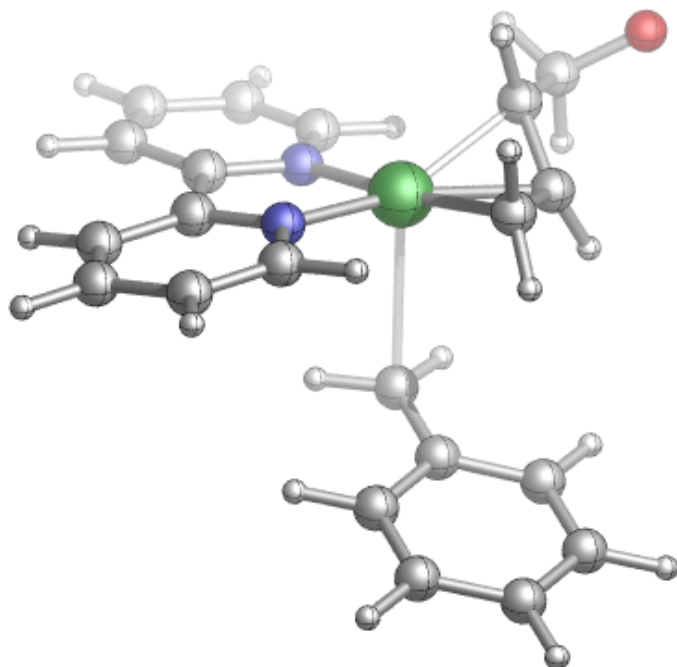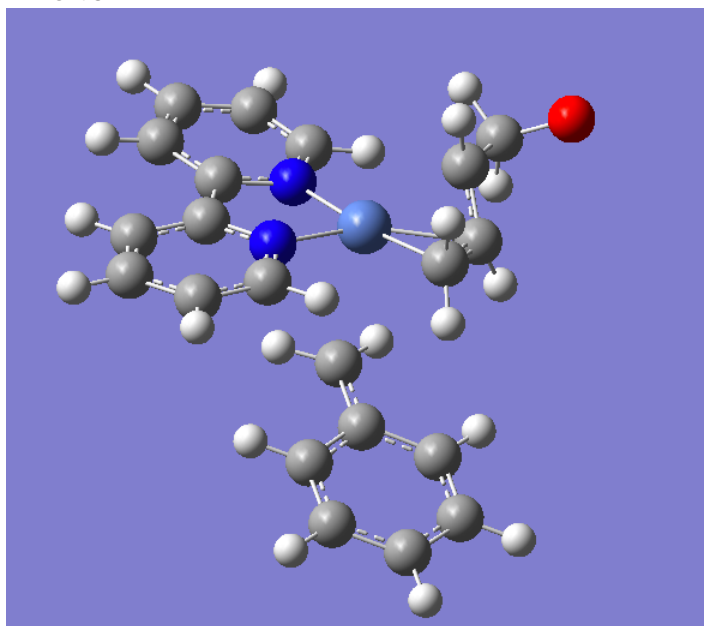HF = -2506.2673435
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.370430155434
ΔG_{solv} = -0.0228725

P_B

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.372712 (Hartree/Particle)
 Thermal correction to Energy=   0.395587
 Thermal correction to Enthalpy=   0.396532
 Thermal correction to Gibbs Free Energy=   0.315690
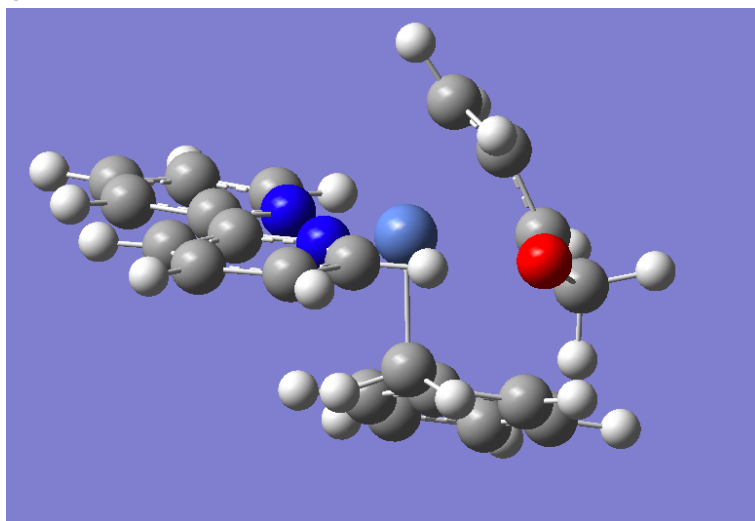 Sum of electronic and zero-point Energies=   -2505.407982
 Sum of electronic and thermal Energies=   -2505.385106
 Sum of electronic and thermal Enthalpies=   -2505.384162
 Sum of electronic and thermal Free Energies=   -2505.465003
C   -2.41018 2.09416 0.98134
C   -0.09   2.17185 1.33364
C   -0.23051 3.07095 2.36716
C   -1.52122 3.51683 2.7207
C   -2.60513 3.01675 2.01818
C   -3.4742   1.49055 0.19483
C   -3.89665 -0.035   -1.53483
C   -5.26562 0.15896 -1.44199
C   -5.74773 1.06623 -0.48293
C   -4.85168 1.73491 0.33606
H   0.88945 1.80428 1.04487
H   0.65011 3.42211 2.89514
H   -1.66351 4.23099 3.52539
H   -3.61165 3.33352 2.27147
H   -3.4462 -0.70864 -2.25771
H   -5.93953 -0.37715 -2.10171
H   -6.81446 1.24453 -0.38165
H   -5.21028 2.43969 1.07855
N   -1.13976 1.67576 0.61941
N   -3.02286 0.60308 -0.73711
Ni   -1.06424 0.50169 -0.8477

```
C          3.45124 -0.36794  1.19085
C          4.15827 -0.9004   2.27103
C          3.85671 -2.1775   2.7428
C          2.84408 -2.91445  2.12387
C          2.13957 -2.37647  1.04798
C          2.42784 -1.09091  0.56417
H          3.70171  0.62575  0.82384
H          4.94722 -0.31663  2.73859
H          4.40536 -2.59662  3.58204
H          2.60094 -3.91194  2.48125
H          1.3504  -2.95983  0.58061
C          1.62848 -0.49347 -0.57212
H          0.59864 -0.33189 -0.19755
H          2.02851  0.4982  -0.84001
C          3.29349 -2.70162 -2.98112
H          2.72396 -3.62272 -2.87313
H          4.24954 -2.78009 -3.49182
C          2.84   -1.53912 -2.51171
H          3.44924 -0.64245 -2.64622
C          1.50648 -1.33015 -1.84771
H          1.08403 -2.3102  -1.58617
C          0.51284 -0.67457 -2.86298
H          0.43051 -1.37577 -3.70942
H          0.99454  0.23825 -3.26706
O         -0.75773 -0.4035  -2.36115
```

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3533175
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.2656535
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.372425835385
ΔG_{solv} = -0.0221931

C-TS$_B$

C-TS_B

UB3LYP/6-31g(d)-gas
Imaginary frequency = -229.10 cm^{-1}
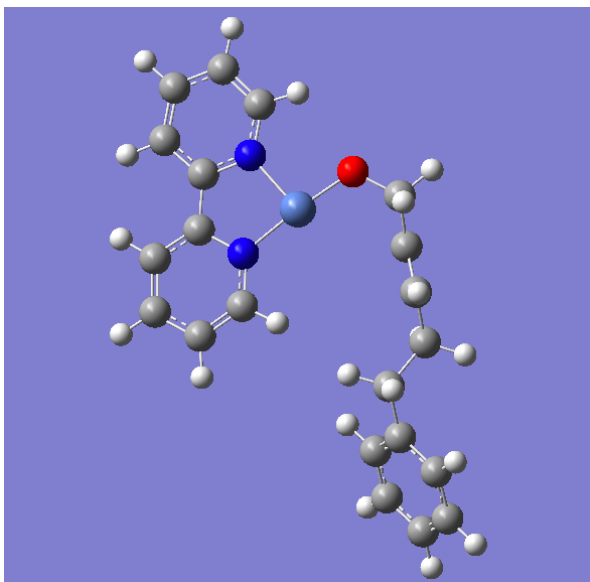Zero-point correction=   0.369235 (Hartree/Particle)
 Thermal correction to Energy=   0.391133
 Thermal correction to Enthalpy=   0.392077
 Thermal correction to Gibbs Free Energy=   0.317630
 Sum of electronic and zero-point Energies=   -2505.303251
 Sum of electronic and thermal Energies=   -2505.281353
 Sum of electronic and thermal Enthalpies=   -2505.280409
 Sum of electronic and thermal Free Energies=   -2505.354856
C   -2.42248 1.29717 1.28299
 C   -0.74205 2.83838 0.79219
 C   -1.17536 3.6922   1.80077
 C   -2.27472 3.31918 2.57813
 C   -2.90506 2.10663 2.31821
 C   -3.0098 -0.00289 0.89711
 C   -2.82347 -1.84296 -0.50009
 C   -3.94979 -2.44874 0.04583
 C   -4.63322 -1.77807 1.06156
 C   -4.15819 -0.54446 1.49058

S65

H	0.10881	3.04021	0.14631
H	-0.65703	4.62993	1.9733
H	-2.63439	3.96122	3.37697
H	-3.75519	1.79629	2.91556
H	-2.26142	-2.32612	-1.29386
H	-4.27943	-3.41649	-0.31768
H	-5.52195	-2.20962	1.51267
H	-4.67711	-0.00622	2.27559
N	-1.35508	1.66711	0.53837
N	-2.35576	-0.65286	-0.09711
Ni	-0.73209	0.46974	-0.93473
C	0.71124	-0.36628	-2.34619
H	1.27783	-1.26669	-2.57809
C	-0.6519	-0.32698	-2.82883
H	-1.13914	-1.29055	-2.98511
C	-1.4373	0.82503	-2.91038
H	-0.99629	1.80771	-3.0314
C	0.73307	-1.07707	-0.27135
H	1.36769	-1.87508	-0.66447
C	0.42133	-1.3514	1.14457
C	0.10659	-2.65276	1.58219
C	0.43527	-0.32517	2.10671
C	-0.16649	-2.91424	2.922
H	0.04502	-3.44979	0.84642
C	0.16198	-0.5857	3.44963
H	0.6829	0.68852	1.7965
C	-0.13812	-1.88326	3.8663
H	-0.40826	-3.92806	3.23236
H	0.18908	0.22686	4.17196
H	-0.34954	-2.08982	4.91221
H	1.24062	-0.12182	-0.41524
C	1.45577	0.95783	-2.23765
H	-2.47208	0.71387	-3.22633
H	1.51421	1.41437	-3.2036
O	2.69285	0.73781	-1.77201
H	0.9326	1.60728	-1.56727

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2794819
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.1862011
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.286377222440
ΔG_{solv} = -0.0366925

CH-TS$_B$
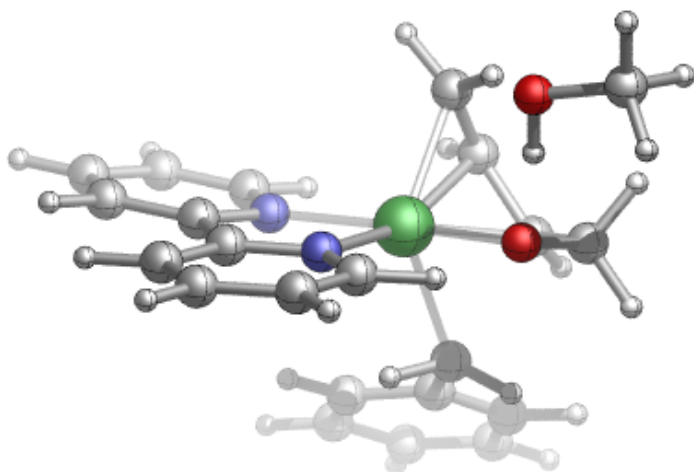
CH-TS$_B$
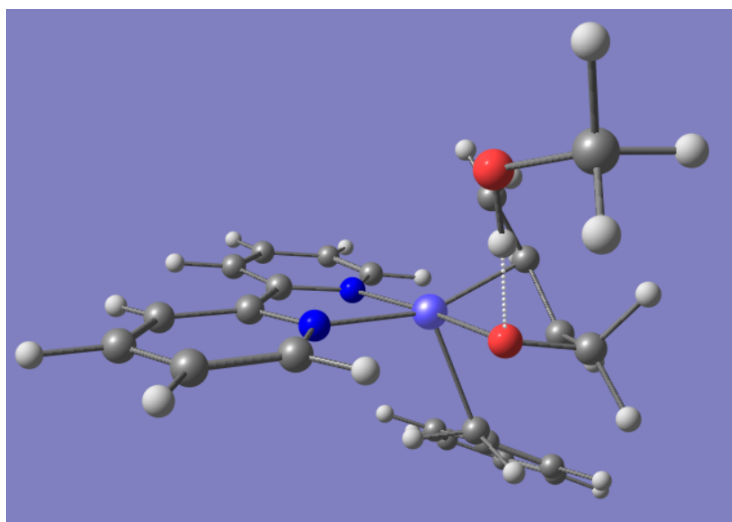
UB3LYP/6-31g(d)-gas
Imaginary frequency = -348.32 cm^{-1}
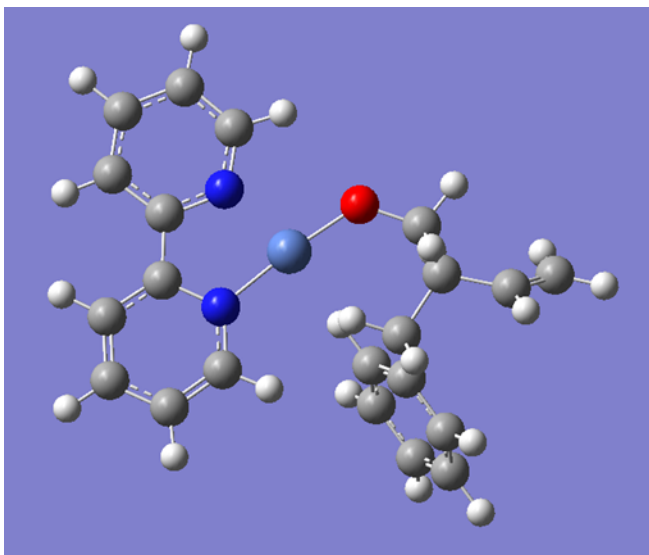Zero-point correction=   0.424888 (Hartree/Particle)
 Thermal correction to Energy=   0.451155
 Thermal correction to Enthalpy=   0.452100
 Thermal correction to Gibbs Free Energy=   0.365281
 Sum of electronic and zero-point Energies=   -2621.033104
 Sum of electronic and thermal Energies=   -2621.006837
 Sum of electronic and thermal Enthalpies=   -2621.005893
 Sum of electronic and thermal Free Energies=   -2621.092711
 C   -0.82961 1.94453 1.64199
 C   1.29757 2.77275 1.20205
 C   1.22882 3.63829 2.29222
 C   0.08009 3.64579 3.07632
 C   -0.96459 2.78253 2.75006

```
C        -1.87408  0.9869   1.20161
C        -2.42957 -0.67735 -0.32054
C        -3.68697 -0.85522  0.24536
C        -4.04097 -0.06219  1.33454
C        -3.12467  0.86818  1.81586
H         2.16266  2.72675  0.55497
H         2.0688   4.2911   2.50308
H        -0.00715  4.30966  3.9313
H        -1.86452  2.76634  3.35405
H        -2.10849 -1.26954 -1.17115
H        -4.3655  -1.59731 -0.16186
H        -5.01532 -0.16323  1.80301
H        -3.38498  1.49947  2.65716
N         0.28811  1.9493   0.87837
N        -1.53882  0.21711  0.13816
Ni        0.24251  0.708   -0.71581
C         1.4421  -0.25802 -2.27185
H         1.67408 -1.27777 -2.57048
C         0.11912  0.17135 -2.67413
H        -0.58201 -0.62343 -2.9321
C        -0.35372  1.4863  -2.56958
H         0.32097  2.33353 -2.62301
C         1.7393  -0.84824 -0.1736
H         2.7823  -0.58143 -0.30842
C         1.47856 -2.30476 -0.14991
C         2.34968 -3.20828 -0.79034
C         0.35758 -2.84613  0.50885
C         2.11295 -4.5819  -0.77385
H         3.23506 -2.82238 -1.29118
C         0.11769 -4.21907  0.52642
H        -0.32464 -2.17749  1.02845
C         0.99284 -5.09673 -0.11789
H         2.80973 -5.25317 -1.2697
H        -0.75214 -4.60685  1.05162
H         0.80838 -6.16742 -0.10235
H         1.41649 -0.40052  0.77103
C         2.50616  0.81155 -2.29862
O         2.10117  1.68633 -1.27629
H        -1.38763  1.68791 -2.84052
H         2.51146  1.31288 -3.28034
H         3.51704  0.40237 -2.13708
H         4.57391  3.71551 -1.07058
C         3.65336  4.35414 -1.05648
O         2.61851  3.91522 -1.84418
H         4.00005  5.36201 -1.36589
H         2.36024  2.80252 -1.56068
```

H   3.41776   4.47063   0.04056

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2621.007
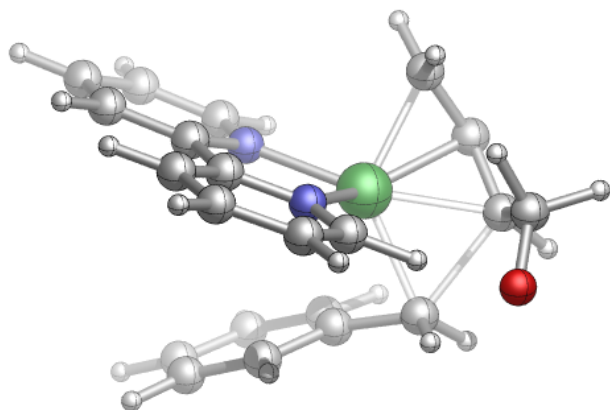
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2621.9977

DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas

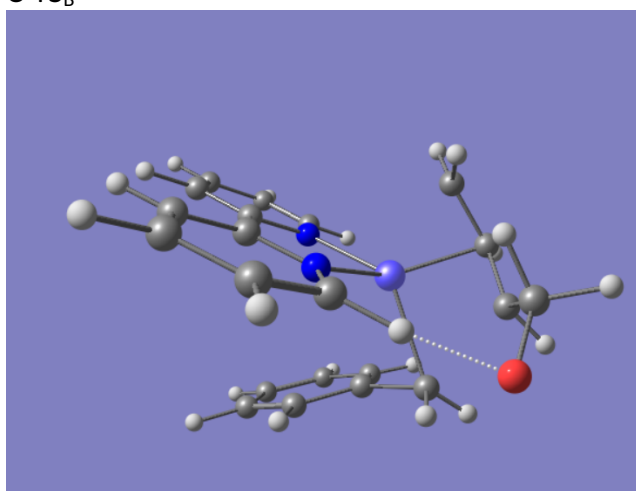HF = -2618.9044

ΔG_{solv} = -0.0229495

C-TS$_L$

C-TS$_L$

UB3LYP/6-31g(d)-gas

Imaginary frequency = -293.16 cm^{-1}

Zero-point correction=		0.368710 (Hartree/Particle)
Thermal correction to Energy=		0.390876
Thermal correction to Enthalpy=		0.391820
Thermal correction to Gibbs Free Energy=		0.316349
Sum of electronic and zero-point Energies=		-2505.302047
Sum of electronic and thermal Energies=		-2505.279881
Sum of electronic and thermal Enthalpies=		-2505.278937
Sum of electronic and thermal Free Energies=		-2505.354409

C	-1.5686	2.18377	1.56507
C	0.48993	3.16267	1.12464
C	0.24254	4.21694	1.99655
C	-0.97821	4.24194	2.6723
C	-1.89019	3.214	2.45568
C	-2.45577	1.03657	1.26535
C	-2.79101	-0.78066	-0.17297
C	-3.99554	-1.0848	0.46584
C	-4.4183	-0.31677	1.5476
C	-3.64613	0.77361	1.9441
H	1.42902	3.09501	0.58206
H	0.98586	4.99473	2.13694
H	-1.21627	5.04881	3.35906
H	-2.84452	3.21489	2.96958
H	-2.42244	-1.27389	-1.11724
H	-4.59119	-1.91573	0.10044
H	-5.34461	-0.54507	2.06815
H	-3.9669	1.39915	2.76996
N	-0.38662	2.17274	0.90088
N	-2.02951	0.24881	0.25039
Ni	-0.19004	0.6344	-0.41963

```
C          1.59975  0.86222 -1.53699
H          1.61552  1.9527  -1.44818
H          2.60094  0.49015 -1.74143
C          0.50411  0.2676  -2.30966
H          0.54351 -0.80218 -2.52213
C         -0.71548  0.86697 -2.56437
H         -0.81131  1.95671 -2.60589
C         -1.84257 -0.02524 -3.10219
H         -1.89372  0.22259 -4.20024
C          1.80391 -0.08757  0.1788
H          2.69434  0.47818  0.45657
H         -2.79166  0.44454 -2.70441
O         -1.66998 -1.32226 -2.81474
C          1.04653 -0.51513  1.40651
C          1.2531   0.0947   2.65814
C          0.19528 -1.64314  1.35905
C          0.60039 -0.36669  3.79975
H          1.93922  0.93537  2.73278
C         -0.46137 -2.09845  2.49761
H          0.04266 -2.15173  0.40924
C         -0.2679  -1.45926  3.7263
H          0.78171  0.12025  4.75502
H         -1.11869 -2.9614   2.42837
H         -0.77126 -1.82063  4.61886
H          2.0981  -0.97851 -0.37641
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.287780
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.1928851
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas

HF = -2503.284994203000
ΔG_{solv} = -0.0445728

CH-TS$_L$

UB3LYP/6-31g(d)-gas

Imaginary frequency = -287.04 cm^{-1}

Zero-point correction=   0.423290 (Hartree/Particle)

 Thermal correction to Energy=   0.449618

 Thermal correction to Enthalpy=   0.450562

 Thermal correction to Gibbs Free Energy=   0.365002

 Sum of electronic and zero-point Energies=   -2620.999177

 Sum of electronic and thermal Energies=   -2620.972849

 Sum of electronic and thermal Enthalpies=   -2620.971905

 Sum of electronic and thermal Free Energies=   -2621.057465

C	-0.7467	1.87713	0.88217
C	1.30271	2.79721	0.30286
C	1.09197	3.9204	1.09392
C	-0.10202	4.00889	1.8107
C	-1.02787	2.97753	1.70112
C	-1.67356	0.74229	0.68273
C	-2.00786	-1.25839	-0.48594
C	-3.26643	-1.4135	0.10074
C	-3.72785	-0.46078	1.004
C	-2.92541	0.64174	1.29295
H	2.21954	2.68646	-0.26828
H	1.8444	4.70059	1.14287
H	-0.30958	4.86713	2.44287
H	-1.96248	3.02845	2.24741
H	-1.59112	-1.93222	-1.27596
H	-3.87313	-2.27225	-0.16897
H	-4.70465	-0.55881	1.47012
H	-3.27511	1.40581	1.97809
N	0.41838	1.79304	0.19053
N	-1.22708	-0.20407	-0.17647
Ni	0.63481	0.04174	-0.88489
C	2.27372	0.4421	-2.17851
H	2.10262	1.52138	-2.19932

```
H           3.31074  0.22226 -2.41555
C           1.26077 -0.39369 -2.80483
H           1.45318 -1.45955 -2.92274
C          -0.03166  0.00455 -3.04031
H          -0.27693  1.06374 -3.16456
C          -1.07361 -1.07397 -3.37052
H          -1.16439 -1.05431 -4.49359
C           2.66877 -0.31479 -0.29355
H           3.16367  0.52236  0.19969
H          -2.05762 -0.61964 -3.04034
C           1.82646 -1.13329  0.62883
C           1.578   -0.73255  1.96286
C           1.34201 -2.39476  0.21334
C           0.84006 -1.53503  2.82364
H           1.97683  0.2165   2.31342
C           0.58807 -3.18757  1.0802
H           1.54273 -2.74972 -0.79271
C           0.33178 -2.76496  2.38383
H           0.66817 -1.2101   3.847
H           0.2088  -4.14304  0.72906
H          -0.24546 -3.39005  3.05967
H           3.40644 -0.95616 -0.76933
H           0.7184  -6.56556 -1.47765
O          -0.0874  -4.79406 -2.26315
O          -0.8563  -2.42246 -2.86325
C           0.5812  -5.97316 -2.42125
H          -0.6177  -3.30446 -3.23375
H           0.0905  -6.69176 -3.12195
H           1.6238  -5.85936 -2.82855
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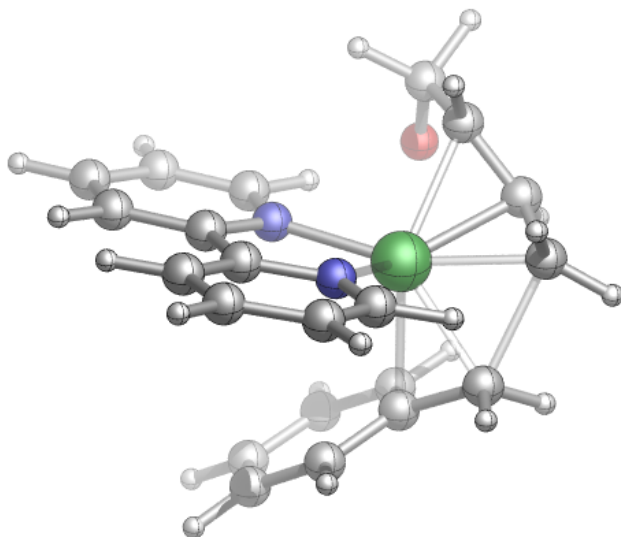UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2620.9982

UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2621.9847

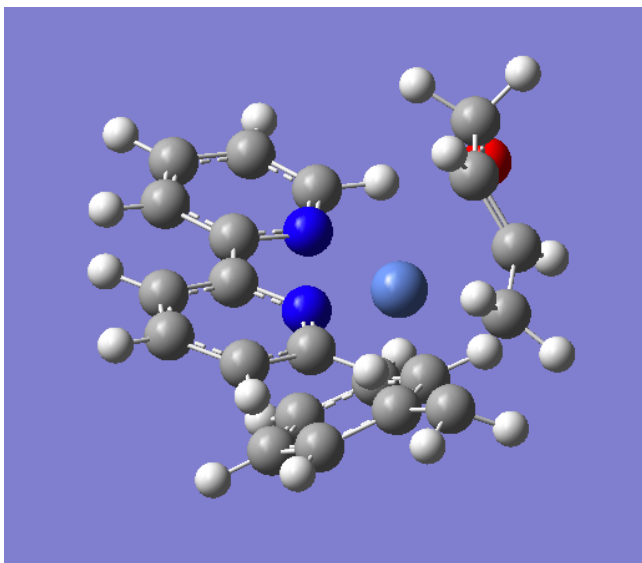DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas

HF = -2618.8747

ΔG_{solv} = -0.0340259

B''-TSL

B''-TSL

UB3LYP/6-31g(d)-gas
Imaginary frequency = -636.59 cm^{-1}
Zero-point correction=   0.365804 (Hartree/Particle)
 Thermal correction to Energy=   0.388564
 Thermal correction to Enthalpy=   0.389508
 Thermal correction to Gibbs Free Energy=   0.310314
 Sum of electronic and zero-point Energies=   -2505.299320
 Sum of electronic and thermal Energies=   -2505.276559
 Sum of electronic and thermal Enthalpies=   -2505.275615
 Sum of electronic and thermal Free Energies=   -2505.354809
C   -0.92081 0.98226 2.85884
 C   0.67014 2.31217 1.794
 C   0.47953 3.35274 2.69422
 C   -0.45476 3.1855 3.71796
 C   -1.15798 1.98782 3.79956
 C   -1.5887 -0.3339 2.85009
 C   -1.72129 -2.37911 1.70945
 C   -2.60446 -2.87359 2.6738
 C   -2.98004 -2.07177 3.74791

```
C          -2.46364 -0.77945  3.84019
H           1.38905  2.39112  0.98607
H           1.05273  4.26801  2.59223
H          -0.63389  3.97557  4.44093
H          -1.89076  1.83878  4.58437
H          -1.33493 -2.98137  0.84436
H          -2.98485 -3.8845   2.56672
H          -3.65853 -2.44172  4.51178
H          -2.72919 -0.1412   4.6758
N          -0.00759  1.15114  1.86035
N          -1.23443 -1.12306  1.80007
Ni          0.04227 -0.29963  0.59114
C           1.83921 -0.03604 -0.58031
H           1.571    0.90726 -1.04641
H           2.68603 -0.02865  0.09911
C           1.08032 -1.2273  -0.79853
H           1.43511 -2.2025  -0.46333
C          -0.23453 -1.18673 -1.25843
H          -0.58624 -0.31939 -1.83027
C          -1.03659 -2.48073 -1.36483
H          -1.07585 -2.68547 -2.47363
C           3.20106 -0.11228 -2.04303
H           3.36256 -1.17159 -1.87679
H          -2.10453 -2.16932 -1.14588
O          -0.57116 -3.48718 -0.62193
C           2.52945  0.31832 -3.23213
C           1.74914 -0.58196 -4.00078
C           2.58448  1.66945 -3.65929
C           1.06791 -0.15095 -5.13345
H           1.68558 -1.62149 -3.69098
C           1.90408  2.09253 -4.79435
H           3.18104  2.37834 -3.08843
C           1.1401   1.18622 -5.5396
H           0.47627 -0.86082 -5.70572
H           1.96966  3.13213 -5.10621
H           0.60908  1.51847 -6.4274
H           3.91701  0.55573 -1.57185
```

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2737072
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1837374
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.267387295916
ΔG_{solv} = -0.0452782

BH-TSL

BH-TSL
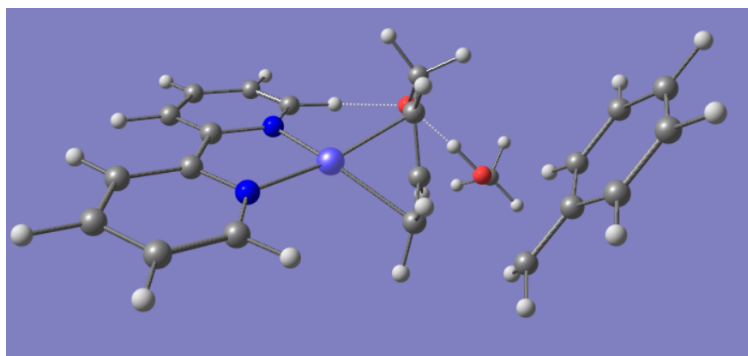
UB3LYP/6-31g(d)-gas

Imaginary frequency = 619.59 cm^{-1}

Zero-point correction=   0.420604 (Hartree/Particle)
 Thermal correction to Energy=   0.447585
 Thermal correction to Enthalpy=   0.448530
 Thermal correction to Gibbs Free Energy=   0.359079
 Sum of electronic and zero-point Energies=   -2620.993664
 Sum of electronic and thermal Energies=   -2620.966683
 Sum of electronic and thermal Enthalpies=   -2620.965739
 Sum of electronic and thermal Free Energies=   -2621.055190
C   -1.126   1.59829 3.24424
 C   0.63832 2.93524 2.49797
 C   0.3049   3.95845 3.37295
 C   -0.80369 3.78481 4.21287
 C   -1.51951 2.5956   4.14501
 C   -1.77827 0.29144 3.10729
 C   -1.69937 -1.75898 1.97797
 C   -2.71252 -2.28077 2.78111
 C   -3.28573 -1.47021 3.76335
 C   -2.80447 -0.17511 3.93525

```
H          1.48883  3.02669  1.83108
H          0.899    4.86555  3.39524
H         -1.09945  4.56601  4.90799
H         -2.38231  2.44077  4.78374
H         -1.1858  -2.35783  1.22191
H         -3.03466 -3.30608  2.63023
H         -4.08284 -1.84731  4.39869
H         -3.21062  0.45783  4.71629
N         -0.04941  1.77845  2.41615
N         -1.25948 -0.49182  2.1152
Ni         0.13765  0.37266  1.09642
C          1.84503  1.0602  -0.07536
H          1.32233  1.94318 -0.43164
H          2.70009  1.21842  0.57513
C          1.3538  -0.2518  -0.32865
H          1.94524 -1.12602 -0.06533
C          0.03523 -0.44104 -0.75688
H         -0.46248  0.38259 -1.28232
C         -0.51307 -1.80804 -1.06598
H         -0.3117  -2.02233 -2.13257
C          3.27408  1.47438 -1.86464
H          3.93114  0.64801 -1.60712
H         -1.62055 -1.78199 -0.97876
O          0.0685  -2.7562  -0.22666
C          2.469    1.38377 -3.04951
C          2.23277  0.12992 -3.67333
C          1.84585  2.52873 -3.61163
C          1.42337  0.03148 -4.80104
H          2.69707 -0.76437 -3.26041
C          1.03989  2.42532 -4.74045
H          2.01541  3.50305 -3.15265
C          0.82275  1.17618 -5.34294
H          1.25962 -0.94158 -5.26115
H          0.57977  3.31852 -5.15929
H          0.19206  1.09798 -6.2251
H          3.59126  2.45445 -1.51331
H          0.07136 -3.66199 -0.73709
H         -0.84    -6.70154 -0.85571
C         -1.0556  -5.64312 -1.1517
O          0.07536 -4.92419 -1.44835
H         -1.7696  -5.7243  -2.01473
H         -1.65254 -5.21138 -0.31179
```
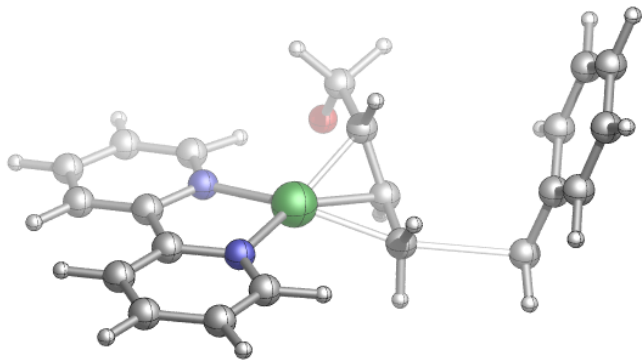UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2620.986

UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
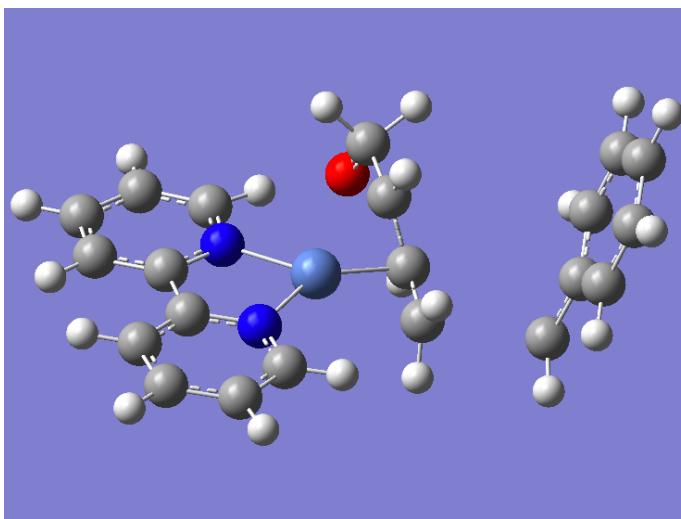HF= -2621.9764

DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2618.8572

ΔG_{solv} = -0.0368533

B-TSB

B-TSB

UB3LYP/6-31g(d)-gas
Imaginary frequency = -469.64 cm^{-1}
Zero-point correction=   0.367811 (Hartree/Particle)
 Thermal correction to Energy=   0.390034
 Thermal correction to Enthalpy=   0.390978
 Thermal correction to Gibbs Free Energy=   0.313856
 Sum of electronic and zero-point Energies=   -2505.299873
 Sum of electronic and thermal Energies=   -2505.277651
 Sum of electronic and thermal Enthalpies=   -2505.276707

Sum of electronic and thermal Free Energies=   -2505.353829

C	-1.80936	0.7111	2.99187
C	-1.90017	1.86364	0.95515
C	-2.54453	2.93768	1.57502
C	-2.8104	2.89256	2.94046
C	-2.43832	1.75954	3.66263
C	-1.44326	-0.57421	3.61927
C	-0.64935	-2.72612	3.19952
C	-0.75578	-3.07952	4.53942
C	-1.22673	-2.12901	5.44609
C	-1.5761	-0.86538	4.97888
H	-1.68401	1.84452	-0.13999
H	-2.82344	3.79752	0.97445
H	-3.30753	3.71876	3.44117
H	-2.65075	1.69117	4.72384
H	-0.29552	-3.42657	2.45206
H	-0.47626	-4.07793	4.85854
H	-1.32186	-2.36744	6.50117
H	-1.94382	-0.11193	5.66614
N	-1.53086	0.77298	1.66148
N	-0.97799	-1.50488	2.74006
Ni	-0.76297	-0.87133	0.95418
C	0.41297	-0.30447	-1.02147
H	1.39382	-0.63414	-0.66391
C	-0.65951	-1.22253	-0.95821
H	-1.58519	-0.92645	-1.44929
C	-0.52708	-2.42792	-0.19993
H	0.45938	-2.89375	-0.13545
C	0.21831	1.20021	-1.2196
H	1.12319	1.57262	-1.76076
C	0.66427	-0.70089	-3.35107
H	-0.28173	-0.171	-3.38089
H	0.41698	1.60604	-0.17461
O	-0.95872	1.53941	-1.74422
C	1.83659	-0.04723	-3.82354
C	1.81382	1.35087	-4.08341
C	3.05041	-0.74892	-4.04597
C	2.94891	1.99907	-4.55637
H	0.88872	1.89324	-3.90404
C	4.17758	-0.09106	-4.51736
H	3.07832	-1.81968	-3.85271
C	4.13389	1.28652	-4.77636
H	2.91443	3.06715	-4.75599
H	5.09646	-0.64603	-4.69033
H	5.01747	1.79841	-5.14845
H	0.6398	-1.7848	-3.29719

H   -1.34407 -3.14984 -0.23024
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2692424
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1777816
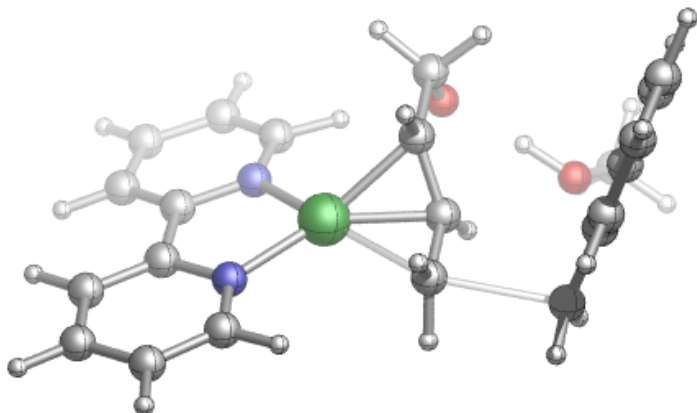DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.270786690197
ΔG_{solv} = -0.0372232

BH-TSB

BH-TSB
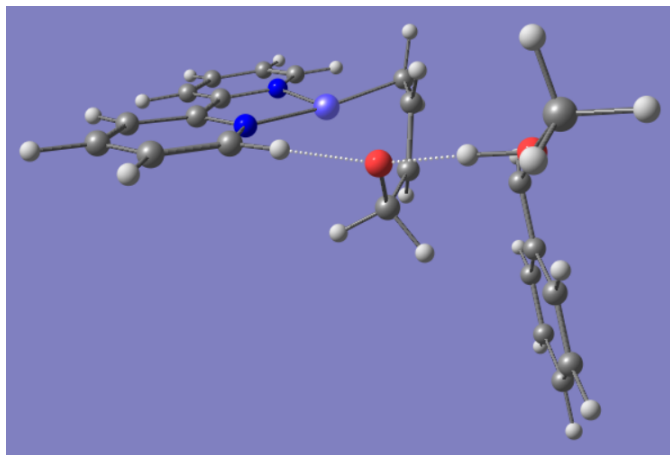
UB3LYP/6-31g(d)-gas
Imaginary frequency = -456.51 cm^{-1}
Zero-point correction=   0.421862 (Hartree/Particle)
 Thermal correction to Energy=   0.448464
 Thermal correction to Enthalpy=   0.449408
 Thermal correction to Gibbs Free Energy=   0.360831
 Sum of electronic and zero-point Energies=   -2620.994637
 Sum of electronic and thermal Energies=   -2620.968035

Sum of electronic and thermal Enthalpies=   -2620.967091
Sum of electronic and thermal Free Energies=   -2621.055668
C   -1.03211 0.71352 3.51861
C   -1.29912 2.15956 1.70403
C   -1.59765 3.22426 2.55114
C   -1.59239 3.01604 3.93116
C   -1.31743 1.74346 4.41893
C   -0.81484 -0.686   3.90093
C   -0.57314 -2.85944 3.08736
C   -0.47287 -3.37895 4.37158
C   -0.54198 -2.50231 5.45979
C   -0.71554 -1.14498 5.21738
H   -1.32425 2.26207 0.62119
H   -1.83566 4.193   2.1253
H   -1.81797 3.82676 4.61795
H   -1.34507 1.54921 5.48556
H   -0.52799 -3.49926 2.21429
H   -0.3434 -4.44657 4.51266
H   -0.46177 -2.87087 6.47766
H   -0.76822 -0.44593 6.04429
N   -0.99552 0.93287 2.17142
N   -0.73596 -1.54429 2.83928
Ni   -0.67977 -0.67589 1.14115
C   0.38881 -0.08032 -0.86912
H   1.32963 -0.46756 -0.48146
C   -0.77566 -0.88654 -0.80638
H   -1.69612 -0.49324 -1.26716
C   -0.70172 -2.14405 -0.139
H   0.24317 -2.6962 -0.14489
C   0.35626 1.39941 -1.18947
H   0.98097 1.5834 -2.07754
C   1.12435 -0.94987 -2.92079
H   0.1719 -0.72452 -3.39399
H   0.82482 1.96238 -0.36987
O   -0.93852 1.92235 -1.3454
C   2.2998 -0.24884 -3.32791
C   2.21495 0.89401 -4.16818
C   3.58696 -0.64497 -2.88115
C   3.35701 1.59583 -4.53752
H   1.24071 1.20467 -4.53862
C   4.7219   0.06157 -3.25324
H   3.67568 -1.52073 -2.24217
C   4.61513 1.18693 -4.08176
H   3.26978 2.46283 -5.18757
H   5.69835 -0.2629 -2.90337
H   5.50666 1.73577 -4.37311

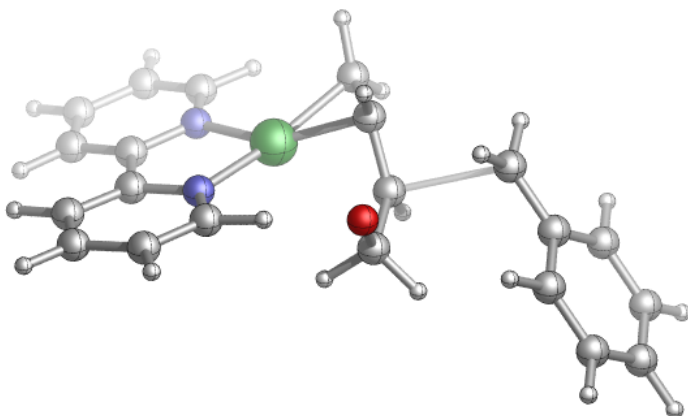|			
H	1.21116	-1.94205	-2.48533
H	-1.58152	-2.78461	-0.16251
H	-1.41267	1.49889	-2.11828
H	-3.56323	-1.33813	-2.97248
C	-3.79634	-0.24442	-3.03711
O	-2.74082	0.52754	-2.63024
H	-4.10729	-0.06473	-4.0946
H	-4.71146	-0.10813	-2.41146

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2620.9837

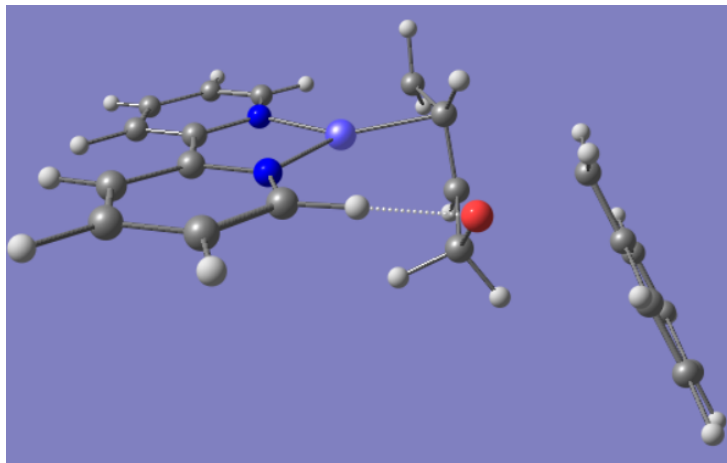UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF= -2621.9729

DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2618.8588

ΔG_{solv} = -0.031814

A''

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.252481 (Hartree/Particle)
 Thermal correction to Energy=   0.268299
 Thermal correction to Enthalpy=   0.269244
 Thermal correction to Gibbs Free Energy=   0.207211
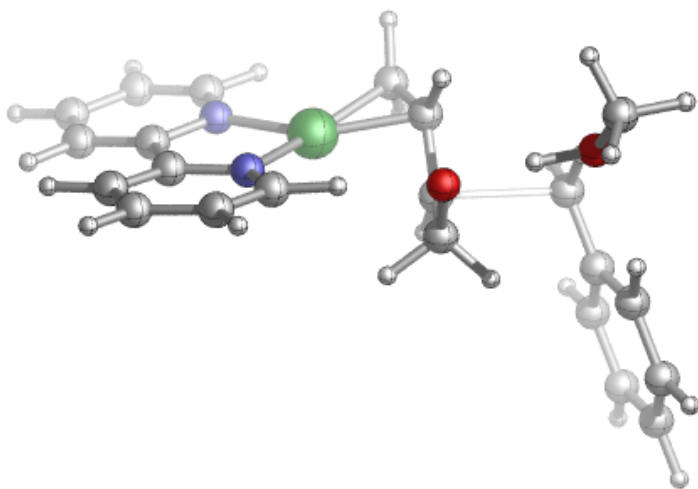 Sum of electronic and zero-point Energies=   -2234.523418
 Sum of electronic and thermal Energies=   -2234.507600
 Sum of electronic and thermal Enthalpies=   -2234.506656

Sum of electronic and thermal Free Energies=   -2234.568688
C   -2.09139 2.31433 0.86226
C   -0.60045 2.29548 2.65039
C   -1.34907 3.2387   3.34487
C   -2.51948 3.72874 2.76326
C   -2.89366 3.25707 1.50751
C   -2.36718 1.74219 -0.47025
C   -1.59   0.23902 -2.07149
C   -2.62395 0.56782 -2.94186
C   -3.56447 1.51936 -2.54539
C   -3.42795 2.11877 -1.29569
H   0.30859 1.87258 3.06297
H   -1.01858 3.57672 4.32156
H   -3.13207 4.46249 3.27829
H   -3.80343 3.61582 1.03871
H   -0.81183 -0.46833 -2.33986
H   -2.68287 0.08483 -3.91175
H   -4.38439 1.79863 -3.20026
H   -4.13605 2.87402 -0.97226
N   -0.94936 1.83577 1.43434
N   -1.46337 0.79615 -0.85248
Ni   -0.13439 0.41052 0.46111
C   1.16771 -0.16166 2.17333
H   1.78899 0.70341 1.93011
C   0.53731 -0.90572 1.06587
H   1.44649 -0.66908 2.95621
H   0.37552 -1.85849 1.18485
C   0.99399 -0.57334 -0.36681
C   0.6564 -1.5233 -1.47899
H   1.97313 -0.06313 -0.37557
H   0.75491 -1.18219 -2.52445
H   -0.19424 -2.2159 -1.35341
O   1.79401 -2.7243 -1.61709
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5095924
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2235.1741033
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.882939502140
ΔG_{solv} = -0.0206952

A''-2

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.252843 (Hartree/Particle)
 Thermal correction to Energy=   0.268511
 Thermal correction to Enthalpy=   0.269455
 Thermal correction to Gibbs Free Energy=   0.208499
 Sum of electronic and zero-point Energies=   -2234.527567
 Sum of electronic and thermal Energies=   -2234.511899
 Sum of electronic and thermal Enthalpies=   -2234.510955
 Sum of electronic and thermal Free Energies=   -2234.571911
C   -2.09139 2.31433 0.86226
 C   -0.60045 2.29548 2.65039
 C   -1.34907 3.2387   3.34487
 C   -2.51948 3.72874 2.76326
 C   -2.89366 3.25707 1.50751
 C   -2.36718 1.74219 -0.47025
 C   -1.59   0.23902 -2.07149
 C   -2.62395 0.56782 -2.94186
 C   -3.56447 1.51936 -2.54539
 C   -3.42795 2.11877 -1.29569
 H   0.30859 1.87258 3.06297
 H   -1.01858 3.57672 4.32156
 H   -3.13207 4.46249 3.27829
 H   -3.80343 3.61582 1.03871
 H   -0.81183 -0.46833 -2.33986
 H   -2.68287 0.08483 -3.91175
 H   -4.38439 1.79863 -3.20026
 H   -4.13605 2.87402 -0.97226
 N   -0.94936 1.83577 1.43434
 N   -1.46337 0.79615 -0.85248
 Ni   -0.13439 0.41052 0.46111
 C   1.63349 0.0152   1.78963

```
H            2.27435   0.84994   1.49639
C            1.2083   -0.94134   0.74956
H            1.78433  -0.3319    2.68677
H            1.04247  -1.86397   1.01291
C            1.89387  -0.84922  -0.62634
C            1.76105  -1.99599  -1.58584
H            2.85325  -0.30568  -0.56929
H            1.17447  -2.88181  -1.28537
H            2.62542  -2.2722   -2.21482
O            1.04532  -0.70447  -1.85607
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5071373
A''-3

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.252625 (Hartree/Particle)
 Thermal correction to Energy=   0.268347
 Thermal correction to Enthalpy=   0.269292
 Thermal correction to Gibbs Free Energy= 0.207703
 Sum of electronic and zero-point Energies=   -2234.520895
 Sum of electronic and thermal Energies=   -2234.505172
 Sum of electronic and thermal Enthalpies=   -2234.504228
 Sum of electronic and thermal Free Energies=   -2234.565817
```
C           -2.09139   2.31433   0.86226
C           -0.60045   2.29548   2.65039
C           -1.34907   3.2387    3.34487
C           -2.51948   3.72874   2.76326
C           -2.89366   3.25707   1.50751
```

C	-2.36718	1.74219	-0.47025
C	-1.59	0.23902	-2.07149
C	-2.62395	0.56782	-2.94186
C	-3.56447	1.51936	-2.54539
C	-3.42795	2.11877	-1.29569
H	0.30859	1.87258	3.06297
H	-1.01858	3.57672	4.32156
H	-3.13207	4.46249	3.27829
H	-3.80343	3.61582	1.03871
H	-0.81183	-0.46833	-2.33986
H	-2.68287	0.08483	-3.91175
H	-4.38439	1.79863	-3.20026
H	-4.13605	2.87402	-0.97226
N	-0.94936	1.83577	1.43434
N	-1.46337	0.79615	-0.85248
Ni	-0.13439	0.41052	0.46111
C	0.78045	-1.52969	1.41108
H	1.08875	-1.05642	2.3462
C	1.14113	-0.87211	0.14025
H	0.75599	-2.503	1.42394
H	1.28424	-1.43213	-0.64332
C	2.13993	0.29844	0.20206
C	2.80085	0.76113	-1.06382
H	2.72334	0.28874	1.13942
H	2.55716	0.25274	-2.01314
H	3.85671	1.08231	-1.03143
O	1.75761	1.61663	-0.40574

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5054061
A-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -329.39 cm^{-1}
Zero-point correction=   0.251353 (Hartree/Particle)
 Thermal correction to Energy=   0.266957
 Thermal correction to Enthalpy=   0.267901
 Thermal correction to Gibbs Free Energy=   0.207241
 Sum of electronic and zero-point Energies=   -2234.525252
 Sum of electronic and thermal Energies=   -2234.509648
 Sum of electronic and thermal Enthalpies=   -2234.508704
 Sum of electronic and thermal Free Energies=   -2234.569364

C	-2.21805	2.2067	1.01322
C	-0.8602	2.24573	2.90975
C	-1.85308	2.85778	3.66243
C	-3.08162	3.13915	3.06051
C	-3.26027	2.80848	1.72103
C	-2.26557	1.84905	-0.4142
C	-1.02128	0.94125	-2.16952
C	-2.06512	1.16928	-3.06505
C	-3.2467	1.7485	-2.60533
C	-3.34417	2.10529	-1.26234
H	0.10485	2.00186	3.33588
H	-1.66162	3.10734	4.70086
H	-3.88259	3.61019	3.62197
H	-4.20318	3.01742	1.2281
H	-0.03147	0.56791	-2.4532
H	-1.93935	0.90042	-4.1089
H	-4.07648	1.9356	-3.28106
H	-4.2424	2.58264	-0.88617
N	-1.02411	1.91274	1.61144
N	-1.12845	1.24983	-0.86255

```
Ni          0.12817   0.87645   0.57706
C           1.17951  -0.03141   1.83021
H           2.04927   0.49458   2.23892
C           1.36142  -0.67741   0.53589
H           0.659    -0.60703   2.5993
H           0.86863  -1.61779   0.2884
C           2.28411  -0.14783  -0.37521
C           2.61845  -0.66706  -1.7188
H           2.77675   0.79031  -0.12996
H           3.04322   0.11678  -2.38177
H           1.76236  -1.1248   -2.25478
O           3.35321  -1.31789  -0.75022
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5046845
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2235.1763672
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2272.466173902212
ΔG_{solv} = -0.014615

A-TS-2
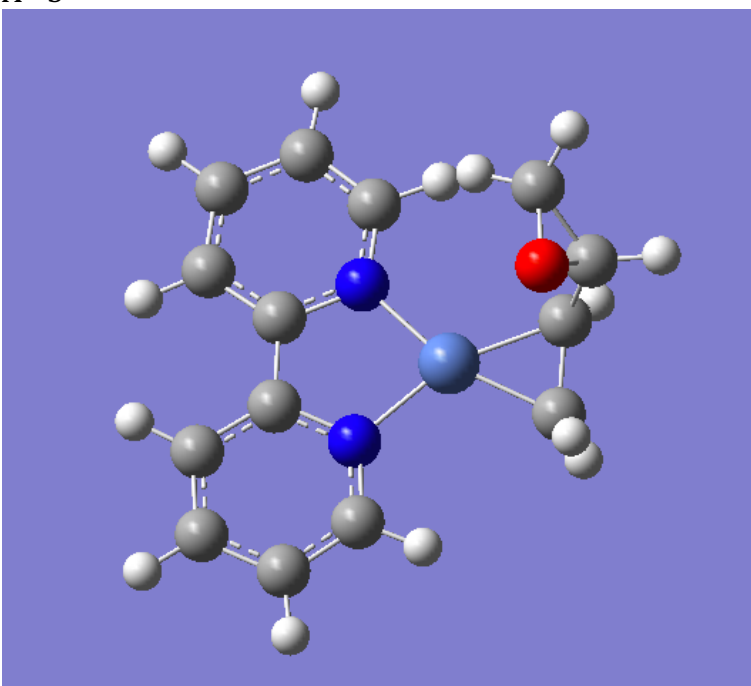

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.251545 (Hartree/Particle)
 Thermal correction to Energy=   0.266822
 Thermal correction to Enthalpy=   0.267766
 Thermal correction to Gibbs Free Energy=   0.208363
 Sum of electronic and zero-point Energies=   -2234.503715
 Sum of electronic and thermal Energies=   -2234.488437
 Sum of electronic and thermal Enthalpies=   -2234.487493

Sum of electronic and thermal Free Energies=   -2234.546896
```
C            -2.09139  2.31433  0.86226
C            -0.60045  2.29548  2.65039
C            -1.34907  3.2387   3.34487
C            -2.51948  3.72874  2.76326
C            -2.89366  3.25707  1.50751
C            -2.36718  1.74219 -0.47025
C            -1.59     0.23902 -2.07149
C            -2.62395  0.56782 -2.94186
C            -3.56447  1.51936 -2.54539
C            -3.42795  2.11877 -1.29569
H             0.30859  1.87258  3.06297
H            -1.01858  3.57672  4.32156
H            -3.13207  4.46249  3.27829
H            -3.80343  3.61582  1.03871
H            -0.81183 -0.46833 -2.33986
H            -2.68287  0.08483 -3.91175
H            -4.38439  1.79863 -3.20026
H            -4.13605  2.87402 -0.97226
N            -0.94936  1.83577  1.43434
N            -1.46337  0.79615 -0.85248
Ni           -0.13439  0.41052  0.46111
C             0.78045 -1.52969  1.41108
H             1.08875 -1.05642  2.3462
C             1.14113 -0.87211  0.14025
H             0.75599 -2.503    1.42394
H             1.28424 -1.43213 -0.64332
C             2.13993  0.29844  0.20206
C             2.80085  0.76113 -1.06382
H             2.72334  0.28874  1.13942
H             2.55716  0.25274 -2.01314
H             3.85671  1.08231 -1.03143
O             1.8792   1.92152 -0.82433
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.4937113
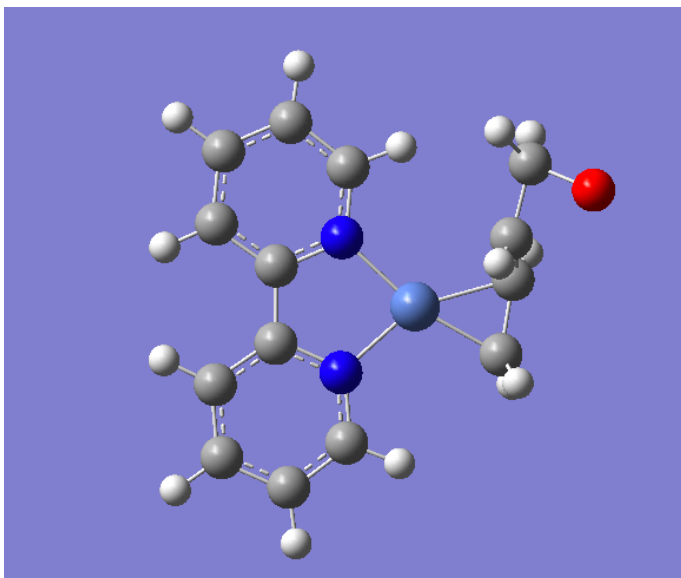A-TS-3

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.249598 (Hartree/Particle)
 Thermal correction to Energy=   0.265678
 Thermal correction to Enthalpy=   0.266622
 Thermal correction to Gibbs Free Energy=   0.204586
 Sum of electronic and zero-point Energies=   -2234.471490
 Sum of electronic and thermal Energies=   -2234.455410
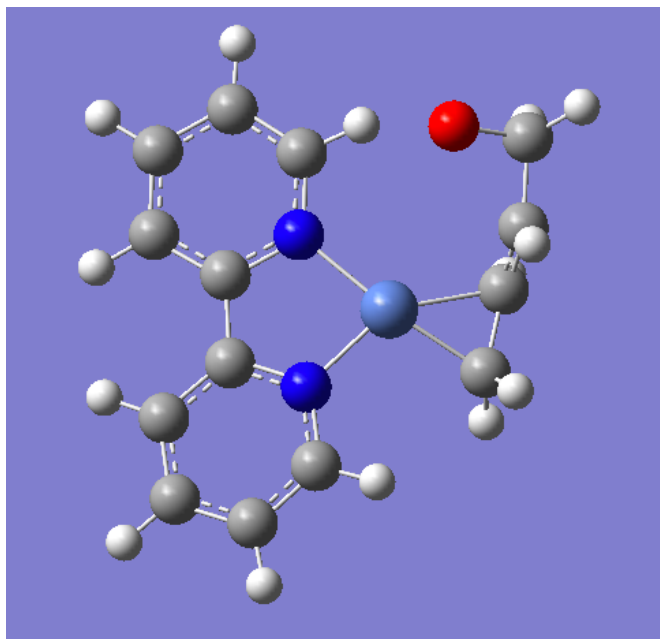 Sum of electronic and thermal Enthalpies=   -2234.454465
 Sum of electronic and thermal Free Energies=   -2234.516502
C   -1.70758 0.53731 0.64911
 C   -0.84761 0.48359 2.81071
 C   -2.11746 0.53539 3.36693
 C   -3.22804 0.55884 2.51601
 C   -3.01465 0.56224 1.14203
 C   -1.33768 0.61935 -0.76877
 C   0.45861 0.52724 -2.24403
 C   -0.34017 0.93312 -3.30687
 C   -1.69949 1.16407 -3.08343
 C   -2.20072 1.01173 -1.79466
 H   0.04099 0.45429 3.43095
 H   -2.2315   0.55472 4.44573
 H   -4.23678 0.57781 2.9166
 H   -3.8542   0.57573 0.45531
 H   1.50788 0.29799 -2.38243
 H   0.10079 1.05222 -4.29077
 H   -2.35245 1.47428 -3.8936
 H   -3.2422   1.224   -1.57912
 N   -0.62699 0.47541 1.47793
 N   -0.0213   0.34151 -0.99906

```
Ni          0.95294 -0.13612  0.60825
C           2.13498 -0.75667  1.97415
H           2.85458  0.02954  2.22291
C           2.35455 -1.50454  0.77786
H           1.75413 -1.28207  2.84949
H           1.99573 -2.53165  0.70416
C           2.78483 -0.84517 -0.40012
C           3.08045 -1.62243 -1.65886
H           3.35209  0.08208 -0.29852
H           2.96316 -1.02099 -2.59654
H           2.37801 -2.48789 -1.76087
O           4.34509 -1.88493 -1.29048
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.4608059
B''

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.251237 (Hartree/Particle)
 Thermal correction to Energy=   0.267198
 Thermal correction to Enthalpy=   0.268142
 Thermal correction to Gibbs Free Energy=   0.207218
 Sum of electronic and zero-point Energies=   -2234.499830
 Sum of electronic and thermal Energies=   -2234.483869
 Sum of electronic and thermal Enthalpies=   -2234.482924
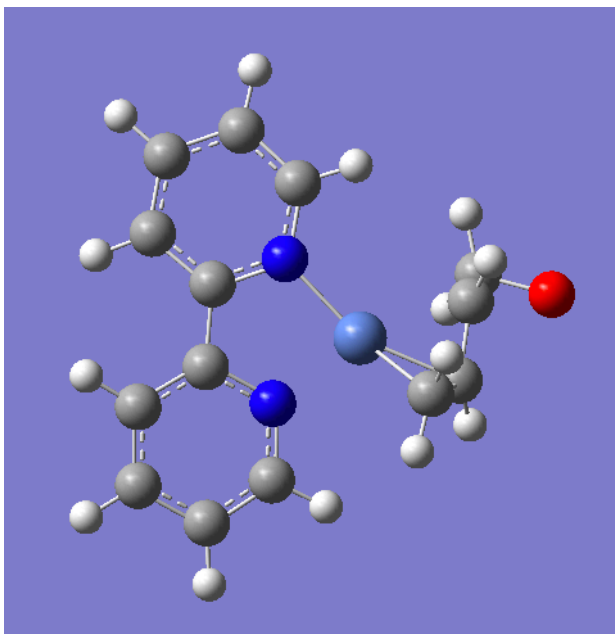 Sum of electronic and thermal Free Energies=   -2234.543848
```
C          -2.09139  2.31433  0.86226
C          -0.60045  2.29548  2.65039
C          -1.34907  3.2387   3.34487
C          -2.51948  3.72874  2.76326
C          -2.89366  3.25707  1.50751
C          -2.36718  1.74219 -0.47025
```

```
C          -1.59    0.23902 -2.07149
C          -2.62395  0.56782 -2.94186
C          -3.56447  1.51936 -2.54539
C          -3.42795  2.11877 -1.29569
H           0.30859  1.87258  3.06297
H          -1.01858  3.57672  4.32156
H          -3.13207  4.46249  3.27829
H          -3.80343  3.61582  1.03871
H          -0.81183 -0.46833 -2.33986
H          -2.68287  0.08483 -3.91175
H          -4.38439  1.79863 -3.20026
H          -4.13605  2.87402 -0.97226
N          -0.94936  1.83577  1.43434
N          -1.46337  0.79615 -0.85248
Ni         -0.13439  0.41052  0.46111
C           0.64814 -1.55952  1.45703
H           1.1168  -1.12328  2.34221
C           0.81569 -0.87001  0.16319
H           0.59959 -2.53195  1.44665
H           0.81451 -1.40784 -0.64849
C           1.84279  0.27536  0.09394
C           2.30199  0.76325 -1.24936
H           2.57003  0.22277  0.92308
H           2.83311  1.72887 -1.31668
H           1.66266  0.58597 -2.13189
O           3.57617 -0.13594 -1.81814
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5213308
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = - 2235.1929384
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2232.8431

ΔG_{solv} = -0.0624885

B''-2

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.250237 (Hartree/Particle)
 Thermal correction to Energy=   0.265860
 Thermal correction to Enthalpy=   0.266804
 Thermal correction to Gibbs Free Energy=   0.206730
 Sum of electronic and zero-point Energies=   -2234.512482
 Sum of electronic and thermal Energies=   -2234.496860
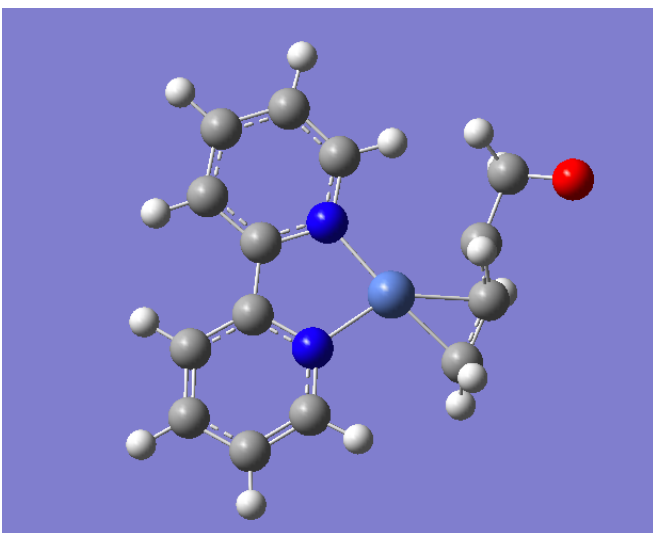 Sum of electronic and thermal Enthalpies=   -2234.495916
 Sum of electronic and thermal Free Energies=   -2234.555990
C   -2.19805 2.1767   1.00322
C   -0.8402   2.20573 2.89975
C   -1.82308 2.84778 3.65243
C   -3.05162 3.13915 3.05051
C   -3.23027 2.79848 1.71103
C   -2.24557 1.83905 -0.4242
C   -0.98128 0.96125 -2.18952
C   -2.05512 1.15928 -3.07505
C   -3.2367   1.7285 -2.60533
C   -3.33417 2.08529 -1.26234
H   0.11485 1.94186 3.33588
H   -1.63162 3.09734 4.68086
H   -3.84259 3.62019 3.60197
H   -4.16318 3.02741 1.2081
H   0.06853 0.67791 -2.4832
H   -1.92935 0.90042 -4.1189
H   -4.06648 1.9156 -3.28106
H   -4.2324   2.55264 -0.88617

```
N          -1.01411  1.85274  1.61144
N          -1.09845  1.26983 -0.89255
Ni          0.19817  0.87645  0.53706
C           1.06951 -0.05141  1.97021
H           1.89927  0.48458  2.42892
C           1.43142 -0.82741  0.77589
H           0.419   -0.52703  2.7293
H           0.87863 -1.72779  0.4984
C           2.12411 -0.12783 -0.17521
C           2.20685 -0.29607 -1.69764
H           2.60778  0.85623  0.09518
H           1.69586 -1.29131 -1.91093
H           3.30641 -0.57579 -1.88126
O           1.73628  0.78243 -2.49592
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
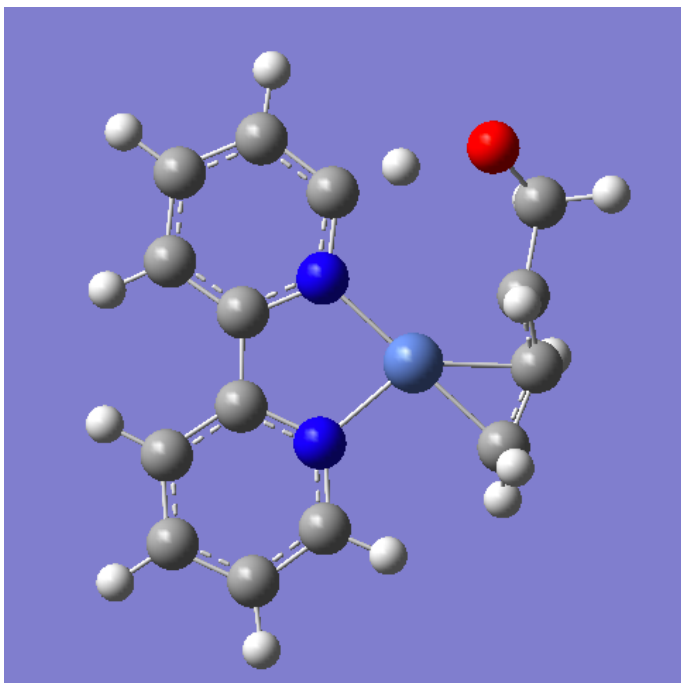HF=-2234.5211117

B''-3

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.255193 (Hartree/Particle)
 Thermal correction to Energy=   0.269634
 Thermal correction to Enthalpy=   0.270578
 Thermal correction to Gibbs Free Energy= 0.214080
 Sum of electronic and zero-point Energies=   -2234.545905
 Sum of electronic and thermal Energies=   -2234.531465
 Sum of electronic and thermal Enthalpies=   -2234.530521
 Sum of electronic and thermal Free Energies=   -2234.587018
```
C          -2.09139  2.31433  0.86226
```

```
C            -0.60045  2.29548  2.65039
C            -1.34907  3.2387   3.34487
C            -2.51948  3.72874  2.76326
C            -2.89366  3.25707  1.50751
C            -2.36718  1.74219 -0.47025
C            -1.59     0.23902 -2.07149
C            -2.62395  0.56782 -2.94186
C            -3.56447  1.51936 -2.54539
C            -3.42795  2.11877 -1.29569
H             0.30859  1.87258  3.06297
H            -1.01858  3.57672  4.32156
H            -3.13207  4.46249  3.27829
H            -3.80343  3.61582  1.03871
H            -0.81183 -0.46833 -2.33986
H            -2.68287  0.08483 -3.91175
H            -4.38439  1.79863 -3.20026
H            -4.13605  2.87402 -0.97226
N            -0.94936  1.83577  1.43434
N            -1.46337  0.79615 -0.85248
Ni           -0.13439  0.41052  0.46111
C             0.98632 -1.70189  1.42354
H             1.19999 -1.04378  2.26895
C             1.16611 -1.17072  0.0586
H             1.17954 -2.64502  1.56932
H             1.41476 -1.79257 -0.6482
C             1.8801   0.18567 -0.08983
C             2.39603  0.59475 -1.43883
H             2.46953  0.43772  0.80914
H             1.80659  0.3427  -2.33776
H             3.4815   0.54721 -1.63517
O             2.28723  2.2367  -1.65742
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5247592

B''-4

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.251518 (Hartree/Particle)
 Thermal correction to Energy=   0.267524
 Thermal correction to Enthalpy=   0.268468
 Thermal correction to Gibbs Free Energy=   0.207388
 Sum of electronic and zero-point Energies=   -2234.493939
 Sum of electronic and thermal Energies=   -2234.477933
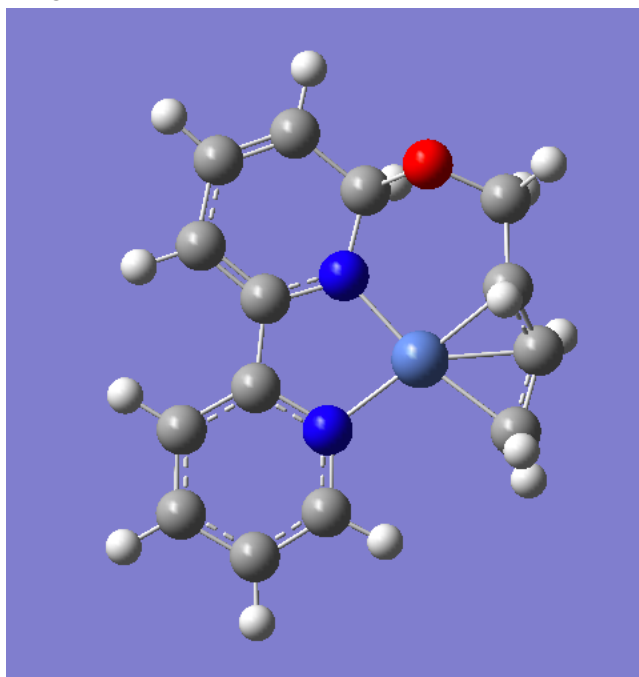 Sum of electronic and thermal Enthalpies=   -2234.476989
 Sum of electronic and thermal Free Energies=   -2234.538070

C	-2.09139	2.31433	0.86226
C	-0.60045	2.29548	2.65039
C	-1.34907	3.2387	3.34487
C	-2.51948	3.72874	2.76326
C	-2.89366	3.25707	1.50751
C	-2.36718	1.74219	-0.47025
C	-1.59	0.23902	-2.07149
C	-2.62395	0.56782	-2.94186
C	-3.56447	1.51936	-2.54539
C	-3.42795	2.11877	-1.29569
H	0.30859	1.87258	3.06297
H	-1.01858	3.57672	4.32156
H	-3.13207	4.46249	3.27829
H	-3.80343	3.61582	1.03871
H	-0.81183	-0.46833	-2.33986
H	-2.68287	0.08483	-3.91175
H	-4.38439	1.79863	-3.20026
H	-4.13605	2.87402	-0.97226
N	-0.94936	1.83577	1.43434
N	-1.46337	0.79615	-0.85248
Ni	-0.13439	0.41052	0.46111

```
C            0.98245 -0.427   2.10699
H            1.10574  0.65611  2.03511
C            1.19576 -1.239    0.89345
H            1.23271 -0.8199   2.96203
H            1.52333 -2.14965  1.00073
C            1.8208  -0.54215 -0.32938
C            2.37662 -1.3819  -1.44258
H            2.34378  0.38821 -0.0465
H            2.59367 -0.90746 -2.41564
H            2.01577 -2.41822 -1.56453
O            3.7039  -1.32877 -0.44704
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2234.5169599

B''-C-TS

UB3LYP/6-31g(d)-gas
Imaginary frequency = -118.30 cm^{-1}
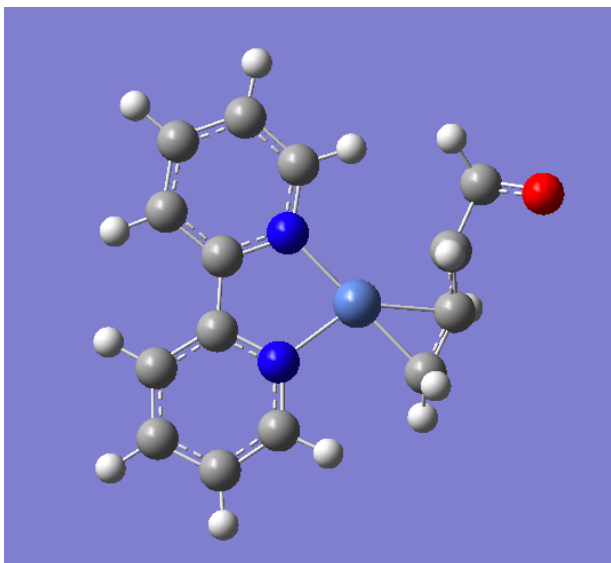Zero-point correction=   0.366489 (Hartree/Particle)
 Thermal correction to Energy=   0.389629
 Thermal correction to Enthalpy=   0.390573
 Thermal correction to Gibbs Free Energy=   0.309400
 Sum of electronic and zero-point Energies=   -2505.299540
 Sum of electronic and thermal Energies=   -2505.276400
 Sum of electronic and thermal Enthalpies=   -2505.275456
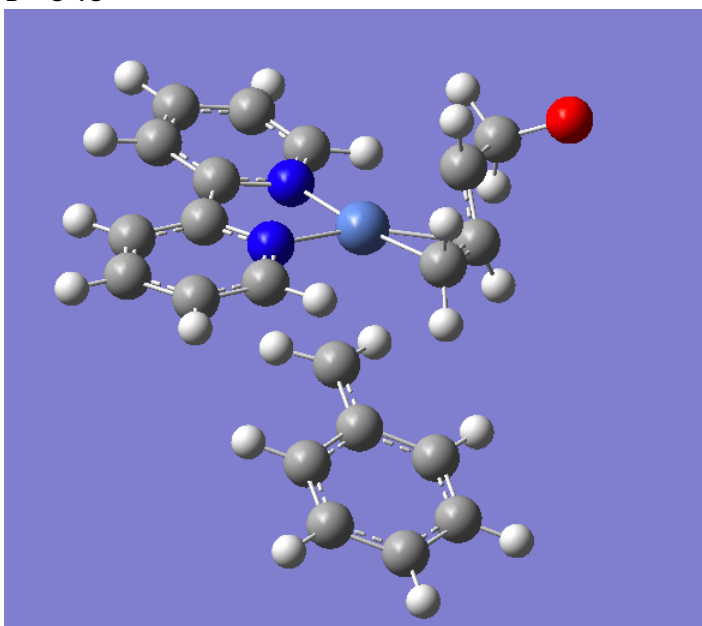 Sum of electronic and thermal Free Energies=   -2505.356629
```
C           -1.6496   1.2818   1.34746
C            0.6055   1.81183  1.79102
C            0.26003  2.60437  2.89104
C           -1.10348  2.7151   3.24415
```

```
C          -2.05844  2.04413  2.46607
C          -2.5476   0.57738  0.44555
C          -2.6721  -0.94304 -1.35147
C          -4.07159 -0.88506 -1.37573
C          -4.72984 -0.05014 -0.44806
C          -3.95693  0.68734  0.46427
H           1.64164  1.68806  1.49557
H           1.03494  3.11664  3.45248
H          -1.4086   3.30577  4.10355
H          -3.11074  2.10083  2.72524
H          -2.13205 -1.57032 -2.04963
H          -4.62223 -1.47773 -2.09914
H          -5.81371  0.02789 -0.44136
H          -4.43693  1.3528   1.17458
N          -0.31562  1.15801  1.01642
N          -1.90476 -0.2391  -0.46238
Ni          0.01751 -0.13324 -0.34789
C           1.56911 -3.00405  1.49008
C           2.95027 -3.02211  1.61029
C           3.61524 -2.01623  2.32751
C           2.87324 -0.98619  2.92492
C           1.49182 -0.95578  2.80895
C           0.79031 -1.96584  2.08432
H           1.05923 -3.78806  0.93559
H           3.52074 -3.82184  1.14543
H           4.69728 -2.03556  2.41998
H           3.38443 -0.20695  3.48482
H           0.92196 -0.15344  3.27132
C          -0.61159 -1.94001  1.96292
H          -1.19995 -1.14607  2.41279
H          -1.14303 -2.71192  1.41599
C           1.9537  -0.27448 -0.22614
H           2.40663  0.58352 -0.72956
H           2.41666 -0.52918  0.72549
C           1.43789 -1.33452 -1.01819
H           1.41227 -2.35578 -0.63945
C           0.64903 -0.99034 -2.12941
H           0.9012  -0.06924 -2.66265
C           0.05869 -2.0586  -3.03744
H          -0.83786 -1.65833 -3.56619
H          -0.2854  -2.91871 -2.41372
O           1.1063  -2.31999 -3.85428
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2944336
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.2038158

DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.253379015522
ΔG_{solv} = -0.0613693

B''-C-TS-2

UB3LYP/6-31g(d)-gas
Imaginary frequency = -119.99 cm^{-1}
Zero-point correction=   0.366492 (Hartree/Particle)
 Thermal correction to Energy=   0.389628
 Thermal correction to Enthalpy=   0.390572
 Thermal correction to Gibbs Free Energy=   0.310125
 Sum of electronic and zero-point Energies=   -2505.299133
 Sum of electronic and thermal Energies=   -2505.275997
 Sum of electronic and thermal Enthalpies=   -2505.275053
 Sum of electronic and thermal Free Energies=   -2505.355500
C   -1.44624   1.86042   0.63873
C   0.8173   2.33916   0.94168
C   0.5457   3.19289   2.00086
C   -0.78572   3.36388   2.40403
C   -1.78449   2.68709   1.71894
C   -2.40812   1.11743 -0.17099
C   -2.65267 -0.55378 -1.77917
C   -4.03709 -0.45944 -1.73709
C   -4.62249   0.4839   -0.88393
C   -3.7985   1.27646 -0.09736
H   1.83307   2.16395   0.60894
H   1.35962   3.70733   2.50029
H   -1.03459   4.0092   3.24103
H   -2.82033   2.78615   2.02434
H   -2.16324 -1.26825 -2.42685
H   -4.63863 -1.11129 -2.36118

H	-5.70129	0.59732	-0.83641
H	-4.22603	2.02352	0.56242
N	-0.14257	1.68519	0.25759
N	-1.83813	0.20979	-1.02441
Ni	0.09928	0.34106	-1.10366
C	-1.66571	-2.70433	-0.67998
C	-2.00321	-3.60505	-1.68006
C	-1.03111	-4.4472	-2.23711
C	0.29008	-4.37403	-1.774
C	0.63764	-3.47563	-0.77573
C	-0.33027	-2.6074	-0.19365
H	-2.42917	-2.06205	-0.2474
H	-3.0309	-3.65882	-2.03011
H	-1.29994	-5.15248	-3.01831
H	1.04836	-5.02853	-2.19708
H	1.66404	-3.42646	-0.41997
C	0.02409	-1.67941	0.8147
H	1.00397	-1.72295	1.27704
H	-0.74041	-1.1094	1.33185
C	2.03296	0.4255	-1.39951
H	2.25682	1.38619	-1.86878
H	2.72273	0.13988	-0.6082
C	1.47293	-0.60596	-2.19659
H	1.64074	-1.65346	-1.95078
C	0.43711	-0.27739	-3.08412
H	0.44685	0.72016	-3.53089
C	-0.20712	-1.32727	-3.97791
H	-1.23152	-0.99581	-4.27446
H	-0.33483	-2.27646	-3.3952
O	0.68155	-1.37695	-4.99063

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2932845
B''-C-TS-3

UB3LYP/6-31g(d)-gas

Imaginary frequency = -11.19 cm^{-1}

Zero-point correction=   0.366544 (Hartree/Particle)
 Thermal correction to Energy=   0.389767
 Thermal correction to Enthalpy=   0.390711
 Thermal correction to Gibbs Free Energy=   0.308380
 Sum of electronic and zero-point Energies=   -2505.301722
 Sum of electronic and thermal Energies=   -2505.278499
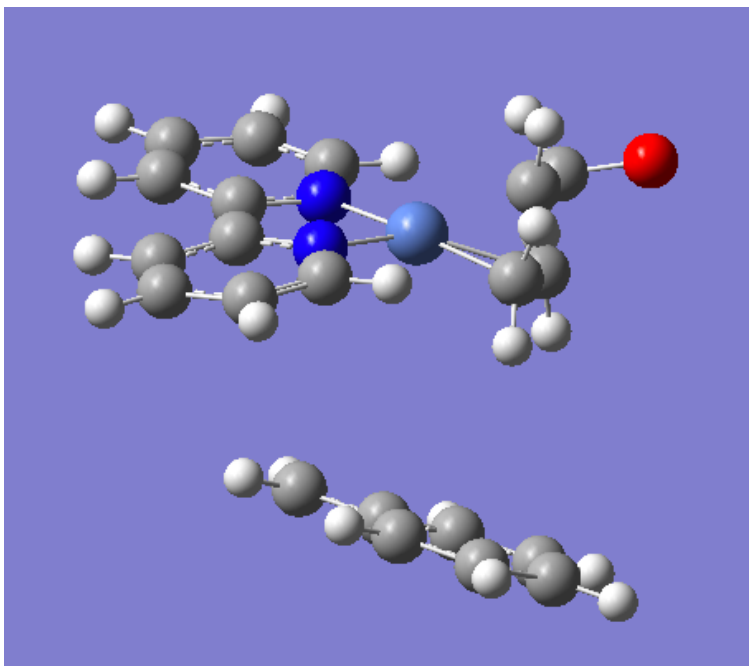 Sum of electronic and thermal Enthalpies=   -2505.277555
 Sum of electronic and thermal Free Energies=   -2505.359886

C	-1.26757	2.01823	0.79284
C	1.01895	2.46656	0.98459
C	0.83673	3.14794	2.17523
C	-0.46025	3.24265	2.70926
C	-1.51114	2.67087	2.0114
C	-2.28891	1.41862	-0.04811
C	-2.67133	0.09481	-1.93252
C	-4.04594	0.18593	-1.77892
C	-4.55844	0.9344	-0.7088
C	-3.67065	1.55552	0.15455
H	2.0039	2.3592	0.54739
H	1.68911	3.59489	2.67564
H	-0.63756	3.75209	3.65152
H	-2.51951	2.71747	2.40818
H	-2.24165	-0.46936	-2.74827
H	-4.6984	-0.3199	-2.48229
H	-5.6296	1.03383	-0.56137
H	-4.03916	2.15917	0.97676

```
N           0.00582   1.9066    0.2869
N          -1.78973   0.68009  -1.0947
Ni          0.13368   0.72433  -1.20296
C           1.25858  -3.15714   1.08437
C           2.5524   -3.52946   0.75359
C           3.64925  -2.81711   1.26093
C           3.43047  -1.72058   2.10819
C           2.14094  -1.33732   2.44404
C           1.00714  -2.04372   1.94145
H           0.41268  -3.7145    0.68954
H           2.7169   -4.37951   0.09671
H           4.66098  -3.11229   0.99862
H           4.27793  -1.16803   2.50618
H           1.97683  -0.48546   3.09965
C          -0.30423  -1.66067   2.27904
H          -0.49205  -0.8132    2.93023
H          -1.16341  -2.2042    1.89973
C           2.06554   0.52607  -1.32097
H           2.48409   1.40408  -1.81946
H           2.62799   0.19604  -0.44962
C           1.42652  -0.4656   -2.11057
H           1.41139  -1.50828  -1.79477
C           0.52783  -0.02996  -3.09843
H           0.7478    0.91655  -3.60025
C          -0.19473  -1.02482  -3.99411
H          -1.13166  -0.57127  -4.39414
H          -0.49356  -1.91271  -3.38685
O           0.74601  -1.26087  -4.93946
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.287344
B''-C-TS-4
```

UB3LYP/6-31g(d)-gas
Imaginary frequency = -44.03 cm^{-1}
Zero-point correction=   0.364680 (Hartree/Particle)
 Thermal correction to Energy=   0.388061
 Thermal correction to Enthalpy=   0.389005
 Thermal correction to Gibbs Free Energy=   0.308596
 Sum of electronic and zero-point Energies=   -2505.342497
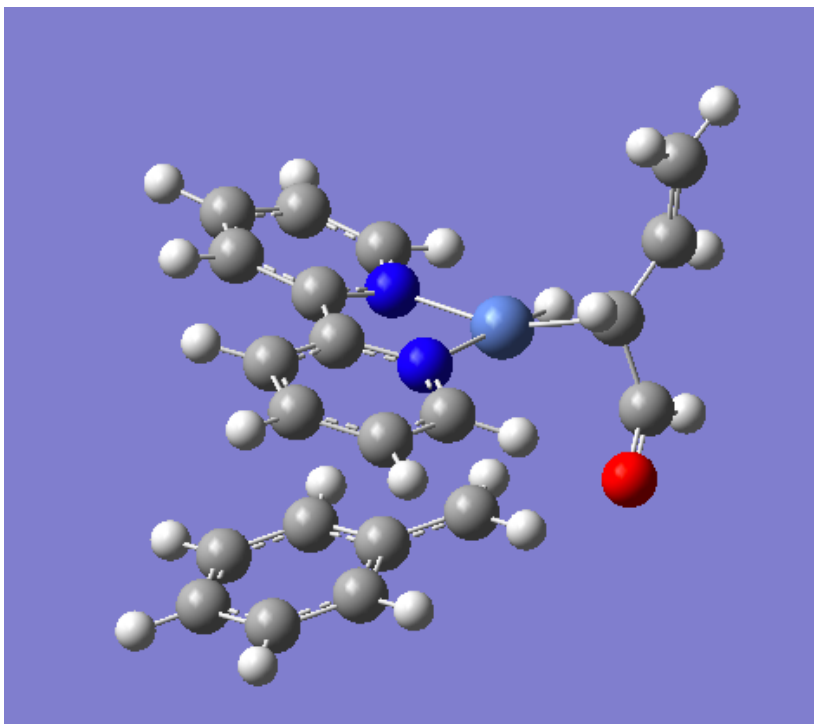 Sum of electronic and thermal Energies=   -2505.319116
 Sum of electronic and thermal Enthalpies=   -2505.318172
 Sum of electronic and thermal Free Energies=   -2505.398581

C	-0.45942	1.34416	0.81609
C	1.86771	1.37529	0.74669
C	1.93417	1.93853	2.01829
C	0.75043	2.23067	2.69379
C	-0.463	1.9162	2.08916
C	-1.66099	0.90211	0.09153
C	-2.40801	-0.24129	-1.79563
C	-3.73669	-0.06332	-1.42992
C	-4.02719	0.63456	-0.25664
C	-2.9742	1.12198	0.51098
H	2.75694	1.08633	0.1914
H	2.90323	2.13967	2.46279
H	0.76888	2.6767	3.68378
H	-1.3976	2.09725	2.608
H	-2.1275	-0.76857	-2.69846
H	-4.52452	-0.46472	-2.05866

H	-5.05449	0.79731	0.05478
H	-3.17073	1.67361	1.42347
N	0.69702	1.10703	0.14008
N	-1.38104	0.22575	-1.05832
Ni	0.43422	0.3	-1.59701
C	1.07656	-1.98021	2.20603
C	0.52778	-2.00833	3.47961
C	-0.80415	-2.40206	3.67354
C	-1.58179	-2.76968	2.5661
C	-1.04233	-2.74689	1.28834
C	0.30891	-2.35141	1.06282
H	2.11087	-1.67966	2.06068
H	1.13835	-1.72792	4.33465
H	-1.22818	-2.42804	4.67363
H	-2.6137	-3.08153	2.70966
H	-1.64895	-3.03972	0.4345
C	0.86959	-2.33031	-0.23299
H	0.30685	-2.69663	-1.08474
H	1.9124	-2.07542	-0.38847
C	1.61385	2.5614	-4.36389
H	1.69047	3.44427	-3.73175
H	1.40012	2.73248	-5.41507
C	1.77338	1.32453	-3.8712
H	1.6816	0.47617	-4.55105
C	2.06495	0.98746	-2.46525
H	2.38848	1.85382	-1.8807
C	2.8495	-0.20267	-2.18754
H	2.78483	-0.99675	-2.964
H	0.16425	-0.48356	-2.81737
O	3.52913	-0.40856	-1.17169

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.293624
B''-C-TS-5

UB3LYP/6-31g(d)-gas

Imaginary frequency = -66.47 cm^{-1}

Zero-point correction=   0.368405 (Hartree/Particle)
 Thermal correction to Energy=   0.390410
 Thermal correction to Enthalpy=   0.391354
 Thermal correction to Gibbs Free Energy=   0.315795
 Sum of electronic and zero-point Energies=   -2505.320022
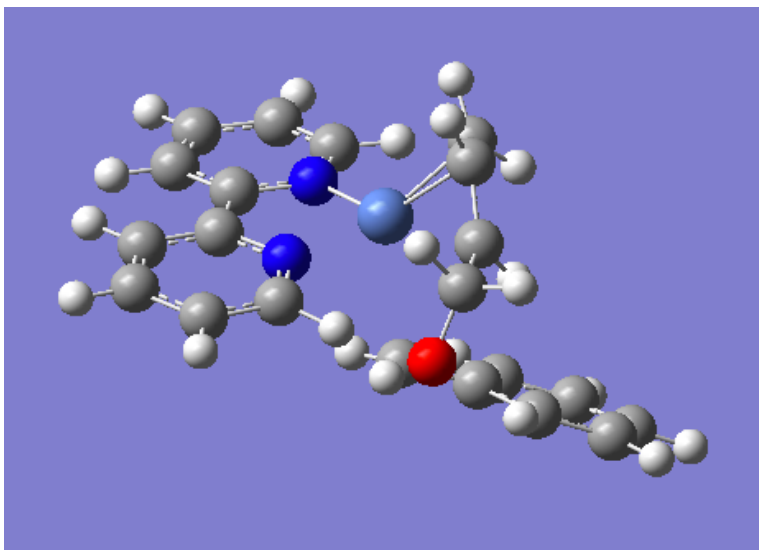 Sum of electronic and thermal Energies=   -2505.298017
 Sum of electronic and thermal Enthalpies=   -2505.297073
 Sum of electronic and thermal Free Energies=   -2505.372632

C	-1.4862	-0.45321	2.43597
C	0.70832	0.16019	2.93673
C	0.34974	0.60516	4.20105
C	-0.98642	0.49914	4.59535
C	-1.90884	-0.03006	3.70141
C	-2.38139	-0.97491	1.39137
C	-2.49679	-1.64944	-0.8469
C	-3.87728	-1.8347	-0.73878
C	-4.51567	-1.58956	0.47415
C	-3.75883	-1.141	1.55384
H	1.73235	0.22042	2.58889
H	1.10434	1.02212	4.8594
H	-1.30396	0.8295	5.57963
H	-2.95299	-0.10967	3.98047
H	-1.93311	-1.71442	-1.81094
H	-4.43442	-2.16057	-1.61143
H	-5.58788	-1.72906	0.5812
H	-4.23582	-0.9229	2.50281
N	-0.17685	-0.36838	2.06743
N	-1.76342	-1.25051	0.21179
Ni	0.22683	-1.04862	0.3095

```
C        1.78677  1.45189  -2.62619
C        2.99535  1.99808  -3.04369
C        3.7467   2.80706  -2.18278
C        3.26794  3.0691   -0.89375
C        2.06013  2.52573  -0.46985
C        1.28452  1.70178  -1.32252
H        1.19774  0.82276  -3.29024
H        3.35519  1.79781  -4.04998
H        4.69008  3.23311  -2.51353
H        3.83903  3.70649  -0.22251
H        1.68596  2.75011   0.52748
C        0.02714  1.12923  -0.90174
H       -0.49207  1.66642  -0.10948
H       -0.60006  0.75935  -1.70531
C        2.02372 -1.74841   0.73849
H        2.77769 -1.0371    0.39995
H        2.18011 -2.12454   1.749
C        1.39561 -2.59391  -0.21948
H        0.96976 -3.55478   0.07171
C        1.02346 -1.99299  -1.42574
H        1.64351 -1.17878  -1.78526
C        0.08686 -2.5457   -2.47825
H       -0.49648 -3.38316  -1.99975
H        0.72291 -3.06249  -3.24172
O       -0.6701  -1.53481  -2.97441
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2855863
B''-C-TS-6

UB3LYP/6-31g(d)-gas

Imaginary frequency = -8.16 cm^{-1}
Zero-point correction=   0.366637 (Hartree/Particle)
 Thermal correction to Energy=   0.390148
 Thermal correction to Enthalpy=   0.391092
 Thermal correction to Gibbs Free Energy=   0.308252
 Sum of electronic and zero-point Energies=   -2505.347559
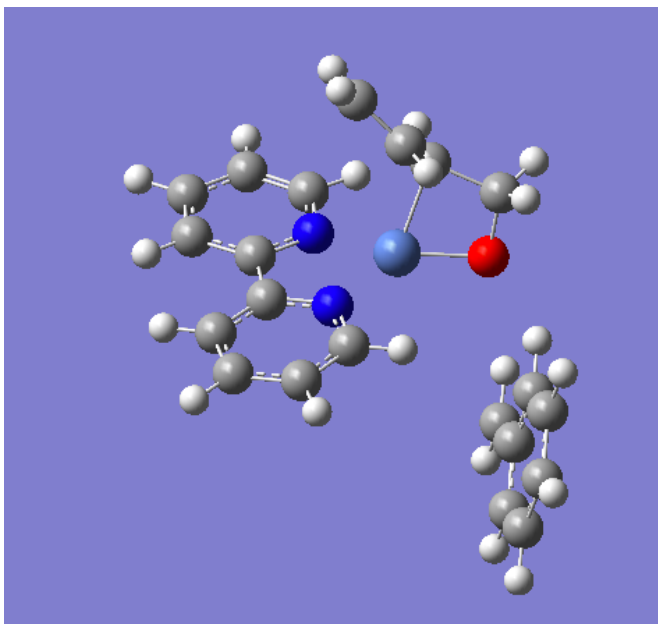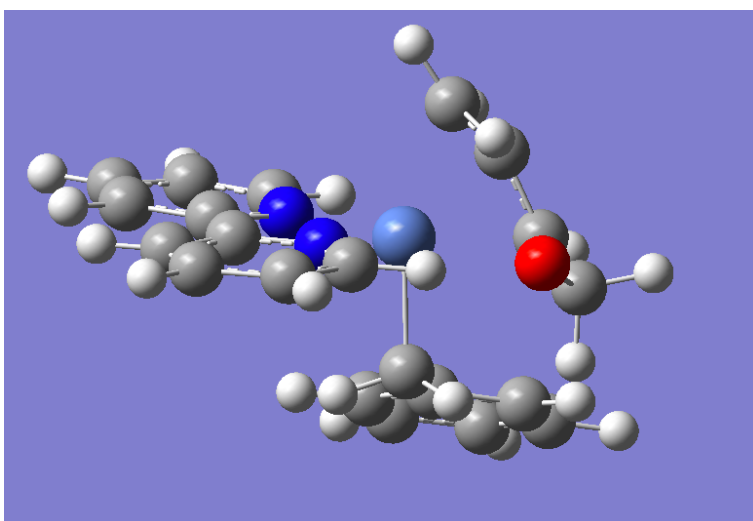 Sum of electronic and thermal Energies=   -2505.324048
 Sum of electronic and thermal Enthalpies=   -2505.323104
 Sum of electronic and thermal Free Energies=   -2505.405945
C   -1.67635   2.0636   0.56997
 C   0.43685   1.45352   1.37487
 C   0.55397   2.62805   2.09657
 C   -0.4992   3.55737   2.05433
 C   -1.61377   3.27006   1.2804
 C   -2.77781   1.66373 -0.29775
 C   -3.44516   0.05064 -1.8648
 C   -4.6806   0.655   -2.03253
 C   -4.96636   1.81497 -1.29127
 C   -4.01389   2.31933 -0.41851
 H   1.21894   0.70321   1.37957
 H   1.44706   2.81346   2.68394
 H   -0.43951   4.48982   2.60727
 H   -2.42862   3.98293   1.20855
 H   -3.14882 -0.8503   -2.39408
 H   -5.40477   0.23468 -2.72231
 H   -5.9275   2.31031 -1.39364
 H   -4.22593   3.20362   0.17327
 N   -0.65335   1.14799   0.63767
 N   -2.5151   0.54067 -1.02508
 Ni   -0.7738   -0.30766 -0.64394
 C   1.81488 -3.33037   0.53152
 C   3.15906 -3.58274   0.30453
 C   4.14146 -3.01686   1.13168
 C   3.75809 -2.18731   2.19458
 C   2.4166   -1.92561   2.43209
 C   1.39961 -2.49196   1.60868
 H   1.05374 -3.74485 -0.1234
 H   3.45334 -4.22255 -0.52347
 H   5.19294 -3.21972   0.94894
 H   4.51564 -1.74962   2.83995
 H   2.1232   -1.29251   3.26669
 C   0.03359 -2.22285   1.83468
 H   -0.27855 -1.61622   2.6787
 H   -0.72474 -2.79192   1.30951
 C   2.48446   1.52869 -1.47587
 H   1.99351   2.44012 -1.81144

```
H          3.48699  1.63442 -1.07137
C          1.89387  0.31973 -1.59106
H          2.45241 -0.55225 -1.2409
C          0.56394  0.04066 -2.10856
H          0.13409  0.85007 -2.7046
C          0.23541 -1.37173 -2.58108
H          1.1252  -2.02339 -2.5398
H         -0.12884 -1.39247 -3.62312
O         -0.76622 -1.82375 -1.66941
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2696041
C

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.368972 (Hartree/Particle)
 Thermal correction to Energy=   0.391340
 Thermal correction to Enthalpy=   0.392284
 Thermal correction to Gibbs Free Energy=   0.316297
 Sum of electronic and zero-point Energies=   -2505.338240
 Sum of electronic and thermal Energies=   -2505.315872
 Sum of electronic and thermal Enthalpies=   -2505.314928
 Sum of electronic and thermal Free Energies=   -2505.390915
```
C         -1.52959 -0.2832   2.37299
C          0.66317  0.22089  2.98422
C          0.26326  0.6746   4.23412
C         -1.09331  0.63081  4.5604
C         -1.99563  0.15047  3.61794
C         -2.38927 -0.76001  1.2763
C         -2.42354 -1.34748 -0.98999
C         -3.81004 -1.52569 -0.93487
C         -4.48983 -1.33293  0.26276
C         -3.76889 -0.93058  1.38643
```

```
H            1.70519  0.22769  2.68906
H            1.00324  1.05034  4.93263
H           -1.44332  0.97224  5.52985
H           -3.05566  0.12324  3.8418
H           -1.82853 -1.35462 -1.94374
H           -4.33707 -1.81067 -1.84006
H           -5.56482 -1.47727  0.32793
H           -4.27553 -0.7549   2.3289
N           -0.20238 -0.25756  2.06901
N           -1.72559 -0.99121  0.10966
Ni           0.23847 -0.93697  0.33881
C            1.67633  1.50578 -2.73846
C            2.84579  2.028   -3.27364
C            3.62099  2.94076 -2.54419
C            3.21083  3.33156 -1.26172
C            2.04348  2.81837 -0.71381
C            1.24056  1.89302 -1.43653
H            1.06449  0.78834 -3.28509
H            3.1614   1.72688 -4.26954
H            4.53515  3.34542 -2.97039
H            3.80754  4.04302 -0.69574
H            1.72245  3.13122  0.27806
C            0.03438  1.35819 -0.9123
H           -0.40418  1.79883 -0.02053
H           -0.58769  0.76477 -1.57417
C            2.01628 -1.61358  0.74633
H            2.78574 -0.88668  0.47812
H            2.16834 -2.07883  1.72067
C            1.43097 -2.39603 -0.29719
H            1.03997 -3.39597 -0.10548
C            1.05503 -1.69432 -1.44099
H            1.63983 -0.81184 -1.69559
C            0.15883 -2.14958 -2.5765
H           -0.45509 -3.01103 -2.18333
H            0.81979 -2.6249  -3.34577
O           -0.57159 -1.09859 -3.03637
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3019133
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2165871
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.305941489868
ΔG_{solv} = -0.0344223

C-2

UB3LYP/6-31g(d)-gas
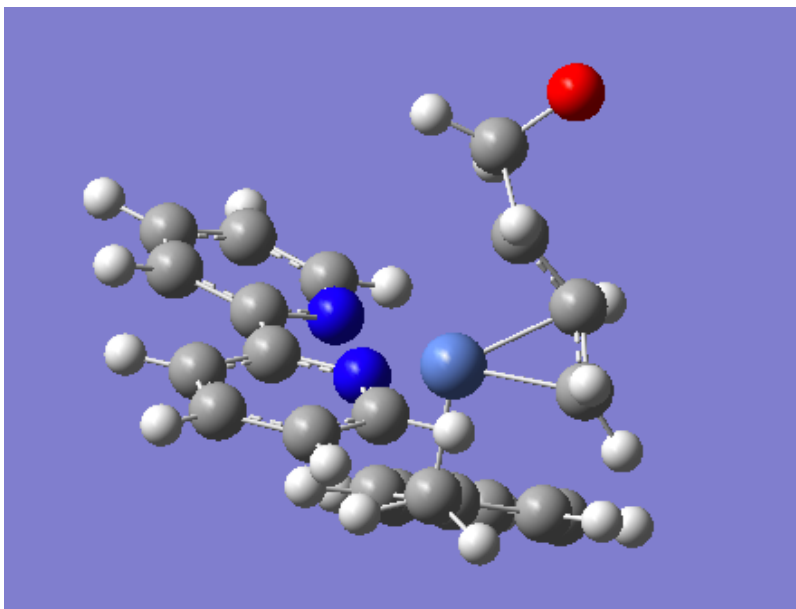Zero-point correction=   0.369826 (Hartree/Particle)
 Thermal correction to Energy=   0.392834
 Thermal correction to Enthalpy=   0.393778
 Thermal correction to Gibbs Free Energy=   0.314718
 Sum of electronic and zero-point Energies=   -2505.325775
 Sum of electronic and thermal Energies=   -2505.302767
 Sum of electronic and thermal Enthalpies=   -2505.301822
 Sum of electronic and thermal Free Energies=   -2505.380882

C	-1.62218	1.16952	1.45613
C	0.64136	1.64826	1.75908
C	0.36976	2.50199	2.81826
C	-0.96166	2.67298	3.22143
C	-1.96043	1.99619	2.53633
C	-2.58406	0.42653	0.64641
C	-2.82861	-1.24468	-0.96177
C	-4.21303	-1.15034	-0.91969
C	-4.79843	-0.207	-0.06653
C	-3.97444	0.58556	0.72004
H	1.65712	1.47305	1.42634
H	1.18368	3.01643	3.31768
H	-1.21053	3.3183	4.05843
H	-2.99628	2.09525	2.84174
H	-2.33918	-1.95915	-1.60946
H	-4.81458	-1.80219	-1.54379
H	-5.87724	-0.09358	-0.01901
H	-4.40198	1.33262	1.37982
N	-0.31851	0.99429	1.07499
N	-2.01407	-0.48111	-0.20702

```
Ni          -0.07667  -0.34984  -0.28626
C           -1.33748  -3.88112   0.24595
C           -1.33127  -5.10311  -0.41138
C           -0.12065  -5.72729  -0.74196
C            1.08931  -5.10658  -0.40124
C            1.09346  -3.8841    0.25448
C           -0.12247  -3.22748   0.60068
H           -2.28203  -3.4096    0.50672
H           -2.27386  -5.57997  -0.66769
H           -0.12019  -6.68497  -1.2546
H            2.0324   -5.5878   -0.64897
H            2.03604  -3.41001   0.51768
C            1.85701  -0.2654   -0.58211
H            2.08088   0.69529  -1.05138
H            2.54679  -0.55102   0.2092
C            1.29698  -1.29685  -1.3792
H            1.4648   -2.34436  -1.13338
C            0.26117  -0.96829  -2.26673
H            0.27091   0.02926  -2.7135
C           -0.38307  -2.01817  -3.16052
H           -1.40746  -1.68671  -3.45706
H           -0.51077  -2.96736  -2.5778
O            0.50561  -2.06785  -4.17323
C           -0.12163  -1.97317   1.25659
H           -0.98792  -2.25324   1.81873
H            0.72022  -1.89755   1.9127
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2895438
C-3

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.369801 (Hartree/Particle)

Thermal correction to Energy=   0.392814
Thermal correction to Enthalpy=   0.393758
Thermal correction to Gibbs Free Energy=   0.314635
Sum of electronic and zero-point Energies=   -2505.325804
Sum of electronic and thermal Energies=   -2505.302790
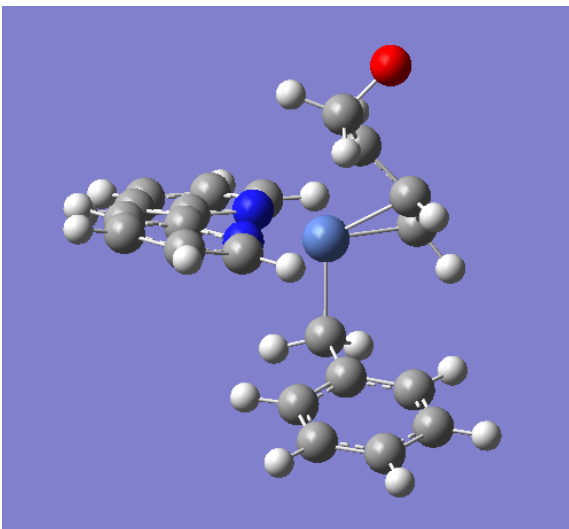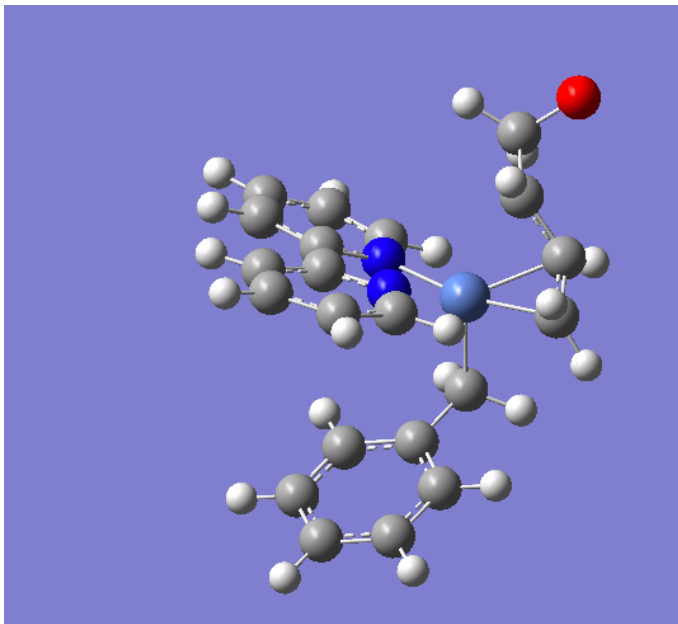Sum of electronic and thermal Enthalpies=   -2505.301846
Sum of electronic and thermal Free Energies=   -2505.380970

```
C         -0.73335  1.60748  1.99082
C          1.55734  1.29446  2.22856
C          1.63974  2.2719   3.21585
C          0.47224  2.92562  3.6044
C         -0.72791  2.59292  2.98322
C         -1.9273   1.23762  1.19858
C         -2.69253  0.00257 -0.61157
C         -3.96139  0.57001 -0.5274
C         -4.21152  1.49454  0.48475
C         -3.18075  1.8392   1.35356
H          2.43529  0.75735  1.88979
H          2.59914  2.50877  3.66284
H          0.49437  3.69226  4.37321
H         -1.64267  3.10406  3.25963
H         -2.43843 -0.71363 -1.38487
H         -4.72725  0.2917  -1.24348
H         -5.18999  1.95403  0.58902
H         -3.34843  2.57701  2.12959
N          0.40107  0.96325  1.64103
N         -1.70834  0.30719  0.24303
Ni         0.24493 -0.41575  0.16021
C          2.52979 -2.75891  1.4011
C          3.78761 -2.99046  1.95334
C          4.08378 -2.56029  3.25021
C          3.10232 -1.89856  3.98924
C          1.84386 -1.66377  3.43316
C          1.52489 -2.08862  2.129
H          2.30972 -3.10079  0.39376
H          4.54141 -3.51229  1.36893
H          5.06509 -2.74427  3.67948
H          3.31281 -1.56961  5.00432
H          1.08084 -1.16316  4.0255
C          0.17688 -1.84665  1.54297
H         -0.52366 -1.48446  2.30456
H         -0.22486 -2.75526  1.09854
C          0.5153  -2.11822 -1.50634
H         -0.5057  -1.99355 -1.80115
H          0.89017 -3.09511 -1.28262
C          1.33528 -1.04309 -1.41534
```

```
H          2.35628 -1.16775 -1.12053
C          0.79575  0.36291 -1.73734
H         -0.23635  0.29478 -2.01127
C          1.89285  1.40864 -1.46455
H          2.69418  0.95174 -0.92232
H          1.48436  2.21198 -0.88777
O          2.54991  1.74104 -2.69039
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
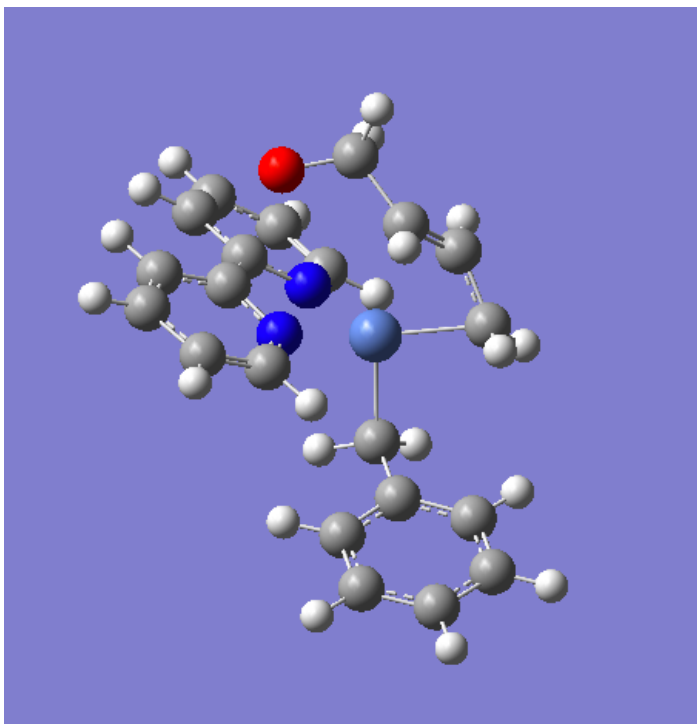HF=-2505.2896038
C-4

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.369649 (Hartree/Particle)
 Thermal correction to Energy=   0.392795
 Thermal correction to Enthalpy=   0.393739
 Thermal correction to Gibbs Free Energy=   0.313549
 Sum of electronic and zero-point Energies=   -2505.325643
 Sum of electronic and thermal Energies=   -2505.302496
 Sum of electronic and thermal Enthalpies=   -2505.301552
 Sum of electronic and thermal Free Energies=   -2505.381742
```
C         -1.44374  1.77606  0.72743
C          0.8198   2.2548   1.03038
C          0.5482   3.10853  2.08955
C         -0.78322  3.27952  2.49273
C         -1.78199  2.60273  1.80763
C         -2.40562  1.03307 -0.08229
C         -2.65016 -0.63814 -1.69047
C         -4.03459 -0.5438  -1.64839
C         -4.61999  0.39954 -0.79523
C         -3.796    1.1921  -0.00867
```

H	1.83557	2.07959	0.69763
H	1.36212	3.62297	2.58898
H	-1.03208	3.92484	3.32973
H	-2.81783	2.70179	2.11304
H	-2.16074	-1.35261	-2.33816
H	-4.63613	-1.19565	-2.27249
H	-5.69879	0.51296	-0.74772
H	-4.22353	1.93916	0.65111
N	-0.14007	1.60083	0.34629
N	-1.83563	0.12543	-0.93572
Ni	0.10178	0.2567	-1.01496
C	2.36732	-2.34947	0.82567
C	3.59835	-2.37253	1.46551
C	3.82681	-1.57897	2.598
C	2.79814	-0.75918	3.08294
C	1.56452	-0.72798	2.44918
C	1.30636	-1.5232	1.29572
H	2.19685	-2.97618	-0.04651
H	4.38909	-3.01458	1.08592
H	4.79127	-1.60161	3.09727
H	2.96604	-0.14545	3.96469
H	0.77069	-0.09141	2.83273
C	0.05361	-1.48258	0.63809
H	-0.78563	-0.96831	1.09309
H	-0.17001	-2.17765	-0.16422
C	2.03546	0.34114	-1.31081
H	2.25932	1.30183	-1.78009
H	2.72524	0.05552	-0.5195
C	1.47543	-0.69031	-2.1079
H	1.64324	-1.73782	-1.86208
C	0.43961	-0.36175	-2.99543
H	0.44935	0.6358	-3.4422
C	-0.20462	-1.41163	-3.88922
H	-1.04484	-0.89038	-3.8283
H	-0.33233	-2.36082	-3.3065
O	-0.19657	-1.38452	-5.26588

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2866806
C-5

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.369916 (Hartree/Particle)
 Thermal correction to Energy=   0.392504
 Thermal correction to Enthalpy=   0.393448
 Thermal correction to Gibbs Free Energy=   0.317174
 Sum of electronic and zero-point Energies=   -2505.337060
 Sum of electronic and thermal Energies=   -2505.314472
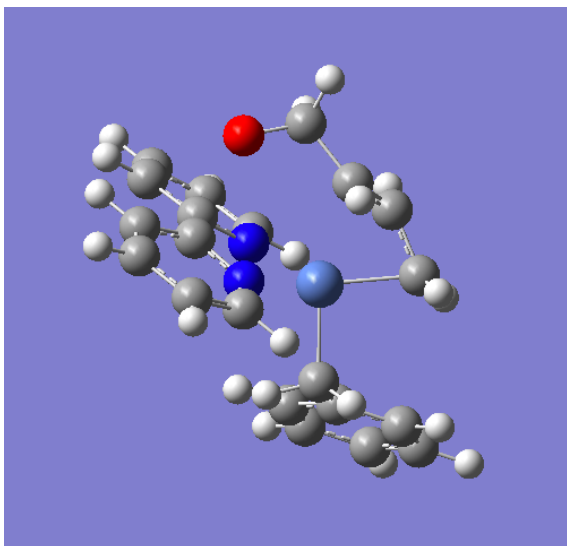 Sum of electronic and thermal Enthalpies=   -2505.313528
 Sum of electronic and thermal Free Energies=   -2505.389802
C   -1.13643 1.77588 0.86103
 C   1.14698 1.6353   1.2649
 C   1.10976 2.71345 2.14195
 C   -0.11655 3.33246 2.38168
 C   -1.25249 2.86166 1.73483
 C   -2.25341 1.23768 0.06375
 C   -2.86749 -0.30137 -1.56745
 C   -4.18843 0.1243 -1.55557
 C   -4.54594 1.14957 -0.67754
 C   -3.57146 1.70469 0.14326
 H   2.07258 1.1099   1.05523
 H   2.02226 3.06247 2.61364
 H   -0.18671 4.17983 3.05741
 H   -2.20864 3.34559 1.89706
 H   -2.54182 -1.11293 -2.21298
 H   -4.91467 -0.33862 -2.21647
 H   -5.56928 1.5096 -0.63179

```
H          -3.83189  2.49891  0.83307
N           0.0504   1.16376  0.65804
N          -1.91835  0.23737 -0.78319
Ni         -0.05189 -0.38076 -0.64957
C           1.7794  -3.35097  0.51076
C           3.04663 -3.77398  0.90613
C           3.69701 -3.15945  1.97752
C           3.05003 -2.12438  2.65361
C           1.7778  -1.70409  2.26261
C           1.0984  -2.29786  1.17333
H           1.28705 -3.82902 -0.32211
H           3.53249 -4.5899   0.37413
H           4.68834 -3.48405  2.28299
H           3.53492 -1.64767  3.5032
H           1.28084 -0.9189   2.82689
C          -0.23554 -1.80478  0.73391
H          -0.80259 -1.40319  1.58291
H          -0.82863 -2.60682  0.27432
C           0.62079 -1.61336 -2.30596
H           1.63756 -1.93435 -2.05621
H          -0.00533 -2.40989 -2.7328
C           0.3645  -0.25858 -2.72754
H          -0.511   -0.08552 -3.36965
C           1.03275  0.80061 -2.40501
H           1.98761  0.72126 -1.86108
C           0.73687  2.21812 -2.86379
H           0.06217  2.20209 -3.76173
H           1.71133  2.65456 -3.21358
O           0.2101   2.89133 -1.85414
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
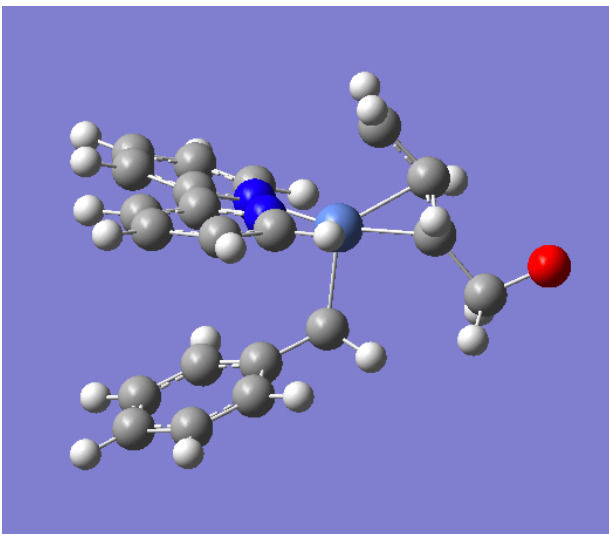HF=-2505.2900261
C-6

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.369732 (Hartree/Particle)
 Thermal correction to Energy=   0.392379
 Thermal correction to Enthalpy=   0.393323
 Thermal correction to Gibbs Free Energy=   0.316313
 Sum of electronic and zero-point Energies=   -2505.337440
 Sum of electronic and thermal Energies=   -2505.314793
 Sum of electronic and thermal Enthalpies=   -2505.313849
 Sum of electronic and thermal Free Energies=   -2505.390859

C	-0.87972	1.89199	0.57811
C	1.2328	1.30693	1.3873
C	1.31204	2.44265	2.17655
C	0.21174	3.31218	2.18774
C	-0.89273	3.03158	1.4067
C	-2.0376	1.42902	-0.2085
C	-2.94316	-0.39549	-1.35897
C	-4.18613	0.20169	-1.46097
C	-4.34363	1.48448	-0.9083
C	-3.27872	2.095	-0.27534
H	2.03496	0.57533	1.36867
H	2.19518	2.63092	2.77691
H	0.2222	4.20157	2.81196
H	-1.7446	3.70001	1.39784
H	-2.75538	-1.38593	-1.76545
H	-5.00445	-0.31134	-1.95404
H	-5.30068	1.99474	-0.97249
H	-3.38169	3.08823	0.14336
N	0.15625	1.01852	0.63578
N	-1.90034	0.18963	-0.74146
Ni	0.02995	-0.43224	-0.72284
C	-2.59033	-2.10808	0.58976

C	-3.81828	-2.6737	0.25448
C	-3.87761	-3.78702	-0.58853
C	-2.68931	-4.32969	-1.08066
C	-1.46089	-3.76194	-0.7413
C	-1.37767	-2.63294	0.09803
H	-2.56019	-1.25106	1.25895
H	-4.73417	-2.24804	0.65761
H	-4.83516	-4.22943	-0.84938
H	-2.71656	-5.20591	-1.72423
H	-0.54176	-4.20674	-1.11574
C	-0.06639	-2.02845	0.45053
H	0.74358	-2.75887	0.35718
H	-0.07684	-1.64287	1.47459
C	0.91622	-1.41062	-2.23665
H	1.95672	-1.38396	-1.90472
H	0.58624	-2.38802	-2.57604
C	0.3282	-0.24107	-2.79864
H	-0.58333	-0.36751	-3.38441
C	0.59174	1.02972	-2.31258
H	1.55181	1.2408	-1.83684
C	-0.30661	2.23637	-2.57613
H	-1.19089	1.85362	-3.1449
H	0.23142	2.89086	-3.30404
O	-0.62714	2.91684	-1.43851

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2893197
C-7

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.369656 (Hartree/Particle)
 Thermal correction to Energy=   0.392606
 Thermal correction to Enthalpy=   0.393551
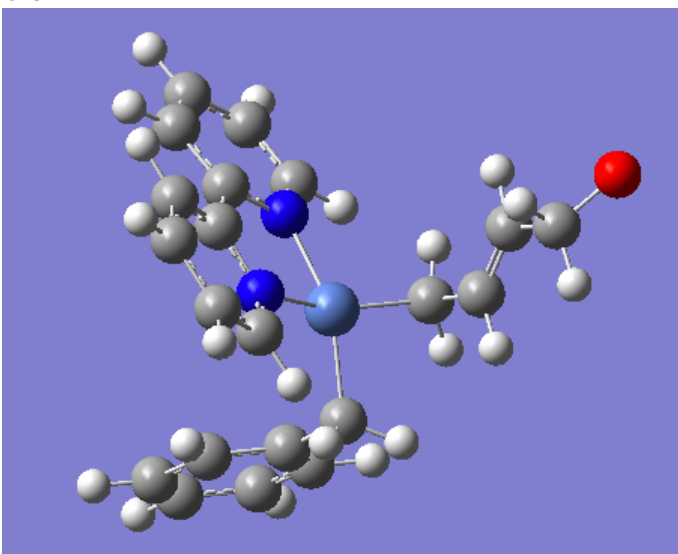
Thermal correction to Gibbs Free Energy=   0.315562
Sum of electronic and zero-point Energies=   -2505.322197
Sum of electronic and thermal Energies=   -2505.299246
Sum of electronic and thermal Enthalpies=   -2505.298302
Sum of electronic and thermal Free Energies=   -2505.376291

C	-1.62298	1.14053	1.48368
C	0.64055	1.61927	1.78663
C	0.36895	2.47301	2.84581
C	-0.96246	2.64399	3.24898
C	-1.96124	1.96721	2.56388
C	-2.58487	0.39754	0.67396
C	-2.82941	-1.27367	-0.93422
C	-4.21384	-1.17933	-0.89214
C	-4.79923	-0.23599	-0.03898
C	-3.97525	0.55658	0.74759
H	1.65632	1.44406	1.45389
H	1.18287	2.98744	3.34524
H	-1.21133	3.28931	4.08598
H	-2.99708	2.06626	2.86929
H	-2.33998	-1.98813	-1.5819
H	-4.81538	-1.83118	-1.51624
H	-5.87804	-0.12257	0.00854
H	-4.40278	1.30363	1.40737
N	-0.31931	0.9653	1.10254
N	-2.01488	-0.5101	-0.17946
Ni	-0.07747	-0.37883	-0.25871
C	2.19289	-2.81107	1.41662
C	3.42392	-2.83413	2.05646
C	3.65238	-2.04057	3.18895
C	2.62371	-1.22078	3.67389
C	1.39009	-1.18958	3.04013
C	1.13193	-1.9848	1.88667
H	2.02242	-3.43778	0.54444
H	4.21466	-3.47618	1.67686
H	4.61684	-2.06321	3.68822
H	2.79161	-0.60705	4.55564
H	0.59626	-0.55301	3.42368
C	1.85621	-0.29439	-0.55456
H	2.08007	0.6663	-1.02383
C	1.29618	-1.32584	-1.35165
H	1.464	-2.37335	-1.10583
C	0.26036	-0.99728	-2.23918
H	0.2701	0.00027	-2.68594
C	-0.12082	-1.94418	1.22904
H	-0.32824	-2.89166	0.77719
H	-0.65255	-1.86624	2.15429

```
C           2.83264 -0.6987   0.56559
H           3.13117  0.17261  1.1102
H           2.34991 -1.3858   1.22873
O           3.98549 -1.32031 -0.00838
H          -0.19258 -1.73542 -2.86758
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2911078
C-8

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.368391 (Hartree/Particle)
 Thermal correction to Energy=   0.391645
 Thermal correction to Enthalpy=   0.392589
 Thermal correction to Gibbs Free Energy=   0.311125
 Sum of electronic and zero-point Energies=   -2505.319608
 Sum of electronic and thermal Energies=   -2505.296354
 Sum of electronic and thermal Enthalpies=   -2505.295410
 Sum of electronic and thermal Free Energies=   -2505.376874
```
C          -0.10058  1.8885   0.88259
C           2.04099  1.17644  1.48799
C           2.17529  2.1877   2.42141
C           1.10034  3.07566  2.61126
C          -0.0363   2.91885  1.83914
C          -1.21775  1.66917 -0.01978
C          -2.1033   0.2744  -1.67241
C          -3.2528   1.03504 -1.77935
C          -3.37668  2.18227 -0.97469
C          -2.35429  2.49465 -0.09667
H           2.83809  0.45937  1.32403
H           3.09425  2.281    2.9905
H           1.15907  3.86965  3.34961
H          -0.88018  3.587    1.97162
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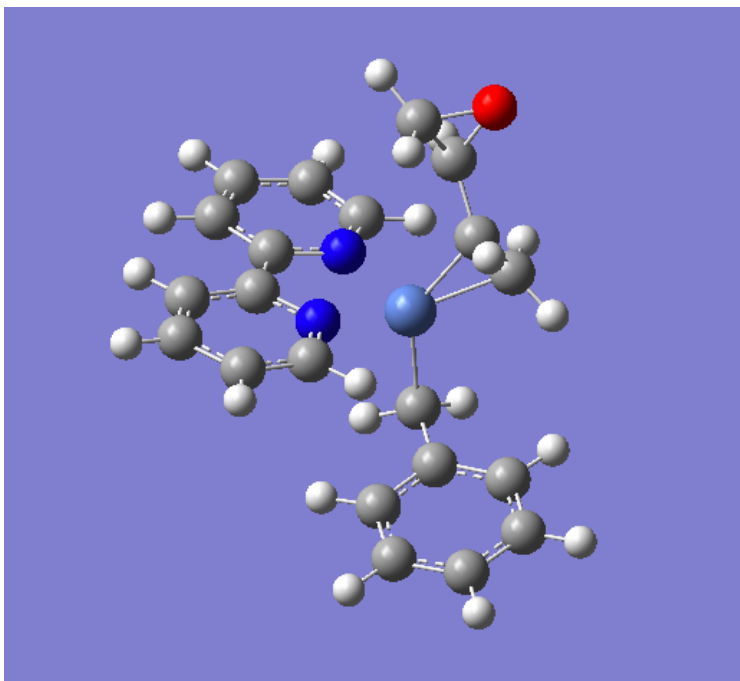
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H          -1.96778 -0.61661 -2.27602
H          -4.03474  0.74162 -2.47174
H          -4.25779  2.81355 -1.03969
H          -2.42704  3.37811  0.52834
N           0.93847  1.00375  0.72698
N          -1.09148  0.56335 -0.82468
Ni          0.59975 -0.46153 -0.53433
C          -0.46078 -1.96343  2.21832
C          -1.67215 -2.45573  2.69521
C          -2.33742 -3.48093  2.01597
C          -1.76531 -4.00964  0.85489
C          -0.55336 -3.51842  0.37751
C           0.1352  -2.47551  1.04093
H           0.05131 -1.17399  2.76428
H          -2.09767 -2.04306  3.60714
H          -3.28202 -3.86681  2.38962
H          -2.26356 -4.8173   0.32347
H          -0.11394 -3.95198 -0.5181
C           1.39934 -1.92063  0.5179
H           1.95631 -2.63223 -0.09841
H           2.04791 -1.54282  1.31383
C           0.79822 -1.34515 -2.29287
H           0.0134  -1.06261 -2.99433
H           0.9662  -2.41642 -2.22316
C           1.86689 -0.45146 -2.07729
H           2.83807 -0.84443 -1.77868
C           1.93329  0.86816 -2.75578
H           0.97485  1.27296 -3.08645
C           3.03285  1.819   -2.52881
H           3.8279   1.5609  -1.82696
H           2.86206  2.88941 -2.6555
O           3.95474  1.95989 -3.59019
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2711397
B'

UB3LYP/6-31g(d)-gas

Zero-point correction=   0.370239 (Hartree/Particle)
 Thermal correction to Energy=   0.393161
 Thermal correction to Enthalpy=   0.394106
 Thermal correction to Gibbs Free Energy=   0.313482
 Sum of electronic and zero-point Energies=   -2505.361098
 Sum of electronic and thermal Energies=   -2505.338175
 Sum of electronic and thermal Enthalpies=   -2505.337231
 Sum of electronic and thermal Free Energies=   -2505.417854

C	-1.08408	1.75012	0.69367
C	1.20805	1.4324	0.92934
C	1.31986	2.51277	1.79753
C	0.17173	3.23828	2.11524
C	-1.04231	2.84826	1.55937
C	-2.32473	1.25743	0.05758
C	-3.19768	-0.16329	-1.55011
C	-4.50409	0.21548	-1.25762
C	-4.71089	1.15569	-0.24603
C	-3.60965	1.68102	0.4217
H	2.06897	0.82662	0.67327
H	2.28763	2.77115	2.21412
H	0.21964	4.09302	2.7832
H	-1.94679	3.40226	1.78355
H	-2.98412	-0.89679	-2.32327
H	-5.33434	-0.21716	-1.80642
H	-5.71495	1.47037	0.0227
H	-3.75112	2.39786	1.22303

```
N            0.04077  1.05826  0.37497
N           -2.13     0.34052 -0.91687
Ni          -0.11549 -0.3651  -0.978
C            1.8752  -3.05474  0.46009
C            3.08711 -3.34317  1.08223
C            3.41955 -2.74473  2.30161
C            2.51274 -1.86055  2.8886
C            1.30057 -1.57219  2.26112
C            0.94589 -2.15456  1.02571
H            1.62974 -3.54356 -0.4801
H            3.77497 -4.04587  0.61733
H            4.36351 -2.97313  2.78918
H            2.74479 -1.39979  3.84657
H            0.59517 -0.89906  2.7439
C           -0.33231 -1.82424  0.35176
H           -1.06937 -1.46494  1.08141
H           -0.74897 -2.69932 -0.15538
C            0.13302 -1.60994 -2.47576
H           -0.70148 -1.50203 -3.17391
H            0.41179 -2.64307 -2.28903
C            1.14787 -0.61584 -2.46573
H            2.17897 -0.84164 -2.19988
C            0.69765  0.72139 -2.57881
H           -0.14932  0.91912 -3.23509
C            1.65112  1.8969  -2.44166
H            2.43771  1.65923 -1.6992
H            1.11032  2.80091 -2.10134
O            1.54377  1.15542 -3.7495
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3023645
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.2104688
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.329788687910
ΔG_{solv} = -0.0193036

B'-2

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.370190 (Hartree/Particle)
 Thermal correction to Energy=   0.393104
 Thermal correction to Enthalpy=   0.394049
 Thermal correction to Gibbs Free Energy=   0.314332
 Sum of electronic and zero-point Energies=   -2505.362509
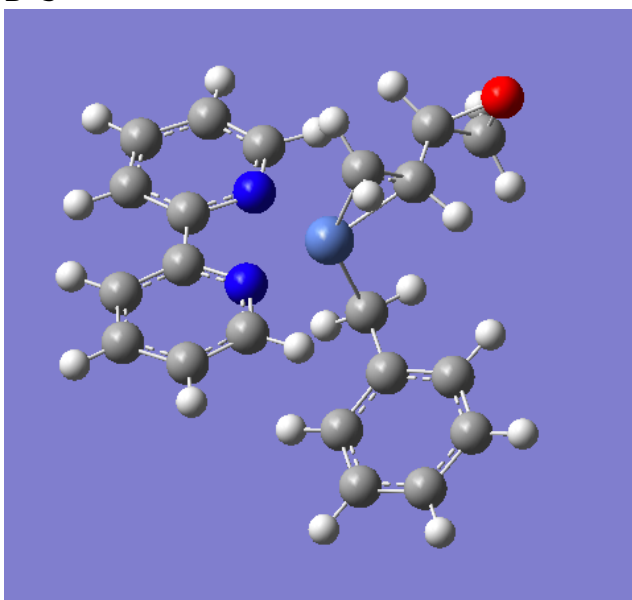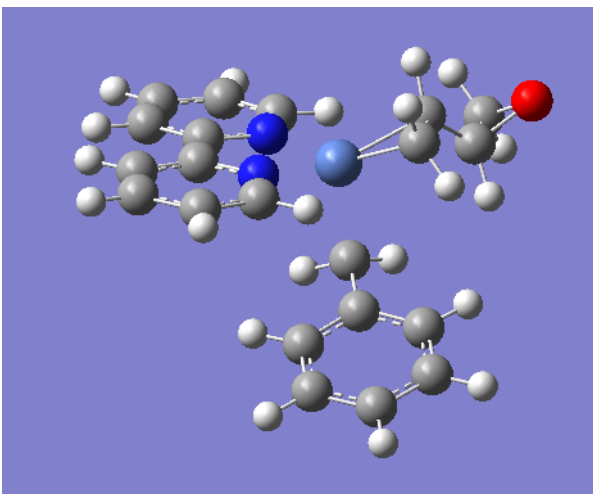 Sum of electronic and thermal Energies=   -2505.339594
 Sum of electronic and thermal Enthalpies=   -2505.338650
 Sum of electronic and thermal Free Energies=   -2505.418367
C   0.46891   2.22078   1.03004
C   2.42025   1.24427   1.8697
C   2.69731   2.33605   2.67462
C   1.7827   3.40079   2.66895
C   0.66014   3.3399   1.8665
C   -0.75638   1.96626   0.25058
C   -1.96456   0.32846 -0.90454
C   -3.08325   1.13605 -1.00517
C   -3.01556   2.42486 -0.44975
C   -1.8607   2.83909   0.18559
H   3.07226   0.37448   1.85222
H   3.58429   2.34796   3.29817
H   1.95008   4.26875   3.30087
H   -0.04972   4.15733   1.84873
H   -1.9545   -0.68152 -1.30391
H   -3.97812   0.77482 -1.49986
H   -3.86893   3.09439 -0.51306
H   -1.78899   3.83421   0.6066
N   1.32855   1.17382   1.09003
N   -0.83642   0.72262 -0.28404
Ni   0.96242 -0.22345 -0.27487
C   -1.56249 -2.67354   0.91222

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C          -2.493   -3.6545   0.57036
C          -2.08543 -4.81463 -0.09164
C          -0.73268 -4.98137 -0.3992
C           0.19419 -3.9985  -0.05708
C          -0.19556 -2.81643  0.60302
H          -1.89095 -1.78046  1.43917
H          -3.54001 -3.51546  0.82973
H          -2.80863 -5.58151 -0.35559
H          -0.39668 -5.88562 -0.9013
H           1.24658 -4.15102 -0.28855
C           0.78318 -1.75973  0.96693
H           1.78773 -2.18279  1.09092
H           0.49149 -1.26713  1.89993
C           1.70888 -1.3298  -1.7777
H           2.75666 -1.43289 -1.48559
H           1.23339 -2.2593  -2.07381
C           1.27443 -0.09672 -2.34676
H           0.34344 -0.09952 -2.91443
C           1.73343  1.12438 -1.87845
H           2.71771  1.18467 -1.40867
C           1.04063  2.46017 -2.12508
H           0.08058  2.23201 -2.65144
H           1.65022  3.00972 -2.88269
O           1.29746  1.76525 -0.6817
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3027151
B'-3

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.370276 (Hartree/Particle)
 Thermal correction to Energy=   0.393202

Thermal correction to Enthalpy=   0.394146
Thermal correction to Gibbs Free Energy=   0.314682
Sum of electronic and zero-point Energies=   -2505.359391
Sum of electronic and thermal Energies=   -2505.336465
Sum of electronic and thermal Enthalpies=   -2505.335521
Sum of electronic and thermal Free Energies=   -2505.414985

C	-1.13741	1.79406	0.98483
C	1.15328	1.48104	1.22257
C	1.23568	2.45849	2.20987
C	0.06818	3.1122	2.59842
C	-1.13197	2.7795	1.97723
C	-2.33136	1.4242	0.19259
C	-3.09659	0.18915	-1.61755
C	-4.36545	0.75659	-1.53338
C	-4.61558	1.68112	-0.52123
C	-3.58481	2.02579	0.34758
H	2.03123	0.94393	0.8838
H	2.19508	2.69535	2.65686
H	0.09031	3.87884	3.36723
H	-2.04673	3.29064	2.25365
H	-2.84249	-0.52705	-2.39085
H	-5.13131	0.47828	-2.24946
H	-5.59405	2.14062	-0.41697
H	-3.75249	2.76359	1.1236
N	-0.00299	1.14983	0.63504
N	-2.1124	0.49377	-0.76296
Ni	-0.15913	-0.22916	-0.84577
C	2.12573	-2.57233	0.39512
C	3.38355	-2.80388	0.94735
C	3.67972	-2.3737	2.24423
C	2.69826	-1.71197	2.98325
C	1.4398	-1.47718	2.42718
C	1.12083	-1.90204	1.12302
H	1.90566	-2.91421	-0.61222
H	4.13735	-3.3257	0.36294
H	4.66103	-2.55769	2.67349
H	2.90875	-1.38302	3.99834
H	0.67678	-0.97658	3.01952
C	-0.22718	-1.66007	0.53699
H	-0.92772	-1.29788	1.29858
H	-0.62892	-2.56868	0.09256
C	1.73109	1.07886	-1.98152
H	1.0737	1.90427	-2.15883
H	2.65957	1.23631	-1.47355
C	1.39179	-0.16528	-2.39812
H	2.04919	-0.99068	-2.22082

```
C           0.05548  -0.39189  -3.12923
H          -0.46579   0.53851  -3.21611
C          -0.04171  -1.86209  -3.57719
H          -1.06855  -2.16239  -3.59496
H           0.4989   -2.48039  -2.89137
O           0.29369  -1.96107  -4.96377
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.3017847
B'-4

UB3LYP/6-31g(d)-gas
Zero-point correction=   0.370248 (Hartree/Particle)
 Thermal correction to Energy=   0.393125
 Thermal correction to Enthalpy=   0.394070
 Thermal correction to Gibbs Free Energy=   0.314670
 Sum of electronic and zero-point Energies=   -2505.353593
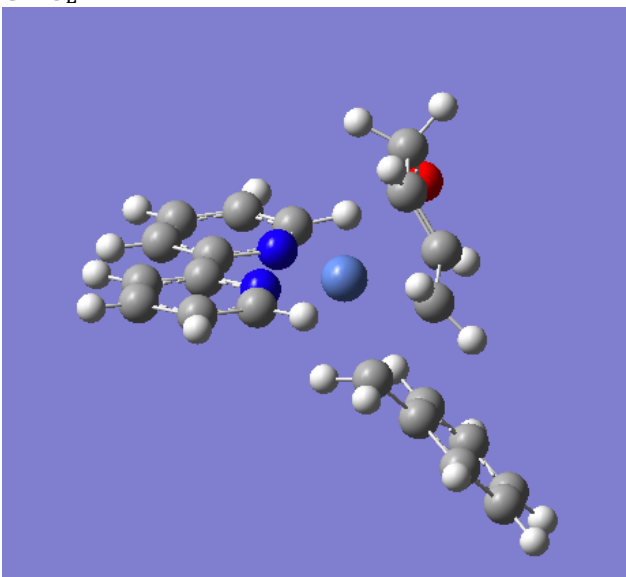 Sum of electronic and thermal Energies=   -2505.330716
 Sum of electronic and thermal Enthalpies=   -2505.329771
 Sum of electronic and thermal Free Energies=   -2505.409171
```
C          -1.0631    1.82374   1.03736
C           1.22759   1.51072   1.27509
C           1.30999   2.48816   2.26239
C           0.14249   3.14188   2.65094
C          -1.05766   2.80918   2.02976
C          -2.25705   1.45388   0.24512
C          -3.02228   0.21883  -1.56503
C          -4.29114   0.78627  -1.48086
C          -4.54127   1.7108   -0.46871
C          -3.5105    2.05546   0.4001
H           2.10555   0.97361   0.93633
H           2.26939   2.72503   2.70938
H           0.16462   3.90852   3.41975
H          -1.97242   3.32032   2.30617
H          -2.76818  -0.49737  -2.33833
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H	-5.057	0.50796	-2.19694
H	-5.51974	2.17029	-0.36445
H	-3.67818	2.79327	1.17612
N	0.07132	1.17951	0.68757
N	-2.03809	0.52345	-0.71044
Ni	-0.08482	-0.19949	-0.79325
C	2.20004	-2.54265	0.44764
C	3.45786	-2.7742	0.99988
C	3.75403	-2.34402	2.29675
C	2.77257	-1.68229	3.03577
C	1.51411	-1.44751	2.4797
C	1.19514	-1.87236	1.17554
H	1.97997	-2.88453	-0.5597
H	4.21166	-3.29603	0.41547
H	4.73534	-2.52801	2.72602
H	2.98306	-1.35335	4.05086
H	0.75109	-0.9469	3.07204
C	-0.15287	-1.63039	0.58951
H	-0.85341	-1.2682	1.3511
H	-0.55461	-2.539	0.14508
C	2.07877	-0.65719	-1.7521
H	2.13387	-1.69386	-1.49289
H	2.7746	0.03618	-1.32788
C	1.13071	-0.21937	-2.61584
H	1.0756	0.8173	-2.87505
C	0.12923	-1.2173	-3.2264
H	0.33424	-2.20001	-2.85608
C	-0.89321	-0.45517	-4.08976
H	-0.80609	0.59468	-3.90237
H	-1.88199	-0.78078	-3.84242
O	-0.49923	-0.51902	-5.46293

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas

HF=-2505.297009
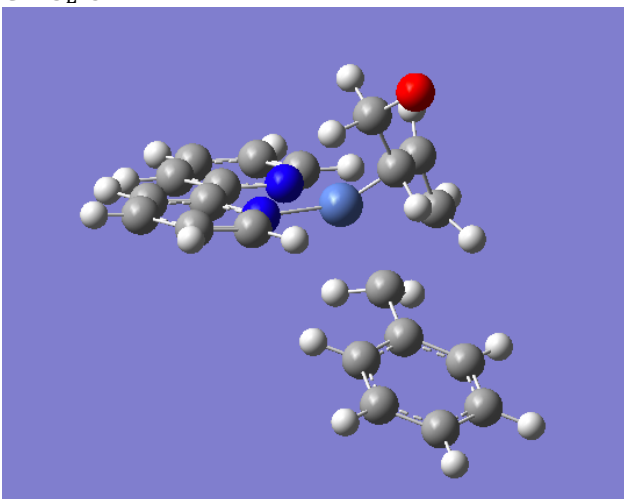
C-TS$_L$-1
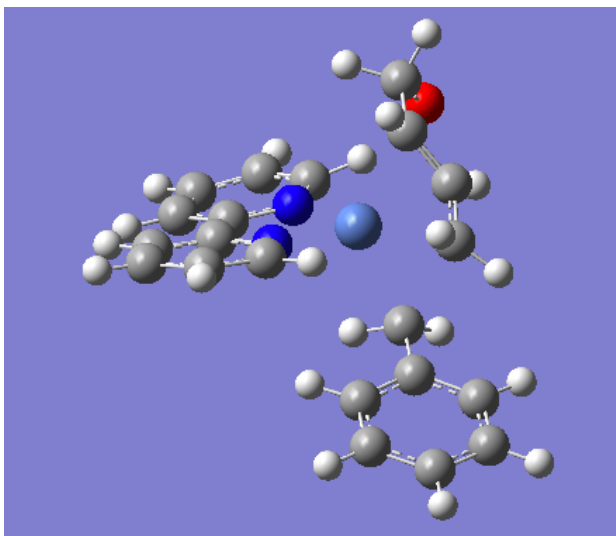
UB3LYP/6-31g(d)-gas

Imaginary frequency = -372.50 cm^{-1}

Zero-point correction=   0.368419 (Hartree/Particle)
 Thermal correction to Energy=   0.390471
 Thermal correction to Enthalpy=   0.391415
 Thermal correction to Gibbs Free Energy=   0.315259
 Sum of electronic and zero-point Energies=   -2505.302546
 Sum of electronic and thermal Energies=   -2505.280494
 Sum of electronic and thermal Enthalpies=   -2505.279550
 Sum of electronic and thermal Free Energies=   -2505.355706

C	-1.45976	1.0688	1.43578
C	0.80377	1.54754	1.73872
C	0.53218	2.40127	2.7979
C	-0.79924	2.57226	3.20107
C	-1.79802	1.89547	2.51598
C	-2.42164	0.32581	0.62606
C	-2.66619	-1.3454	-0.98213
C	-4.05061	-1.25106	-0.94005
C	-4.63601	-0.30772	-0.08689
C	-3.81203	0.48484	0.69968
H	1.81954	1.37233	1.40598
H	1.3461	2.91571	3.29733
H	-1.04811	3.21758	4.03807
H	-2.83386	1.99453	2.82138
H	-2.17676	-2.05987	-1.62981
H	-4.65216	-1.90291	-1.56414
H	-5.71482	-0.1943	-0.03937
H	-4.23956	1.2319	1.35946
N	-0.15609	0.89357	1.05464
N	-1.85166	-0.58183	-0.22737
Ni	-0.09138	-0.15237	-0.29102

```
C        1.40658  0.18509 -1.935
H        0.90422  1.14578 -1.80097
H        2.43233  0.54569 -1.8985
C        1.20205 -0.77633 -2.95809
H        2.03807 -1.42333 -3.21946
C       -0.09025 -1.29006 -3.1442
H       -1.05817 -0.98736 -2.73639
C       -0.38933 -2.31718 -4.22665
H       -1.20326 -1.90427 -4.87025
H       -0.88647 -2.96965 -3.46247
O        0.63006 -2.8819  -4.90469
C        1.79629 -1.3945  -0.32846
H        1.67602 -1.63567  0.70705
C        3.2946  -1.23918 -0.6487
C        4.05806 -0.2889   0.02994
C        3.88844 -2.04856 -1.6171
C        5.41491 -0.14764 -0.2603
H        3.58942  0.34958  0.79281
C        5.2459  -1.90806 -1.90685
H        3.28689 -2.7977  -2.15195
C        6.00914 -0.9577  -1.22875
H        6.01661  0.60179  0.27413
H        5.71394 -2.54664 -2.67015
H        7.079   -0.84618 -1.45738
H        1.48655 -2.28206 -0.58223
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2785411
C-TS$_L$-2
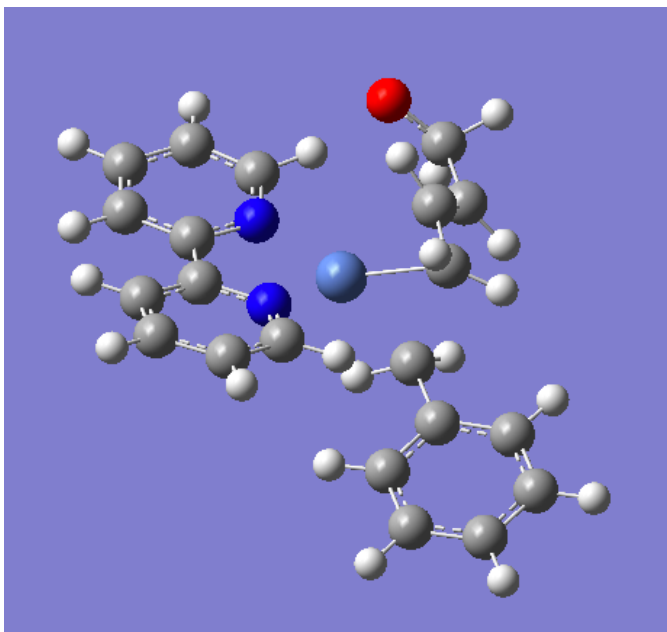

UB3LYP/6-31g(d)-gas
Imaginary frequency = -371.89 cm^{-1}

Zero-point correction=   0.372838 (Hartree/Particle)
Thermal correction to Energy=   0.393787
Thermal correction to Enthalpy=   0.394731
Thermal correction to Gibbs Free Energy= 0.322265
Sum of electronic and zero-point Energies=   -2505.320583
Sum of electronic and thermal Energies=   -2505.299634
Sum of electronic and thermal Enthalpies=   -2505.298690
Sum of electronic and thermal Free Energies=   -2505.371156

C	-1.00887	0.76959	0.9193
C	0.95985	1.84477	0.30467
C	0.82981	2.78452	1.32068
C	-0.26802	2.68807	2.17709
C	-1.19467	1.67128	1.97328
C	-1.96964	-0.29399	0.55778
C	-2.53694	-1.84132	-1.11276
C	-3.7095	-2.17213	-0.42601
C	-3.98906	-1.57106	0.79729
C	-3.11558	-0.60034	1.29042
H	1.81113	1.86631	-0.36859
H	1.57289	3.56656	1.43479
H	-0.40504	3.399	2.98643
H	-2.06442	1.58931	2.61478
H	-2.31825	-2.15008	-2.16778
H	-4.39147	-2.89228	-0.86713
H	-4.88339	-1.8311	1.35702
H	-3.33206	-0.09382	2.22474
N	0.07426	0.85393	0.10338
N	-1.67365	-0.93729	-0.60047
Ni	0.10196	-0.52445	-1.37993
C	1.76253	-0.7881	-2.68121
H	2.1678	0.22457	-2.60622
H	2.54856	-1.49445	-2.92374
C	0.48766	-0.97926	-3.33515
H	0.15873	-1.97837	-3.62657
C	-0.50762	-0.0183	-3.36826
H	-0.26549	1.05033	-3.35161
C	-1.89165	-0.45982	-3.87015
H	-1.97828	0.01892	-4.88624
C	1.86433	-1.64896	-0.77148
H	1.19413	-1.61143	0.09645
C	3.23936	-1.28678	-0.34376
C	3.46652	-0.44167	0.75833
C	4.37014	-1.78998	-1.01499
C	4.75744	-0.09606	1.15612
H	2.61683	-0.07286	1.32633
C	5.66202	-1.44752	-0.62012

H	4.23464	-2.47645	-1.84776
C	5.86423	-0.59166	0.46457
H	4.89901	0.55307	2.01686
H	6.51376	-1.85812	-1.15632
H	6.87101	-0.32607	0.775
H	1.8084	-2.65362	-1.19011
O	-2.8171	0.30385	-3.09217
H	-2.03791	-1.51973	-3.85993

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2824389
C-TS$_L$-3

UB3LYP/6-31g(d)-gas
Imaginary frequency = -371.87 cm^{-1}
Zero-point correction=   0.367897 (Hartree/Particle)
 Thermal correction to Energy=   0.390308
 Thermal correction to Enthalpy=   0.391252
 Thermal correction to Gibbs Free Energy=   0.313707
 Sum of electronic and zero-point Energies=   -2505.285711
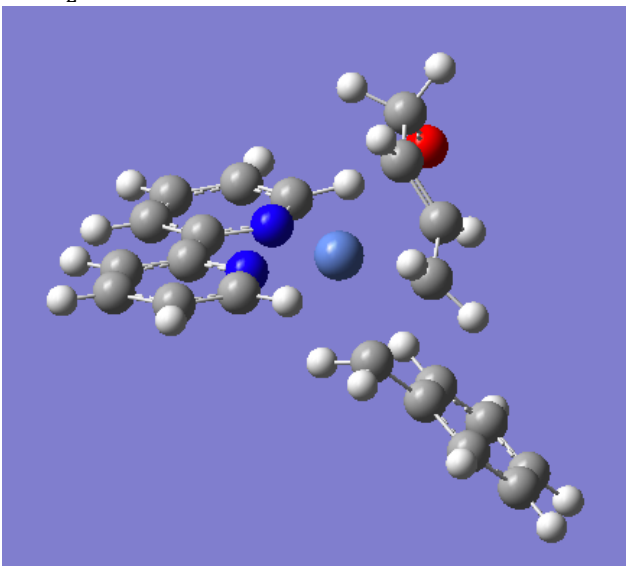 Sum of electronic and thermal Energies=   -2505.263300
 Sum of electronic and thermal Enthalpies=   -2505.262356
 Sum of electronic and thermal Free Energies=   -2505.339901

C	-1.88171	1.04522	1.34899
C	-0.24139	2.48591	0.48394
C	-0.66074	3.52516	1.29052
C	-1.73951	3.31456	2.17007
C	-2.34356	2.06702	2.19093
C	-2.4771	-0.27864	1.26072
C	-2.49572	-2.28282	0.05787
C	-3.45708	-2.83922	0.88286
C	-3.94539	-2.06607	1.95382
C	-3.44889	-0.78775	2.14251
H	0.59888	2.60357	-0.1909

```
H        -0.15483   4.48364   1.23802
H        -2.09775   4.11229   2.81295
H        -3.19183   1.88452   2.84239
H        -2.08651  -2.84194  -0.77981
H        -3.81905  -3.8452    0.69877
H        -4.6939   -2.46856   2.62982
H        -3.79281  -0.18627   2.97728
N        -0.82043   1.2557     0.48987
N        -2.01282  -1.03494   0.21756
Ni       -0.45958  -0.14557  -0.75594
C         0.49173  -1.59695  -1.99981
H         1.55745  -1.61563  -2.22436
H         0.04368  -2.58378  -2.11171
C        -0.25169  -0.50987  -2.63122
H        -1.20267  -0.7056   -3.12654
C         0.19981   0.81156  -2.40439
H         1.27439   0.98961  -2.3215
C        -0.57827   1.99405  -2.95909
O        -0.14652   2.43733  -4.16757
H        -0.49526   2.84847  -2.24476
H        -1.67032   1.76318  -2.9546
C         1.04378  -1.66985  -0.05001
H         0.42463  -1.43754   0.81874
C         2.42202  -1.1337     0.08621
C         2.6741    0.07099    0.7678
C         3.52053  -1.81519   -0.4677
C         3.96853   0.57112    0.89182
H         1.84321   0.61034    1.21524
C         4.81656  -1.31259   -0.35137
H         3.35568  -2.75926   -0.98297
C         5.04707  -0.1155     0.32786
H         4.13739   1.49938    1.43197
H         5.64795  -1.86147   -0.78633
H         6.05615   0.27645    0.42149
H         1.04179  -2.75614   -0.13945
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas

HF=-2505.2776618

C-TS$_L$-4

UB3LYP/6-31g(d)-gas
Imaginary frequency = -409.97 cm^{-1}
Zero-point correction=   0.367346 (Hartree/Particle)
 Thermal correction to Energy=   0.389708
 Thermal correction to Enthalpy=   0.390652
 Thermal correction to Gibbs Free Energy=   0.313773
 Sum of electronic and zero-point Energies=   -2505.292666
 Sum of electronic and thermal Energies=   -2505.270304
 Sum of electronic and thermal Enthalpies=   -2505.269360
 Sum of electronic and thermal Free Energies=   -2505.346240

C	-1.45976	1.0688	1.43578
C	0.80377	1.54754	1.73872
C	0.53218	2.40127	2.7979
C	-0.79924	2.57226	3.20107
C	-1.79802	1.89547	2.51598
C	-2.42164	0.32581	0.62606
C	-2.66619	-1.3454	-0.98213
C	-4.05061	-1.25106	-0.94005
C	-4.63601	-0.30772	-0.08689
C	-3.81203	0.48484	0.69968
H	1.81954	1.37233	1.40598
H	1.3461	2.91571	3.29733
H	-1.04811	3.21758	4.03807
H	-2.83386	1.99453	2.82138
H	-2.17676	-2.05987	-1.62981
H	-4.65216	-1.90291	-1.56414
H	-5.71482	-0.1943	-0.03937
H	-4.23956	1.2319	1.35946
N	-0.15609	0.89357	1.05464

```
N          -1.85166 -0.58183 -0.22737
Ni         -0.09138 -0.15237 -0.29102
C           1.46627  0.07254 -1.93851
H           2.45424 -0.2411  -2.2832
H           1.5396   1.15792 -1.94859
C           0.31301 -0.40294 -2.61437
H          -0.61306  0.15649 -2.49074
C           0.48455 -1.10309 -3.81809
H           1.37745 -1.50466 -4.30418
C          -0.70351 -1.65135 -4.59531
H          -0.4112  -2.64958 -5.00185
H          -0.50825 -0.90548 -5.40919
O          -1.93326 -1.60825 -4.04426
C           1.79629 -1.3945  -0.32846
H           1.67602 -1.63567  0.70705
C           3.2946  -1.23918 -0.6487
C           4.05806 -0.2889   0.02994
C           3.88844 -2.04856 -1.6171
C           5.41491 -0.14764 -0.2603
H           3.58942  0.34958  0.79281
C           5.2459  -1.90806 -1.90685
H           3.28689 -2.7977  -2.15195
C           6.00914 -0.9577  -1.22875
H           6.01661  0.60179  0.27413
H           5.71394 -2.54664 -2.67015
H           7.079   -0.84618 -1.45738
H           1.48655 -2.28206 -0.58223
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2709984
C-TS$_L$-5

UB3LYP/6-31g(d)-gas

Imaginary frequency = -384.55 cm^{-1}
Zero-point correction=   0.368151 (Hartree/Particle)
 Thermal correction to Energy=   0.390247
 Thermal correction to Enthalpy=   0.391191
 Thermal correction to Gibbs Free Energy=   0.314859
 Sum of electronic and zero-point Energies=   -2505.304542
 Sum of electronic and thermal Energies=   -2505.282446
 Sum of electronic and thermal Enthalpies=   -2505.281502
 Sum of electronic and thermal Free Energies=   -2505.357834
C   -1.00887 0.76959 0.9193
 C   0.95985 1.84477 0.30467
 C   0.82981 2.78452 1.32068
 C   -0.26802 2.68807 2.17709
 C   -1.19467 1.67128 1.97328
 C   -1.96964 -0.29399 0.55778
 C   -2.53694 -1.84132 -1.11276
 C   -3.7095 -2.17213 -0.42601
 C   -3.98906 -1.57106 0.79729
 C   -3.11558 -0.60034 1.29042
 H   1.81113 1.86631 -0.36859
 H   1.57289 3.56656 1.43479
 H   -0.40504 3.399   2.98643
 H   -2.06442 1.58931 2.61478
 H   -2.31825 -2.15008 -2.16778
 H   -4.39147 -2.89228 -0.86713
 H   -4.88339 -1.8311   1.35702
 H   -3.33206 -0.09382 2.22474
 N   0.07426 0.85393 0.10338
 N   -1.67365 -0.93729 -0.60047
 Ni   0.10196 -0.52445 -1.37993
 C   1.76253 -0.7881 -2.68121
 H   2.1678   0.22457 -2.60622
 H   2.54856 -1.49445 -2.92374
 C   0.48766 -0.97926 -3.33515
 H   0.15873 -1.97837 -3.62657
 C   -0.50762 -0.0183 -3.36826
 H   -0.26549 1.05033 -3.35161
 C   -1.89165 -0.45982 -3.87015
 H   -1.97828 0.01892 -4.88624
 H   -2.62351 0.1441 -3.25491
 O   -2.07463 -1.7858 -3.85737
 C   1.86433 -1.64896 -0.77148
 H   1.19413 -1.61143 0.09645
 C   1.80404 -3.01301 -1.35586
 C   2.95914 -3.67622 -1.77105
 C   0.56286 -3.64001 -1.46345

```
C          2.87265  -4.96624  -2.29443
H          3.93765  -3.18188  -1.68573
C          0.47625  -4.93038  -1.98753
H         -0.34757  -3.11756  -1.13563
C          1.63106  -5.59319  -2.40303
H          3.78293  -5.48903  -2.62188
H         -0.50249  -5.42452  -2.07231
H          1.56313  -6.61015  -2.81612
H          2.85518  -1.38797  -0.46326
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2824389

C-TS$_L$-6
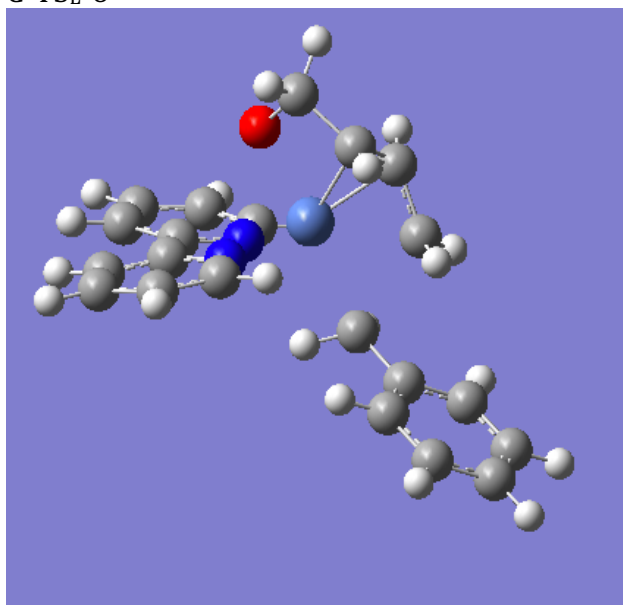
UB3LYP/6-31g(d)-gas
Imaginary frequency = -248.89 cm^{-1}
Zero-point correction=   0.369766 (Hartree/Particle)
 Thermal correction to Energy=   0.392117
 Thermal correction to Enthalpy=   0.393062
 Thermal correction to Gibbs Free Energy=   0.315549
 Sum of electronic and zero-point Energies=   -2505.317044
 Sum of electronic and thermal Energies=   -2505.294692
 Sum of electronic and thermal Enthalpies=   -2505.293748
 Sum of electronic and thermal Free Energies=   -2505.371260
```
C         -1.00887   0.76959   0.9193
C          0.95985   1.84477   0.30467
C          0.82981   2.78452   1.32068
C         -0.26802   2.68807   2.17709
C         -1.19467   1.67128   1.97328
C         -1.96964  -0.29399   0.55778
C         -2.53694  -1.84132  -1.11276
C         -3.7095   -2.17213  -0.42601
```

```
C          -3.98906 -1.57106  0.79729
C          -3.11558 -0.60034  1.29042
H           1.81113  1.86631 -0.36859
H           1.57289  3.56656  1.43479
H          -0.40504  3.399    2.98643
H          -2.06442  1.58931  2.61478
H          -2.31825 -2.15008 -2.16778
H          -4.39147 -2.89228 -0.86713
H          -4.88339 -1.8311   1.35702
H          -3.33206 -0.09382  2.22474
N           0.07426  0.85393  0.10338
N          -1.67365 -0.93729 -0.60047
Ni          0.10196 -0.52445 -1.37993
C           1.76253 -0.7881  -2.68121
H           2.1678   0.22457 -2.60622
H           2.54856 -1.49445 -2.92374
C           0.48766 -0.97926 -3.33515
H           0.15873 -1.97837 -3.62657
C          -0.50762 -0.0183  -3.36826
H          -0.26549  1.05033 -3.35161
C          -1.89165 -0.45982 -3.87015
H          -2.09789 -1.4093  -3.29999
H          -1.70575 -0.84231 -4.91801
O          -2.836    0.48156 -3.7524
C           1.86433 -1.64896 -0.77148
H           1.19413 -1.61143  0.09645
C           3.23936 -1.28678 -0.34376
C           3.46652 -0.44167  0.75833
C           4.37014 -1.78998 -1.01499
C           4.75744 -0.09606  1.15612
H           2.61683 -0.07286  1.32633
C           5.66202 -1.44752 -0.62012
H           4.23464 -2.47645 -1.84776
C           5.86423 -0.59166  0.46457
H           4.89901  0.55307  2.01686
H           6.51376 -1.85812 -1.15632
H           6.87101 -0.32607  0.775
H           1.8084  -2.65362 -1.19011
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2655221
C-TS$_L$-7
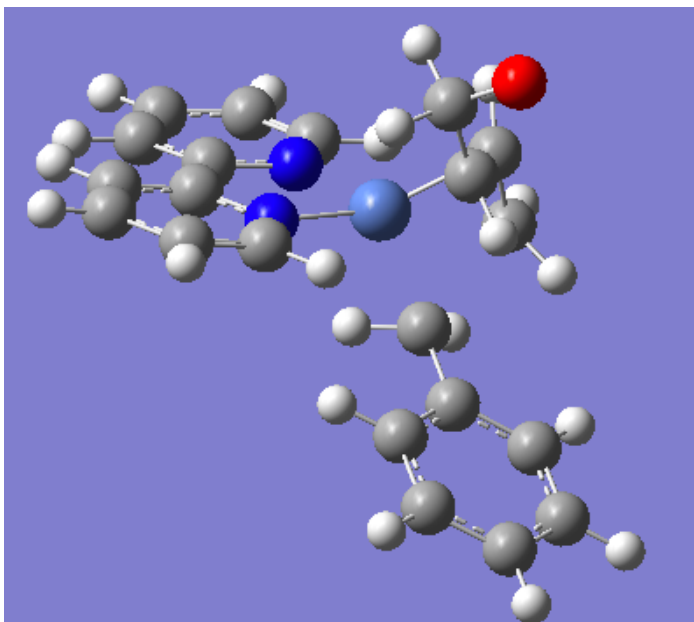
UB3LYP/6-31g(d)-gas

Imaginary frequency = -371.49 cm^{-1}

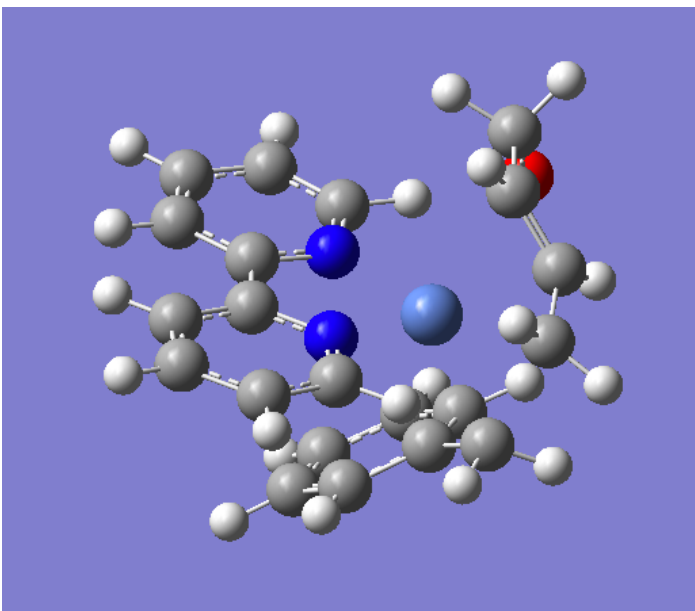|	
Zero-point correction=	0.367747 (Hartree/Particle)
Thermal correction to Energy=	0.390174
Thermal correction to Enthalpy=	0.391119
Thermal correction to Gibbs Free Energy=	0.313602
Sum of electronic and zero-point Energies=	-2505.285876
Sum of electronic and thermal Energies=	-2505.263449
Sum of electronic and thermal Enthalpies=	-2505.262505
Sum of electronic and thermal Free Energies=	-2505.340021

```
C        -1.89363  1.05288  1.33965
C        -0.196    2.45558  0.52408
C        -0.62332  3.51064  1.30635
C        -1.73605  3.32661  2.14799
C        -2.36411  2.09072  2.15737
C        -2.49981 -0.26644  1.25377
C        -2.47448 -2.31451  0.13252
C        -3.51275 -2.81705  0.89775
C        -4.06366 -1.99287  1.8953
C        -3.55105 -0.71997  2.07308
H         0.67039  2.55007 -0.12049
H        -0.09717  4.45867  1.26499
H        -2.09973  4.13461  2.77489
H        -3.23221  1.92961  2.78756
H        -2.01402 -2.91836 -0.64525
H        -3.88419 -3.82111  0.72231
H        -4.875   -2.34974  2.52271
H        -3.95206 -0.07693  2.84896
N        -0.79907  1.23812  0.51957
```

```
N        -1.96966 -1.07393  0.28046
Ni       -0.40226 -0.19977 -0.68863
C         0.49487 -1.6282  -1.99765
H         1.55315 -1.64242 -2.25492
H         0.04221 -2.61364 -2.09917
C        -0.27309 -0.53825 -2.58851
H        -1.24784 -0.73439 -3.03508
C         0.18646  0.77301 -2.39291
H         1.2636   0.9431  -2.32768
C        -0.60167  1.96295 -2.9166
O        -0.1732   2.44522 -4.10731
H        -0.53715  2.79136 -2.16802
H        -1.69073  1.71467 -2.92442
C         1.10134 -1.71964 -0.04958
H         0.49505 -2.23583  0.69828
C         1.98636 -0.70022  0.57187
C         1.60399 -0.01396  1.73937
C         3.23846 -0.38936  0.01116
C         2.43488  0.94293  2.3181
H         0.64794 -0.24609  2.20186
C         4.06852  0.57418  0.58409
H         3.57215 -0.92388 -0.87585
C         3.66987  1.24768  1.73948
H         2.1189   1.45179  3.22535
H         5.03186  0.79288  0.13049
H         4.31614  1.99697  2.18834
H         1.67549 -2.48816 -0.56807
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2772145
C-TS$_L$-8
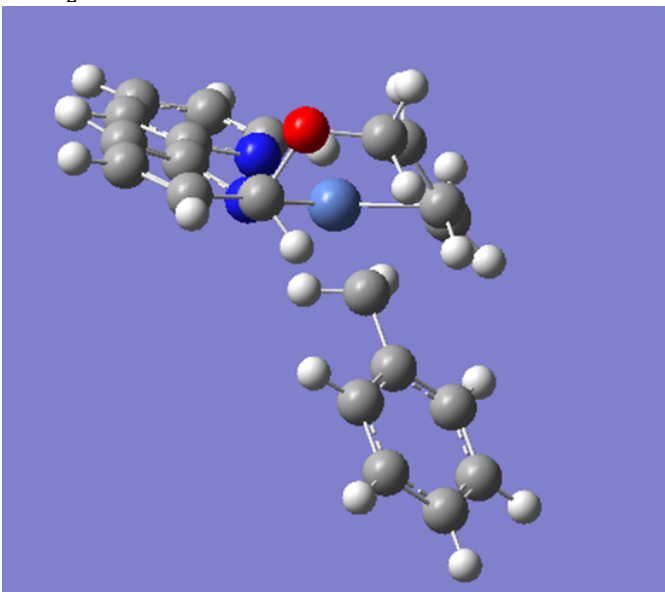
UB3LYP/6-31g(d)-gas
Imaginary frequency = -378.75 cm^{-1}
Zero-point correction=   0.372723 (Hartree/Particle)
 Thermal correction to Energy=   0.393717
 Thermal correction to Enthalpy=   0.394661
 Thermal correction to Gibbs Free Energy=   0.321651
 Sum of electronic and zero-point Energies=   -2505.324950
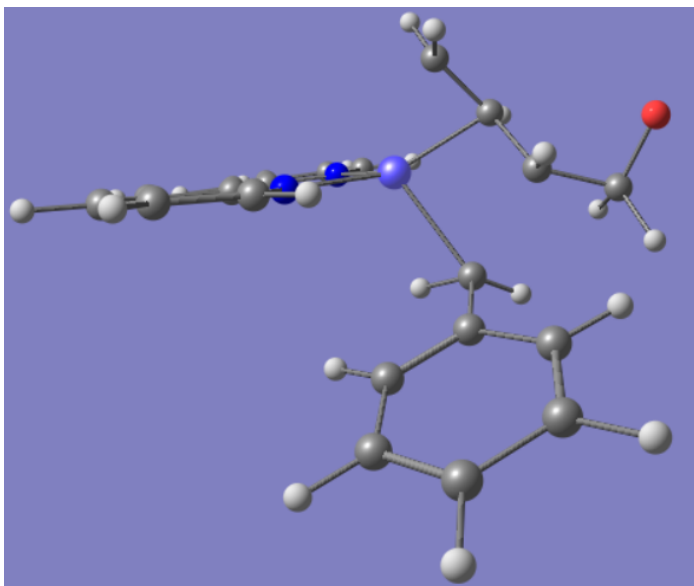 Sum of electronic and thermal Energies=   -2505.303957
 Sum of electronic and thermal Enthalpies=   -2505.303013
 Sum of electronic and thermal Free Energies=   -2505.376023
C   -1.80402 1.39559 1.05496
C   -0.50118 2.65698 -0.49201
C   -0.76882 3.84795 0.3943
C   -1.71565 3.7753   1.36116
C   -2.34886 2.52549 1.63255
C   -2.35841 0.06283 1.30424
C   -2.31033 -2.17308 0.65345
C   -3.31009 -2.52949 1.54315
C   -3.83627 -1.52844 2.36989
C   -3.35154 -0.23644 2.25473
H   0.58715 2.67109 -0.6746
H   -0.26748 4.78129 0.15198
H   -1.98698 4.65338 1.94434
H   -3.18857 2.47352 2.31442
H   -1.86555 -2.91885 -0.00136
H   -3.65959 -3.55535 1.59332
H   -4.60911 -1.76043 3.09739
H   -3.72627 0.54686 2.9023
N   -0.71756 1.41189 0.2252
N   -1.84096 -0.9161   0.51934
Ni   -0.28455 -0.28614 -0.68162
C   0.81573 -1.51801 -2.20464
H   0.04735 -2.12486 -2.69117
H   1.807   -1.87351 -2.49438
C   0.66651 -0.05611 -2.41185
H   1.5692   0.55345 -2.37877
C   -0.55778 0.5595 -2.63152
H   -1.39165 -0.03611 -3.00648
C   -0.63719 2.05961 -2.8416
O   -1.2538   2.79415 -1.79209
C   1.02771 -2.14921 -0.55836
H   0.23209 -2.19537 0.18669
C   2.32531 -1.66914 0.02819
C   2.38882 -0.4735   0.76181
C   3.50982 -2.39251 -0.17332
C   3.60116 -0.02244 1.28353

H	1.48371	0.10996	0.91956
C	4.72429	-1.93937	0.34261
H	3.47554	-3.32652	-0.73124
C	4.77344	-0.75158	1.07409
H	3.62851	0.90229	1.85373
H	5.62968	-2.51827	0.17971
H	5.71741	-0.39839	1.48033
H	1.14703	-3.16735	-0.93913
H	0.3803	2.45106	-2.99987
H	-1.24552	2.28436	-3.72295

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas

HF=-2505.281191

C-TS$_L$

UB3LYP/6-31g(d)-gas

Imaginary frequency = -293.16 cm^{-1}

Zero-point correction=   0.368710 (Hartree/Particle)
 Thermal correction to Energy=   0.390876
 Thermal correction to Enthalpy=   0.391820
 Thermal correction to Gibbs Free Energy=   0.316349
 Sum of electronic and zero-point Energies=   -2505.302047
 Sum of electronic and thermal Energies=   -2505.279881
 Sum of electronic and thermal Enthalpies=   -2505.278937
 Sum of electronic and thermal Free Energies=   -2505.354409

C	-1.5686	2.18377	1.56507
C	0.48993	3.16267	1.12464
C	0.24254	4.21694	1.99655
C	-0.97821	4.24194	2.6723
C	-1.89019	3.214	2.45568

C	-2.45577	1.03657	1.26535
C	-2.79101	-0.78066	-0.17297
C	-3.99554	-1.0848	0.46584
C	-4.4183	-0.31677	1.5476
C	-3.64613	0.77361	1.9441
H	1.42902	3.09501	0.58206
H	0.98586	4.99473	2.13694
H	-1.21627	5.04881	3.35906
H	-2.84452	3.21489	2.96958
H	-2.42244	-1.27389	-1.11724
H	-4.59119	-1.91573	0.10044
H	-5.34461	-0.54507	2.06815
H	-3.9669	1.39915	2.76996
N	-0.38662	2.17274	0.90088
N	-2.02951	0.24881	0.25039
Ni	-0.19004	0.6344	-0.41963
C	1.59975	0.86222	-1.53699
H	1.61552	1.9527	-1.44818
H	2.60094	0.49015	-1.74143
C	0.50411	0.2676	-2.30966
H	0.54351	-0.80218	-2.52213
C	-0.71548	0.86697	-2.56437
H	-0.81131	1.95671	-2.60589
C	-1.84257	-0.02524	-3.10219
H	-1.89372	0.22259	-4.20024
C	1.80391	-0.08757	0.1788
H	2.69434	0.47818	0.45657
H	-2.79166	0.44454	-2.70441
O	-1.66998	-1.32226	-2.81474
C	1.04653	-0.51513	1.40651
C	1.2531	0.0947	2.65814
C	0.19528	-1.64314	1.35905
C	0.60039	-0.36669	3.79975
H	1.93922	0.93537	2.73278
C	-0.46137	-2.09845	2.49761
H	0.04266	-2.15173	0.40924
C	-0.2679	-1.45926	3.7263
H	0.78171	0.12025	4.75502
H	-1.11869	-2.9614	2.42837
H	-0.77126	-1.82063	4.61886
H	2.0981	-0.97851	-0.37641

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.287780
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.1928851
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas

HF = -2503.284994203000

ΔG$_{solv}$ = -0.0445728
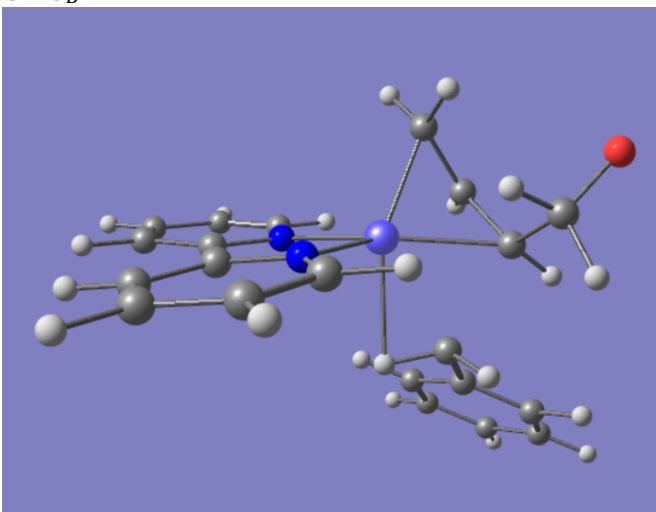
C-TS$_B$-1

UB3LYP/6-31g(d)-gas

Imaginary frequency = -385.66 cm^{-1}

Zero-point correction=   0.368199 (Hartree/Particle)
 Thermal correction to Energy=   0.390811
 Thermal correction to Enthalpy=   0.391755
 Thermal correction to Gibbs Free Energy=   0.314247
 Sum of electronic and zero-point Energies=   -2505.289391
 Sum of electronic and thermal Energies=   -2505.266778
 Sum of electronic and thermal Enthalpies=   -2505.265834
 Sum of electronic and thermal Free Energies=   -2505.343342

C	-1.00887	0.76959	0.9193
C	0.95985	1.84477	0.30467
C	0.82981	2.78452	1.32068
C	-0.26802	2.68807	2.17709
C	-1.19467	1.67128	1.97328
C	-1.96964	-0.29399	0.55778
C	-2.53694	-1.84132	-1.11276
C	-3.7095	-2.17213	-0.42601
C	-3.98906	-1.57106	0.79729
C	-3.11558	-0.60034	1.29042
H	1.81113	1.86631	-0.36859
H	1.57289	3.56656	1.43479
H	-0.40504	3.399	2.98643
H	-2.06442	1.58931	2.61478
H	-2.31825	-2.15008	-2.16778
H	-4.39147	-2.89228	-0.86713
H	-4.88339	-1.8311	1.35702

H	-3.33206	-0.09382	2.22474
N	0.07426	0.85393	0.10338
N	-1.67365	-0.93729	-0.60047
Ni	0.10196	-0.52445	-1.37993
C	1.76253	-0.7881	-2.68121
H	2.54856	-1.49445	-2.92374
C	0.48766	-0.97926	-3.33515
H	0.15873	-1.97837	-3.62657
C	-0.50762	-0.0183	-3.36826
H	-0.26549	1.05033	-3.35161
C	1.86433	-1.64896	-0.77148
H	1.19413	-1.61143	0.09645
C	3.23936	-1.28678	-0.34376
C	3.46652	-0.44167	0.75833
C	4.37014	-1.78998	-1.01499
C	4.75744	-0.09606	1.15612
H	2.61683	-0.07286	1.32633
C	5.66202	-1.44752	-0.62012
H	4.23464	-2.47645	-1.84776
C	5.86423	-0.59166	0.46457
H	4.89901	0.55307	2.01686
H	6.51376	-1.85812	-1.15632
H	6.87101	-0.32607	0.775
H	1.8084	-2.65362	-1.19011
C	2.33337	0.63829	-2.57558
H	1.7578	1.20153	-1.87103
H	3.35115	0.59185	-2.24867
O	2.27244	1.27213	-3.85598
H	-1.47113	-0.32567	-3.71766

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
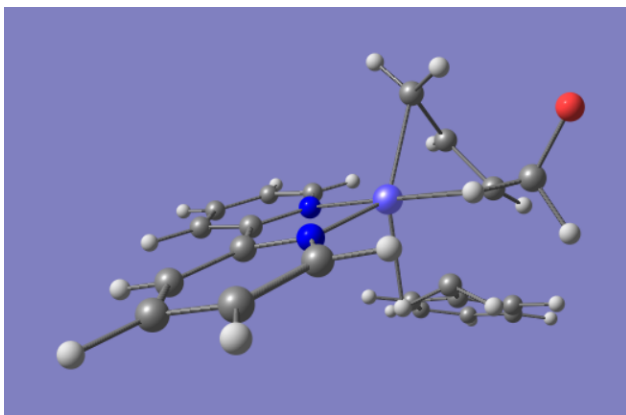
HF=-2505.2814078

C-TS$_B$-2

UB3LYP/6-31g(d)-gas

Imaginary frequency = -486.76 cm^{-1}

Zero-point correction=   0.367873 (Hartree/Particle)
Thermal correction to Energy=   0.390488
Thermal correction to Enthalpy=   0.391432
Thermal correction to Gibbs Free Energy=   0.313474
Sum of electronic and zero-point Energies=   -2505.289900
Sum of electronic and thermal Energies=   -2505.267284
Sum of electronic and thermal Enthalpies=   -2505.266340
Sum of electronic and thermal Free Energies=   -2505.344298

C	-2.05201	1.2627	1.01432
C	0.12903	1.84547	1.58725
C	-0.30184	2.57254	2.6896
C	-1.67084	2.63119	2.96109
C	-2.55195	1.96683	2.11523
C	-2.8959	0.5622	0.02994
C	-2.89613	-0.63169	-1.97151
C	-4.27758	-0.77177	-1.94982
C	-4.98735	-0.21479	-0.88207
C	-4.28983	0.45778	0.11419
H	1.18438	1.75227	1.35519
H	0.42339	3.07428	3.32126
H	-2.04524	3.18557	3.81619
H	-3.61853	2.00386	2.30588
H	-2.29974	-1.04307	-2.78015
H	-4.78123	-1.30354	-2.7499
H	-6.06803	-0.30416	-0.82766
H	-4.82429	0.89516	0.94971
N	-0.71539	1.20263	0.75831
N	-2.21232	0.01442	-1.01088

```
Ni        -0.23167  0.25064 -0.91324
C          1.68574 -0.5193  -2.121
C          0.56718  0.19892 -2.73684
H         -0.00079 -0.35406 -3.4839
C          0.25061  1.52411 -2.44288
H          1.01213  2.19167 -2.04043
C          1.04762 -1.47011 -0.40421
H          0.02428 -1.60205 -0.00379
C          2.00969 -1.28016  0.71609
C          1.56448 -1.05017  2.03315
C          3.40181 -1.34855  0.50802
C          2.46069 -0.89216  3.09013
H          0.49524 -1.02179  2.23262
C          4.29826 -1.18851  1.56364
H          3.77945 -1.54609 -0.49101
C          3.83654 -0.95537  2.86126
H          2.08139 -0.72964  4.09655
H          5.36625 -1.25173  1.36995
H          4.53797 -0.83391  3.68237
H          1.23737 -2.38701 -0.96312
H         -0.55726  2.01776 -2.97733
H          2.45055  0.11705 -1.67329
C          2.26818 -1.6098  -3.02398
H          3.0339  -2.20599 -2.45764
H          1.43535 -2.34927 -3.23601
O          2.69643 -0.86235 -4.03127
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.2812 cm^{-1}

C-TS$_B$-3
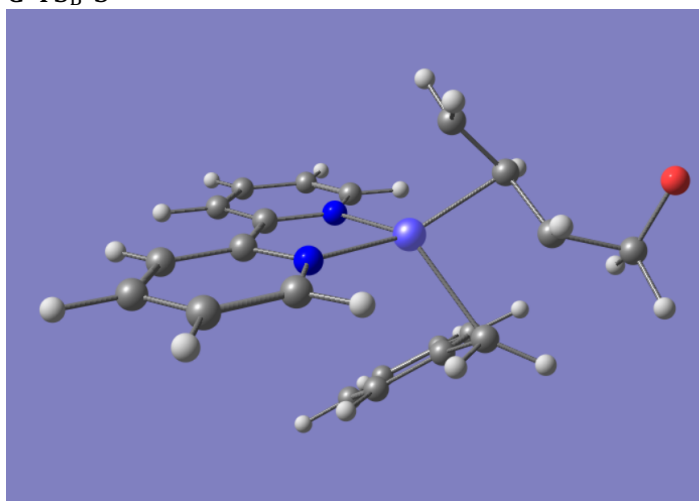
UB3LYP/6-31g(d)-gas
Imaginary frequency = -444.04 cm^{-1}

Zero-point correction=   0.367858 (Hartree/Particle)
Thermal correction to Energy=   0.390523
Thermal correction to Enthalpy=   0.391467
Thermal correction to Gibbs Free Energy=   0.313912
Sum of electronic and zero-point Energies=   -2505.290812
Sum of electronic and thermal Energies=   -2505.268147
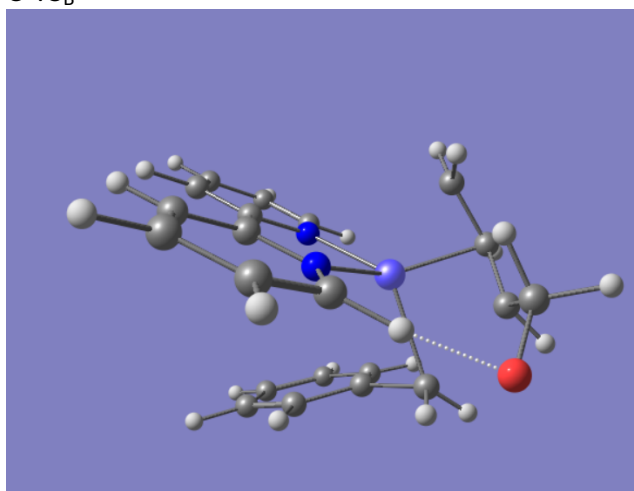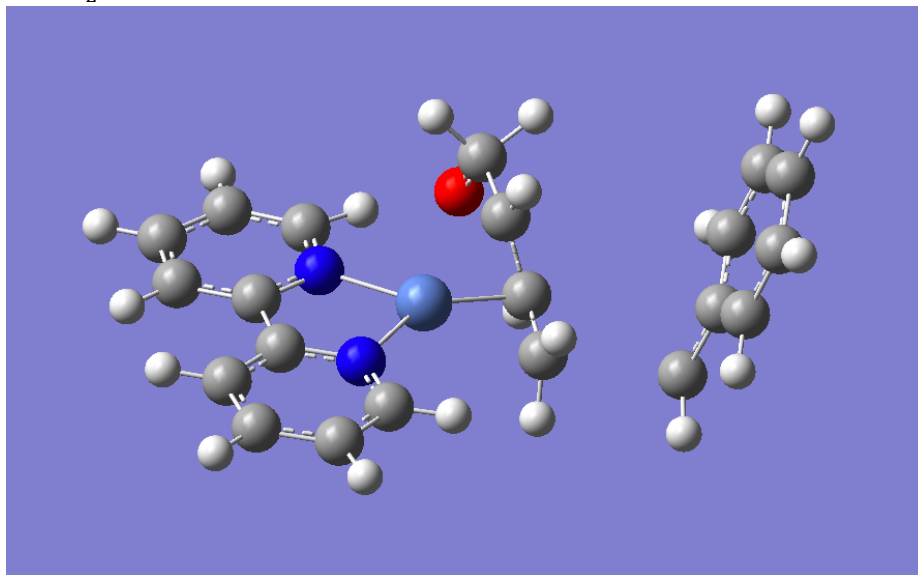Sum of electronic and thermal Enthalpies=   -2505.267203
Sum of electronic and thermal Free Energies=   -2505.344757
C   -1.80262 1.15196 1.48108
C   0.24825 2.16667 1.047
C   0.07471 3.07472 2.08389
C   -1.08954 3.00123 2.85224
C   -2.03429 2.02761 2.54747
C   -2.75312 0.11388 1.04501
C   -3.18037 -1.52622 -0.55407
C   -4.39705 -1.85446 0.02948
C   -4.79559 -1.15932 1.17502
C   -3.96665 -0.16738 1.68503
H   1.14851 2.17281 0.44246
H   0.84044 3.81646 2.2843
H   -1.25867 3.69054 3.6738
H   -2.94672 1.95574 3.12837
H   -2.82679 -2.03452 -1.4459
H   -5.01368 -2.6344 -0.40415
H   -5.73839 -1.38801 1.66251
H   -4.26059 0.38102 2.57283
N   -0.66248 1.2239   0.73891
N   -2.37001 -0.57095 -0.06606
Ni   -0.58797 -0.03076 -0.79573
C   0.93249 -0.76107 -2.49107
C   -0.47474 -0.43678 -2.73965
H   -1.09968 -1.25757 -3.08959
C   -1.00215 0.84574 -2.59602
H   -0.35081 1.71676 -2.66284
C   1.15868 -1.34658 -0.52829
H   1.86423 -1.426   -1.37858
C   0.64901 -2.69841 -0.16556
C   0.88441 -3.81836 -0.98711
C   -0.06787 -2.91267 1.02875
C   0.4254 -5.08889 -0.63863
H   1.46054 -3.69278 -1.90153
C   -0.52927 -4.18121 1.37629
H   -0.24747 -2.0747   1.6961
C   -0.29039 -5.27823 0.54479
H   0.63711 -5.93399 -1.2899
H   -1.0753 -4.31341 2.30714

```
H          -0.64892 -6.26657  0.81984
H           1.75749 -0.90303  0.26789
H          -2.04246  1.03039 -2.85257
H           1.60819  0.09549 -2.48591
C           1.4491  -1.91931 -3.3487
H           2.48555 -2.20327 -3.01931
H           0.81515 -2.82602 -3.10374
O           1.31453 -1.38447 -4.55408
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.270998
C-TS$_B$-4

UB3LYP/6-31g(d)-gas
Imaginary frequency = -327.692 cm^{-1}
Zero-point correction=   0.367979 (Hartree/Particle)
 Thermal correction to Energy=   0.390539
 Thermal correction to Enthalpy=   0.391484
 Thermal correction to Gibbs Free Energy=   0.314033
 Sum of electronic and zero-point Energies=   -2505.293742
 Sum of electronic and thermal Energies=   -2505.271182
 Sum of electronic and thermal Enthalpies=   -2505.270238
 Sum of electronic and thermal Free Energies=   -2505.347689
```
C          -1.8928   1.10853  1.38535
C           0.00439  2.32527  0.79091
C          -0.16019  3.19905  1.85603
C          -1.2387   3.00344  2.72622
C          -2.10858  1.94809  2.48632
C          -2.7653  -0.01762  1.02582
C          -3.07434 -1.79771 -0.4453
C          -4.25948 -2.17443  0.17019
C          -4.71271 -1.42119  1.25977
C          -3.96036 -0.33569  1.6869
H           0.82765  2.43483  0.09181
```

H	0.54307	4.0126	1.99898
H	-1.39503	3.66122	3.57575
H	-2.94692	1.77356	3.15124
H	-2.68611	-2.34475	-1.29945
H	-4.81343	-3.0323	-0.19584
H	-5.63982	-1.67705	1.76367
H	-4.30191	0.26522	2.52219
N	-0.83538	1.29944	0.5443
N	-2.33445	-0.75082	-0.03834
Ni	-0.68394	-0.03203	-0.92368
C	0.94339	-0.44871	-2.34082
H	1.64738	-1.18959	-2.70708
C	-0.44759	-0.63321	-2.78057
H	-0.78234	-1.64267	-3.02428
C	-1.33518	0.44143	-2.8217
H	-0.96073	1.44065	-3.02578
C	1.0059	-1.38599	-0.48709
H	1.01722	-0.45188	0.09117
C	2.31794	-2.06283	-0.35221
C	3.50485	-1.33272	-0.15603
C	2.41892	-3.46569	-0.39621
C	4.73561	-1.97253	-0.02132
H	3.45701	-0.24778	-0.09535
C	3.64796	-4.10807	-0.26279
H	1.51772	-4.05906	-0.53414
C	4.81626	-3.3655	-0.0776
H	5.63489	-1.38102	0.13375
H	3.69298	-5.19356	-0.30122
H	5.77509	-3.86583	0.02693
H	0.1812	-1.98696	-0.10377
C	1.59107	0.95986	-2.46019
H	0.97777	1.71654	-1.88721
H	2.56435	0.91397	-1.92004
O	1.63455	1.12188	-3.77615
H	-2.36629	0.2564	-3.1127

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.273915

C-TS$_B$-5
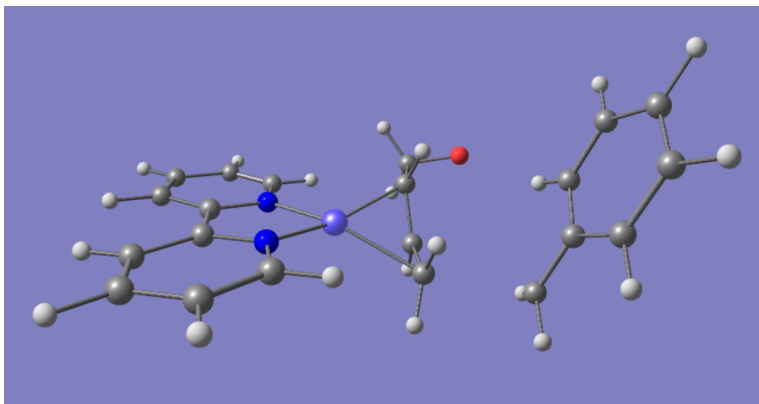
UB3LYP/6-31g(d)-gas

Imaginary frequency = -343.95 cm^{-1}

Zero-point correction=   0.367045 (Hartree/Particle)
 Thermal correction to Energy=   0.389313
 Thermal correction to Enthalpy=   0.390257
 Thermal correction to Gibbs Free Energy=   0.313588
 Sum of electronic and zero-point Energies=   -2505.294430
 Sum of electronic and thermal Energies=   -2505.272162
 Sum of electronic and thermal Enthalpies=   -2505.271218
 Sum of electronic and thermal Free Energies=   -2505.347887

C	-1.11231	1.98772	1.96309
C	0.82866	3.14897	1.39528
C	0.72374	3.95527	2.52379
C	-0.34078	3.75117	3.4052
C	-1.26974	2.75431	3.12378
C	-2.03918	0.9216	1.53266
C	-2.4228	-0.77706	0.00359
C	-3.65558	-1.0861	0.56743
C	-4.08931	-0.34001	1.66453
C	-3.2718	0.6733	2.15058
H	1.62705	3.22425	0.66095
H	1.46683	4.72439	2.70835
H	-0.44429	4.35639	4.3012
H	-2.09557	2.57063	3.80216
H	-2.04458	-1.33721	-0.84495
H	-4.25532	-1.89067	0.15474
H	-5.04923	-0.54164	2.13084
H	-3.59395	1.27555	2.99253
N	-0.07209	2.18724	1.12231
N	-1.62313	0.19946	0.46147
Ni	0.13045	0.98614	-0.46614
C	1.32849	-0.0145	-2.01822
H	1.73593	-0.97749	-2.31842
C	-0.0647	0.1966	-2.34574
H	-0.67389	-0.70203	-2.44483

```
C          -0.70592  1.43943 -2.34939
H          -0.16462  2.35985 -2.53549
C           1.73289 -0.58905 -0.21064
H           2.76903 -0.28156 -0.3236
C           1.53273 -2.05284 -0.24736
C           2.40357 -2.89352 -0.9713
C           0.47474 -2.6729   0.44639
C           2.21771 -4.27391 -1.01254
H           3.25158 -2.45335 -1.49172
C           0.28486 -4.05354  0.40575
H          -0.19411 -2.05797  1.04226
C           1.15223 -4.86463 -0.32897
H           2.91306 -4.89252 -1.57496
H          -0.53873 -4.49908  0.95929
H           1.00753 -5.94124 -0.3592
H           1.35935 -0.17655  0.73038
C           2.23278  1.21164 -2.00619
H          -1.77445  1.4587  -2.55297
H           1.67178  2.06544 -1.68806
O           2.71136  1.4258  -3.23935
H           3.0467   1.04793 -1.33118
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.2764

C-TS_B

UB3LYP/6-31g(d)-gas
Imaginary frequency = -229.10 cm⁻¹
Zero-point correction=   0.369235 (Hartree/Particle)
 Thermal correction to Energy=   0.391133
 Thermal correction to Enthalpy=   0.392077
 Thermal correction to Gibbs Free Energy=   0.317630
 Sum of electronic and zero-point Energies=   -2505.303251
 Sum of electronic and thermal Energies=   -2505.281353

```
C          -0.70592  1.43943 -2.34939
H          -0.16462  2.35985 -2.53549
C           1.73289 -0.58905 -0.21064
H           2.76903 -0.28156 -0.3236
C           1.53273 -2.05284 -0.24736
C           2.40357 -2.89352 -0.9713
C           0.47474 -2.6729   0.44639
C           2.21771 -4.27391 -1.01254
H           3.25158 -2.45335 -1.49172
C           0.28486 -4.05354  0.40575
H          -0.19411 -2.05797  1.04226
C           1.15223 -4.86463 -0.32897
H           2.91306 -4.89252 -1.57496
H          -0.53873 -4.49908  0.95929
H           1.00753 -5.94124 -0.3592
H           1.35935 -0.17655  0.73038
C           2.23278  1.21164 -2.00619
H          -1.77445  1.4587  -2.55297
H           1.67178  2.06544 -1.68806
O           2.71136  1.4258  -3.23935
H           3.0467   1.04793 -1.33118
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.2764

C-TS$_B$

UB3LYP/6-31g(d)-gas
Imaginary frequency = -229.10 cm^{-1}
Zero-point correction=   0.369235 (Hartree/Particle)
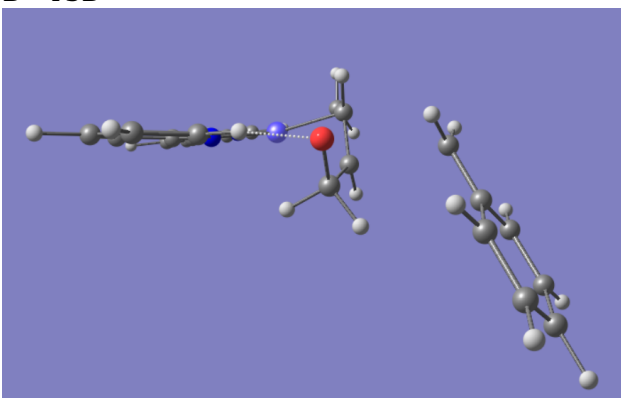 Thermal correction to Energy=   0.391133
 Thermal correction to Enthalpy=   0.392077
 Thermal correction to Gibbs Free Energy=   0.317630
 Sum of electronic and zero-point Energies=   -2505.303251
 Sum of electronic and thermal Energies=   -2505.281353

Sum of electronic and thermal Enthalpies=   -2505.280409
Sum of electronic and thermal Free Energies=   -2505.354856
C   -2.42248 1.29717 1.28299
C   -0.74205 2.83838 0.79219
C   -1.17536 3.6922   1.80077
C   -2.27472 3.31918 2.57813
C   -2.90506 2.10663 2.31821
C   -3.0098 -0.00289 0.89711
C   -2.82347 -1.84296 -0.50009
C   -3.94979 -2.44874 0.04583
C   -4.63322 -1.77807 1.06156
C   -4.15819 -0.54446 1.49058
H   0.10881 3.04021 0.14631
H   -0.65703 4.62993 1.9733
H   -2.63439 3.96122 3.37697
H   -3.75519 1.79629 2.91556
H   -2.26142 -2.32612 -1.29386
H   -4.27943 -3.41649 -0.31768
H   -5.52195 -2.20962 1.51267
H   -4.67711 -0.00622 2.27559
N   -1.35508 1.66711 0.53837
N   -2.35576 -0.65286 -0.09711
Ni   -0.73209 0.46974 -0.93473
C   0.71124 -0.36628 -2.34619
H   1.27783 -1.26669 -2.57809
C   -0.6519 -0.32698 -2.82883
H   -1.13914 -1.29055 -2.98511
C   -1.4373   0.82503 -2.91038
H   -0.99629 1.80771 -3.0314
C   0.73307 -1.07707 -0.27135
H   1.36769 -1.87508 -0.66447
C   0.42133 -1.3514   1.14457
C   0.10659 -2.65276 1.58219
C   0.43527 -0.32517 2.10671
C   -0.16649 -2.91424 2.922
H   0.04502 -3.44979 0.84642
C   0.16198 -0.5857   3.44963
H   0.6829   0.68852 1.7965
C   -0.13812 -1.88326 3.8663
H   -0.40826 -3.92806 3.23236
H   0.18908 0.22686 4.17196
H   -0.34954 -2.08982 4.91221
H   1.24062 -0.12182 -0.41524
C   1.45577 0.95783 -2.23765
H   -2.47208 0.71387 -3.22633
H   1.51421 1.41437 -3.2036

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O   2.69285   0.73781 -1.77201
H   0.9326   1.60728 -1.56727
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2794819
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2506.1862011
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.286377222440
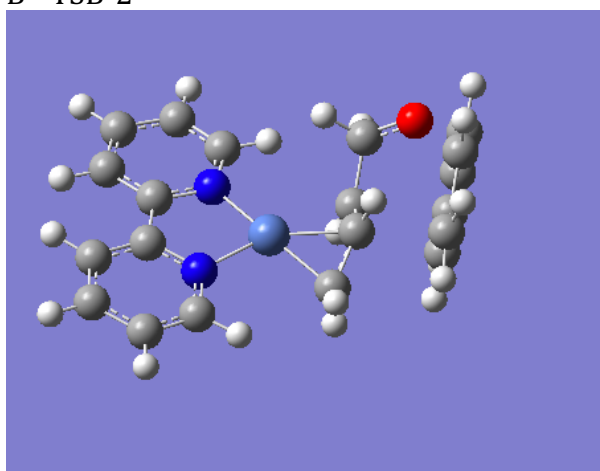ΔG_{solv} = -0.0366925

B''-TS$_L$

UB3LYP/6-31g(d)-gas
Imaginary frequency = -636.59 cm^{-1}
Zero-point correction=   0.365804 (Hartree/Particle)
 Thermal correction to Energy=   0.388564
 Thermal correction to Enthalpy=   0.389508
 Thermal correction to Gibbs Free Energy=   0.310314
 Sum of electronic and zero-point Energies=   -2505.299320
 Sum of electronic and thermal Energies=   -2505.276559
 Sum of electronic and thermal Enthalpies=   -2505.275615
 Sum of electronic and thermal Free Energies=   -2505.354809
C   -0.92081   0.98226   2.85884
C   0.67014   2.31217   1.794
C   0.47953   3.35274   2.69422
C   -0.45476   3.1855   3.71796
C   -1.15798   1.98782   3.79956
C   -1.5887   -0.3339   2.85009
C   -1.72129 -2.37911   1.70945
C   -2.60446 -2.87359   2.6738

```
C          -2.98004 -2.07177  3.74791
C          -2.46364 -0.77945  3.84019
H           1.38905  2.39112  0.98607
H           1.05273  4.26801  2.59223
H          -0.63389  3.97557  4.44093
H          -1.89076  1.83878  4.58437
H          -1.33493 -2.98137  0.84436
H          -2.98485 -3.8845   2.56672
H          -3.65853 -2.44172  4.51178
H          -2.72919 -0.1412   4.6758
N          -0.00759  1.15114  1.86035
N          -1.23443 -1.12306  1.80007
Ni          0.04227 -0.29963  0.59114
C           1.83921 -0.03604 -0.58031
H           1.571    0.90726 -1.04641
H           2.68603 -0.02865  0.09911
C           1.08032 -1.2273  -0.79853
H           1.43511 -2.2025  -0.46333
C          -0.23453 -1.18673 -1.25843
H          -0.58624 -0.31939 -1.83027
C          -1.03659 -2.48073 -1.36483
H          -1.07585 -2.68547 -2.47363
C           3.20106 -0.11228 -2.04303
H           3.36256 -1.17159 -1.87679
H          -2.10453 -2.16932 -1.14588
O          -0.57116 -3.48718 -0.62193
C           2.52945  0.31832 -3.23213
C           1.74914 -0.58196 -4.00078
C           2.58448  1.66945 -3.65929
C           1.06791 -0.15095 -5.13345
H           1.68558 -1.62149 -3.69098
C           1.90408  2.09253 -4.79435
H           3.18104  2.37834 -3.08843
C           1.1401   1.18622 -5.5396
H           0.47627 -0.86082 -5.70572
H           1.96966  3.13213 -5.10621
H           0.60908  1.51847 -6.4274
H           3.91701  0.55573 -1.57185
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2737072
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1837374
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.267387295916
ΔG_{solv} = -0.0452782

B''-TSL-2

UB3LYP/6-31g(d)-gas
Imaginary frequency = -587.27 cm^{-1}
Zero-point correction=   0.366803 (Hartree/Particle)
 Thermal correction to Energy=   0.389962
 Thermal correction to Enthalpy=   0.390906
 Thermal correction to Gibbs Free Energy=   0.310188
 Sum of electronic and zero-point Energies=   -2505.285504
 Sum of electronic and thermal Energies=   -2505.262346
 Sum of electronic and thermal Enthalpies=   -2505.261402
 Sum of electronic and thermal Free Energies=   -2505.342119

C	-1.13555	0.9784	3.13108
C	0.43215	2.32358	2.05098
C	0.24767	3.35842	2.95902
C	-0.67091	3.18005	3.99505
C	-1.36553	1.97763	4.08032
C	-1.79637	-0.34133	3.12417
C	-1.93433	-2.38063	1.97353
C	-2.8029	-2.88466	2.94612
C	-3.16789	-2.09087	4.02985
C	-2.65622	-0.79674	4.12298
H	1.1391	2.41115	1.23344
H	0.81351	4.27787	2.85356
H	-0.84463	3.96527	4.7246
H	-2.08618	1.82002	4.87463
H	-1.55618	-2.97619	1.10031
H	-3.1803	-3.89657	2.83793
H	-3.8346	-2.4684	4.80035
H	-2.91389	-0.16456	4.96565
N	-0.23722	1.15793	2.12098
N	-1.45185	-1.12296	2.06531
Ni	-0.19356	-0.28773	0.84543
C	1.59434	-0.01393	-0.33685
H	1.3201	0.93041	-0.7973
H	2.44569	-0.0067	0.33687

```
C        0.83763 -1.20673 -0.55461
H        1.19789 -2.18206 -0.2257
C       -0.48027 -1.16865 -1.00576
H       -0.8386  -0.30022 -1.57182
C       -1.2794  -2.46449 -1.11135
O       -1.32664 -2.66469 -2.22068
C        3.18263 -0.09223 -2.06942
H        3.35043 -1.15141 -1.90868
C        2.50027  0.33984 -3.25184
C        1.71925 -0.56117 -4.01891
C        2.54542  1.69305 -3.67363
C        1.0281  -0.12891 -5.14509
H        1.66314 -1.60232 -3.71312
C        1.85503  2.11742 -4.80213
H        3.14227  2.40258 -3.10387
C        1.09063  1.21031 -5.54602
H        0.43619 -0.83939 -5.71631
H        1.91308  3.15866 -5.10999
H        0.55181  1.54357 -6.42873
H        3.89895  0.57727 -1.60094
H       -0.78047 -3.26201 -0.60152
H       -2.2485  -2.38918 -0.66406

C       -1.13392  0.98313  3.13145
C        0.2665   2.37938  1.89052
C        0.18006  3.39099  2.83243
C       -0.58321  3.1698   3.98831
C       -1.23954  1.95627  4.13435
C       -1.8115  -0.31349  3.15335
C       -2.05793 -2.34834  2.03802
C       -2.97543 -2.80536  2.9727
C       -3.31985 -1.97003  4.04314
C       -2.73293 -0.71509  4.12936
H        0.86187  2.49866  0.99175
H        0.70313  4.32724  2.66937
H       -0.65994  3.93201  4.75759
H       -1.82899  1.76067  5.02339
H       -1.76139 -2.95971  1.19433
H       -3.41036 -3.79288  2.86184
H       -4.03673 -2.29297  4.79192
H       -2.99464 -0.0454   4.94112
N       -0.36736  1.19414  2.01554
N       -1.47165 -1.13647  2.114
Ni      -0.21298 -0.35341  0.87121
C        1.65776 -0.04242 -0.29443
H        1.26996  0.83326 -0.8044
```

H   2.49738   0.10715   0.37555
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.2689

B''-TSL-3
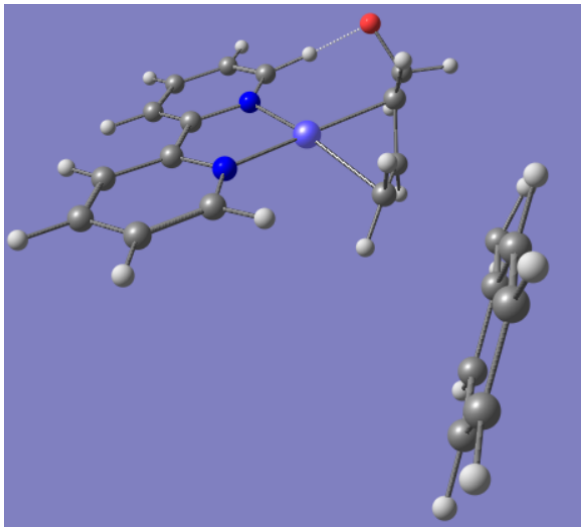
UB3LYP/6-31g(d)-gas
Imaginary frequency = -690.20 cm^{-1}
Zero-point correction=
0.365903 (Hartree/Particle)
 Thermal correction to Energy=
0.388736
Thermal correction to Enthalpy=   0.389680
Thermal correction to Gibbs Free Energy=   0.309870
Sum of electronic and zero-point Energies=   -2505.294342
Sum of electronic and thermal Energies=   -2505.271510
Sum of electronic and thermal Enthalpies=   -2505.270566
Sum of electronic and thermal Free Energies=   -2505.350376

C   -1.30688   0.97795   2.4599
C   -0.57325   2.03894   0.5226
C   -0.70569   3.29597   1.09769
C   -1.14757   3.38255   2.41843
C   -1.4485   2.2111   3.10334
C   -1.61961 -0.32063   3.07059
C   -1.78021 -2.6172   2.65712
C   -2.23093 -2.83573   3.96382
C   -2.36273 -1.76406   4.83954
C   -2.06743 -0.48102   4.38205
H   -0.21584   1.9269   -0.49492
H   -0.46151   4.18095   0.52
H   -1.25603   4.34629   2.90679
H   -1.79422   2.25384   4.12959
H   -1.83246 -3.37628   1.83445
H   -2.49217 -3.84477   4.26653
H   -2.70712 -1.91176   5.85965
H   -2.18738   0.37444   5.03754
N   -0.86432   0.896   1.1749
N   -1.45375 -1.37986   2.23271
Ni   -0.63504 -0.90297   0.52471

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```
C          0.8627  -0.61283 -0.96595
H          0.17276 -0.20868 -1.70321
H          1.59993  0.06699 -0.55613
C          0.7145  -1.95441 -0.48194
H          1.51791 -2.40096  0.10553
C         -0.49859 -2.66369 -0.596
H         -1.22527 -2.34672 -1.35095
C         -0.74657 -4.06211 -0.0521
C          2.31375 -0.68497 -2.77826
H          1.76754 -1.48293 -3.26861
C          2.26474  0.64318 -3.31625
C          1.28095  1.01444 -4.26747
C          3.16363  1.64877 -2.88047
C          1.20875  2.31287 -4.75814
H          0.57962  0.26147 -4.61986
C          3.08715  2.94601 -3.37533
H          3.93166  1.3899  -2.15474
C          2.11021  3.28896 -4.317
H          0.44978  2.56822 -5.49351
H          3.79645  3.69518 -3.03204
H          2.05516  4.30185 -4.70617
H          3.18266 -0.99119 -2.20425
O         -2.00181 -4.14632  0.44186
H         -0.51611 -4.78164 -0.88264
H          0.07115 -4.25204  0.7066
```
UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF = -2505.2704

B''-TSB

UB3LYP/6-31g(d)-gas
Imaginary frequency = -469.64 cm^{-1}
Zero-point correction=   0.367811 (Hartree/Particle)
 Thermal correction to Energy=   0.390034
 Thermal correction to Enthalpy=   0.390978
 Thermal correction to Gibbs Free Energy=   0.313856

Sum of electronic and zero-point Energies=   -2505.299873
Sum of electronic and thermal Energies=   -2505.277651
Sum of electronic and thermal Enthalpies=   -2505.276707
Sum of electronic and thermal Free Energies=   -2505.353829

```
C          -1.80936  0.7111   2.99187
C          -1.90017  1.86364  0.95515
C          -2.54453  2.93768  1.57502
C          -2.8104   2.89256  2.94046
C          -2.43832  1.75954  3.66263
C          -1.44326 -0.57421  3.61927
C          -0.64935 -2.72612  3.19952
C          -0.75578 -3.07952  4.53942
C          -1.22673 -2.12901  5.44609
C          -1.5761  -0.86538  4.97888
H          -1.68401  1.84452 -0.13999
H          -2.82344  3.79752  0.97445
H          -3.30753  3.71876  3.44117
H          -2.65075  1.69117  4.72384
H          -0.29552 -3.42657  2.45206
H          -0.47626 -4.07793  4.85854
H          -1.32186 -2.36744  6.50117
H          -1.94382 -0.11193  5.66614
N          -1.53086  0.77298  1.66148
N          -0.97799 -1.50488  2.74006
Ni         -0.76297 -0.87133  0.95418
C           0.41297 -0.30447 -1.02147
H           1.39382 -0.63414 -0.66391
C          -0.65951 -1.22253 -0.95821
H          -1.58519 -0.92645 -1.44929
C          -0.52708 -2.42792 -0.19993
H           0.45938 -2.89375 -0.13545
C           0.21831  1.20021 -1.2196
H           1.12319  1.57262 -1.76076
C           0.66427 -0.70089 -3.35107
H          -0.28173 -0.171  -3.38089
H           0.41698  1.60604 -0.17461
O          -0.95872  1.53941 -1.74422
C           1.83659 -0.04723 -3.82354
C           1.81382  1.35087 -4.08341
C           3.05041 -0.74892 -4.04597
C           2.94891  1.99907 -4.55637
H           0.88872  1.89324 -3.90404
C           4.17758 -0.09106 -4.51736
H           3.07832 -1.81968 -3.85271
C           4.13389  1.28652 -4.77636
H           2.91443  3.06715 -4.75599
```

H	5.09646	-0.64603	-4.69033
H	5.01747	1.79841	-5.14845
H	0.6398	-1.7848	-3.29719
H	-1.34407	-3.14984	-0.23024

UM06/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2692424
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1777816
DLPNO-CCSD(T)/def2-TZVPP//uB3LYP/6-31G(d)-gas
HF = -2503.270786690197
ΔG_{solv} = -0.0372232

B''-TSB-2

UB3LYP/6-31g(d)-gas
Imaginary frequency = -570.54 cm^{-1}
Zero-point correction=   0.366566 (Hartree/Particle)
 Thermal correction to Energy=   0.389164
 Thermal correction to Enthalpy=   0.390108
 Thermal correction to Gibbs Free Energy=   0.312030
 Sum of electronic and zero-point Energies=   -2505.286375
 Sum of electronic and thermal Energies=   -2505.263777
 Sum of electronic and thermal Enthalpies=   -2505.262833
 Sum of electronic and thermal Free Energies=   -2505.340911

C	-1.53132	0.76541	2.57804
C	0.25036	1.86711	1.5835
C	-0.27739	3.11203	1.91509
C	-1.49347	3.17274	2.59292
C	-2.12467	1.9817	2.93018
C	-2.09251	-0.54683	2.92656
C	-1.83772	-2.84207	2.67807
C	-2.91561	-3.10236	3.51483
C	-3.60643	-2.02692	4.07587
C	-3.1847	-0.73617	3.7785

```
H           1.19501  1.79191  1.06501
H           0.26598  4.00908  1.63876
H          -1.94243  4.12622  2.85456
H          -3.0735   1.99674  3.45384
H          -1.27884 -3.64832  2.22169
H          -3.20014 -4.12881  3.72031
H          -4.45126 -2.19025  4.73788
H          -3.68876  0.11581  4.21966
N          -0.35572  0.70321  1.89024
N          -1.4282  -1.59647  2.36662
Ni          0.08838 -1.10889  1.27661
C           1.32509 -0.67475 -0.53293
H           0.38987 -0.27134 -0.92389
C           1.41472 -1.96639  0.02001
H           2.41562 -2.23678  0.36197
C           0.30545 -2.79282  0.28662
H          -0.5512  -2.8161  -0.39227
C           2.62892  0.19303 -0.43564
H           2.7359   0.42393  0.67156
C           1.63484 -1.17853 -2.79413
H           0.86696 -1.94682 -2.84965
H           2.33583  1.18272 -0.89708
O           3.70376 -0.3808  -0.94942
C           1.46392  0.04053 -3.51623
C           0.28304  0.32637 -4.24963
C           2.49918  1.01716 -3.50697
C           0.15529  1.51085 -4.96409
H          -0.5197  -0.40843 -4.26459
C           2.36152  2.19462 -4.23254
H           3.38075  0.80335 -2.90345
C           1.19484  2.4505  -4.96392
H          -0.75237  1.70632 -5.53058
H           3.16526  2.92726 -4.22435
H           1.09204  3.37625 -5.5246
H           2.63198 -1.44334 -2.4591
H           0.5214  -3.75162  0.75616
```
UM06 /6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2505.2732996
UB3LYP-D3/6-311+g(d,p)-SMD-water//UB3LYP/6-31G(d)-gas
HF=-2506.1816811

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^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-5-phenylpent-2-en-1-ol (**1a**)

JKM-04-272-2.2.fid
1H NMR

JKM-04-272-2_13C.2.fid
13C NMR
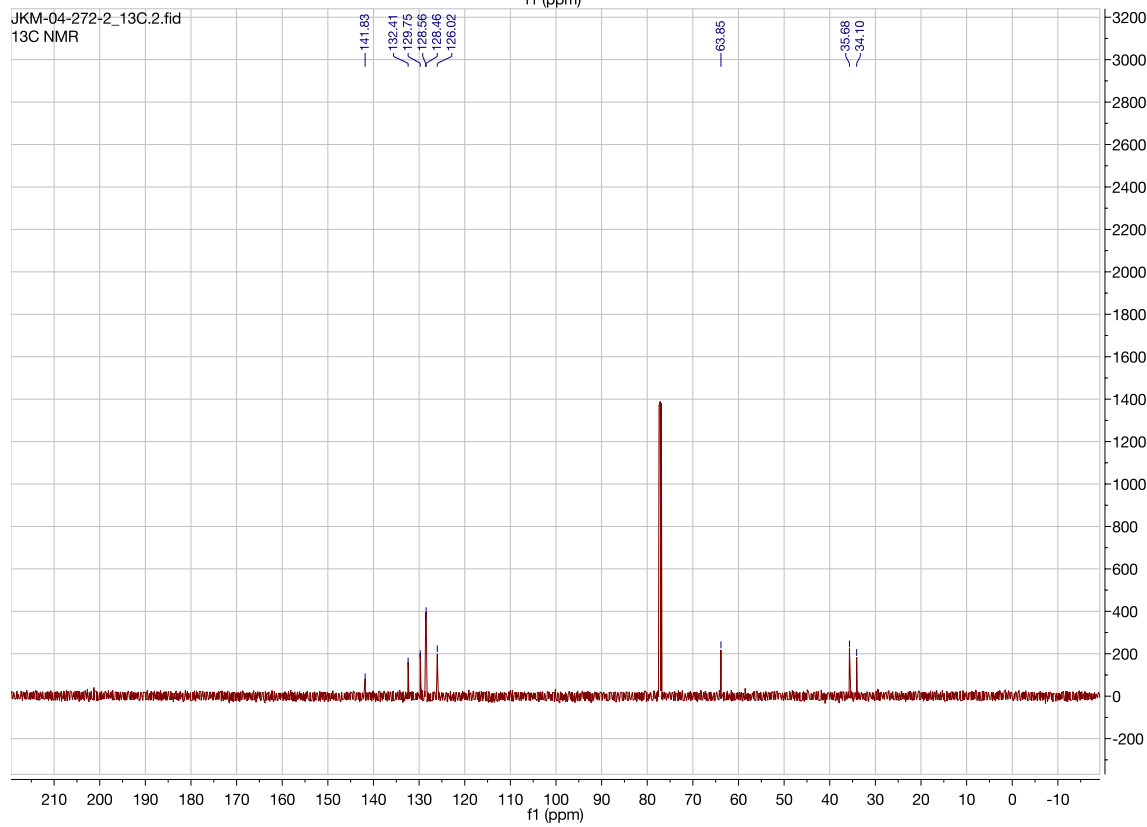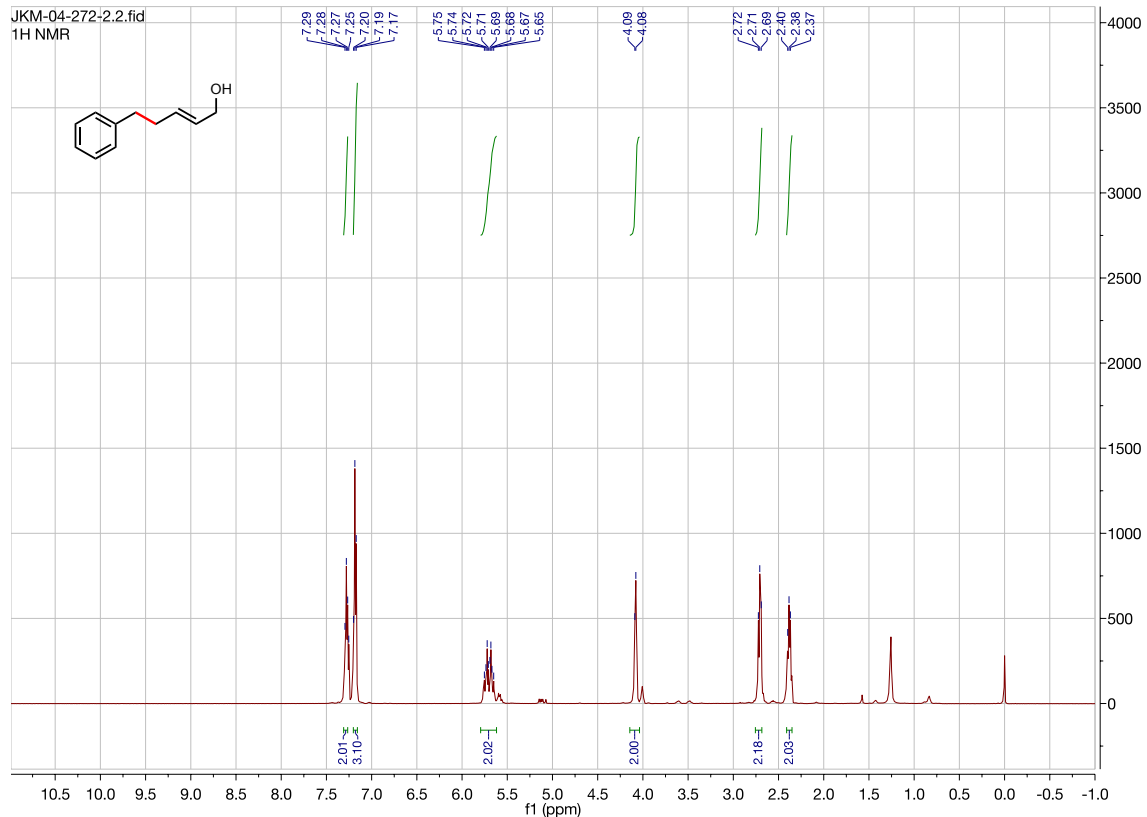
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-5-(3,5-dimethoxyphenyl)pent-2-en-1-ol (**1b**)
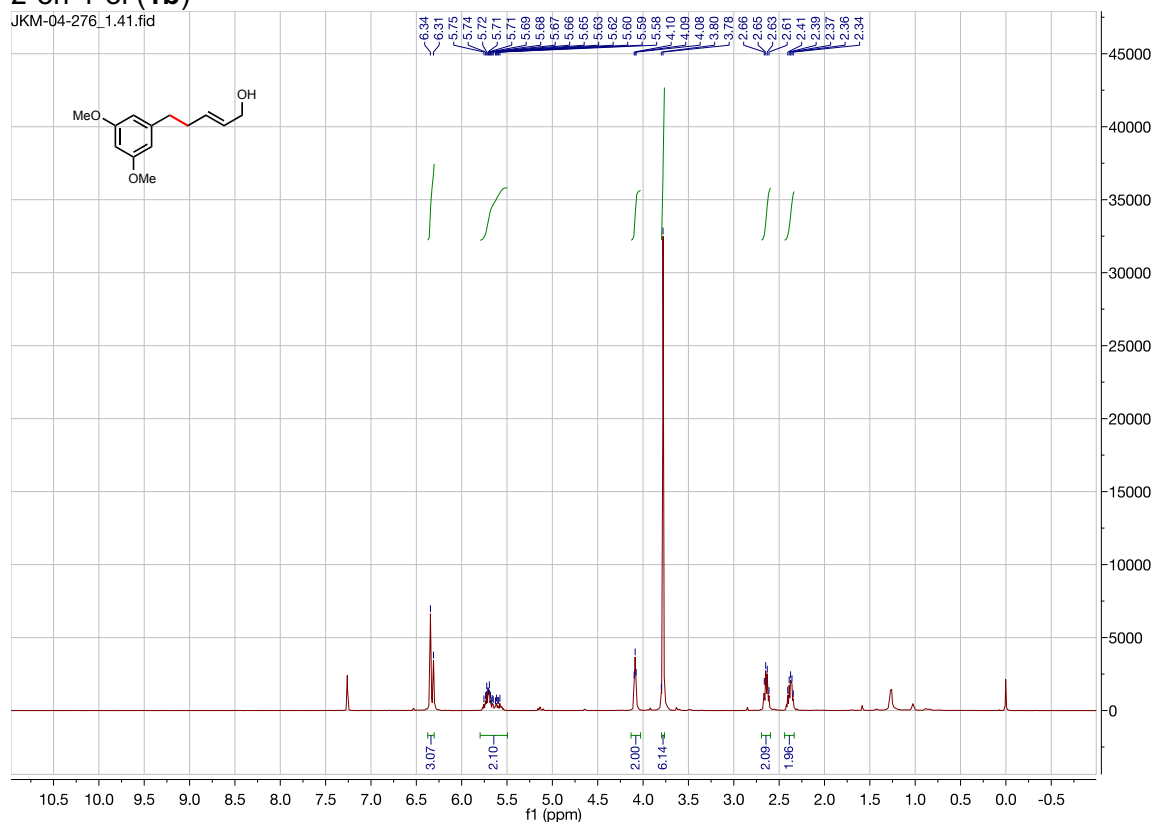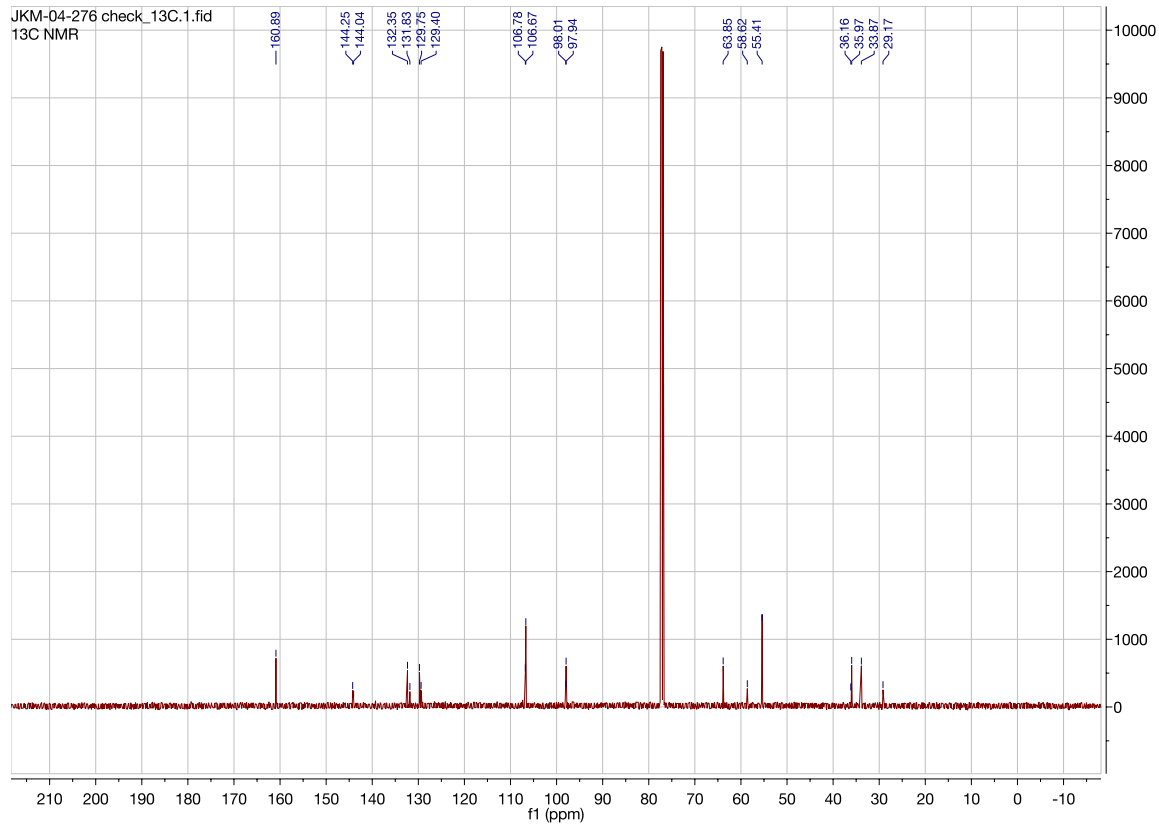
Note: Mixture of E/Z isomers.

^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-5-(3-chlorophenyl)pent-2-en-1-ol (**1c**)

JKM-05-064.1.fid
1H NMR

7.34
7.33
7.19
7.18
7.16
7.15
7.14
5.77
5.76
5.74
5.73
5.70
5.69
5.68
5.66
4.10
4.09
2.84
2.82
2.81
2.38
2.37

organic impurity co-eluting
with desired product; does
not appear in carbon NMR

1.04
3.08
2.00
1.98
2.01
2.00

f1 (ppm)
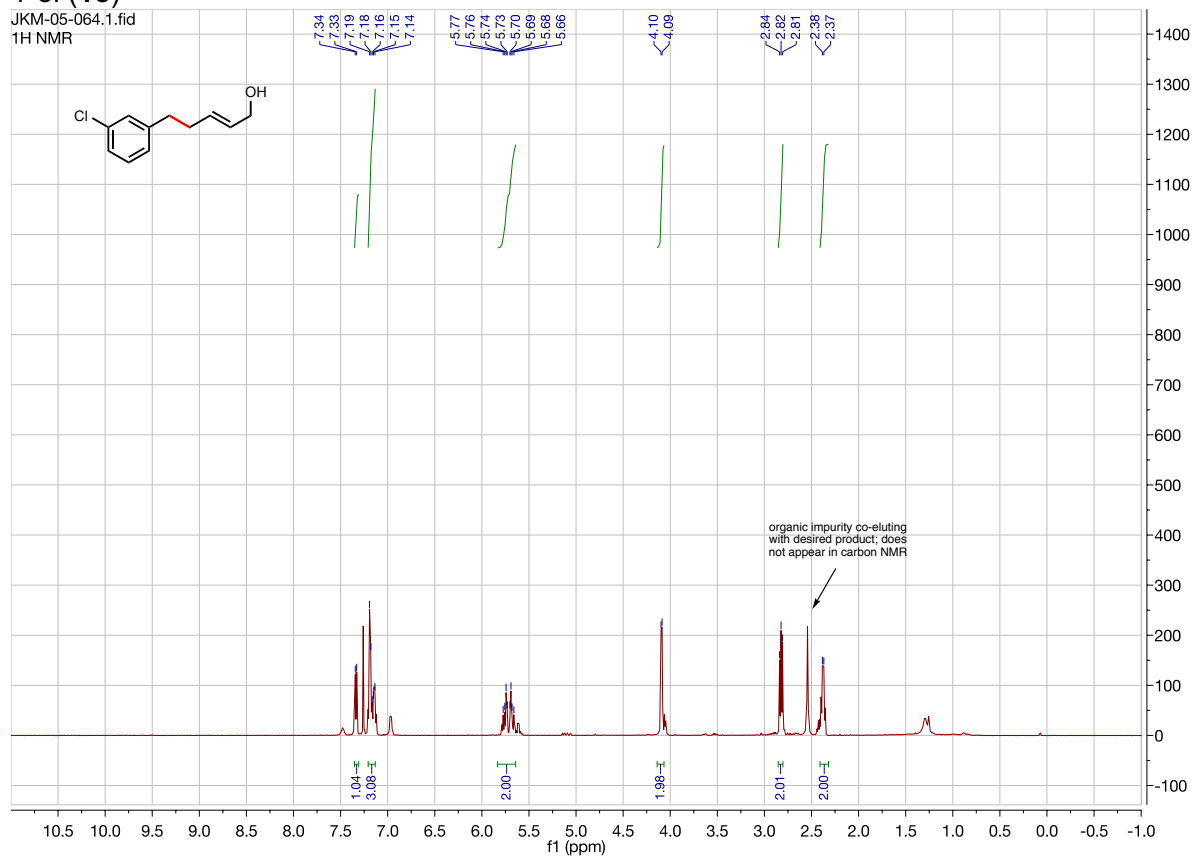
JKM-05-064_13C.1.fid
13C NMR

139.36
131.99
130.54
130.00
129.63
127.55
126.85
100.14
63.80
33.40
32.35

f1 (ppm)
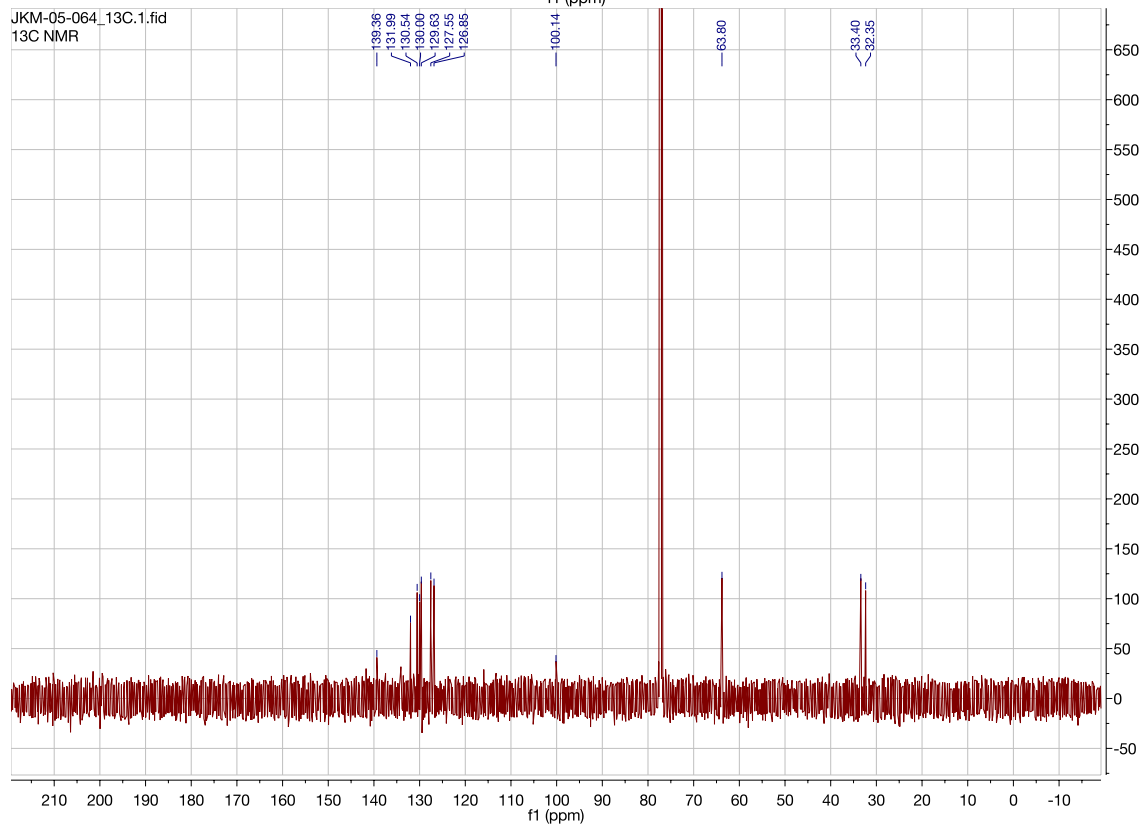
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (E)-5-(4-fluorophenyl)pent-2-en-1-ol (1d)

JKM-05-178 check_1.1.fid
1H NMR

Matsui_5_178_13C_CDCl3_Cryoprobe_1.fid
Matsui_5_178_13C_CDCl3_Cryoprobe
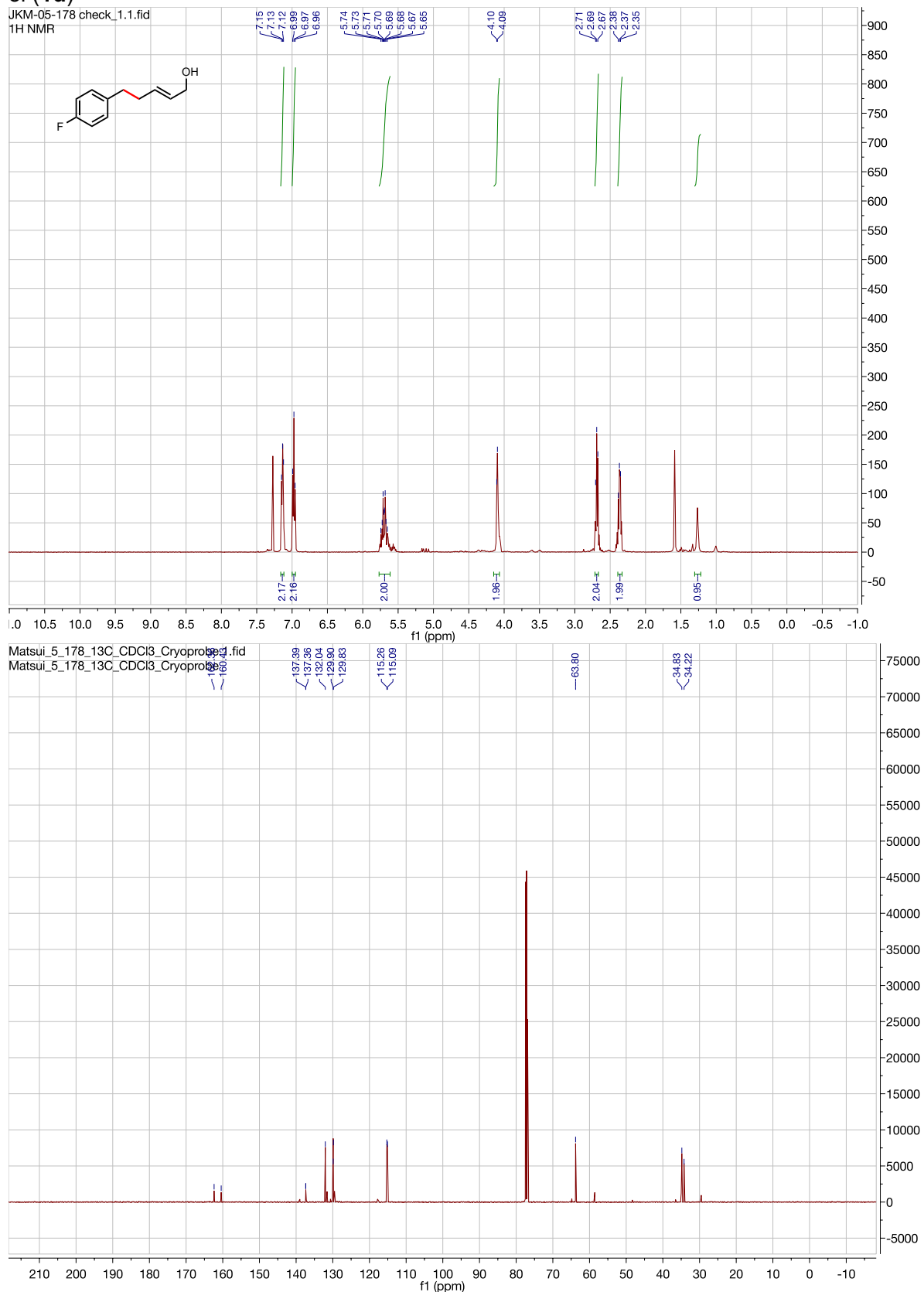
^{19}F NMR (CDCl$_3$, 471 MHz) of (*E*)-5-(4-fluorophenyl)pent-2-en-1-ol (**1d**)

JKM-05-178 check_19F_1.1.fid
F19 NMR

−117.36
−117.70

f1 (ppm)
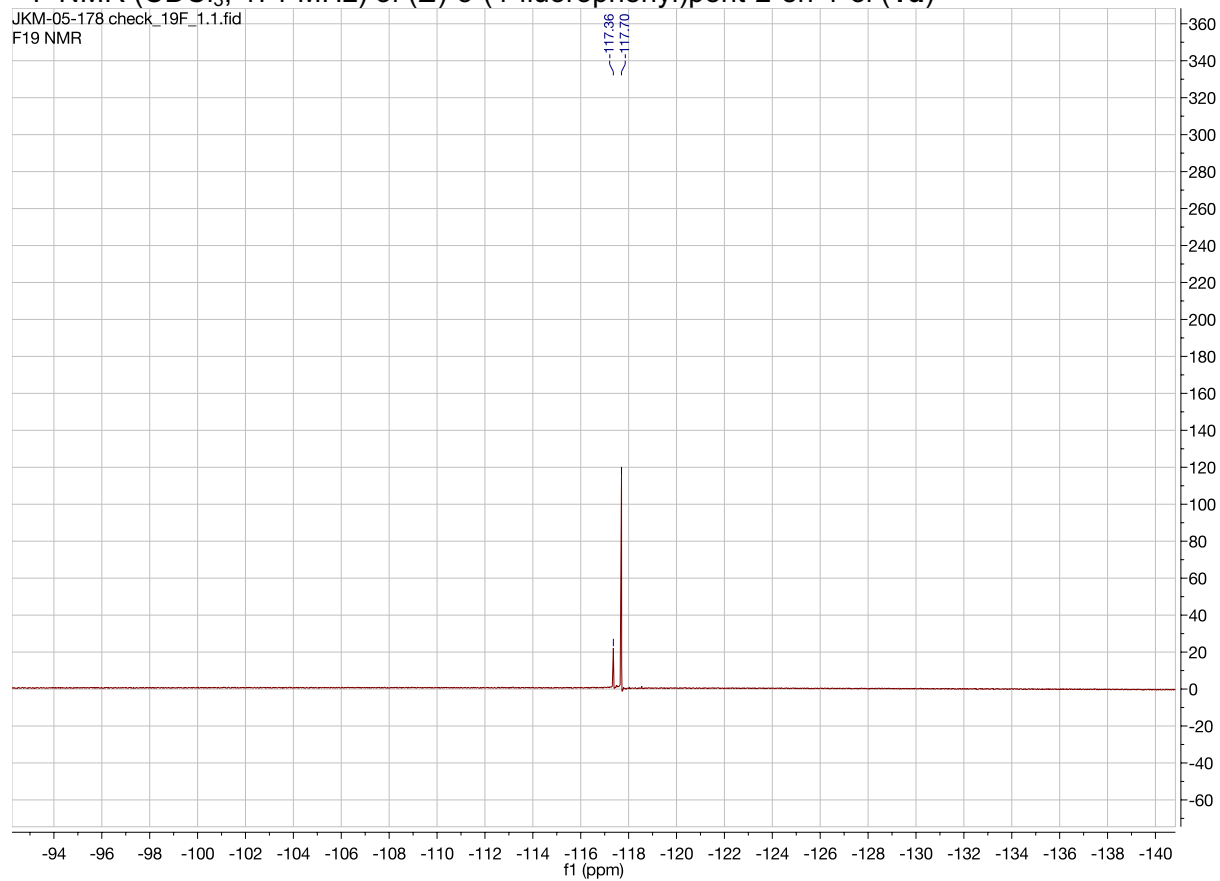
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-5-(2,4-difluorophenyl)pent-2-en-1-ol (**1e**)
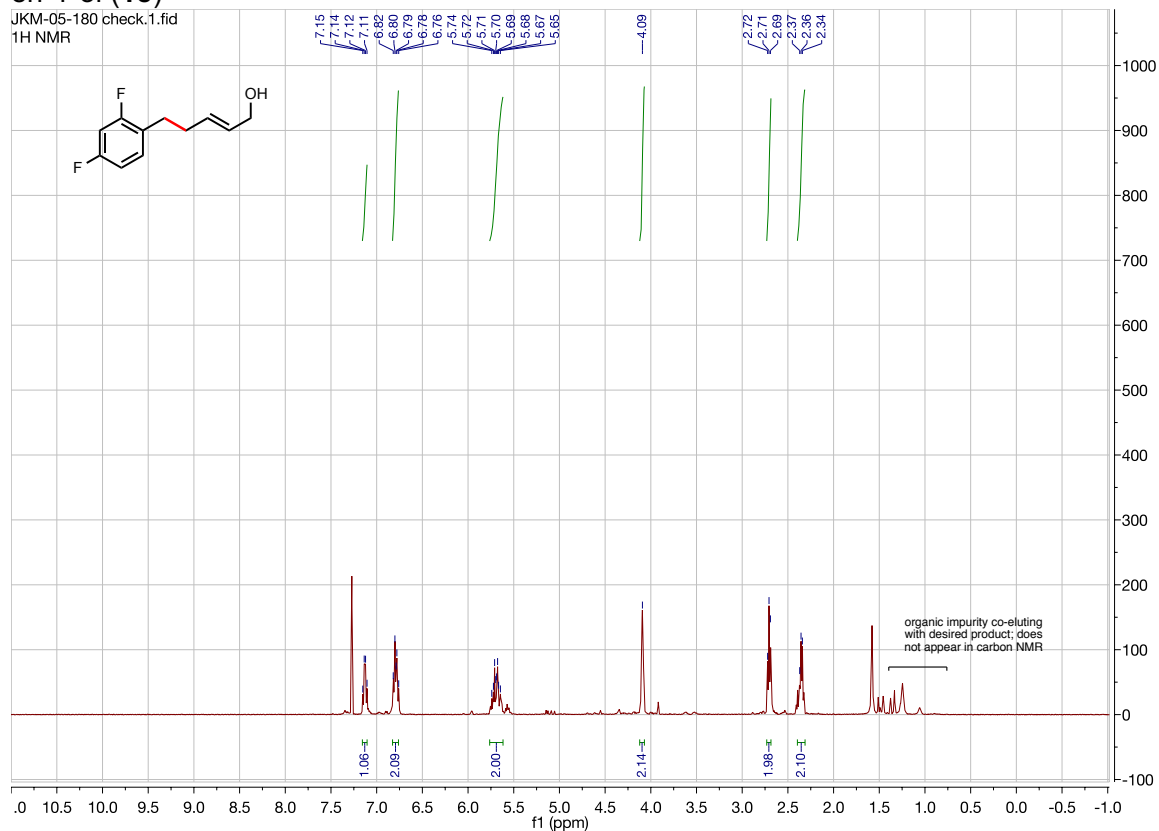
¹⁹F NMR (CDCl₃, 471 MHz) of (*E*)-5-(2,4-difluorophenyl)pent-2-en-1-ol (**1e**)
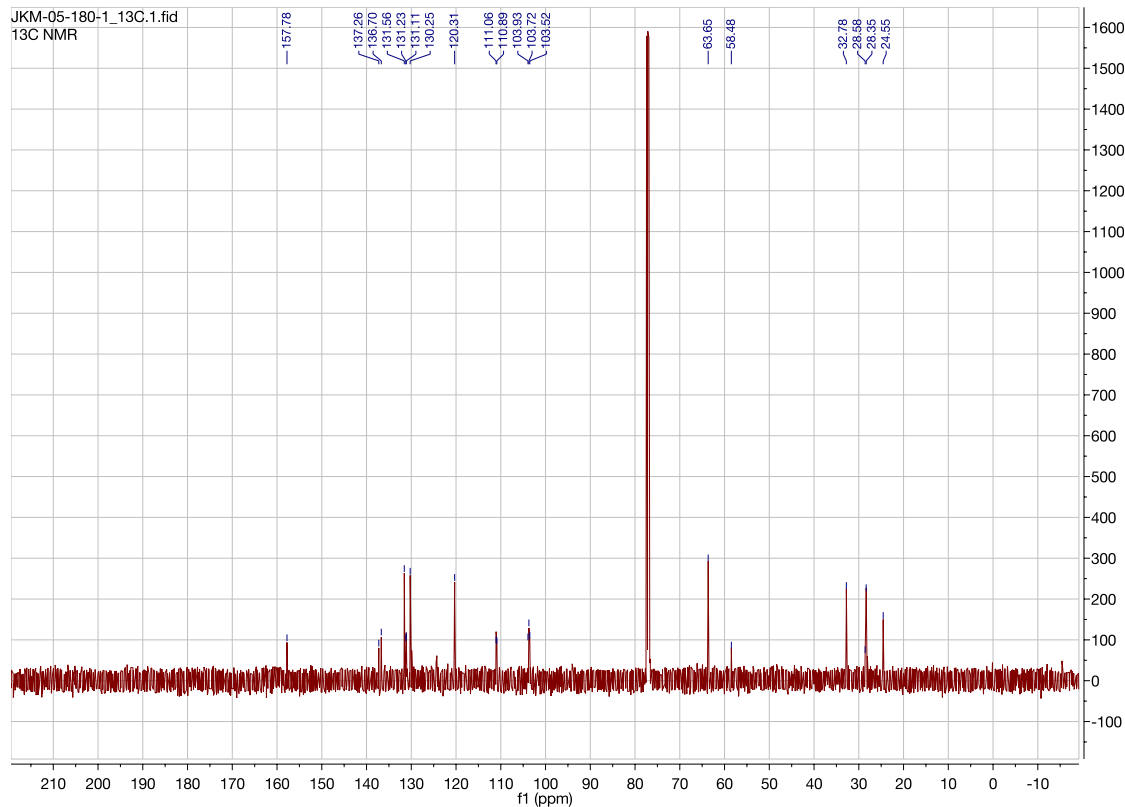
^{19}F NMR (CDCl$_3$, 471 MHz) of (*E*)-5-(2,4-difluorophenyl)pent-2-en-1-ol (**1e**)
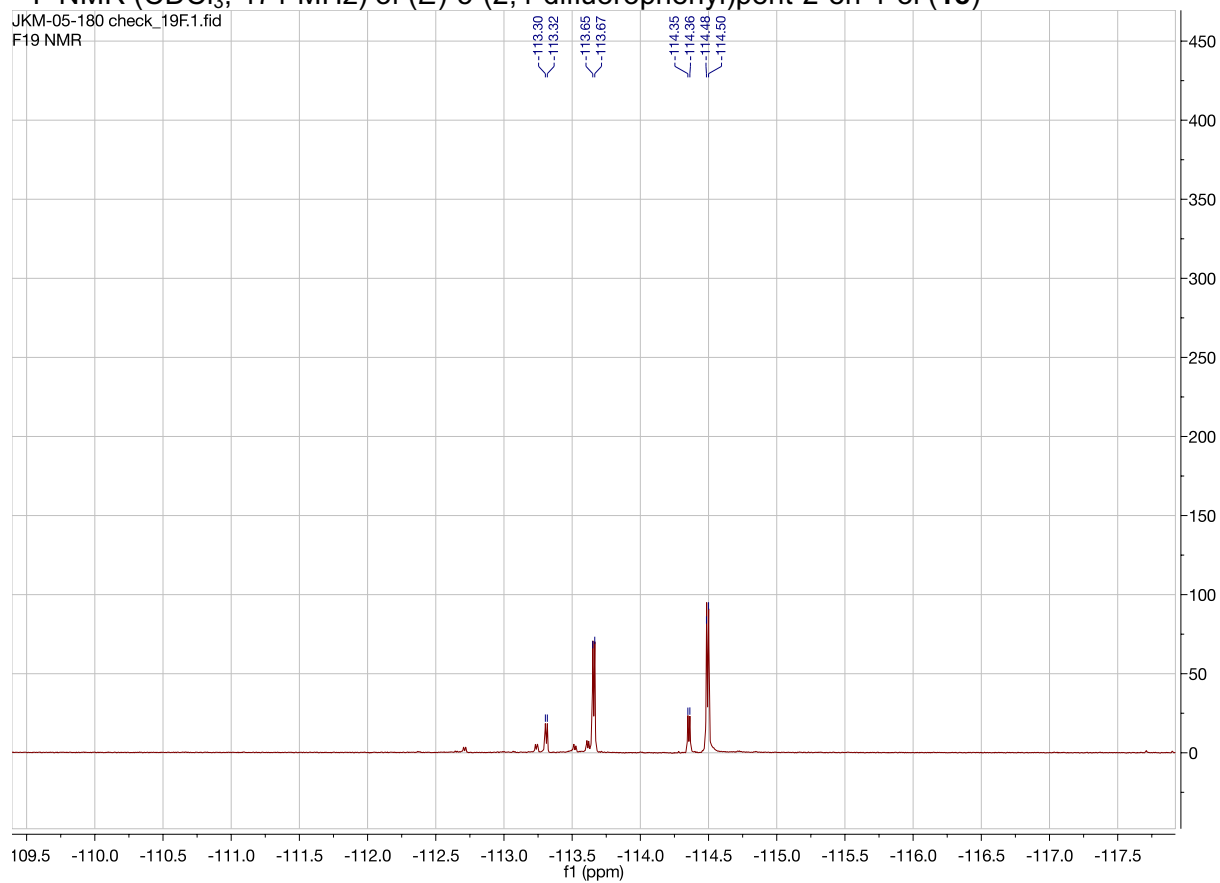
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of methyl (*E*)-4-(5-hydroxypent-3-en-1-yl)benzoate (**1f**)
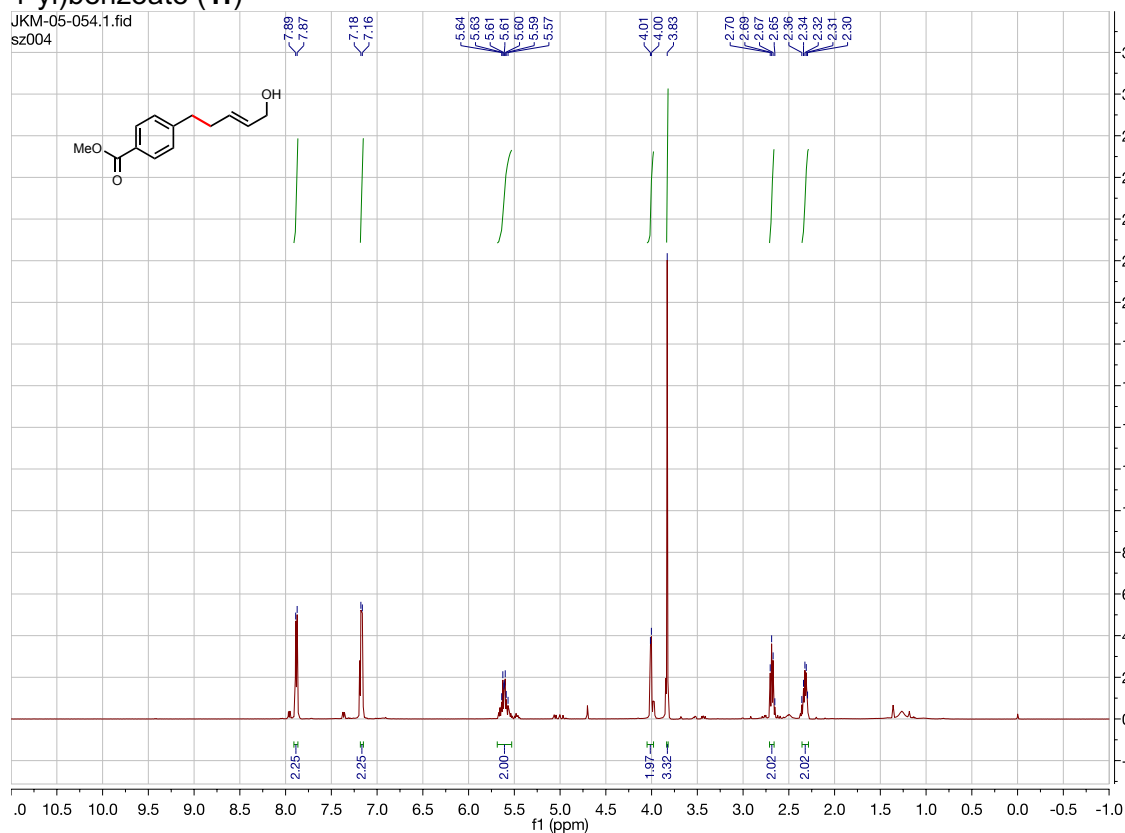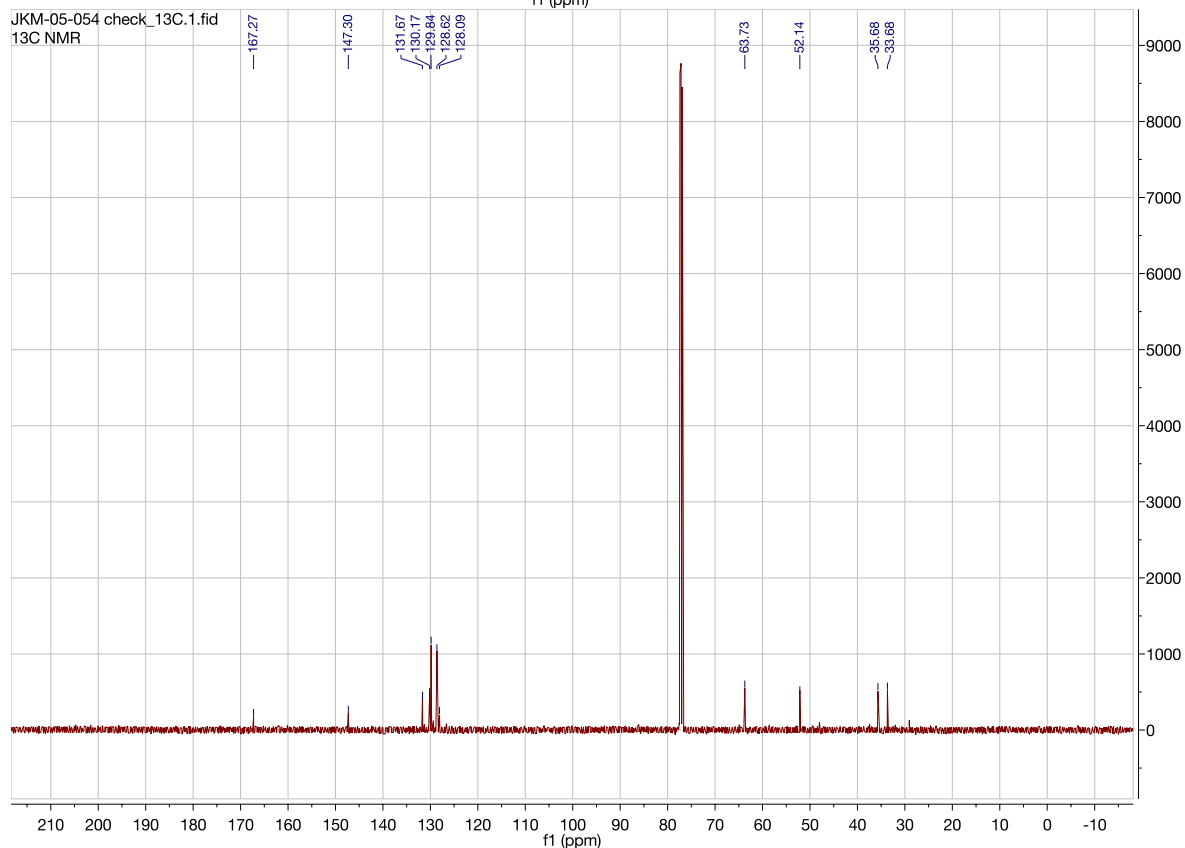
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (*E*)-5-(cyclopentyloxy)pent-2-en-1-ol (**1h**)
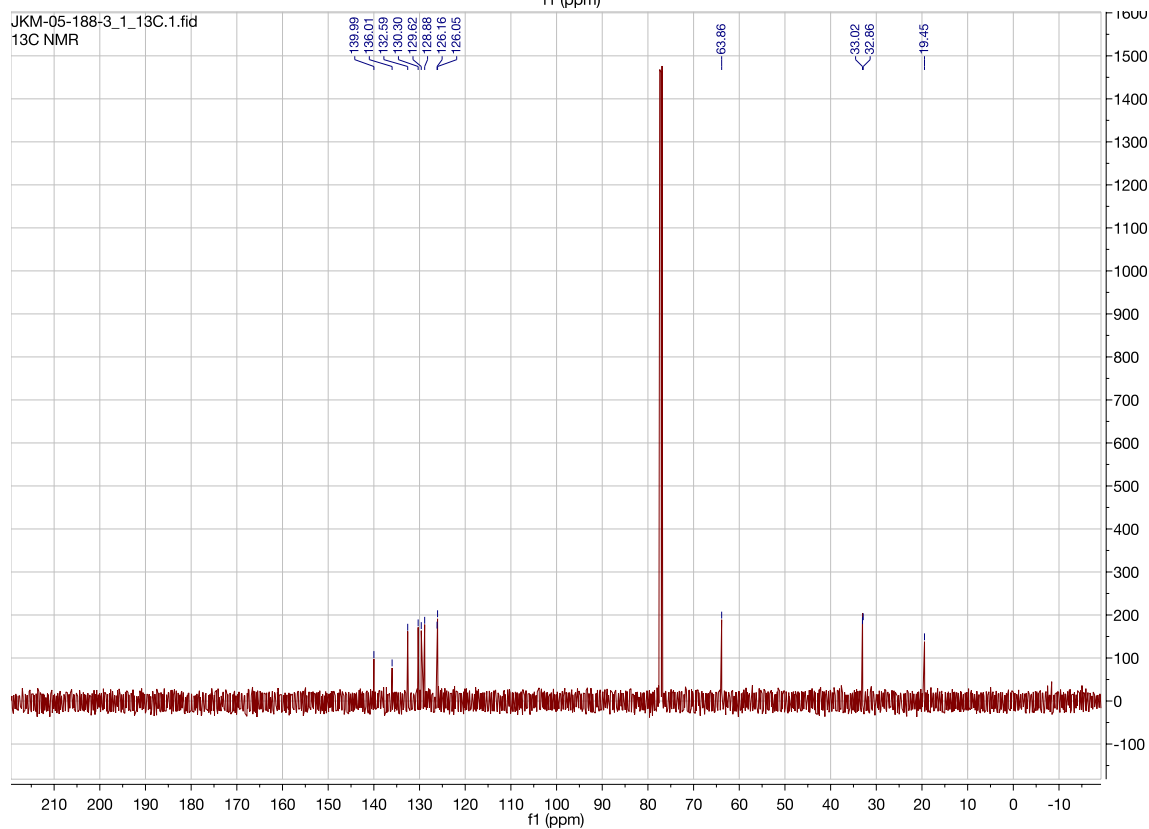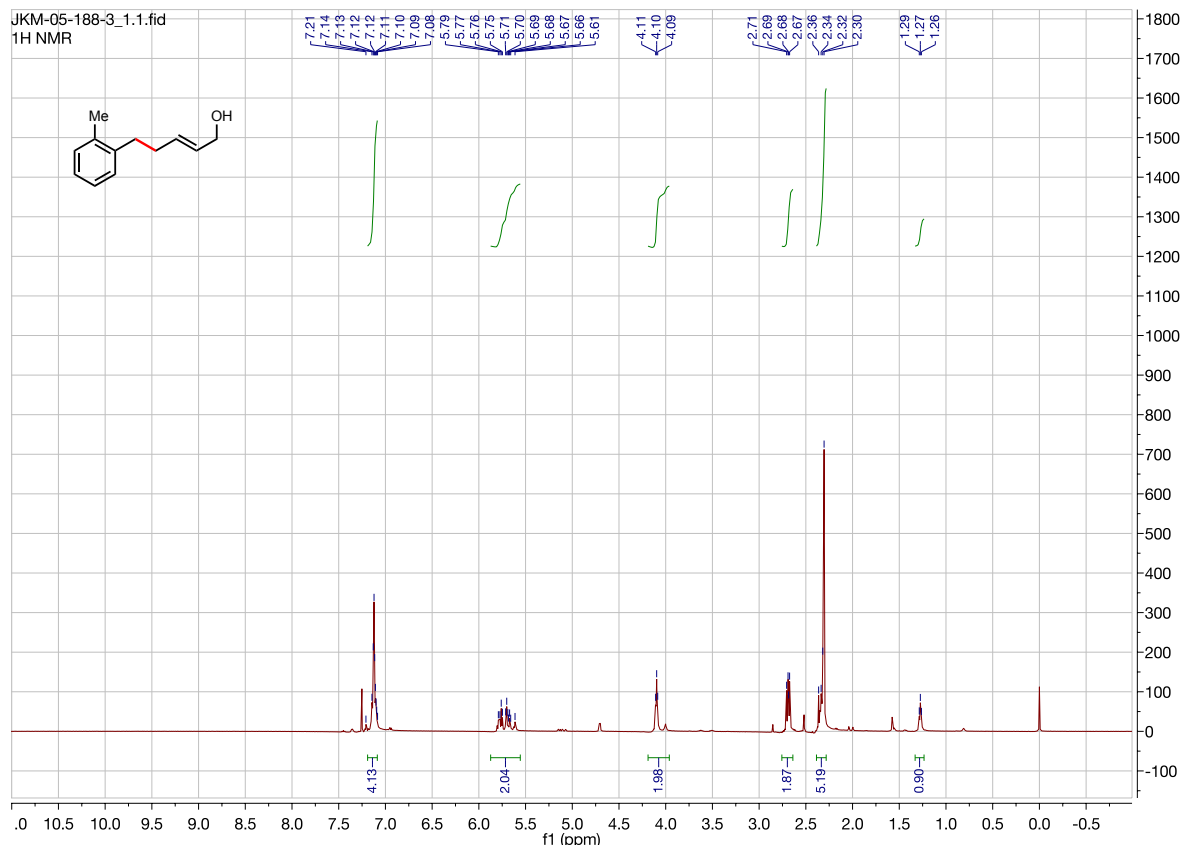
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (*E*)-5-(cyclopentyloxy)pent-2-en-1-ol (**1h**)

JKM-05-100.1.fid
1H NMR

¹H peaks: 5.90, 5.89, 5.87, 5.85, 5.65, 5.63, 5.61, 5.60, 4.10, 4.09, 3.90, 3.42, 3.41, 3.40, 2.39, 2.38, 2.36, 1.74, 1.73, 1.70, 1.68, 1.65, 1.62, 1.52, 1.51, 1.50

Integrations: 1.00, 1.05, 2.30, 1.18, 2.09, 2.13, 7.20, 2.26
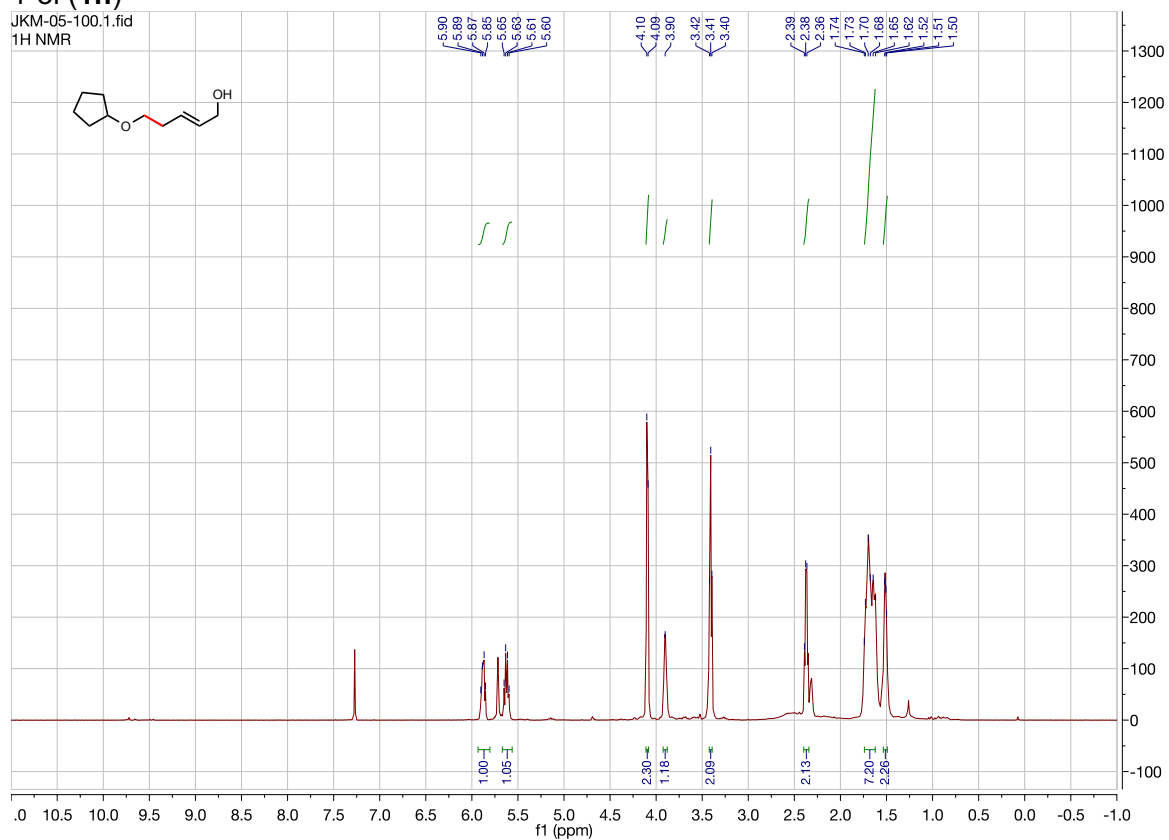
JKM-05-100_13C.1.fid
13C NMR

¹³C peaks: 131.07, 130.54, 81.93, 67.24, 57.58, 32.23, 28.40, 23.58
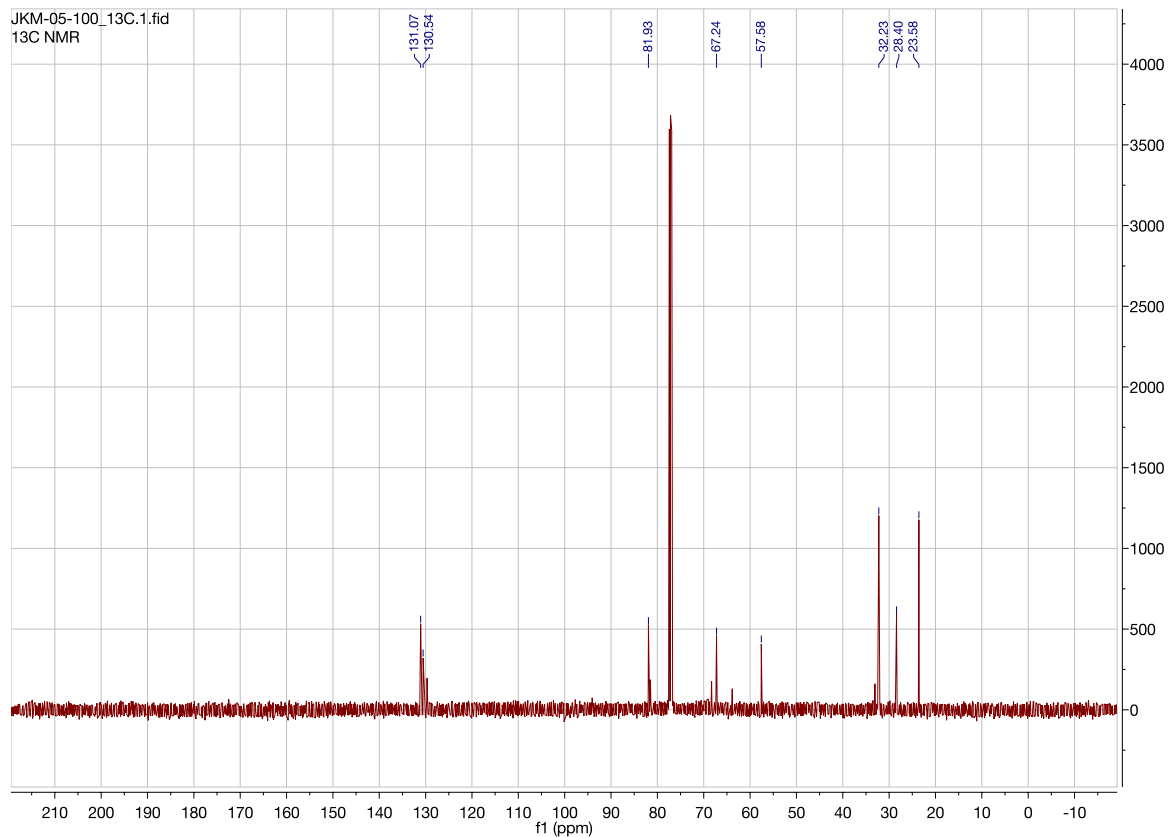
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (*E*)-5-((4-methoxybenzyl)oxy)pent-2-en-1-ol (**1i**)
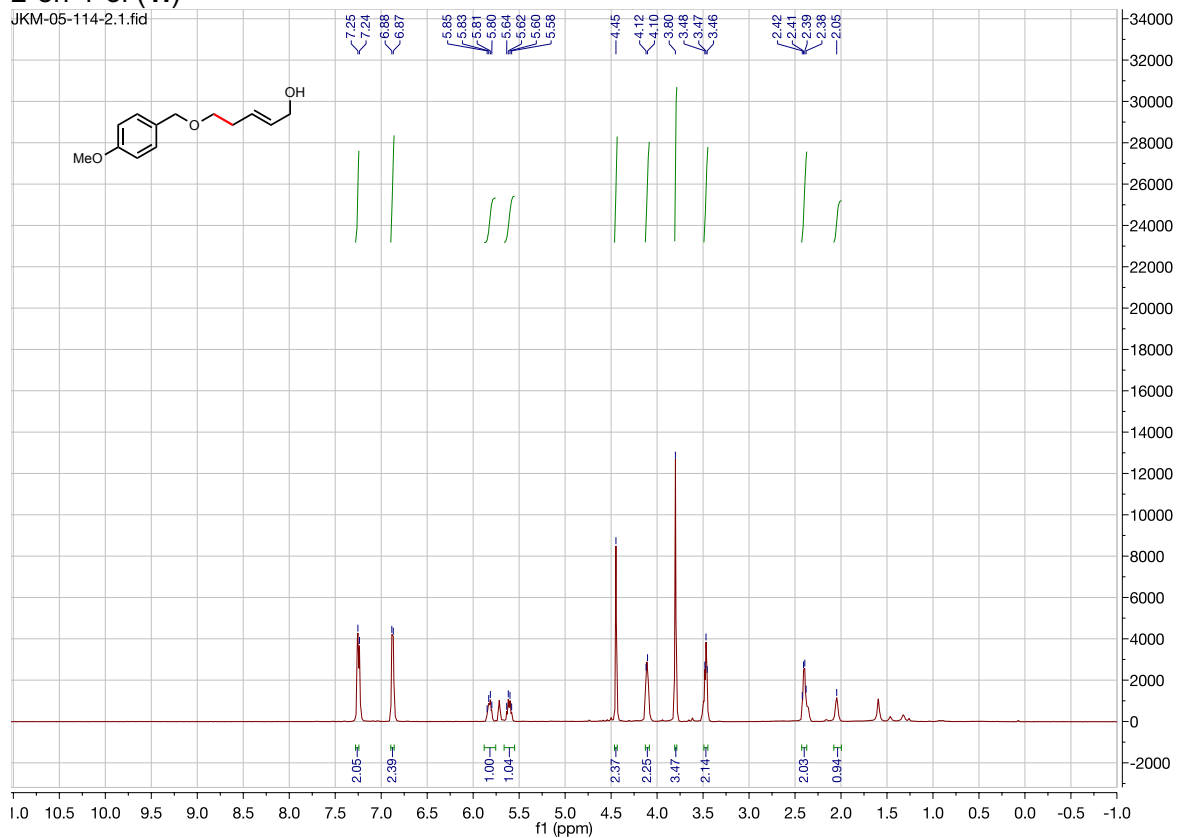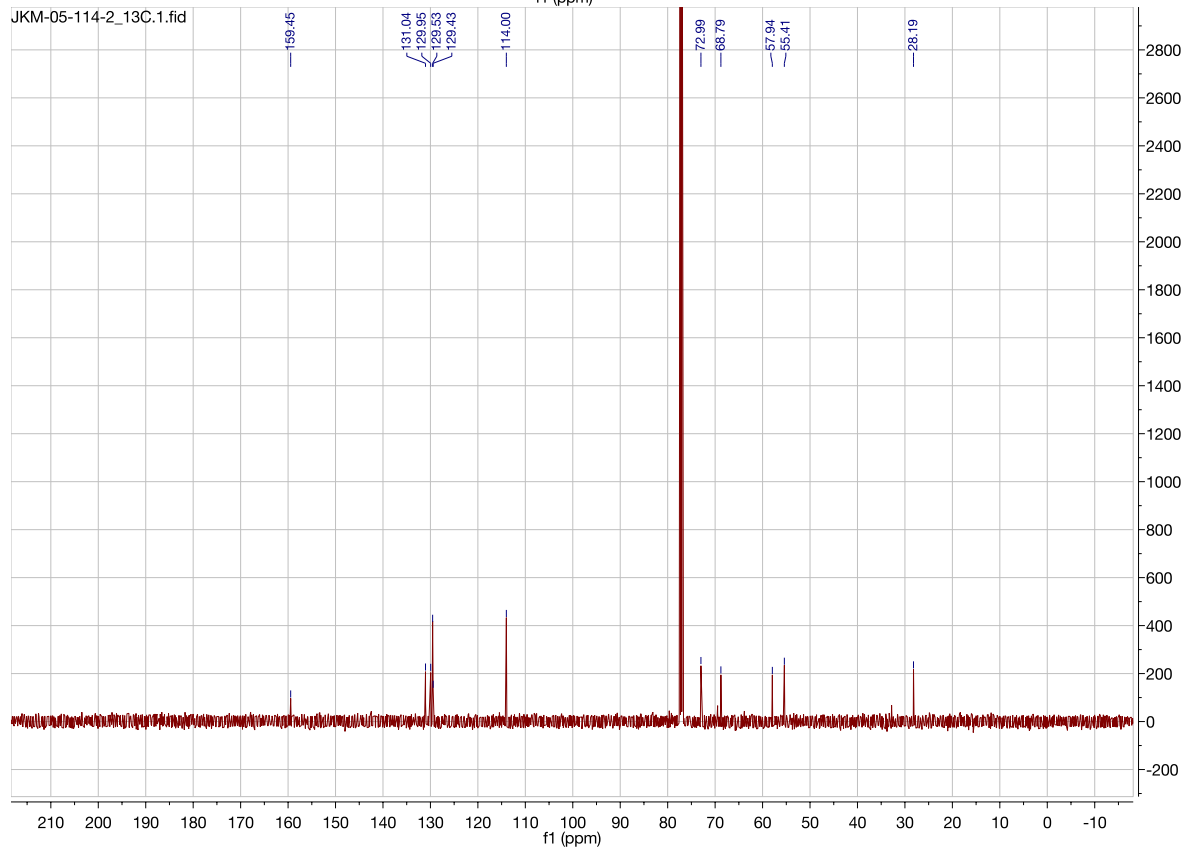
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-5-(((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methoxy)pent-2-en-1-ol (**1j**)
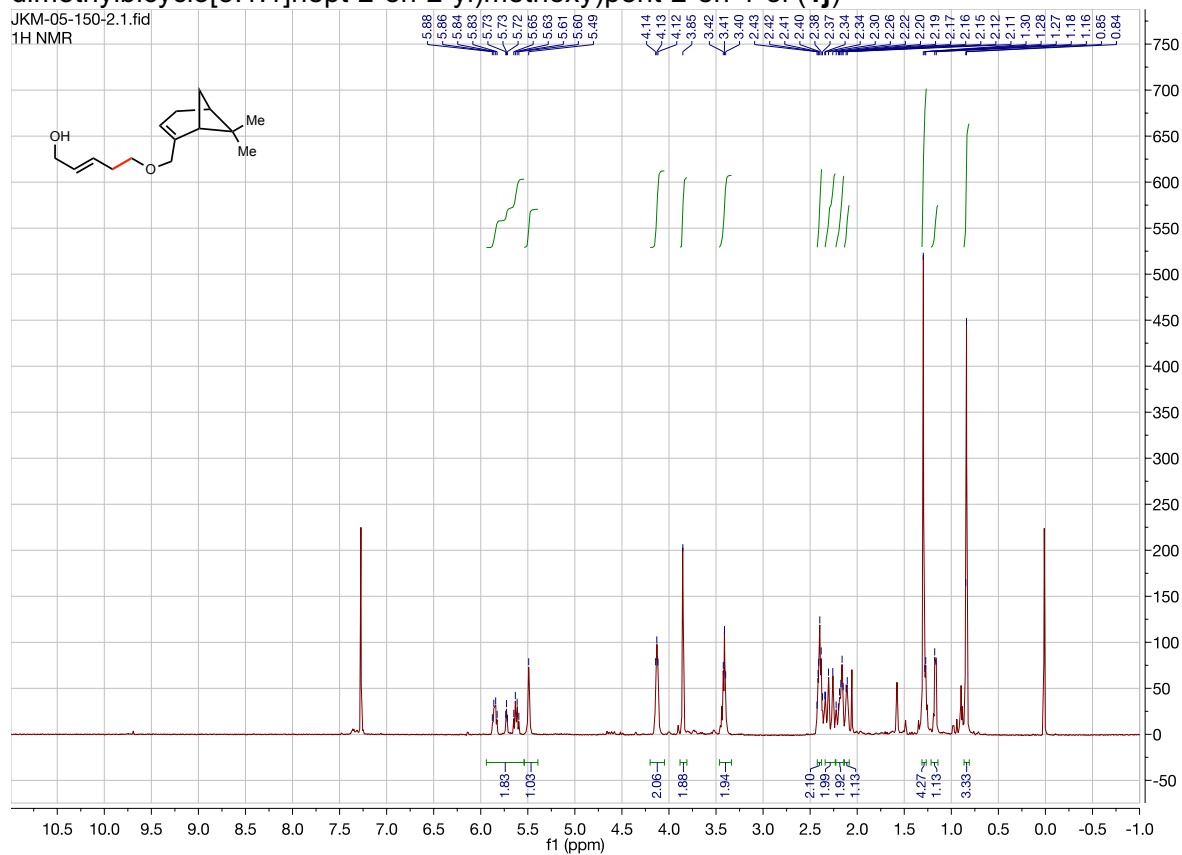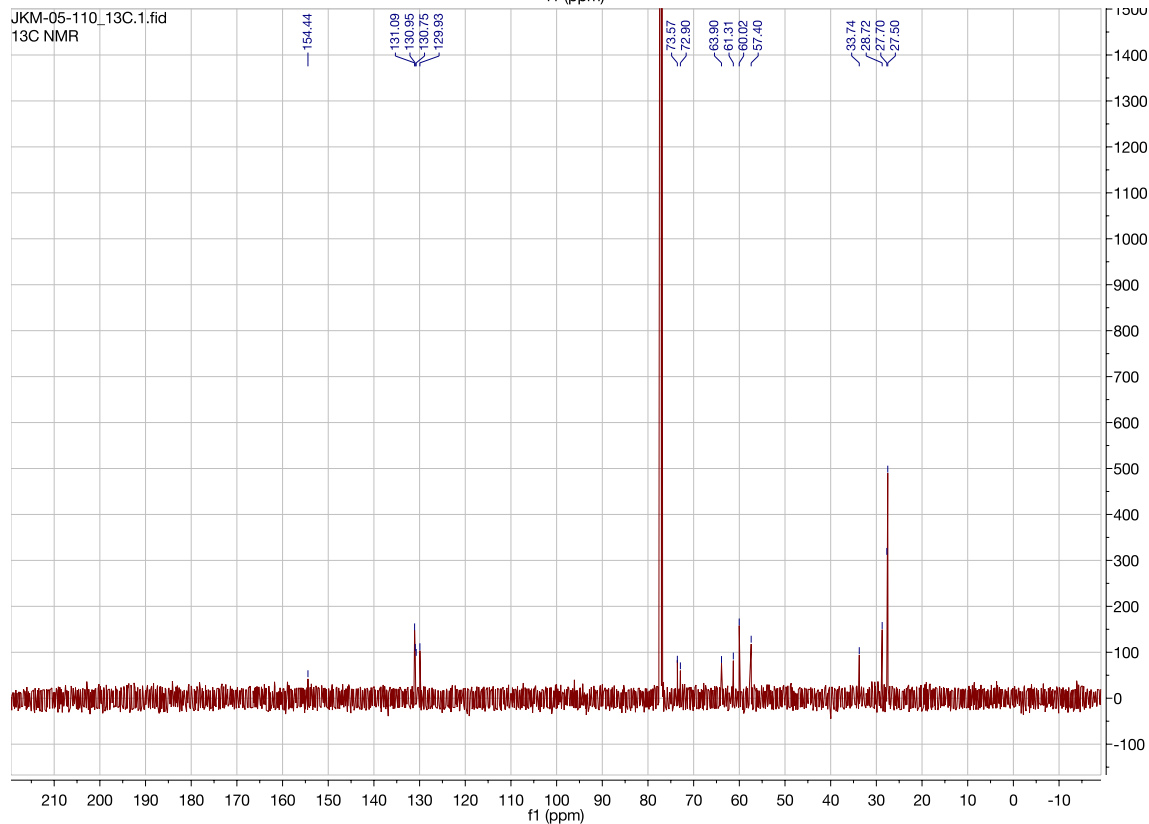
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (*E*)-5-(*tert*-Butoxy)pent-2-en-1-ol (**1k**)
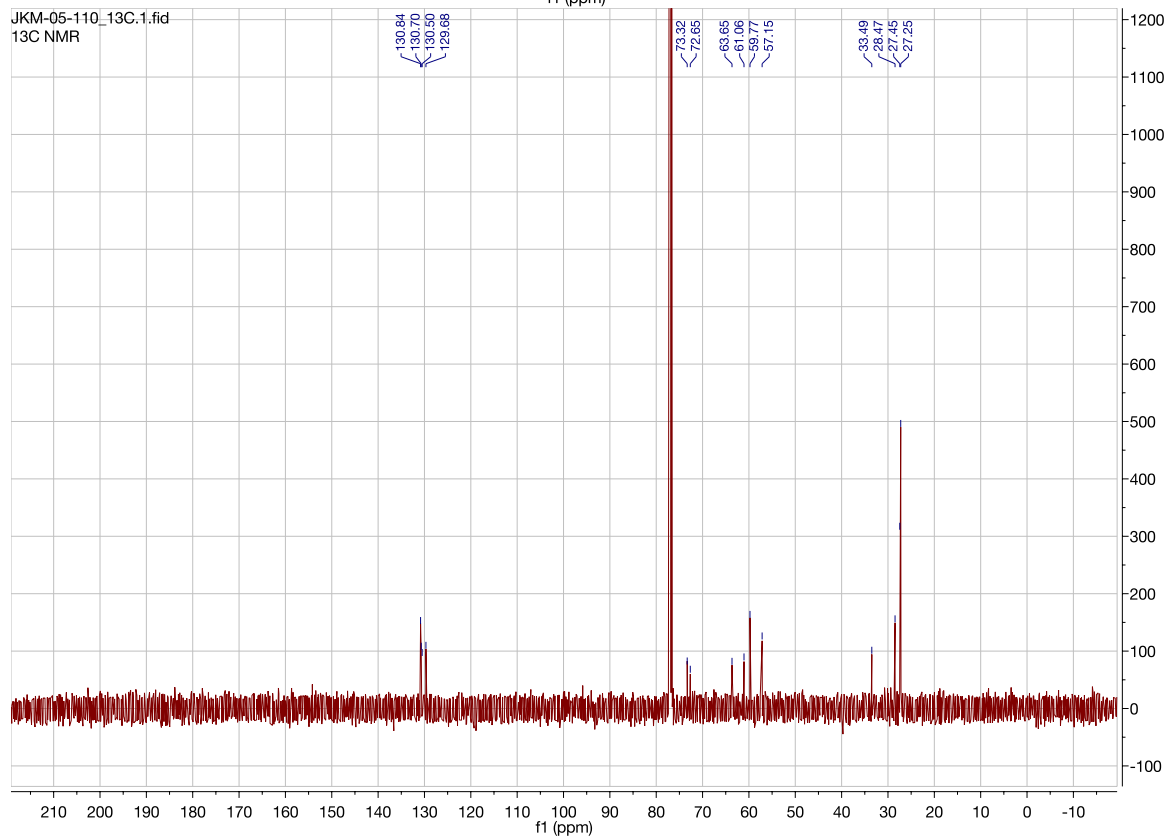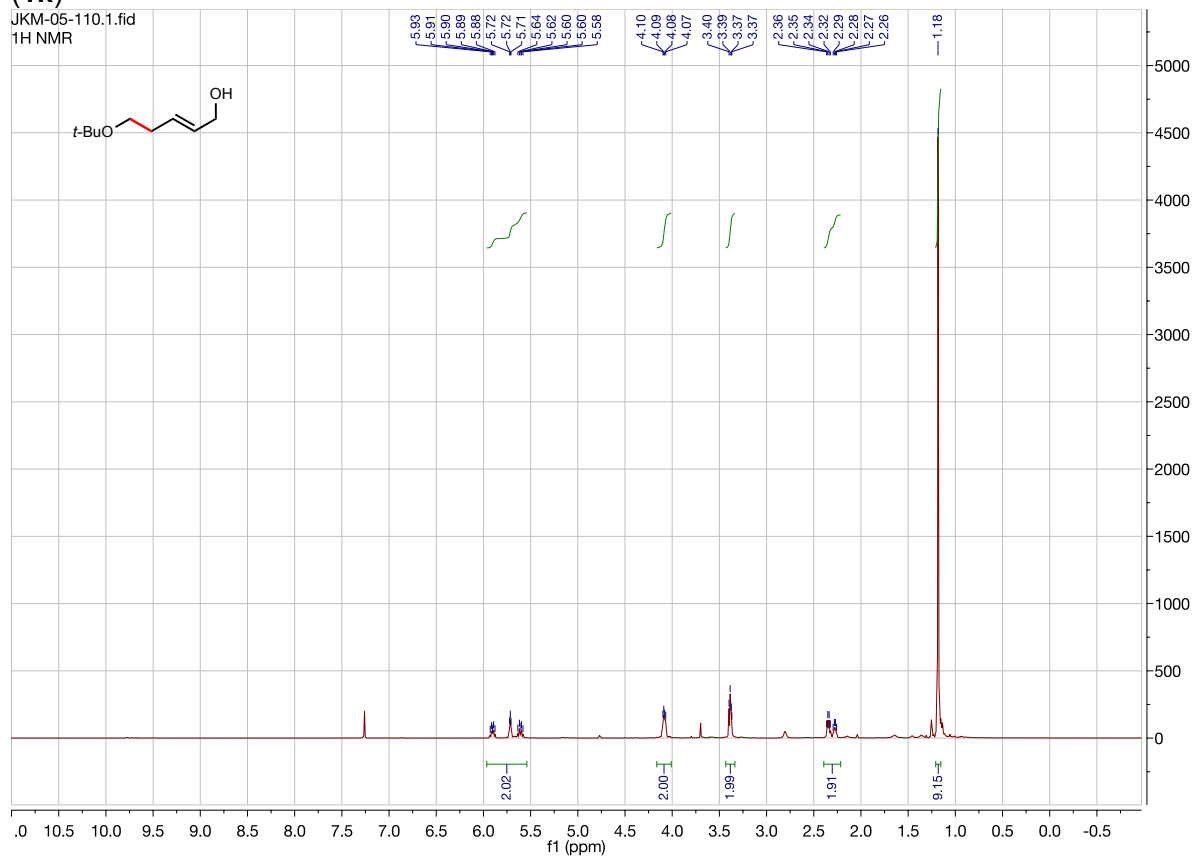
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*Z*)-2-methyl-5-phenylpent-2-en-1-ol (**2f**)

JKM-05-126-2.1.fid
1H NMR
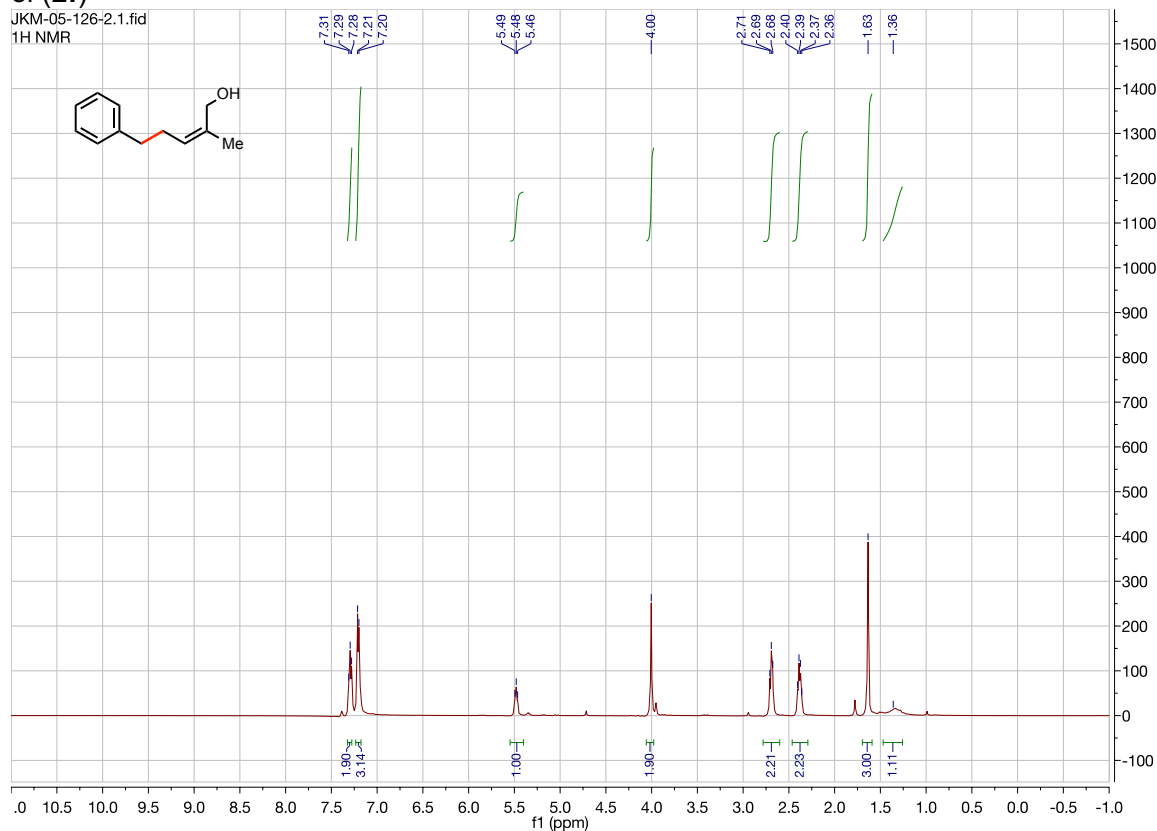
JKM-05-126-2_13C.1.fid
13C NMR
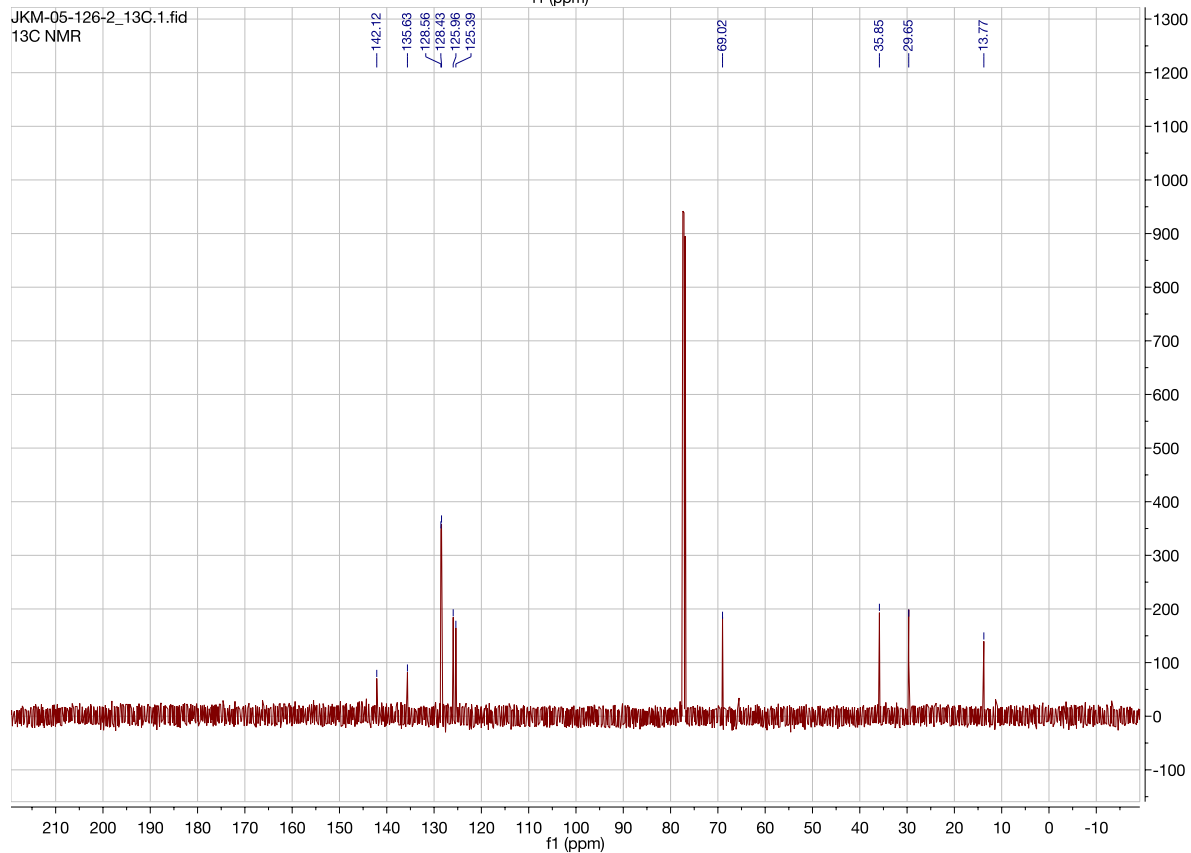
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (E)-4-(tetrahydro-2H-pyran-4-yl)but-2-en-1-ol (2a)
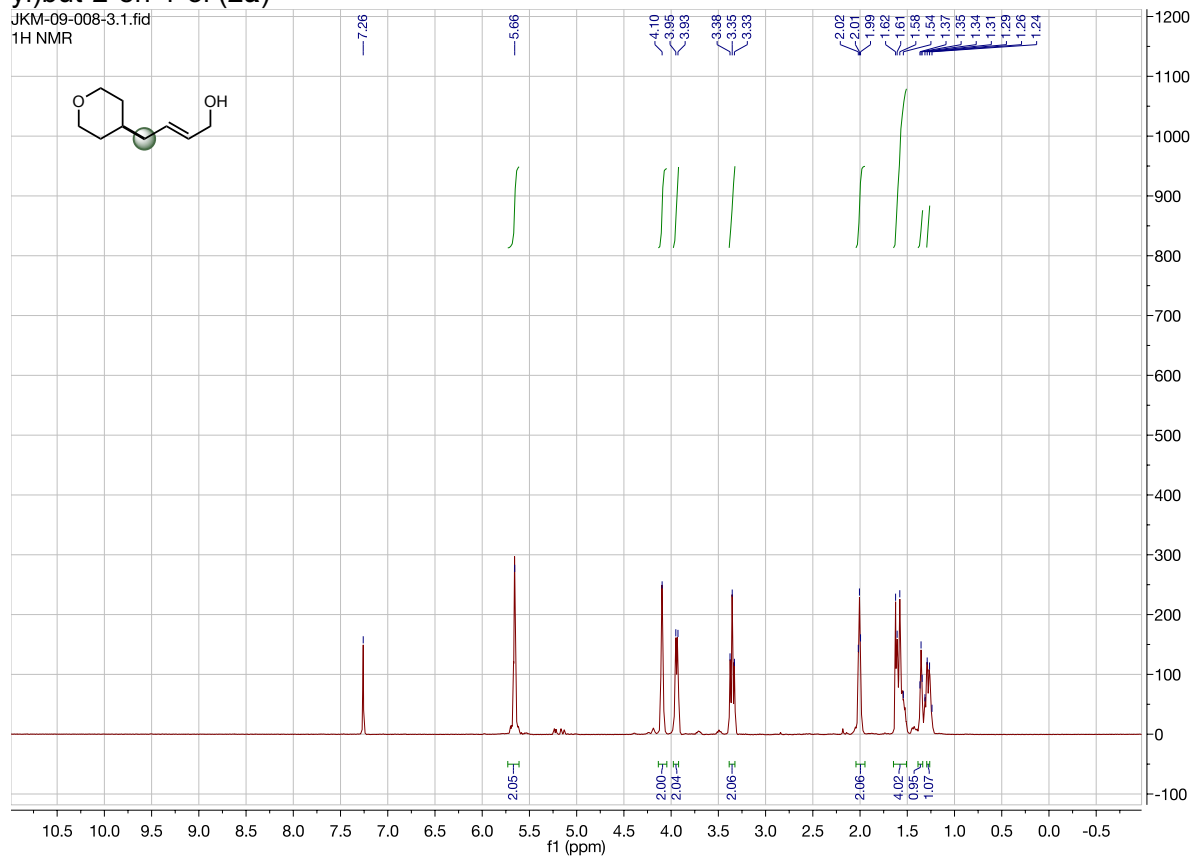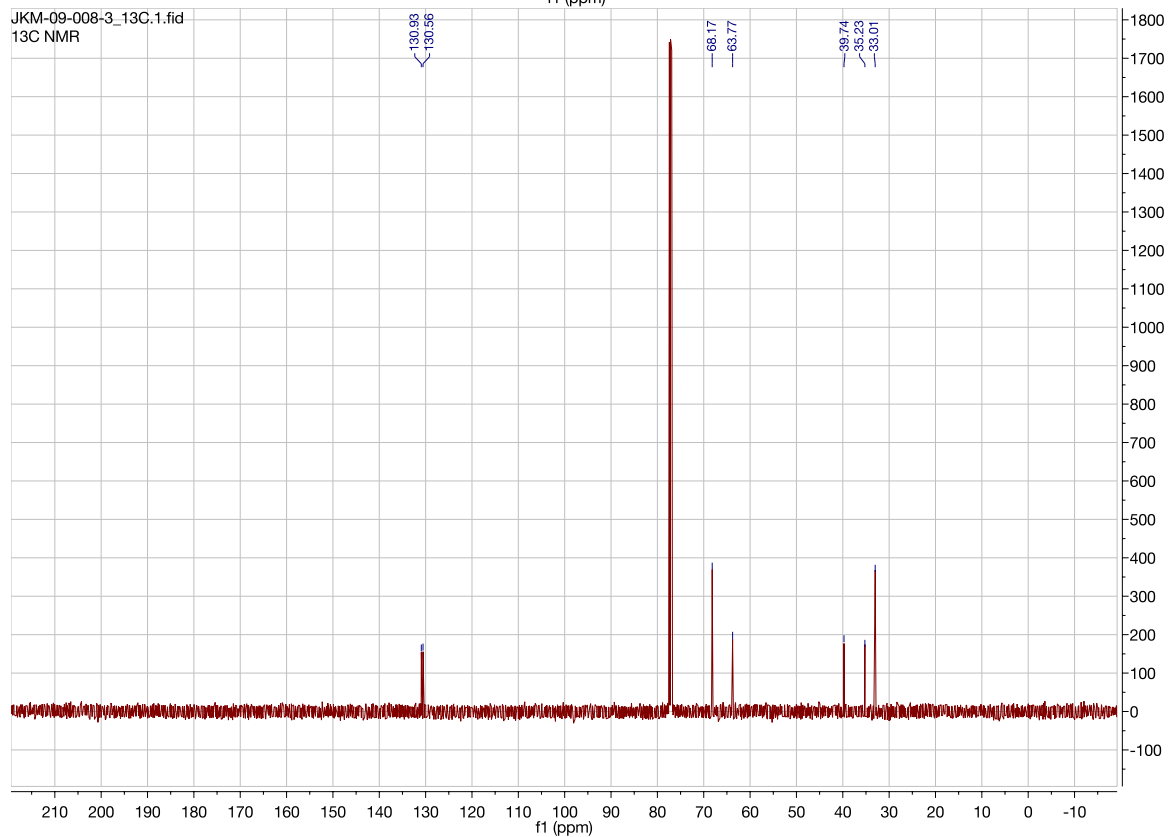
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of *(E)*-4-(cyclohex-3-en-1-yl)but-2-en-1-ol (**2c**)
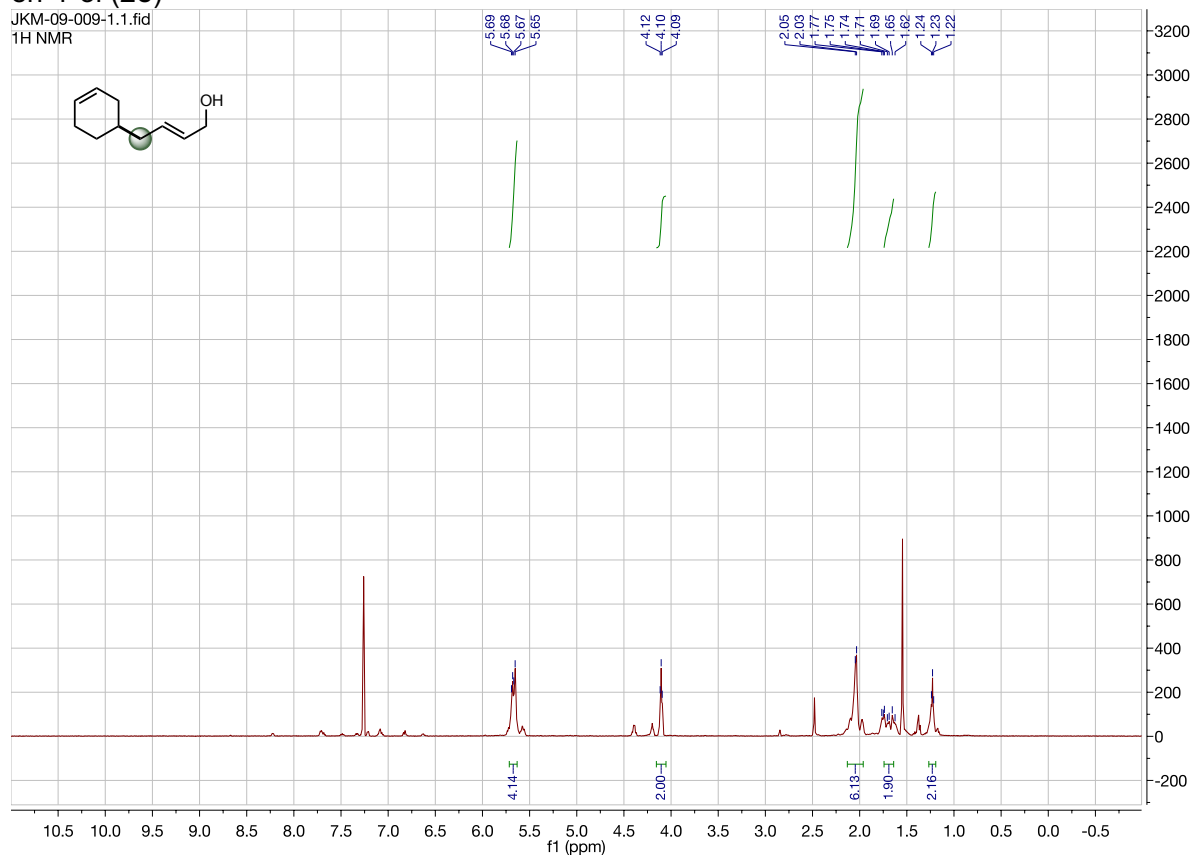
Note: Trace photocatalyst is present in the aryl region (<5%) by integration.
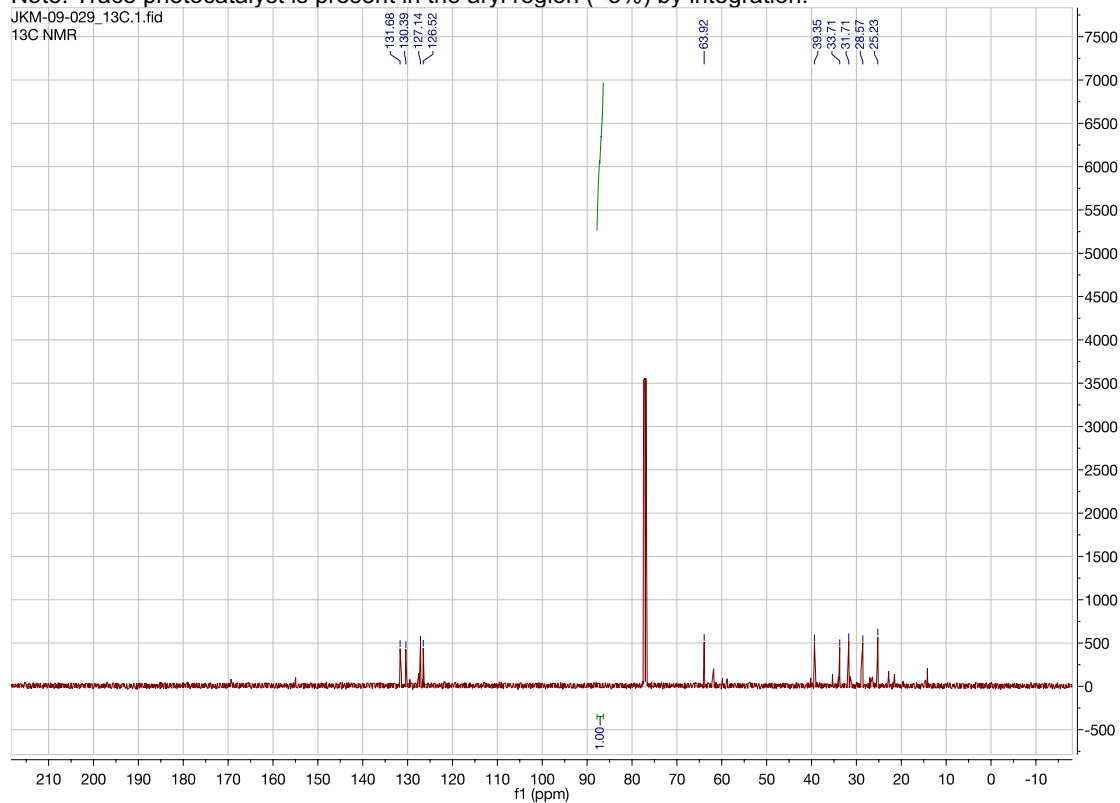
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (E)-6-(benzo[d][1,3]dioxol-5-yl)-5-methylhex-2-en-1-ol (**2d**)

Note: Major E isomer.

JKM-09-017 check.1.fid
1H NMR
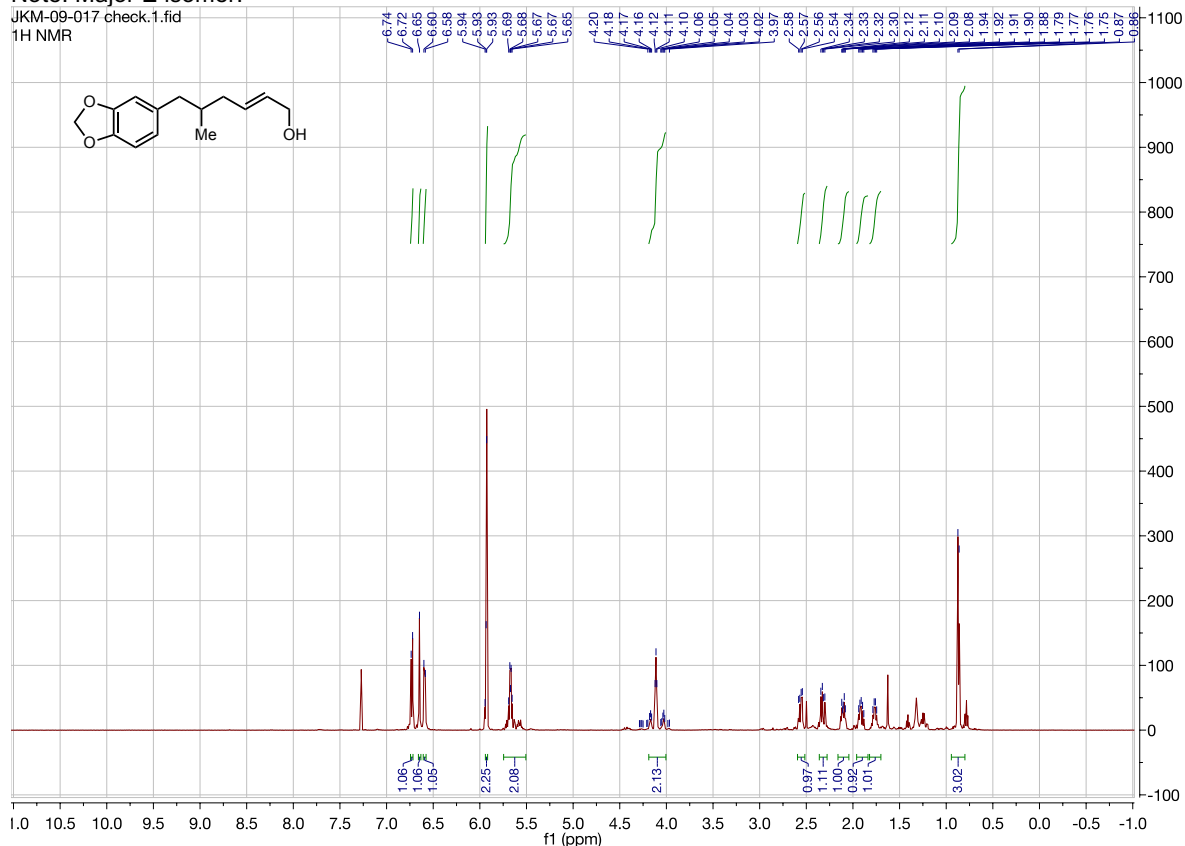
JKM-09-017-1_13C.1.fid
13C NMR
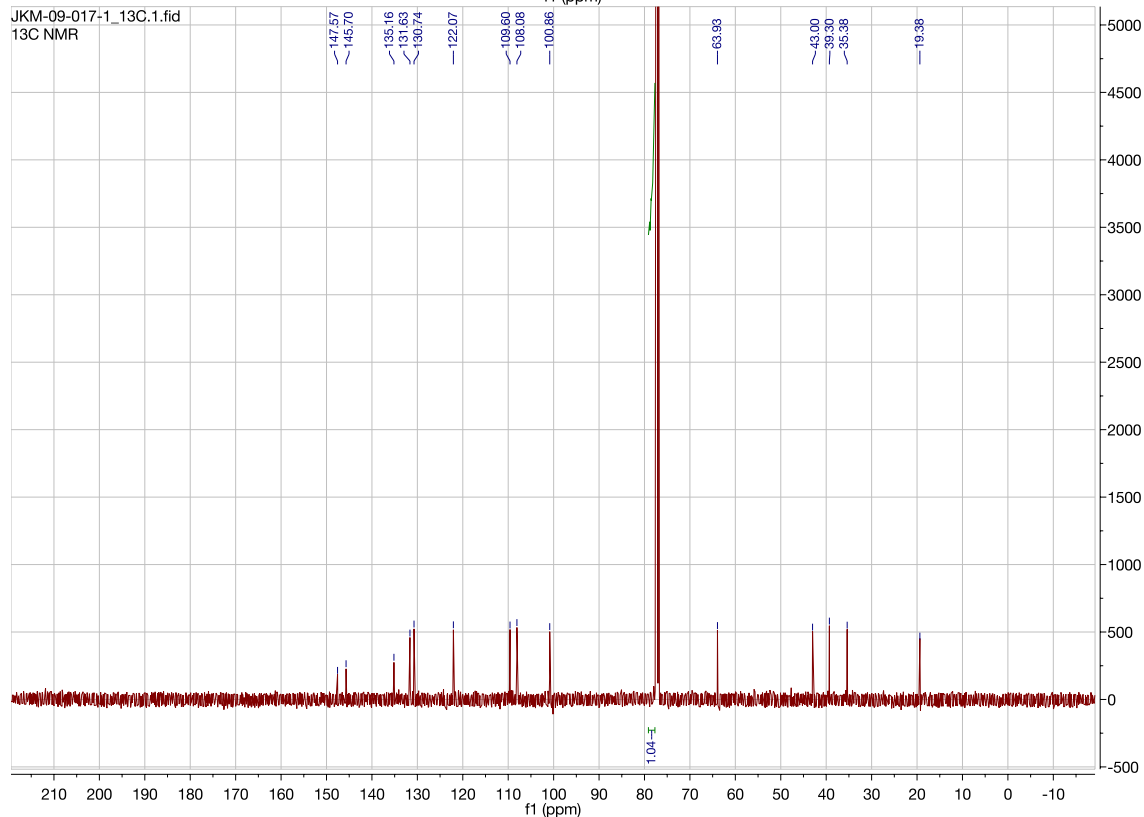
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of benzyl (E)-4-(4-hydroxybut-2-en-1-yl)piperidine-1-carboxylate (**2e**)

¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (*E*)-2-methyl-4-(tetrahydro-2H-pyran-4-yl)but-2-en-1-ol (**2g**)

^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of *(E)*-6-(benzo[d][1,3]dioxol-5-yl)-2,5-dimethylhex-2-en-1-ol (**2h**)

^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (E)-4-((3aS,5R,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)but-2-en-1-ol **(2i)**

JKM-09-018_check 1.1.fid
1H NMR
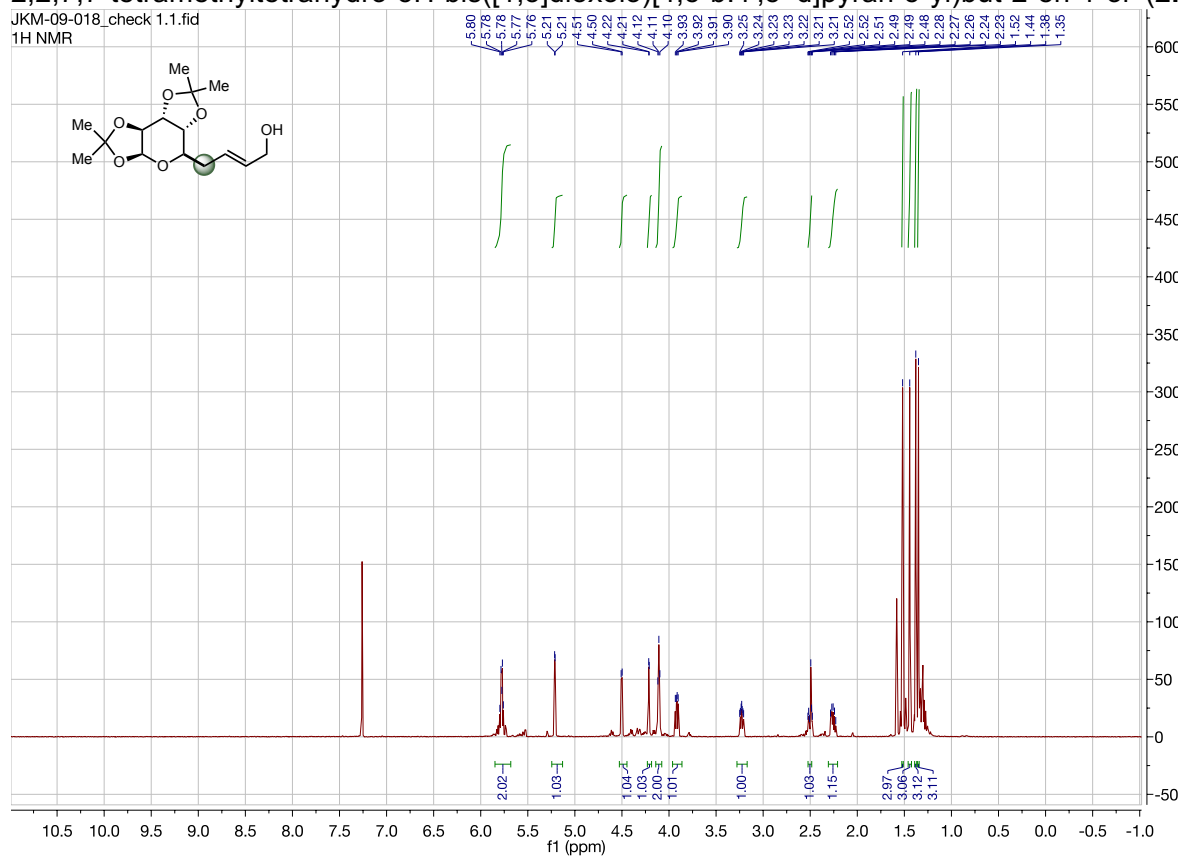
JKM-09-018_check_13C.1.fid
13C NMR
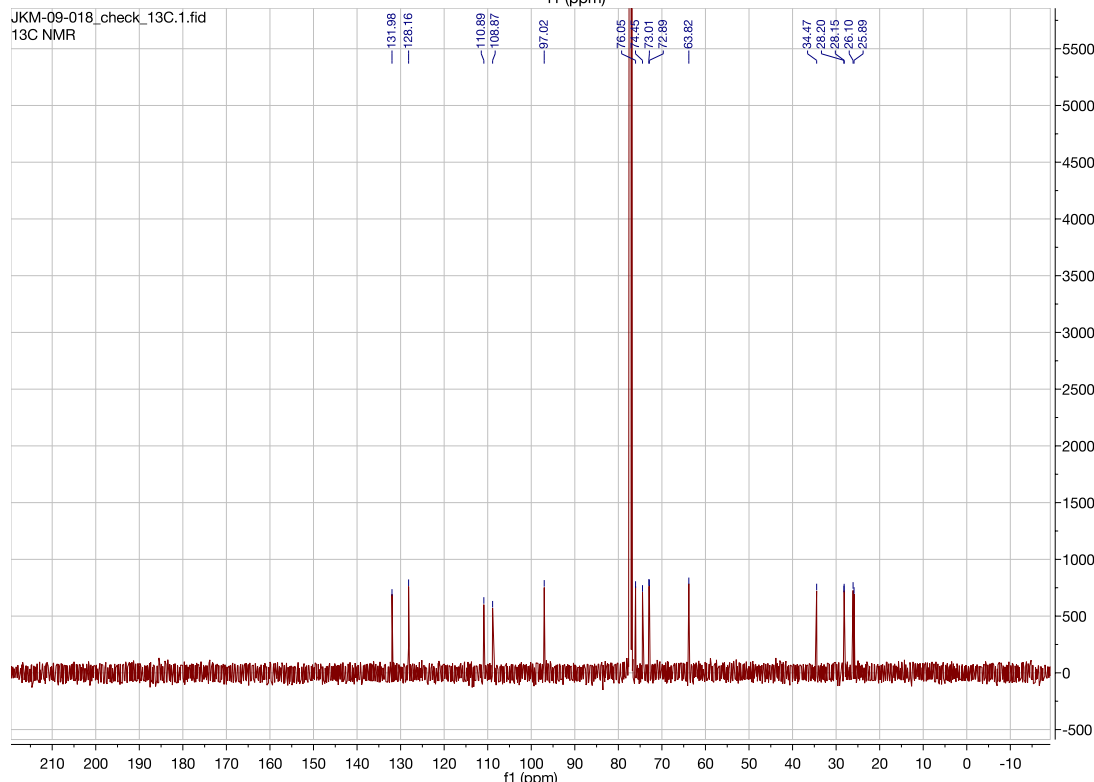
Note: Major isomer highlighted in both proton and carbon NMR.

^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-2-methyl-4-((3a*S*,5*R*,5a*R*,8a*R*,8b*S*)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)but-2-en-1-ol (**2j**)
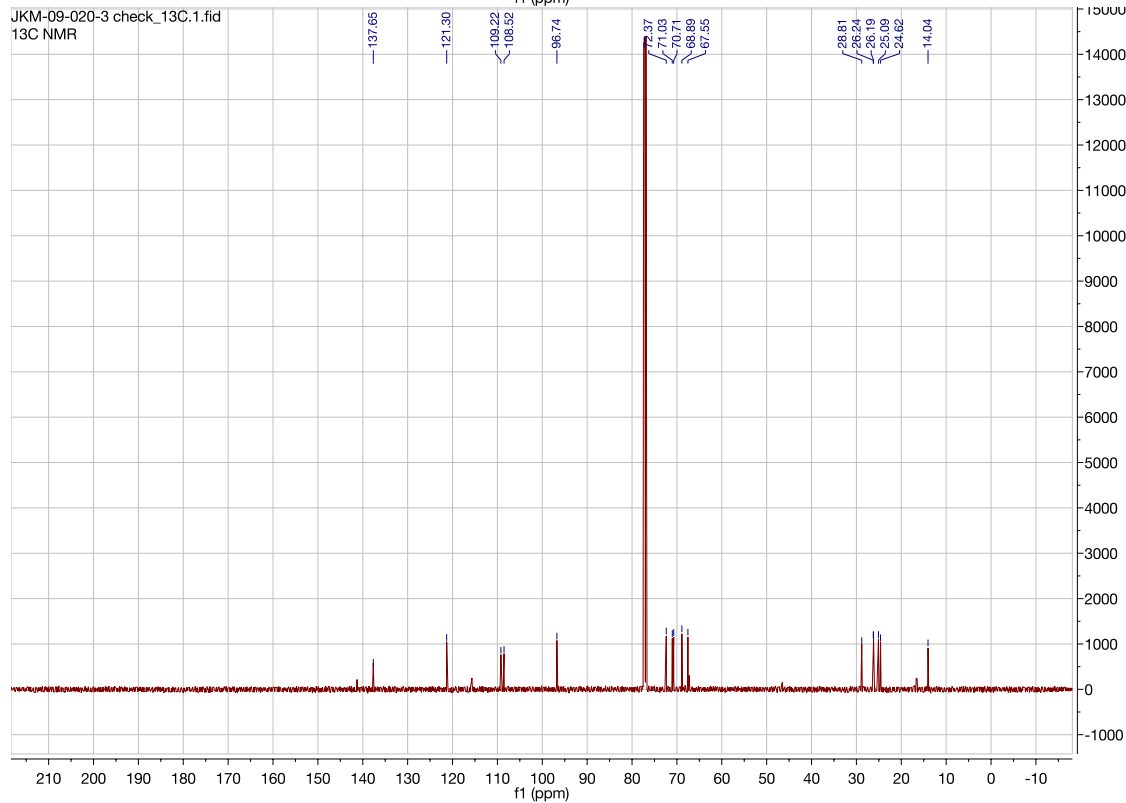
Note: Major isomer highlighted in both proton and carbon NMR.

¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (*E*)-2-methyl-5-phenylhex-2-en-1-ol (**2k**)

JKM-09-032-1.1.fid
1H NMR
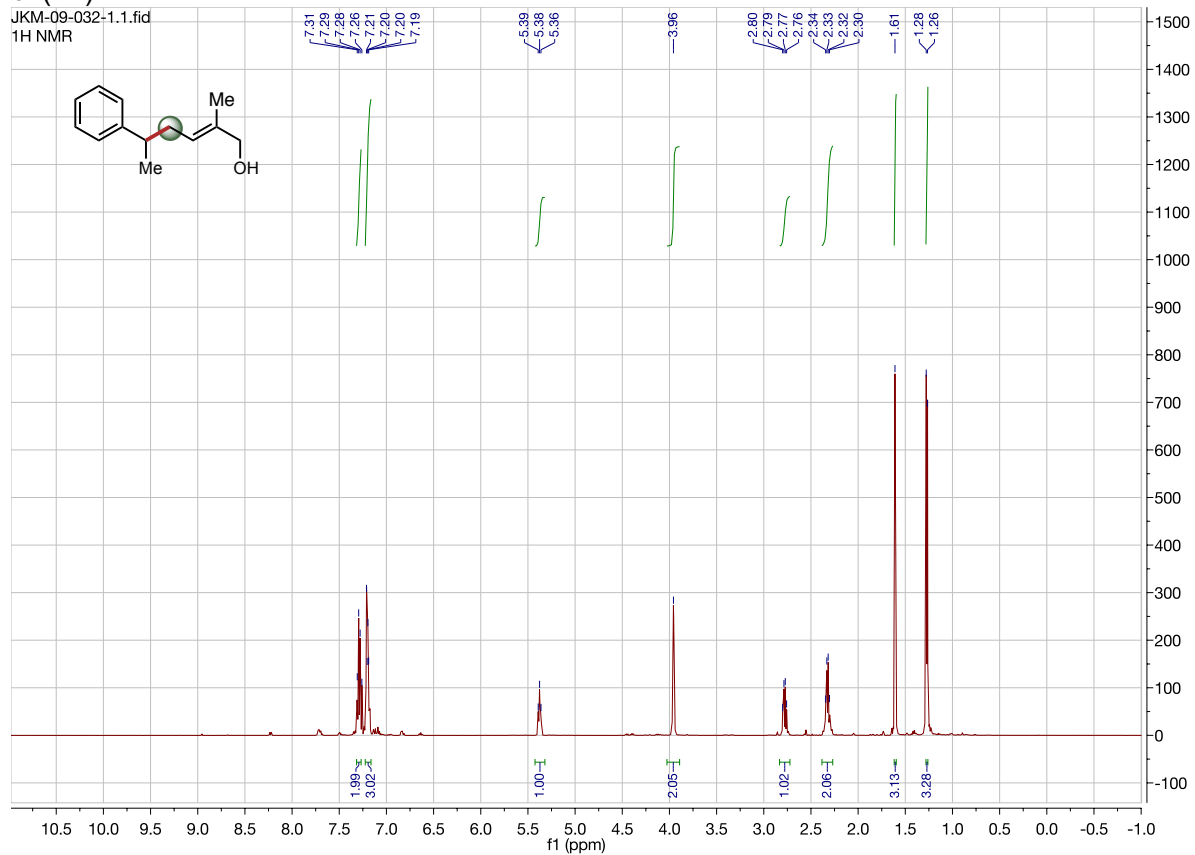
JKM-09-032-1_13C.1.fid
13C NMR
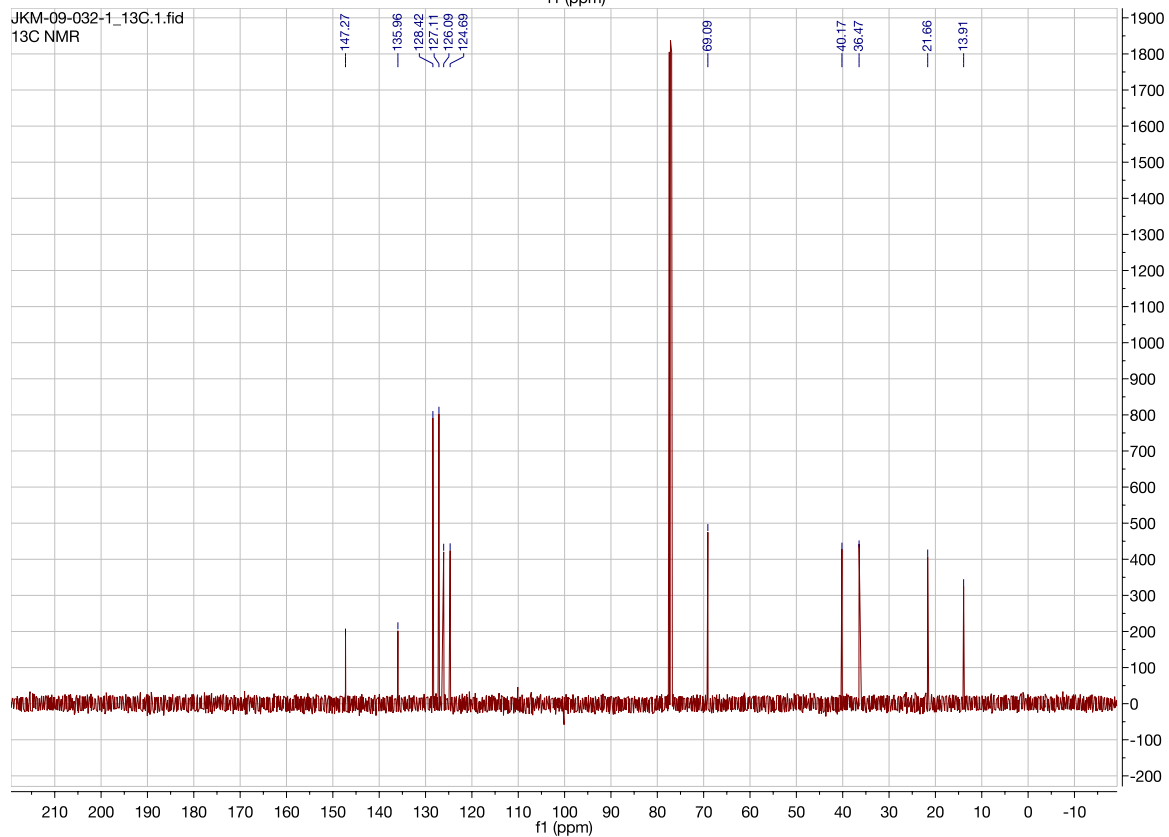
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (*E*)-2-methyl-4-(tetrahydro-2H-pyran-4-yl)oct-2-en-1-ol (**2l**)
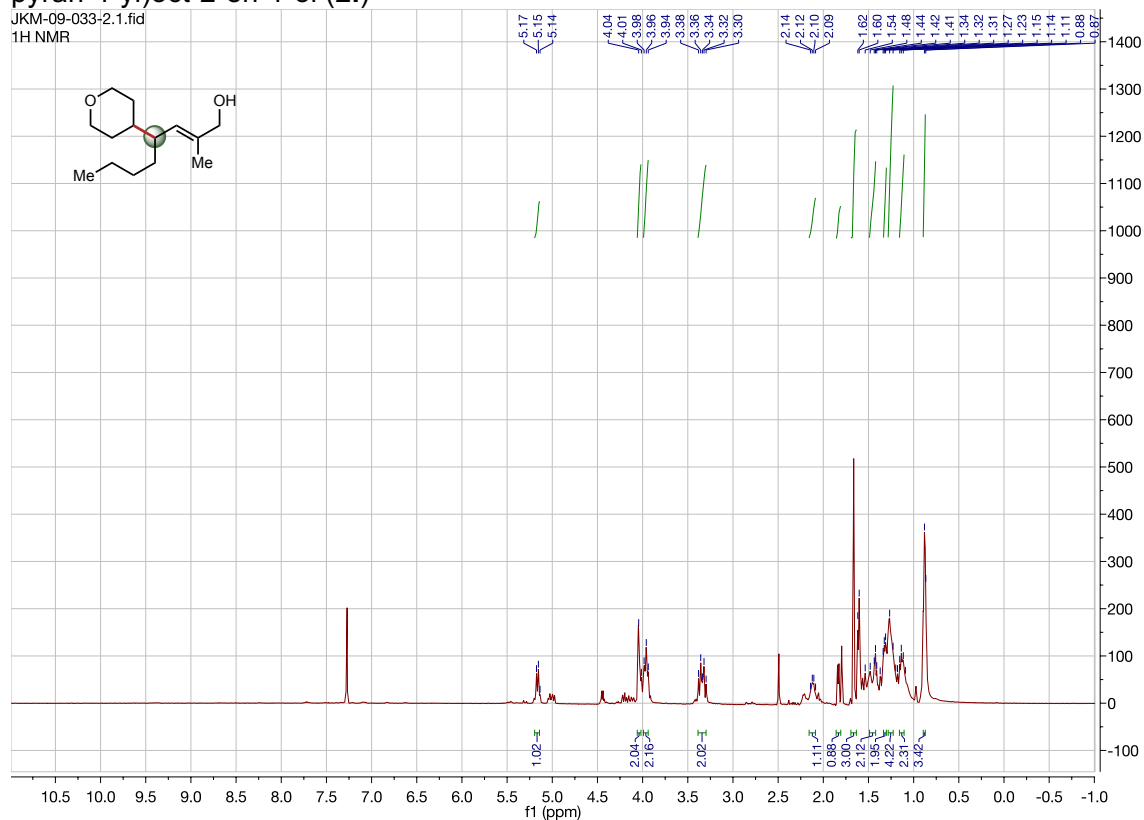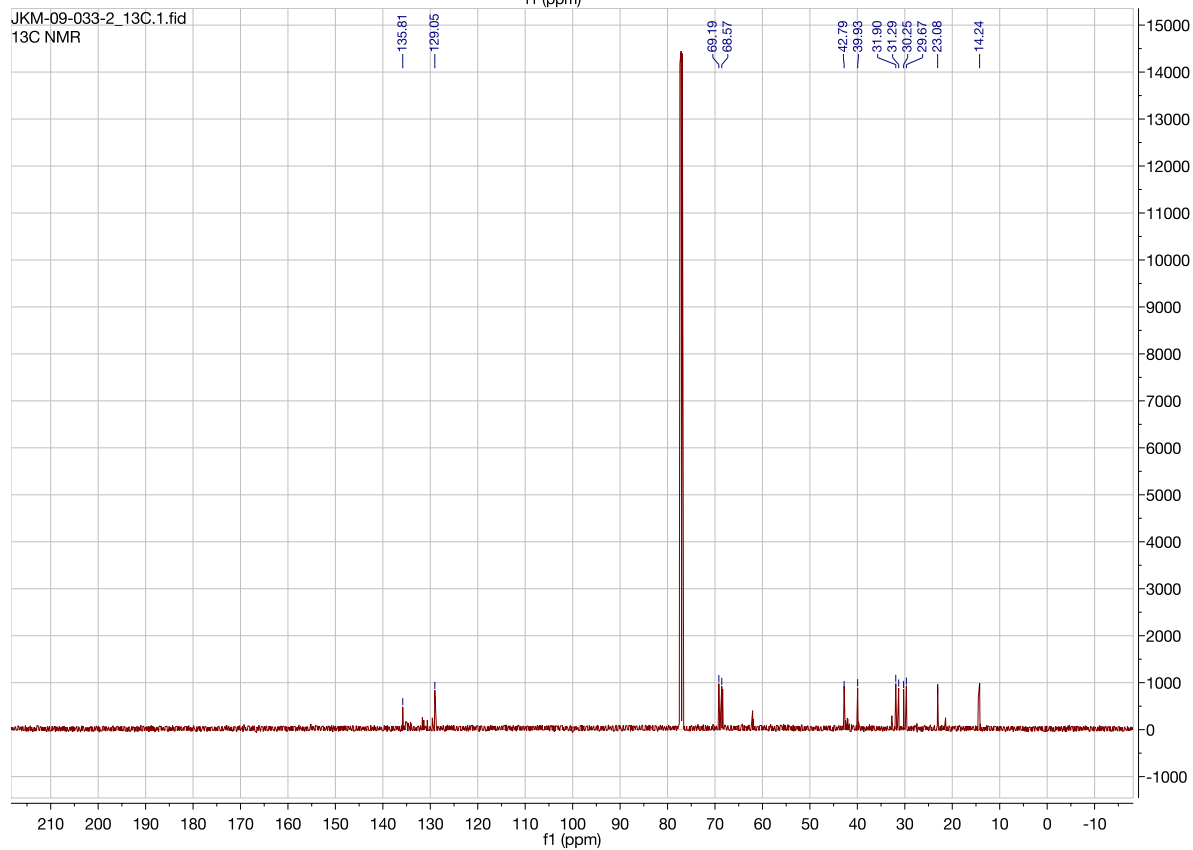
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (3a*R*,5*R*,5a*S*,8a*S*,8b*R*)-5-Allyl-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran (**4a**)

JKM-07-216-1_1.1.fid
1H NMR
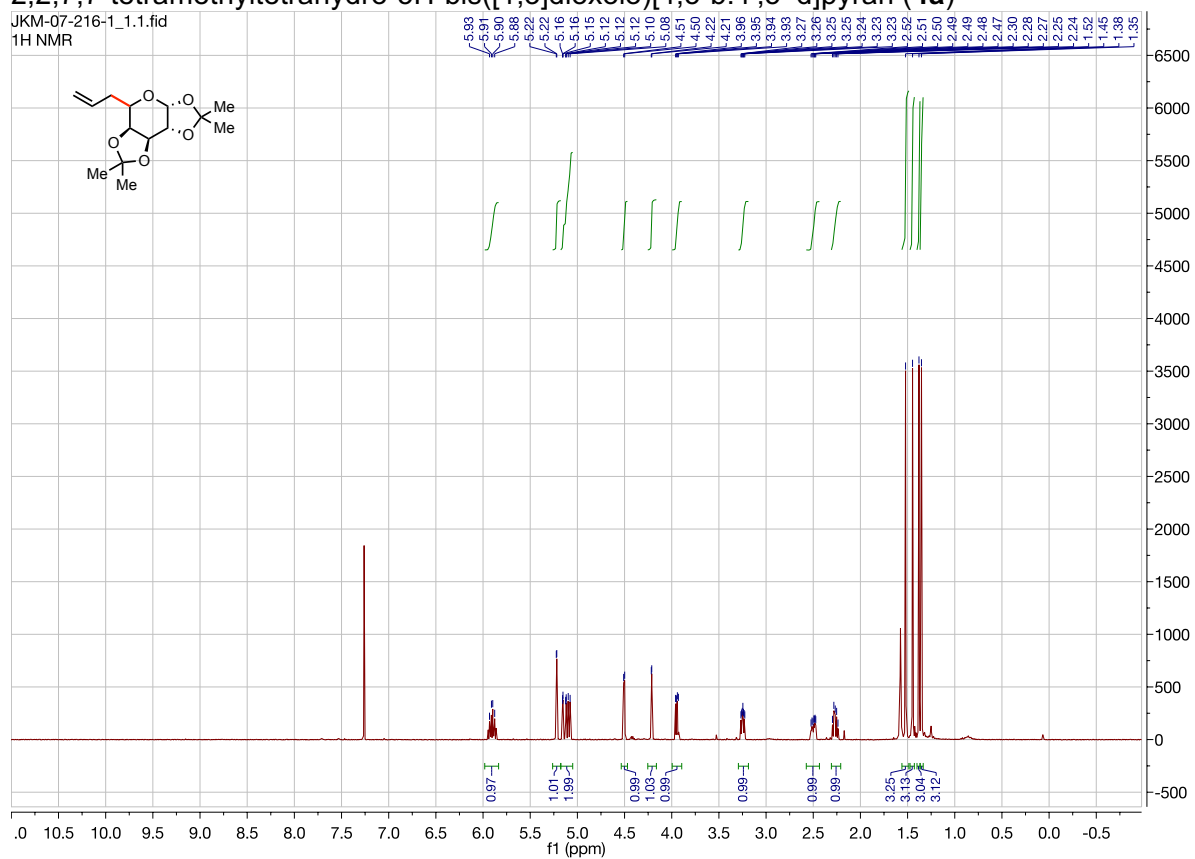
JKM-07-216-1_1_13C.1.fid
13C NMR
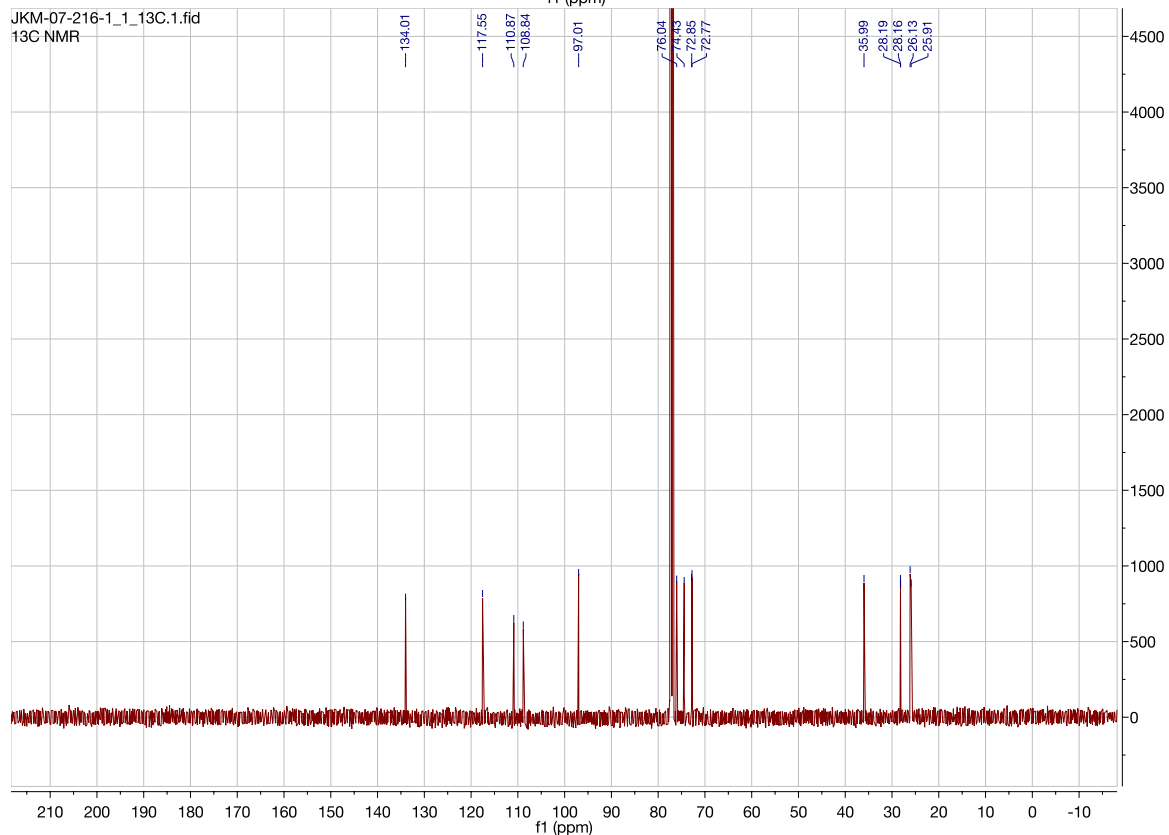
¹H NMR (CDCl₃, 500 MHz) and ¹³C NMR (CDCl₃, 126 MHz) of (3a*R*,4*R*,6*R*,6a*R*)-4-allyl-6-methoxy-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxole (**4b**)
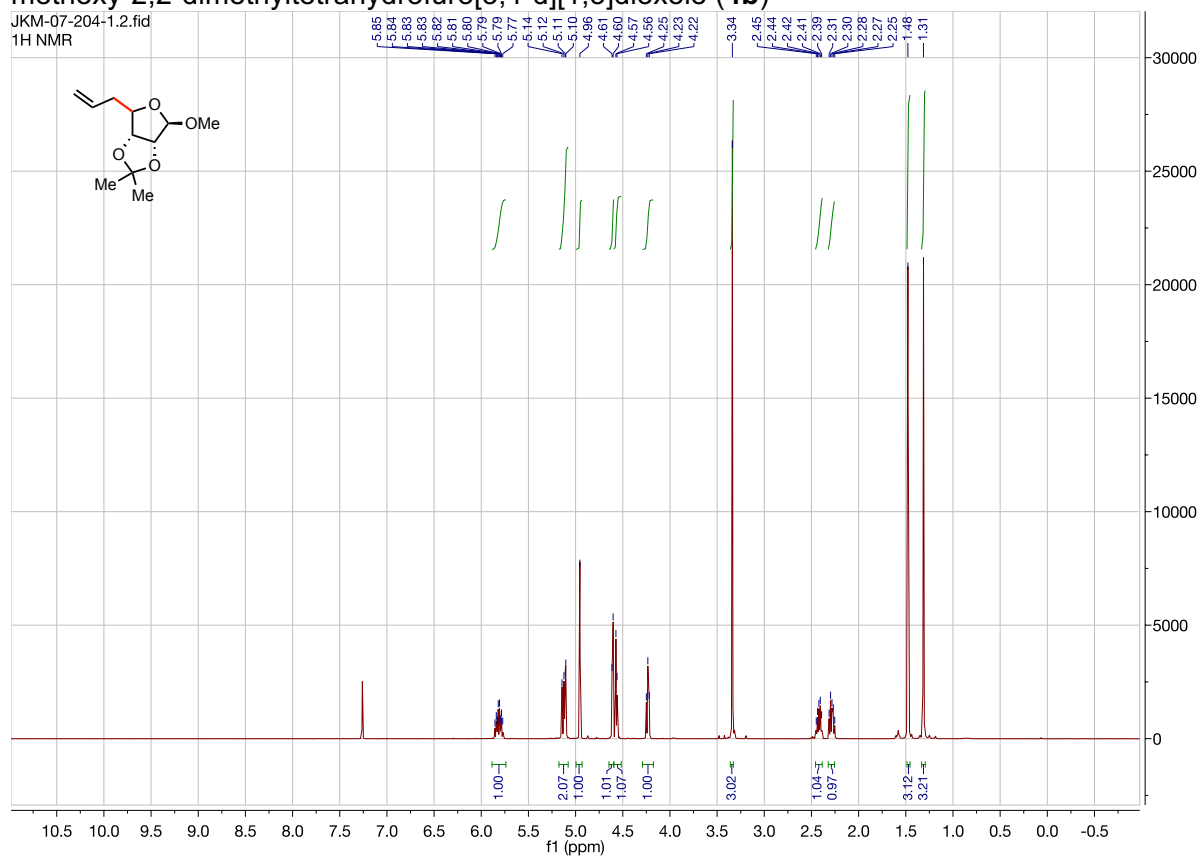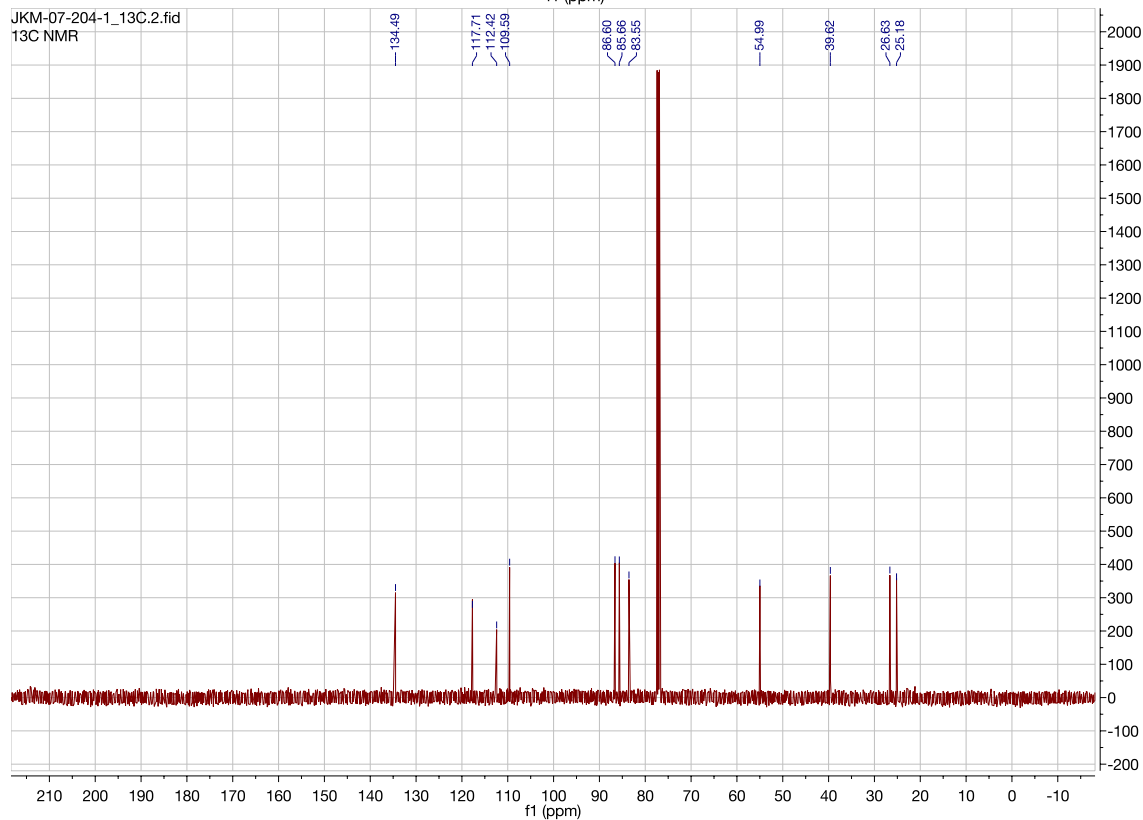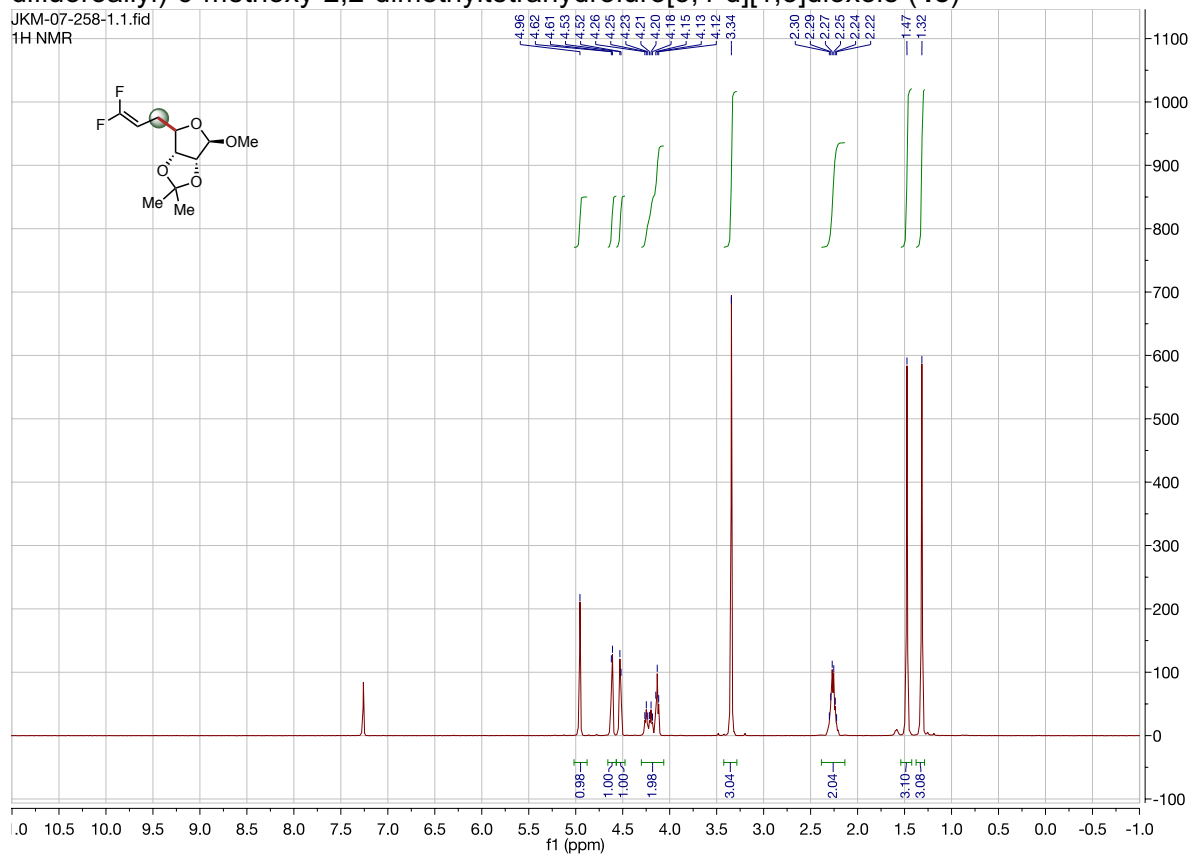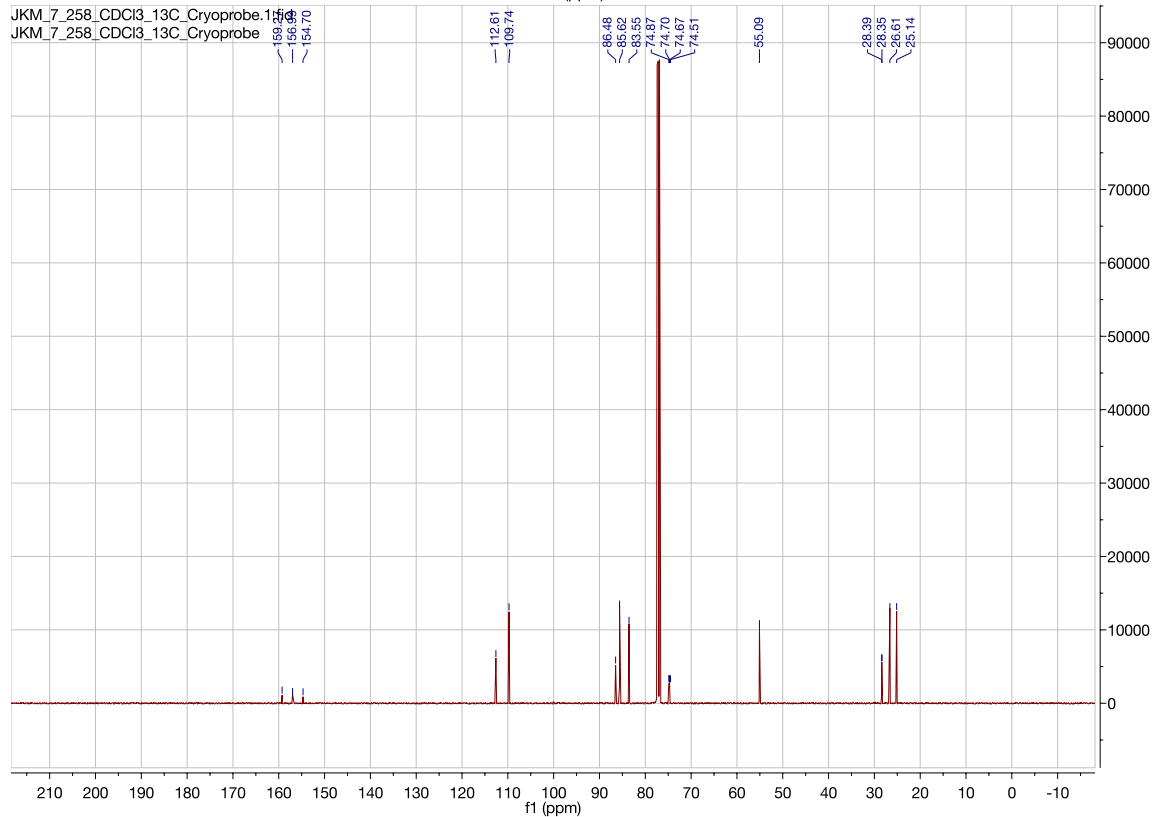
^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of (3a*R*,4*R*,6*R*,6a*R*)-4-(3,3-difluoroallyl)-6-methoxy-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxole (**4c**)
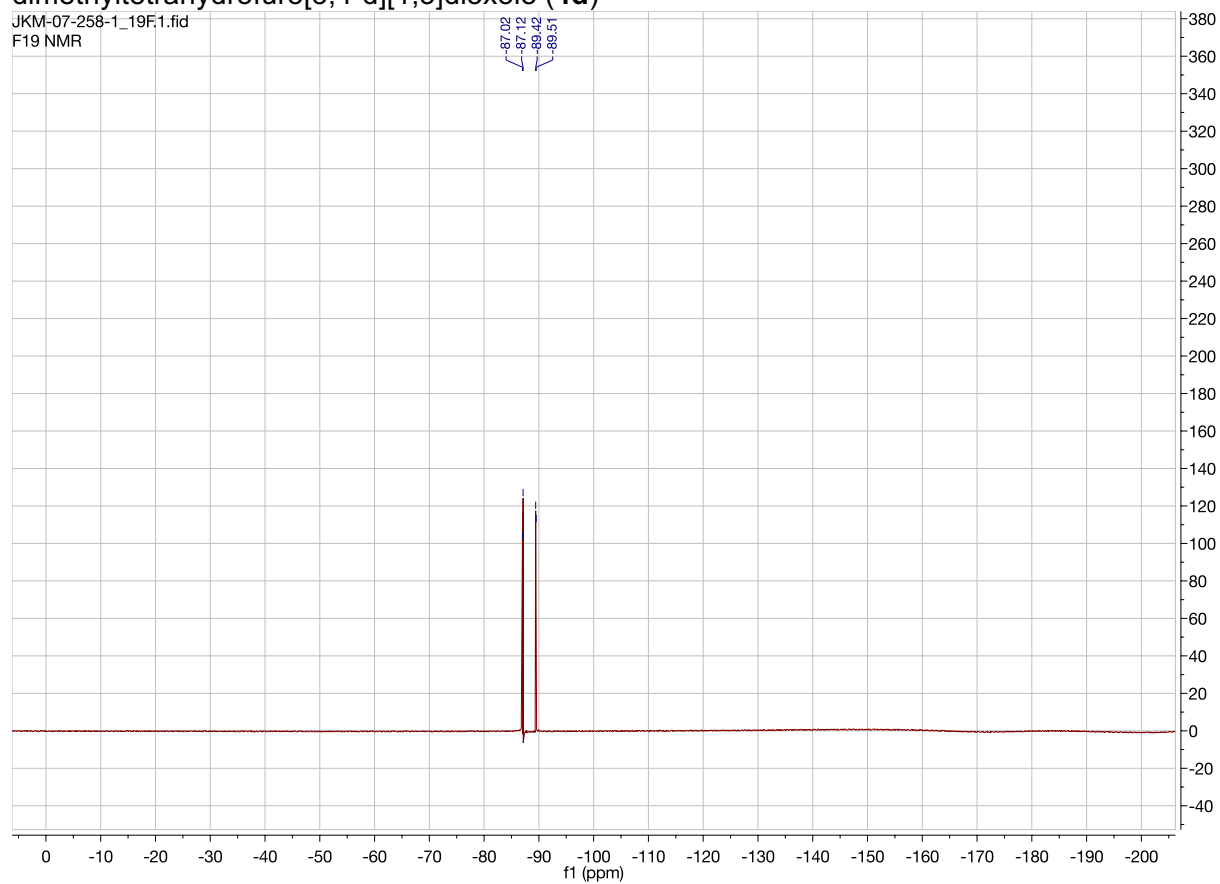
JKM-07-258-1.1.fid
1H NMR

JKM_7_258_CDCl3_13C_Cryoprobe.1.fid
JKM_7_258_CDCl3_13C_Cryoprobe

¹⁹F NMR (CDCl₃, 471 MHz) of (3a*R*,4*R*,6*R*,6a*R*)-4-(3,3-difluoroallyl)-6-methoxy-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxole (**4d**)

^{1}H NMR (CDCl$_3$, 500 MHz) and ^{13}C NMR (CDCl$_3$, 126 MHz) of 5-(4-methoxyphenyl)-1-phenylpent-2-en-1-ol (**5a**)

RA71002 re F3.1.fid
1H NMR