

Z-Selective Cross-Metathesis and Homodimerization of 3E-1,3-Dienes: Reaction Optimization, Computational Analysis, and Synthetic Applications

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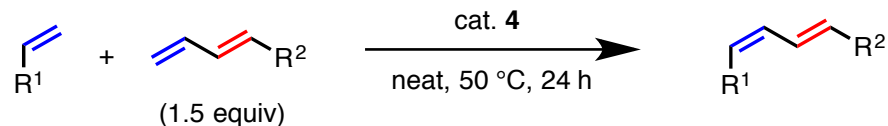
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General experimental procedures

All reactions were carried out in dry glassware under an argon atmosphere using standard Schlenk techniques or in a Vacuum Atmospheres Glovebox under a nitrogen atmosphere, unless otherwise specified. All solvents were purified by passage through solvent purification columns and further degassed by bubbling argon. NMR solvents were dried over CaH_2 and vacuum transferred to a dry Schlenk flask and subsequently degassed with bubbling argon. CDCl_3 was used as received. All α -olefins were filtered through a plug of neutral alumina prior to use. Ruthenium complexes **1** - **5** were obtained from Materia Inc. Ruthenium complex **6**¹ and (2*E*)-7-(acetyloxy)-2-Heptenal² were prepared according to their previously reported procedures. Other commercially available reagents and silica gel were used as received. Semi-preparative HPLC was performed using an Agilent 1200 series, a UV detector, and two ACE C18 columns (21.2mm x 250 mm, 5 μm) or an Agilent Eclipse XDB-C18 column (9.4 mm x 250 mm, 5 μm). ^1H and ^{13}C NMR spectra were recorded on either a Bruker Ascend 400 spectrometer (400 MHz and 101 MHz, respectively) or a Varian Inova 500 MHz (500 MHz and 126 MHz, respectively) and are internally referenced to CDCl_3 . High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High Resolution Mass Spectrometer. All HRMS were by positive-ion EI or FAB.

General procedure for cross-metathesis between 3*E*-1,3-dienes and terminal olefins:



Scheme S1: General depiction of cross-metathesis between 3*E*-1,3-dienes and terminal olefins

In a nitrogen-filled glovebox, a 4 mL screw-top vial was charged with the appropriate terminal olefin (0.50 mmol), the appropriate 3*E*-1,3-diene (0.75 mmol), and catalyst **4** (0.01–0.02 mmol). The vial was sealed with a septum cap, removed from the glovebox, wrapped at the interface with Teflon tape, and heated to 50 °C. The reaction vessel was equipped with an argon inlet and a mineral oil bubbler outlet, both of which were connected via 18G × 11/2” needles through the septum. The reaction mixture was kept under constant flow of argon (1–2 bubbles/s) for the duration of the reaction. The solution was maintained at 50 °C for 24 h, cooled to ambient temperature and quenched with excess butyl or ethyl vinyl ether (~0.1 mL). The solution was loaded onto a column loaded with silica gel. Elution first with hexanes (50 mL) to remove excess 3*E*-1,3-diene, followed by 20:1 hexanes:ethyl ether to elute the product, collected in a separate flask. The resulting solution was concentrated *in vacuo* to provide pure cross-metathesis product.

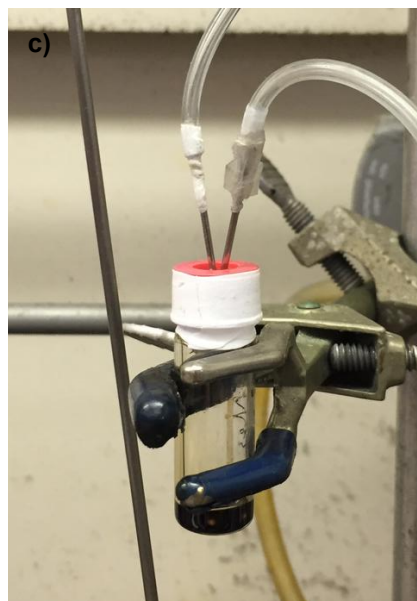
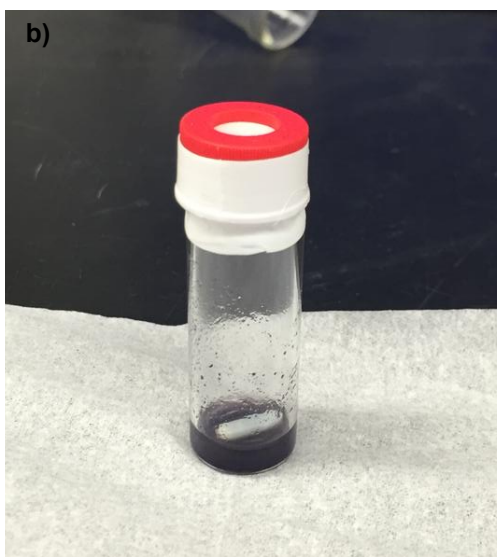
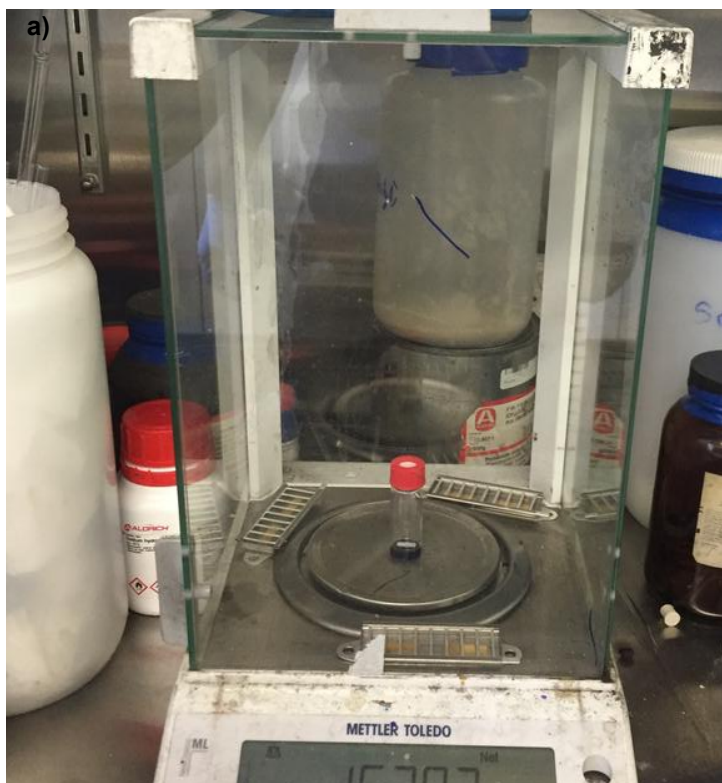


Figure S1: Photographic depiction of reaction setup following general procedure.

a) Weighing starting materials in glovebox. b) Sealing the vial with Teflon tape c) Connecting Ar inlet and outlet with needles

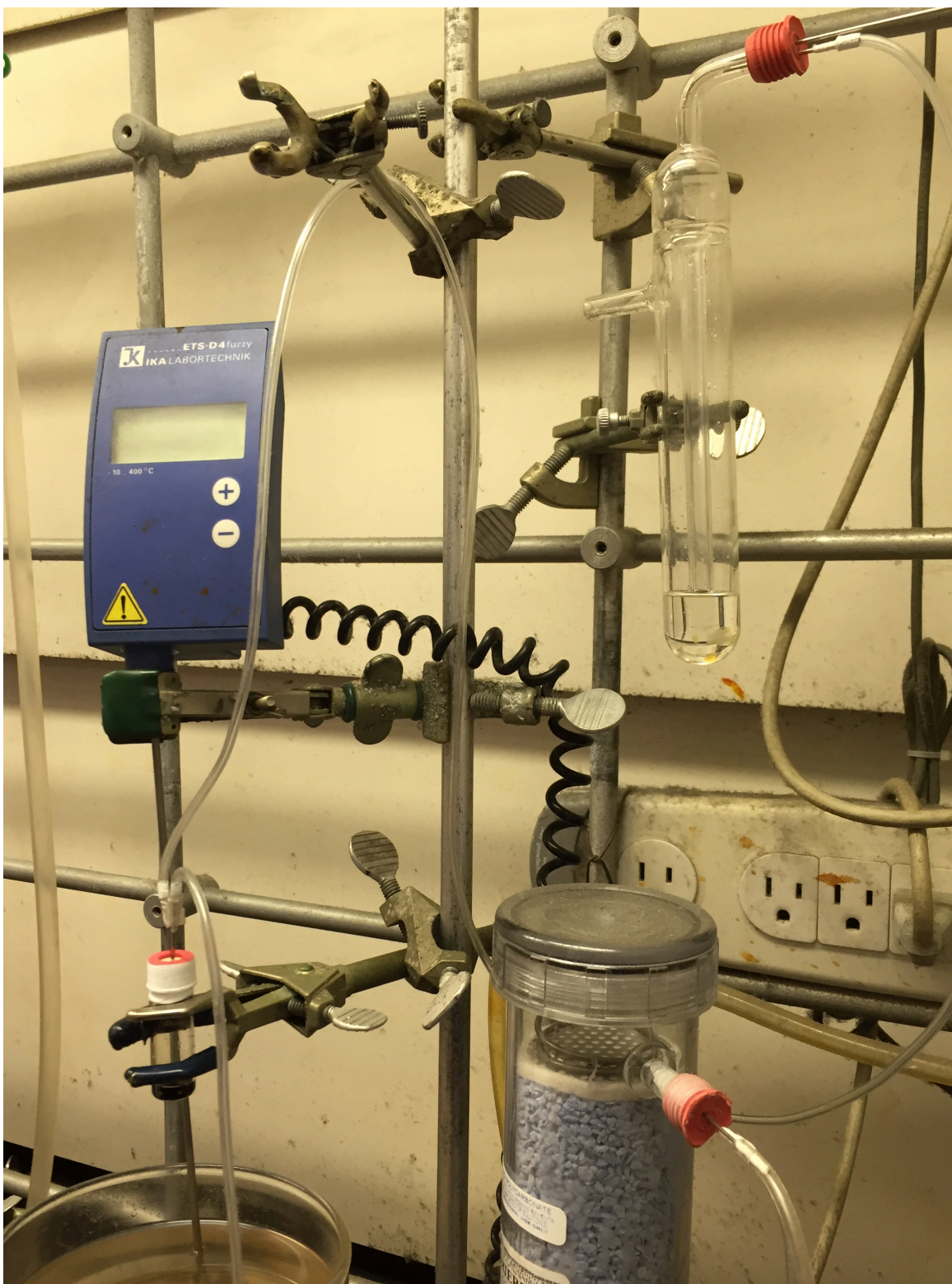
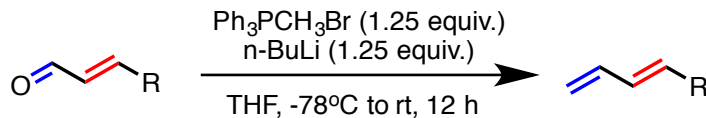


Figure S2: Photographic depiction of reaction setup following general procedure.

General Wittig olefination procedure for the synthesis of 3*E*-1,3-dienes:

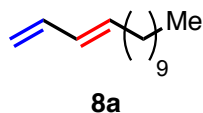


Scheme S2: General depiction of Wittig olefination for the synthesis of 3*E*-1,3-dienes

A flame-dried 100 mL Schlenk flask equipped with a Teflon-coated magnetic stir bar under Ar were charged with methyltriphenylphosphonium bromide (1.34 g, 3.75 mmol) and anhydrous THF (20 mL). *n*-Butyllithium solution (2.5 M in hexanes) (1.5 mL, 3.75 mmol) was added at 0 °C. The resulting yellow solution was allowed to warm to room temperature and stir until it became homogeneous (approximately 1 h). The solution was cooled to -78°C in a dry ice/acetone bath, and the appropriate *trans*-enal was added (3.0 mmol). The solution was allowed to warm to room temperature and stir overnight (approximately 12 h). Et_2O (30 mL) was added, and the resulting heterogeneous solution was cooled to -20°C for 30 min. The solution was filtered through a pad of Celite to remove the triphenylphosphine oxide precipitate, and the Celite was washed twice with Et_2O that had been cooled to 0 °C. The filtrate was concentrated in vacuo, and the resulting yellow oil was purified by silica gel column chromatography using a gradient solvent system (100:1 hexane: Et_2O → 10:1 hexane: Et_2O) as the eluent. The pure product was thus obtained as white solid or colorless oil. To prevent polymerization during prolonged storage, all 3*E*-1,3-dienes were kept under an Ar atmosphere at -20°C .

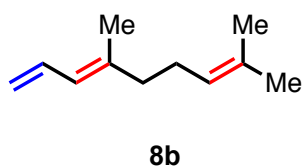
Characterization of 3*E*-1,3-dienes

(*E*)-tetradeca-1,3-diene (8a)



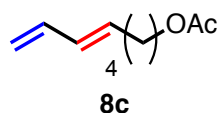
The title compound was prepared from (*E*)-tridec-2-enal (1.96 g, 10.00 mmol) according to the general Wittig procedure and was obtained as a colorless liquid (1.50 g, 77% yield); Analytical data were in agreement with previously reported data.³

(*E*)-4,8-dimethylnona-1,3,7-triene (8b)



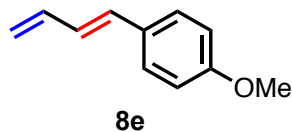
The title compound was prepared from (*E*)-3,7-dimethylocta-2,6-dienal (4.00 g, 26.30 mmol) according to the general Wittig procedure and was obtained as a colorless liquid (1.40 g, 35% yield); Analytical data were in agreement with previously reported data.⁴

(*E*)-octa-5,7-dien-1-yl acetate (8c)



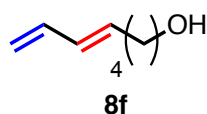
The title compound was prepared from (2*E*)-7-(acetyloxy)-2-Heptenal (1.70 g, 10.00 mmol) according to the general Wittig procedure and was obtained as a colorless liquid (927 mg, 55% yield); ¹H NMR (400 MHz, Chloroform-*d*) δ 6.31 (dt, *J* = 16.9, 10.2 Hz, 1H), 6.12 – 6.00 (m, 1H), 5.68 (dt, *J* = 14.6, 7.0 Hz, 1H), 5.10 (d, *J* = 17.0 Hz, 1H), 4.97 (d, *J* = 10.6 Hz, 1H), 4.09 – 4.03 (m, 2H), 2.12 (q, *J* = 6.5, 5.8 Hz, 2H), 2.04 (d, *J* = 4.6 Hz, 3H), 1.68 – 1.60 (m, 2H), 1.46 (p, *J* = 7.1, 6.6 Hz, 2H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 171.37, 137.27, 134.70, 131.56, 115.21, 64.52, 32.21, 28.24, 25.62, 21.17; HRMS (EI+) *m/z* calcd for C₁₀H₁₆O [M⁺] 168.1150, found 168.1140.

(*E*)-1-(buta-1,3-dien-1-yl)-4-methoxybenzene (8e)



The title compound was prepared from *trans*-4-Methoxy-cinnamaldehyde (972 mg, 6.00 mmol) according to the general Wittig procedure and was obtained as a white solid (815 mg, 81% yield); **¹H NMR** (400 MHz, Chloroform-*d*) δ 7.39 – 7.32 (m, 2H), 6.90 – 6.84 (m, 2H), 6.72 – 6.63 (m, 1H), 6.56 – 6.43 (m, 2H), 5.33 – 5.25 (m, 1H), 5.15 – 5.10 (m, 1H), 3.82 (s, 3H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ 159.39, 137.49, 132.52, 130.04, 127.77, 116.59, 114.19, 55.43; **HRMS** (FAB+) *m/z* calcd for C₁₁H₁₂O [M]⁺ 168.0888, found 168.0887.

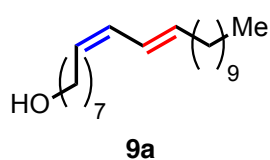
(*E*)-octa-5,7-dien-1-ol (8f)



To a 500 mL round-bottom flask equipped with a Teflon-coated magnetic stir bar were added (*E*)-octa-5,7-dien-1-yl acetate (**8c**) (252 mg, 1.50 mmol), sodium hydroxide (60.0 mg, 1.50 mmol), H₂O (50 mL), and MeOH (50 mL). The reaction mixture was stirred at 60 °C for 5 h. The flask was allowed to cool to room temperature, and the reaction was extracted with ethyl acetate (3 × 150 mL). The combined organic layers were washed with water (100 mL) and brine (2 × 100 mL), dried over Na₂SO₄, filtered, and concentrated in vacuo. Purification by silica gel column chromatography using a gradient solvent system (4:1 hexane:EtOAc → 1:1 hexane:EtOAc) as the eluent provided product as colorless liquid (157 mg, 82% yield); **¹H NMR** (400 MHz, Chloroform-*d*) δ 6.30 (dt, *J* = 17.0, 10.3 Hz, 1H), 6.13 – 6.02 (m, 1H), 5.70 (dt, *J* = 14.7, 6.9 Hz, 1H), 5.15 – 5.05 (m, 1H), 5.01 – 4.93 (m, 1H), 3.65 (t, *J* = 6.5 Hz, 2H), 2.20 – 2.06 (m, 2H), 1.65 – 1.55 (m, 2H), 1.48 (dtd, *J* = 11.0, 8.4, 7.8, 5.6 Hz, 2H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ 137.33, 135.03, 131.41, 115.07, 62.96, 32.37, 25.43; **HRMS** (FAB+) *m/z* calcd for C₈H₁₅O [M]⁺ 127.1123, found 127.1122.

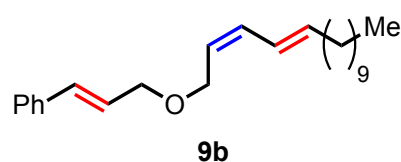
Characterization of cross-metathesis products between 3*E*-1,3-dienes and terminal olefins

(8*Z*,10*E*)-henicosa-8,10-dien-1-ol (**9a**)



The title compound was prepared from non-8-en-1-ol (**7a**) (71 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (6.8 mg, 0.01 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 10:1 hexane:Et₂O provided the product as a colorless oil (130 mg, 84% yield). ¹H NMR (500 MHz, Chloroform-*d*) δ 6.34 – 6.22 (m, 2H), 5.93 (t, *J* = 10.9 Hz, 1H), 5.64 (dt, *J* = 14.6, 7.0 Hz, 1H), 5.28 (dt, *J* = 10.7, 7.6 Hz, 1H), 3.61 (t, *J* = 6.7 Hz, 2H), 2.14 (q, *J* = 6.8 Hz, 2H), 2.08 (q, *J* = 7.1 Hz, 2H), 1.55 (p, *J* = 6.7 Hz, 2H), 1.40 – 1.24 (m, 24H), 0.87 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (126 MHz, Chloroform-*d*) δ 134.84, 129.98, 128.79, 125.66, 63.04, 33.01, 32.86, 32.03, 29.77, 29.75, 29.64, 29.55, 29.46, 29.42, 29.38, 29.3, 27.77, 25.82, 22.80, 14.22; HRMS (FAB+) *m/z* Calcd for C₂₁H₄₀O [M]⁺ 308.3079, found 308.3077.

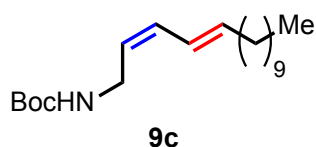
((*E*)-3-(((2*Z*,4*E*)-pentadeca-2,4-dien-1-yl)oxy)prop-1-en-1-yl)benzene (**9b**)



The title compound was prepared from (*E*)-(3-(allyloxy)prop-1-en-1-yl)benzene (**7b**) (35 mg, 0.20 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (58 mg, 0.30 mmol), and catalyst **4** (4.0 mg, 0.006 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (56 mg, 82% yield). ¹H NMR (500 MHz, Chloroform-*d*) δ 7.43 – 7.39 (m, 2H), 7.33 (td, *J* = 6.9, 6.4, 1.7 Hz, 2H), 7.28 – 7.24 (m, 1H), 6.63 (dd, *J* = 15.9, 5.6 Hz, 1H), 6.36 – 6.29 (m, 2H),

6.16 (t, $J = 11.2$ Hz, 1H), 5.78 (dt, $J = 14.5, 7.0$ Hz, 1H), 5.49 (dt, $J = 11.0, 6.9$ Hz, 1H), 4.22 (dd, $J = 6.9, 1.3$ Hz, 2H), 4.18 (dd, $J = 6.1, 1.4$ Hz, 2H), 2.11 (q, $J = 7.3$ Hz, 2H), 1.43 – 1.37 (m, 2H), 1.28 (s, 14H), 0.91 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (126 MHz, Chloroform- d) δ 137.57, 136.86, 132.69, 132.20, 128.65, 127.76, 126.61, 126.27, 125.15, 124.83, 70.66, 65.87, 33.02, 32.05, 29.76, 29.75, 29.64, 29.48, 29.40, 29.36, 22.83, 14.27; HRMS (EI+) m/z calcd for $\text{C}_{24}\text{H}_{36}\text{O}$ $[\text{M}]^+$ 340.2766, found 340.2768.

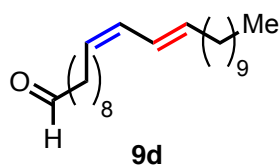
tert-butyl ((2Z,4E)-pentadeca-2,4-dien-1-yl)carbamate (9c)



The title compound was prepared from *tert*-butyl allylcarbamate (**7c**) (79 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure.

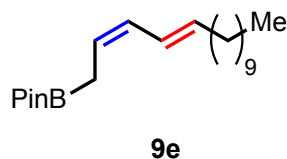
Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (97 mg, 60% yield). ^1H NMR (400 MHz, Chloroform- d) δ 6.35 – 6.21 (m, 1H), 6.04 (t, $J = 10.9$ Hz, 1H), 5.74 (dt, $J = 14.6, 7.0$ Hz, 1H), 5.29 (dt, $J = 10.5, 7.2$ Hz, 1H), 4.49 (s, 1H), 3.87 (s, 2H), 2.09 (q, $J = 7.0$ Hz, 2H), 1.45 (s, 9H), 1.38 (t, $J = 7.1$ Hz, 2H), 1.26 (s, 14H), 0.88 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (101 MHz, Chloroform- d) δ 155.94, 137.58, 131.57, 124.78, 124.73, 38.06, 33.03, 32.07, 29.78, 29.76, 29.66, 29.50, 29.41, 29.37, 28.57, 22.85, 14.27; HRMS (FAB+) m/z Calcd for $\text{C}_{20}\text{H}_{36}\text{NO}_2$ $[(\text{M}+\text{H})-\text{H}_2]^+$ 322.2746, found 322.2772.

(10*Z*,12*E*)-tricos-10,12-dienal (9d)



The title compound was prepared from undec-10-enal (**7d**) (84 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (99 mg, 59% yield). **¹H NMR** (400 MHz, Chloroform-*d*) δ 9.76 (t, *J* = 1.9 Hz, 1H), 6.35 – 6.23 (m, 1H), 5.94 (t, *J* = 11.1 Hz, 1H), 5.65 (dt, *J* = 14.6, 7.0 Hz, 1H), 5.29 (dt, *J* = 10.7, 7.6 Hz, 1H), 2.41 (td, *J* = 7.4, 1.9 Hz, 2H), 2.15 (q, *J* = 6.6 Hz, 2H), 2.09 (q, *J* = 7.4 Hz, 2H), 1.62 (p, *J* = 7.3 Hz, 2H), 1.37 – 1.24 (m, 26H), 0.91 – 0.85 (m, 3H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ 203.03, 134.92, 130.09, 128.82, 125.71, 44.07, 33.06, 32.07, 29.85, 29.79, 29.69, 29.59, 29.50, 29.46, 29.45, 29.42, 29.32, 29.31, 27.82, 22.85, 22.24, 14.27; **HRMS** (EI+) *m/z* Calcd for C₂₃H₄₂O [M]⁺ 334.3236, found 334.3246.

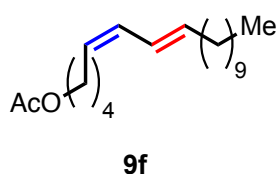
4,4,5,5-tetramethyl-2-((2*Z*,4*E*)-pentadeca-2,4-dien-1-yl)-1,3,2-dioxaborolane (9e)



The title compound was prepared from 2-allyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**7e**) (84 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. ¹H NMR yield (60%) was determined by characteristic olefin chemical shifts (5.4 - 6.3 ppm) with reference to nitrobenzene internal standard (61.5 mg, 0.50 mmol). Attempts were made to purify this product via silica gel chromatography, but were proved to be unsuccessful due to the instability of the compound on silica gel and its tendency to co-elute with the Hoveyda styrene generated in situ upon catalyst activation. In the interest of completeness, below we have included ¹H NMR spectra of the crude reaction mixture and of a ~94% pure sample of the product. **¹H NMR** (400

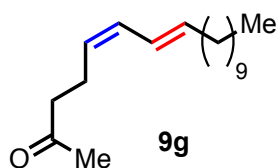
MHz, Chloroform-*d*) δ 6.34 – 6.25 (m, 1H), 5.96 (t, J = 10.9 Hz, 1H), 5.64 (dt, J = 14.6, 7.0 Hz, 1H), 5.47 – 5.38 (m, 1H), 2.08 (q, J = 7.0 Hz, 2H), 1.81 (d, J = 8.1 Hz, 2H), 1.41 – 1.37 (m, 2H), 1.28 (d, J = 15.5 Hz, 14H), 1.25 (s, 12H), 0.88 (t, J = 6.8 Hz, 3H). **HRMS** (FAB+) m/z Calcd for C₂₁H₃₉BO₂ [M]⁺ 334.3043, found 334.3041.

(5*Z*,7*E*)-octadeca-5,7-dien-1-yl acetate (9f)



The title compound was prepared from hex-5-en-1-yl acetate (**7f**) (71 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (107 mg, 69% yield). **¹H NMR** (400 MHz, Chloroform-*d*) δ 6.34 – 6.21 (m, 1H), 5.96 (t, J = 11.0 Hz, 1H), 5.67 (dt, J = 14.6, 7.0 Hz, 1H), 5.27 (dt, J = 10.8, 7.6 Hz, 1H), 4.06 (t, J = 6.7 Hz, 2H), 2.19 (qd, J = 7.5, 1.3 Hz, 2H), 2.09 (q, J = 7.3 Hz, 2H), 2.04 (s, 3H), 1.69 – 1.61 (m, 2H), 1.49 – 1.42 (m, 2H), 1.39 – 1.23 (m, 16H), 0.93 – 0.82 (m, 3H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ 171.31, 135.37, 129.37, 129.11, 125.51, 64.57, 33.05, 32.06, 29.78, 29.77, 29.67, 29.55, 29.49, 29.41, 28.32, 27.36, 26.17, 22.84, 21.14, 14.26; **HRMS** (EI+) m/z Calcd for C₂₀H₃₆O₂ [M]⁺ 308.2715, found 308.2713.

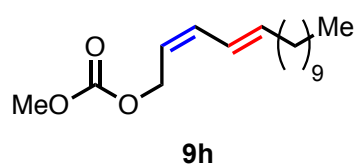
(5*Z*,7*E*)-octadeca-5,7-dien-2-one (9g)



The title compound was prepared from hex-5-en-2-one (**7g**) (49 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (55 mg, 41% yield). **¹H NMR**

(400 MHz, Chloroform-*d*) δ 6.29 (ddq, $J = 14.9, 11.0, 1.3$ Hz, 1H), 5.96 (t, $J = 11.1$ Hz, 1H), 5.68 (dt, $J = 14.6, 7.0$ Hz, 1H), 5.23 (dt, $J = 10.7, 7.3$ Hz, 1H), 2.54 – 2.48 (m, 2H), 2.47 – 2.39 (m, 2H), 2.14 (s, 3H), 2.09 (q, $J = 6.9$ Hz, 2H), 1.40 – 1.35 (m, 2H), 1.26 (s, 14H), 0.91 – 0.84 (m, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 208.42, 135.96, 129.89, 127.42, 125.23, 43.68, 33.04, 32.06, 30.09, 29.77, 29.77, 29.66, 29.49, 29.41, 22.84, 22.22, 14.26; **HRMS** (EI+) m/z Calcd for $\text{C}_{18}\text{H}_{32}\text{O}$ $[\text{M}]^+$ 264.2453, found 264.2442.

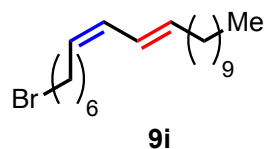
Methyl-((2Z,4E)-pentadeca-2,4-dien-1-yl) carbonate (**9h**)



The title compound was prepared from allyl methyl carbonate (**7h**) (58 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure.

Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (60 mg, 42% yield). ^1H NMR (400 MHz, Chloroform-*d*) δ 6.35 – 6.27 (m, 1H), 6.17 (t, $J = 11.1$ Hz, 1H), 5.80 (dt, $J = 14.5, 7.0$ Hz, 1H), 5.43 (dt, $J = 10.8, 7.2$ Hz, 1H), 4.79 (dd, $J = 7.2, 1.1$ Hz, 2H), 3.78 (s, 3H), 2.11 (q, $J = 7.0$ Hz, 2H), 1.42 – 1.37 (m, 2H), 1.26 (s, 14H), 0.91 – 0.85 (m, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.94, 139.07, 133.96, 124.57, 121.00, 64.00, 54.91, 33.03, 32.06, 29.76, 29.74, 29.64, 29.49, 29.39, 29.25, 22.84, 14.27; **HRMS** (FAB+) m/z Calcd for $\text{C}_{17}\text{H}_{29}\text{O}_3$ $[(\text{M}+\text{H})-\text{H}_2]^+$ 281.2117, found 281.2135.

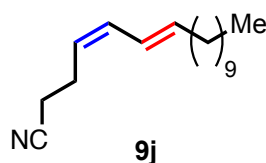
(7Z,9E)-1-bromoicosa-7,9-diene (9i)



The title compound was prepared from 8-bromooct-1-ene (**7i**) (31 mg, 0.17 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (49 mg, 0.25 mmol), and catalyst **4** (4.5 mg, 0.007 mmol) according to the general procedure. Purification by silica gel

column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (20 mg, 34% yield). **¹H NMR** (400 MHz, Chloroform-*d*) δ 6.34 – 6.23 (m, 1H), 5.95 (t, *J* = 10.9 Hz, 1H), 5.66 (dt, *J* = 14.5, 7.0 Hz, 1H), 5.28 (dt, *J* = 10.7, 7.6 Hz, 1H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.16 (q, *J* = 7.1 Hz, 2H), 2.09 (q, *J* = 7.1 Hz, 2H), 1.86 (p, *J* = 6.9 Hz, 2H), 1.48 – 1.33 (m, 8H), 1.26 (s, 14H), 0.88 (t, *J* = 6.8 Hz, 3H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ 135.11, 129.77, 128.99, 125.61, 34.16, 33.06, 32.92, 32.07, 29.78, 29.68, 29.63, 29.57, 29.50, 29.42, 28.48, 28.19, 27.67, 22.85, 14.29; **HRMS** (FAB+) *m/z* Calcd for C₂₀H₃₇Br [M]⁺ 356.2079, found 356.2068.

(4Z,6E)-heptadeca-4,6-dienenitrile (9j)

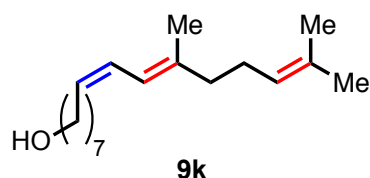


The title compound was prepared from pent-4-enenitrile (**7j**) (41 mg, 0.50 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel

column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (15 mg, 12% yield). **¹H NMR** (400 MHz, Chloroform-*d*) δ 6.28 – 6.19 (m, 1H), 6.09 (t, *J* = 10.9 Hz, 1H), 5.77 (dt, *J* = 14.5, 7.0 Hz, 1H), 5.27 (dt, *J* = 10.6, 7.5 Hz, 1H), 2.53 (q, *J* = 7.3 Hz, 2H), 2.43 – 2.37 (m, 2H), 2.10 (q, *J* = 7.1 Hz, 2H), 1.43 – 1.35 (m, 2H), 1.26 (s, 14H), 0.90 – 0.86 (m, 3H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ

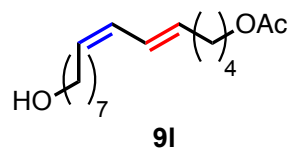
137.69, 131.94, 124.53, 124.03, 119.46, 33.07, 32.06, 29.77, 29.75, 29.65, 29.49, 29.40, 29.36, 23.80, 22.84, 17.71, 14.28. **HRMS** (FAB+) m/z Calcd for $C_{17}H_{30}N$ $[M+H]^+$ 248.2378, found 248.2360.

(8Z,10E)-11,15-dimethylhexadeca-8,10,14-trien-1-ol (9k)



The title compound was prepared from non-8-en-1-ol (**7a**) (28 mg, 0.20 mmol), (E)-4,8-dimethylnona-1,3,7-triene (**8b**) (45 mg, 0.3 mmol), and catalyst **4** (2.7 mg, 0.004 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane ((E)-4,8-dimethylnona-1,3,7-triene (**8b**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (53 mg, >95% yield). **¹H NMR** (500 MHz, Chloroform-*d*) δ 6.17 (tt, J = 11.2, 1.5 Hz, 1H), 6.06 (dt, J = 11.4, 1.1 Hz, 1H), 5.34 (dt, J = 10.8, 7.5 Hz, 1H), 5.16 – 5.06 (m, 1H), 3.62 (t, J = 6.7 Hz, 2H), 2.18 – 2.14 (m, 2H), 2.12 – 2.05 (m, 4H), 1.74 (s, 3H), 1.68 (s, 3H), 1.61 (s, 3H), 1.57 – 1.53 (m, 2H), 1.40 – 1.31 (m, 8H); **¹³C NMR** (126 MHz, Chloroform-*d*) δ 138.59, 131.72, 130.08, 124.79, 124.23, 120.04, 63.14, 40.40, 32.89, 29.79, 29.44, 29.37, 27.63, 26.81, 25.82, 17.84, 16.57; **HRMS** (FAB+) m/z calcd for $C_{18}H_{31}O$ $[(M+H)-H_2]^+$ 263.2375, found 263.2375.

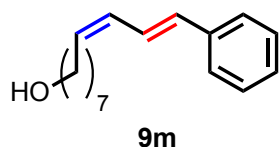
(5E,7Z)-15-hydroxypentadeca-5,7-dien-1-yl acetate (9l)



The title compound was prepared from non-8-en-1-ol (**7a**) (71 mg, 0.50 mmol), (E)-octa-5,7-dien-1-yl acetate (**8c**) (126 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using 5:1 hexane:Et₂O provided the product as a colorless oil (105 mg, 75% yield). **¹H NMR** (400 MHz, Chloroform-*d*) δ 6.29 (ddt, J = 14.9, 11.0, 1.1 Hz, 1H), 5.92 (t, J = 10.9 Hz, 1H), 5.61 (dt, J = 14.5, 7.0 Hz, 1H), 5.29 (q, J = 7.8 Hz, 1H), 4.05 (td, J = 6.6, 1.3 Hz,

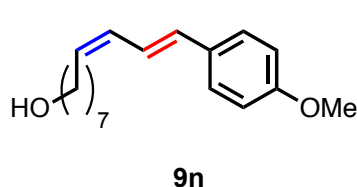
2H), 3.61 (td, $J = 6.6, 1.8$ Hz, 2H), 2.16 – 2.10 (m, 4H), 2.03 (d, $J = 1.2$ Hz, 3H), 1.67 – 1.41 (m, 8H), 1.33 – 1.28 (m, 6H); ^{13}C NMR (101 MHz, Chloroform- d) δ 171.41, 133.76, 130.51, 128.54, 126.26, 64.53, 63.07, 32.85, 32.48, 29.71, 29.38, 29.28, 28.20, 27.75, 25.80, 25.78, 21.12; HRMS (FAB+) m/z Calcd for $\text{C}_{17}\text{H}_{31}\text{O}_3$ $[\text{M}+\text{H}]^+$ 283.2273, found 283.2273.

(8Z,10E)-11-phenylundeca-8,10-dien-1-ol (9m)



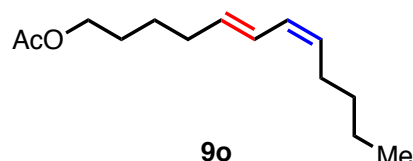
The title compound was prepared from non-8-en-1-ol (**7a**) (71 mg, 0.50 mmol), (*E*)-buta-1,3-dien-1-ylbenzene (**8d**) (120 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. The crude mixture was purified by semi-preparative scale HPLC (9.4 mm x 250 mm, 5 μm Agilent Eclipse XDB-C18 column, detection at 230 nm, flow rate 3 mL/min, H₂O/MeCN, gradient: ramp 90-100% MeCN over 4 min, 100% MeCN for 8 min, t_R (min) = 8.4 min to afford a colorless liquid (19 mg, 15% yield). ^1H NMR (400 MHz, Chloroform- d) δ 7.41 (dd, $J = 8.4, 1.1$ Hz, 2H), 7.31 (td, $J = 7.0, 6.6, 1.6$ Hz, 2H), 7.24 – 7.19 (m, 1H), 7.06 (ddd, $J = 15.6, 11.1, 1.1$ Hz, 1H), 6.52 (d, $J = 15.6$ Hz, 1H), 6.20 – 6.11 (m, 1H), 5.53 (dtt, $J = 10.9, 7.7, 1.0$ Hz, 1H), 3.64 (q, $J = 6.5$ Hz, 2H), 2.33 – 2.24 (m, 2H), 1.58 (d, $J = 6.8$ Hz, 2H), 1.48 – 1.41 (m, 2H), 1.42 – 1.33 (m, 6H); ^{13}C NMR (101 MHz, Chloroform- d) δ 137.79, 133.42, 132.11, 128.86, 128.72, 127.48, 126.44, 124.60, 63.22, 32.92, 29.76, 29.44, 29.35, 28.12, 25.84; HRMS (FAB+) m/z Calcd for $\text{C}_{17}\text{H}_{24}\text{O}$ $[\text{M}]^+$ 244.1827, found 244.1835.

(8Z,10E)-11-(4-methoxyphenyl)undeca-8,10-dien-1-ol (9n)



The title compound was prepared from non-8-en-1-ol (**7a**) (71 mg, 0.50 mmol), (*E*)-1-(buta-1,3-dien-1-yl)-4-methoxybenzene (**8e**) (120 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using 5:1 hexane:Et₂O provided the product as a white solid (34 mg, 25% yield). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 8.7 Hz, 2H), 6.96 – 6.88 (m, 1H), 6.88 – 6.82 (m, 2H), 6.47 (d, *J* = 15.5 Hz, 1H), 6.13 (t, *J* = 10.9 Hz, 1H), 5.46 (dt, *J* = 10.6, 7.7 Hz, 1H), 3.81 (s, 3H), 3.64 (t, *J* = 6.6 Hz, 2H), 2.27 (q, *J* = 6.7 Hz, 2H), 1.60 – 1.54 (m, 2H), 1.45 – 1.40 (m, 2H), 1.35 (s, 6H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 159.19, 132.25, 131.64, 130.61, 129.00, 127.62, 122.68, 114.17, 63.21, 55.45, 32.91, 29.80, 29.44, 29.35, 28.08, 25.83; HRMS (FAB+) *m/z* Calcd for C₁₈H₂₆O₂ [M]⁺ 274.1933, found 274.1948.

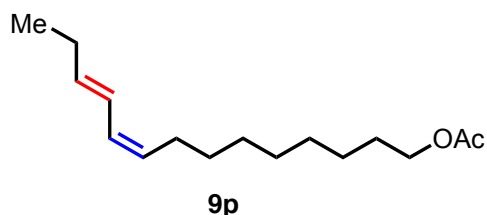
(5E,7Z)-dodeca-5,7-dien-1-yl acetate (9o)



The title compound was prepared from hex-1-ene (**7k**) (42 mg, 0.50 mmol), (*E*)-octa-5,7-dien-1-yl acetate (**8c**) (126 mg, 0.75 mmol), DCE (0.50 mL, 1.0 M), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. The crude mixture was purified by preparative scale HPLC (21.2 mm x 250 mm, 5 μm ACE C18 column, detection at 230 nm, flow rate 30 mL/min, H₂O/MeCN, gradient: ramp 65-100% MeCN over 12 min, 100% MeCN for 13 min, t_R (min) = 17.5 min) to afford a colorless liquid (36 mg, 30% yield). ¹H NMR (400 MHz, Chloroform-*d*) δ 6.37 – 6.26 (m, 1H), 5.94 (t, *J* = 10.9 Hz, 1H), 5.62 (dt, *J* = 14.6, 7.0 Hz, 1H), 5.32 (dt, *J* = 10.7, 7.6 Hz, 1H), 4.06 (t, *J* = 6.7 Hz, 2H), 2.19 – 2.10 (m, 4H), 2.04 (s, 3H), 1.68 – 1.61 (m, 2H), 1.46 (p, *J* = 7.6 Hz, 2H), 1.40 – 1.29 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (101 MHz, Chloroform-*d*) δ 171.37,

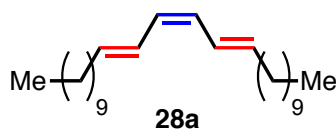
133.73, 130.67, 128.50, 126.32, 64.56, 32.53, 32.02, 28.25, 27.55, 25.84, 22.47, 21.16, 14.12; **HRMS** (FAB+) m/z Calcd for $C_{14}H_{24}O_2$ $[M]^+$ 224.1776, found 224.1783.

(9Z,11E)-tetradeca-9,11-dien-1-yl acetate (9p)



The title compound was prepared from dec-9-en-1-yl acetate (**7l**) (99 mg, 0.50 mmol), (*E*)-hexa-1,3-diene (**8g**) (62 mg, 0.75 mmol), DCE (0.50 mL, 1.0 M), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. The crude mixture was purified by preparative scale HPLC (21.2 mm x 250 mm, 5 μ m ACE C18 column, detection at 230 nm, flow rate 50 mL/min, H₂O/MeCN, gradient: ramp 70-100% MeCN over 6 min, 100% MeCN for 9 min, t_R (min) = 10.8 min) to afford a colorless liquid (70 mg, 56% yield). **¹H NMR** (400 MHz, Chloroform-*d*) δ 6.29 (ddq, J = 15.1, 11.0, 1.5 Hz, 1H), 5.94 (t, J = 10.9 Hz, 1H), 5.69 (dt, J = 15.0, 6.6 Hz, 1H), 5.29 (dt, J = 10.7, 7.6 Hz, 1H), 4.04 (t, J = 6.8 Hz, 2H), 2.13 (dq, J = 15.0, 7.1 Hz, 4H), 2.04 (s, 3H), 1.63 – 1.59 (m, 2H), 1.39 – 1.27 (m, 10H), 1.01 (t, J = 7.5 Hz, 3H); **¹³C NMR** (101 MHz, Chloroform-*d*) δ 171.40, 136.30, 130.21, 128.74, 124.79, 64.79, 29.82, 29.51, 29.35, 29.29, 28.73, 27.79, 26.03, 21.18, 13.81; **HRMS** (FAB+) m/z Calcd for $C_{16}H_{28}O_2$ $[M]^+$ 252.2089, found 252.2101.

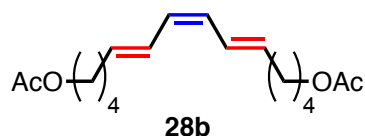
(11E,13Z,15E)-hexacos-11,13,15-triene (28a)



The title compound was prepared from (*E*)-tetradeca-1,3-diene (**8a**) (146 mg, 0.75 mmol), DCE (0.50 mL, 1.0 M) and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane provided a mixture of the starting (*E*)-tetradeca-1,3-diene (**8a**) and the desired product as a colorless liquid (62% yield by ¹H NMR). The product identity was assigned based on analogy to the

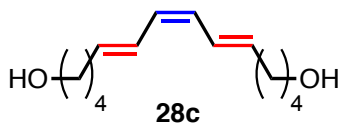
^1H NMR spectra of **28b** and **28c**, and no attempt was made to purify this mixture further. ^1H NMR (500 MHz, Chloroform-*d*) δ 6.53 – 6.42 (m, 2H), 5.88 – 5.81 (m, 2H), 5.69 (dt, J = 14.7, 7.1 Hz, 2H), 2.12 (q, J = 6.9 Hz, 4H), 1.42 – 1.37 (m, 4H), 1.27 (s, 28H), 0.89 (t, J = 6.9 Hz, 6H).

(5*E*,7*Z*,9*E*)-tetradeca-5,7,9-triene-1,14-diyl diacetate (28b)



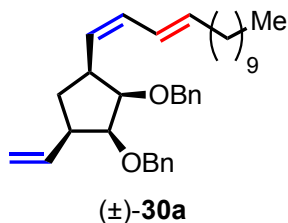
The title compound was prepared from (*E*)-octa-5,7-dien-1-yl acetate (**8c**) (126 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using 1:1 hexane:Et₂O provided the product as a colorless oil (85 mg, 74% yield). ^1H NMR (400 MHz, Chloroform-*d*) δ 6.55 – 6.41 (m, 2H), 5.89 – 5.79 (m, 2H), 5.66 (dt, J = 14.6, 7.1 Hz, 2H), 4.05 (t, J = 6.7 Hz, 4H), 2.15 (qd, J = 7.4, 1.1 Hz, 4H), 2.03 (s, 6H), 1.65 – 1.59 (m, 4H), 1.46 (dd, J = 8.9, 6.2 Hz, 4H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.34, 134.80, 127.84, 126.34, 64.48, 32.57, 28.22, 25.75, 21.13; HRMS (FAB+) m/z calcd for C₁₈H₂₇O₄ [(M+H)-H₂]⁺ 307.1909, found 307.1900.

(5*E*,7*Z*,9*E*)-tetradeca-5,7,9-triene-1,14-diol (28c)



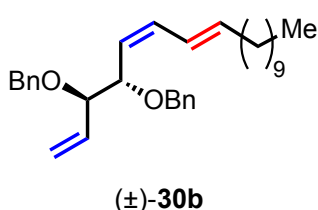
The title compound was prepared from (*E*)-octa-5,7-dien-1-ol (**8f**) (95 mg, 0.75 mmol), and catalyst **4** (13.5 mg, 0.02 mmol) according to the general procedure. Purification by silica gel column chromatography using 1:4 hexane:Et₂O provided the product as a colorless oil (48 mg, 57% yield). ^1H NMR (400 MHz, Chloroform-*d*) δ 6.57 – 6.42 (m, 2H), 5.91 – 5.80 (m, 2H), 5.69 (dt, J = 14.6, 7.0 Hz, 2H), 3.66 (q, J = 6.2 Hz, 4H), 2.20 – 2.13 (m, 4H), 1.64 – 1.60 (m, 2H), 1.59 – 1.53 (m, 2H), 1.53 – 1.45 (m, 4H), 1.26 (t, J = 5.2 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 135.07, 127.84, 126.25, 63.00, 32.75, 32.41, 25.57; HRMS (FAB+) m/z calcd for C₁₄H₂₄O₂ [M]⁺ 224.1776, found 224.1766.

((((1*S*,2*R*,3*S*,5*R*)-3-((1*Z*,3*E*)-tetradeca-1,3-dien-1-yl)-5-vinylcyclopentane-1,2-diyl)bis(methylene))bis(oxy))bis(methylene))dibenzene (30a)



The title compound was prepared from (5*R*,6*S*)-5,6-bis-((benzyloxy)methyl)-bicyclo[2.2.1]hept-2-ene (**29a**) (33 mg, 0.10 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (29 mg, 0.15 mmol), and catalyst **4** (1.4 mg, 0.002 mmol) according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (53 mg, >95% yield). ¹H NMR (500 MHz, Chloroform-*d*) δ 7.40 – 7.25 (m, 10H), 6.37 – 6.28 (m, 1H), 5.99 – 5.85 (m, 2H), 5.68 (dt, *J* = 14.5, 7.0 Hz, 1H), 5.36 – 5.26 (m, 1H), 5.00 (ddd, *J* = 17.1, 2.0, 1.0 Hz, 1H), 4.93 (dd, *J* = 10.1, 2.1 Hz, 1H), 4.43 – 4.33 (m, 4H), 3.54 – 3.44 (m, 4H), 3.23 (p, *J* = 9.0 Hz, 1H), 2.77 (p, *J* = 8.5 Hz, 1H), 2.48 (dp, *J* = 13.3, 6.9 Hz, 2H), 2.09 (q, *J* = 7.0 Hz, 2H), 2.03 (dt, *J* = 12.9, 8.2 Hz, 1H), 1.62 – 1.55 (m, 1H), 1.42 – 1.35 (m, 2H), 1.28 (s, 14H), 0.90 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (126 MHz, Chloroform-*d*) δ 140.88, 138.74, 138.71, 135.34, 132.10, 128.94, 128.40, 128.36, 127.97, 127.58, 127.54, 125.84, 114.27, 73.34, 69.01, 68.88, 45.97, 45.86, 45.73, 39.12, 38.93, 33.08, 32.07, 29.79, 29.78, 29.69, 29.59, 29.50, 29.46, 22.85, 14.29; HRMS (FAB+) *m/z* Calcd for C₃₀H₄₅O₂ [M-Bn]⁺ 437.3420, found 437.3412.

((((3*R*,4*S*,5*Z*,7*E*)-octadeca-1,5,7-triene-3,4-diyl)bis(oxy))bis(methylene))dibenzene (30b)



The title compound was prepared from (3*R*,4*S*)-3,4-bis(benzyloxy)cyclobut-1-ene (**29b**) (27 mg, 0.10 mmol), (*E*)-tetradeca-1,3-diene (**8a**) (29 mg, 0.15 mmol), and catalyst **4** (1.4 mg, 0.002 mmol)

according to the general procedure. Purification by silica gel column chromatography using pure hexane (to elute unreacted (*E*)-tetradeca-1,3-diene (**8a**)) followed by 20:1 hexane:Et₂O provided the product as a colorless oil (41 mg, 89% yield). **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.32 (dt, *J* = 10.6, 7.6 Hz, 8H), 7.29 – 7.24 (m, 2H), 6.25 (t, *J* = 11.0 Hz, 1H), 6.17 – 6.09 (m, 1H), 5.88 (ddd, *J* = 17.3, 10.4, 7.7 Hz, 1H), 5.75 (dt, *J* = 14.5, 7.0 Hz, 1H), 5.35 – 5.25 (m, 3H), 4.65 (dd, *J* = 12.3, 2.7 Hz, 2H), 4.49 – 4.41 (m, 2H), 4.36 (dd, *J* = 9.4, 4.5 Hz, 1H), 3.87 (dd, *J* = 7.7, 4.5 Hz, 1H), 2.06 (q, *J* = 7.0 Hz, 2H), 1.40 – 1.33 (m, 2H), 1.28 (s, 14H), 0.89 (t, *J* = 7.0 Hz, 3H); **¹³C NMR** (126 MHz, Chloroform-*d*) δ 138.82, 138.81, 137.80, 135.60, 133.60, 128.32, 128.31, 127.94, 127.71, 127.47, 127.43, 125.97, 125.56, 118.97, 82.77, 76.31, 70.54, 70.12, 32.97, 32.07, 29.80, 29.79, 29.69, 29.51, 29.43, 29.37, 22.85, 14.28; **HRMS** (FAB+) *m/z*. Calcd for C₃₂H₄₅O₂ [M+H]⁺ 461.3420, found 461.3423.

Computational Details

DFT calculations were performed with Gaussian 09.⁵ Computed structures are illustrated using CYLView.⁶

Geometries were optimized with the B3LYP⁷ functional in the gas phase, using a mixed basis set of LANL2DZ (with ECP) for Ru and 6-31G(d) for all other atoms. Thermal corrections were calculated from unscaled vibrational frequencies at the same level of theory using a standard state of 298.15 K and 1 mol/L.

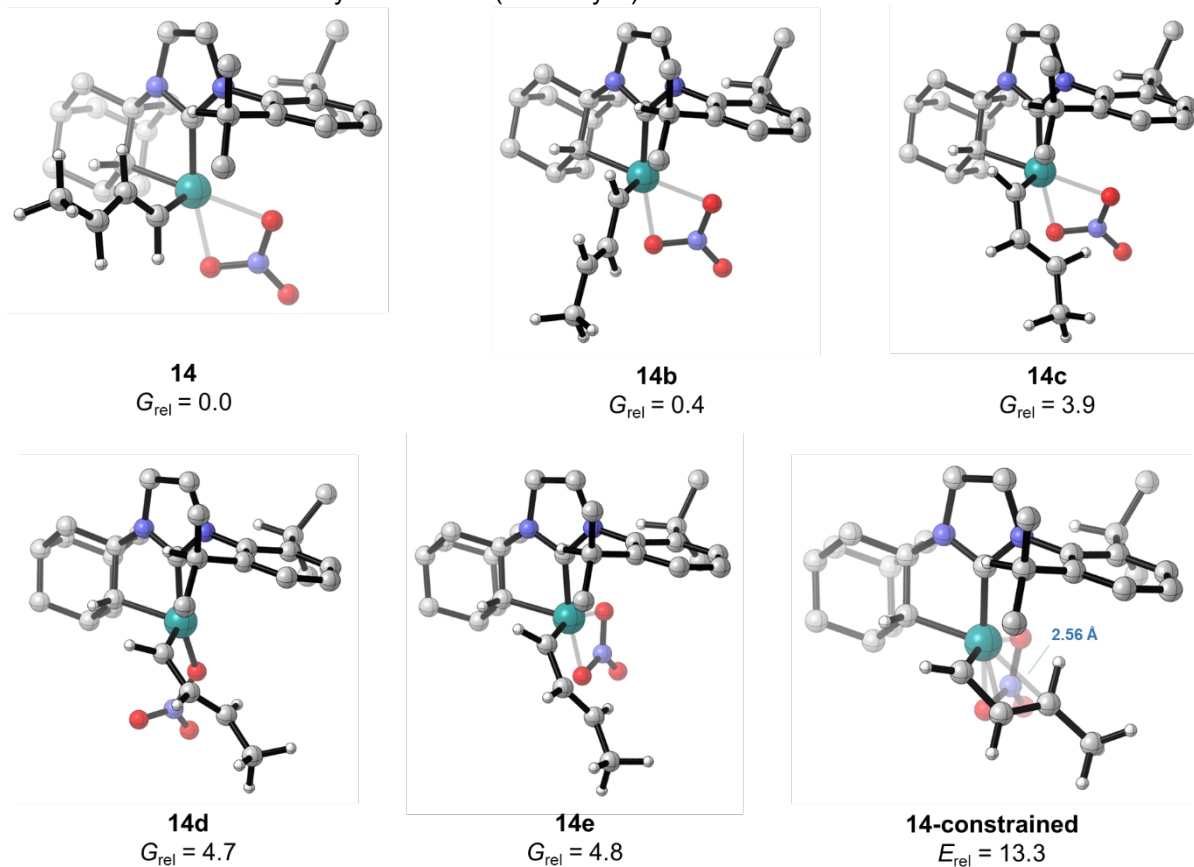
Gibbs free energies in Gaussian were calculated at the default pressure of 1 atm and corrected to the standard state in solution, 1 mol/L. The correction was made by adding $RT \ln(c_{\text{soln}}/c_{\text{gas}})$, or about 1.84 kcal/mol, to the free energy of all structures, where c_{soln} is the standard molar concentration in solution (1 mol/L) and c_{gas} is the standard molar concentration in the gas phase (0.0446 mol/L).

Electronic energies were obtained from single point energy calculations performed with the M06⁸ functional and a mixed basis set of SDD for Ru and 6-311+G(d,p) for all other atoms. The SMD⁹ solvation model for n-octanol was used in M06 single point energy calculations. This solvent was chosen to model reactions run neat with alkenes containing a polar functional group.

IRC calculations were performed to link each transition state to the relevant intermediates. These calculations confirmed that the nitrate ligand is bidentate in alkylidene ruthenium complexes, but shifts to monodentate coordination upon metallacyclobutane formation. We also found stable olefin π -complexes in some cases; these complexes are shown below in the SI (highlighted in red), but omitted from main text.

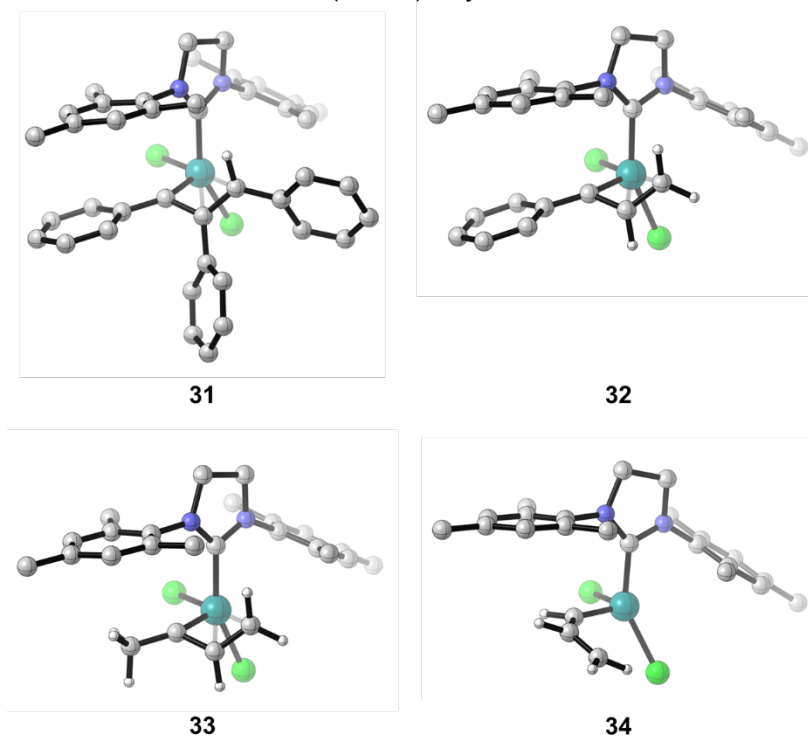
Vinylcarbene Conformations

Figure S3: Conformations of vinylcarbene **14** (Pathway A)



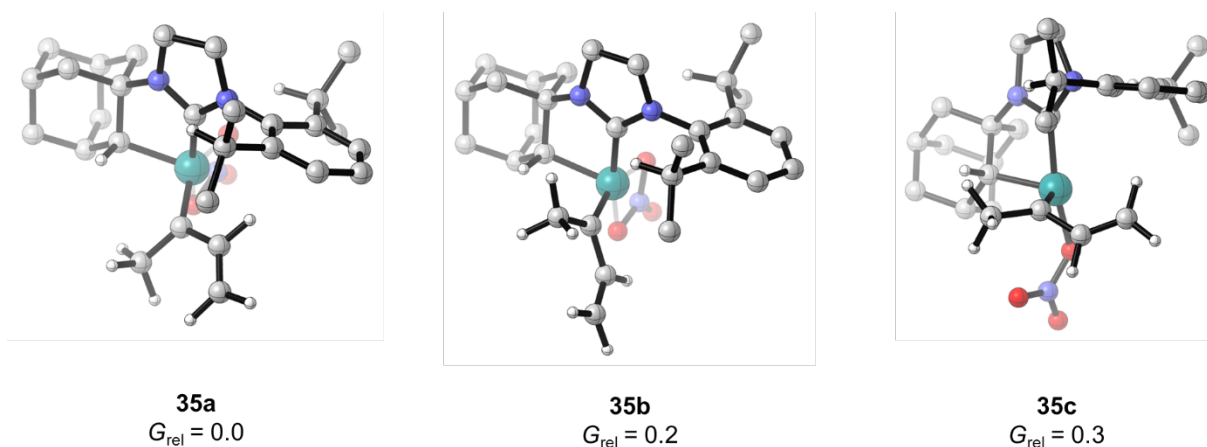
Conformational searches were performed and we were unable to locate an η^3 -vinylcarbene complex as a local minimum. To estimate the relative energy of such a complex the Ru–C3 distance was constrained to 2.56 Å (the distance computed for η^3 -vinylcarbene complex **31**, see below), and all other coordinates were optimized. The resulting complex, **14-constrained**, is 13.3 kcal/mol higher in energy than **14**.

Figure S4: S-cis conformations of non-chelated (SIMes) vinylcarbenes **31–34**



Vinylcarbene **31** is known to exist as an η^3 -vinylcarbene complex based on an x-ray crystal structure. Likewise, our calculations confirm the η^3 -vinylcarbene structure to be the lowest-energy conformation for **31**. Additionally, our calculations indicate that η^3 -vinylcarbene complexes are favored for 1-phenyl-1-vinylcarbene **32** and 1-methyl-1-vinylcarbene **33**. However, we were unable to locate an η^3 coordination mode for the parent vinylcarbene complex **34**. Substitution at the 1-position appears to be required for an η^3 coordination mode.

Figure S5: Lowest-energy conformations of chelated 1-methyl-1-vinylcarbene **35**



We also examined the conformations of **35**, the 1-methyl analogue of vinylcarbene complex **14**. Here also, we were unable to locate an η^3 -vinylcarbene complex as a local minimum. Since an η^3 coordination mode would place the alkene ligand *trans* to the adamantly ligand, we speculate that η^3 coordination of chelated catalysts may be less favorable due to the strong *trans* effect of the chelating alkyl ligand.

Additional Intermediates on Diene-First Pathway A

Scheme S3: Complete Pathway A including olefin π -complexes

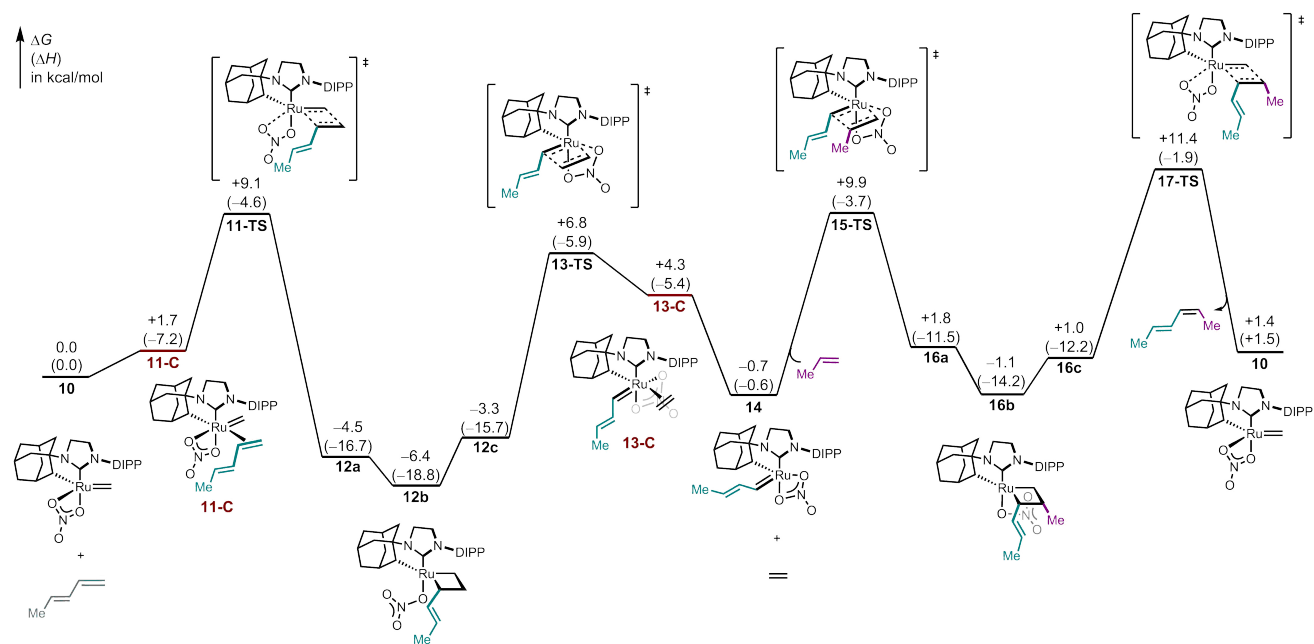


Figure S6: Conformations of 2-vinylmetallacyclobutane **12**

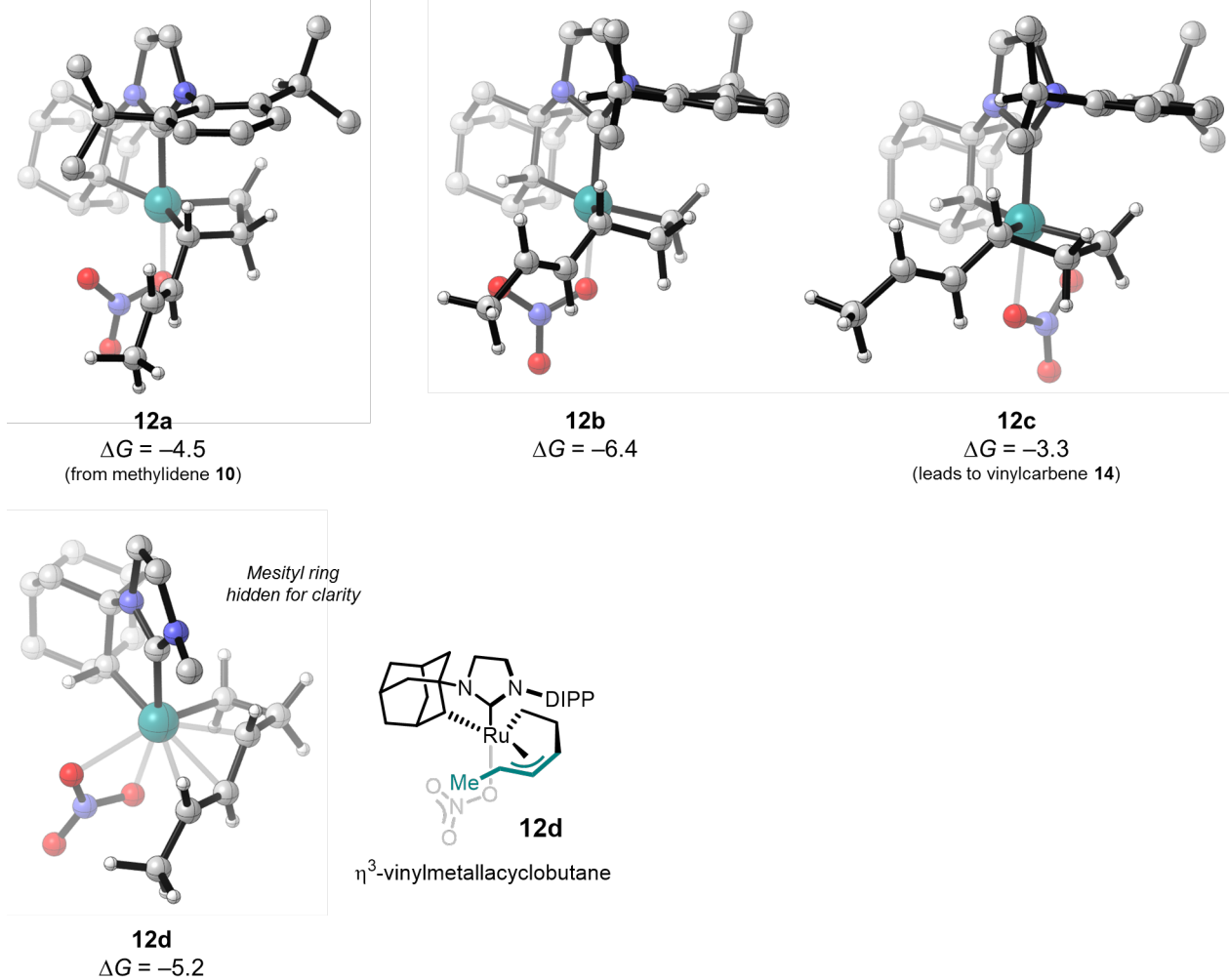
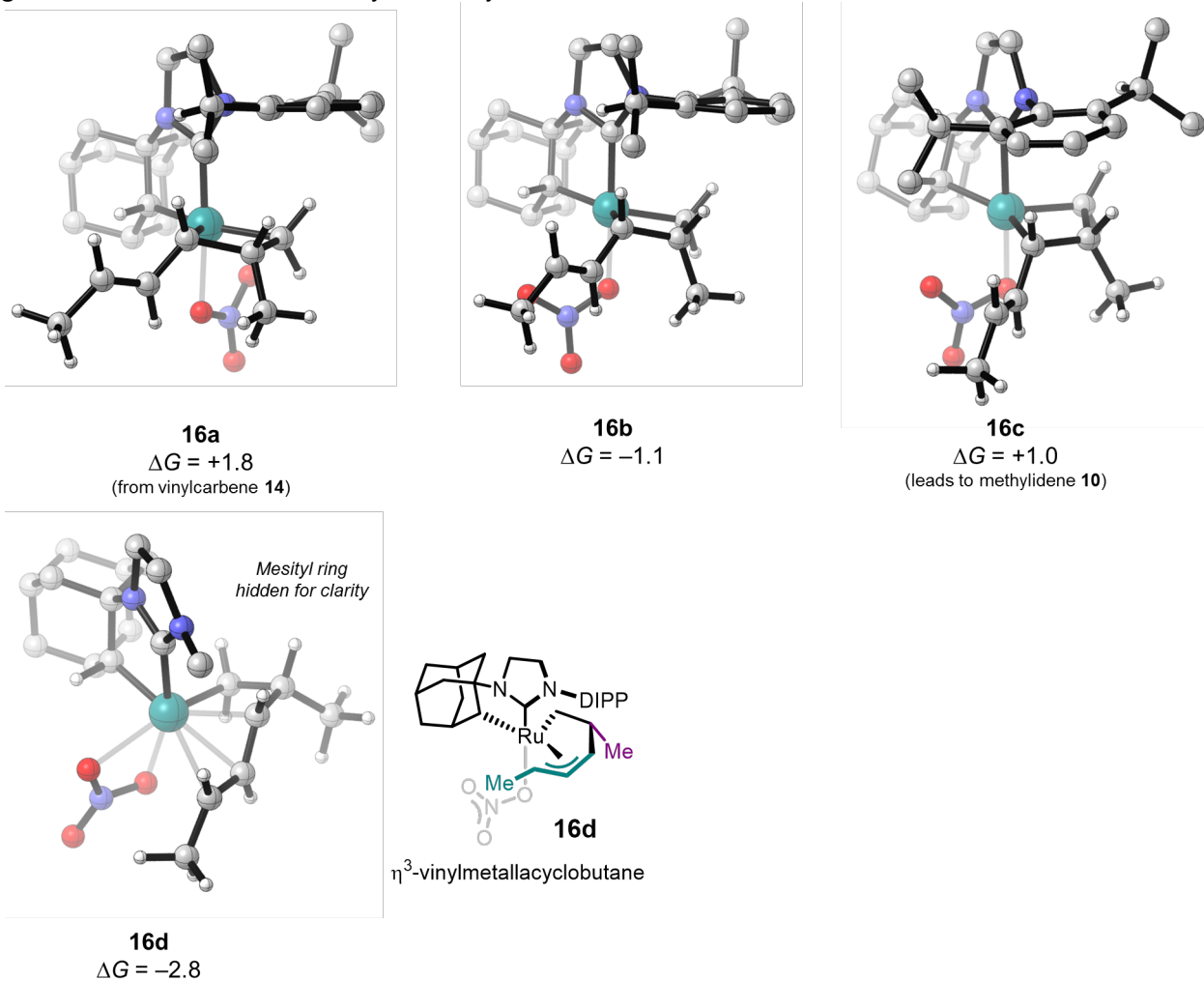


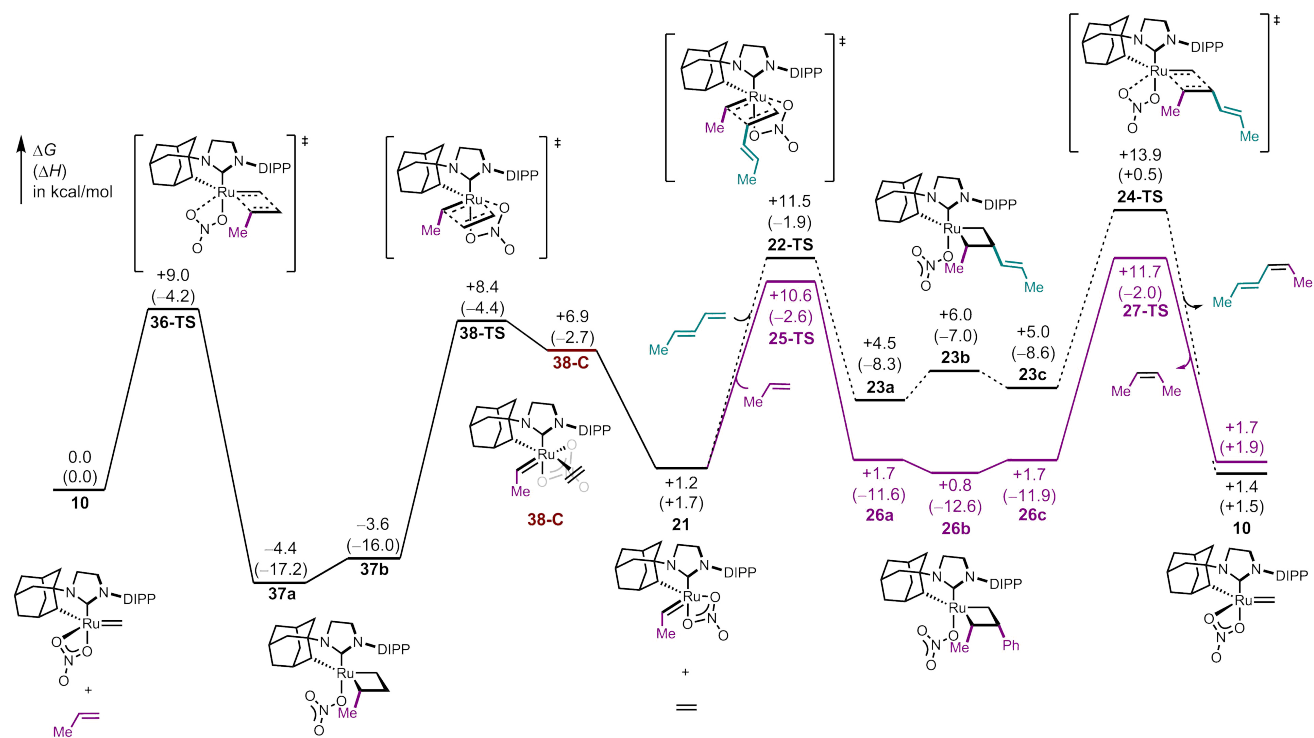
Figure S7: Conformations of 2-vinylmetallacyclobutane **16**



Although we were able to locate η^3 -vinylmetallacyclobutane intermediates **12d** and **16d**, they are similar in energy to other conformations of the metallacycles **12** and **16**, and we do not believe they impact the overall reactivity.

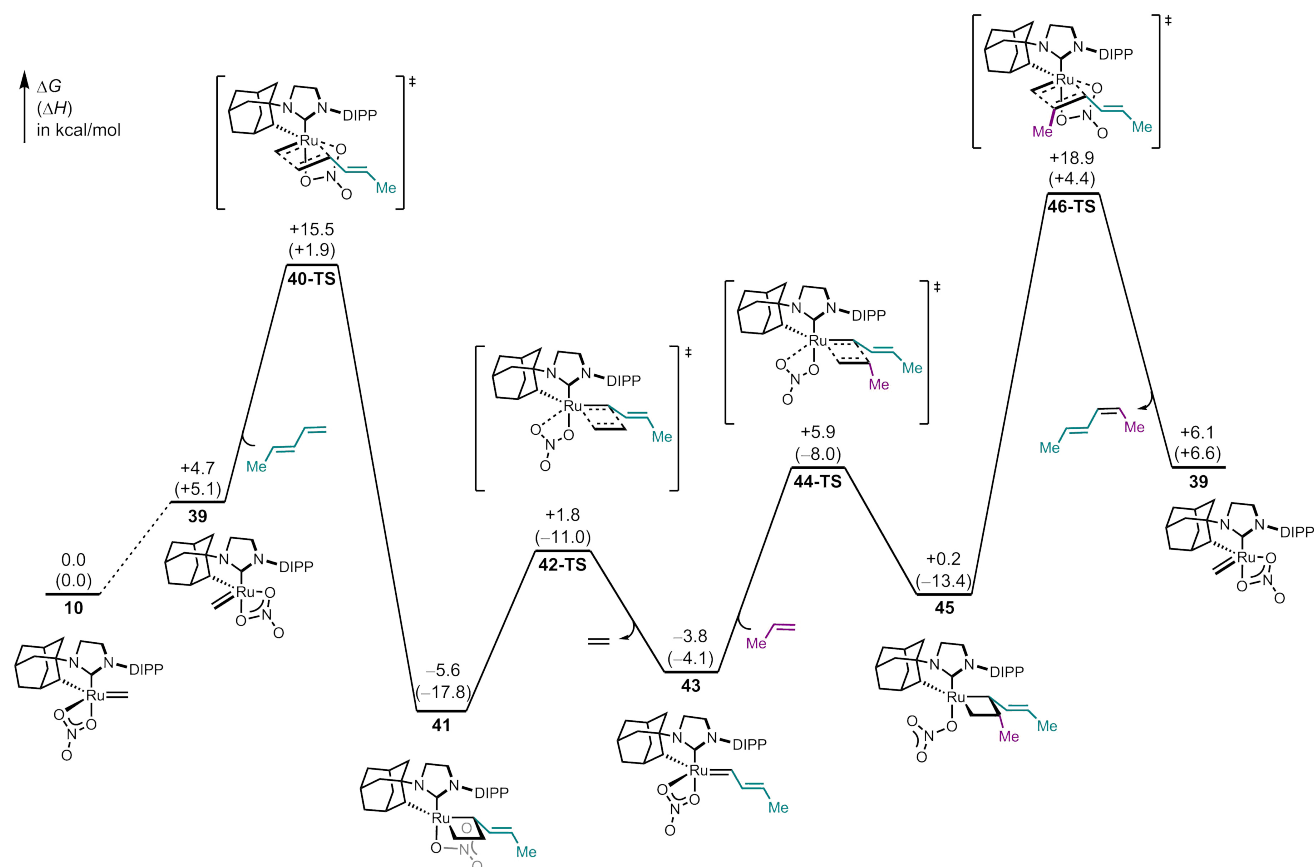
Additional Intermediates on Alkene-First Pathway B

Scheme S4: Complete Pathway B including olefin π -complexes



Reaction Pathway C Starting from Diastereomeric Methylidene Complex 39

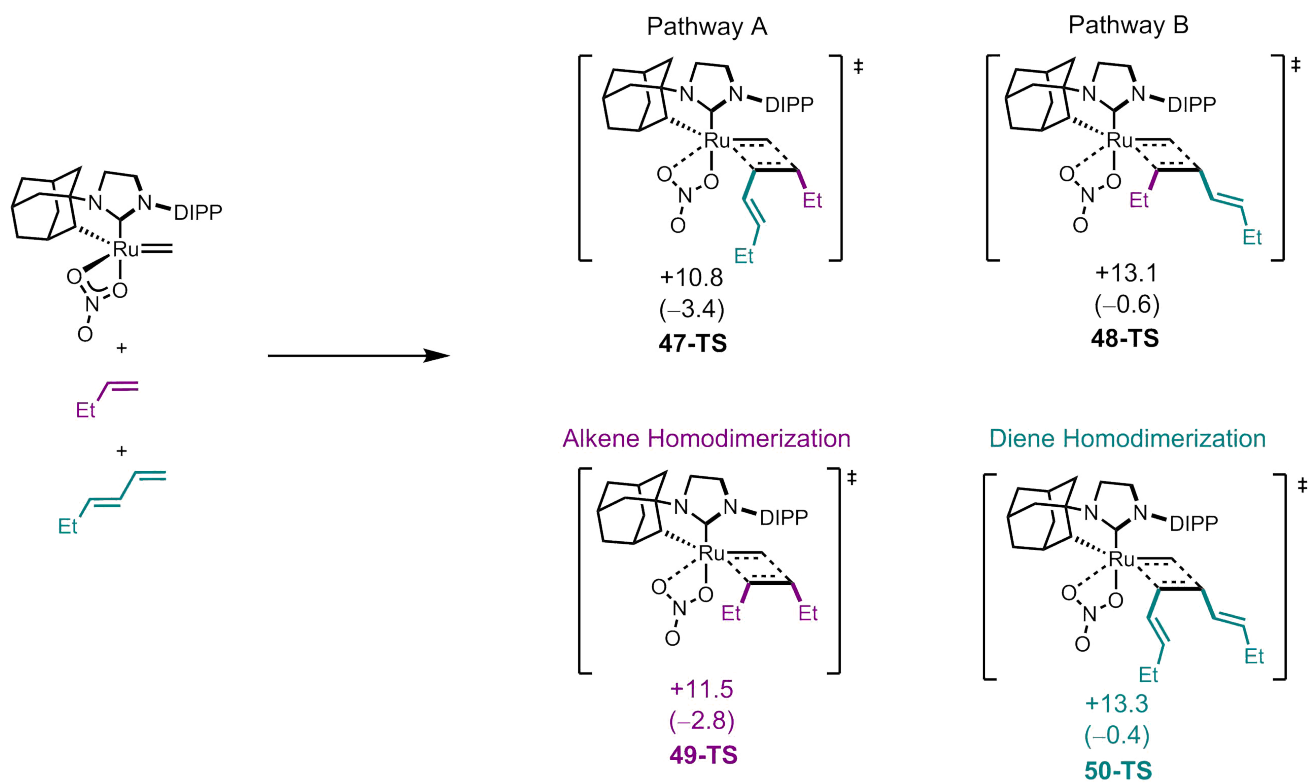
Scheme S5: Diastereomeric Pathway C



We also calculated the reaction of the diastereomer of methylidene complex 10. Methylidene 39 is about 5 kcal/mol less stable than 10, but may be accessible via non-productive metathesis pathways. Nevertheless, cross-metathesis starting from 39 is disfavored by about 7 kcal/mol in the rate-limiting transition state 46-TS (compared to 17-TS, Scheme S3).

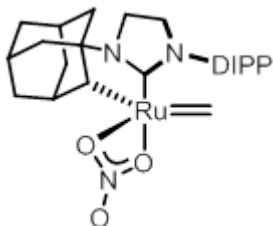
Calculations using larger substrate models

Scheme S6: Rate-limiting transition states using larger substrates 1-butene and *E*-1,3-hexadiene



Cartesian coordinates (Å), energies (hartree), and thermal corrections for optimized structures

Diene-First Pathway A

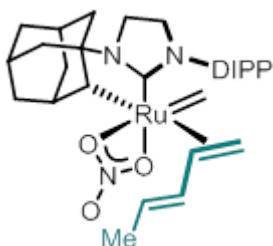


10

SCF Energy (M06, n-octanol): -1497.167761
 SCF Energy (B3LYP, gas-phase): -1496.738551
 Enthalpy Correction: 0.633713
 Free-Energy Correction: 0.542099

Ru	0.49185500	1.07399500	-0.51155600
O	-1.03909200	2.59279600	-0.18073100
O	0.78301500	3.22779200	-1.19104700
N	0.94790800	-1.44230800	0.83146400
N	-1.21684100	-1.31659000	0.46622500
C	-0.03544500	-0.66976300	0.30321100
C	0.47701800	-2.77490700	1.21970600
H	0.86780400	-3.07448600	2.19661300
H	0.78658400	-3.52759700	0.48178800
C	-1.05071100	-2.57345300	1.22855600
H	-1.59505700	-3.39241400	0.75016500
H	-1.44201600	-2.44990200	2.24599300
C	2.33810800	-1.06350100	0.55687100
C	2.87725500	-1.81060600	-0.68949400
H	2.19204600	-1.65547100	-1.52979100
H	2.91303600	-2.89049000	-0.48570600
C	4.28559600	-1.29482000	-1.04425300
H	4.65338700	-1.83140900	-1.92882900
C	5.23092000	-1.54830800	0.14719600
H	5.30623700	-2.62647600	0.34828700
H	6.24397200	-1.19690400	-0.09094500
C	4.69743600	-0.80786800	1.39087600
H	5.36687300	-0.98587400	2.24260900
C	3.28696600	-1.34180500	1.74545100
H	2.90188600	-0.84750900	2.64722900
H	3.34399300	-2.41915600	1.96123800
C	4.63963700	0.70550100	1.08474800
H	4.29887200	1.26048700	1.96946500
H	5.64773800	1.07273900	0.84667100
C	3.67851400	0.96551000	-0.10658800
H	3.63196700	2.04164700	-0.31326100
C	2.28965000	0.45886200	0.30582900
H	2.03893100	0.93761300	1.28216000
C	4.20502200	0.21608900	-1.34607800
H	3.54329700	0.39529500	-2.20193500
H	5.19844400	0.59835200	-1.61786800
C	-2.53014400	-0.76409400	0.25758800
C	-3.22684100	-1.09507700	-0.92556400
C	-4.52309200	-0.59232500	-1.08967500
H	-5.07778800	-0.83026700	-1.99297300
C	-5.11337900	0.20751200	-0.11613900
C	-4.41588800	0.51280400	1.04839100
H	-4.88651900	1.13520600	1.80383200
C	-3.11827600	0.03401000	1.26544400
C	-2.62872000	-1.99201500	-2.00438800
H	-1.58422300	-2.18051600	-1.73673700
C	-2.41809000	0.35784400	2.58341300

H	-1.38435400	0.00325700	2.51768100
C	0.58112200	0.37312500	-2.19038700
H	0.23554400	-0.61167400	-2.52170500
H	0.96304600	1.02500800	-2.98957700
H	-6.11910900	0.59184800	-0.26417100
C	-3.34927900	-3.35475700	-2.06077200
H	-4.40262300	-3.23502400	-2.34059300
H	-2.87836600	-4.00935900	-2.80409200
H	-3.32272400	-3.86656000	-1.09158600
C	-2.63323700	-1.31655600	-3.38912100
H	-2.11918900	-1.94999800	-4.12227200
H	-3.65275000	-1.15170600	-3.75621600
H	-2.12714600	-0.34654000	-3.35730100
C	-3.09216700	-0.38040800	3.75968700
H	-3.12092500	-1.46485800	3.60100100
H	-2.55250400	-0.18649100	4.69440900
H	-4.12605600	-0.04158200	3.89474600
C	-2.35760500	1.87250800	2.86297600
H	-3.35720800	2.29043600	3.03087200
H	-1.76932800	2.06152500	3.76933200
H	-1.90273500	2.41230400	2.02825600
N	-0.36240600	3.56682400	-0.73695400
O	-0.80660900	4.69119600	-0.79926900

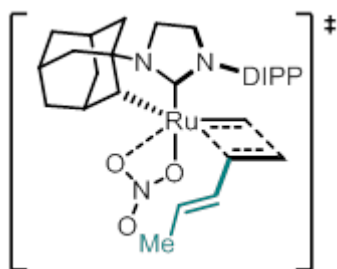


11-C

SCF Energy (M06, n-octanol):	-1692.379703
SCF Energy (B3LYP, gas-phase):	-1692.043911
Enthalpy Correction:	0.757079
Free-Energy Correction:	0.646719

Ru	0.48882900	0.66171900	-0.51660900
O	0.01362300	2.37823800	0.93703500
O	0.80676600	2.84151000	-1.03740600
N	1.41178300	-1.65296800	0.93005300
N	-0.73662400	-1.97947000	0.60813900
C	0.28902000	-1.11279200	0.37735900
C	1.21625100	-3.03323200	1.37960500
H	1.69612300	-3.21805600	2.34503900
H	1.62680000	-3.74555000	0.64993200
C	-0.31655700	-3.11568500	1.45520200
H	-0.71750700	-4.05788400	1.07172300
H	-0.68265800	-2.97759300	2.48065600
C	2.70330400	-1.05865600	0.56587000
C	3.30086700	-1.76722000	-0.67500000
H	2.55951400	-1.77588400	-1.48026400
H	3.53149600	-2.81349800	-0.42807400
C	4.57938400	-1.04097600	-1.13500000
H	4.98828400	-1.55185400	-2.01699600
C	5.61367500	-1.06952600	0.00821100
H	5.88311600	-2.10794000	0.24886600
H	6.53745500	-0.56339700	-0.30291800
C	5.02443000	-0.36772900	1.24905600
H	5.75644300	-0.38783800	2.06707900
C	3.74563300	-1.11378900	1.70735300
H	3.32810000	-0.64784400	2.60956300
H	3.99713900	-2.15464900	1.96094000
C	4.69517400	1.09708900	0.88364200

H	4.31434500	1.63457600	1.76214300
H	5.61275100	1.61215500	0.56608700
C	3.64129600	1.13083800	-0.25667100
H	3.39958400	2.16979500	-0.50601600
C	2.38863900	0.42275200	0.27955400
H	2.12295000	0.89199200	1.24352900
C	4.22293700	0.41654800	-1.49268500
H	3.49865700	0.43524400	-2.31588300
H	5.11896200	0.94910900	-1.83983600
C	-2.13284100	-1.73773500	0.37156200
C	-2.73833300	-2.32181200	-0.76547000
C	-4.10867900	-2.11222500	-0.96451600
H	-4.59521700	-2.54729100	-1.83299000
C	-4.85979600	-1.36092200	-0.06497500
C	-4.25257900	-0.81776800	1.06368100
H	-4.85198000	-0.25214300	1.77143700
C	-2.88520000	-0.99717600	1.31270200
C	-1.96395500	-3.20368500	-1.74215900
H	-0.90443400	-3.14282300	-1.47496300
C	-2.28446800	-0.45486400	2.60836000
H	-1.19962200	-0.58853500	2.56410200
C	0.73932000	-0.12039100	-2.16782600
H	0.52280000	-1.14229900	-2.50995500
H	1.07853500	0.52842500	-2.99220300
C	-2.15747800	1.30840800	-2.12054600
H	-1.58931400	1.68770600	-2.96603100
H	-2.38552400	0.24930100	-2.10846700
C	-2.63174100	2.13720400	-1.16803300
H	-3.21687000	1.71695700	-0.35075400
C	-2.42967300	3.57569400	-1.15063400
H	-1.85026100	4.00135500	-1.97001300
C	-2.88444400	4.38019800	-0.17443500
H	-3.44654700	3.93389900	0.64788100
C	-2.64400500	5.85547200	-0.09135300
H	-3.58460400	6.41033600	0.02861000
H	-2.01718700	6.09014600	0.77939100
H	-2.12965300	6.23040300	-0.98177100
N	0.44073600	3.27753000	0.11357800
O	0.49887900	4.45575300	0.41461500
C	-2.09444800	-2.73364800	-3.20341300
H	-1.48301900	-3.36549000	-3.85864100
H	-3.12861300	-2.79488300	-3.56121800
H	-1.75853400	-1.69882700	-3.32244700
C	-2.39765400	-4.67896100	-1.61181200
H	-3.44930600	-4.80857700	-1.89390600
H	-1.79413100	-5.31700600	-2.26845800
H	-2.28535600	-5.04484400	-0.58473900
C	-2.81005000	-1.25597100	3.81966000
H	-2.32391600	-0.91650800	4.74184500
H	-3.89122300	-1.12073700	3.94280000
H	-2.62434600	-2.33098100	3.71142000
C	-2.53887100	1.05097800	2.80955100
H	-3.61048000	1.27622000	2.87257300
H	-2.08015800	1.38119600	3.74883600
H	-2.09964500	1.64418600	2.00352000
H	-5.92178100	-1.20787700	-0.23799500

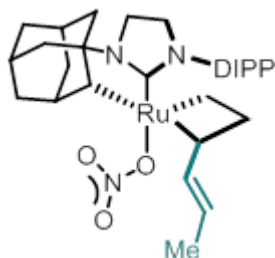


11-TS

SCF Energy (M06, n-octanol):	-1692.376027
SCF Energy (B3LYP, gas-phase):	-1692.037055
Enthalpy Correction:	0.757467
Free-Energy Correction:	0.654734

Ru	0.61246000	0.64556400	-0.59162700
O	1.71661300	2.52825500	-1.06588500
O	1.00811400	2.35860000	0.98283000
N	0.81638900	-1.95868700	0.64653000
N	-1.34193300	-1.67266000	0.38548600
C	-0.11661300	-1.07931000	0.19887300
C	0.27188100	-3.27738600	0.96896600
H	0.70816400	-3.68378100	1.88558800
H	0.46307300	-3.98840500	0.15242400
C	-1.21915200	-2.95744900	1.11238500
H	-1.86747300	-3.71978200	0.67435900
H	-1.50862600	-2.82214600	2.16267600
C	2.23453100	-1.66914200	0.40920900
C	2.71664700	-2.30084200	-0.92011600
H	2.05301400	-1.98734000	-1.73234200
H	2.66218500	-3.39746500	-0.85226200
C	4.16449700	-1.86048600	-1.21193100
H	4.49242500	-2.30230100	-2.16260500
C	5.07877800	-2.34924300	-0.07033700
H	5.06328700	-3.44745100	-0.01647300
H	6.11884800	-2.05383100	-0.26431700
C	4.60133200	-1.74002600	1.26402200
H	5.24449900	-2.09202300	2.08161700
C	3.14651400	-2.19157300	1.54611600
H	2.79938600	-1.79262900	2.50830600
H	3.11090700	-3.28976200	1.61133900
C	4.67696500	-0.20117100	1.16582600
H	4.38097500	0.25790800	2.11844700
H	5.71537800	0.10407500	0.97259200
C	3.74700300	0.29904200	0.02907800
H	3.81030900	1.38962500	-0.03685700
C	2.31385800	-0.13039700	0.38785300
H	2.10774100	0.20958300	1.41290900
C	4.21043600	-0.32081200	-1.30467800
H	3.56732000	0.02822400	-2.12192000
H	5.23307300	0.00890500	-1.53476700
C	-2.62483600	-1.02298400	0.38418500
C	-3.54587400	-1.33562000	-0.64539500
C	-4.79934100	-0.71169300	-0.62324800
H	-5.51940300	-0.93043700	-1.40651700
C	-5.14243800	0.17947800	0.38966300
C	-4.24489500	0.43585100	1.42162700
H	-4.53592300	1.10479300	2.22641500
C	-2.97972100	-0.16648300	1.45498300
C	-3.24132700	-2.37762000	-1.72139800
H	-2.16883700	-2.59374100	-1.67562000
C	-2.08641300	0.05208300	2.67729400
H	-1.11886400	-0.41990300	2.48678200
C	0.49000700	-0.03119400	-2.34833300
H	0.01321900	-0.94492200	-2.72428100
C	-1.30790400	1.98580500	-0.98064400
H	-1.90178100	1.68559600	-0.12344500

C	-1.26963500	1.10363500	-2.08420600
H	-1.92059200	0.24150700	-2.05875200
H	1.00811500	0.51964300	-3.14593900
N	1.63811500	3.05191200	0.10930100
O	2.13533000	4.13722200	0.36453700
C	-3.55893700	-1.90479700	-3.15317400
H	-3.26233900	-2.67572500	-3.87385600
H	-4.63037400	-1.72278500	-3.29449400
H	-3.02842300	-0.98330900	-3.41209600
C	-4.00455300	-3.68923500	-1.43190900
H	-3.72632800	-4.46493300	-2.15532800
H	-3.79699000	-4.07068500	-0.42636900
H	-5.08753800	-3.53416800	-1.50573800
C	-2.70894400	-0.63343500	3.91420600
H	-3.66008000	-0.16276500	4.18959200
H	-2.90815000	-1.69647900	3.73556900
H	-2.03430600	-0.55197000	4.77442100
C	-1.80369700	1.53619800	2.97807600
H	-1.25131900	2.01684300	2.16666400
H	-2.72767600	2.09858000	3.15927200
H	-1.18874900	1.61865900	3.88165900
H	-6.11775900	0.65884600	0.38514600
C	-1.03346300	3.40936000	-1.12905300
H	-0.56638400	3.72430800	-2.06168400
C	-1.30555600	4.33091300	-0.18869700
H	-1.75069200	4.00277700	0.75090000
C	-1.00042700	5.79217100	-0.30769700
H	-0.24103400	6.08214400	0.43094800
H	-0.61338900	6.04373200	-1.30056300
H	-1.88955500	6.40784100	-0.11475600
H	-1.09835800	1.54194900	-3.06537600



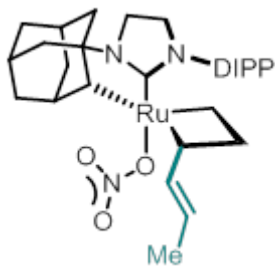
12a

SCF Energy (M06, n-octanol):	-1692.397781
SCF Energy (B3LYP, gas-phase):	-1692.051345
Enthalpy Correction:	0.760023
Free-Energy Correction:	0.654882

Ru	0.68610100	0.64706100	-0.60045700
O	1.80391000	2.72939800	0.67906700
O	1.84152500	2.28692700	-1.45913000
N	0.71693100	-1.99446700	0.56844900
N	-1.41610700	-1.64856800	0.21748700
C	-0.17530600	-1.06505000	0.14231900
C	0.14553100	-3.33166100	0.73344900
H	0.51666500	-3.82349500	1.63676200
H	0.38887700	-3.96774100	-0.12921600
C	-1.35052600	-3.00858900	0.80223800
H	-1.96901500	-3.70665300	0.23272100
H	-1.71908800	-2.98918300	1.83569100
C	2.14468900	-1.70521500	0.43040700
C	2.68722400	-2.20191400	-0.93617100
H	2.07616300	-1.77914100	-1.74328700
H	2.59785300	-3.29649100	-0.99467000
C	4.16009500	-1.78038900	-1.10097200
H	4.53129300	-2.13793300	-2.07056800
C	4.99464300	-2.40413100	0.03651400

H	4.95068900	-3.50145200	-0.01784700
H	6.05013300	-2.12083600	-0.07137100
C	4.45709900	-1.91509100	1.39779100
H	5.04875400	-2.35820100	2.20973500
C	2.98350400	-2.35359100	1.55695900
H	2.58995200	-2.04093600	2.53323700
H	2.91690300	-3.45095700	1.51012100
C	4.55589800	-0.37729900	1.45756800
H	4.20644500	-0.00817500	2.43096200
H	5.60562100	-0.06768400	1.35698800
C	3.71166000	0.25529100	0.31792300
H	3.79836500	1.34115200	0.38460800
C	2.25091500	-0.17141700	0.53948800
H	1.93013400	0.13462800	1.54642300
C	4.24980300	-0.24210900	-1.03895000
H	3.67758400	0.21237200	-1.85661500
H	5.29363400	0.07671600	-1.16377300
C	-2.68310000	-0.96976100	0.28418900
C	-3.58831300	-1.09619400	-0.79519500
C	-4.81839000	-0.43185900	-0.70407500
H	-5.52729900	-0.50504500	-1.52368400
C	-5.15473800	0.31139800	0.42367400
C	-4.27575500	0.37489600	1.50154000
H	-4.56263200	0.92802200	2.39152200
C	-3.03395900	-0.27217900	1.46600700
C	-3.30150600	-1.99498000	-1.99696100
H	-2.24009500	-2.26118700	-1.96339300
C	-2.14746000	-0.24998400	2.71276000
H	-1.20901000	-0.75936000	2.47851100
C	0.03252200	0.22482400	-2.43508600
C	-1.01054400	1.84486100	-0.58256900
C	-0.96565800	1.40182300	-2.09257800
H	-0.47035100	-0.71706000	-2.66138500
H	0.74274400	0.51001700	-3.21651400
H	-1.97804000	1.05781700	-2.31806200
H	-0.70833700	2.27130100	-2.69930300
H	-1.84035600	1.39581900	-0.04475200
C	-0.90785500	3.28899500	-0.34303600
H	-0.17409100	3.84215500	-0.92580800
C	-1.69502900	3.96017800	0.51613100
H	-2.44917700	3.40833400	1.07888100
C	-1.61712800	5.43450000	0.77680400
H	-2.57548200	5.92999300	0.56717600
H	-1.38614500	5.63366600	1.83265800
H	-0.84204200	5.91052900	0.16792700
H	-6.11172000	0.82420800	0.47125300
C	-2.82289900	-1.02317200	3.86670000
H	-3.74901500	-0.53108300	4.18593100
H	-3.07912900	-2.04887000	3.57659800
H	-2.15488600	-1.07111700	4.73465900
C	-1.77345300	1.17278200	3.16995600
H	-2.66144400	1.76062700	3.43153100
H	-1.14000900	1.12174300	4.06326200
H	-1.21958700	1.71390800	2.39823100
C	-4.12065500	-3.30108300	-1.89397700
H	-5.19583000	-3.09434300	-1.95439900
H	-3.86283000	-3.98209400	-2.71382700
H	-3.94093100	-3.82390200	-0.94799800
C	-3.56817900	-1.32125900	-3.35561200
H	-2.97855400	-0.40832600	-3.48144100
H	-3.30265800	-2.00557100	-4.16971300
H	-4.62494500	-1.06005100	-3.48222000
N	2.18803400	3.06508100	-0.47122800

O 2.84976900 4.07156800 -0.69891200

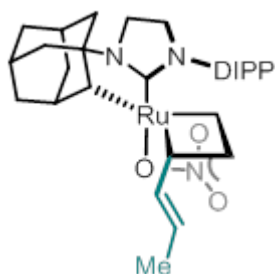


12b

SCF Energy (M06, n-octanol): -1692.400995
 SCF Energy (B3LYP, gas-phase): -1692.048723
 Enthalpy Correction: 0.759859
 Free-Energy Correction: 0.654990

Ru	0.70024800	0.61553500	-0.61101100
O	2.82747500	2.77878000	-0.04248700
O	1.90221400	1.93113600	-1.84939900
N	0.44650000	-1.50149600	1.35504800
N	-1.63565100	-1.07298200	0.81515100
C	-0.33398600	-0.74217800	0.53594800
C	-0.30072800	-2.53521300	2.07575600
H	0.04501300	-2.63878600	3.10749900
H	-0.20400800	-3.51083600	1.57766900
C	-1.72260200	-1.97914200	1.98500100
H	-2.48510700	-2.74532400	1.83310200
H	-1.98219400	-1.40636800	2.88367500
C	1.87207900	-1.60091400	1.03149700
C	2.10514600	-2.72835500	-0.01071800
H	1.45841200	-2.54585600	-0.87925000
H	1.81866600	-3.69948000	0.41742100
C	3.58267200	-2.75636700	-0.44248600
H	3.73105300	-3.56483000	-1.17068600
C	4.46706300	-3.00454200	0.79726400
H	4.23027800	-3.98214400	1.24134100
H	5.52524200	-3.03466100	0.50527300
C	4.23928600	-1.87901500	1.82790100
H	4.87006600	-2.05283800	2.70948600
C	2.75630300	-1.87466600	2.26890900
H	2.57987700	-1.09856800	3.02513000
H	2.50255000	-2.84343900	2.72469800
C	4.60424800	-0.52567000	1.18267800
H	4.48220200	0.29271500	1.90377100
H	5.66108100	-0.53113900	0.88125200
C	3.70659200	-0.26963200	-0.05872800
H	3.96715800	0.69711200	-0.48972700
C	2.25390400	-0.24081900	0.43406900
H	2.15516500	0.54200900	1.21282000
C	3.93481800	-1.39911000	-1.08248400
H	3.32166100	-1.22948100	-1.97738300
H	4.98355900	-1.39739000	-1.40906400
C	-2.82978000	-0.74303900	0.08075600
C	-3.13602600	-1.47695400	-1.09629300
C	-4.31211600	-1.15488900	-1.78486800
H	-4.56056300	-1.68759300	-2.69706500
C	-5.18156800	-0.17408900	-1.31616900
C	-4.89953200	0.48975100	-0.12783500
H	-5.60003400	1.23013400	0.24610600
C	-3.73158600	0.21795400	0.59782300
C	-2.28659900	-2.65610800	-1.57771500
H	-1.26248000	-2.50366000	-1.22473000
C	-3.52073500	0.90813200	1.94506000
H	-2.47024500	0.77910900	2.22905400

C	-0.35008000	0.42306300	-2.29451300
H	-1.03344000	-0.40713400	-2.44019600
C	-0.65540300	2.09758300	-0.24039200
H	-1.40670100	1.80190000	0.48796100
C	-1.05832200	1.71094200	-1.71709500
H	-2.13309300	1.51466000	-1.70379000
H	0.25319300	0.64258600	-3.17855800
C	-0.16069700	3.46386800	-0.02200400
H	0.39303100	3.92772300	-0.83568500
C	-0.34742100	4.15523500	1.11557200
H	-0.89958600	3.68655000	1.93238100
C	0.18136300	5.53352000	1.37537200
H	0.88004600	5.52980400	2.22343800
H	0.71470300	5.92848500	0.50518100
H	-0.62608900	6.23226600	1.63554200
C	-4.39514000	0.24149900	3.03121400
H	-4.20219400	0.69354100	4.01141500
H	-5.45953200	0.37349600	2.80389900
H	-4.20800900	-0.83450400	3.10901500
C	-3.80924000	2.42186700	1.91363500
H	-4.87355200	2.62869700	1.75577700
H	-3.53377800	2.87167900	2.87457100
H	-3.24634700	2.93382900	1.12780800
C	-2.80687700	-3.97743600	-0.96661600
H	-2.80737600	-3.95840500	0.12751000
H	-3.83470800	-4.17453900	-1.29357600
H	-2.18286100	-4.81968400	-1.28851600
C	-2.22754100	-2.80824300	-3.11003600
H	-1.48290200	-3.56731300	-3.37435100
H	-3.18590400	-3.14121600	-3.52483200
H	-1.94998300	-1.87668400	-3.61203500
H	-6.08811000	0.05835600	-1.86857200
H	-0.81596800	2.55643200	-2.36329300
N	2.69118300	2.81279400	-1.28088000
O	3.24677200	3.63468900	-2.00877000



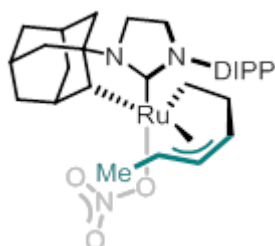
12c

SCF Energy (M06, n-octanol):	-1692.396138
SCF Energy (B3LYP, gas-phase):	-1692.052351
Enthalpy Correction:	0.759864
Free-Energy Correction:	0.655095

Ru	-0.60364000	0.73308600	0.62143300
O	-2.09621400	-0.00380700	2.66298700
O	-1.82888700	2.02931500	1.91453000
N	-0.44247100	-1.18745200	-1.54193100
N	1.64709900	-0.91983200	-0.93430500
C	0.35969600	-0.55178900	-0.64456100
C	0.25981800	-2.16206300	-2.38072000
H	-0.03191200	-2.07110900	-3.43076300
H	0.04426100	-3.18800600	-2.05313000
C	1.72367400	-1.77334100	-2.14241800
H	2.37402200	-2.63361800	-1.96589500
H	2.13533000	-1.20045300	-2.98195100
C	-1.88851900	-1.21471200	-1.31438400
C	-2.30044800	-2.50887500	-0.56324700

H	-1.72613900	-2.57720800	0.36914000
H	-2.05377300	-3.38846100	-1.17421800
C	-3.81121600	-2.48707500	-0.25732600
H	-4.08509400	-3.41722500	0.25757200
C	-4.60399600	-2.36892300	-1.57491700
H	-4.40977400	-3.23865600	-2.21897600
H	-5.68158800	-2.36196200	-1.36371700
C	-4.20103600	-1.06944100	-2.30146700
H	-4.76850100	-0.97630900	-3.23674700
C	-2.69275300	-1.12170700	-2.63479700
H	-2.38400600	-0.22427800	-3.18721600
H	-2.48507700	-1.99022300	-3.27716200
C	-4.49859300	0.14103000	-1.39020400
H	-4.24609200	1.07742200	-1.90614100
H	-5.57280400	0.18094100	-1.16293200
C	-3.69004400	0.01996300	-0.06721600
H	-3.90420800	0.88823600	0.56337900
C	-2.20703000	0.01224400	-0.45671300
H	-2.00142000	0.93021600	-1.06155300
C	-4.11276100	-1.27950400	0.64886400
H	-3.58435900	-1.36559700	1.60166600
H	-5.18761500	-1.23764100	0.87266000
C	2.83177400	-0.76395300	-0.13148500
C	3.04726900	-1.65825500	0.94814200
C	4.22393600	-1.51829900	1.69419300
H	4.40411400	-2.18404300	2.53288800
C	5.17300100	-0.55160900	1.37418000
C	4.97236300	0.27933900	0.27688200
H	5.73384200	1.00752000	0.01386700
C	3.81183700	0.18595300	-0.50337700
C	2.09401200	-2.81062800	1.27011800
H	1.15906500	-2.63910000	0.73004400
C	3.68839000	1.04383900	-1.76099100
H	2.65318200	0.97400600	-2.11167000
C	0.73418800	0.68856700	2.14049700
H	1.50487600	-0.07428500	2.15704900
C	0.54587500	2.28067500	0.02462200
H	1.26234200	2.08870600	-0.77366300
C	1.18576000	2.02001800	1.46964600
H	2.26746200	1.97471800	1.31611700
H	0.26427200	0.82512000	3.11377100
C	-0.15905500	3.56487500	-0.15321300
H	-0.79997400	3.88772300	0.66693200
C	-0.08372400	4.31621100	-1.26489400
H	0.55982700	3.98308100	-2.08244600
C	-0.82390000	5.60334400	-1.48606000
H	-1.48317300	5.53989400	-2.36337100
H	-1.44042000	5.86435700	-0.61944300
H	-0.13253300	6.43637000	-1.67630300
C	4.60428900	0.49589700	-2.87820800
H	4.46510100	1.06702100	-3.80392500
H	5.65931200	0.57527600	-2.59048900
H	4.40156100	-0.55864800	-3.09402500
C	3.99842000	2.53366400	-1.52030500
H	5.04790700	2.69075000	-1.24648900
H	3.81368900	3.10595700	-2.43687300
H	3.37646400	2.95899600	-0.72716500
C	2.68945800	-4.14619300	0.77146500
H	2.92640800	-4.11718300	-0.29820000
H	3.61651200	-4.38573700	1.30578600
H	1.98296700	-4.96741300	0.94052200
C	1.73341500	-2.92347100	2.76359700
H	1.02073700	-3.74326000	2.90937500

H	2.61080700	-3.14185600	3.38340400
H	1.26831400	-2.00843800	3.13981100
H	6.07797900	-0.45936300	1.96874900
H	0.91923100	2.86194900	2.11128700
N	-2.37826100	1.22179200	2.77607600
O	-3.12741400	1.66446800	3.63676900

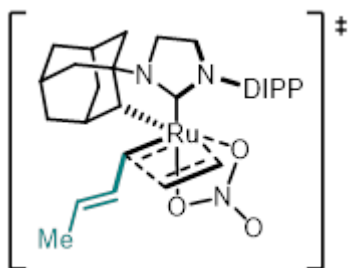


12d

SCF Energy (M06, n-octanol):	-1692.401982
SCF Energy (B3LYP, gas-phase):	-1692.059214
Enthalpy Correction:	0.760995
Free-Energy Correction:	0.657941

O	-0.92976900	2.50152100	-1.06173300
O	-1.67555300	2.79193900	0.96135400
N	-0.75812200	-1.74368900	-0.69075800
N	1.39588500	-1.42210400	-0.42727500
C	0.15281000	-0.86340000	-0.19710300
C	-0.18919400	-3.03189300	-1.08401800
H	-0.61158700	-3.38976000	-2.02742900
H	-0.38241700	-3.79015900	-0.31291700
C	1.29703200	-2.68908900	-1.18854000
H	1.94535600	-3.45494300	-0.75588600
H	1.60769500	-2.52629900	-2.22769500
C	-2.18961500	-1.51077000	-0.51468400
C	-2.78313800	-2.44412700	0.57193000
H	-2.19688300	-2.37739000	1.49260700
H	-2.71948900	-3.48753300	0.23008200
C	-4.25857300	-2.07958200	0.83013700
H	-4.65934300	-2.73363700	1.61607600
C	-5.05816600	-2.28296400	-0.47233200
H	-5.01363900	-3.33627300	-0.78487500
H	-6.11707200	-2.04244600	-0.30777300
C	-4.47575300	-1.37221800	-1.57240200
H	-5.03722600	-1.51459100	-2.50524300
C	-2.99535700	-1.75723100	-1.82020800
H	-2.56789800	-1.15582600	-2.63252700
H	-2.94166800	-2.81284400	-2.12735800
C	-4.59375100	0.10024900	-1.11527200
H	-4.23895900	0.77662600	-1.90343000
H	-5.65115700	0.34273100	-0.93680600
C	-3.76621200	0.31433200	0.18387200
H	-3.84375800	1.35996800	0.50025700
C	-2.30570500	-0.01626400	-0.18485000
H	-2.11396900	0.51208100	-1.13269200
C	-4.35414200	-0.60570800	1.27526100
H	-3.84105000	-0.45973800	2.22966000
H	-5.40809500	-0.34188000	1.44181100
C	2.66696800	-0.74680400	-0.49532600
C	3.65111200	-1.03811400	0.48139400
C	4.89395300	-0.40042300	0.38239400
H	5.65723700	-0.60136500	1.12829700
C	5.17216800	0.47953300	-0.65904400
C	4.21595500	0.71003100	-1.64300600
H	4.45424000	1.36926200	-2.47266400
C	2.95711500	0.09487800	-1.59805800
C	3.42732600	-2.06695800	1.58961800

H	2.35589800	-2.29218200	1.62085900
C	2.00275300	0.29537700	-2.77650500
H	1.04494100	-0.17255500	-2.53296700
H	6.14082900	0.96911600	-0.71503600
C	2.56199500	-0.40285400	-4.03683200
H	3.49591000	0.06776900	-4.36596900
H	2.77466500	-1.46363300	-3.86063200
H	1.84322700	-0.33125100	-4.86147100
C	1.70996600	1.77642900	-3.08085100
H	2.62327700	2.32808900	-3.33340900
H	1.03446500	1.85059900	-3.94081400
H	1.22001800	2.27141300	-2.23986500
C	4.17713100	-3.37893300	1.26807300
H	5.26138300	-3.21578300	1.25752200
H	3.95980500	-4.14141300	2.02557100
H	3.89730300	-3.78229800	0.28894200
C	3.84289800	-1.56545600	2.98668600
H	3.35157800	-0.62339800	3.24769000
H	3.57382600	-2.30988100	3.74498900
H	4.92538000	-1.40874700	3.05597200
N	-1.56546600	3.25275700	-0.23527500
O	-2.03205000	4.33063500	-0.55853100
Ru	-0.55515700	0.86657500	0.62499900
C	-1.26827500	0.11094300	2.51316800
H	-1.74328000	-0.86275200	2.47821000
H	-1.99416700	0.87765000	2.80024800
C	0.02091100	0.11791100	3.33210900
C	0.91449900	0.59983100	2.21499000
H	0.01017200	0.78737400	4.20308700
H	0.30971000	-0.87901800	3.68276800
C	1.04202600	2.00655800	1.96109200
H	1.70518300	-0.04922600	1.86369800
C	1.63527500	2.49989800	0.82742500
H	2.25467800	1.84020300	0.22761500
C	1.61544600	3.94708400	0.43855400
H	1.25826400	4.07348900	-0.59009700
H	0.97047300	4.53567700	1.09822500
H	2.62951000	4.36936100	0.47790500
H	0.47969700	2.69303400	2.59392100



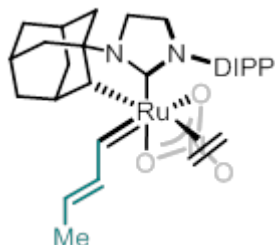
13-TS

SCF Energy (M06, n-octanol):	-1692.378773
SCF Energy (B3LYP, gas-phase):	-1692.040871
Enthalpy Correction:	0.758122
Free-Energy Correction:	0.653919

Ru	-0.55369000	0.72226900	0.66808800
O	-1.77180500	-0.29984000	2.46559100
O	-1.81711900	1.84549800	2.11576900
N	-0.48909000	-1.13030600	-1.56172300
N	1.61608300	-0.90641900	-0.99017400
C	0.33597100	-0.52989800	-0.66590300
C	0.18266400	-2.09290100	-2.43812300
H	-0.12029400	-1.96149600	-3.48059800
H	-0.05437300	-3.12375400	-2.14184600

C	1.65932900	-1.74640200	-2.20832000
H	2.28683000	-2.62684700	-2.04666200
H	2.08163400	-1.17648700	-3.04505800
C	-1.93873500	-1.12044500	-1.33193700
C	-2.36650400	-2.38851400	-0.54799600
H	-1.79770700	-2.43841100	0.38847700
H	-2.13043300	-3.28950600	-1.13286300
C	-3.87773800	-2.34016700	-0.24589500
H	-4.16550200	-3.25328200	0.29207100
C	-4.66834100	-2.24402400	-1.56611500
H	-4.48461400	-3.13129200	-2.18954800
H	-5.74616200	-2.21864800	-1.35617700
C	-4.24686000	-0.96730000	-2.32128400
H	-4.81351600	-0.88767900	-3.25872800
C	-2.73884300	-1.05830400	-2.65514800
H	-2.41542400	-0.18401100	-3.23597300
H	-2.55625500	-1.95017700	-3.27400000
C	-4.53201300	0.26671600	-1.43461200
H	-4.27463500	1.18854400	-1.97407700
H	-5.60753700	0.31624200	-1.21168100
C	-3.71571800	0.17004100	-0.11588600
H	-3.92061700	1.05345700	0.50012100
C	-2.22661200	0.14974200	-0.51809900
H	-2.08504100	1.00002200	-1.20477000
C	-4.16397300	-1.10556100	0.62968100
H	-3.64275800	-1.19444400	1.58541200
H	-5.23998200	-1.04350600	0.84542900
C	2.81305100	-0.77908300	-0.20494300
C	3.05287000	-1.71459900	0.83339900
C	4.23912600	-1.59389200	1.56812200
H	4.43731000	-2.29165600	2.37655200
C	5.17481700	-0.60623000	1.27382700
C	4.95218000	0.26517500	0.21215300
H	5.70508900	1.00847600	-0.03348900
C	3.78103100	0.19206500	-0.55386200
C	2.11531500	-2.88937100	1.11837500
H	1.18991100	-2.72848500	0.55856900
C	3.62845900	1.09174000	-1.77868600
H	2.59035100	1.01534000	-2.11883900
C	0.93467500	0.68828700	2.27454400
H	1.60031400	-0.15949600	2.18524100
C	0.23850300	2.24665600	-0.18364400
H	1.06314500	2.19100700	-0.90134000
C	1.29579200	1.90342800	1.63781000
H	2.23457600	1.94000200	1.09534400
H	0.36540700	0.73927100	3.19725900
C	-0.36224300	3.57050200	-0.10068000
H	-1.15861500	3.71719300	0.62878500
C	-0.02891500	4.58026600	-0.93182000
H	0.77240600	4.41770100	-1.65541900
C	-0.69129400	5.92402100	-0.96504200
H	-1.15163200	6.11421900	-1.94469300
H	-1.47006000	6.00884400	-0.20050900
H	0.03992900	6.72843300	-0.80430800
C	4.53824200	0.59632400	-2.92472000
H	4.37848400	1.19474500	-3.82967200
H	5.59576500	0.68170100	-2.64789500
H	4.34689700	-0.45340200	-3.17171300
C	3.91672600	2.57751200	-1.49207700
H	4.96258800	2.74255200	-1.20935300
H	3.72592900	3.17540400	-2.39115600
H	3.28695500	2.97023500	-0.68762200
C	2.74814900	-4.20562900	0.61478600

H	3.01578400	-4.15238500	-0.44674100
H	3.66283800	-4.44111600	1.17180400
H	2.05045300	-5.04075300	0.74787700
C	1.72252700	-3.02899500	2.60164000
H	1.05008900	-3.88546300	2.72594700
H	2.59449000	-3.20275200	3.24293000
H	1.19816900	-2.14288200	2.96905300
H	6.08733200	-0.52920500	1.85898600
H	0.97007200	2.83797300	2.08375800
N	-2.23806500	0.83869800	2.80909300
O	-3.02952000	0.97998500	3.72708900

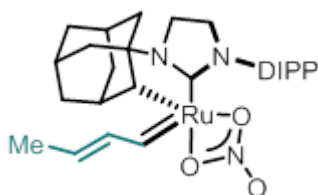


13-C

SCF Energy (M06, n-octanol):	-1692.378784
SCF Energy (B3LYP, gas-phase):	-1692.045588
Enthalpy Correction:	0.759023
Free-Energy Correction:	0.649855

Ru	-0.50754100	0.68887000	0.63996800
O	-1.39359700	-0.48416700	2.44933000
O	-1.74909600	1.65258100	2.25855200
N	-0.55612600	-1.09664800	-1.64918100
N	1.55701900	-0.96950300	-1.08427300
C	0.30153100	-0.54124300	-0.74981300
C	0.07361400	-2.09681100	-2.51617300
H	-0.24005400	-1.97813300	-3.55705100
H	-0.18764100	-3.11449400	-2.19477600
C	1.56381100	-1.79302500	-2.31074900
H	2.17227600	-2.69126000	-2.17171500
H	1.98792100	-1.22047900	-3.14613600
C	-1.98935300	-1.08947100	-1.32912300
C	-2.35526800	-2.31575900	-0.45244700
H	-1.72397300	-2.32187000	0.44337200
H	-2.15841400	-3.24510700	-1.00703500
C	-3.84222600	-2.25271500	-0.04953200
H	-4.08813300	-3.13491300	0.55638400
C	-4.72166400	-2.23010200	-1.31452500
H	-4.57571200	-3.14968900	-1.89995100
H	-5.78309700	-2.19537600	-1.03375100
C	-4.35898000	-0.99532300	-2.16427300
H	-4.98896300	-0.96577700	-3.06353000
C	-2.87600100	-1.10349000	-2.59523900
H	-2.59727700	-0.26416900	-3.24629800
H	-2.73096600	-2.02950500	-3.17245400
C	-4.59227700	0.28244900	-1.32385200
H	-4.38494400	1.17691700	-1.92689500
H	-5.64987500	0.33518500	-1.02769700
C	-3.68279300	0.26328400	-0.06356300
H	-3.84976900	1.17670000	0.51911700
C	-2.22609200	0.23541300	-0.58185800
H	-2.18121000	1.01392200	-1.35129100
C	-4.07211600	-0.97285000	0.77708700
H	-3.49200700	-1.02669400	1.70011400
H	-5.13093300	-0.89850300	1.06273000
C	2.78334200	-0.78610400	-0.36433400
C	3.16298800	-1.76898100	0.58110000
C	4.37528900	-1.59500400	1.26064600

H	4.68126200	-2.32875900	2.00134800
C	5.19464900	-0.49852500	1.00443400
C	4.82494000	0.43465600	0.03985300
H	5.48414800	1.27147000	-0.17279700
C	3.62467100	0.30596300	-0.67147000
C	2.31910900	-3.01106700	0.86179600
H	1.42989600	-2.96495000	0.22626800
C	3.30030300	1.29119400	-1.79000500
H	2.27021800	1.10406300	-2.10804600
C	-0.18556100	2.14672900	-0.50402000
H	0.04913200	2.04969200	-1.57657200
C	1.24523400	1.97273800	2.26695900
H	1.90772100	2.53209000	1.61370100
C	1.45798100	0.66661000	2.52284600
H	0.84798700	0.12283900	3.23632200
H	2.30175400	0.14047500	2.09592900
C	-0.41101900	3.52411100	-0.12338500
H	-0.69591900	3.73221500	0.90792800
C	-0.32706300	4.55517700	-0.99800400
H	-0.04903600	4.33587500	-2.03057800
C	-0.59081500	5.99135800	-0.67170600
H	0.29174200	6.61159700	-0.88274100
H	-1.40416900	6.39036200	-1.29373200
H	-0.86458500	6.12568000	0.37935500
H	6.12853000	-0.37891100	1.54731800
C	3.08947600	-4.29655100	0.49434500
H	3.96855300	-4.43329200	1.13481400
H	2.44646800	-5.17517300	0.62222200
H	3.43838100	-4.27781500	-0.54485700
C	1.82159900	-3.07397100	2.31913400
H	1.23822200	-3.98858400	2.47747900
H	2.65549800	-3.08518000	3.03101800
H	1.17720500	-2.22346700	2.55838700
C	4.22139000	1.04868500	-3.00525300
H	4.15596800	0.01462800	-3.36213100
H	3.94821200	1.71327400	-3.83368600
H	5.27013800	1.24348500	-2.75091900
C	3.38060900	2.76133600	-1.34209900
H	3.11173300	3.42293700	-2.17418500
H	2.69155500	2.96367600	-0.51723900
H	4.39160900	3.03648400	-1.02023400
N	-1.93800800	0.57538000	2.93666600
O	-2.59354500	0.55946600	3.96323800
H	0.45621900	2.52831500	2.76181900



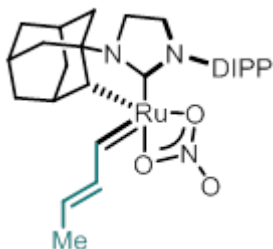
14

SCF Energy (M06, n-octanol):	-1613.828636
SCF Energy (B3LYP, gas-phase):	-1613.455204
Enthalpy Correction:	0.700146
Free-Energy Correction:	0.598624

Ru	-0.55034600	0.20646600	1.09175700
O	0.64128500	-1.12095900	2.43791000
O	-1.11657800	-0.12049600	3.24773800
N	-0.85398500	0.14924300	-1.78724600
N	1.28538700	-0.19341500	-1.37239900
C	0.08299400	0.07206800	-0.79546100
C	-0.33585800	-0.31481500	-3.07837600
H	-0.66975000	0.32398100	-3.90100000

H	-0.66273500	-1.34330900	-3.28841300
C	1.18401000	-0.23286000	-2.84772700
H	1.72919400	-1.08983200	-3.25098000
H	1.61317700	0.68107500	-3.27849400
C	-2.24436500	-0.02253100	-1.32951300
C	-2.55583700	-1.52622300	-1.09296700
H	-1.79581200	-1.95732800	-0.42414300
H	-2.49814400	-2.08219400	-2.03980100
C	-3.95495600	-1.68753100	-0.47034200
H	-4.16218700	-2.75446100	-0.31389700
C	-5.00182300	-1.09052300	-1.43334500
H	-4.99139800	-1.63630900	-2.38764800
H	-6.00971900	-1.20303400	-1.01177000
C	-4.69422300	0.40312400	-1.66821700
H	-5.44039000	0.82934400	-2.35171400
C	-3.28993300	0.54924400	-2.30679900
H	-3.06636200	1.60527200	-2.50721400
H	-3.26746200	0.01921100	-3.27143900
C	-4.74971900	1.14124200	-0.31147900
H	-4.57128900	2.21549200	-0.45428000
H	-5.75547700	1.03842800	0.12099200
C	-3.68521200	0.55254900	0.65169000
H	-3.72252700	1.08533500	1.60997600
C	-2.30365100	0.75583800	0.00274400
H	-2.21794300	1.81674500	-0.25810000
C	-3.99006400	-0.94152700	0.87977000
H	-3.25731900	-1.37456000	1.57496000
H	-4.97665800	-1.05950500	1.34866000
C	2.49328400	-0.61489000	-0.70941000
C	2.64660800	-1.98384000	-0.38282600
C	3.85023700	-2.38912500	0.20582100
H	3.98574400	-3.43283300	0.47362300
C	4.87633800	-1.48255900	0.45156700
C	4.71602800	-0.14533900	0.10446200
H	5.52567700	0.55453200	0.28989800
C	3.53033500	0.31520200	-0.48143900
C	1.58598000	-3.03782700	-0.69268000
H	0.67824400	-2.52086900	-1.01787900
C	3.41713600	1.78063100	-0.88478200
H	2.37403100	1.97034200	-1.15456100
C	-0.12178400	1.98125800	1.33776700
H	-0.21950800	2.28513400	2.39388700
C	2.03903200	-3.94884700	-1.85378400
H	2.93669400	-4.51670300	-1.58218500
H	1.25146100	-4.66943600	-2.10515500
H	2.27533000	-3.37455800	-2.75754800
C	1.20884900	-3.88204900	0.54012600
H	0.38152800	-4.55788900	0.29060400
H	2.04694300	-4.50486100	0.87406200
H	0.90712200	-3.24646400	1.37711300
C	4.28817800	2.08316800	-2.12219200
H	4.16319000	3.12647400	-2.43692600
H	5.35091800	1.92455700	-1.90362400
H	4.02694500	1.43865500	-2.96940300
C	3.77085600	2.73369000	0.27170900
H	4.82658600	2.65321800	0.55521400
H	3.59016300	3.77327000	-0.02608900
H	3.16360700	2.52205300	1.15657000
H	5.80241000	-1.81944000	0.90987200
C	0.19992100	3.05884000	0.43480900
H	0.27735100	2.83450200	-0.62787100
C	0.34856200	4.33795900	0.84987400
H	0.26205200	4.54791000	1.91723000

C	0.62370500	5.51138200	-0.03731200
H	-0.16463400	6.27069600	0.05930600
H	1.56374500	6.00519600	0.24627100
H	0.69177800	5.21923800	-1.09022000
N	-0.13866200	-0.92689900	3.46008900
O	0.04825600	-1.47584100	4.52455300

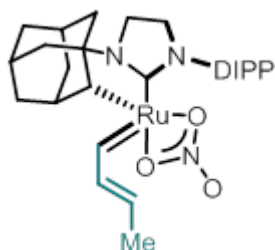


14b

SCF Energy (M06, n-octanol):	-1613.827824
SCF Energy (B3LYP, gas-phase):	-1613.459057
Enthalpy Correction:	0.700296
Free-Energy Correction:	0.598456

Ru	-0.58408400	0.70472700	0.54396800
O	0.40601200	0.58083200	2.52604800
O	-1.30205800	1.91535100	2.33908600
N	-0.79588400	-1.36245100	-1.44363800
N	1.34632700	-1.20959200	-0.96692700
C	0.12260000	-0.68159700	-0.70191300
C	-0.23965100	-2.57642800	-2.04641600
H	-0.60144800	-2.72410100	-3.06773400
H	-0.50044200	-3.46718600	-1.45609800
C	1.26863400	-2.27363800	-1.99229900
H	1.87273100	-3.13649200	-1.70198900
H	1.64161600	-1.89891400	-2.95404200
C	-2.20100600	-1.15267600	-1.06297300
C	-2.56857800	-2.01905700	0.17188200
H	-1.84400100	-1.83277700	0.97953700
H	-2.49699800	-3.08754700	-0.07804300
C	-3.99206400	-1.67810400	0.65253600
H	-4.24080000	-2.30103200	1.52185100
C	-4.98765900	-1.96125000	-0.49162800
H	-4.96668900	-3.02815300	-0.75606100
H	-6.01120500	-1.73295700	-0.16537400
C	-4.62219900	-1.09906900	-1.71778600
H	-5.33204400	-1.29669300	-2.53177100
C	-3.19550100	-1.46366700	-2.19899500
H	-2.92834100	-0.88092000	-3.09039900
H	-3.16151200	-2.52772900	-2.47913200
C	-4.69173100	0.39233400	-1.31874300
H	-4.46963900	1.02878700	-2.18595900
H	-5.71372700	0.63757600	-0.99567100
C	-3.68088000	0.68187000	-0.17797400
H	-3.73078200	1.74279700	0.09647200
C	-2.27329100	0.34984500	-0.70656300
H	-2.12889700	0.89928800	-1.64319000
C	-4.04449000	-0.18671700	1.04333800
H	-3.35116200	0.01729600	1.87042200
H	-5.04973400	0.07093200	1.40427100
C	2.59149600	-0.89757800	-0.31642500
C	2.92077800	-1.57055400	0.88412200
C	4.15670000	-1.28670500	1.47757800
H	4.42780500	-1.78343700	2.40428800
C	5.04549000	-0.38442100	0.90178700
C	4.71578900	0.24753000	-0.29292400
H	5.42239800	0.93909800	-0.74255200
C	3.49090600	0.00490100	-0.92677800

C	2.01972900	-2.63116700	1.51296800
H	1.03886000	-2.56919000	1.03162100
C	3.19512900	0.67512200	-2.26513900
H	2.13657200	0.51184600	-2.49405100
C	0.03663400	2.10143000	-0.49193400
H	0.55423100	1.94697100	-1.44658400
C	2.58239500	-4.04481900	1.24816400
H	3.56086900	-4.17267200	1.72638100
H	1.90858900	-4.80859000	1.65481900
H	2.71307200	-4.24265000	0.17762000
C	1.79761700	-2.41676100	3.02220000
H	1.08010700	-3.15608300	3.39892000
H	2.72531400	-2.54907100	3.59149000
H	1.40665400	-1.41695900	3.22689100
C	4.02448000	0.03191300	-3.39732300
H	3.77319700	0.48280100	-4.36502600
H	5.09787400	0.17767500	-3.22749500
H	3.84709200	-1.04714500	-3.46805800
C	3.43015600	2.19718600	-2.23169900
H	4.49114400	2.44116600	-2.10555100
H	3.10347000	2.64981800	-3.17593200
H	2.87822400	2.66979300	-1.41367900
H	5.99899600	-0.17893600	1.38118900
C	-0.13835700	3.48957000	-0.12320400
H	-0.62615400	3.70629500	0.82610400
C	0.26546400	4.51377600	-0.91060700
H	0.75715500	4.28143600	-1.85688900
C	0.09018400	5.96602100	-0.59139300
H	1.06048400	6.48130000	-0.55835400
H	-0.50244900	6.47194700	-1.36652900
H	-0.40884900	6.11095300	0.37183000
N	-0.39818700	1.42424200	3.10515700
O	-0.29274600	1.70811300	4.27918800



14c

SCF Energy (M06, n-octanol):	-1613.822199
SCF Energy (B3LYP, gas-phase):	-1613.452106
Enthalpy Correction:	0.700186
Free-Energy Correction:	0.598426

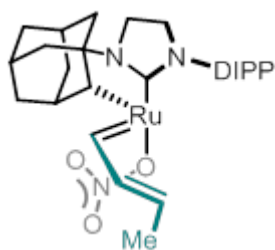
Ru	-0.56347000	0.89880700	0.07759300
O	0.59129800	1.75529200	1.83723400
O	-1.25537700	2.71503700	1.20258900
N	-0.97413800	-1.85255000	-0.69860700
N	1.18299100	-1.64463500	-0.33570200
C	0.00654000	-0.96780100	-0.37568300
C	-0.51884000	-3.24404600	-0.63764400
H	-0.91124100	-3.83529400	-1.46964300
H	-0.83465200	-3.72077000	0.30171200
C	1.00899100	-3.06571300	-0.70703000
H	1.55137300	-3.71580900	-0.01593700
H	1.39419300	-3.24146800	-1.71943900
C	-2.35104400	-1.38165700	-0.49800100
C	-2.77809300	-1.53550500	0.98681000
H	-2.03433500	-1.04847300	1.63593200
H	-2.79762100	-2.59840200	1.26859300
C	-4.16476700	-0.90017000	1.20478600

H	-4.45690900	-1.01992900	2.25646100
C	-5.18990600	-1.61087400	0.29709100
H	-5.26027800	-2.67482700	0.56509000
H	-6.18818900	-1.17777800	0.44628100
C	-4.76502800	-1.45749800	-1.17815100
H	-5.49529100	-1.95984400	-1.82620000
C	-3.37777400	-2.11314900	-1.38539500
H	-3.07115000	-2.04187800	-2.43721600
H	-3.43428800	-3.18271200	-1.13083400
C	-4.70584600	0.04637100	-1.52875600
H	-4.43871500	0.17908800	-2.58598100
H	-5.70037200	0.49479800	-1.39171900
C	-3.66399800	0.75872600	-0.62625300
H	-3.62515800	1.82454000	-0.88368600
C	-2.29081900	0.11241100	-0.89031000
H	-2.11587700	0.13840200	-1.97352800
C	-4.09158800	0.59885100	0.84736200
H	-3.38121200	1.11613700	1.50523600
H	-5.07109600	1.06973300	1.00895900
C	2.47892500	-1.12407900	0.00854900
C	2.88595200	-1.15194400	1.36294900
C	4.16904800	-0.68495500	1.67300500
H	4.50117800	-0.69027700	2.70695200
C	5.02760200	-0.22057300	0.68154000
C	4.61790800	-0.22245800	-0.64833300
H	5.29991200	0.12950100	-1.41702500
C	3.34396100	-0.67388700	-1.01413500
C	2.01057600	-1.72207400	2.47683400
H	1.00775100	-1.88016900	2.06766100
C	2.95721700	-0.70798900	-2.48999700
H	1.88202200	-0.90581200	-2.55081200
C	0.06688700	1.55779600	-1.53101300
H	0.09146800	0.92244400	-2.42740800
C	2.54743300	-3.09354000	2.94052400
H	3.54661900	-2.99537600	3.38127300
H	1.88728400	-3.52691600	3.70141300
H	2.62380200	-3.80630700	2.11077300
C	1.86706600	-0.76588500	3.67615500
H	1.16972400	-1.19124100	4.40843900
H	2.82374000	-0.61598300	4.19067300
H	1.49005300	0.21110500	3.36261100
C	3.69042400	-1.85090800	-3.22451100
H	3.37137800	-1.90312100	-4.27252400
H	4.77519500	-1.69116100	-3.21169600
H	3.49657600	-2.82472600	-2.76068100
C	3.21560200	0.63323400	-3.20223900
H	4.28655100	0.85806300	-3.26701800
H	2.82928600	0.59477700	-4.22793100
H	2.72779400	1.46257200	-2.68180200
H	6.01962400	0.13720000	0.94466400
C	0.43874900	2.93697900	-1.79671600
H	0.28836500	3.28190700	-2.82477800
C	0.99386600	3.79480400	-0.91211300
H	1.21952300	3.43079200	0.08778100
C	1.37515800	5.20876000	-1.21543400
H	0.85039500	5.89926200	-0.54070700
H	2.44883500	5.37320100	-1.05003800
H	1.13621900	5.48733900	-2.24710300
N	-0.30446700	2.66337700	2.06919500
O	-0.24413400	3.40557400	3.02786700



Ru	-0.55353700	0.78565600	0.07295700
O	-2.51778400	3.28988100	-0.76895800
O	-1.45993900	2.41915700	0.96949000
N	-0.60097900	-2.09890600	-0.30340900
N	1.51053200	-1.61623700	0.03009100
C	0.27048000	-1.08809300	-0.11673700
C	-0.00689300	-3.42500100	-0.10294500
H	-0.26074300	-4.10505600	-0.92140300
H	-0.36200700	-3.87375900	0.83421700
C	1.50230500	-3.09320500	-0.05634100
H	2.01005100	-3.52921700	0.80985100
H	2.02356100	-3.42878800	-0.95979700
C	-2.02935900	-1.75973700	-0.26770300
C	-2.56187800	-1.82238500	1.18760700
H	-1.93720000	-1.18571700	1.83234100
H	-2.48156300	-2.84847500	1.57554900
C	-4.02672400	-1.34621500	1.23483600
H	-4.39197300	-1.40361500	2.26868900
C	-4.88182800	-2.25657700	0.32969600
H	-4.85489500	-3.29274800	0.69709000
H	-5.93136500	-1.93507600	0.35916600
C	-4.35228100	-2.18888300	-1.11782400
H	-4.96169600	-2.83426000	-1.76419300
C	-2.88794100	-2.68821000	-1.15221900
H	-2.50094300	-2.67772700	-2.17977400
H	-2.84122000	-3.72778000	-0.79336900
C	-4.42623700	-0.72898400	-1.61598000
H	-4.08429400	-0.66475200	-2.65787200
H	-5.47074000	-0.38717200	-1.60189300
C	-3.55600000	0.18601100	-0.71341700
H	-3.60595600	1.21754200	-1.07202800
C	-2.10305700	-0.31245700	-0.81373600
H	-1.83363300	-0.35679500	-1.87966900
C	-4.09103300	0.10972500	0.73189900
H	-3.50561400	0.76435500	1.38883100
H	-5.12754400	0.47174300	0.76517500
C	2.71872000	-0.88468800	0.28645200
C	2.99805900	-0.45757600	1.60458500
C	4.19486900	0.23395700	1.83190800
H	4.42744400	0.57921500	2.83548700
C	5.09632500	0.47501300	0.79967700
C	4.81361200	0.02743200	-0.48795100
H	5.52640900	0.21464400	-1.28596700
C	3.62482500	-0.65405700	-0.77360200
C	2.06961200	-0.74576700	2.78119000
H	1.20531700	-1.29875300	2.40159900
C	3.35815200	-1.14061000	-2.19574500
H	2.32120300	-1.48964700	-2.24022200
C	0.15565400	1.40066400	-1.51647400
H	-0.05692800	0.87880000	-2.46108500
C	2.75944900	-1.64054500	3.83144400
H	3.62177300	-1.13825500	4.28509400

H	2.05969000	-1.89092000	4.63741500
H	3.11770900	-2.57682000	3.38787600
C	1.53404700	0.54605700	3.42882100
H	0.85159300	0.30482100	4.25235000
H	2.34545600	1.15902600	3.83850000
H	0.98347100	1.15980700	2.70603200
C	4.27835400	-2.32476500	-2.56040400
H	4.03999100	-2.70432100	-3.56121400
H	5.33085900	-2.01729600	-2.56132600
H	4.17972900	-3.15290700	-1.84946300
C	3.49789300	-0.01631100	-3.23925300
H	4.53033000	0.34470700	-3.31217700
H	3.20847400	-0.38385600	-4.23078800
H	2.86058900	0.83657100	-2.98925300
H	6.02215200	1.00816100	0.99917300
C	0.98175400	2.58617000	-1.66993000
H	1.44809700	2.73328200	-2.64815500
C	1.17952900	3.53983200	-0.72933000
H	0.67328200	3.44334800	0.23071600
C	2.00786300	4.76834100	-0.92628500
H	1.39352500	5.67158700	-0.80859000
H	2.79852000	4.83225800	-0.16560000
H	2.47578800	4.79440300	-1.91580800
N	-2.29279200	3.32553400	0.44365900
O	-2.76203000	4.14758700	1.22429000

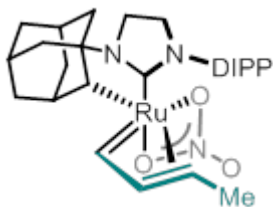


14e

SCF Energy (M06, n-octanol):	-1613.820649
SCF Energy (B3LYP, gas-phase):	-1613.452269
Enthalpy Correction:	0.700874
Free-Energy Correction:	0.598247

Ru	-0.46121700	0.94162300	-0.09227500
O	-1.21226600	1.27113200	2.09981300
O	-1.29693200	2.87239900	0.62928700
N	-0.76492100	-1.91690900	-0.49107100
N	1.34476700	-1.58319500	0.02278800
C	0.16074800	-0.96505200	-0.22119700
C	-0.28153300	-3.27318900	-0.21135100
H	-0.54856300	-3.96873500	-1.01237800
H	-0.70667700	-3.65348600	0.72722600
C	1.24115300	-3.05208400	-0.10351200
H	1.68621300	-3.54657600	0.76497200
H	1.76894600	-3.39700900	-1.00046700
C	-2.17056900	-1.49031800	-0.46733600
C	-2.75753900	-1.61195600	0.96132900
H	-2.12698700	-1.05755200	1.66475900
H	-2.76375500	-2.66626500	1.27424100
C	-4.19322000	-1.05094400	0.98852000
H	-4.59872900	-1.14969000	2.00387100
C	-5.07207100	-1.83894500	-0.00243400
H	-5.12077600	-2.89786800	0.28972900
H	-6.10086200	-1.45456100	0.01647300
C	-4.48596200	-1.70446300	-1.42246700
H	-5.11046900	-2.25901100	-2.13548900
C	-3.05668700	-2.29844600	-1.44136700
H	-2.62962500	-2.25037900	-2.45178100

H	-3.09441500	-3.35940100	-1.15105400
C	-4.45409400	-0.20945300	-1.81511100
H	-4.08143800	-0.09290300	-2.84173000
H	-5.47552700	0.19661100	-1.79812900
C	-3.55072600	0.57985800	-0.82576200
H	-3.52602900	1.63695600	-1.11598600
C	-2.13710400	-0.02075300	-0.94682600
H	-1.89670400	-0.05617300	-2.01696800
C	-4.14885400	0.43799500	0.58932600
H	-3.56049000	0.99418100	1.32389700
H	-5.16325000	0.86013000	0.60199300
C	2.59669700	-0.94478600	0.32162200
C	2.88337800	-0.58459800	1.65911200
C	4.13087600	-0.00730100	1.93042000
H	4.37344000	0.27946300	2.94944900
C	5.06909300	0.19453700	0.92306600
C	4.77525800	-0.18081800	-0.38467000
H	5.51657200	-0.02589500	-1.16342800
C	3.54136500	-0.75433300	-0.71350100
C	1.91806500	-0.85195300	2.81098600
H	0.95461900	-1.14570400	2.38495700
C	3.27294200	-1.17862800	-2.15500700
H	2.21441100	-1.44703700	-2.23383600
C	0.17533700	1.33707700	-1.81493800
H	0.06214500	0.63398300	-2.65622200
C	2.42159700	-2.02425900	3.68003600
H	3.37928500	-1.78135700	4.15589700
H	1.69963100	-2.24865700	4.47397900
H	2.56999400	-2.93482900	3.08748800
C	1.66450700	0.39517700	3.67767700
H	0.92376900	0.16769500	4.45206200
H	2.57665300	0.73637800	4.18111800
H	1.26784900	1.22029300	3.07978800
C	4.11068700	-2.41853700	-2.53374500
H	3.86863000	-2.75203500	-3.55004400
H	5.18278400	-2.19049500	-2.50305200
H	3.93468400	-3.25602400	-1.84932600
C	3.52586000	-0.03941800	-3.16033600
H	4.58739400	0.22925600	-3.21074500
H	3.21937100	-0.34942400	-4.16653300
H	2.96361000	0.85882700	-2.89019500
H	6.03225400	0.64011500	1.15792700
C	0.83622000	2.56383300	-2.23524100
H	1.21732800	2.59396800	-3.26039300
C	1.00285500	3.67762200	-1.47997900
H	0.59149200	3.69693700	-0.47198700
C	1.68405500	4.92356600	-1.94661300
H	0.99803400	5.78089000	-1.90344600
H	2.52847300	5.17467900	-1.28928700
H	2.05888700	4.82943100	-2.97110800
N	-1.48487900	2.50333600	1.85383800
O	-1.89797400	3.26905100	2.70224500

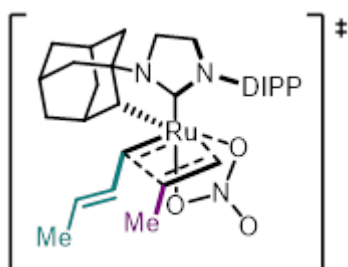


14-constained

SCF Energy (M06, n-octanol):	-1613.807519
SCF Energy (B3LYP, gas-phase):	-1613.430740

Ru	-0.47726200	0.81070200	-0.66921700
O	-1.09310500	2.12171800	1.16831100
O	-1.47699800	2.81376200	-0.85328400
N	-0.81436800	-1.88616900	0.37741100
N	1.31581700	-1.40734700	0.60936700
C	0.12854500	-0.95004700	0.13502900
C	-0.32889300	-2.97489300	1.23309700
H	-0.63022200	-3.95335400	0.84815500
H	-0.72546700	-2.87088200	2.25148300
C	1.19752100	-2.76381900	1.18456900
H	1.66992900	-2.80830900	2.17032700
H	1.69232700	-3.49536000	0.53489200
C	-2.21951700	-1.47683500	0.23724400
C	-2.75564200	-0.91335400	1.57827500
H	-2.10204900	-0.10445900	1.92237400
H	-2.74978100	-1.70165300	2.34554500
C	-4.19038100	-0.38380000	1.38576000
H	-4.56038300	0.00694700	2.34274600
C	-5.10084900	-1.53069200	0.90471600
H	-5.13686400	-2.33085600	1.65816300
H	-6.12918200	-1.16748900	0.77380400
C	-4.56361300	-2.08090500	-0.43233800
H	-5.21045000	-2.89569700	-0.78429100
C	-3.13429500	-2.63567800	-0.21658100
H	-2.74319200	-3.07065800	-1.14590700
H	-3.16156600	-3.43859200	0.53614200
C	-4.55008900	-0.94102300	-1.47629300
H	-4.21381600	-1.32168000	-2.45025000
H	-5.57261800	-0.56222500	-1.61695800
C	-3.61445400	0.20412600	-0.99850000
H	-3.60477500	1.00601100	-1.74615000
C	-2.20034700	-0.39782100	-0.86710000
H	-2.00330400	-0.93477100	-1.80734900
C	-4.16271500	0.74620500	0.33779700
H	-3.55111300	1.57284200	0.70799400
H	-5.17680100	1.14183300	0.18654600
C	2.58626600	-0.74234600	0.52325800
C	2.97252500	0.12637700	1.57043200
C	4.22316600	0.75157700	1.47664200
H	4.54064300	1.42675900	2.26607900
C	5.07037200	0.51275300	0.39880800
C	4.68377300	-0.36776500	-0.60834800
H	5.35824400	-0.55779400	-1.43818400
C	3.44199000	-1.01340800	-0.56961100
C	2.11130200	0.35788600	2.80959700
H	1.15075000	-0.14070400	2.65036400
C	3.07572000	-2.00974300	-1.66686800
H	2.01038200	-2.24159000	-1.56619300
C	0.09552200	0.40147000	-2.38944100
H	-0.15610500	-0.38278600	-3.11358100
C	2.76918600	-0.28151600	4.05111400
H	3.72436000	0.20196300	4.28803600
H	2.11602400	-0.17674900	4.92528000
H	2.96884000	-1.34912300	3.90038600
C	1.81058400	1.84777900	3.05941700
H	1.19409100	1.95740800	3.95887500
H	2.72793600	2.42792700	3.21539700
H	1.25267000	2.28895100	2.22870800
C	3.86946700	-3.32365100	-1.49996200
H	3.56056200	-4.05867700	-2.25282300
H	4.94469800	-3.14815500	-1.62417500
H	3.72328400	-3.76855100	-0.50931000
C	3.28415100	-1.44303700	-3.08391700

H	4.34561800	-1.28058800	-3.30452400
H	2.90182900	-2.14949100	-3.83012400
H	2.76258900	-0.49025300	-3.21230700
H	6.03780000	1.00561400	0.34785800
C	0.92139600	1.53705000	-2.73123000
H	0.96151800	1.98174000	-3.72853700
C	1.45648000	2.16793500	-1.65519900
H	1.53518200	1.63301100	-0.69572900
C	2.10204400	3.51956200	-1.66836300
H	1.54300100	4.20948700	-1.02121200
H	3.12817100	3.48066900	-1.27974000
H	2.12202500	3.94631600	-2.67632600
N	-1.52604300	3.06392200	0.40863400
O	-1.96094400	4.11388600	0.84624000

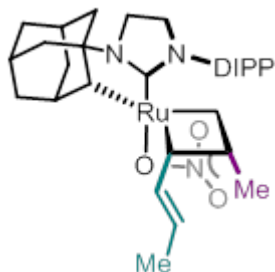


15-TS

SCF Energy (M06, n-octanol):	-1731.672626
SCF Energy (B3LYP, gas-phase):	-1731.354204
Enthalpy Correction:	0.787843
Free-Energy Correction:	0.681266

Ru	-0.58079400	0.74447600	0.52407200
O	-1.86814900	0.04675600	2.47034200
O	-1.81851500	2.10788300	1.77933700
N	-0.56138100	-1.39979000	-1.42863700
N	1.55448300	-1.13789400	-0.91863400
C	0.28415700	-0.69830900	-0.62976200
C	0.08382600	-2.48663500	-2.16831700
H	-0.25186100	-2.51754800	-3.20825300
H	-0.13929700	-3.45942600	-1.70811600
C	1.56123500	-2.10556500	-2.04007400
H	2.20948200	-2.95544600	-1.81404200
H	1.93586500	-1.62241600	-2.95126900
C	-2.00751100	-1.32738600	-1.19758100
C	-2.46350400	-2.46147600	-0.24167300
H	-1.89347900	-2.39414100	0.69292400
H	-2.25126900	-3.44179100	-0.69307500
C	-3.97287800	-2.33264200	0.04825900
H	-4.28091300	-3.15133400	0.71215200
C	-4.76268400	-2.41046900	-1.27327400
H	-4.60099000	-3.38170300	-1.76356700
H	-5.83931600	-2.32998300	-1.07142900
C	-4.31289700	-1.26525800	-2.20368300
H	-4.87849400	-1.30831500	-3.14416000
C	-2.80878500	-1.43579300	-2.51725000
H	-2.46637700	-0.65988300	-3.21518200
H	-2.64659400	-2.41019200	-3.00288500
C	-4.56457900	0.09099000	-1.50821000
H	-4.28083200	0.91686500	-2.17498900
H	-5.63783800	0.20378900	-1.29851000
C	-3.75217700	0.16586800	-0.18468500
H	-3.93509900	1.13335400	0.29651400
C	-2.26323700	0.04647100	-0.56538200
H	-2.07766600	0.80046800	-1.35084100
C	-4.23260100	-0.97847400	0.73423600

H	-3.71623200	-0.93876800	1.69551700
H	-5.30758700	-0.86208100	0.93151200
C	2.77043600	-0.96028700	-0.17181900
C	3.00245100	-1.77727400	0.96487200
C	4.21325700	-1.62394300	1.65145100
H	4.40699100	-2.23137800	2.53056800
C	5.18043600	-0.72046800	1.22016400
C	4.96156200	0.03145800	0.07058600
H	5.73593500	0.70824600	-0.27855300
C	3.76638300	-0.07819000	-0.65309400
C	2.02616000	-2.86826800	1.40969400
H	1.07840600	-2.70863600	0.88852100
C	3.61702500	0.68675500	-1.96683500
H	2.56711800	0.62296400	-2.27122100
C	0.88996000	0.79252200	2.08609000
H	1.51501000	-0.09026400	2.06020500
C	0.33498200	2.11876800	-0.45514800
H	1.16794500	1.92987500	-1.13745800
C	1.34991300	1.96082600	1.38754900
H	2.27691500	1.82083900	0.83621200
C	1.18441800	3.32002200	2.03797600
H	1.91369300	3.41039200	2.85445100
H	1.35986500	4.14144900	1.33757000
H	0.18265000	3.42957300	2.46206900
H	0.36682700	0.94914800	3.02704000
C	-0.25073900	3.44387800	-0.60813200
H	-1.06394600	3.71357600	0.06442500
C	0.11367300	4.30617100	-1.57995600
H	0.93029300	4.02725300	-2.24886600
C	-0.53612700	5.63181900	-1.84148500
H	-0.97501300	5.66769100	-2.84847100
H	-1.33004400	5.84051200	-1.11718200
H	0.19750500	6.44868500	-1.79344600
C	4.47054900	0.02811800	-3.07318600
H	4.31424600	0.53469900	-4.03313000
H	5.53814600	0.08925600	-2.83082600
H	4.22309600	-1.03097400	-3.20278400
C	3.97751400	2.17997500	-1.85078400
H	5.03865800	2.32634400	-1.61941600
H	3.78076300	2.68737600	-2.80263600
H	3.39322600	2.68335300	-1.07419500
C	2.56116200	-4.25852300	0.99932300
H	2.76278100	-4.32066800	-0.07603600
H	3.49729100	-4.48846000	1.52200300
H	1.83417000	-5.03868100	1.25406800
C	1.71660600	-2.85333200	2.91882300
H	0.98355900	-3.63399400	3.15164400
H	2.60866300	-3.05384600	3.52355100
H	1.29459200	-1.89720900	3.24016600
H	6.11269500	-0.61751700	1.76910200
N	-2.27817500	1.24289900	2.62607400
O	-3.05470900	1.57004100	3.50999400



16a

SCF Energy (M06, n-octanol):	-1731.686644
SCF Energy (B3LYP, gas-phase):	-1731.363260
Enthalpy Correction:	0.789495
Free-Energy Correction:	0.682258

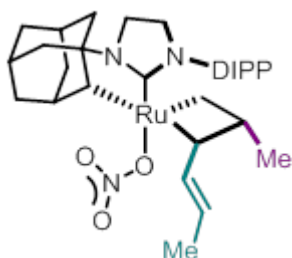
Ru	-0.61400100	0.74768600	0.47260900
O	-2.12859600	0.36146100	2.61940100
O	-1.81078900	2.24634900	1.56409600
N	-0.52335700	-1.44486000	-1.41513100
N	1.58074300	-1.15195100	-0.87423200
C	0.30584700	-0.71842400	-0.61622400
C	0.14474600	-2.53797200	-2.12542700
H	-0.17346400	-2.59185100	-3.17011600
H	-0.07276300	-3.50477800	-1.65066200
C	1.61565600	-2.13661100	-1.98087200
H	2.27076500	-2.97475700	-1.73270400
H	1.99669900	-1.66245200	-2.89368600
C	-1.96567800	-1.40660800	-1.17039100
C	-2.39494300	-2.56281400	-0.22719700
H	-1.81382300	-2.49919100	0.70129700
H	-2.17008900	-3.53099000	-0.69646100
C	-3.90246500	-2.46278200	0.08049100
H	-4.18965400	-3.29725700	0.73356200
C	-4.70408500	-2.53218600	-1.23469000
H	-4.53178300	-3.49286200	-1.74132500
H	-5.77958300	-2.47250700	-1.02107500
C	-4.28367200	-1.36604200	-2.15305000
H	-4.85803600	-1.40433800	-3.08803700
C	-2.78069400	-1.49874200	-2.48379900
H	-2.45986500	-0.70130200	-3.16734400
H	-2.59624200	-2.45834700	-2.98904700
C	-4.54675900	-0.02426800	-1.43721400
H	-4.27803600	0.81561000	-2.09240500
H	-5.61756600	0.07584100	-1.21254700
C	-3.72951700	0.04120700	-0.11481500
H	-3.91953200	0.99948000	0.37805500
C	-2.24860900	-0.06039600	-0.50073300
H	-2.01926500	0.75552000	-1.23005000
C	-4.17533800	-1.12520200	0.79185600
H	-3.64509700	-1.07706100	1.74579600
H	-5.24825900	-1.02800700	1.00756500
C	2.77946300	-0.95135400	-0.10316700
C	2.96904800	-1.71404800	1.07806500
C	4.16562400	-1.54522600	1.78552100
H	4.32845500	-2.11065300	2.69801400
C	5.15799600	-0.67977000	1.33380600
C	4.97830800	0.01947500	0.14501400
H	5.77001100	0.66933000	-0.21595000
C	3.79837200	-0.10569800	-0.60075100
C	1.96568600	-2.76832700	1.54959000
H	1.01931500	-2.59277000	1.03128500
C	3.68750100	0.61243600	-1.94444900
H	2.64379200	0.55091300	-2.27036500
C	0.72121000	0.85298400	1.98619600
H	1.43528800	0.04839700	2.13168500
C	0.58425700	2.16870100	-0.30941400
H	1.27480500	1.85302200	-1.09166600

SCF Energy (M06, n-octanol):	-1731.691230
SCF Energy (B3LYP, gas-phase):	-1731.359576
Enthalpy Correction:	0.789790
Free-Energy Correction:	0.682336

S56

H	1.92098000	-3.74384700	0.17948800
C	3.65438000	-2.69828300	-0.62211900
H	3.80841200	-3.44107100	-1.41615000
C	4.55841900	-3.03080700	0.58274200
H	4.34600600	-4.04656300	0.94616000
H	5.61328300	-3.01484500	0.27788500
C	4.32194000	-1.99941700	1.70609200
H	4.96592800	-2.23358300	2.56388500
C	2.84436400	-2.05822700	2.16130800
H	2.66379700	-1.35037600	2.98100800
H	2.61267600	-3.06538400	2.53901600
C	4.65389300	-0.59064900	1.17157500
H	4.52388800	0.16223900	1.95960600
H	5.70723700	-0.54986800	0.86087200
C	3.73800300	-0.25028900	-0.03528200
H	3.97554200	0.75385600	-0.38636000
C	2.29007600	-0.29075200	0.46923200
H	2.17786700	0.42813200	1.30579100
C	3.97339900	-1.28631000	-1.15201000
H	3.34435300	-1.05355500	-2.02127400
H	5.01731800	-1.23766900	-1.49024600
C	-2.78902200	-0.88685600	0.11681300
C	-3.08536800	-1.55115300	-1.10310500
C	-4.27833800	-1.22152600	-1.75826300
H	-4.51979400	-1.70117000	-2.70121300
C	-5.17240100	-0.30152500	-1.21812400
C	-4.89858100	0.29017700	0.00968800
H	-5.61779000	0.98105000	0.43874800
C	-3.71522800	0.00754500	0.70550300
C	-2.20758700	-2.67046600	-1.66919800
H	-1.18510400	-2.51523900	-1.31303200
C	-3.51088500	0.61037100	2.09463500
H	-2.45477500	0.49077800	2.36069700
C	-0.35021100	0.49954700	-2.18577500
H	-1.00530200	-0.34312100	-2.38368200
C	-0.67281800	2.03347100	-0.04052500
H	-1.41299100	1.67236200	0.67063900
C	-1.11711500	1.73300000	-1.54003200
H	-2.15202700	1.39523200	-1.43645500
C	-1.03558800	2.95710900	-2.46254800
H	-1.48677400	2.71572700	-3.43144100
H	-1.57591500	3.81006900	-2.03683200
H	0.00418200	3.24639400	-2.63502800
H	0.23937100	0.79309400	-3.05880600
C	-0.18450900	3.37260000	0.31750600
H	0.40467000	3.91867700	-0.41270700
C	-0.40996600	3.94438800	1.51410800
H	-0.99608200	3.39990600	2.25683200
C	0.11611900	5.28329600	1.93539700
H	0.77301300	5.18725500	2.81107500
H	0.69283900	5.75748500	1.13527400
H	-0.69816400	5.96169900	2.22674200
C	-4.35636500	-0.15149100	3.14039100
H	-4.16605600	0.23976700	4.14694500
H	-5.42613100	-0.03391600	2.93105100
H	-4.13941400	-1.22468800	3.14508200
C	-3.84145400	2.11391500	2.16761400
H	-4.91237400	2.30056100	2.03065400
H	-3.57079600	2.50537900	3.15509400
H	-3.29936600	2.69284600	1.41436500
C	-2.68738800	-4.04399200	-1.14656700
H	-2.67930600	-4.09943300	-0.05365200
H	-3.71217600	-4.24610900	-1.47987100

H	-2.04374200	-4.84495200	-1.52939300
C	-2.15709300	-2.71583100	-3.20881400
H	-1.39521800	-3.43501600	-3.52964900
H	-3.10995400	-3.04472900	-3.63941500
H	-1.90802500	-1.74490900	-3.64716500
H	-6.09152400	-0.06155200	-1.74596100
N	2.65061800	2.89296700	-1.06135000
O	3.12419800	3.79980900	-1.74619800

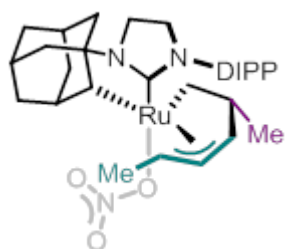


16c

SCF Energy (M06, n-octanol):	-1731.687893
SCF Energy (B3LYP, gas-phase):	-1731.362112
Enthalpy Correction:	0.789682
Free-Energy Correction:	0.682226

Ru	0.68770100	0.64202400	-0.50640600
O	1.76443700	2.58033500	0.99187300
O	1.82160400	2.38387100	-1.18140500
N	0.77716100	-2.11279300	0.33470200
N	-1.37144600	-1.75780500	0.10483400
C	-0.13850200	-1.15291500	0.05533300
C	0.22760200	-3.46771000	0.37218000
H	0.63421900	-4.04818000	1.20483400
H	0.44917900	-4.00451400	-0.56106600
C	-1.26964300	-3.17602400	0.52504300
H	-1.89739300	-3.81387300	-0.10174900
H	-1.60402800	-3.28257700	1.56514300
C	2.19861900	-1.77745600	0.24186200
C	2.76591000	-2.08152100	-1.17083900
H	2.15283300	-1.57187300	-1.92435400
H	2.70264400	-3.16117100	-1.37058800
C	4.23087600	-1.60848200	-1.25922500
H	4.62016000	-1.82961600	-2.26181200
C	5.06922000	-2.35461700	-0.20096100
H	5.05399600	-3.43641200	-0.39713800
H	6.11821900	-2.03445500	-0.25794100
C	4.50609100	-2.05873400	1.20495600
H	5.09981000	-2.58991900	1.96064800
C	3.04272600	-2.54784300	1.28514500
H	2.63151900	-2.37603600	2.28878500
H	3.00400200	-3.63065100	1.09321800
C	4.56439300	-0.54029800	1.46567700
H	4.19142800	-0.31114800	2.47285000
H	5.60692100	-0.19528300	1.42414700
C	3.71925000	0.21557200	0.40419000
H	3.77961300	1.28484500	0.61350700
C	2.26683300	-0.26772500	0.54605800
H	1.92789800	-0.10007100	1.57913400
C	4.28622800	-0.09018900	-0.99728400
H	3.71655500	0.45534800	-1.75860400
H	5.32493300	0.26160100	-1.06244100
C	-2.63433000	-1.10324500	0.32517500
C	-3.61055600	-1.13116600	-0.69800600

C	-4.83453900	-0.49281200	-0.45878700
H	-5.59644300	-0.49167600	-1.23285400
C	-5.09663800	0.13140800	0.75743100
C	-4.14678600	0.09667200	1.77469800
H	-4.37424800	0.55499500	2.73318900
C	-2.90769200	-0.53073500	1.59178000
C	-3.40195000	-1.90240100	-2.00024200
H	-2.33742400	-2.14900500	-2.06973100
C	-1.94031000	-0.62231900	2.77350000
H	-1.02555700	-1.11532900	2.43438300
C	0.02624400	0.38802300	-2.36585700
C	-1.02827600	1.80688900	-0.36976100
C	-1.05414000	1.46678200	-1.91979700
H	-0.42750100	-0.54830600	-2.69817700
H	0.71615900	0.79256000	-3.11374900
H	-2.01760200	0.96327100	-2.03207600
H	-1.83380000	1.29793200	0.15228600
C	-0.93765700	3.21560800	0.03250800
H	-0.21236900	3.85137100	-0.46704700
C	-1.72768000	3.76274100	0.97424400
H	-2.47275100	3.13454400	1.46447800
C	-1.66050200	5.19156300	1.42296400
H	-2.62497300	5.70068500	1.28661800
H	-1.42195700	5.25530800	2.49393100
H	-0.89505300	5.75001900	0.87472800
H	-6.05017700	0.62674900	0.92022600
C	-2.54384200	-1.49048700	3.89851100
H	-3.43799100	-1.02329100	4.32768400
H	-2.83386300	-2.48345100	3.53544100
H	-1.81672700	-1.62223300	4.70842400
C	-1.51951500	0.75415900	3.32222700
H	-2.38063300	1.32185500	3.69495400
H	-0.82519300	0.62413900	4.16068300
H	-1.01599500	1.35591000	2.56097500
C	-4.19719400	-3.22683900	-1.96767400
H	-5.27581600	-3.03306500	-1.92868900
H	-3.99461600	-3.81996700	-2.86741100
H	-3.94329600	-3.83624400	-1.09337000
C	-3.77677000	-1.10515900	-3.26322500
H	-3.22082300	-0.16542500	-3.33362000
H	-3.55070000	-1.69674400	-4.15791900
H	-4.84595800	-0.86606000	-3.29338500
N	2.14740200	3.05257300	-0.11022800
O	2.78880600	4.09168500	-0.21715200
C	-0.98283900	2.70189900	-2.82711400
H	-1.15324400	2.40466500	-3.86823200
H	-1.74275600	3.44107500	-2.55090400
H	0.00159100	3.17385900	-2.76549600



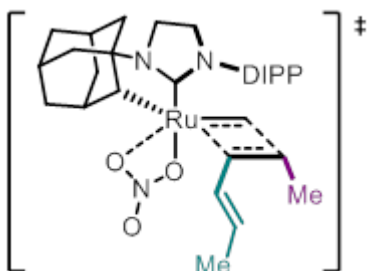
16d

SCF Energy (M06, n-octanol):	-1731.697313
SCF Energy (B3LYP, gas-phase):	-1731.374154
Enthalpy Correction:	0.790833
Free-Energy Correction:	0.685616

O	0.92663900	2.39242800	1.32509800
O	1.69274000	2.82068300	-0.66543900

N	0.75949500	-1.79689400	0.70644900
N	-1.39491300	-1.44199300	0.50025400
C	-0.15062600	-0.88570700	0.27361300
C	0.18384200	-3.09587300	1.05063000
H	0.62319600	-3.50427500	1.96508500
H	0.34829600	-3.81772000	0.23862900
C	-1.29390000	-2.73869600	1.20907000
H	-1.96453900	-3.47865400	0.76602900
H	-1.57323800	-2.61108900	2.26205100
C	2.19033800	-1.56006400	0.53115200
C	2.76928900	-2.40727400	-0.63064000
H	2.17660000	-2.26225900	-1.53854200
H	2.69976400	-3.47481200	-0.37468000
C	4.24734200	-2.03299900	-0.86719800
H	4.63983200	-2.62717100	-1.70328900
C	5.05189900	-2.34245900	0.41154200
H	5.00085500	-3.41612800	0.64313300
H	6.11169400	-2.09815400	0.25860400
C	4.48311100	-1.51448300	1.58192300
H	5.04973000	-1.73102900	2.49729700
C	3.00266600	-1.90930200	1.80845000
H	2.58299000	-1.36908700	2.66664800
H	2.94481400	-2.98498200	2.03417000
C	4.60271600	-0.01129500	1.24038000
H	4.25161700	0.60118500	2.08080200
H	5.65983000	0.24321900	1.07771500
C	3.77191100	0.30535800	-0.03569600
H	3.85362200	1.37186000	-0.27061400
C	2.30940700	-0.04719600	0.30839300
H	2.11971500	0.41241800	1.29106800
C	4.35886500	-0.52910100	-1.19377300
H	3.85785700	-0.29883300	-2.13764700
H	5.41681100	-0.26384300	-1.33037800
C	-2.66562100	-0.76946500	0.59634000
C	-3.65893400	-1.04523800	-0.37629300
C	-4.90348200	-0.41587300	-0.25215200
H	-5.67324800	-0.60568100	-0.99434100
C	-5.17450900	0.44268000	0.80880900
C	-4.20860800	0.65892000	1.78638400
H	-4.44134800	1.30052400	2.63114900
C	-2.94752800	0.05015400	1.71728600
C	-3.44119900	-2.04636800	-1.51108500
H	-2.37075900	-2.27508100	-1.55035700
C	-1.98306400	0.23011100	2.89045100
H	-1.01841400	-0.20794900	2.61923200
H	-6.14467100	0.92658000	0.88468300
C	-2.51142100	-0.52301600	4.13221000
H	-3.45254200	-0.08603600	4.48679100
H	-2.70121300	-1.58209600	3.92305100
H	-1.78518100	-0.46191300	4.95113000
C	-1.71867300	1.70567300	3.24242200
H	-2.63749600	2.22481600	3.53987300
H	-1.02110700	1.76533300	4.08550500
H	-1.26341000	2.24153500	2.40729600
C	-4.19747200	-3.36256700	-1.22449200
H	-5.28097200	-3.19487900	-1.21145000
H	-3.98253100	-4.10650100	-2.00084800
H	-3.92139700	-3.79210000	-0.25546700
C	-3.85516200	-1.50523300	-2.89383600
H	-3.35406100	-0.56232100	-3.13235700
H	-3.59616200	-2.23290300	-3.67170700
H	-4.93602800	-1.33474500	-2.95574000
N	1.57759300	3.19477700	0.56060200

O	2.05311500	4.24062300	0.96514700
Ru	0.55924800	0.88136100	-0.46815400
C	1.25194700	0.25632300	-2.40917300
H	1.89337800	-0.61641700	-2.43471300
H	1.81252900	1.14397700	-2.72697000
C	-0.07046000	0.07077800	-3.14783200
C	-0.93812000	0.63702000	-2.04420500
H	-0.29257000	-1.00141900	-3.22885100
C	-0.99991200	2.04810100	-1.79321500
H	-1.76354100	0.04157500	-1.67657200
C	-1.57631800	2.54462900	-0.64987200
H	-2.22282600	1.89675500	-0.06479700
C	-1.51137100	3.98453500	-0.23943800
H	-1.17440700	4.08500300	0.79876600
H	-0.83113400	4.55744100	-0.87679800
H	-2.50841200	4.44417000	-0.29545600
H	-0.41645800	2.72510400	-2.41464700
C	-0.19161900	0.69829300	-4.54117000
H	0.51558200	0.22642800	-5.23429100
H	-1.20215500	0.57669400	-4.95254000
H	0.03700700	1.77027800	-4.52036100



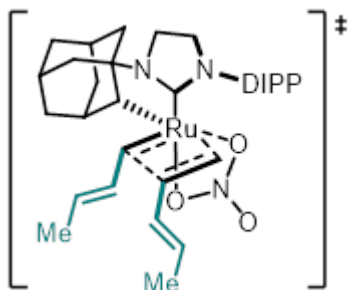
17-TS

SCF Energy (M06, n-octanol):	-1731.669122
SCF Energy (B3LYP, gas-phase):	-1731.347965
Enthalpy Correction:	0.787243
Free-Energy Correction:	0.680175

Ru	0.62018500	0.65453100	-0.50130800
O	1.60802300	2.60252800	-0.96692300
O	1.01951700	2.34092800	1.11031100
N	0.96031500	-1.97846800	0.64859600
N	-1.20966700	-1.79433400	0.40225400
C	-0.01829000	-1.12891300	0.24065000
C	0.48670400	-3.33614500	0.91689000
H	0.94309100	-3.75365500	1.81870200
H	0.71792900	-4.00371600	0.07457000
C	-1.02022500	-3.10415400	1.06607500
H	-1.62496900	-3.87738800	0.58631800
H	-1.32215600	-3.03741100	2.11935800
C	2.35916800	-1.61534000	0.39938000
C	2.84254700	-2.17584700	-0.96096900
H	2.14989000	-1.86334900	-1.74928400
H	2.83947100	-3.27550400	-0.93290500
C	4.26321900	-1.66007500	-1.26235200
H	4.59200500	-2.05188800	-2.23445800
C	5.22021600	-2.14832600	-0.15614000
H	5.25309900	-3.24739700	-0.14204100
H	6.24247200	-1.80044000	-0.35732700
C	4.74228600	-1.60916900	1.20772200
H	5.41702300	-1.95937100	2.00026100
C	3.31537700	-2.13640000	1.49965400
H	2.96942900	-1.78850100	2.48194700
H	3.32960000	-3.23678900	1.52517400
C	4.74648200	-0.06543300	1.16392200
H	4.45028000	0.34594300	2.13796700

H	5.76607200	0.29309300	0.96188800
C	3.77231700	0.43275700	0.06335000
H	3.78487000	1.52680300	0.03689200
C	2.36733800	-0.07565100	0.43292400
H	2.16421800	0.21933100	1.47199500
C	4.23892000	-0.11744600	-1.29949500
H	3.56853000	0.23102300	-2.09467400
H	5.24209000	0.26586100	-1.53246200
C	-2.52230800	-1.21018500	0.43738500
C	-3.42633500	-1.49817400	-0.61348400
C	-4.70527800	-0.93010000	-0.55824300
H	-5.41394300	-1.12975800	-1.35686900
C	-5.08911400	-0.12207500	0.50838600
C	-4.20691000	0.10396100	1.56096000
H	-4.52848100	0.70617600	2.40596800
C	-2.91671700	-0.44310900	1.56065400
C	-3.07807700	-2.46823800	-1.74237000
H	-1.99723500	-2.63981500	-1.70637600
C	-2.03065900	-0.26085400	2.79425600
H	-1.04769300	-0.68834000	2.57920700
C	0.45412100	0.01851900	-2.26846500
H	-0.01450800	-0.89989100	-2.64433200
C	-1.36620100	1.88159100	-0.77605500
H	-1.96486300	1.40912500	-0.00473900
C	-1.28134300	1.19317000	-2.02258200
H	-1.89641300	0.30143400	-2.06398200
C	-1.17901800	1.97107300	-3.32622800
H	-1.10442400	1.30008800	-4.18693000
H	-2.07681200	2.59061100	-3.45547500
H	-0.31083300	2.63569500	-3.33840000
H	0.96626200	0.57401900	-3.06457700
N	1.56368700	3.08966500	0.22816600
O	2.01233600	4.19539100	0.48589800
C	-3.41792200	-1.93924400	-3.14871500
H	-3.09618200	-2.66328900	-3.90634600
H	-4.49561100	-1.78904700	-3.27988700
H	-2.92095700	-0.98830400	-3.36406300
C	-3.78310500	-3.82454300	-1.51838100
H	-3.47328300	-4.55075400	-2.27937000
H	-3.55599000	-4.24567900	-0.53311800
H	-4.87201600	-3.71325000	-1.58369300
C	-2.62587400	-1.03236000	3.99305800
H	-3.59403600	-0.61394800	4.29266100
H	-2.78424400	-2.09163100	3.75928200
H	-1.95380300	-0.97028200	4.85692100
C	-1.79572700	1.21383000	3.17127100
H	-1.26311900	1.75310700	2.38384200
H	-2.73765700	1.73537300	3.38083300
H	-1.18236600	1.27045500	4.07800300
H	-6.08420000	0.31434300	0.52933800
C	-1.23699100	3.33248100	-0.67683500
H	-0.71418900	3.85072100	-1.47663300
C	-1.71582800	4.05750700	0.34983100
H	-2.22440200	3.54182200	1.16467000
C	-1.57985800	5.54324800	0.48390300
H	-0.98352000	5.79715800	1.37086500
H	-1.08517100	5.98328500	-0.38794300
H	-2.55823300	6.02759900	0.60964500

Diene Homodimerization

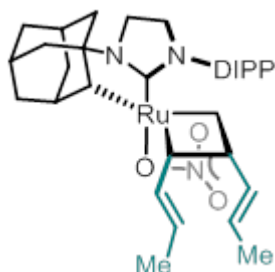


18-TS

SCF Energy (M06, n-octanol):	-1809.032243
SCF Energy (B3LYP, gas-phase):	-1808.752596
Enthalpy Correction:	0.823264
Free-Energy Correction:	0.710459

Ru	0.51751000	0.73213600	-0.33376200
O	1.83017000	0.75681400	-2.42321700
O	1.34455300	2.55614200	-1.30238800
N	1.05589800	-1.67406400	1.19900600
N	-1.09197100	-1.79158800	0.77535500
C	0.04057200	-1.04801000	0.54837500
C	0.69227300	-2.98217900	1.74895600
H	1.07714600	-3.11089700	2.76415900
H	1.09315000	-3.79344600	1.12577800
C	-0.83727300	-2.91612900	1.70555700
H	-1.29956500	-3.83475100	1.33634100
H	-1.26195800	-2.69165800	2.69185600
C	2.43952000	-1.26074100	0.94919100
C	3.06762400	-2.12114600	-0.17913500
H	2.44043400	-2.04898700	-1.07620300
H	3.09456000	-3.17732300	0.12622200
C	4.49579300	-1.62814300	-0.48775900
H	4.92958000	-2.25846300	-1.27535300
C	5.35988700	-1.72010800	0.78560600
H	5.43508900	-2.76337600	1.12527400
H	6.38158800	-1.37974000	0.56976700
C	4.73529400	-0.84492900	1.89162000
H	5.35175900	-0.89863400	2.79890100
C	3.32058200	-1.37865900	2.21637900
H	2.86404400	-0.80187200	3.03187300
H	3.39241400	-2.42400500	2.55292000
C	4.65691100	0.61839400	1.40249800
H	4.24673700	1.26120900	2.19344700
H	5.66826800	0.98840900	1.18201400
C	3.77098100	0.70347800	0.12778200
H	3.71838600	1.74655800	-0.20343000
C	2.36871600	0.21145800	0.52811700
H	2.06784300	0.79272400	1.42123100
C	4.42144500	-0.16716500	-0.96869500
H	3.84590200	-0.10023600	-1.89480300
H	5.43261400	0.20749200	-1.18067400
C	-2.35174800	-1.75892900	0.08214800
C	-2.45153100	-2.38223100	-1.18848000
C	-3.69672200	-2.37778900	-1.82918100
H	-3.79305300	-2.83797600	-2.80809600
C	-4.81673100	-1.80815900	-1.23024100
C	-4.71502200	-1.25415800	0.04160900
H	-5.60157300	-0.84427600	0.51650000
C	-3.49300500	-1.22661500	0.72718900
C	-1.28265600	-3.12623700	-1.83706300
H	-0.36946900	-2.86046600	-1.29790400

C	-3.45503200	-0.70567800	2.16268900
H	-2.40390400	-0.59176900	2.44789000
C	-0.99606900	0.73749000	-1.80207700
H	-1.46448600	-0.22713500	-1.94932600
C	-0.66482300	1.66033700	0.87953100
H	-1.37566000	1.14280400	1.52761200
C	-1.66445300	1.65196000	-0.87930900
H	-2.54421800	1.22608400	-0.40091800
H	-0.59593100	1.17636200	-2.71417600
C	-0.36707100	3.01978400	1.31862600
H	0.28932300	3.61971700	0.69030300
C	-0.80648000	3.52854200	2.48636600
H	-1.46860200	2.92168000	3.10720700
C	-0.44420400	4.88007400	3.02616800
H	0.06777100	4.79882000	3.99529800
H	0.21291400	5.42363300	2.33958700
H	-1.34123500	5.49127800	3.19856400
C	-4.09727300	-1.73106800	3.12327900
H	-4.01159500	-1.39141700	4.16241000
H	-5.16269600	-1.86129400	2.89932300
H	-3.62276000	-2.71523000	3.04613800
C	-4.13450700	0.66608800	2.33700700
H	-5.21026100	0.61610000	2.13399100
H	-4.01535900	1.01314900	3.37015600
H	-3.70301200	1.42456700	1.67648200
C	-1.48493200	-4.65184600	-1.69981100
H	-1.62062700	-4.95640800	-0.65578500
H	-2.37121700	-4.98094000	-2.25532500
H	-0.61822400	-5.19044400	-2.10087200
C	-1.05106900	-2.76120600	-3.31588800
H	-0.17864700	-3.30457100	-3.69625800
H	-1.90511700	-3.03550100	-3.94584600
H	-0.85887000	-1.69301400	-3.44771600
H	-5.77278300	-1.81434400	-1.74686600
C	-1.80026400	3.07081800	-1.27677700
H	-0.95721700	3.49440800	-1.82001400
C	-2.88155900	3.81942500	-1.02496200
H	-3.71428900	3.37801500	-0.47317100
C	-3.05641800	5.24627500	-1.45821600
H	-3.93292100	5.36279000	-2.11060000
H	-3.21883900	5.90657300	-0.59492100
H	-2.17830500	5.60983700	-2.00223600
N	1.94153100	2.01920300	-2.31995000
O	2.56649200	2.70193600	-3.11722800



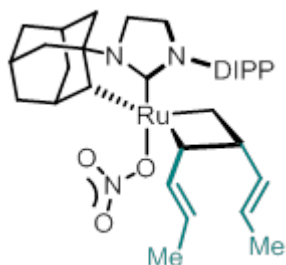
19a

SCF Energy (M06, n-octanol):	-1809.041065
SCF Energy (B3LYP, gas-phase):	-1808.758160
Enthalpy Correction:	0.824779
Free-Energy Correction:	0.710981

Ru	0.55200400	0.73982300	-0.27040500
O	1.91898300	1.07530100	-2.48933700
O	1.33111900	2.64016200	-1.08557700
N	1.06112300	-1.75903400	1.10372600

N	-1.09368200	-1.82350700	0.70657000
C	0.04095700	-1.07973600	0.51152800
C	0.68918800	-3.09475000	1.57696700
H	1.08656100	-3.29153100	2.57650400
H	1.06944500	-3.87040300	0.89831900
C	-0.84023300	-3.00769100	1.56001100
H	-1.31885300	-3.89571700	1.14057800
H	-1.24806600	-2.84081000	2.56427400
C	2.44232500	-1.35785800	0.83329100
C	3.03911000	-2.19162200	-0.33244300
H	2.39278000	-2.08777600	-1.21291900
H	3.06033300	-3.25544700	-0.05678000
C	4.46522900	-1.70377600	-0.65745500
H	4.87593300	-2.31727400	-1.46998100
C	5.35465200	-1.83689600	0.59495300
H	5.42762600	-2.88933400	0.90490900
H	6.37453700	-1.49972200	0.36660000
C	4.76264600	-0.98685200	1.73810700
H	5.39761900	-1.07110400	2.62988400
C	3.34966500	-1.51161600	2.07890600
H	2.91553900	-0.94975700	2.91661000
H	3.41066900	-2.56583800	2.38696400
C	4.68507800	0.48937100	1.29345400
H	4.29247200	1.11229700	2.10872400
H	5.69205700	0.86308700	1.06205400
C	3.77964600	0.61673200	0.03478500
H	3.72620900	1.66843800	-0.26317600
C	2.38735200	0.12046600	0.44266800
H	2.05726000	0.71060100	1.33322400
C	4.39534200	-0.23066000	-1.09839700
H	3.79829700	-0.12473700	-2.00736000
H	5.40426700	0.14173600	-1.32296800
C	-2.37311200	-1.71470700	0.05610200
C	-2.51915700	-2.23502500	-1.25581800
C	-3.78206300	-2.16184800	-1.85604100
H	-3.91495600	-2.54225600	-2.86439200
C	-4.87422400	-1.62340200	-1.18176100
C	-4.72622500	-1.16895200	0.12430200
H	-5.59105500	-0.77965200	0.65334200
C	-3.48456000	-1.21249600	0.77325700
C	-1.38309900	-2.94304500	-1.99645000
H	-0.44619000	-2.71201800	-1.48258400
C	-3.39729500	-0.79058200	2.23899000
H	-2.33697900	-0.70402700	2.49913300
C	-0.90892800	0.85431400	-1.66170400
H	-1.47606800	-0.03130800	-1.92904900
C	-0.82262800	1.67911700	0.86076600
H	-1.38070700	1.07286800	1.57424900
C	-1.61266700	1.72276300	-0.56383300
H	-2.55691300	1.22021600	-0.33753800
H	-0.60245700	1.42491700	-2.53879300
C	-4.02240600	-1.87110500	3.14912800
H	-3.90468300	-1.59972100	4.20503700
H	-5.09498400	-1.97687900	2.94764600
H	-3.56152400	-2.85284200	2.99582400
C	-4.05706700	0.57262900	2.52293300
H	-5.14191200	0.53662000	2.37245800
H	-3.88444900	0.86053300	3.56650200
H	-3.65474300	1.36495800	1.88473100
C	-1.58792800	-4.47349700	-1.94120600
H	-1.67519000	-4.84009100	-0.91213500
H	-2.50239800	-4.76485000	-2.47154100
H	-0.74529900	-4.99043400	-2.41541600

C	-1.21473900	-2.49264600	-3.46021700
H	-0.35375500	-3.00406000	-3.90555600
H	-2.09077700	-2.74125200	-4.07026300
H	-1.03861900	-1.41648400	-3.53862200
H	-5.84460000	-1.57535100	-1.66865300
N	1.92930000	2.30239300	-2.19296500
O	2.46504300	3.15920900	-2.88338300
C	-1.85910600	3.12481500	-1.05334900
H	-0.98033300	3.67018700	-1.39384500
C	-3.06718200	3.69178500	-1.10870100
H	-3.93557700	3.12207400	-0.76985600
C	-3.34270700	5.08147800	-1.61045700
H	-3.81038000	5.70078200	-0.83246300
H	-2.42225400	5.58027100	-1.93193400
H	-4.03724700	5.06913200	-2.46174900
C	-0.37998100	2.95486300	1.45683400
H	0.10819700	3.67179000	0.79986900
C	-0.49761500	3.24254700	2.76434700
H	-0.98688100	2.51930400	3.42075600
C	-0.00599000	4.50225500	3.41637000
H	-0.82759900	5.05037800	3.89870600
H	0.72835400	4.28489700	4.20492400
H	0.46713600	5.17079100	2.68942400



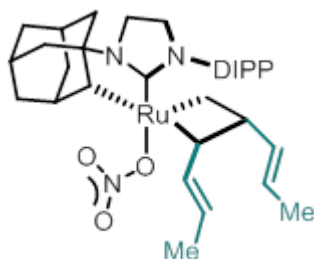
19b

SCF Energy (M06, n-octanol):	-1809.045689
SCF Energy (B3LYP, gas-phase):	-1808.754534
Enthalpy Correction:	0.825099
Free-Energy Correction:	0.711503

Ru	0.64175300	0.65756400	-0.32618200
O	2.34637400	3.12095900	0.61112000
O	1.36474000	2.48247600	-1.25331600
N	1.10980600	-1.84133700	1.06950500
N	-1.06220700	-1.84014000	0.76245000
C	0.08896300	-1.14225300	0.49734900
C	0.70516600	-3.15631500	1.57324300
H	1.17624100	-3.38323700	2.53313100
H	0.97109500	-3.94997200	0.86011900
C	-0.80828900	-2.96750300	1.69091000
H	-1.38549600	-3.84856000	1.40446500
H	-1.09452200	-2.68398000	2.71126200
C	2.47412400	-1.51454600	0.64706400
C	2.83762700	-2.30765100	-0.63787900
H	2.07011200	-2.11824400	-1.39950600
H	2.83470800	-3.38607100	-0.42507100
C	4.22046300	-1.87483400	-1.15758900
H	4.46475400	-2.45272400	-2.05885800
C	5.27738700	-2.14287700	-0.06618700
H	5.32746700	-3.21841600	0.15621400
H	6.27171700	-1.84404400	-0.42388200
C	4.91806300	-1.34822200	1.20673400
H	5.67075300	-1.53568100	1.98366700
C	3.53611600	-1.80782400	1.73088600
H	3.27564800	-1.27449000	2.65452300
H	3.56792000	-2.88166000	1.96878900

C	4.88445000	0.15631200	0.86435300
H	4.66319900	0.75326300	1.75829000
H	5.87187900	0.47579900	0.50289200
C	3.81242700	0.42950500	-0.22596100
H	3.78631900	1.49809900	-0.44068800
C	2.46290500	-0.01022200	0.35611700
H	2.28407700	0.54401700	1.30078800
C	4.17100000	-0.37125300	-1.49280800
H	3.43263900	-0.18229400	-2.28333200
H	5.14415700	-0.03849900	-1.87859700
C	-2.36017500	-1.70409600	0.15397500
C	-2.56258000	-2.21987200	-1.15406300
C	-3.84006100	-2.10540800	-1.71555600
H	-4.01653300	-2.47534400	-2.72025800
C	-4.89599900	-1.53872800	-1.00717200
C	-4.69562600	-1.09355100	0.29427900
H	-5.53231300	-0.68090900	0.84969400
C	-3.43600900	-1.17205200	0.90431700
C	-1.47143000	-2.96935200	-1.92328600
H	-0.50002900	-2.60784100	-1.57433600
C	-3.29613200	-0.75278500	2.36713400
H	-2.22748700	-0.66384600	2.59072600
C	-0.56588400	0.62351500	-1.91033600
H	-1.07249900	-0.28457900	-2.22270700
C	-0.94218000	1.61098000	0.53481100
H	-1.51136900	0.95508700	1.19020500
C	-1.48295200	1.52602200	-0.96967100
H	-2.42254000	0.97510200	-0.87356400
H	-0.15507700	1.19123500	-2.74946800
C	-3.88699100	-1.83696300	3.29614500
H	-3.73553400	-1.56600400	4.34782500
H	-4.96529800	-1.94434900	3.12926000
H	-3.42942800	-2.81750000	3.12724000
C	-3.94901000	0.60764300	2.67979500
H	-5.03943700	0.56645800	2.58051300
H	-3.73070300	0.89505700	3.71490000
H	-3.58017100	1.40220200	2.02459400
C	-1.54770200	-4.48428500	-1.62661400
H	-1.44850600	-4.70504100	-0.55922100
H	-2.50783100	-4.89509700	-1.96073400
H	-0.74969600	-5.01817800	-2.15627200
C	-1.51531400	-2.75703700	-3.44891000
H	-0.62227500	-3.19821000	-3.90558500
H	-2.38364400	-3.24576100	-3.90584800
H	-1.54269200	-1.69788500	-3.72206500
H	-5.87849700	-1.46098600	-1.46501800
N	1.95392100	3.41027400	-0.53416800
O	2.07210300	4.52754800	-1.03858500
C	-1.71444300	2.87113800	-1.60752200
H	-0.82109200	3.44933300	-1.83618200
C	-2.92602700	3.33747700	-1.92160100
H	-3.80468700	2.73016600	-1.69114400
C	-3.19087800	4.65937000	-2.58590800
H	-3.71543600	4.52744800	-3.54245400
H	-3.83164700	5.29789800	-1.96219000
H	-2.25990800	5.20158800	-2.78163000
C	-0.71841200	2.93017000	1.14297500
H	-0.36397400	3.73652600	0.50836800
C	-0.91711200	3.17886300	2.44947200
H	-1.27525100	2.37143900	3.09138700
C	-0.65839600	4.49478300	3.11913400
H	0.10176700	4.39176900	3.90594600
H	-0.30246500	5.24404200	2.40537200

H	-1.56447100	4.88175100	3.60639800
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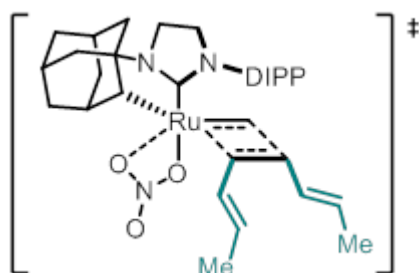


19c

SCF Energy (M06, n-octanol):	-1809.042001
SCF Energy (B3LYP, gas-phase):	-1808.756902
Enthalpy Correction:	0.825033
Free-Energy Correction:	0.711698

Ru	0.66333300	0.67091500	-0.19388900
O	1.52521000	2.15555200	1.79186200
O	1.49659200	2.69298900	-0.32126900
N	1.19761900	-2.16008400	-0.24118000
N	-0.99139100	-2.08909400	-0.26018900
C	0.13984300	-1.31396000	-0.17183700
C	0.83893600	-3.52877900	-0.61092600
H	1.39595300	-4.26758700	-0.02822900
H	1.03880700	-3.70902600	-1.67665400
C	-0.66165700	-3.53418100	-0.30074800
H	-1.25600400	-4.04811200	-1.05980500
H	-0.87808100	-3.99296900	0.67266300
C	2.54607600	-1.59275800	-0.29435600
C	3.01213700	-1.36420400	-1.75705900
H	2.26628700	-0.76136000	-2.28856100
H	3.08381100	-2.33080500	-2.27679500
C	4.38026200	-0.65280500	-1.76578400
H	4.69623800	-0.49362800	-2.80522900
C	5.41359200	-1.53712200	-1.03858900
H	5.53051900	-2.49573700	-1.56414100
H	6.39726700	-1.04869500	-1.04248100
C	4.95377600	-1.77644600	0.41454600
H	5.68553100	-2.40828800	0.93511800
C	3.58557700	-2.49600600	0.41171800
H	3.25603700	-2.70279500	1.43855500
H	3.67626300	-3.46213900	-0.10704200
C	4.82807200	-0.41921600	1.13539000
H	4.52909800	-0.56778400	2.18160300
H	5.80388400	0.08597000	1.15006200
C	3.78571500	0.47488500	0.40995900
H	3.72074100	1.42677900	0.94017400
C	2.43508800	-0.25759500	0.46796700
H	2.18240500	-0.47069900	1.51623400
C	4.24660900	0.70330200	-1.04398700
H	3.53133700	1.35069000	-1.56511500
H	5.21298200	1.22582500	-1.04958400
C	-2.30456400	-1.73558900	0.21119800
C	-3.36039800	-1.61783400	-0.72290400
C	-4.63044200	-1.27444800	-0.24148400
H	-5.45543800	-1.16658800	-0.93958500
C	-4.85723800	-1.07815700	1.11782100
C	-3.81965200	-1.25870800	2.02840000
H	-4.01515500	-1.13812300	3.09036800
C	-2.53062100	-1.60575200	1.60362200
C	-3.17344800	-1.93587700	-2.20554400
H	-2.09672800	-1.98959100	-2.39744400
C	-1.45303000	-1.88349300	2.65341200
H	-0.51378400	-2.09857300	2.13733100
C	-0.08570000	0.83599100	-2.02993300

C	-1.19153300	1.45576700	0.32262700
C	-1.25731900	1.60408000	-1.26268500
H	-0.45556300	-0.02429400	-2.59249200
H	0.48745600	1.51706600	-2.66724800
H	-2.17127000	1.05886500	-1.51121700
H	-1.88747800	0.69557400	0.66513600
C	-1.28454100	2.67613100	1.13117800
H	-0.70202700	3.54113400	0.82723600
C	-2.07417600	2.78056000	2.21495200
H	-2.67867000	1.92146100	2.50932400
C	-2.18970700	4.00325100	3.07451400
H	-3.22652900	4.36513500	3.11883700
H	-1.88950100	3.78550900	4.10912200
H	-1.55669300	4.81612900	2.70470000
H	-5.84834300	-0.80449400	1.46976900
C	-1.82086500	-3.13097700	3.48566700
H	-2.73255300	-2.96515000	4.07143500
H	-1.99259200	-4.00814300	2.85085300
H	-1.01359600	-3.37061400	4.18766800
C	-1.18089700	-0.68135600	3.57750000
H	-2.07444400	-0.39755200	4.14653500
H	-0.39961800	-0.93941300	4.30203500
H	-0.84033000	0.19251000	3.01566100
C	-3.78589400	-3.31592900	-2.53470000
H	-4.87339300	-3.30307600	-2.39481800
H	-3.58473400	-3.58792000	-3.57776400
H	-3.38348100	-4.10693900	-1.89230200
C	-3.76104600	-0.87217200	-3.15129000
H	-3.32982900	0.11761700	-2.97414400
H	-3.55434600	-1.14481200	-4.19270000
H	-4.84891900	-0.78885500	-3.04700900
N	1.78142700	3.01722000	0.90832600
O	2.26537400	4.11564700	1.15273900
C	-1.34090700	3.02879600	-1.74220800
H	-0.43860100	3.62501700	-1.61432700
C	-2.42118800	3.55602600	-2.32446300
H	-3.31432600	2.93828000	-2.44402800
C	-2.51841200	4.96326800	-2.84312900
H	-2.74409000	4.97824200	-3.91845500
H	-3.32635900	5.51661200	-2.34504900
H	-1.58449400	5.51310700	-2.68549500



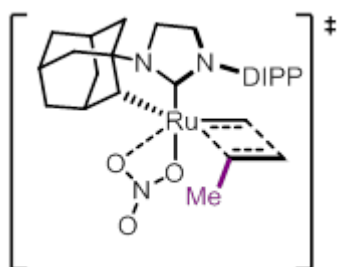
20-TS

SCF Energy (M06, n-octanol):	-1809.026229
SCF Energy (B3LYP, gas-phase):	-1808.746274
Enthalpy Correction:	0.823052
Free-Energy Correction:	0.711103

Ru	-0.61014300	0.69661300	0.12091100
O	-1.42459900	2.74746600	-0.14055000
O	-1.08402500	1.69034900	-2.00908500
N	-1.19639700	-2.12649200	0.29747400
N	0.99600000	-2.05994500	0.30177600
C	-0.13687700	-1.28472200	0.20503900
C	-0.83468600	-3.49413600	0.66617000
H	-1.39830500	-4.23328800	0.09011100
H	-1.02562200	-3.67250300	1.73394400
C	0.66308000	-3.50398500	0.34251000
H	1.26170900	-4.02223800	1.09483700
H	0.86867400	-3.96133300	-0.63405900
C	-2.55254600	-1.56914300	0.32853300
C	-3.05686800	-1.37431600	1.77988400
H	-2.32397700	-0.78843800	2.34412600
H	-3.15185900	-2.35189700	2.27528800
C	-4.42032900	-0.65416400	1.76329900
H	-4.76328000	-0.50770300	2.79639400
C	-5.43887700	-1.52279100	0.99755400
H	-5.57153400	-2.48860900	1.50616800
H	-6.42130700	-1.03158000	0.98378100
C	-4.94179200	-1.74102600	-0.44638500
H	-5.65986100	-2.36604300	-0.99388200
C	-3.57342300	-2.46469100	-0.41625300
H	-3.21708200	-2.65690100	-1.43691800
H	-3.68488000	-3.43890200	0.08359100
C	-4.80735500	-0.36938100	-1.14177400
H	-4.49087600	-0.49877300	-2.18529100
H	-5.78682700	0.12926800	-1.16361100
C	-3.77505000	0.50664300	-0.38348300
H	-3.69685800	1.47633300	-0.88416100
C	-2.42700800	-0.23256700	-0.42784500
H	-2.20946900	-0.47877000	-1.47716100
C	-4.26217100	0.71278000	1.06455800
H	-3.55038800	1.34199000	1.61228900
H	-5.22475800	1.24284100	1.06323800
C	2.30721500	-1.70411900	-0.17219000
C	3.36322600	-1.57931200	0.76199200
C	4.63636100	-1.24896600	0.28056700
H	5.46044100	-1.13837300	0.97918900
C	4.86660700	-1.06430100	-1.07973200
C	3.82734000	-1.23844100	-1.98907200
H	4.02346000	-1.12222900	-3.05130800
C	2.53516500	-1.57558700	-1.56448800
C	3.16803500	-1.85946100	2.25071200
H	2.09025600	-1.85977900	2.44594000
C	1.45859700	-1.84361400	-2.61684800
H	0.51155400	-2.03258000	-2.10479300
C	-0.38376100	0.83032700	1.99276500
H	0.07240500	0.11919200	2.69262400

C	1.47290400	1.63145500	-0.18843000
H	2.08190700	0.79484700	-0.51124800
C	1.32896800	1.76313300	1.23968200
H	1.93193400	1.05311700	1.79882200
H	-0.85064400	1.67730300	2.50819300
N	-1.49522400	2.74999200	-1.43254700
O	-1.92503200	3.71639200	-2.04355300
C	3.81132500	-0.80233500	3.16801200
H	3.54598100	-1.00251700	4.21256500
H	4.90522900	-0.81748300	3.10274600
H	3.48068400	0.21197600	2.92351400
C	3.71965800	-3.25595500	2.61563100
H	3.52039900	-3.48636400	3.66908400
H	3.27339700	-4.04738200	2.00410800
H	4.80462000	-3.29677800	2.46176000
C	1.80607800	-3.10768300	-3.43297000
H	2.72533700	-2.96652500	-4.01356600
H	1.95501800	-3.98207300	-2.78851500
H	0.99897000	-3.33745500	-4.13839800
C	1.22098300	-0.64534400	-3.55549900
H	0.90362800	0.24473700	-3.00609900
H	2.12215100	-0.39698800	-4.12947900
H	0.43164900	-0.88984800	-4.27578900
H	5.86019600	-0.80078100	-1.43248400
C	1.51191600	2.78735700	-1.08556000
H	0.93863800	3.66917900	-0.81114000
C	2.23619100	2.81608100	-2.21739800
H	2.81616500	1.93412600	-2.49215000
C	2.30768200	3.98223900	-3.15652400
H	1.95503800	3.70024100	-4.15827400
H	1.69244500	4.81789500	-2.80773000
H	3.34020600	4.33957700	-3.27601900
C	1.17164200	3.08698700	1.88397500
H	0.50484100	3.79267300	1.39311700
C	1.79853000	3.43792600	3.01490300
H	2.45116800	2.71216700	3.50502600
C	1.68396300	4.77913300	3.67914700
H	2.66246900	5.27326500	3.75228200
H	1.00888400	5.44289800	3.12895500
H	1.30460600	4.68286400	4.70599400

Alkene-First Pathway B



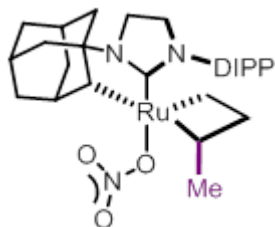
36-TS

SCF Energy (M06, n-octanol):	-1615.013610
SCF Energy (B3LYP, gas-phase):	-1614.634107
Enthalpy Correction:	0.721613
Free-Energy Correction:	0.623964

Ru	0.61699400	0.83955000	-0.63388500
O	1.87044700	2.57518200	-1.21720100
O	1.24257100	2.59584100	0.86606200
N	0.62189900	-1.75827000	0.63963700
N	-1.50979900	-1.31840400	0.38056900

C	-0.24453800	-0.81677200	0.18791400
C	-0.01558500	-3.03113500	0.97575300
H	0.39247600	-3.45988300	1.89506700
H	0.12217400	-3.76076400	0.16504200
C	-1.47865000	-2.60250400	1.11913200
H	-2.18227000	-3.31915400	0.68955900
H	-1.75480500	-2.43604300	2.16872500
C	2.06026100	-1.57156000	0.42335500
C	2.52298600	-2.25634200	-0.88676700
H	1.90042200	-1.90838600	-1.71791400
H	2.38780200	-3.34508700	-0.80591500
C	4.00517000	-1.92663700	-1.15156600
H	4.32024200	-2.40637700	-2.08803900
C	4.85681100	-2.46255300	0.01721000
H	4.76120400	-3.55583300	0.08611700
H	5.91930300	-2.24537400	-0.15788700
C	4.39654200	-1.79954900	1.33192200
H	4.99529600	-2.18400500	2.16841400
C	2.90816400	-2.14040400	1.58753400
H	2.56963500	-1.70196600	2.53550600
H	2.79213500	-3.23197900	1.66789900
C	4.58563600	-0.27198400	1.21352700
H	4.30307800	0.22236900	2.15235900
H	5.64716400	-0.04586800	1.03870800
C	3.71921100	0.27611300	0.04860500
H	3.86750100	1.35761000	-0.02923900
C	2.25032300	-0.04313700	0.37999600
H	2.04956100	0.32865000	1.39531500
C	4.16772000	-0.39632300	-1.26456500
H	3.57585500	-0.01172700	-2.10413300
H	5.21799800	-0.14793300	-1.47111400
C	-2.74184300	-0.57667000	0.39220000
C	-3.69606900	-0.82390400	-0.62433700
C	-4.90213700	-0.11326300	-0.58648300
H	-5.64629100	-0.28200200	-1.35956500
C	-5.16851400	0.80053300	0.42932700
C	-4.24034900	0.99529400	1.44758200
H	-4.46953100	1.68819500	2.25224200
C	-3.02026000	0.30561600	1.46447600
C	-3.48055400	-1.88456100	-1.70315400
H	-2.42578300	-2.17708400	-1.67151500
C	-2.08762800	0.48326800	2.66413500
H	-1.16712700	-0.07525600	2.47331000
C	0.46731700	0.13483000	-2.36854200
H	-0.09560200	-0.73321400	-2.73377600
C	-1.20704000	2.25994900	-0.93602900
H	-1.84870900	1.92796800	-0.12667800
C	-1.22540700	1.47984100	-2.10241600
H	-1.91029800	0.64472800	-2.15884400
H	1.03369500	0.63253600	-3.16820400
N	1.92715600	3.15027400	-0.06348500
O	2.59160800	4.15730600	0.11843700
C	-3.78276000	-1.38836800	-3.13033900
H	-3.54574800	-2.17488900	-3.85616900
H	-4.84141900	-1.13597700	-3.25868100
H	-3.19656300	-0.50233800	-3.39342400
C	-4.33157100	-3.13881200	-1.40381700
H	-4.12079800	-3.93060700	-2.13254400
H	-4.13646400	-3.53678200	-0.40213400
H	-5.40175800	-2.90656300	-1.46045800
C	-2.73662100	-0.10667700	3.93536700
H	-3.63932700	0.44909500	4.21505200
H	-3.02571100	-1.15502400	3.79674800

H	-2.03787400	-0.05342700	4.77832000
C	-1.67529500	1.94866600	2.90327700
H	-1.10048300	2.34922900	2.06431900
H	-2.54577600	2.59376500	3.07133500
H	-1.04026700	2.01432000	3.79415800
H	-6.10780900	1.34711400	0.43710200
H	-0.96578300	1.95493100	-3.04629200
C	-0.92254600	3.74152100	-0.97724300
H	-1.86036100	4.28024100	-1.17659000
H	-0.53587200	4.10527600	-0.02221600
H	-0.20930500	3.99863900	-1.76479000

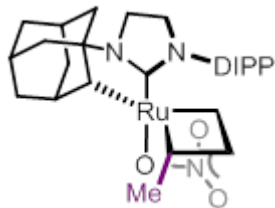


37a

SCF Energy (M06, n-octanol):	-1615.037139
SCF Energy (B3LYP, gas-phase):	-1614.650609
Enthalpy Correction:	0.724438
Free-Energy Correction:	0.626095

Ru	0.69815300	0.88115700	-0.43060500
O	2.14320300	2.72654900	1.04008100
O	2.00018800	2.47568600	-1.12864900
N	0.47054800	-1.85324300	0.47556100
N	-1.62053700	-1.27828200	0.18486200
C	-0.33203400	-0.81067000	0.14043000
C	-0.22602300	-3.13896900	0.54282100
H	0.10051000	-3.73264000	1.40097500
H	-0.04829700	-3.72659800	-0.36883200
C	-1.68337300	-2.68165900	0.65625800
H	-2.36949400	-3.26784200	0.03995200
H	-2.04308200	-2.71216400	1.69230600
C	1.91720100	-1.70048000	0.30935300
C	2.35791100	-2.10982400	-1.12205300
H	1.77064000	-1.54531700	-1.85748500
H	2.14740800	-3.17688300	-1.28399500
C	3.86207300	-1.83208500	-1.30981400
H	4.15929300	-2.12580700	-2.32518300
C	4.65874900	-2.65500000	-0.27650100
H	4.49264000	-3.72992100	-0.43740500
H	5.73503000	-2.47597900	-0.40087600
C	4.22282800	-2.25511300	1.14846000
H	4.78765400	-2.84049500	1.88595100
C	2.71556700	-2.54561700	1.32931900
H	2.39310000	-2.29351300	2.34830600
H	2.52454400	-3.61864900	1.17877400
C	4.49124000	-0.75121000	1.35697100
H	4.21454600	-0.44958400	2.37601300
H	5.56465500	-0.54488700	1.24356600
C	3.68699600	0.08153200	0.32207200
H	3.89417600	1.13837600	0.49442800
C	2.19499900	-0.20552900	0.55497600
H	1.92816300	0.04327500	1.59382800
C	4.12356800	-0.32681300	-1.09921900
H	3.57852800	0.26857900	-1.84168100
H	5.19145800	-0.10951400	-1.23702200
C	-2.83924700	-0.51407800	0.23665600
C	-3.68511900	-0.49665700	-0.89734200
C	-4.87775600	0.23458500	-0.81928700
H	-5.53903600	0.27143600	-1.68021300

C	-5.23801900	0.90485700	0.34594700
C	-4.42190200	0.82896300	1.47089600
H	-4.72740800	1.32946200	2.38536000
C	-3.21867800	0.11205700	1.44957400
C	-3.38208800	-1.30770700	-2.15601900
H	-2.34634700	-1.65489800	-2.08398900
C	-2.40745900	-0.01657500	2.74034000
H	-1.47114500	-0.53223700	2.50842900
C	-0.05401100	0.82653100	-2.27373400
C	-0.82218000	2.21001400	-0.12718800
C	-0.95636500	1.98493600	-1.67779800
H	-0.62945300	-0.02867200	-2.62917500
H	0.64644600	1.19779600	-3.02679500
H	-1.99896000	1.71412400	-1.86162000
H	-0.69631900	2.91875300	-2.18014900
H	-1.65819600	1.76859300	0.40809200
H	-6.16525900	1.47040200	0.38359000
C	-3.17468000	-0.87286600	3.77186800
H	-4.10225000	-0.37828700	4.08315600
H	-3.44633300	-1.85454800	3.36721200
H	-2.56303200	-1.03004100	4.66798400
C	-2.02640300	1.34166600	3.36001700
H	-2.91186300	1.92891700	3.62886600
H	-1.44650200	1.18272800	4.27646100
H	-1.41513500	1.93889000	2.67862000
C	-4.29472400	-2.55207400	-2.22512600
H	-5.34661800	-2.26038800	-2.32801700
H	-4.03236300	-3.17360400	-3.08948800
H	-4.21318900	-3.17004500	-1.32406100
C	-3.51114300	-0.49521500	-3.45819600
H	-2.86481900	0.38747600	-3.45463600
H	-3.22669900	-1.11621000	-4.31560400
H	-4.53995800	-0.15808200	-3.62844500
N	2.49281700	3.11557100	-0.10261900
O	3.26081500	4.05175300	-0.29533100
C	-0.58734500	3.64377500	0.30285600
H	-1.53322500	4.20211300	0.22152800
H	-0.25592400	3.69922600	1.34338900
H	0.15443200	4.15084900	-0.31818200



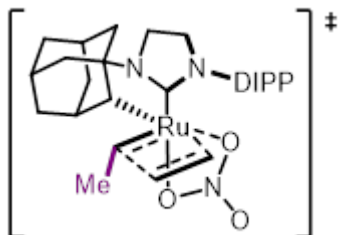
37b

SCF Energy (M06, n-octanol):	-1615.034796
SCF Energy (B3LYP, gas-phase):	-1614.650622
Enthalpy Correction:	0.723936
Free-Energy Correction:	0.625105

Ru	-0.60430700	1.12534700	-0.07794400
O	-2.15107300	1.67384600	1.99556400
O	-1.80214100	2.94312000	0.25407700
N	-0.48655700	-1.66816300	-0.83560500
N	1.60677000	-1.15385500	-0.43614400
C	0.32828600	-0.66077700	-0.41793700
C	0.19309700	-2.95711200	-0.98562100
H	-0.09927100	-3.45973700	-1.91161300
H	-0.04255200	-3.62372800	-0.14478800
C	1.66356200	-2.52620900	-0.99147400
H	2.30347600	-3.16481700	-0.37813800
H	2.07600000	-2.50280400	-2.00734000

C	-1.93406000	-1.53490300	-0.66191900
C	-2.39069700	-2.18042800	0.67412200
H	-1.82584600	-1.72797900	1.49886600
H	-2.16557300	-3.25631200	0.66519000
C	-3.90312700	-1.95978700	0.87967900
H	-4.20907000	-2.43829100	1.81919700
C	-4.67954100	-2.58285100	-0.29767200
H	-4.50467100	-3.66760000	-0.34258000
H	-5.75856100	-2.43936300	-0.15261300
C	-4.23204700	-1.91809400	-1.61570700
H	-4.78894900	-2.35084200	-2.45722500
C	-2.72388400	-2.17823500	-1.82779900
H	-2.38342000	-1.74834600	-2.77926400
H	-2.53789800	-3.26157500	-1.87196500
C	-4.50022300	-0.39895400	-1.54251700
H	-4.21316400	0.08293000	-2.48718100
H	-5.57465500	-0.21655600	-1.40378200
C	-3.70769700	0.22326800	-0.35730400
H	-3.89914000	1.30022400	-0.32173700
C	-2.22093500	-0.03171400	-0.63647400
H	-1.98207700	0.38895400	-1.64470000
C	-4.17864500	-0.44694000	0.95002200
H	-3.66577800	0.00371300	1.80309600
H	-5.25455500	-0.26792200	1.08275600
C	2.79359400	-0.61204400	0.17196300
C	2.98270200	-0.77794200	1.56827200
C	4.16448100	-0.28525100	2.13531800
H	4.32633600	-0.38923200	3.20398300
C	5.14251700	0.32513100	1.35520100
C	4.96555400	0.42997100	-0.02032200
H	5.74816100	0.87866100	-0.62506000
C	3.80136000	-0.04280800	-0.64137200
C	1.99391700	-1.54097900	2.45207800
H	1.05394100	-1.64104700	1.90281400
C	3.69987100	0.00196100	-2.16477500
H	2.66220100	-0.21829800	-2.43696900
C	0.71175500	1.87834300	1.26447700
H	1.45406200	1.22505400	1.70983400
C	0.59056500	2.07131600	-1.37551700
H	1.31643200	1.46108700	-1.91337400
C	1.21619500	2.62139300	-0.00949800
H	2.29748300	2.47217000	-0.07885800
H	0.23542100	2.52874300	1.99702200
C	4.59649600	-1.08533800	-2.79758300
H	4.48027400	-1.09278400	-3.88796300
H	5.65326500	-0.89728300	-2.57394000
H	4.35428900	-2.08543300	-2.42213300
C	4.05271100	1.37825300	-2.76086500
H	5.11023600	1.62527200	-2.61496700
H	3.86622500	1.37670800	-3.84099400
H	3.45595000	2.18047000	-2.31638500
C	2.52588400	-2.96290600	2.74018000
H	2.73060400	-3.52105300	1.81961200
H	3.45984400	-2.92252600	3.31310300
H	1.79608300	-3.53303400	3.32715200
C	1.66560400	-0.83027700	3.77876500
H	0.90788200	-1.40309500	4.32541200
H	2.54379500	-0.75048400	4.42991000
H	1.26857300	0.17531300	3.61599000
H	6.05068400	0.70213300	1.81794700
H	0.96968900	3.68252400	0.06691900
N	-2.39439400	2.75967300	1.39976700
O	-3.14474400	3.61901400	1.84343400

C	-0.01975500	3.13473300	-2.27392900
H	0.75211800	3.83762700	-2.62492100
H	-0.46757200	2.67565000	-3.16431900
H	-0.79309000	3.71127700	-1.75796000

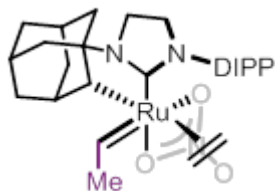


38-TS

SCF Energy (M06, n-octanol):	-1615.014318
SCF Energy (B3LYP, gas-phase):	-1614.635548
Enthalpy Correction:	0.721930
Free-Energy Correction:	0.623669

Ru	-0.54237200	1.16438300	-0.06039900
O	-1.72189600	1.30250900	1.99593900
O	-1.79089400	2.91849100	0.54272400
N	-0.53311700	-1.63108200	-0.81978800
N	1.58048500	-1.16288400	-0.46995200
C	0.31065900	-0.64173500	-0.43156000
C	0.11067300	-2.93776600	-0.97166400
H	-0.19575800	-3.42643500	-1.90062200
H	-0.14916700	-3.60234600	-0.13634500
C	1.59666100	-2.55521100	-0.97298400
H	2.20431600	-3.19215500	-0.32466000
H	2.02715300	-2.58586400	-1.98140800
C	-1.98218400	-1.45099100	-0.66206000
C	-2.44266200	-1.97780900	0.72193100
H	-1.87362800	-1.46415500	1.50611700
H	-2.23181500	-3.05443600	0.80390200
C	-3.95280800	-1.72350900	0.90876700
H	-4.26529800	-2.11940000	1.88419300
C	-4.73893700	-2.42859400	-0.21398400
H	-4.57773200	-3.51583600	-0.17325000
H	-5.81604100	-2.26014600	-0.08004100
C	-4.28403800	-1.87479900	-1.57980800
H	-4.84909200	-2.36415200	-2.38455400
C	-2.77992800	-2.18180100	-1.76704900
H	-2.43257900	-1.84306900	-2.75259600
H	-2.62370300	-3.27046900	-1.72068200
C	-4.53547100	-0.34976300	-1.62191500
H	-4.25280100	0.05270300	-2.60458200
H	-5.60920400	-0.15216500	-1.49267700
C	-3.72117200	0.35261700	-0.49973800
H	-3.90168000	1.43325900	-0.54257900
C	-2.23040000	0.06209900	-0.78451400
H	-2.07844000	0.30966500	-1.84510600
C	-4.20936900	-0.20563200	0.85518300
H	-3.70125400	0.28511000	1.68709000
H	-5.28490800	-0.00679400	0.96483400
C	2.78068800	-0.63154100	0.11353900
C	3.01203800	-0.82812100	1.49827100
C	4.20020800	-0.32694500	2.04535100
H	4.39309500	-0.45443100	3.10680100
C	5.14574800	0.31756600	1.25286200
C	4.93171400	0.44577800	-0.11627500
H	5.69311100	0.91591500	-0.73200800
C	3.75882300	-0.03298600	-0.71523900
C	2.06497800	-1.63568400	2.38791100
H	1.16016100	-1.85112200	1.81308700

C	3.61215300	0.02439600	-2.23450800
H	2.57029000	-0.21125000	-2.47551800
C	0.99355000	2.07176100	1.33636200
H	1.61951500	1.28687400	1.73744800
C	0.20058000	1.88831000	-1.63904800
H	1.04428800	1.44879000	-2.18584200
C	1.35218700	2.69074700	0.13720700
H	2.25764000	2.37903700	-0.37140200
H	0.38270700	2.61141100	2.05130200
C	4.50329000	-1.04716400	-2.90088600
H	4.35191600	-1.05254900	-3.98696600
H	5.56427000	-0.84640100	-2.71032800
H	4.28499300	-2.05124800	-2.52156800
C	3.92683500	1.40809800	-2.83346500
H	4.97820500	1.68350400	-2.69458700
H	3.73254500	1.40229400	-3.91227800
H	3.31339800	2.19694000	-2.38655100
C	2.71454900	-2.98563300	2.76494300
H	3.02643700	-3.55135500	1.87934400
H	3.60393800	-2.83501100	3.38826400
H	2.00900400	-3.60349000	3.33273500
C	1.61893700	-0.89021700	3.66066000
H	0.95981400	-1.53414000	4.25411600
H	2.47019000	-0.61860000	4.29578000
H	1.06258500	0.02081000	3.42445100
H	6.05975900	0.70037400	1.69902400
H	0.99513100	3.69421200	-0.07328900
N	-2.19463600	2.44839300	1.67504000
O	-2.97622500	3.05985500	2.38455300
C	-0.37696000	3.08633700	-2.33964800
H	0.39563600	3.80612300	-2.64840600
H	-0.85648200	2.72856500	-3.26526600
H	-1.13522700	3.59993800	-1.74249900

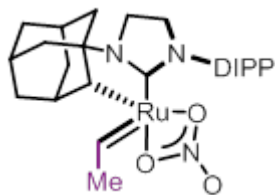


38-C

SCF Energy (M06, n-octanol):	-1615.012338
SCF Energy (B3LYP, gas-phase):	-1614.637651
Enthalpy Correction:	0.722785
Free-Energy Correction:	0.619274

Ru	-0.52728400	1.13734400	0.02240700
O	-1.51145400	1.12085800	2.15270700
O	-1.81219200	2.80651000	0.81311400
N	-0.57100900	-1.60652400	-0.93345500
N	1.54334500	-1.20869600	-0.52947300
C	0.28996600	-0.66016200	-0.47615600
C	0.04977900	-2.91911700	-1.13192100
H	-0.27520600	-3.37689900	-2.07002700
H	-0.20829700	-3.60213400	-0.31058900
C	1.53926100	-2.55671700	-1.13664900
H	2.15445200	-3.24756500	-0.55393800
H	1.94918100	-2.50963400	-2.15416600
C	-2.00955400	-1.41218300	-0.71541100
C	-2.42755700	-1.94402400	0.67981400
H	-1.82269100	-1.45150200	1.44964000
H	-2.23495300	-3.02541800	0.74179200
C	-3.92478100	-1.66352200	0.92412500
H	-4.20819800	-2.05912700	1.90837200
C	-4.76576700	-2.34537700	-0.17231000

H	-4.62342800	-3.43562100	-0.14472800
H	-5.83392800	-2.15824900	0.00264000
C	-4.35083100	-1.78963400	-1.54967600
H	-4.95358700	-2.26218700	-2.33687300
C	-2.86022000	-2.12245400	-1.79347500
H	-2.54296500	-1.78681200	-2.78993300
H	-2.72135700	-3.21369300	-1.75522700
C	-4.57625400	-0.25979700	-1.57136100
H	-4.32684900	0.14496900	-2.56183000
H	-5.64009600	-0.04471400	-1.39658500
C	-3.70555700	0.42152800	-0.47794400
H	-3.86911800	1.50523000	-0.50470900
C	-2.23311900	0.10631000	-0.83277600
H	-2.14343400	0.32834600	-1.90222800
C	-4.15386800	-0.14031000	0.88975300
H	-3.61222300	0.32670000	1.71339200
H	-5.22057400	0.07868100	1.03889300
C	2.78251100	-0.68668900	-0.03035100
C	3.18729200	-1.05199500	1.27677400
C	4.41703100	-0.57226000	1.74439400
H	4.74295200	-0.82846000	2.74881300
C	5.23064300	0.22633700	0.94507400
C	4.83504000	0.54143500	-0.35153200
H	5.48989100	1.14218200	-0.97631700
C	3.61606400	0.08479100	-0.87033600
C	2.35138500	-1.96290500	2.17450100
H	1.42872000	-2.20857100	1.64082000
C	3.26245000	0.37199600	-2.32603700
H	2.22003800	0.07738300	-2.47799100
C	-0.16373700	1.75677800	-1.69084100
H	0.06086100	1.09931000	-2.54780000
C	1.16544800	3.01596700	0.81240100
H	1.83566100	3.20651200	-0.02050700
C	1.38125100	1.98118700	1.65309800
H	0.77475600	1.84282800	2.54196400
H	2.23195200	1.32503800	1.52645500
H	6.17948400	0.59210900	1.32849500
C	3.09272800	-3.28538100	2.46183800
H	4.00286800	-3.11369100	3.04831300
H	2.45153200	-3.96468100	3.03560100
H	3.38839100	-3.79530800	1.53743900
C	1.93454900	-1.27853000	3.49067000
H	1.35151800	-1.97260300	4.10714400
H	2.80510800	-0.96383200	4.07795600
H	1.31334600	-0.39848300	3.30212200
C	4.13613100	-0.47675900	-3.27439300
H	4.04473400	-1.54710100	-3.05830500
H	3.84187500	-0.31345600	-4.31804800
H	5.19554800	-0.21050900	-3.17861000
C	3.37665400	1.86388600	-2.68709000
H	3.03672400	2.03078200	-3.71602600
H	2.76459000	2.48057500	-2.02205100
H	4.41040900	2.22210600	-2.62294500
N	-2.04965400	2.27227400	1.96070500
O	-2.74472600	2.81837300	2.79873900
H	0.38199200	3.74440500	0.98832300
C	-0.35819300	3.17705000	-2.13820600
H	-0.62008700	3.85766000	-1.32416000
H	0.54181900	3.55349400	-2.64910300
H	-1.16515500	3.20681100	-2.88816900

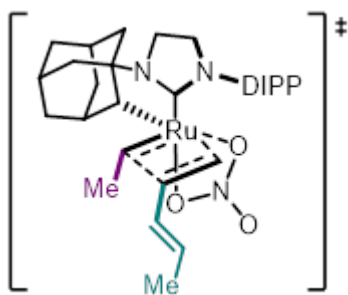


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SCF Energy (M06, n-octanol): -1536.462676
 SCF Energy (B3LYP, gas-phase): -1536.047585
 Enthalpy Correction: 0.663652
 Free-Energy Correction: 0.567398

Ru	-0.55334800	0.83277400	-0.85476700
O	0.66674400	2.57262900	-0.18989200
O	-1.11460800	2.95537500	-1.38565500
N	-0.82980500	-1.75319300	0.41222200
N	1.32002500	-1.26669200	0.45821500
C	0.10439500	-0.83615000	0.02555700
C	-0.28839600	-2.74113300	1.35018400
H	-0.64965500	-3.74919000	1.12800900
H	-0.56619800	-2.49693800	2.38571500
C	1.22467100	-2.59179600	1.11025500
H	1.81281100	-2.61423700	2.03069400
H	1.60816900	-3.36989300	0.43752800
C	-2.21736900	-1.25898400	0.41149600
C	-2.48874500	-0.39018200	1.67070700
H	-1.72324400	0.39718900	1.74535400
H	-2.40610600	-1.00020500	2.58187100
C	-3.88949000	0.24516300	1.58304100
H	-4.06925800	0.85196300	2.48031300
C	-4.94260200	-0.87856500	1.49713300
H	-4.90907700	-1.49920700	2.40395400
H	-5.95102800	-0.44673800	1.44324300
C	-4.67389700	-1.74248200	0.24674700
H	-5.42473400	-2.54091300	0.18215500
C	-3.26807000	-2.38465600	0.35308700
H	-3.07033000	-3.02583700	-0.51599200
H	-3.22056100	-3.02176300	1.24950800
C	-4.76051900	-0.84499400	-1.00770400
H	-4.60623100	-1.44436400	-1.91517400
H	-5.76759200	-0.40972700	-1.07914800
C	-3.69234200	0.27749800	-0.92863900
H	-3.75395800	0.90757200	-1.82467400
C	-2.30757800	-0.39332700	-0.86285700
H	-2.23683700	-1.08830500	-1.70802900
C	-3.96056500	1.13471400	0.32494500
H	-3.22563700	1.94878900	0.38987200
H	-4.94975400	1.60768100	0.25587400
C	2.54405700	-0.50890800	0.51749400
C	2.75800800	0.35264000	1.62049300
C	3.97740000	1.03628600	1.69397300
H	4.15906700	1.70943800	2.52654300
C	4.96125700	0.86807100	0.72500600
C	4.74294400	-0.00080700	-0.33872800
H	5.52058900	-0.13666100	-1.08474000
C	3.53936600	-0.70559100	-0.46388200
C	1.74936200	0.52161500	2.75484900
H	0.81203200	0.04589000	2.45075900
C	3.36284500	-1.68213700	-1.62054500
H	2.31185100	-1.98506300	-1.64050700
C	-0.21154700	0.34353100	-2.57893900
H	-0.33965200	1.19488300	-3.27118900
C	2.23872500	-0.19398400	4.03255900
H	3.16805500	0.25493300	4.40265400
H	1.48852400	-0.11416900	4.82856200
H	2.43628600	-1.25824300	3.85754900

C	1.42882800	1.99878200	3.05479000
H	0.63196200	2.06182800	3.80607200
H	2.29917700	2.52706200	3.46140100
H	1.10551400	2.52348800	2.15190100
C	4.21425900	-2.95174300	-1.40836600
H	4.04751500	-3.66968000	-2.22065300
H	5.28357500	-2.70973500	-1.38899600
H	3.97209800	-3.44747900	-0.46134400
C	3.68534300	-1.03943400	-2.98258400
H	4.74931800	-0.79259800	-3.07267700
H	3.44225300	-1.73226400	-3.79704000
H	3.11502500	-0.11690600	-3.13056800
H	5.90002200	1.41011900	0.80238900
N	-0.11733200	3.45052100	-0.74516500
O	0.08560700	4.64153300	-0.65128800
C	0.05720600	-0.95380400	-3.26698000
H	-0.82258900	-1.20638000	-3.88297900
H	0.90425800	-0.87252200	-3.96154500
H	0.23422200	-1.78236700	-2.57770000

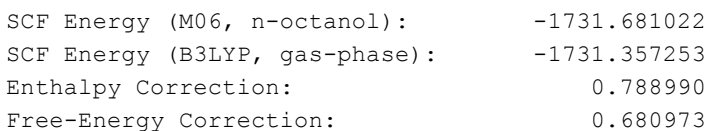


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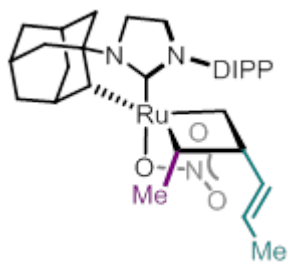
SCF Energy (M06, n-octanol):	-1731.668852
SCF Energy (B3LYP, gas-phase):	-1731.349296
Enthalpy Correction:	0.787022
Free-Energy Correction:	0.679921

Ru	-0.50567800	0.92899700	-0.01253400
O	-1.75878400	1.35199000	2.04197900
O	-1.39138500	2.89701800	0.55596000
N	-0.99016700	-1.78111400	-0.92961400
N	1.16251400	-1.74150100	-0.51424000
C	0.01168400	-0.99371900	-0.45787400
C	-0.59418900	-3.17184200	-1.16294000
H	-0.97268800	-3.53966800	-2.12049700
H	-0.97897300	-3.82697000	-0.36941100
C	0.93426700	-3.06434200	-1.13938300
H	1.41305300	-3.85484000	-0.55606700
H	1.35917500	-3.08041000	-2.15052600
C	-2.38377400	-1.35877600	-0.75402200
C	-2.95526100	-1.92926700	0.57077900
H	-2.31494800	-1.60800200	1.40152300
H	-2.94346600	-3.02852100	0.54321800
C	-4.39579900	-1.42433900	0.78656100
H	-4.79075300	-1.85275700	1.71735000
C	-5.27918100	-1.85752500	-0.40037000
H	-5.31905800	-2.95443200	-0.47001500
H	-6.30945900	-1.50931600	-0.24739600
C	-4.70969400	-1.26371600	-1.70532700
H	-5.34116200	-1.56021100	-2.55354100
C	-3.28303100	-1.81699800	-1.92654000
H	-2.86436100	-1.44855100	-2.87289300
H	-3.32314800	-2.91498100	-1.99117800
C	-4.67838400	0.27731200	-1.59433500
H	-4.30975100	0.71771700	-2.53104300
H	-5.69938200	0.65562400	-1.44355100

C	-3.77115300	0.70405300	-0.40604400
H	-3.75144900	1.79780100	-0.34306800
C	-2.35696000	0.17420300	-0.71417000
H	-2.10950100	0.51663500	-1.73544300
C	-4.36793100	0.11176700	0.88879000
H	-3.77972600	0.42216100	1.75524900
H	-5.38852000	0.49491600	1.02926300
C	2.42536900	-1.50648800	0.13195200
C	2.55387800	-1.80358100	1.51323000
C	3.80271700	-1.60685800	2.11563500
H	3.92185500	-1.81486900	3.17485900
C	4.89866400	-1.16202400	1.38174500
C	4.76974300	-0.93024200	0.01620500
H	5.63881500	-0.61624500	-0.55454400
C	3.54274500	-1.10654900	-0.63801000
C	1.41382300	-2.40007500	2.34113700
H	0.48921400	-2.30509800	1.76564000
C	3.47519200	-0.94508500	-2.15558000
H	2.41849600	-0.93964600	-2.44327300
C	1.05015800	1.34716900	1.38896600
H	1.54399800	0.45208700	1.74248800
C	0.56254500	1.56750200	-1.45964700
H	1.31481900	0.95909000	-1.97088700
C	1.65786800	2.03356100	0.26926700
H	2.52814100	1.53395500	-0.15067600
H	0.63000200	1.96770800	2.17739500
C	4.14955200	-2.14666000	-2.85426700
H	4.04166000	-2.06945500	-3.94280200
H	5.22118400	-2.18015400	-2.62457100
H	3.71526800	-3.10029900	-2.53537700
C	4.10029700	0.36847400	-2.66248200
H	5.17851600	0.40695500	-2.47074000
H	3.95923700	0.45623100	-3.74602900
H	3.64506100	1.24616400	-2.19289900
C	1.66658300	-3.90455800	2.58457600
H	1.80666000	-4.45483800	1.64720700
H	2.56660400	-4.05664600	3.19214100
H	0.82095500	-4.35306700	3.11915200
C	1.17911000	-1.68554000	3.68591800
H	0.32577700	-2.14168200	4.20054000
H	2.04474900	-1.77038000	4.35304300
H	0.95465500	-0.62415700	3.55086800
H	5.85769700	-1.01441500	1.87110100
N	-1.93769100	2.56027300	1.68076900
O	-2.57946400	3.36391000	2.33965400
C	1.72218900	3.50750300	0.27932600
H	0.87938800	4.01779700	0.74249100
C	2.74676600	4.21628700	-0.21623500
H	3.58164300	3.68557300	-0.67945600
C	2.85911000	5.71269400	-0.16527500
H	1.97886600	6.16423200	0.30402000
H	3.74613500	6.02759800	0.40165700
H	2.96457500	6.13939700	-1.17235600
C	0.21095500	2.81541600	-2.22346000
H	1.09640700	3.41875600	-2.46627900
H	-0.24233600	2.50213700	-3.17696000
H	-0.50675400	3.44771100	-1.69416200

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C	1.60501600	1.95511000	-0.08819800
H	2.56098600	1.43007700	-0.17122500
H	0.60343300	2.16441400	1.90638900
C	4.05710100	-2.47422300	-2.75509500
H	3.93852400	-2.48349500	-3.84518600
H	5.13010600	-2.51694500	-2.53389500
H	3.60273500	-3.38695900	-2.35460700
C	4.07247100	0.05023500	-2.77204500
H	5.15656600	0.06632000	-2.61223000
H	3.90325000	0.06153500	-3.85500900
H	3.65800200	0.97357900	-2.35624000
C	1.54366600	-3.65712000	2.79715500
H	1.58968700	-4.25719000	1.88151500
H	2.46163600	-3.85292300	3.36396400
H	0.69658800	-4.01473700	3.39444400
C	1.27634300	-1.36851800	3.82209800
H	0.39324100	-1.71268000	4.37214500
H	2.14449100	-1.52642300	4.47239700
H	1.16545500	-0.29354200	3.65510200
H	5.87220500	-0.96186300	1.82490100
N	-1.94213700	2.90306100	1.34642600
O	-2.49264900	3.90082500	1.79246000
C	1.81879900	3.44092900	0.01686500
H	0.92372600	4.03661200	0.18919900
C	3.01389900	4.03199100	-0.07078200
H	3.89992100	3.41483200	-0.23769600
C	3.25219600	5.51127100	0.05116200
H	3.72749200	5.91566400	-0.85331500
H	2.31532300	6.05465500	0.21325400
H	3.92612300	5.73976500	0.88833600
C	0.41907200	2.63785600	-2.40138600
H	1.30842400	3.17060400	-2.76778300
H	-0.09075100	2.20854600	-3.27320200
H	-0.24625000	3.37514000	-1.94456600



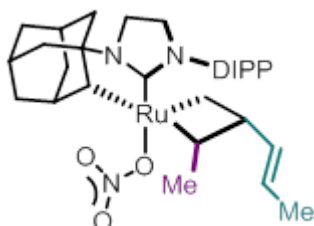
23b

SCF Energy (M06, n-octanol):	-1731.679373
SCF Energy (B3LYP, gas-phase):	-1731.355041
Enthalpy Correction:	0.789370
Free-Energy Correction:	0.681747

Ru	-0.63350600	0.77904500	-0.18845200
O	-2.35346200	2.61875400	1.41704500
O	-1.54066000	2.72204800	-0.62215200
N	-0.96957800	-2.02959800	0.41822400
N	1.20243800	-1.76566500	0.53472900
C	0.02395900	-1.12313800	0.24572300
C	-0.53505900	-3.28196100	1.03976500
H	-0.96023900	-4.15348800	0.53385700
H	-0.84148100	-3.31561300	2.09348900
C	0.98770400	-3.18990400	0.88587400
H	1.52527300	-3.44602600	1.80243600
H	1.35800800	-3.83632800	0.08296600
C	-2.37004200	-1.62970600	0.26984900
C	-3.04311000	-1.40157900	1.64873000
H	-2.46896600	-0.65490900	2.21174400
H	-3.02957900	-2.33708700	2.22612900

C	-4.49567400	-0.91932900	1.45412800
H	-4.95979400	-0.78155800	2.43926000
C	-5.28860500	-1.96554500	0.64656000
H	-5.32891500	-2.92254400	1.18667000
H	-6.32550500	-1.62845400	0.51613100
C	-4.62018300	-2.16174600	-0.72976200
H	-5.18471100	-2.89967900	-1.31498800
C	-3.18332000	-2.68790200	-0.51719900
H	-2.69099600	-2.88125500	-1.47988900
H	-3.21841100	-3.64146500	0.03021200
C	-4.58493500	-0.81599100	-1.48767500
H	-4.13568500	-0.95286700	-2.48121500
H	-5.60921400	-0.45241200	-1.64759700
C	-3.77976700	0.23246800	-0.66874400
H	-3.75410800	1.18270700	-1.21231400
C	-2.35195500	-0.31910000	-0.52981400
H	-1.96517200	-0.53290100	-1.55236200
C	-4.47631700	0.41996400	0.69522500
H	-3.95980400	1.18516900	1.27834700
H	-5.50481800	0.77054500	0.53170000
C	2.53879600	-1.37913900	0.15392600
C	3.42550500	-0.89211600	1.14407400
C	4.72823100	-0.55038100	0.75608100
H	5.42069300	-0.16460400	1.49812900
C	5.15492300	-0.70640100	-0.55867400
C	4.29093300	-1.24496300	-1.50717100
H	4.64530000	-1.39842900	-2.52226300
C	2.97945100	-1.60820700	-1.17547000
C	3.04165800	-0.80544200	2.61980300
H	1.95243800	-0.89330300	2.68571900
C	2.12467900	-2.31913400	-2.22842200
H	1.09997800	-2.38750900	-1.85085500
C	0.51913000	1.66114400	1.18942800
C	0.87414900	1.27035300	-1.41900400
C	1.40007100	2.00312500	-0.07586000
H	1.02713200	1.03537500	1.91996500
H	0.04882600	2.53191100	1.64360100
H	2.37627300	1.54300700	0.10050700
H	1.56303000	0.46363400	-1.65809700
H	6.16753200	-0.42930600	-0.83949900
C	2.64995700	-3.75534400	-2.45606300
H	3.65229600	-3.73582000	-2.89987400
H	2.71858300	-4.32565700	-1.52337600
H	1.99055300	-4.30014100	-3.14201600
C	2.05910100	-1.58584100	-3.58266800
H	3.04515400	-1.51553200	-4.05540800
H	1.40792100	-2.13828300	-4.26997200
H	1.65997700	-0.57339800	-3.48406300
C	3.65747100	-1.98571200	3.40411200
H	4.75264400	-1.93236400	3.39247700
H	3.33081700	-1.96304000	4.45050200
H	3.37224900	-2.95446900	2.97947900
C	3.44970700	0.52417800	3.28379900
H	3.07281400	1.39157300	2.73380900
H	3.04861200	0.57023400	4.30267700
H	4.53875000	0.62194400	3.36026100
N	-2.25027600	3.25274800	0.34343700
O	-2.77058700	4.34701100	0.14575500
C	1.52797300	3.49405000	-0.24075900
H	0.59452300	4.03975400	-0.36433100
C	2.69421500	4.14542600	-0.22637800
H	3.61827200	3.57617300	-0.10100700
C	2.84734200	5.63412800	-0.36800900

H	3.47114300	5.89059300	-1.23544800
H	1.87654100	6.12542400	-0.49140400
H	3.33924900	6.07062500	0.51218200
C	0.58748600	2.13273300	-2.63541100
H	1.49814900	2.66158200	-2.95190000
H	0.26956200	1.49725500	-3.47156700
H	-0.19188500	2.87410200	-2.45076000

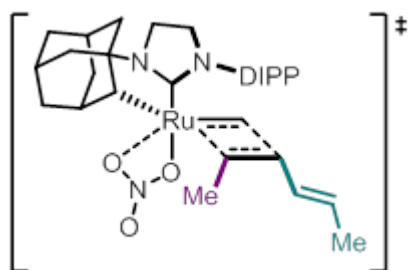


23c

SCF Energy (M06, n-octanol):	-1731.682031
SCF Energy (B3LYP, gas-phase):	-1731.356683
Enthalpy Correction:	0.789553
Free-Energy Correction:	0.682847

Ru	0.69147100	0.76042300	0.05520200
O	1.97336300	1.99360800	2.13018300
O	1.71114700	2.68576900	0.07307700
N	0.91140200	-2.10170600	-0.29793900
N	-1.25556300	-1.79905300	-0.26851200
C	-0.05037000	-1.15828700	-0.12731800
C	0.40362900	-3.38240300	-0.79161400
H	0.88203600	-4.22844700	-0.29095400
H	0.57719000	-3.47942600	-1.87263700
C	-1.08521000	-3.25908800	-0.45840800
H	-1.73795700	-3.62548800	-1.25436900
H	-1.34266800	-3.78918800	0.46699300
C	2.30373900	-1.66644300	-0.41381900
C	2.66837200	-1.36054600	-1.89221800
H	1.94836500	-0.63982800	-2.30061800
H	2.58831400	-2.27919400	-2.49126500
C	4.10004700	-0.79714600	-1.97618700
H	4.34395500	-0.58701300	-3.02592700
C	5.08681700	-1.83996000	-1.41214800
H	5.05276600	-2.75948600	-2.01385600
H	6.11414600	-1.45650900	-1.47131900
C	4.72723700	-2.14902700	0.05646300
H	5.42773700	-2.89208300	0.45988900
C	3.29442800	-2.72387800	0.12724300
H	3.03064900	-2.97862300	1.16221800
H	3.23767600	-3.64902000	-0.46564400
C	4.80951700	-0.84933700	0.88192000
H	4.58558500	-1.05106300	1.93785500
H	5.83153800	-0.44724600	0.84311300
C	3.81325900	0.20129500	0.32064200
H	3.89206000	1.10727200	0.92303800
C	2.39962900	-0.39145700	0.44378100
H	2.19846800	-0.65020700	1.49441500
C	4.17661200	0.50122900	-1.14816800
H	3.49705900	1.26030900	-1.55404600
H	5.19068400	0.92014300	-1.20147100
C	-2.55931800	-1.34712100	0.14336500
C	-3.50717200	-0.99424700	-0.84664000
C	-4.78078700	-0.58942700	-0.42536600
H	-5.52240700	-0.30634700	-1.16663500
C	-5.11862000	-0.55663600	0.92417900
C	-4.19177500	-0.95994300	1.88103600
H	-4.47430300	-0.96082900	2.92990600
C	-2.90483300	-1.37598100	1.51703800

C	-3.21735100	-1.12033900	-2.34155100
H	-2.13988400	-1.27503800	-2.45811200
C	-1.95901600	-1.89741200	2.60019800
H	-0.98400300	-2.08797500	2.14291800
C	-0.21728100	1.32380100	-1.61887200
C	-0.97012600	1.56848200	0.92465500
C	-1.24161000	1.99223900	-0.58556200
H	-0.70476400	0.61121800	-2.28543800
H	0.34817500	2.07968100	-2.17249700
H	-2.21107500	1.53909100	-0.81017300
H	-1.68374300	0.80525200	1.22328300
H	-6.11094800	-0.23517600	1.22904400
C	-2.48105600	-3.23382600	3.17256700
H	-3.43277700	-3.09298000	3.69834200
H	-2.64821000	-3.97939100	2.38677400
H	-1.76240400	-3.64847300	3.88916500
C	-1.72738700	-0.88941300	3.74206700
H	-2.65942500	-0.64727900	4.26548600
H	-1.03674400	-1.31418100	4.47965500
H	-1.29122600	0.04311500	3.37489500
C	-3.93858100	-2.35593300	-2.92463200
H	-5.02703700	-2.23602100	-2.86832800
H	-3.67029700	-2.49583100	-3.97854600
H	-3.68224600	-3.27344400	-2.38345000
C	-3.59857000	0.13270900	-3.15261000
H	-3.09087700	1.02975800	-2.78615700
H	-3.31901900	-0.00435800	-4.20367600
H	-4.67789900	0.32168500	-3.12592700
N	2.18177000	2.89015200	1.27396800
O	2.79385100	3.92563600	1.50972700
C	-1.28335500	3.48158700	-0.79978500
H	-0.33316000	4.00224400	-0.69282400
C	-2.38951700	4.15489200	-1.12827900
H	-3.33022700	3.60923400	-1.23380100
C	-2.45456000	5.63665200	-1.37217600
H	-3.15964200	6.12315200	-0.68423700
H	-1.47455900	6.10727800	-1.24055800
H	-2.80479400	5.85928200	-2.38960300
C	-0.90828900	2.66852700	1.96428200
H	-1.92204000	3.06559500	2.12479900
H	-0.54741800	2.27359000	2.91822900
H	-0.27051400	3.50641900	1.68217600



24-TS

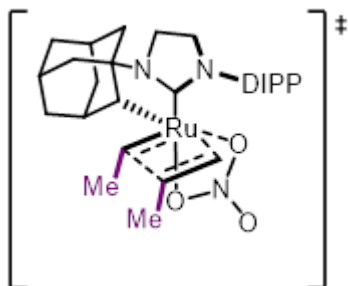
SCF Energy (M06, n-octanol):	-1731.665291
SCF Energy (B3LYP, gas-phase):	-1731.345432
Enthalpy Correction:	0.787282
Free-Energy Correction:	0.680299

Ru	0.63090800	0.78158500	0.17293500
O	1.68863900	2.65915800	0.68321700
O	1.44157200	1.33080900	2.38753300
N	0.91935900	-2.02374400	-0.49237100
N	-1.24983500	-1.75690300	-0.36387300
C	-0.04653800	-1.11141100	-0.20937600
C	0.40403100	-3.27233700	-1.05420200

H	0.91898800	-4.14482200	-0.64328000
H	0.52284000	-3.28523900	-2.14707100
C	-1.06710100	-3.20017700	-0.63910700
H	-1.75402800	-3.53957400	-1.41779600
H	-1.26488000	-3.78186300	0.27090300
C	2.31120200	-1.57688900	-0.60242900
C	2.66616500	-1.20426200	-2.06454200
H	1.93692100	-0.48068000	-2.44483300
H	2.60766800	-2.09899600	-2.70186000
C	4.08714700	-0.61025900	-2.11893000
H	4.32475000	-0.33715800	-3.15594300
C	5.09397700	-1.66532200	-1.61739900
H	5.07174300	-2.55043000	-2.26942700
H	6.11543700	-1.26347700	-1.65840800
C	4.74357800	-2.05807600	-0.16710600
H	5.45336000	-2.81508200	0.19227800
C	3.31587000	-2.65415900	-0.12483100
H	3.05922700	-2.96777600	0.89563900
H	3.27320500	-3.54846700	-0.76505500
C	4.82488700	-0.80098300	0.72483100
H	4.61842400	-1.06050000	1.77155500
H	5.84451100	-0.39128200	0.69155100
C	3.80408600	0.26000900	0.23420100
H	3.88103500	1.14590900	0.87135000
C	2.40217100	-0.36560400	0.34318300
H	2.27661500	-0.74722100	1.36624800
C	4.14258500	0.64307300	-1.22083200
H	3.43655400	1.40135200	-1.58066600
H	5.14558600	1.08953800	-1.26579900
C	-2.53665600	-1.33625200	0.11882700
C	-3.52524200	-0.95513200	-0.81976700
C	-4.77981600	-0.56439400	-0.33447700
H	-5.55284900	-0.26052600	-1.03448400
C	-5.05895900	-0.57106400	1.02925000
C	-4.09325900	-1.00342800	1.93364800
H	-4.33111700	-1.03463600	2.99315400
C	-2.82313100	-1.40951300	1.50366200
C	-3.29376200	-1.04402000	-2.32789900
H	-2.22128700	-1.19445700	-2.48893000
C	-1.83306300	-1.96698700	2.52725400
H	-0.88671500	-2.16774500	2.01746300
C	0.19540200	1.31685500	-1.58461500
H	-0.40253500	0.79829600	-2.34323300
C	-1.24198300	1.73531800	0.96980800
H	-1.85998400	0.88274600	1.22767900
C	-1.35401900	2.14406100	-0.40312700
H	-2.07665900	1.57356000	-0.97992700
H	0.65984500	2.23183000	-1.97018100
N	1.91797300	2.42331700	1.93409300
O	2.55013900	3.20924000	2.62289600
C	-3.70365600	0.22577500	-3.09664600
H	-3.47904300	0.10573200	-4.16287600
H	-4.77731600	0.42786800	-3.01044600
H	-3.16683200	1.11077500	-2.74136600
C	-4.03861400	-2.26509200	-2.91232900
H	-3.81126600	-2.38092800	-3.97876200
H	-3.76344700	-3.19509600	-2.40289600
H	-5.12389400	-2.14563000	-2.81119400
C	-2.34998800	-3.30509900	3.09962700
H	-3.27022200	-3.16053300	3.67802900
H	-2.56985500	-4.03055500	2.30773200
H	-1.60204500	-3.74630700	3.76872800
C	-1.52041500	-0.98256400	3.67050300

H	-1.05012300	-0.06909100	3.29755000
H	-2.42346300	-0.70590800	4.22729600
H	-0.82465400	-1.44541600	4.37971000
H	-6.03670500	-0.25805200	1.38579600
C	-1.21177000	3.56186800	-0.80094800
H	-0.42841600	4.13137900	-0.30545800
C	-1.99555000	4.15900800	-1.70931600
H	-2.77318300	3.57327800	-2.20394100
C	-1.90076200	5.60306100	-2.10792500
H	-2.83925800	6.13640400	-1.90339300
H	-1.09531200	6.11530600	-1.57137000
H	-1.71129900	5.70599700	-3.18544600
C	-1.12173200	2.74985100	2.08713200
H	-2.10503300	3.21637600	2.24928800
H	-0.81869700	2.27353500	3.02157600
H	-0.41236200	3.55033400	1.87054300

Alkene Homodimerization

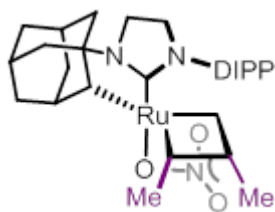


25-TS

SCF Energy (M06, n-octanol):	-1654.308711
SCF Energy (B3LYP, gas-phase):	-1653.948443
Enthalpy Correction:	0.751638
Free-Energy Correction:	0.650159

Ru	-0.56225200	1.07978100	-0.05384200
O	-1.82372800	1.32945000	1.99864300
O	-1.79192300	2.87021400	0.46489200
N	-0.58975600	-1.71405200	-0.83502200
N	1.53130400	-1.28779500	-0.48071900
C	0.26942700	-0.74569700	-0.42750200
C	0.03331300	-3.02660700	-1.01998900
H	-0.28974800	-3.49223000	-1.95499100
H	-0.22674200	-3.70360500	-0.19466600
C	1.52256100	-2.66314800	-1.03006900
H	2.13203900	-3.32845200	-0.41318700
H	1.93690900	-2.66450200	-2.04573000
C	-2.03491900	-1.51948000	-0.67097300
C	-2.50127300	-2.08454700	0.69633800
H	-1.92239000	-1.60510100	1.49502100
H	-2.30559400	-3.16602300	0.74257500
C	-4.00678000	-1.81464600	0.89482500
H	-4.32281600	-2.23636300	1.85822800
C	-4.80375700	-2.47475600	-0.24752600
H	-4.65723100	-3.56481200	-0.23960300
H	-5.87835600	-2.29609100	-0.10705800
C	-4.34317600	-1.88649300	-1.59698800
H	-4.91560200	-2.34407600	-2.41504900
C	-2.84345000	-2.20505900	-1.79719300
H	-2.49364000	-1.83930100	-2.77210300
H	-2.69907900	-3.29622300	-1.78490500
C	-4.57336100	-0.35784600	-1.59347800
H	-4.28438200	0.06985800	-2.56356800
H	-5.64392400	-0.14814100	-1.45793200
C	-3.75027400	0.29939600	-0.45027300
H	-3.91695600	1.38271200	-0.46137200
C	-2.26443100	-0.00244500	-0.73841700
H	-2.09124100	0.29491300	-1.78640000
C	-4.24173600	-0.29250300	0.88850800
H	-3.71999000	0.17033300	1.72859400
H	-5.31358600	-0.08110400	1.00970700
C	2.74503300	-0.80652100	0.12030400
C	2.96291800	-1.04127300	1.50183400
C	4.16468900	-0.59438400	2.06528000
H	4.34717800	-0.75213500	3.12443300
C	5.13624900	0.03451200	1.29196700
C	4.93389600	0.20002100	-0.07461100
H	5.71376500	0.65771600	-0.67637400
C	3.74865300	-0.22498000	-0.69006500
C	1.98229300	-1.83139400	2.37052600
H	1.06298400	-1.97925900	1.79742700

C	3.61666900	-0.12753100	-2.20871500
H	2.56931400	-0.31953800	-2.46409200
C	0.94502700	1.83946700	1.32645700
H	1.55957800	1.02555100	1.68559500
C	0.30471800	1.80966000	-1.57315600
H	1.15792000	1.33856600	-2.07199100
C	1.38260800	2.56403700	0.18259200
H	2.28970900	2.18800000	-0.28339500
H	0.40716200	2.38555200	2.09771800
C	4.47550500	-1.21339600	-2.89401500
H	4.33467400	-1.18585700	-3.98116800
H	5.54099500	-1.05552900	-2.68897200
H	4.21823800	-2.21840400	-2.54264200
C	3.98493400	1.25842700	-2.77110400
H	5.04617400	1.48889100	-2.62531200
H	3.79146400	1.28862200	-3.84966000
H	3.40205600	2.05779500	-2.30266200
C	2.56438400	-3.22582900	2.69271100
H	2.83263500	-3.77777300	1.78450100
H	3.46989700	-3.14234000	3.30517800
H	1.83568100	-3.82441700	3.25187200
C	1.58732100	-1.11140900	3.67432300
H	0.88048900	-1.73039100	4.23868500
H	2.45397300	-0.93232200	4.32111500
H	1.10229400	-0.15135100	3.47834500
H	6.06053500	0.37545000	1.75078100
N	-2.24210800	2.46969600	1.60987100
O	-3.01770900	3.15010000	2.26271900
C	-0.28073700	2.93997200	-2.37510800
H	0.48177500	3.62801500	-2.76675700
H	-0.77403600	2.48928700	-3.25183200
H	-1.03503600	3.51038900	-1.82714600
C	1.17720800	4.06282100	0.11944800
H	1.36619900	4.47653100	-0.87487700
H	0.16307300	4.33081200	0.42647300
H	1.88244900	4.54270800	0.81172800



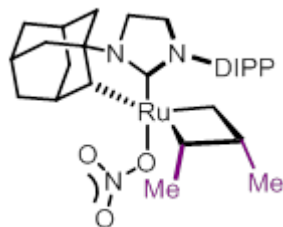
26a

SCF Energy (M06, n-octanol):	-1654.325170
SCF Energy (B3LYP, gas-phase):	-1653.961117
Enthalpy Correction:	0.753715
Free-Energy Correction:	0.652423

Ru	-0.60825300	1.03891700	-0.09977800
O	-2.14195300	1.65602900	1.97265200
O	-1.78279300	2.88134800	0.20178000
N	-0.56228300	-1.76795800	-0.81113400
N	1.54445300	-1.30597800	-0.42009200
C	0.28014500	-0.77593800	-0.40862700
C	0.08228200	-3.07781700	-0.93366600
H	-0.23285300	-3.59765000	-1.84238400
H	-0.15919600	-3.71517400	-0.07184500
C	1.56117800	-2.68329800	-0.96601200
H	2.19631000	-3.33226500	-0.35894600
H	1.95621300	-2.67594000	-1.98912900
C	-2.00556000	-1.59492700	-0.63882200
C	-2.47727700	-2.20734900	0.70768600
H	-1.90066400	-1.75607600	1.52487000

H	-2.27887200	-3.28839100	0.71542300
C	-3.98368200	-1.94651600	0.91004700
H	-4.30060400	-2.40164900	1.85749100
C	-4.77562800	-2.56995600	-0.25667200
H	-4.62758200	-3.65923100	-0.28335300
H	-5.85075300	-2.39752000	-0.11404100
C	-4.31270700	-1.93859600	-1.58579100
H	-4.88050000	-2.37165400	-2.41983300
C	-2.81158600	-2.23800000	-1.79385500
H	-2.46116500	-1.83244000	-2.75235700
H	-2.65150100	-3.32601000	-1.81998900
C	-4.54326000	-0.41247000	-1.53814800
H	-4.24450400	0.04635400	-2.49071800
H	-5.61263100	-0.20049100	-1.40267900
C	-3.73530500	0.20996200	-0.36334200
H	-3.90088600	1.29154100	-0.34628700
C	-2.25520600	-0.08546500	-0.63704700
H	-2.00297000	0.31711000	-1.65015900
C	-4.22213500	-0.42645700	0.95507200
H	-3.69793000	0.02531000	1.80062000
H	-5.29323700	-0.21863900	1.08470500
C	2.74911400	-0.79626900	0.18045000
C	2.93134600	-0.94461400	1.57967600
C	4.13323500	-0.49222800	2.13791500
H	4.29119300	-0.58430100	3.20816100
C	5.13590500	0.06237900	1.34745300
C	4.96167500	0.15337800	-0.02930500
H	5.76069100	0.56141900	-0.64128700
C	3.77773100	-0.27943700	-0.64197800
C	1.91034300	-1.64711500	2.47701900
H	0.96010200	-1.69467100	1.93848200
C	3.67256900	-0.24483100	-2.16554500
H	2.62641000	-0.42846800	-2.43219100
C	0.72536200	1.77311000	1.22541300
H	1.43140800	1.10273000	1.70474800
C	0.61170700	1.93885400	-1.40929800
H	1.31060600	1.29589900	-1.94595100
C	1.30468600	2.47501800	-0.05308700
H	2.33670700	2.12073500	-0.13211900
H	0.26986500	2.46602000	1.93407400
C	4.52710800	-1.36797400	-2.79367400
H	4.40431600	-1.38044700	-3.88329800
H	5.59114100	-1.21496400	-2.57790400
H	4.25288700	-2.35597100	-2.40848400
C	4.07143600	1.11345400	-2.77414200
H	5.13678600	1.32599100	-2.63067000
H	3.88432000	1.10798700	-3.85418400
H	3.50206300	1.93931100	-2.33709200
C	2.36300900	-3.09584900	2.76665500
H	2.52034600	-3.67113300	1.84738700
H	3.30665900	-3.10581600	3.32508600
H	1.61056600	-3.61892600	3.36870500
C	1.63724300	-0.91425200	3.80403800
H	0.84330100	-1.43260700	4.35354600
H	2.52055400	-0.89467800	4.45293300
H	1.31048600	0.11640700	3.64143600
H	6.05979900	0.40776600	1.80371300
N	-2.36936700	2.73282200	1.35636200
O	-3.09960400	3.61633400	1.78655500
C	-0.01244100	2.95768400	-2.35127800
H	0.74624500	3.63770500	-2.76720600
H	-0.47132600	2.43582300	-3.20078700
H	-0.78396000	3.56330400	-1.86917100

C	1.26633900	4.00212200	0.09385800
H	1.84491700	4.30359900	0.97436100
H	1.69995600	4.50129200	-0.77986000
H	0.23983700	4.35495200	0.22261000

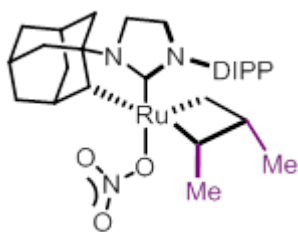


26b

SCF Energy (M06, n-octanol):	-1654.327210
SCF Energy (B3LYP, gas-phase):	-1653.960872
Enthalpy Correction:	0.754214
Free-Energy Correction:	0.652989

Ru	0.71900300	0.86789800	-0.23159000
O	2.19449500	2.49947900	1.47112100
O	1.99770800	2.56062600	-0.70761700
N	0.53100000	-1.96562600	0.34052400
N	-1.56780400	-1.39378100	0.11002000
C	-0.28688600	-0.90183600	0.12115800
C	-0.14587300	-3.26088200	0.25740000
H	0.18813900	-3.94370500	1.04337500
H	0.04252400	-3.73812900	-0.71464100
C	-1.60916800	-2.84248800	0.41616700
H	-2.28485400	-3.36274900	-0.26687500
H	-1.97010500	-2.99931300	1.43964900
C	1.97131400	-1.78515300	0.15691100
C	2.36841500	-2.04252700	-1.32137200
H	1.75846700	-1.40459100	-1.97385800
H	2.15275800	-3.08706800	-1.58864700
C	3.86481600	-1.74274300	-1.52646600
H	4.13132700	-1.93194200	-2.57474100
C	4.69533100	-2.66004900	-0.60556600
H	4.52581200	-3.71442700	-0.86743600
H	5.76678000	-2.46440800	-0.74602100
C	4.30424800	-2.40477800	0.86504200
H	4.89414600	-3.05642800	1.52299300
C	2.80397000	-2.72257300	1.06254100
H	2.51221000	-2.57416300	2.11068300
H	2.61353300	-3.77701400	0.81308400
C	4.57623400	-0.92716500	1.21131100
H	4.33532100	-0.72872300	2.26394800
H	5.64455900	-0.70471300	1.08060600
C	3.73383100	-0.00153400	0.29219900
H	3.94349600	1.03452400	0.56069200
C	2.25160400	-0.32421600	0.54904000
H	2.02593300	-0.19085800	1.61851000
C	4.12736500	-0.26474300	-1.17604500
H	3.55817100	0.39613900	-1.84120800
H	5.18972600	-0.02692500	-1.32252100
C	-2.81478500	-0.67846600	0.19781000
C	-3.61392100	-0.54726600	-0.96314400
C	-4.84444700	0.11302600	-0.84650400
H	-5.46985700	0.23447400	-1.72604900
C	-5.28648500	0.60540300	0.37741600
C	-4.51315500	0.41964400	1.51949600
H	-4.88077500	0.78043600	2.47580600
C	-3.27575000	-0.23382400	1.46193300
C	-3.22105200	-1.16351400	-2.30490900
H	-2.16769000	-1.45378600	-2.24085700
C	-2.51313000	-0.49548900	2.76183400

H	-1.53258300	-0.90810800	2.50635100
C	-0.07022400	1.08532700	-2.03866900
H	-0.62883900	0.28482000	-2.52389300
C	-0.82264900	2.10139000	0.29822100
H	-1.63908900	1.55231800	0.75989900
C	-1.01213400	2.12727000	-1.27564000
H	-2.02479500	1.73962300	-1.41995000
H	0.61154600	1.58906300	-2.73145700
C	-3.25845600	-1.54006000	3.62248200
H	-2.67264800	-1.78741500	4.51559100
H	-4.22894700	-1.15405100	3.95591900
H	-3.44801300	-2.46829100	3.07172300
C	-2.26170600	0.77925800	3.58985800
H	-3.19929800	1.24274800	3.91749000
H	-1.68691600	0.53107900	4.48949600
H	-1.69439700	1.52372700	3.02564200
C	-4.04679400	-2.44099100	-2.57590700
H	-3.95010900	-3.17308300	-1.76661100
H	-5.11244300	-2.20351100	-2.67711800
H	-3.71907900	-2.91836000	-3.50698100
C	-3.36685200	-0.19330800	-3.49275500
H	-2.99288300	-0.66592700	-4.40840200
H	-4.41376200	0.07665200	-3.67184800
H	-2.80329000	0.73122800	-3.33704600
H	-6.24284900	1.11711300	0.44485700
N	2.50509200	3.05672000	0.38977900
O	3.24946600	4.02865700	0.31472100
C	-0.59951900	3.41477800	1.02038300
H	-1.54953700	3.97020700	1.06861600
H	-0.27204100	3.23447500	2.04820100
H	0.13917000	4.06015500	0.54487600
C	-0.86732900	3.52057900	-1.90169800
H	-1.12353100	3.47500800	-2.96623700
H	-1.53487200	4.24624400	-1.42422000
H	0.16118800	3.88040100	-1.81464600



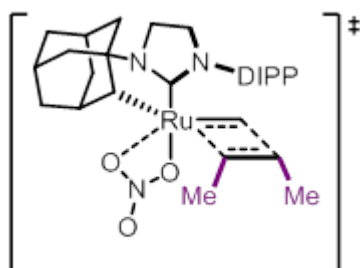
26c

SCF Energy (M06, n-octanol):	-1654.326015
SCF Energy (B3LYP, gas-phase):	-1653.960799
Enthalpy Correction:	0.754060
Free-Energy Correction:	0.653245

Ru	0.70396800	0.86762100	-0.25366800
O	2.04019000	2.38957300	1.52627100
O	2.00105400	2.57534700	-0.64999400
N	0.52404400	-1.99119000	0.09688300
N	-1.58035300	-1.40228400	-0.01758800
C	-0.29779900	-0.91439000	0.00740800
C	-0.15581100	-3.27243900	-0.09436800
H	0.20484100	-4.03299300	0.60329500
H	-0.00497200	-3.64404000	-1.11797700
C	-1.61140800	-2.87336400	0.16175700
H	-2.31478300	-3.33524000	-0.53506500
H	-1.92993700	-3.11786700	1.18310400
C	1.96792400	-1.78327400	-0.01753400
C	2.44171000	-1.87986700	-1.49358200
H	1.85554100	-1.18724100	-2.11032100
H	2.25731300	-2.89481400	-1.87478200

C	3.94303900	-1.54141500	-1.58645300
H	4.26320900	-1.61240900	-2.63434300
C	4.74246200	-2.54477700	-0.73016000
H	4.60672800	-3.56603100	-1.11414400
H	5.81583600	-2.32071100	-0.79176100
C	4.27264300	-2.45844800	0.73692700
H	4.83737400	-3.17396600	1.34910500
C	2.76987300	-2.80791000	0.81960100
H	2.42365500	-2.78198000	1.86134900
H	2.60659100	-3.82857600	0.44242000
C	4.50240600	-1.02615000	1.25941100
H	4.19945000	-0.94949700	2.31220400
H	5.57251600	-0.78000500	1.21594100
C	3.69772900	-0.01165800	0.40177300
H	3.88008000	0.99037500	0.79295200
C	2.20911500	-0.36764700	0.54008600
H	1.92419900	-0.34975200	1.60243400
C	4.16937100	-0.10851200	-1.06317900
H	3.62832000	0.61958400	-1.67920200
H	5.23548700	0.14832100	-1.12810700
C	-2.80250300	-0.69138800	0.25327600
C	-3.72498800	-0.49233600	-0.80109400
C	-4.92423500	0.17215400	-0.51257000
H	-5.64354500	0.34411000	-1.30799400
C	-5.21739900	0.60386700	0.77744500
C	-4.32270500	0.35124600	1.81342300
H	-4.57371100	0.66529800	2.82258300
C	-3.10904100	-0.30861100	1.58262000
C	-3.49313200	-1.04543200	-2.20623800
H	-2.45142300	-1.37707000	-2.26350100
C	-2.20461100	-0.63464100	2.77203600
H	-1.26943700	-1.05301200	2.38968000
C	-0.05604700	1.06201400	-2.07947000
C	-0.85410100	2.10936100	0.22673100
C	-1.00386500	2.12216300	-1.34911900
H	-0.61776000	0.26104600	-2.56367800
H	0.63538800	1.55133900	-2.77321000
H	-2.01635900	1.74188300	-1.51117400
H	-1.67915700	1.56279300	0.67548500
H	-6.15186500	1.12062800	0.97937400
C	-2.86380000	-1.69958600	3.67564000
H	-3.78553000	-1.31634600	4.12897100
H	-3.12503000	-2.60622200	3.11782300
H	-2.18492400	-1.98335300	4.48838500
C	-1.82770100	0.60527900	3.60546000
H	-2.70895800	1.07863300	4.05386300
H	-1.15869600	0.31500600	4.42371100
H	-1.30934000	1.35356200	3.00084900
C	-4.39675300	-2.27356200	-2.45549400
H	-5.45556100	-1.98844800	-2.44883900
H	-4.17634700	-2.72144800	-3.43175200
H	-4.26141800	-3.04418300	-1.68845600
C	-3.71011200	-0.00541800	-3.32132600
H	-3.06510500	0.86895900	-3.19351800
H	-3.48335100	-0.45063300	-4.29706100
H	-4.74819800	0.34441500	-3.35620000
N	2.43596600	3.00558900	0.50192000
O	3.19334300	3.96799700	0.54030200
C	-0.65462400	3.43295500	0.93688900
H	-1.60449500	3.99052500	0.93810200
H	-0.36921200	3.27068900	1.97975500
H	0.10262700	4.06923200	0.47791600
C	-0.83420900	3.50588600	-1.98956200

H	-1.06188700	3.44712400	-3.05998200
H	-1.50925200	4.24254900	-1.54035000
H	0.19366800	3.86168700	-1.87964700



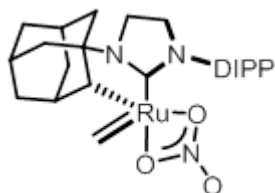
27-TS

SCF Energy (M06, n-octanol):	-1654.307801
SCF Energy (B3LYP, gas-phase):	-1653.946927
Enthalpy Correction:	0.751656
Free-Energy Correction:	0.651000

Ru	0.63032000	0.87519800	-0.36822200
O	1.84920200	2.69855800	-0.71347300
O	1.35221200	2.36623300	1.37804100
N	0.67307900	-1.90270900	0.45906600
N	-1.46250800	-1.46362100	0.25083700
C	-0.20810500	-0.91042800	0.16914800
C	0.05804600	-3.22729800	0.55749700
H	0.45989600	-3.79818200	1.39909800
H	0.22912000	-3.80528400	-0.36170300
C	-1.41831800	-2.86110500	0.73689900
H	-2.09421300	-3.49672800	0.15963100
H	-1.72669300	-2.90121200	1.78991700
C	2.10367500	-1.66795700	0.23611500
C	2.52005000	-2.10817700	-1.18934200
H	1.86915200	-1.62233100	-1.92402700
H	2.38998700	-3.19498400	-1.29799400
C	3.99053400	-1.72599500	-1.44543700
H	4.27227500	-2.03211200	-2.46203000
C	4.88492200	-2.45017700	-0.41911800
H	4.79262400	-3.53948800	-0.53811100
H	5.94009600	-2.19842300	-0.59122000
C	4.47185600	-2.03031300	1.00670200
H	5.10226400	-2.54881000	1.74136300
C	2.99444100	-2.42263800	1.25288300
H	2.69079500	-2.15731000	2.27422900
H	2.88260000	-3.51254600	1.14793900
C	4.65110200	-0.50359200	1.14998200
H	4.40220800	-0.18231000	2.17008100
H	5.70459600	-0.23902700	0.97965900
C	3.74111200	0.23113000	0.12992100
H	3.88454300	1.31052000	0.23767700
C	2.28509100	-0.15395900	0.45076000
H	2.11088000	0.03872900	1.51897500
C	4.14417700	-0.19770000	-1.29555800
H	3.52033600	0.32086600	-2.03386700
H	5.18525400	0.09380500	-1.49203800
C	-2.71574300	-0.76742300	0.34802800
C	-3.61247400	-0.81848900	-0.74583100
C	-4.83608500	-0.14725900	-0.62662200
H	-5.53845500	-0.16410700	-1.45511000
C	-5.17530600	0.53142100	0.54064500
C	-4.30448500	0.52418300	1.62651700
H	-4.59163700	1.03058900	2.54371400
C	-3.06859800	-0.13276800	1.56360200
C	-3.32421700	-1.64718600	-1.99746400
H	-2.26832900	-1.93524300	-1.96619700

C	-2.18895700	-0.18649200	2.81338800
H	-1.25509400	-0.69386600	2.55625600
C	0.36537800	0.48614700	-2.18821600
H	-0.24204300	-0.29959900	-2.65421400
C	-1.20549200	2.25603900	-0.32288900
H	-1.89309000	1.67263500	0.27814400
C	-1.18245300	1.92947700	-1.70356900
H	-1.89369900	1.16533700	-1.99985400
H	0.93174600	1.07183000	-2.92356400
N	1.97254000	3.07598600	0.51693200
O	2.64055100	4.05199000	0.81977200
C	-3.55866500	-0.88675600	-3.31630000
H	-3.29510500	-1.52591000	-4.16703200
H	-4.60801400	-0.59630200	-3.44037500
H	-2.95150500	0.02154100	-3.38111900
C	-4.16916600	-2.94055300	-1.98915800
H	-3.91115800	-3.57451500	-2.84583500
H	-4.01437600	-3.52375900	-1.07493600
H	-5.23898700	-2.70865700	-2.05251900
C	-2.87918900	-1.01214000	3.92103100
H	-3.79993200	-0.52629900	4.26485500
H	-3.14746500	-2.01648700	3.57283400
H	-2.21469300	-1.11717700	4.78653500
C	-1.80266600	1.20799200	3.34264300
H	-1.21131600	1.76459400	2.61089200
H	-2.68588200	1.80337500	3.60214900
H	-1.19481600	1.10666600	4.24905100
H	-6.12803900	1.04959300	0.61087000
C	-1.00931900	3.67478700	0.16145200
H	-1.94828200	4.23208800	0.01926500
H	-0.76615800	3.70298000	1.22536700
H	-0.22659600	4.20782900	-0.38144700
C	-0.86582300	2.97974300	-2.75173000
H	0.09830800	3.45868500	-2.56036900
H	-0.84641700	2.55202600	-3.75822700
H	-1.63820100	3.76132800	-2.73338300

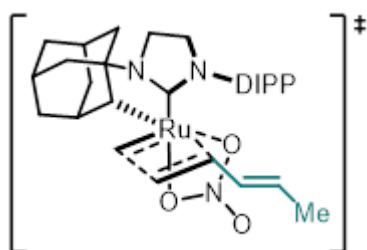
Diastereomeric Pathway C

**39**

SCF Energy (M06, n-octanol): -1497.159821
SCF Energy (B3LYP, gas-phase): -1496.729610
Enthalpy Correction: 0.633925
Free-Energy Correction: 0.541623

Ru	-0.59213000	0.78999100	-0.89605300
O	0.23766000	2.60608000	-0.02367900
O	-1.30120900	2.86397800	-1.54242400
N	-0.76711200	-1.71220800	0.49630400
N	1.37430500	-1.20537900	0.45674300
C	0.14340700	-0.80170400	0.05195700
C	-0.19308100	-2.64645800	1.46783600
H	-0.55656000	-3.66595800	1.31306000
H	-0.43495300	-2.34572300	2.49785200
C	1.30973100	-2.50363000	1.16555800
H	1.93105400	-2.48604500	2.06391300
H	1.66981700	-3.30757600	0.51119000
C	-2.17463900	-1.29074000	0.42174500
C	-2.53034800	-0.34713100	1.60320300
H	-1.80759000	0.48267800	1.64387700
H	-2.44508300	-0.88616300	2.55781800
C	-3.95810800	0.20498300	1.42745700
H	-4.19807300	0.86448100	2.27164800
C	-4.95065900	-0.97490900	1.39155800
H	-4.91703500	-1.52742400	2.34131200
H	-5.97655400	-0.60029700	1.27643600
C	-4.59815400	-1.91041200	0.21558000
H	-5.30538300	-2.74959100	0.18680900
C	-3.16708700	-2.46977900	0.41170600
H	-2.90819600	-3.16000300	-0.40195100
H	-3.11842100	-3.03765000	1.35333400
C	-4.68584800	-1.11145900	-1.10447200
H	-4.47011400	-1.76592800	-1.95969900
H	-5.70983600	-0.73505600	-1.23914800
C	-3.67937000	0.06877100	-1.07488900
H	-3.74177000	0.62872400	-2.01591400
C	-2.26931800	-0.52633000	-0.91924700
H	-2.11764900	-1.26175900	-1.71396900
C	-4.03366300	0.99685700	0.10539000
H	-3.34940500	1.85553100	0.13091600
H	-5.04472800	1.40530600	-0.02783800
C	2.61362700	-0.48062300	0.34814100
C	2.95541700	0.43623000	1.37079900
C	4.18494400	1.09881700	1.27349000
H	4.46570800	1.81311000	2.04163600
C	5.05569100	0.85538500	0.21615800
C	4.71471400	-0.07051000	-0.76483000
H	5.40814000	-0.26546400	-1.57756700
C	3.49558800	-0.75812100	-0.72018600
C	2.07756800	0.67509200	2.59736900
H	1.10349700	0.21232100	2.41095900
C	3.18873200	-1.80934100	-1.78244400
H	2.12797200	-2.06863500	-1.69897200
C	0.05592500	0.31329300	-2.52288100
H	0.70051100	-0.53726600	-2.75917000

C	2.69053000	-0.00632200	3.84066700
H	3.65989900	0.43982300	4.09244200
H	2.03121100	0.11407800	4.70866300
H	2.85479600	-1.07911500	3.68448800
C	1.82400000	2.16865100	2.87703300
H	1.12975600	2.27405500	3.71981000
H	2.74763100	2.69112500	3.15326000
H	1.39076100	2.66834300	2.00717100
C	4.00657200	-3.09540000	-1.53529400
H	3.74627100	-3.86596000	-2.27099000
H	5.08144400	-2.89705500	-1.62238400
H	3.82825200	-3.50533900	-0.53484700
C	3.42997400	-1.29708200	-3.21550200
H	4.49517600	-1.13035200	-3.41213100
H	3.07727000	-2.03578200	-3.94496900
H	2.90520200	-0.35451600	-3.39991500
H	6.00466000	1.38224200	0.16075700
N	-0.49934600	3.43094900	-0.72583200
O	-0.41239800	4.63021900	-0.58618100
H	-0.18818900	0.97271900	-3.36921300

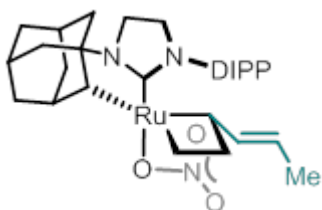


40-TS

SCF Energy (M06, n-octanol):	-1692.365370
SCF Energy (B3LYP, gas-phase):	-1692.027744
Enthalpy Correction:	0.757100
Free-Energy Correction:	0.654337

Ru	-0.56721300	0.52168200	-0.89645800
O	-1.76173500	1.87149800	0.56117300
O	-1.91052400	2.16737000	-1.58714300
N	-0.52501700	-2.06308000	0.40552900
N	1.57592100	-1.44224700	0.40724200
C	0.30826400	-1.05120600	0.04245100
C	0.12228500	-3.08385000	1.23209600
H	-0.20629700	-4.09020300	0.96098500
H	-0.09875000	-2.92333800	2.29743300
C	1.59370800	-2.83723400	0.90332700
H	2.25928200	-2.93871000	1.76299300
H	1.94622500	-3.51429100	0.11487400
C	-1.97750900	-1.86466300	0.35026800
C	-2.51333800	-1.34829400	1.71018900
H	-1.98892900	-0.42362100	1.97729900
H	-2.31023100	-2.08925500	2.49755400
C	-4.03080600	-1.08609200	1.61401100
H	-4.39732600	-0.73886600	2.58923100
C	-4.76108300	-2.38434300	1.21669100
H	-4.60788600	-3.16185900	1.97947500
H	-5.84280100	-2.20250900	1.15858900
C	-4.23116500	-2.86849300	-0.14774000
H	-4.75369700	-3.78860700	-0.44238900
C	-2.72117200	-3.17270400	-0.01245900
H	-2.31761200	-3.57257500	-0.95242200
H	-2.57596500	-3.94216400	0.76116300
C	-4.47218100	-1.77150000	-1.21006200
H	-4.13628200	-2.11947800	-2.19660100
H	-5.55024400	-1.57198200	-1.29151100
C	-3.71495000	-0.47357700	-0.81193300

H	-3.88833900	0.29541000	-1.57312300
C	-2.21329600	-0.83976200	-0.77234400
H	-2.01259800	-1.36981900	-1.71116400
C	-4.27840700	-0.00194700	0.54779000
H	-3.82126300	0.93663700	0.86445700
H	-5.35781500	0.18018700	0.44784200
C	2.80382100	-0.69746800	0.41212000
C	3.06739200	0.19217800	1.48602800
C	4.30679300	0.84384100	1.51159800
H	4.52757500	1.53830800	2.31562600
C	5.26904100	0.61285900	0.53223700
C	5.00728600	-0.28447300	-0.49694100
H	5.76805200	-0.46948100	-1.24984800
C	3.78002800	-0.95605200	-0.57981900
C	2.07559800	0.40782000	2.63166600
H	1.06873700	0.22520400	2.24435500
C	3.55947900	-1.96024400	-1.71025000
H	2.50187700	-2.24378000	-1.70492800
C	1.01107400	2.34502900	-0.56456700
H	1.36236900	2.02461600	0.41007800
C	0.22238700	0.09094100	-2.54544300
H	1.01816200	-0.62285200	-2.78612100
C	1.51479200	1.68328000	-1.69002000
H	2.32787800	0.98145600	-1.56908900
C	4.39851200	-3.23682300	-1.48499000
H	4.18825500	-3.97830500	-2.26495000
H	5.47081900	-3.01024100	-1.51887600
H	4.19079300	-3.69667600	-0.51291800
C	3.86807600	-1.37330000	-3.10198300
H	4.93024100	-1.12827400	-3.21347900
H	3.61786400	-2.10308200	-3.88079200
H	3.29315400	-0.46248400	-3.29765600
C	2.33071200	-0.59724500	3.77682000
H	2.24877600	-1.63618800	3.44368200
H	3.33528400	-0.46073200	4.19498700
H	1.60512600	-0.44648700	4.58486400
C	2.09240500	1.83708400	3.20667400
H	1.24545400	1.96822700	3.88885400
H	3.00446900	2.03673100	3.78147900
H	2.01618900	2.60023100	2.42595200
H	6.22496700	1.12786900	0.57674800
H	1.45235800	2.19086900	-2.64980500
N	-2.29254700	2.52114400	-0.41142200
O	-3.11147900	3.40832300	-0.23313600
C	0.40865300	3.66910900	-0.65103200
H	0.21400800	4.05325800	-1.65200000
C	0.08098600	4.42038600	0.41446200
H	0.24602700	4.01338500	1.41226000
C	-0.55887700	5.77247800	0.34484100
H	0.00069000	6.51507800	0.92975300
H	-0.63504500	6.13014400	-0.68725400
H	-1.57423100	5.73076800	0.76121900
H	-0.16158000	0.60082600	-3.44135700

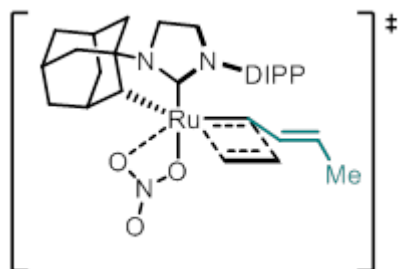


41

SCF Energy (M06, n-octanol):	-1692.399534
SCF Energy (B3LYP, gas-phase):	-1692.055053
Enthalpy Correction:	0.759883
Free-Energy Correction:	0.654916

Ru	-0.61833900	0.34531500	-0.81261100
O	-1.75546900	-0.71983300	-3.07023900
O	-1.96772500	1.29690600	-2.24980600
N	-0.26279500	-1.26677300	1.55376800
N	1.78205300	-0.64685000	1.07615700
C	0.48186900	-0.58493400	0.64839700
C	0.46972600	-1.62932000	2.76730900
H	0.22949400	-2.64279300	3.10012800
H	0.23538900	-0.93422800	3.58598200
C	1.92011400	-1.48678600	2.29003800
H	2.57021900	-1.00419400	3.02392000
H	2.36170300	-2.45587900	2.02552000
C	-1.72050300	-1.22822800	1.42058600
C	-2.32567300	-0.02195500	2.18740600
H	-1.83602300	0.90340800	1.85863200
H	-2.13168600	-0.13124500	3.26442900
C	-3.84287000	0.05861800	1.92471500
H	-4.25792800	0.91275300	2.47576800
C	-4.51050000	-1.24540700	2.40670200
H	-4.36404100	-1.36977000	3.48933900
H	-5.59417300	-1.20023000	2.23431800
C	-3.90857200	-2.44463900	1.64486000
H	-4.38235500	-3.37468800	1.98538900
C	-2.39080100	-2.52528700	1.92736700
H	-1.94785000	-3.39091300	1.41706900
H	-2.22151000	-2.65602000	3.00676500
C	-4.15244600	-2.25756100	0.13277000
H	-3.75694300	-3.11523700	-0.42741100
H	-5.23227700	-2.21545000	-0.06694700
C	-3.47710200	-0.94794500	-0.35762000
H	-3.65598000	-0.83933300	-1.42928700
C	-1.97010500	-1.08408300	-0.09253200
H	-1.58420800	-1.97661000	-0.60699800
C	-4.07996100	0.24532300	0.41221100
H	-3.62985100	1.18329100	0.06559600
H	-5.15719500	0.31330900	0.20771200
C	2.96717000	-0.42013400	0.29049700
C	3.76974100	0.70906300	0.57433600
C	4.93166600	0.90116900	-0.18463000
H	5.55894700	1.76620700	0.00995100
C	5.30186700	-0.00196400	-1.17649400
C	4.52753500	-1.13553300	-1.40693200
H	4.84026000	-1.84979200	-2.16323400
C	3.35766400	-1.37958700	-0.67613000
C	3.45335700	1.67037300	1.71825200
H	2.43948100	1.44779600	2.06667700
C	2.59773400	-2.68700800	-0.90718300
H	1.68035900	-2.66282900	-0.31243000
C	-0.00282800	2.16289600	-0.19391300
H	0.65836000	2.18880400	0.67454400
C	0.85392100	0.59750100	-2.17018200
H	1.79475600	0.07181200	-2.04338000
C	0.83685900	2.02648000	-1.55991600
H	1.86457500	2.29414300	-1.30171000
C	3.43935100	-3.88829600	-0.42241300
H	2.86524900	-4.81771400	-0.51474300
H	4.35148200	-3.99880500	-1.02042400
H	3.74444000	-3.77804900	0.62468800
C	2.17082200	-2.89610000	-2.37326500
H	3.03454600	-2.93374200	-3.04739900
H	1.63688300	-3.84840100	-2.47111200
H	1.50112000	-2.10367200	-2.71738600

C	4.42018400	1.43908300	2.90064300
H	4.40680900	0.39799500	3.24230200
H	5.45208600	1.67676200	2.61597300
H	4.15036300	2.07954800	3.74883100
C	3.48546800	3.15209000	1.29888500
H	3.20124100	3.78736700	2.14586700
H	4.48662700	3.46360600	0.98009700
H	2.79211000	3.35830900	0.47799400
H	6.20398600	0.16781800	-1.75819200
H	0.41620400	2.72936500	-2.28044000
N	-2.25608500	0.42779100	-3.18256100
O	-2.99268000	0.76157300	-4.10295000
C	-1.01296400	3.23795100	-0.16320200
H	-1.64086100	3.34187500	-1.04711300
C	-1.21360500	4.04543300	0.89240800
H	-0.57676900	3.92923200	1.77248400
C	-2.25810700	5.12094700	0.96704700
H	-2.94844200	4.95028000	1.80515600
H	-1.80487300	6.10824600	1.13360800
H	-2.84942100	5.16909200	0.04668300
H	0.47332100	0.54339200	-3.19004000

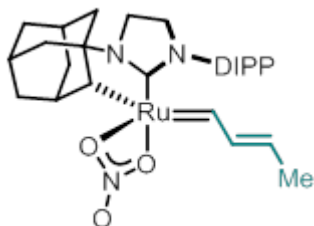


42-TS

SCF Energy (M06, n-octanol):	-1692.386772
SCF Energy (B3LYP, gas-phase):	-1692.046883
Enthalpy Correction:	0.758093
Free-Energy Correction:	0.653890

Ru	0.56254300	0.27158700	0.88669100
O	1.88428900	0.89585300	2.54854400
O	1.25242600	-1.17473300	2.77189700
N	0.31641500	-1.11538300	-1.64321600
N	-1.74445100	-0.55152200	-1.16142000
C	-0.45331500	-0.51699400	-0.69988200
C	-0.39602000	-1.40856700	-2.88734700
H	-0.13904900	-2.39720400	-3.27760000
H	-0.15519500	-0.66279500	-3.65802400
C	-1.85538200	-1.31041900	-2.42832200
H	-2.49803700	-0.78714800	-3.14075000
H	-2.29237700	-2.29844200	-2.23457600
C	1.77588700	-1.06819000	-1.50474200
C	2.36840800	0.15935600	-2.24198600
H	1.86565000	1.06884600	-1.89637500
H	2.18800400	0.06974000	-3.32346300
C	3.88226600	0.25025000	-1.96621800
H	4.29152700	1.12651700	-2.48685300
C	4.56928400	-1.02909700	-2.48492500
H	4.42860700	-1.12109900	-3.57168800
H	5.65181100	-0.97642400	-2.30628100
C	3.97777400	-2.25750600	-1.76251900
H	4.46096700	-3.17149500	-2.13267100
C	2.46022500	-2.34268100	-2.05436200
H	2.02379800	-3.22841600	-1.57407900
H	2.30101800	-2.44311800	-3.13888500
C	4.22573900	-2.11417300	-0.24500200
H	3.84756100	-2.99540800	0.28968700

H	5.30699700	-2.06220100	-0.05286400
C	3.52403400	-0.83519600	0.28437000
H	3.71088600	-0.74392100	1.35869300
C	2.01741000	-0.99074100	0.01411200
H	1.69155800	-1.95047500	0.44176300
C	4.10748800	0.39145500	-0.44655100
H	3.63549200	1.30982300	-0.07798400
H	5.18277400	0.47500200	-0.23547300
C	-2.94586500	-0.35936400	-0.39516300
C	-3.72872200	0.79429200	-0.63383900
C	-4.90756200	0.95774600	0.10500500
H	-5.52059300	1.83992500	-0.05588500
C	-5.31350500	0.00323900	1.03306500
C	-4.55815600	-1.15151200	1.21694200
H	-4.89838200	-1.90442700	1.92220200
C	-3.37168700	-1.36770500	0.50390100
C	-3.37344500	1.80922200	-1.71918600
H	-2.35667900	1.58668400	-2.05911900
C	-2.62945800	-2.69371800	0.67930400
H	-1.70149000	-2.64824800	0.10259600
C	0.37029400	2.03983300	0.15583200
H	-0.31062000	2.27908200	-0.66980500
C	-1.05610500	0.58762000	2.28502700
H	-1.93491000	0.00338100	2.04417300
C	-0.94215600	1.90158700	1.73224600
H	-1.76584700	2.25543900	1.12095800
N	1.94484000	-0.20893300	3.22472600
O	2.63482500	-0.29378000	4.22921700
C	-3.38911000	3.26909500	-1.22883000
H	-3.09840300	3.94116200	-2.04481700
H	-4.38575900	3.57674300	-0.89279100
H	-2.69278900	3.42998200	-0.39987900
C	-4.32147900	1.65546500	-2.92917100
H	-4.02172900	2.32838800	-3.74147100
H	-4.32354200	0.63133500	-3.31843100
H	-5.35332500	1.90252200	-2.65235300
C	-3.47337800	-3.85794900	0.11523600
H	-4.39893400	-3.99143600	0.68761000
H	-3.75532500	-3.68829600	-0.93052600
H	-2.90994400	-4.79682900	0.16871100
C	-2.22913200	-2.98262100	2.13949200
H	-1.54004000	-2.22830900	2.52838700
H	-3.10317500	-3.02826100	2.79996900
H	-1.72219000	-3.95264200	2.19829100
H	-6.22864900	0.15039700	1.60041600
H	-0.44855300	2.65899000	2.33348500
H	-0.64057900	0.41392200	3.27346200
C	1.29958500	3.12574900	0.46175100
H	1.97387700	2.98207800	1.30531000
C	1.39046000	4.24586500	-0.28221500
H	0.70447500	4.37313400	-1.12229300
C	2.38476800	5.34638300	-0.06397900
H	3.03131500	5.47661300	-0.94301100
H	1.87961500	6.30912000	0.09561100
H	3.02347300	5.14574500	0.80203100

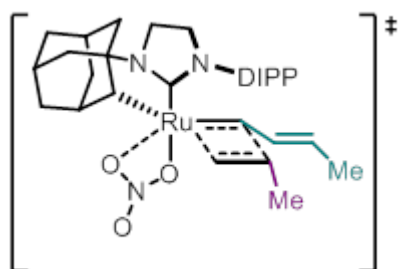


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SCF Energy (M06, n-octanol): -1613.834302
 SCF Energy (B3LYP, gas-phase): -1613.466877
 Enthalpy Correction: 0.700216
 Free-Energy Correction: 0.599364

Ru	-0.44378100	0.48414000	-0.87306500
O	1.12568200	1.02448200	-2.33659000
O	-0.86737400	1.84131100	-2.65280600
N	-0.69877700	-1.74436900	0.94915200
N	1.41224700	-1.13324500	1.00312800
C	0.20261900	-0.86177400	0.44768500
C	-0.15555400	-2.55380300	2.04334500
H	-0.43885800	-3.60634800	1.94962400
H	-0.51609100	-2.18797500	3.01467800
C	1.35901900	-2.32918100	1.87157000
H	1.87655800	-2.14606100	2.81740900
H	1.84495600	-3.17727800	1.37332600
C	-2.11906800	-1.50089500	0.67647000
C	-2.77089100	-0.69511400	1.82862200
H	-2.18799500	0.21377800	2.00869800
H	-2.75169400	-1.28963200	2.75351000
C	-4.22353300	-0.33418000	1.46298900
H	-4.67169200	0.23573200	2.28780300
C	-5.02493600	-1.63109700	1.23319300
H	-5.04868800	-2.23115700	2.15414300
H	-6.06711000	-1.39275100	0.98098500
C	-4.37830200	-2.43600800	0.08656200
H	-4.94513700	-3.36118500	-0.08141000
C	-2.92385500	-2.80445700	0.47146300
H	-2.45527500	-3.40421600	-0.32012700
H	-2.92860600	-3.41554000	1.38666300
C	-4.39471300	-1.57750800	-1.19759700
H	-3.97479500	-2.14357300	-2.04019300
H	-5.43270300	-1.33259900	-1.46346600
C	-3.57678500	-0.27660000	-0.97291200
H	-3.58262200	0.32419100	-1.89064700
C	-2.13539300	-0.68867800	-0.63653400
H	-1.79734100	-1.38269100	-1.44371300
C	-4.21818500	0.52160100	0.17974800
H	-3.66390100	1.45191400	0.34890900
H	-5.24710500	0.79949300	-0.08824700
C	2.68246300	-0.60395600	0.57992500
C	3.28569100	0.41275400	1.35228300
C	4.54589000	0.87981700	0.96016100
H	5.02749600	1.66416300	1.53746700
C	5.19155000	0.35679700	-0.15588300
C	4.58663700	-0.65269200	-0.89821400
H	5.09929100	-1.05645000	-1.76640900
C	3.32881200	-1.15835600	-0.54870500
C	2.62624200	0.99203900	2.59949400
H	1.61882100	0.56923400	2.66828200
C	2.73268300	-2.30119400	-1.36748900
H	1.70722500	-2.46850700	-1.02290600
C	-0.66856500	1.76408400	0.44609200
H	-0.34092200	1.60612500	1.48225300
H	6.16784300	0.73530000	-0.44696500
C	3.39140700	0.58413400	3.87551100
H	4.40915300	0.99201200	3.87560400

H	2.88009900	0.96156800	4.76937100
H	3.47405800	-0.50543600	3.96559400
C	2.47761100	2.52314500	2.51899900
H	1.93436200	2.89778600	3.39536600
H	3.45263200	3.02384300	2.49961600
H	1.92889700	2.82143600	1.62024800
C	3.52095100	-3.60943000	-1.14392000
H	3.56615400	-3.88519800	-0.08376600
H	3.05431000	-4.43684700	-1.69190800
H	4.55282300	-3.51243100	-1.50153600
C	2.65363300	-1.97166700	-2.87114600
H	3.65160100	-1.87777300	-3.31527800
H	2.13472200	-2.77837600	-3.40337600
H	2.11949300	-1.03350300	-3.04337800
N	0.34189300	1.76314300	-3.07057900
O	0.73972700	2.32130700	-4.07028200
C	-1.23668800	3.07582400	0.20318600
H	-1.55931900	3.31125500	-0.80997700
C	-1.37149100	4.00755100	1.17455000
H	-1.03251500	3.76147400	2.18276800
C	-1.95235500	5.37483600	0.98450000
H	-2.82443600	5.52855400	1.63567300
H	-1.22441200	6.15317300	1.25349600
H	-2.26409500	5.54089800	-0.05149700

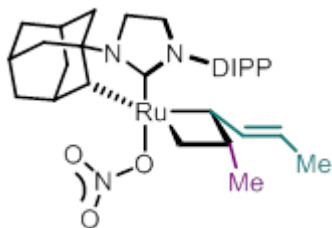


44-TS

SCF Energy (M06, n-octanol):	-1731.679930
SCF Energy (B3LYP, gas-phase):	-1731.359476
Enthalpy Correction:	0.788290
Free-Energy Correction:	0.682205

Ru	0.57330000	0.42213000	0.73595000
O	1.88740800	1.47717100	2.17796900
O	1.30852200	-0.47109800	2.95753300
N	0.35387200	-1.55741000	-1.36734600
N	-1.71680500	-0.91360700	-1.05472500
C	-0.42916700	-0.75420900	-0.60520900
C	-0.34199500	-2.14669800	-2.51182800
H	-0.07321300	-3.19721000	-2.65260800
H	-0.09855700	-1.60344000	-3.43582100
C	-1.80652600	-1.95681800	-2.10270300
H	-2.44557000	-1.62775700	-2.92594600
H	-2.23666100	-2.87410200	-1.68054200
C	1.81046300	-1.46995600	-1.22546800
C	2.40915300	-0.45256800	-2.22951700
H	1.89835900	0.51033800	-2.11829500
H	2.24046300	-0.80057200	-3.25945900
C	3.91921000	-0.29010400	-1.96728500
H	4.33299600	0.43599700	-2.67989600
C	4.61604800	-1.65338900	-2.15217400
H	4.48915100	-2.00719600	-3.18553700
H	5.69597700	-1.55261200	-1.97901100
C	4.01879600	-2.67330300	-1.16044400
H	4.50931300	-3.64701000	-1.29161400
C	2.50537200	-2.83558500	-1.44022700
H	2.06608300	-3.58096300	-0.76405900

H	2.35948100	-3.19703500	-2.46962000
C	4.24414000	-2.16477800	0.27986400
H	3.86011900	-2.89219700	1.00719200
H	5.32215900	-2.06113300	0.46907400
C	3.53357000	-0.79897300	0.47470500
H	3.70771100	-0.45294800	1.49768100
C	2.03069900	-1.02200500	0.23206000
H	1.69562000	-1.84411700	0.88137000
C	4.12586700	0.21598900	-0.52435800
H	3.65162200	1.19584300	-0.39401800
H	5.19867000	0.34988900	-0.32719600
C	-2.92552800	-0.58811900	-0.34621300
C	-3.74525500	0.45607800	-0.83492200
C	-4.92721400	0.74708400	-0.14130200
H	-5.57004800	1.54926600	-0.49268900
C	-5.29905800	0.01942400	0.98537500
C	-4.50673500	-1.03888300	1.42110600
H	-4.82008400	-1.61873200	2.28477200
C	-3.31729100	-1.37721300	0.76292000
C	-3.42486100	1.20617100	-2.12687200
H	-2.39907200	0.95008900	-2.41184200
C	-2.53436200	-2.60604100	1.23091700
H	-1.61763700	-2.67799900	0.63918100
C	0.29553400	1.96476700	-0.38236200
H	-0.40043200	1.97253200	-1.22893400
C	-1.05286800	0.99777100	1.98447000
H	-1.90670500	0.34118300	1.87644000
C	-1.01556300	2.19161300	1.16860500
H	-1.84619500	2.26074300	0.47046900
C	-0.63005700	3.50081400	1.83484700
H	-0.45595600	4.30182400	1.11110000
H	-1.44919600	3.81271600	2.49604200
H	0.26982600	3.37588800	2.44291900
N	1.96981400	0.59826500	3.12961200
O	2.65445400	0.81236000	4.11940600
C	-3.49848800	2.73841200	-1.98827300
H	-3.22090600	3.21290100	-2.93681600
H	-4.50989400	3.07825600	-1.73821200
H	-2.81970400	3.11333500	-1.21594100
C	-4.36163500	0.74051600	-3.26348800
H	-4.08621700	1.21990600	-4.21051100
H	-4.32106200	-0.34494000	-3.40645900
H	-5.40346900	1.00347000	-3.04486600
C	-3.35402500	-3.89028300	0.97834400
H	-4.26438000	-3.90778600	1.58904000
H	-3.66036200	-3.97902200	-0.07057500
H	-2.76238900	-4.77611400	1.23719500
C	-2.10183000	-2.52835200	2.70850500
H	-1.41881700	-1.69377900	2.88754700
H	-2.96273000	-2.42173000	3.37891800
H	-1.57793000	-3.44920900	2.98972700
H	-6.21655200	0.26531600	1.51341900
C	1.25244900	3.06875900	-0.42172600
H	1.95727800	3.15211900	0.40418200
C	1.33850600	3.92966800	-1.45551000
H	0.62345100	3.83617600	-2.27551900
C	2.36618300	5.01353500	-1.59017800
H	2.98259900	4.86713800	-2.48820100
H	1.89133700	5.99881700	-1.69664600
H	3.03254400	5.04603600	-0.72216100
H	-0.67863200	1.08596700	3.00292700

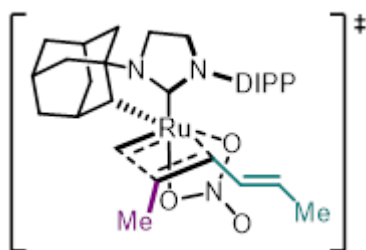


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SCF Energy (M06, n-octanol): -1731.690010
 SCF Energy (B3LYP, gas-phase): -1731.366153
 Enthalpy Correction: 0.789787
 Free-Energy Correction: 0.683192

Ru	-0.62824500	0.44574600	-0.67244300
O	-1.75701500	-0.07663900	-3.12525500
O	-1.97060800	1.69914300	-1.86508200
N	-0.30876600	-1.67709000	1.25370000
N	1.74780200	-0.99004400	0.94706400
C	0.45194200	-0.81079500	0.53820100
C	0.40910600	-2.32438300	2.35214000
H	0.15506800	-3.38460500	2.43539100
H	0.17543800	-1.83846500	3.31012600
C	1.86469400	-2.09273700	1.93069800
H	2.51358900	-1.80472300	2.76148400
H	2.29686000	-2.97845700	1.44904300
C	-1.76505100	-1.58608100	1.13025600
C	-2.35487500	-0.58743800	2.16187100
H	-1.84928400	0.38214100	2.06579800
H	-2.16633900	-0.95395000	3.18162300
C	-3.86925600	-0.42277500	1.92633100
H	-4.27330900	0.28320900	2.66378000
C	-4.55935500	-1.79294600	2.08561900
H	-4.41868200	-2.17253700	3.10785700
H	-5.64142300	-1.69041800	1.92887900
C	-3.97352800	-2.78698500	1.06131600
H	-4.46216900	-3.76392200	1.17235100
C	-2.45765300	-2.95563300	1.31551900
H	-2.02709100	-3.68279400	0.61433900
H	-2.29366400	-3.34076600	2.33318000
C	-4.20956400	-2.24328900	-0.36308000
H	-3.82671300	-2.95026300	-1.11104100
H	-5.28793200	-2.13674100	-0.54625200
C	-3.51144700	-0.86638100	-0.52996700
H	-3.68861600	-0.50526100	-1.54491000
C	-2.00745700	-1.08634200	-0.30715700
H	-1.63542000	-1.84012900	-1.01662300
C	-4.09735900	0.12044800	0.50075200
H	-3.63180100	1.10679400	0.38595500
H	-5.17264900	0.25215000	0.31835400
C	2.94555100	-0.60175000	0.24805600
C	3.76264900	0.41208500	0.80113300
C	4.94025400	0.75440000	0.12335600
H	5.57960100	1.53495300	0.52569100
C	5.31109500	0.10559200	-1.05043900
C	4.52082900	-0.92406600	-1.55339800
H	4.83355100	-1.44472900	-2.45397500
C	3.33592200	-1.31155100	-0.91467700
C	3.44377900	1.08238100	2.13628800
H	2.42324700	0.79863900	2.41347900
C	2.56334800	-2.51684900	-1.45512600
H	1.62484400	-2.60183300	-0.90042400
C	0.00640100	2.06597300	0.34295500
H	0.63305700	1.87917100	1.21781800
C	0.85502900	0.97616700	-1.92772100
H	1.76925200	0.39152500	-1.95951100
C	0.93723500	2.21546200	-0.98105500

H	1.94862100	2.19421800	-0.56737400
C	0.68765200	3.52151400	-1.74706800
H	0.73910400	4.38836300	-1.07935800
H	1.44740200	3.64313200	-2.52742800
H	-0.29473100	3.50818300	-2.22607100
C	3.36849400	-3.81442800	-1.22140300
H	2.78549300	-4.68738600	-1.53759600
H	4.30126900	-3.80913800	-1.79759000
H	3.63606000	-3.94693600	-0.16672900
C	2.18826600	-2.38996300	-2.94467600
H	3.07511400	-2.29973000	-3.58247800
H	1.64352800	-3.28512100	-3.26616400
H	1.54449500	-1.52613100	-3.12936200
C	4.39371200	0.56660700	3.23956900
H	4.36715200	-0.52556700	3.32402000
H	5.43082400	0.85399100	3.02968500
H	4.11892900	0.99036800	4.21286300
C	3.49781500	2.62069700	2.07725900
H	3.20816600	3.04291500	3.04659000
H	4.50685400	2.98458300	1.85203900
H	2.81907300	3.02369200	1.31969800
H	6.22571100	0.38998600	-1.56387700
N	-2.25308800	1.06766100	-2.97503700
O	-2.98035200	1.60894300	-3.79970400
H	0.47145000	1.20457800	-2.92357700
C	-1.00419500	3.10784600	0.61199900
H	-1.63902300	3.41477900	-0.21620900
C	-1.20793300	3.64667000	1.82696100
H	-0.56910600	3.33352400	2.65610600
C	-2.26127000	4.66635000	2.14976800
H	-2.95286600	4.29715900	2.92025000
H	-1.81644800	5.58920900	2.54776300
H	-2.85053200	4.92744900	1.26443900



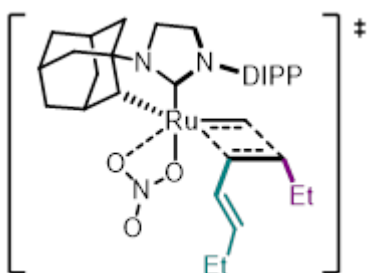
46-TS

SCF Energy (M06, n-octanol): -1731.659119
 SCF Energy (B3LYP, gas-phase): -1731.339581
 Enthalpy Correction: 0.787374
 Free-Energy Correction: 0.682014

Ru	-0.58028300	0.53526700	-0.81668400
O	-1.82401300	1.83668300	0.64905500
O	-1.83818900	2.26236600	-1.48251800
N	-0.64640000	-2.09926800	0.37781900
N	1.47620600	-1.56128700	0.42822800
C	0.22704000	-1.10329800	0.07205900
C	-0.04779900	-3.18749800	1.15306800
H	-0.41152100	-4.16430700	0.82464000
H	-0.27431500	-3.07724800	2.22381100
C	1.43493700	-2.98035700	0.84933200
H	2.08799100	-3.15372400	1.70700800
H	1.76807500	-3.62707800	0.02771600
C	-2.09047300	-1.86086000	0.28883000
C	-2.65862100	-1.39609400	1.65405500
H	-2.12120200	-0.49897400	1.98190000
H	-2.49947300	-2.17870100	2.41072600
C	-4.16573100	-1.09209800	1.52104900
H	-4.55631000	-0.78106500	2.49914100
C	-4.91179900	-2.35271300	1.04111200
H	-4.80149000	-3.16829100	1.77084800
H	-5.98661600	-2.14214100	0.95749800
C	-4.34899100	-2.78627900	-0.32747400
H	-4.88231900	-3.67892800	-0.68132800
C	-2.85161400	-3.13177600	-0.16054000
H	-2.42738500	-3.49515800	-1.10625500
H	-2.74795800	-3.94080100	0.57857500
C	-4.52774100	-1.63692500	-1.34560000
H	-4.16517200	-1.94863000	-2.33486900
H	-5.59723800	-1.40708700	-1.45497700
C	-3.75592500	-0.37670500	-0.86240300
H	-3.88622600	0.43036500	-1.59236700
C	-2.26536200	-0.77689500	-0.78764100
H	-2.03597200	-1.25960000	-1.74659700
C	-4.35651000	0.04415800	0.49817500
H	-3.89349400	0.95866700	0.87105900
H	-5.42878500	0.25022200	0.37081100
C	2.73500900	-0.87011900	0.47635600
C	3.03397900	-0.06033300	1.60304300
C	4.29731900	0.54060800	1.66760300
H	4.54384300	1.17422600	2.51332100
C	5.25108400	0.33340500	0.67504700
C	4.95704600	-0.49169700	-0.40438400
H	5.71232100	-0.66250000	-1.16599400
C	3.70508200	-1.10978800	-0.52701700
C	2.05392200	0.11963500	2.76444700
H	1.04055500	-0.01419500	2.37437400
C	3.45722400	-2.04662800	-1.70839500
H	2.38799900	-2.28149300	-1.73124100
C	1.01445700	2.23011700	-0.32457000
H	1.37367300	1.77847700	0.59320500
C	0.30374600	0.17390500	-2.43698100

H	1.08943800	-0.55315800	-2.66607000
C	1.54862400	1.72276200	-1.53549400
H	2.33600900	0.98772500	-1.41122600
C	1.66724800	2.60002300	-2.76994000
H	2.36797900	3.42276300	-2.57043800
H	2.05008300	2.03540200	-3.62488600
H	0.70880800	3.04091800	-3.05797600
C	4.23425400	-3.36968500	-1.53357700
H	4.00449100	-4.06164100	-2.35257300
H	5.31589600	-3.19019700	-1.54016600
H	3.98989700	-3.86700700	-0.58898200
C	3.81735600	-1.41080800	-3.06590500
H	4.89343900	-1.22398200	-3.15440400
H	3.53537600	-2.08546800	-3.88255500
H	3.29987000	-0.45886600	-3.22162400
C	2.28776900	-0.95324100	3.85127600
H	2.18026300	-1.97002800	3.46168800
H	3.29668300	-0.86371100	4.27166100
H	1.56859300	-0.82972400	4.66958200
C	2.11568500	1.51445400	3.41552300
H	1.27490400	1.63504700	4.10751500
H	3.03450000	1.65408600	3.99728000
H	2.06254500	2.31926100	2.67623100
H	6.22613000	0.80752600	0.74965900
N	-2.27198600	2.56306500	-0.30864200
O	-3.06086000	3.47596500	-0.12233500
C	0.47823100	3.58257900	-0.20767600
H	0.31781300	4.14139100	-1.12659400
C	0.15376900	4.16802900	0.95908300
H	0.26936400	3.60037700	1.88202000
C	-0.42655300	5.54213100	1.09312200
H	-1.45386900	5.48262200	1.47705000
H	0.14706600	6.15656600	1.80050500
H	-0.45943300	6.06183000	0.12991700
H	-0.04257000	0.70872800	-3.33143200

Transition states with larger substrate models



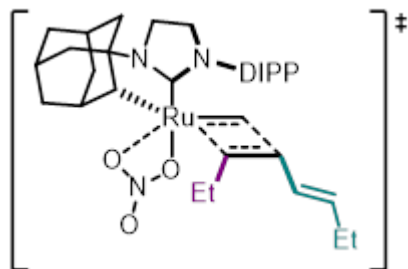
47-TS

SCF Energy (M06, n-octanol):	-1809.974472
SCF Energy (B3LYP, gas-phase):	-1810.253184
Enthalpy Correction:	0.847557
Free-Energy Correction:	0.734437

Ru	0.61872000	0.52289000	-0.51711100
O	1.35481100	2.55276400	-1.07638500
O	0.90352400	2.30902400	1.03578200
N	1.31458200	-2.04609900	0.60841700
N	-0.87353900	-2.11447000	0.47086500
C	0.22558800	-1.31598200	0.25542900
C	1.01703200	-3.45057700	0.88706100
H	1.56200500	-3.81478700	1.76243100
H	1.28443500	-4.08328500	0.02874500
C	-0.49790400	-3.39764700	1.10966000
H	-1.02904300	-4.23385400	0.64940200

H	-0.75458500	-3.37390700	2.17676100
C	2.64989300	-1.51246700	0.32096700
C	3.16092000	-2.00593000	-1.05536000
H	2.41347200	-1.78096500	-1.82309800
H	3.29441500	-3.09764100	-1.03279500
C	4.49729200	-1.31750900	-1.39294400
H	4.84469800	-1.66381100	-2.37578400
C	5.53879800	-1.68422300	-0.31651000
H	5.71020900	-2.77040400	-0.30930500
H	6.50299200	-1.21006700	-0.54487600
C	5.03651500	-1.21096400	1.06317700
H	5.77131100	-1.47694900	1.83474500
C	3.69461100	-1.91162000	1.39175900
H	3.33543300	-1.61019100	2.38461500
H	3.84687600	-3.00159300	1.41230900
C	4.84910500	0.32124500	1.02692700
H	4.53364400	0.69242500	2.01089700
H	5.81032800	0.80248300	0.79610600
C	3.78936600	0.69582700	-0.04300200
H	3.66850500	1.78336900	-0.06335500
C	2.46823200	0.01761400	0.36291700
H	2.26098200	0.28210000	1.40972400
C	4.28131700	0.21023000	-1.42117900
H	3.55148500	0.47676100	-2.19534900
H	5.22284000	0.71451700	-1.67938600
C	-2.23393700	-1.67154800	0.62232500
C	-3.19175100	-2.05478400	-0.34748800
C	-4.51410200	-1.62658800	-0.17508600
H	-5.26485200	-1.90113700	-0.91032000
C	-4.88661000	-0.86227300	0.92706400
C	-3.94354500	-0.54024100	1.89852300
H	-4.25089900	0.02702500	2.77257000
C	-2.60773000	-0.94719400	1.78079700
C	-2.84397500	-2.97883600	-1.51424300
H	-1.75231700	-3.00860600	-1.59651200
C	-1.64255500	-0.66259900	2.93297100
H	-0.64316100	-0.99230700	2.63690200
C	0.46645900	-0.14344600	-2.27162400
H	0.09970300	-1.11359000	-2.62959500
C	-1.51911500	1.47684600	-0.71231400
H	-2.02963800	0.94279200	0.08248600
C	-1.40019900	0.78832200	-1.95765800
H	-1.89113500	-0.17960500	-1.95800500
C	-1.48447200	1.53774300	-3.28616900
H	-0.78076300	2.37686200	-3.29126100
H	-1.18077000	0.87404600	-4.10333600
H	0.88084300	0.46954200	-3.08226200
N	1.32489400	3.07220200	0.10402900
O	1.67750200	4.22698300	0.30181600
C	-3.40144300	-2.50855400	-2.87133600
H	-3.05173400	-3.17471500	-3.66850300
H	-4.49701900	-2.52718200	-2.89082000
H	-3.08185000	-1.49182900	-3.11989000
C	-3.34094200	-4.41379200	-1.22783800
H	-3.02765300	-5.09735400	-2.02605800
H	-2.95651700	-4.80070300	-0.27808900
H	-4.43574300	-4.44131900	-1.17214500
C	-2.05110600	-1.47456300	4.18188300
H	-3.02376900	-1.14707900	4.56763900
H	-2.12759000	-2.54651200	3.96530400
H	-1.31306200	-1.33943900	4.98115200
C	-1.52953000	0.83363400	3.28095100
H	-1.13649300	1.41714500	2.44458000

H	-2.49776700	1.25468800	3.57794500
H	-0.84269000	0.96666700	4.12486500
H	-5.91665800	-0.53413300	1.03848400
C	-1.55065600	2.93362100	-0.60557200
H	-1.08315700	3.51146100	-1.39933000
C	-2.10887400	3.59285900	0.42545900
H	-2.56076600	3.01686800	1.23491300
C	-2.11999100	5.08465300	0.59227600
H	-1.71140100	5.56057000	-0.30785200
H	-3.15803200	5.43661000	0.69559400
C	-2.91221800	2.04141700	-3.56228200
H	-3.24256300	2.74521400	-2.79216000
H	-2.95692800	2.54870700	-4.53292200
H	-3.62717800	1.21007400	-3.58643400
C	-1.31251900	5.53438500	1.82577100
H	-1.35631700	6.62378800	1.94057400
H	-1.71073400	5.08371200	2.74321200
H	-0.26505100	5.23446300	1.72563600

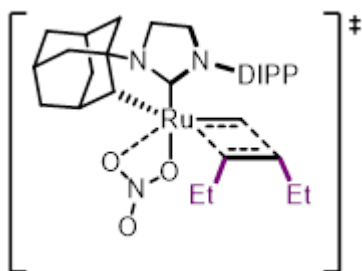


48-TS

SCF Energy (M06, n-octanol):	-1809.971257
SCF Energy (B3LYP, gas-phase):	-1810.248762
Enthalpy Correction:	0.847613
Free-Energy Correction:	0.733726

Ru	0.61801500	0.63750400	0.29723200
O	1.36145600	2.56116600	1.10574100
O	1.34313100	0.96852700	2.58688900
N	1.34401300	-1.94299500	-0.79886200
N	-0.83914800	-2.04943200	-0.67273700
C	0.24673200	-1.25479900	-0.39181100
C	1.03459100	-3.15186700	-1.56206900
H	1.68299900	-3.98604500	-1.28065400
H	1.15409800	-2.97264100	-2.64015000
C	-0.42868400	-3.38047800	-1.17636500
H	-1.05393700	-3.69057400	-2.01674200
H	-0.52953900	-4.12860700	-0.37911700
C	2.64820900	-1.27500500	-0.79316600
C	2.94714800	-0.61374500	-2.16294300
H	2.11594400	0.04324100	-2.44098600
H	3.03105400	-1.38747700	-2.94034600
C	4.25826700	0.19147000	-2.07574400
H	4.45451100	0.66791000	-3.04576100
C	5.41503200	-0.76668800	-1.72539000
H	5.53380400	-1.52285400	-2.51486500
H	6.36188800	-0.21277700	-1.66849200
C	5.12387000	-1.44625300	-0.37120600
H	5.94125500	-2.13555600	-0.12079200
C	3.80608700	-2.25115800	-0.46966000
H	3.59742100	-2.76576700	0.47763200
H	3.90537300	-3.02221400	-1.24886800
C	5.00491800	-0.36040300	0.71861400
H	4.83588200	-0.82058500	1.70112900
H	5.94842400	0.19993900	0.78529100
C	3.83393600	0.60099400	0.37929700
H	3.77025000	1.36781500	1.15675000

C	2.54467900	-0.23829300	0.34022500
H	2.47148300	-0.79868800	1.28310800
C	4.11519500	1.26976300	-0.98143400
H	3.30145200	1.96114900	-1.23224900
H	5.03716000	1.86459100	-0.92230400
C	-2.16936700	-1.93285400	-0.13982800
C	-3.22436200	-1.57325400	-1.01238100
C	-4.51795300	-1.48528000	-0.48276000
H	-5.34253600	-1.20356400	-1.13125600
C	-4.76877700	-1.76537400	0.85758700
C	-3.72840200	-2.17220400	1.68811400
H	-3.93884700	-2.41940700	2.72474100
C	-2.41550100	-2.28032100	1.21074100
C	-3.00724600	-1.36821600	-2.51106500
H	-1.92788700	-1.29722200	-2.68113800
C	-1.32818700	-2.81914400	2.14099100
H	-0.37058900	-2.77251600	1.61514100
C	0.11144600	1.36073000	-1.37163600
H	-0.39951600	0.87928100	-2.21381800
C	-1.39303700	1.14515600	1.16703300
H	-1.88395000	0.18068600	1.24611300
C	-1.54020500	1.77061300	-0.11946500
H	-2.16520800	1.21813900	-0.81556900
H	0.43509100	2.38125800	-1.60641000
N	1.63106900	2.17994200	2.31208800
O	2.12892700	2.94521400	3.12344900
C	-3.64932500	-0.08155400	-3.06220400
H	-3.41661000	0.02530500	-4.12804600
H	-4.74097100	-0.09513800	-2.96669400
H	-3.28104400	0.81225600	-2.54933600
C	-3.53472700	-2.58720700	-3.30062100
H	-3.31028000	-2.48135800	-4.36871400
H	-3.09028700	-3.52534500	-2.95093900
H	-4.62192300	-2.68112000	-3.19340700
C	-1.60079900	-4.29943400	2.48650300
H	-2.52423500	-4.40842500	3.06748800
H	-1.70396800	-4.91646400	1.58628100
H	-0.77927400	-4.70689000	3.08720500
C	-1.16680100	-1.98995500	3.42942600
H	-0.87373900	-0.95995500	3.21042500
H	-2.09133800	-1.96954400	4.01845300
H	-0.38447400	-2.42918500	4.05897500
H	-5.77907900	-1.68598500	1.25005600
C	-1.58542000	3.24259900	-0.26922400
H	-0.89818500	3.81508000	0.35027800
C	-2.41930200	3.87862800	-1.10404700
H	-3.09431700	3.29056100	-1.73136900
C	-2.50661800	5.37094200	-1.26914900
H	-3.52071500	5.70868100	-1.00697900
H	-1.82281700	5.86029100	-0.56461200
C	-1.45613000	1.94341000	2.45707000
H	-0.97728900	1.37473300	3.25877700
H	-0.90539600	2.88375800	2.37311100
C	-2.91710400	2.24187600	2.84617800
H	-3.49550000	1.31643900	2.95556300
H	-2.95717800	2.77904600	3.80101800
H	-3.41150900	2.85883000	2.08743300
C	-2.19227200	5.82879800	-2.70465200
H	-2.87101600	5.36023400	-3.42784800
H	-2.29882400	6.91521800	-2.80173100
H	-1.16777500	5.56049100	-2.98578800

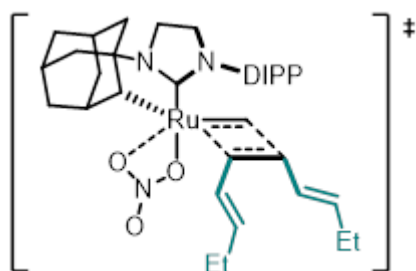


49-TS

SCF Energy (M06, n-octanol):	-1732.570489
SCF Energy (B3LYP, gas-phase):	-1732.890950
Enthalpy Correction:	0.812054
Free-Energy Correction:	0.705038

Ru	0.64608200	0.80557900	-0.15302600
O	1.69398000	2.75897200	-0.18516100
O	1.32168900	2.02608400	1.82797000
N	0.94064800	-2.06744400	0.08056500
N	-1.22978600	-1.78769200	0.01239500
C	-0.02919100	-1.11859100	0.02507400
C	0.44373800	-3.43212300	-0.09518500
H	0.92718800	-4.13103100	0.59275500
H	0.62227100	-3.78159200	-1.12217400
C	-1.04757300	-3.24567000	0.19668000
H	-1.69431000	-3.80914600	-0.47978200
H	-1.30152100	-3.52632600	1.22747500
C	2.34295500	-1.66597200	-0.06597000
C	2.80102500	-1.74867800	-1.54391700
H	2.10749100	-1.17849300	-2.17106400
H	2.77436300	-2.79394100	-1.88543200
C	4.22972200	-1.18661100	-1.67789000
H	4.54015900	-1.23684800	-2.73031300
C	5.18651100	-2.03369300	-0.81455600
H	5.19673700	-3.07418800	-1.17021200
H	6.21370100	-1.65520500	-0.90472600
C	4.73364600	-1.97575200	0.65918200
H	5.40756000	-2.58437200	1.27677100
C	3.29841600	-2.54210300	0.78115900
H	2.96989500	-2.53509900	1.82891600
H	3.28682300	-3.58798000	0.43858300
C	4.77084600	-0.50814900	1.13577900
H	4.48926600	-0.44182300	2.19508400
H	5.79589700	-0.11974000	1.05242300
C	3.80107300	0.34839300	0.27916000
H	3.84662500	1.38523300	0.62512000
C	2.38593900	-0.22413800	0.47211100
H	2.18796900	-0.28090700	1.55235600
C	4.24255800	0.27976100	-1.19637300
H	3.57189900	0.88931300	-1.81417400
H	5.25243900	0.69880300	-1.30538700
C	-2.53149200	-1.24731200	0.29478700
C	-3.48119600	-1.17005600	-0.75182800
C	-4.75017900	-0.65668400	-0.45534200
H	-5.49341200	-0.58071100	-1.24382200
C	-5.08051100	-0.25266500	0.83523700
C	-4.15235700	-0.38775500	1.86381600
H	-4.43004000	-0.10004100	2.87400900
C	-2.87034900	-0.90029700	1.62498700
C	-3.19144300	-1.70533700	-2.15337600
H	-2.11280600	-1.88073100	-2.22212600
C	-1.92286300	-1.11147000	2.80651600
H	-0.96641400	-1.47582300	2.42190400
C	0.39383600	0.74319900	-2.01316100
H	-0.15031600	0.01190400	-2.62301300
C	-1.30584800	1.96394000	0.14682600
H	-1.94487900	1.20307900	0.58186300

C	-1.25079800	1.96345600	-1.27435000
H	-1.89416900	1.22881200	-1.75174900
H	0.92267700	1.48885800	-2.61976400
N	1.83779500	2.92850900	1.08851900
O	2.43287200	3.89547400	1.53806500
C	-3.57741800	-0.73250900	-3.28285600
H	-3.29942600	-1.15892700	-4.25372800
H	-4.65650300	-0.54285800	-3.30806800
H	-3.07146600	0.23283300	-3.18495400
C	-3.90710200	-3.05747500	-2.37071200
H	-3.63931900	-3.48196500	-3.34564000
H	-3.64572900	-3.78859100	-1.59800900
H	-4.99615100	-2.93168100	-2.34693000
C	-2.48206000	-2.18921200	3.76046000
H	-3.41763300	-1.86094300	4.22826700
H	-2.68816300	-3.12972200	3.23621100
H	-1.76345600	-2.39533300	4.56217200
C	-1.62314000	0.18764000	3.57815600
H	-1.12256200	0.92357700	2.94361800
H	-2.53672200	0.63985700	3.98189100
H	-0.95872100	-0.02521700	4.42362800
H	-6.06872200	0.14884900	1.04335700
C	-1.25829800	3.24422900	0.95966100
H	-0.83005300	3.03844200	1.94397800
H	-0.60890800	3.98712400	0.48846000
C	-1.02429700	3.24813600	-2.06572100
H	-0.01601400	3.62949100	-1.87282000
H	-1.71227900	4.00863100	-1.67072300
C	-2.67206600	3.82963100	1.14791900
H	-2.63351700	4.73273500	1.76796400
H	-3.13604200	4.09798900	0.19126400
H	-3.33267600	3.10795300	1.64304600
C	-1.27491800	3.11348100	-3.57177200
H	-1.15179500	4.08150700	-4.06952000
H	-0.58300100	2.40741200	-4.04332100
H	-2.29575000	2.76579500	-3.77488700



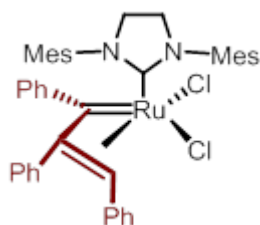
50-TS

SCF Energy (M06, n-octanol):	-1887.373081
SCF Energy (B3LYP, gas-phase):	-1887.609875
Enthalpy Correction:	0.883151
Free-Energy Correction:	0.763473

Ru	0.59504200	0.59387200	-0.07721800
O	1.15621200	2.72155200	0.27393900
O	1.03108300	1.52603900	2.08514200
N	1.52753800	-2.12360200	-0.38177600
N	-0.65428200	-2.33554300	-0.32270100
C	0.37380900	-1.42589000	-0.22875000
C	1.32668900	-3.51104700	-0.79817800
H	2.00010900	-4.19433400	-0.27354200
H	1.49848400	-3.62122200	-1.87839500
C	-0.14410200	-3.72303700	-0.42651900
H	-0.69945600	-4.28911800	-1.17757200
H	-0.25206600	-4.23465800	0.53880500
C	2.79387900	-1.39152500	-0.47374200
C	3.16998600	-1.10148300	-1.94810400
H	2.33168900	-0.60197400	-2.44509900
H	3.35411400	-2.04732800	-2.47857600
C	4.42849600	-0.21378400	-1.99857100
H	4.68047600	-0.00336000	-3.04671400
C	5.59832900	-0.95888600	-1.32401000
H	5.81794600	-1.88980200	-1.86668600
H	6.50949800	-0.34639800	-1.36047900
C	5.23139000	-1.26721300	0.14225100
H	6.05873800	-1.80445800	0.62483200
C	3.96834500	-2.16088300	0.17979000
H	3.70798300	-2.41649000	1.21540000
H	4.17199900	-3.10293500	-0.35160700
C	4.97075900	0.06219700	0.88228900
H	4.74583500	-0.12610000	1.94043800
H	5.87715800	0.68366000	0.85328100
C	3.78451100	0.81080900	0.21740600
H	3.61376700	1.75245600	0.74826000
C	2.54843200	-0.09878900	0.32938300
H	2.43873800	-0.39360800	1.38261900
C	4.14240000	1.10696100	-1.25306400
H	3.31851300	1.64595400	-1.73644800
H	5.02535400	1.75944200	-1.29853000
C	-1.98960900	-2.15743300	0.18191700
C	-3.07039100	-2.12577300	-0.73162000
C	-4.36250800	-1.95206900	-0.21968600
H	-5.20706200	-1.91374200	-0.90131800
C	-4.58560300	-1.83508700	1.14937800
C	-3.51769700	-1.92908700	2.03702400
H	-3.70570700	-1.87421800	3.10560900
C	-2.20510600	-2.10936000	1.58102500
C	-2.87520400	-2.35920200	-2.22878000
H	-1.80847700	-2.23712800	-2.44493700
C	-1.08741300	-2.31839400	2.60361000
H	-0.13688200	-2.39062000	2.06892900
C	0.22899100	0.78724200	-1.92355600

H	-0.15715900	0.05542700	-2.64326600
C	-1.55961300	1.27857800	0.38227600
H	-2.00575000	0.36798400	0.76704700
C	-1.53956900	1.39523100	-1.05731200
H	-2.07696500	0.59366700	-1.55547400
H	0.55090100	1.71417100	-2.41175600
N	1.26261800	2.66389100	1.56026100
O	1.55946400	3.65085200	2.21937700
C	-3.64948700	-1.37198500	-3.12202900
H	-3.39365200	-1.54199200	-4.17427100
H	-4.73374400	-1.49988700	-3.02738400
H	-3.41697500	-0.32958500	-2.88370500
C	-3.27527300	-3.80459300	-2.60256400
H	-3.06641200	-4.00073700	-3.66104700
H	-2.73683300	-4.54827000	-2.00560500
H	-4.34705700	-3.96552600	-2.43561400
C	-1.29775300	-3.64889500	3.35959700
H	-2.21043400	-3.62146000	3.96646800
H	-1.38489800	-4.49935000	2.67314900
H	-0.45495000	-3.83960100	4.03427600
C	-0.94452400	-1.15195900	3.59908300
H	-0.69329200	-0.21613200	3.09355200
H	-1.86306800	-1.00062600	4.17916200
H	-0.14009500	-1.36901900	4.31150400
H	-5.59504300	-1.69191300	1.52562800
C	-1.68444100	2.44066900	1.25903700
H	-1.34734900	3.40257400	0.88177600
C	-2.18734800	2.38670200	2.50502900
H	-2.51472200	1.42432300	2.90143900
C	-2.27733500	3.55704700	3.44116700
H	-2.06913700	4.48478800	2.89389300
H	-3.30208000	3.64110000	3.83320600
C	-1.64987700	2.71868100	-1.71827800
H	-1.05576800	3.52632600	-1.29503000
C	-2.42716000	2.95689800	-2.78296100
H	-3.00596400	2.13591600	-3.21326900
C	-2.57092600	4.28930800	-3.46593700
H	-3.62123800	4.61388400	-3.41576000
H	-1.98540500	5.04446300	-2.92677500
C	-1.29350800	3.42754200	4.62143800
H	-0.26280000	3.39398100	4.25518200
H	-1.39533200	4.27797400	5.30592400
H	-1.48139800	2.51090200	5.19385600
C	-2.13792100	4.25053200	-4.94238700
H	-2.71755000	3.50926800	-5.50613500
H	-2.28681100	5.22525200	-5.42087300
H	-1.07869500	3.98483100	-5.03286700

Other Vinylcarbene Complexes

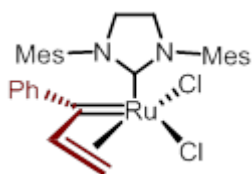


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SCF Energy (M06, n-octanol):	-2749.758820
SCF Energy (B3LYP, gas-phase):	-2749.584244
Enthalpy Correction:	0.779107
Free-Energy Correction:	0.651433

Ru	0.51251200	-0.02714000	-0.77498600
Cl	0.91954700	-1.71801800	-2.44297300
Cl	1.44474700	1.57026700	-2.29611400
N	0.04260000	-2.07116400	1.60591600
N	2.12706100	-1.80261400	0.97559600
C	-1.32017000	0.21459100	-0.66641400
C	-1.11020200	1.50556000	-0.01139500
C	-0.26658900	1.52998500	1.10052300
C	-2.54340600	-0.25895300	-1.29323900
C	-2.52781100	-1.16725900	-2.37221700
H	-1.57128700	-1.50942500	-2.75199500
C	-3.72119200	-1.59499800	-2.94699800
H	-3.69414000	-2.28458100	-3.78637500
C	-4.94809800	-1.13719100	-2.45633800
H	-5.87663200	-1.47136900	-2.91221500
C	-4.97817100	-0.23970800	-1.38482400
H	-5.92828300	0.12795500	-1.00613600
C	-3.78900100	0.19976500	-0.81036700
H	-3.81436100	0.90304200	0.01550500
C	-1.67687600	2.73864200	-0.64297200
C	-2.28367000	3.69946700	0.18531900
H	-2.26012400	3.56793100	1.26299700
C	-2.92124900	4.81142700	-0.36226600
H	-3.38837900	5.54112500	0.29397900
C	-2.95861800	4.98522100	-1.74741200
H	-3.45137700	5.85415100	-2.17571400
C	-2.35966200	4.03620700	-2.57842900
H	-2.37836900	4.16608300	-3.65704300
C	-1.72972700	2.91724000	-2.03474200
H	-1.24622100	2.19748400	-2.68500800
C	0.43065600	2.70870700	1.64486600
C	0.57295400	2.83375400	3.03944500
H	0.14771600	2.07159700	3.68876700
C	1.23843100	3.92356000	3.59989600
H	1.32881800	4.00462500	4.68007900
C	1.79024900	4.90403800	2.77307400
H	2.31458900	5.75201700	3.20560000
C	1.67545300	4.78126100	1.38466200
H	2.11969300	5.52990100	0.73416500
C	1.00421100	3.69813300	0.82192900
H	0.95256900	3.58771200	-0.25614400
C	0.84851200	-1.43751600	0.70853800
C	-1.39081000	-2.20010400	1.59680400
C	-2.14863900	-1.55498200	2.58958500
C	-3.53658300	-1.75254300	2.60483200
H	-4.12732800	-1.24491400	3.36516700
C	-4.17412500	-2.58589200	1.68771800
C	-3.38301100	-3.25754500	0.74714400
H	-3.85867900	-3.93074900	0.03766300
C	-1.99945500	-3.09293700	0.68515900

C	-1.53441100	-0.69355100	3.67123200
H	-1.77102400	-1.09647200	4.66390200
H	-1.93371200	0.32708700	3.63786700
H	-0.44758900	-0.62918300	3.58643000
C	-5.67352000	-2.76394700	1.69659900
H	-6.12514000	-2.33469200	2.59667600
H	-5.95254700	-3.82314100	1.64898100
H	-6.12625100	-2.27141900	0.82665300
C	-1.19268900	-3.87755900	-0.32032800
H	-0.47023600	-4.54217100	0.17209200
H	-0.62455600	-3.23013300	-0.99593900
H	-1.85128200	-4.50602000	-0.92687700
C	3.32598300	-1.37765600	0.29491500
C	3.91896100	-0.14101900	0.59965000
C	5.09974100	0.21026300	-0.06953300
H	5.55239200	1.17515400	0.14966800
C	5.70506000	-0.63523600	-0.99586200
C	5.12088400	-1.88773700	-1.22751800
H	5.59308700	-2.57283600	-1.92812100
C	3.94395900	-2.28496500	-0.59636700
C	3.36451900	0.81142300	1.63095200
H	2.51887800	0.39138200	2.17880900
H	3.01965600	1.73898400	1.16394000
H	4.14096400	1.08040700	2.35743300
C	6.95050900	-0.21718500	-1.74050800
H	7.64906000	-1.05352700	-1.85740400
H	7.47343000	0.59541200	-1.22564100
H	6.69922300	0.13950200	-2.74774700
C	3.37058200	-3.65466100	-0.86642800
H	3.95985100	-4.16852000	-1.63152600
H	2.34053600	-3.58069100	-1.22537000
H	3.37804500	-4.28891600	0.03054300
C	0.79457100	-3.01825800	2.46184200
H	0.58046800	-4.04785900	2.15086500
H	0.49654700	-2.90789900	3.50798400
C	2.24600200	-2.61575500	2.20097100
H	2.66667700	-2.00378100	3.00982900
H	2.90938100	-3.46838300	2.03859900
H	-0.27651100	0.66498800	1.74937700

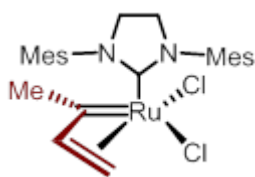


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SCF Energy (M06, n-octanol):	-2287.894386
SCF Energy (B3LYP, gas-phase):	-2287.486239
Enthalpy Correction:	0.607318
Free-Energy Correction:	0.499915

Ru	0.51402100	-1.00638000	-0.26107600
Cl	0.61771200	-1.28082700	2.14364800
Cl	1.50896100	-3.17000500	-0.49812700
N	-0.34384100	2.02966000	-0.00029900
N	1.81207900	1.65189600	0.13159100
C	-1.25215100	-1.25824100	-0.77447500
C	-0.65121900	-1.45938100	-2.07440900
C	0.25997600	-0.53745600	-2.57419000
C	-2.52725900	-1.70196100	-0.26711200
C	-2.73213100	-1.96174000	1.10500900
H	-1.90229400	-1.82249100	1.79045400
C	-3.96754700	-2.42138100	1.54882700
H	-4.11328600	-2.63617400	2.60377500
C	-5.01701300	-2.61728400	0.64402300

H	-5.97840200	-2.98064700	0.99792300
C	-4.82845800	-2.35702500	-0.71717600
H	-5.64039300	-2.51586300	-1.42166600
C	-3.59265800	-1.90658800	-1.17160500
H	-3.43741900	-1.70623300	-2.22803000
C	0.60297800	1.05821600	-0.01106100
C	-1.77586700	1.88972900	0.02858900
C	-2.51696600	2.09629400	-1.14871500
C	-3.91345200	2.00860300	-1.08150000
H	-4.48991300	2.16013600	-1.99217300
C	-4.58092200	1.74034400	0.11325100
C	-3.81549100	1.59391300	1.27601900
H	-4.31843900	1.41252000	2.22320100
C	-2.42174800	1.67321300	1.26564300
C	-1.87754200	2.42017200	-2.48056100
H	-2.42241800	3.22839300	-2.98119500
H	-1.89916200	1.55388600	-3.15278000
H	-0.83414800	2.72860200	-2.37961600
C	-6.08364600	1.59753300	0.15494000
H	-6.56023700	2.10032700	-0.69306400
H	-6.50197300	2.01440400	1.07772700
H	-6.37154900	0.53872700	0.11626600
C	-1.65092400	1.53739900	2.55618100
H	-1.06686200	2.44016600	2.77815300
H	-0.95044500	0.69535300	2.52969100
H	-2.33768100	1.38267400	3.39376500
C	3.09729300	0.99834900	0.10516800
C	3.73659800	0.74650500	-1.12331900
C	4.98444000	0.11157200	-1.10474600
H	5.47353600	-0.10338100	-2.05283600
C	5.61603300	-0.24337100	0.08650100
C	4.98903200	0.09469700	1.29161500
H	5.48347400	-0.13905200	2.23163100
C	3.74271400	0.72070600	1.33177500
C	3.17771900	1.19091700	-2.45602800
H	2.17965300	1.62303200	-2.37122800
H	3.12100700	0.35231400	-3.15760700
H	3.83410100	1.94537400	-2.90875200
C	6.93651900	-0.97557100	0.08175100
H	7.57717200	-0.65477000	0.91060600
H	7.48215300	-0.81600500	-0.85415700
H	6.78031100	-2.05655300	0.19103200
C	3.13348400	1.09792200	2.65955300
H	3.81799600	0.84660300	3.47509400
H	2.19410000	0.56180000	2.82563300
H	2.92701100	2.17430200	2.72379900
C	0.22441000	3.37337500	0.25772800
H	-0.08588600	3.72503000	1.24783100
H	-0.13954600	4.08882900	-0.48575400
C	1.73494100	3.12537300	0.16759400
H	2.17875800	3.54268900	-0.74492900
H	2.28683600	3.52058300	1.02464100
H	0.08840000	0.52738000	-2.52168700
H	-0.59996100	-2.49016900	-2.43477500
H	0.99063200	-0.87680900	-3.30215500

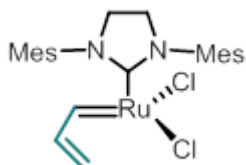


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SCF Energy (M06, n-octanol): -2096.250354
 SCF Energy (B3LYP, gas-phase): -2095.746593
 Enthalpy Correction: 0.550615
 Free-Energy Correction: 0.449992

Ru	0.30300500	1.25620200	0.00633800
Cl	0.44143200	1.07387700	-2.39818800
Cl	1.69833600	3.19614300	-0.10015800
N	-1.17032400	-1.52463800	0.25418400
N	1.01934300	-1.63109200	0.17836500
C	-1.38007800	1.90770600	0.31417300
C	-0.84496600	2.28665500	1.60260100
C	-0.15728800	1.36362500	2.37588300
C	-0.03609900	-0.78578300	0.14353800
C	-2.53890100	-1.10112100	0.11477700
C	-3.32947600	-0.91799900	1.26322900
C	-4.67715100	-0.56612000	1.09847400
H	-5.28941700	-0.41870100	1.98596700
C	-5.25430800	-0.41751000	-0.16217500
C	-4.45038900	-0.65256100	-1.28546100
H	-4.88752000	-0.56865700	-2.27818600
C	-3.10344200	-1.00315600	-1.17854400
C	-2.80099500	-1.09977200	2.66842500
H	-3.50576800	-1.68486300	3.26983700
H	-2.67326200	-0.13409000	3.17181300
H	-1.83499800	-1.60975400	2.68821600
C	-6.70558000	-0.02779100	-0.32144500
H	-7.23100500	-0.03575000	0.63860900
H	-7.22994500	-0.71119000	-0.99970100
H	-6.80200500	0.98001100	-0.74510200
C	-2.29715300	-1.27192500	-2.42515600
H	-1.87860700	-2.28645200	-2.42905100
H	-1.45874800	-0.57338100	-2.52651900
H	-2.92898100	-1.17787500	-3.31342700
C	2.41169700	-1.25887500	0.14004400
C	3.07822400	-0.89621700	1.32514600
C	4.43407700	-0.55525900	1.24613600
H	4.95039600	-0.25770600	2.15667300
C	5.13633000	-0.59063900	0.04226300
C	4.45853600	-1.01877900	-1.10569000
H	4.99746300	-1.08173100	-2.04824200
C	3.10713300	-1.36412300	-1.08593700
C	2.41587500	-0.90522000	2.68394300
H	1.36224100	-1.18435100	2.63395300
H	2.47579200	0.08201200	3.15391400
H	2.92348600	-1.61333600	3.35106900
C	6.58539100	-0.17201700	-0.02910100
H	7.14997000	-0.79662600	-0.73026300
H	7.07095500	-0.23286900	0.95043400
H	6.67238200	0.86585300	-0.37561500
C	2.43266200	-1.84199000	-2.34800000
H	3.15824500	-1.90780800	-3.16402300
H	1.64026600	-1.14991900	-2.65089500
H	1.98594900	-2.83703900	-2.22421600
C	-0.89660900	-2.98053600	0.28104200
H	-1.26148600	-3.44602300	-0.64123200
H	-1.41310900	-3.44870700	1.12435800
C	0.63183500	-3.03673800	0.40422200
H	0.96506800	-3.35835600	1.39889400
H	1.09783600	-3.69101900	-0.33757000

H	-0.49627600	0.34588100	2.49840900
H	-0.63800800	3.35047800	1.75365600
H	0.56919400	1.72609100	3.09701200
C	-2.50870400	2.45203100	-0.47289400
H	-3.46006200	2.05759200	-0.09130700
H	-2.53489500	3.54620900	-0.35855300
H	-2.41027500	2.20365400	-1.53068700

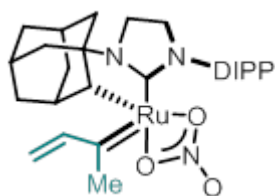


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SCF Energy (M06, n-octanol):	-2056.940529
SCF Energy (B3LYP, gas-phase):	-2056.430229
Enthalpy Correction:	0.520586
Free-Energy Correction:	0.420141

Ru	0.35457800	1.11981800	-0.49360500
Cl	0.46918900	0.26125400	-2.69248100
Cl	1.73369100	3.05707400	-0.45131400
N	-1.18662300	-1.42383200	0.48459100
N	1.00442800	-1.52843300	0.53309300
C	-1.35784700	1.74190700	-0.72566300
C	-2.11146900	2.51883900	0.24740500
C	-1.57113900	3.37136200	1.14135000
C	-0.05034500	-0.73973700	0.21205800
C	-2.54979400	-1.00455500	0.32058800
C	-3.22293500	-0.45893300	1.42963700
C	-4.57587900	-0.13120600	1.29155200
H	-5.10294700	0.28885400	2.14559400
C	-5.26451800	-0.33026500	0.09095000
C	-4.56759800	-0.88913600	-0.98585300
H	-5.09066900	-1.06558400	-1.92329000
C	-3.21752900	-1.24441700	-0.89672600
C	-2.51198500	-0.20550000	2.73799500
H	-1.97137500	-1.08885100	3.09700200
H	-3.22592200	0.08528100	3.51448400
H	-1.78024500	0.60493600	2.63721100
C	-6.71837900	0.05821400	-0.04655400
H	-7.21574300	0.10209200	0.92780800
H	-7.26494900	-0.65243700	-0.67599600
H	-6.82153600	1.04730600	-0.51213500
C	-2.51566300	-1.86931800	-2.07785100
H	-2.17643800	-2.88912100	-1.85388900
H	-1.63466600	-1.29196200	-2.37843600
H	-3.19263200	-1.93239500	-2.93499700
C	2.38251300	-1.11478300	0.49428300
C	2.89663100	-0.28889500	1.51357100
C	4.24962600	0.06267000	1.46033100
H	4.65137700	0.70839000	2.23808700
C	5.09066300	-0.38443300	0.43978200
C	4.55358900	-1.22708600	-0.54012300
H	5.19700600	-1.59377500	-1.33667600
C	3.21036200	-1.60695500	-0.53717800
C	2.03986100	0.24391300	2.63989200
H	1.21294500	-0.42585500	2.89366700
H	1.60717600	1.21726000	2.37345200
H	2.64300100	0.39588100	3.54085800
C	6.53625000	0.04842600	0.37985000
H	7.16785000	-0.72080200	-0.07729200
H	6.93190200	0.26832900	1.37702000
H	6.64336300	0.95978500	-0.22265800
C	2.67168100	-2.50592000	-1.62316900

H	3.46628800	-2.77396700	-2.32561700
H	1.87577700	-2.00309100	-2.18260700
H	2.25961600	-3.44035600	-1.22080400
C	-0.91383300	-2.80693100	0.93653100
H	-1.20532700	-3.51868800	0.15547300
H	-1.48898400	-3.03611400	1.83820100
C	0.60251400	-2.79191600	1.17715700
H	0.86166700	-2.76947300	2.24389400
H	1.11522800	-3.64280900	0.72096500
H	-0.50210900	3.56534300	1.16507900
H	-1.84606300	1.56158700	-1.69035600
H	-3.19734900	2.41170500	0.20399300
H	-2.19992700	3.93876100	1.82241300

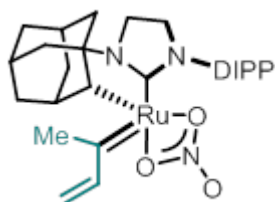


35a

SCF Energy (M06, n-octanol):	-1613.821061
SCF Energy (B3LYP, gas-phase):	-1613.447044
Enthalpy Correction:	0.700402
Free-Energy Correction:	0.597143

O	-1.37417500	2.38951000	0.85565500
O	-1.85243300	2.54205400	-1.25233800
N	-0.57780700	-1.54610900	0.99354500
N	1.53172100	-0.94996200	0.94897600
C	0.29525400	-0.66846600	0.45599500
C	0.02029100	-2.46287400	1.96837800
H	-0.05885700	-3.50086200	1.62445800
H	-0.47895600	-2.39023900	2.94090000
C	1.48112800	-1.96883300	2.02194300
H	1.73106800	-1.50380800	2.98349000
H	2.20130600	-2.77012800	1.83808300
C	-2.01238600	-1.42496300	0.69404900
C	-2.72818200	-0.62708100	1.81396100
H	-2.23837800	0.34350800	1.94703700
H	-2.64574900	-1.17505300	2.76433400
C	-4.21053700	-0.41916700	1.44796000
H	-4.70438400	0.14160300	2.25192200
C	-4.89470600	-1.78889400	1.27079300
H	-4.86102900	-2.35642100	2.21178000
H	-5.95486600	-1.65231300	1.01807400
C	-4.18390000	-2.57324800	0.14902900
H	-4.66725600	-3.55009000	0.01547200
C	-2.70457300	-2.80006300	0.54469000
H	-2.18676900	-3.39327100	-0.22072200
H	-2.65921700	-3.36604500	1.48720100
C	-4.27391200	-1.76581500	-1.16567600
H	-3.81154500	-2.32689600	-1.98907300
H	-5.32958200	-1.61696000	-1.43298900
C	-3.56781000	-0.39311400	-0.99177300
H	-3.64192000	0.17174500	-1.92865100
C	-2.09055600	-0.69081100	-0.67259800
H	-1.72539100	-1.40111900	-1.42518500
C	-4.28413400	0.38214800	0.13307200
H	-3.83662300	1.36969700	0.27279300
H	-5.33356900	0.54677300	-0.14741200
C	2.76567500	-0.27573600	0.65900500
C	3.01488100	1.01029600	1.19218000
C	4.24974100	1.60984300	0.90732900
H	4.46149200	2.59957000	1.30089800

C	5.21350300	0.95883300	0.14417600
C	4.95928100	-0.31645200	-0.35294500
H	5.71972600	-0.82134800	-0.94209700
C	3.73908800	-0.95803900	-0.11117300
C	2.02524100	1.74367200	2.09367300
H	1.07242700	1.20920800	2.06621300
C	3.51432400	-2.36488500	-0.66257000
H	2.47456800	-2.64143900	-0.46107100
C	4.42848100	-3.38968800	0.04214500
H	4.20878200	-4.40539800	-0.30787000
H	5.48459700	-3.18559800	-0.17005200
H	4.30530300	-3.36982000	1.13107600
C	3.70642200	-2.44109300	-2.18934000
H	4.73901400	-2.21369500	-2.47979000
H	3.48169900	-3.45390700	-2.54467500
H	3.04629000	-1.74055500	-2.70860500
C	2.51778600	1.74490700	3.55637200
H	2.67990000	0.72686600	3.93012300
H	3.46541500	2.28797100	3.65525000
H	1.78128500	2.23272600	4.20548900
C	1.74554200	3.18137200	1.61590900
H	0.94186100	3.62452100	2.21180200
H	2.63080500	3.82119000	1.71128600
H	1.42524500	3.19978700	0.56902000
H	6.16517500	1.44287600	-0.05904700
N	-1.96581300	3.05291300	-0.07699800
O	-2.58681100	4.07687800	0.13611600
Ru	-0.61461500	0.79355000	-0.63137800
C	0.06412100	0.54199700	-2.35769200
C	1.49472100	0.71097700	-2.60166200
C	-0.85336800	0.47872000	-3.55431500
C	2.09773500	0.73445100	-3.80921900
H	2.12418800	0.81991800	-1.72058000
H	-0.79248800	-0.52396000	-4.00595700
H	-0.58595200	1.20573900	-4.33194700
H	-1.89350800	0.65016800	-3.27072000
H	1.55074900	0.61696200	-4.74011700
H	3.17395900	0.85851700	-3.89383100



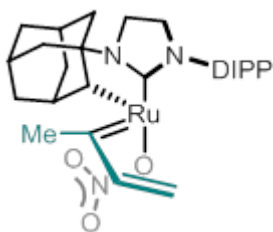
35b

SCF Energy (M06, n-octanol):	-1613.824309
SCF Energy (B3LYP, gas-phase):	-1613.449028
Enthalpy Correction:	0.701063
Free-Energy Correction:	0.600762

O	-1.01794700	1.13816700	-2.23275200
O	-1.25833800	-0.91021700	-2.92781000
N	-0.65191400	0.35548200	1.86834000
N	1.45105000	0.59595600	1.25253300
C	0.23488500	0.13658700	0.85808700
C	-0.09122600	1.20828300	2.92364100
H	-0.34911100	0.83869500	3.92024600
H	-0.46150900	2.23837200	2.83310700
C	1.42053900	1.11700800	2.63481400
H	1.92960700	2.08244700	2.69867000
H	1.92420700	0.41761300	3.31383300
C	-2.07012500	0.33000000	1.47127600

C	-2.50721900	1.71030000	0.91495000
H	-1.83069200	2.01065500	0.10699500
H	-2.44190500	2.47063800	1.70666700
C	-3.95365000	1.63275800	0.38725300
H	-4.24981000	2.61853500	0.00561400
C	-4.89560500	1.21442700	1.53307400
H	-4.87290900	1.96328800	2.33784100
H	-5.93173300	1.16496400	1.17183900
C	-4.46058200	-0.16304500	2.07370700
H	-5.13100600	-0.47159600	2.88682000
C	-3.01720900	-0.06176900	2.62644200
H	-2.69746600	-1.02056400	3.05535200
H	-2.98289200	0.68601400	3.43317700
C	-4.52912900	-1.19630000	0.92579900
H	-4.26579400	-2.19604900	1.29663100
H	-5.55953100	-1.25697000	0.54793100
C	-3.56511600	-0.78141500	-0.22188200
H	-3.61425300	-1.52505800	-1.02628400
C	-2.14929600	-0.76901000	0.38711600
H	-2.02816800	-1.72299000	0.90807000
C	-4.00841200	0.59682800	-0.75280900
H	-3.36737900	0.92621800	-1.57527100
H	-5.03137200	0.52664100	-1.14779100
C	2.63086900	0.68361300	0.43280800
C	2.81204300	1.82987000	-0.37886900
C	3.97575200	1.90823600	-1.15486100
H	4.13351800	2.77518200	-1.78952500
C	4.93728700	0.90359500	-1.11980100
C	4.75783500	-0.19966600	-0.29102600
H	5.52274600	-0.96970000	-0.25640600
C	3.61153000	-0.33235400	0.50204300
C	1.83829700	3.00633600	-0.38226100
H	0.93364200	2.70050700	0.15156400
C	3.48778700	-1.52227000	1.44762000
H	2.45330900	-1.55921900	1.80265800
C	4.40425900	-1.33701900	2.67671000
H	4.27337600	-2.16430700	3.38484600
H	5.45922700	-1.31457300	2.37823700
H	4.19316800	-0.40046400	3.20499900
C	3.78798800	-2.86679900	0.75966500
H	4.83710200	-2.94056700	0.45128300
H	3.59851200	-3.69433600	1.45407600
H	3.16463400	-3.01353100	-0.12763600
C	2.44576200	4.20604100	0.37788700
H	2.73539100	3.93930100	1.40129700
H	3.34284400	4.57983100	-0.12993400
H	1.72393000	5.02960400	0.43193000
C	1.40777600	3.43090300	-1.79848300
H	0.68485400	4.25257300	-1.73484200
H	2.25727600	3.78914700	-2.39156600
H	0.92602200	2.60918300	-2.33413100
H	5.83232100	0.98541000	-1.73093500
N	-1.33864500	0.34518700	-3.20115900
O	-1.69906700	0.75498300	-4.28596100
Ru	-0.43764400	-0.62584600	-0.85517200
C	0.06697300	-2.39307700	-0.41186300
C	0.41654400	-3.20357300	-1.58568100
C	0.08547300	-3.09858700	0.92144800
C	0.79747900	-4.49811600	-1.58080800
H	0.34352100	-2.70359200	-2.55109300
H	1.02441300	-3.64226600	1.08389500
H	-0.71767300	-3.85037600	0.95332800
H	-0.06717300	-2.41359800	1.75688000

H	0.88482100	-5.08196300	-0.66905400
H	1.02860700	-5.01645200	-2.50752400



35c

SCF Energy (M06, n-octanol):	-1613.818753
SCF Energy (B3LYP, gas-phase):	-1613.430501
Enthalpy Correction:	0.699911
Free-Energy Correction:	0.595317

O	2.54363200	3.35684800	0.49892800
O	1.77041500	2.23699300	-1.24214700
N	0.43089900	-1.95546200	0.34726600
N	-1.66577000	-1.36773900	0.12647700
C	-0.38948300	-0.90536300	0.14486100
C	-0.25202300	-3.25287500	0.31168600
H	0.03009700	-3.87579500	1.16520900
H	-0.00142600	-3.80097200	-0.60636500
C	-1.73468200	-2.82837400	0.35483100
H	-2.33990100	-3.30714300	-0.42100400
H	-2.19670700	-3.04099000	1.32596000
C	1.88068100	-1.73141500	0.28147800
C	2.39943200	-1.92933500	-1.16622500
H	1.83078300	-1.27969700	-1.84847600
H	2.22503100	-2.96594200	-1.49048100
C	3.90095900	-1.58771900	-1.23868800
H	4.25604300	-1.74427300	-2.26569700
C	4.67922600	-2.50562400	-0.27396300
H	4.56302200	-3.55853000	-0.56918100
H	5.75195200	-2.27625000	-0.32434600
C	4.16331700	-2.29477400	1.16472200
H	4.71833700	-2.94358800	1.85515900
C	2.66403800	-2.66916200	1.22552700
H	2.28043600	-2.56354600	2.24901800
H	2.53514200	-3.72225800	0.93236200
C	4.35990900	-0.81618700	1.56445800
H	4.02725500	-0.65618300	2.59924300
H	5.42901900	-0.56372500	1.53046500
C	3.56489500	0.10458900	0.59984500
H	3.70471300	1.14921400	0.89551200
C	2.07480300	-0.26464100	0.73480400
H	1.81994600	-0.23033900	1.80134500
C	4.09487900	-0.11313200	-0.83405000
H	3.57669700	0.54747300	-1.53711700
H	5.16089800	0.14820500	-0.87861600
C	-2.85774900	-0.62526800	-0.16713000
C	-3.21775400	-0.41529300	-1.51859400
C	-4.41007700	0.27192400	-1.78203300
H	-4.70226100	0.45621900	-2.81208600
C	-5.23138800	0.71327200	-0.74851900
C	-4.87006200	0.47840800	0.57523100
H	-5.51866900	0.82507600	1.37457000
C	-3.68128900	-0.18859300	0.89504700
C	-2.37217200	-0.91697000	-2.68621300
H	-1.51239100	-1.45375000	-2.27460000
C	-3.32220100	-0.42968200	2.35815300
H	-2.29243600	-0.80065200	2.39022500
C	-4.23661300	-1.50111200	2.98845100
H	-3.93704000	-1.70175500	4.02399800

H	-5.28081300	-1.16672100	3.00138300
H	-4.20187000	-2.44632800	2.43484500
C	-3.36576900	0.86673000	3.19024300
H	-4.38882700	1.24699900	3.29342000
H	-2.98354000	0.67912100	4.20047000
H	-2.76071900	1.65397100	2.73133500
C	-3.15677600	-1.91249900	-3.56430600
H	-3.54081200	-2.75289600	-2.97428600
H	-4.01284000	-1.43362200	-4.05355000
H	-2.50974700	-2.31666500	-4.35163300
C	-1.81508100	0.24589400	-3.53036100
H	-1.18754600	-0.13939700	-4.34259400
H	-2.62056100	0.83631500	-3.98266700
H	-1.20318400	0.92059900	-2.92107900
H	-6.15513000	1.23918000	-0.97484100
N	2.60304000	3.13230400	-0.71873700
O	3.36641000	3.69423400	-1.49627000
Ru	0.58828800	0.88577200	-0.20657600
C	-0.06569400	1.88290000	1.19814000
C	-0.89152700	3.02200700	0.76298200
C	0.39234000	1.89422200	2.63282600
C	-1.92628600	2.98115900	-0.09389600
H	-0.58527400	3.98846200	1.17337500
H	-0.29904500	2.44628800	3.28236900
H	1.36808300	2.39846800	2.66861600
H	0.52346700	0.88611700	3.03301900
H	-2.30416500	2.04707400	-0.49557000
H	-2.43865200	3.89144500	-0.39334200

Alkenes



ethene

SCF Energy (M06, n-octanol):	-78.538857
SCF Energy (B3LYP, gas-phase):	-78.587458
Enthalpy Correction:	0.055207
Free-Energy Correction:	0.031969

C	0.66547000	-0.00006400	-0.00000600
H	1.23896400	0.92416400	0.00000800
H	1.23968100	-0.92371500	0.00002500
C	-0.66554500	-0.00005900	-0.00000400
H	-1.23936000	-0.92391800	0.00000600
H	-1.23883500	0.92420700	0.00002300

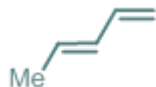


propene

SCF Energy (M06, n-octanol):	-117.836374
SCF Energy (B3LYP, gas-phase):	-117.907562
Enthalpy Correction:	0.085110
Free-Energy Correction:	0.058033

C	1.29328800	0.15060400	0.00000000
H	2.07406800	0.90663400	0.00000000
C	0.00000000	0.47469000	0.00000000
H	-0.27890700	1.52975700	0.00000000

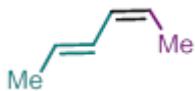
C	-1.13904800	-0.50467900	0.00000000
H	-0.77952200	-1.53936200	0.00000000
H	-1.78145800	-0.36674800	0.88045800
H	-1.78145800	-0.36674800	-0.88045800
H	1.62184100	-0.88722600	0.00000000



(E)-penta-1,3-diene

SCF Energy (M06, n-octanol):	-195.198056
SCF Energy (B3LYP, gas-phase):	-195.308285
Enthalpy Correction:	0.120884
Free-Energy Correction:	0.087985

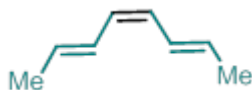
C	-1.36083200	0.39574600	-0.00006500
C	-2.53089300	-0.26036600	0.00001600
H	-1.36245300	1.48648300	0.00010900
H	-2.57444600	-1.34743000	0.00009800
C	-0.05300300	-0.24487400	0.00001100
H	-0.04485200	-1.33619900	-0.00025900
C	1.11478500	0.41955700	-0.00004500
H	1.09326400	1.51085200	-0.00002500
C	2.47224000	-0.21726900	0.00003000
H	3.05530400	0.08702300	0.88049600
H	3.05580800	0.08795500	-0.87972400
H	2.40474300	-1.31044400	-0.00054700
H	-3.48115000	0.26499600	0.00017300



(2Z,4E)-hexa-2,4-diene

SCF Energy (M06, n-octanol):	-234.493331
SCF Energy (B3LYP, gas-phase):	-234.625085
Enthalpy Correction:	0.150894
Free-Energy Correction:	0.114007

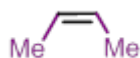
C	-0.46241000	-0.03242600	-0.00007600
C	-1.73829500	0.39157100	-0.00006600
H	-0.27290900	-1.10533600	0.00002100
H	-1.93090500	1.46604700	0.00008900
C	-2.94547300	-0.49831700	0.00004400
H	-3.57776900	-0.31419800	0.88000000
H	-3.57747200	-0.31461400	-0.88020500
H	-2.66569000	-1.55742700	0.00033100
C	0.68675100	0.86203700	0.00003900
H	0.44567800	1.92559500	0.00002300
C	1.98890300	0.51853500	-0.00002800
H	2.71912200	1.32770600	0.00010100
C	2.57371400	-0.86486500	-0.00000600
H	3.21323100	-1.01834700	0.88033100
H	3.21423300	-1.01811600	-0.87962000
H	1.81334000	-1.65051700	-0.00051500



(2E,4Z,6E)-octa-2,4,6-triene

SCF Energy (M06, n-octanol):	-311.856289
SCF Energy (B3LYP, gas-phase):	-312.029564
Enthalpy Correction:	0.186578
Free-Energy Correction:	0.143970

C	-0.67830200	1.19048200	0.00001500
C	0.67830100	1.19047600	-0.00000300
H	-1.18004800	2.15795400	-0.00008300
H	1.18005600	2.15794300	0.00010000
C	1.55645000	0.03531300	0.00001200
H	1.09936800	-0.95379200	-0.00006300
C	2.90023300	0.11823600	0.00005700
H	3.36087900	1.10778600	-0.00003000
C	3.83868400	-1.05067200	-0.00002700
H	4.49736700	-1.03449300	0.87982600
H	4.49722900	-1.03458500	-0.87999600
H	3.29754200	-2.00300300	0.00006300
C	-1.55645300	0.03532100	-0.00002300
H	-1.09936600	-0.95378200	0.00005200
C	-2.90023600	0.11823700	-0.00007100
H	-3.36088900	1.10778500	0.00000700
C	-3.83868000	-1.05067700	0.00003500
H	-4.49718300	-1.03462100	0.88003800
H	-4.49740400	-1.03447700	-0.87978400
H	-3.29753000	-2.00300400	-0.00010600



(Z)-but-2-ene

SCF Energy (M06, n-octanol):	-157.131025
SCF Energy (B3LYP, gas-phase):	-157.221726
Enthalpy Correction:	0.115112
Free-Energy Correction:	0.083868

C	-0.66950300	0.66430600	-0.00004200
C	0.66914700	0.66427500	0.00000300
H	1.16974300	1.63339400	0.00011000
C	1.59339500	-0.52181700	-0.00004600
H	1.06097700	-1.47701200	-0.00019500
H	2.25092000	-0.50504400	-0.88010900
H	2.25062600	-0.50524200	0.88023400
C	-1.59321200	-0.52198800	0.00003200
H	-2.25190800	-0.50480000	-0.87921000
H	-1.05993700	-1.47683100	-0.00172800
H	-2.24949100	-0.50672400	0.88115500
H	-1.16989600	1.63360300	0.00006800



1-butene

SCF Energy (M06, n-octanol):	-157.2180532
SCF Energy (B3LYP, gas-phase):	-157.1272270
Enthalpy Correction:	0.115231
Free-Energy Correction:	0.084472

C	-1.86133200	0.01723000	-0.28037400
H	-2.74072200	-0.61897300	-0.22307800
C	-0.72357600	-0.29513200	0.34170700
H	-0.67346300	-1.22033900	0.91981200
C	0.54047400	0.52134100	0.30814900
H	0.36659400	1.44442900	-0.25936500
H	0.80195100	0.82775700	1.33225900
H	-1.95808400	0.92699400	-0.87023900
C	1.72883800	-0.24733700	-0.29500900
H	2.64085400	0.36016900	-0.27626000

H	1.92991100	-1.16895900	0.26475600
H	1.52654000	-0.52769000	-1.33472200



(E)-hexa-1,3-diene

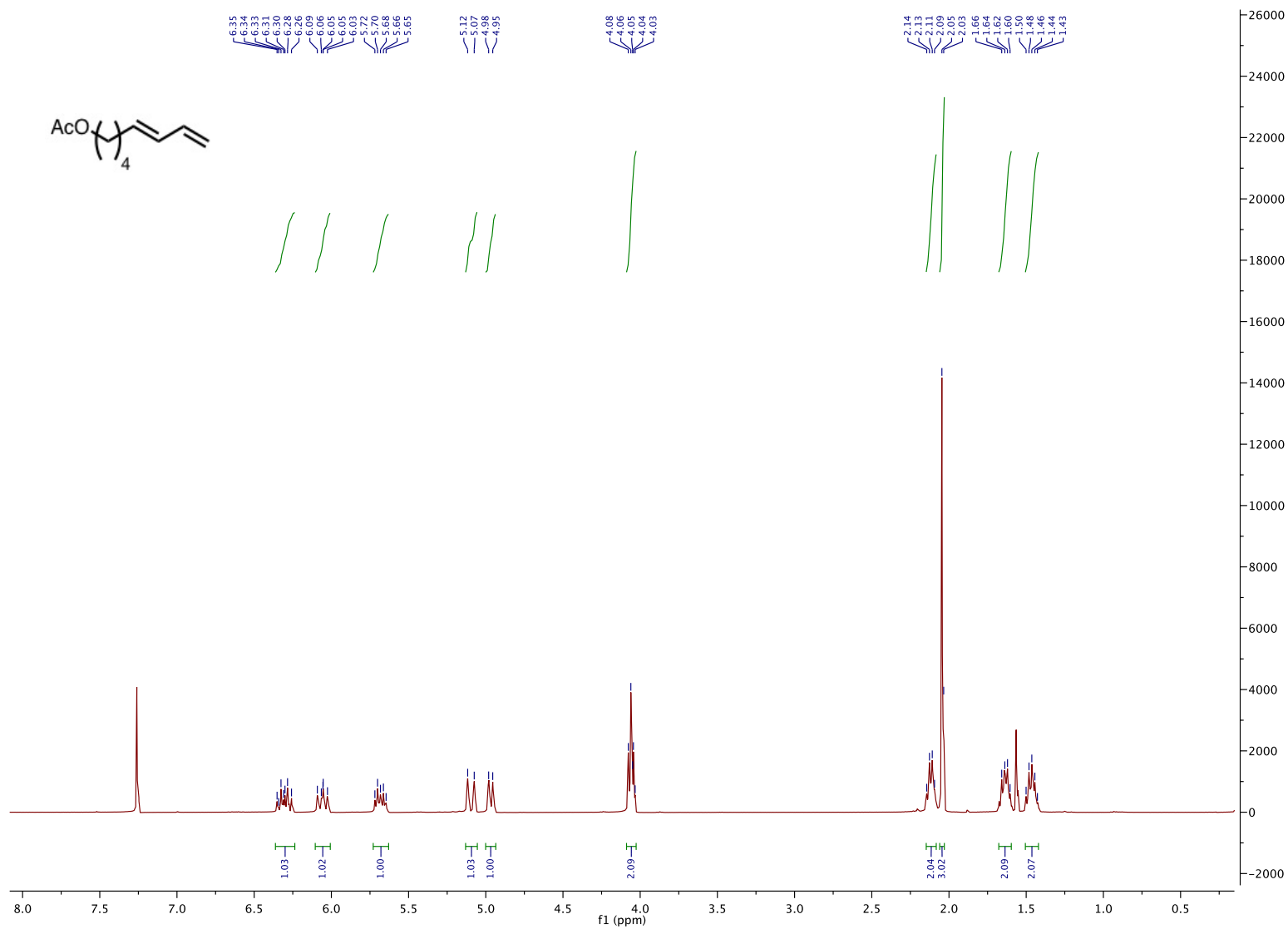
SCF Energy (M06, n-octanol):	-234.6211067
SCF Energy (B3LYP, gas-phase):	-234.4888887
Enthalpy Correction:	0.151012
Free-Energy Correction:	0.114442

C	-1.96072100	-0.40489300	-0.04878800
C	-3.13269300	0.16555500	0.26854800
H	-1.93672300	-1.46489300	-0.30470500
H	-3.20074600	1.21939300	0.53009300
C	-0.68284900	0.29313000	-0.08002200
H	-0.70174300	1.35439700	0.17412300
C	0.48830500	-0.28334200	-0.39907200
H	0.49680000	-1.34699300	-0.64819000
C	1.82045300	0.41035900	-0.42902800
H	2.23978700	0.35013100	-1.44510200
H	1.68660200	1.47745200	-0.21045000
H	-4.05987500	-0.39945900	0.27822600
C	2.83395500	-0.20034600	0.55590000
H	2.99532500	-1.26504400	0.34820000
H	3.80381300	0.30512400	0.48419100
H	2.47806300	-0.11288900	1.58838600

References

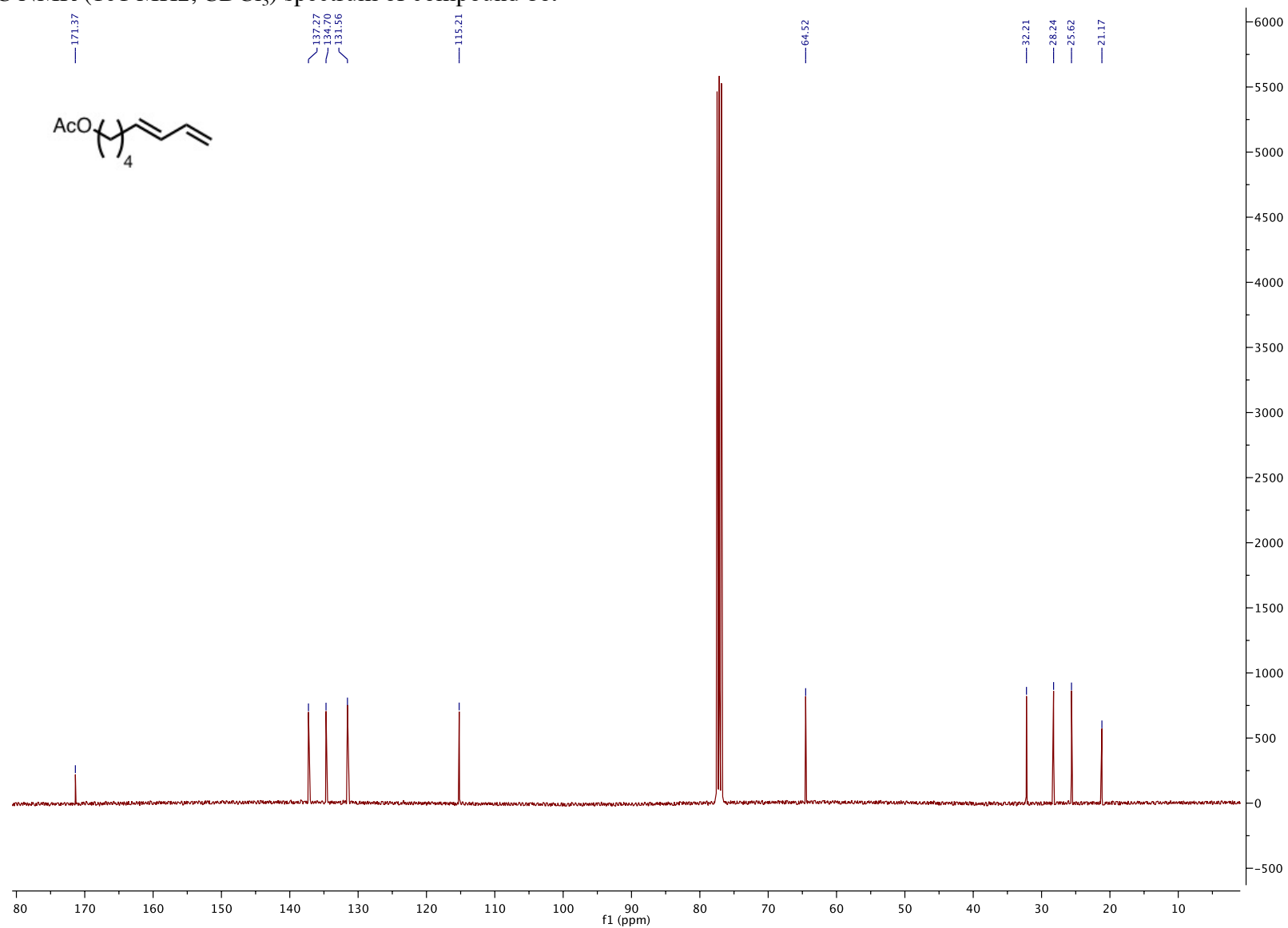
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- (2) Aponick, A.; Li, C.-Y.; Biannic B. *Org. Lett.* **2008**, *10*, 669–671.
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- (4) Lebel, H.; Davi, M.; Díez-González, S.; Nolan S. P. *J. Org. Chem.* **2007**, *72*, 144–149.
- (5) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.
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- (8) (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215–241. (b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157–167.
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¹H NMR (400 MHz, CDCl₃) spectrum of compound **8c**.



S131

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **8c**.



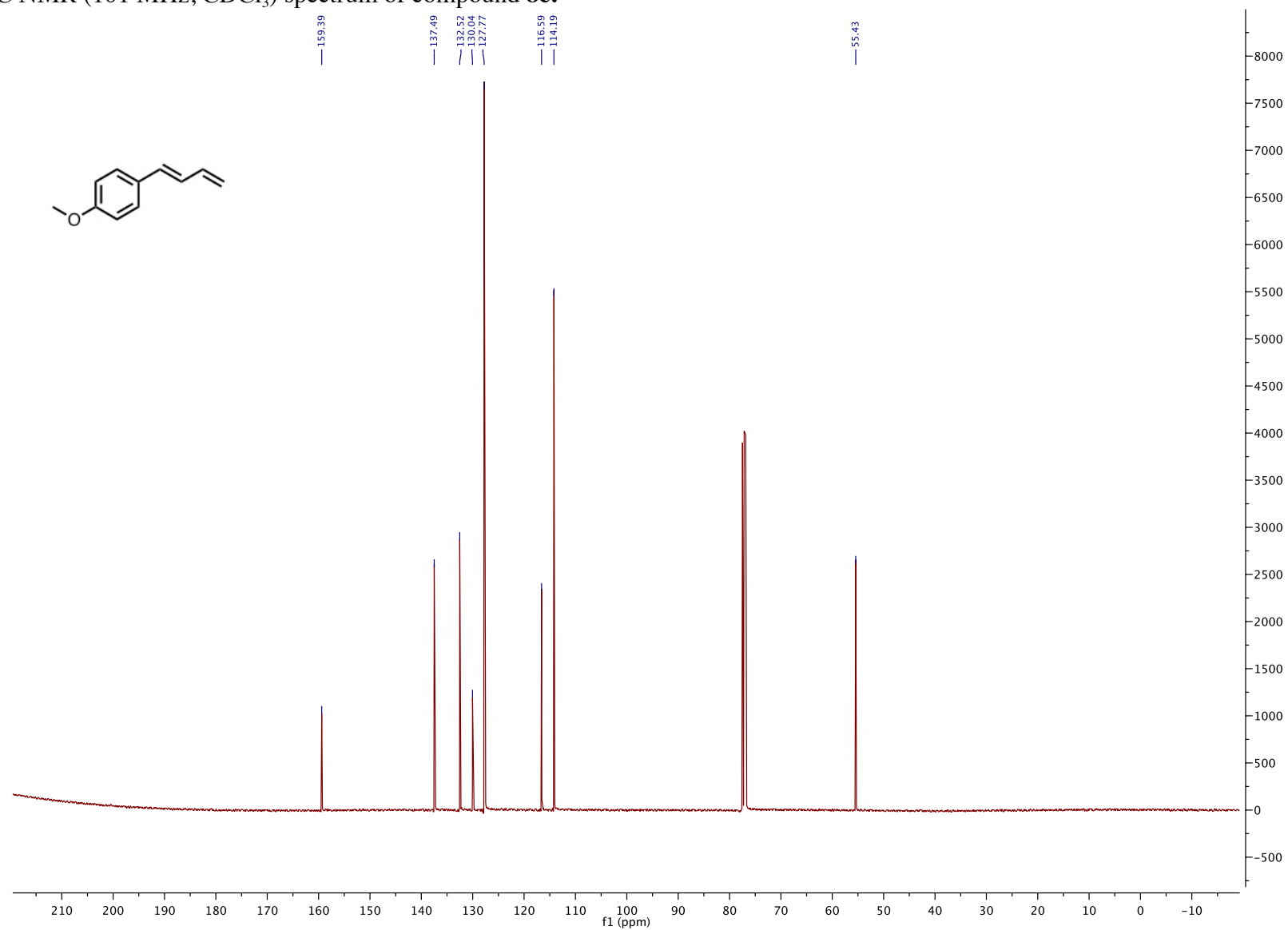
S132

Chemical structure: COc1ccc(C=CC#CCO)cc1

¹H NMR spectrum (ppm) showing peaks and integration values:

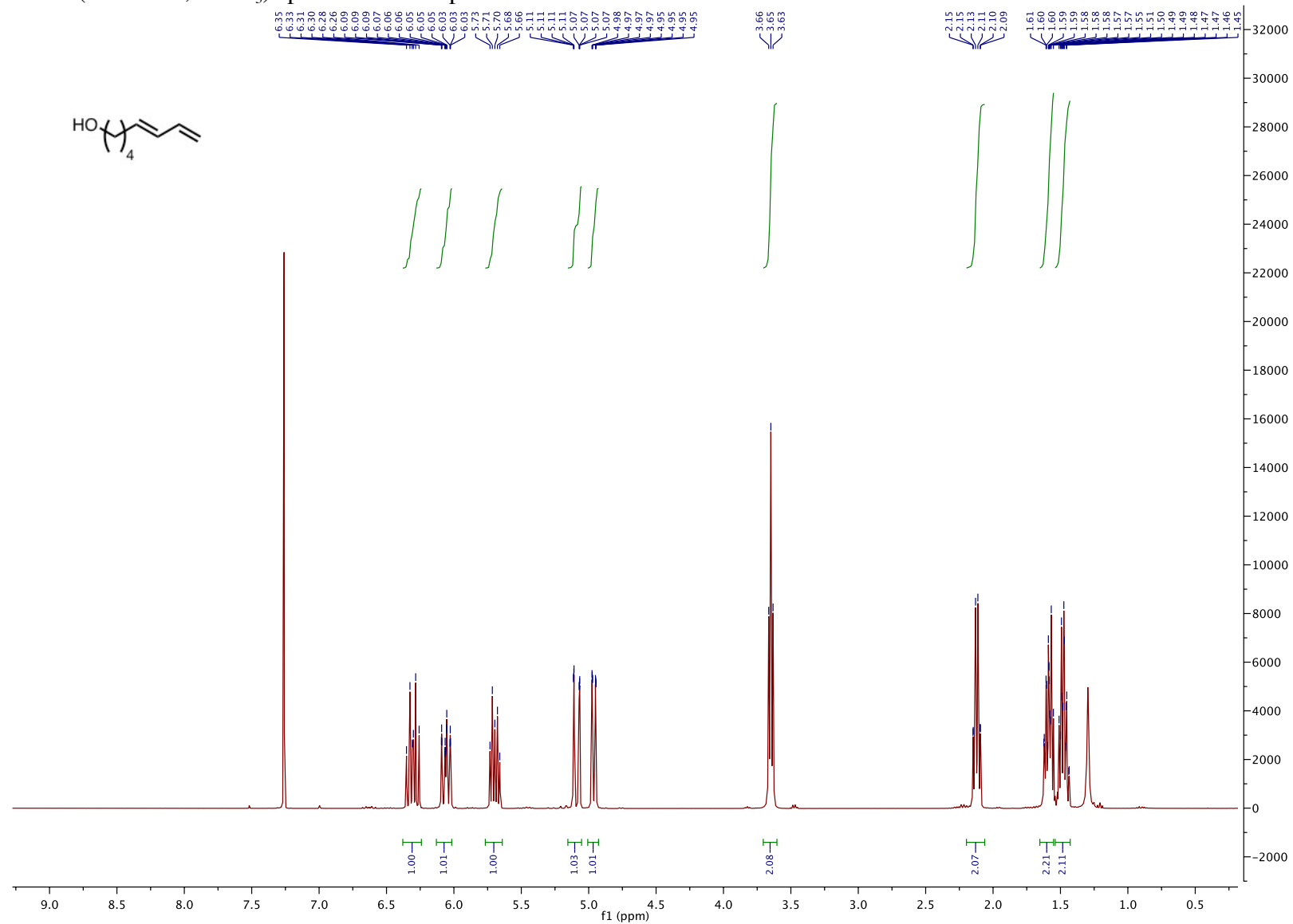
Chemical Shift (ppm)	Integration
~7.3	2.00
~6.8	1.99
~6.6	1.03
~6.4	1.98
~5.1	1.00
~5.0	0.99
~3.8	2.99

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **8e**.



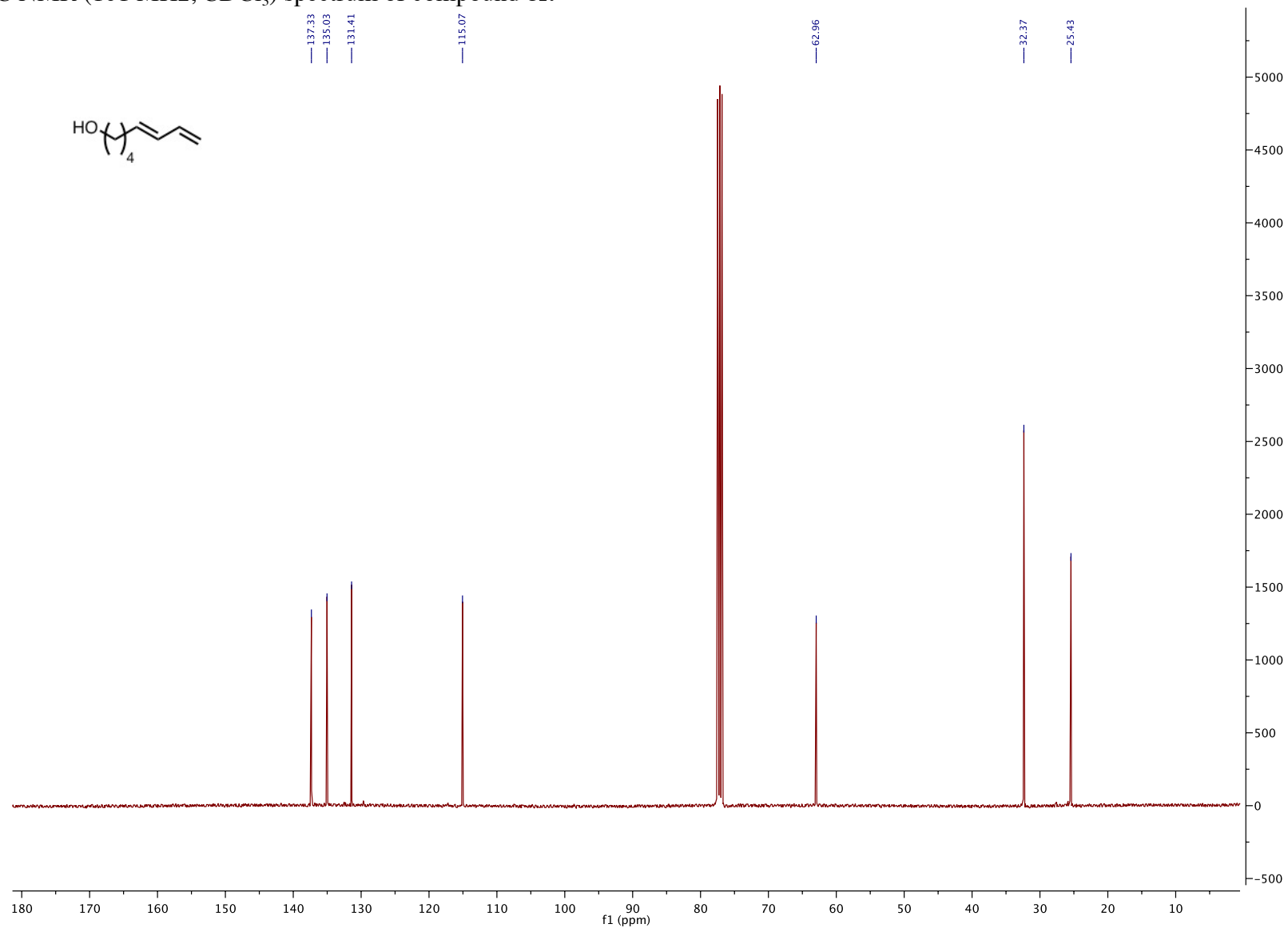
S134

^1H NMR (400 MHz, CDCl_3) spectrum of compound **8f**.



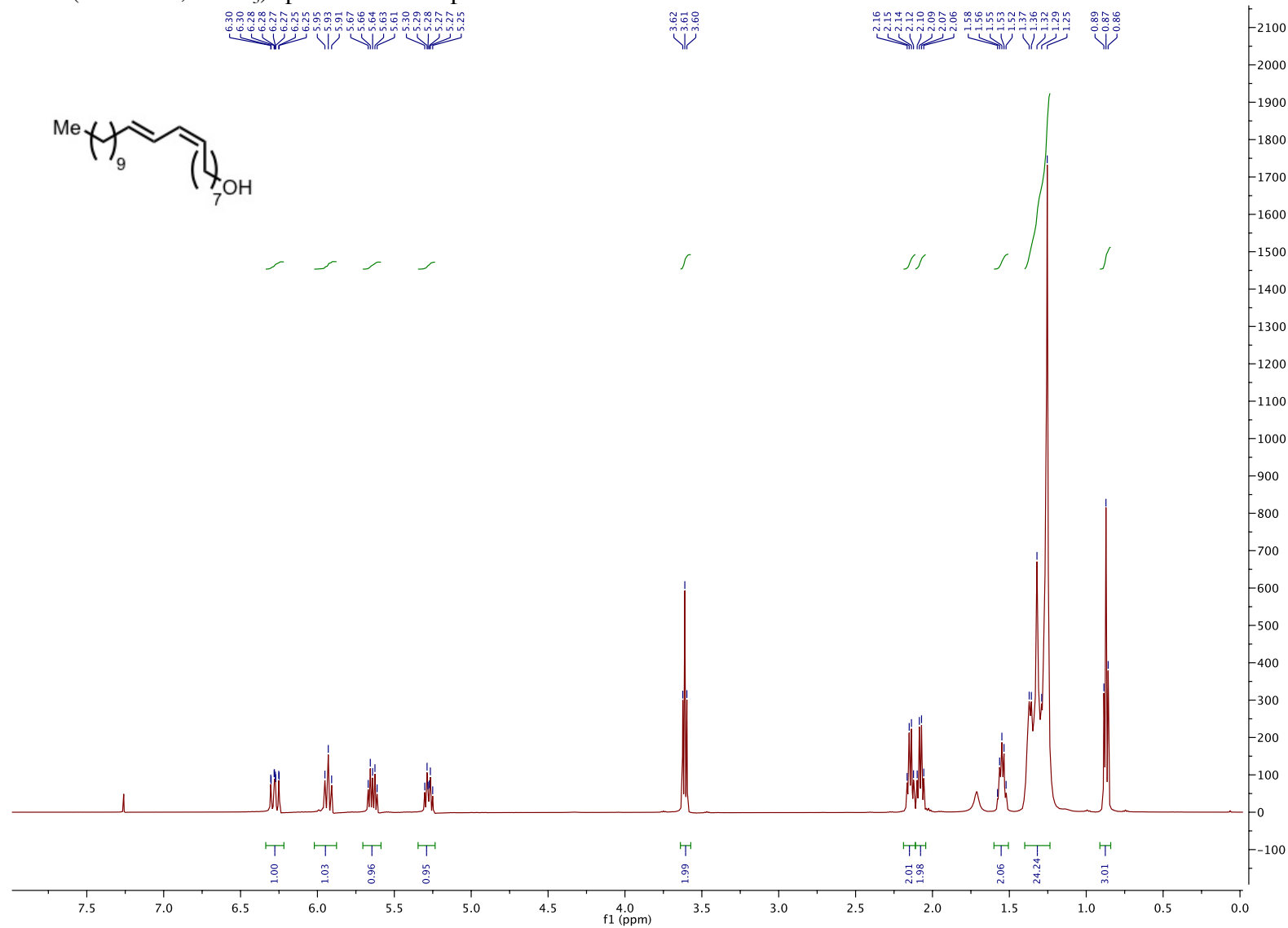
S135

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **8f**.

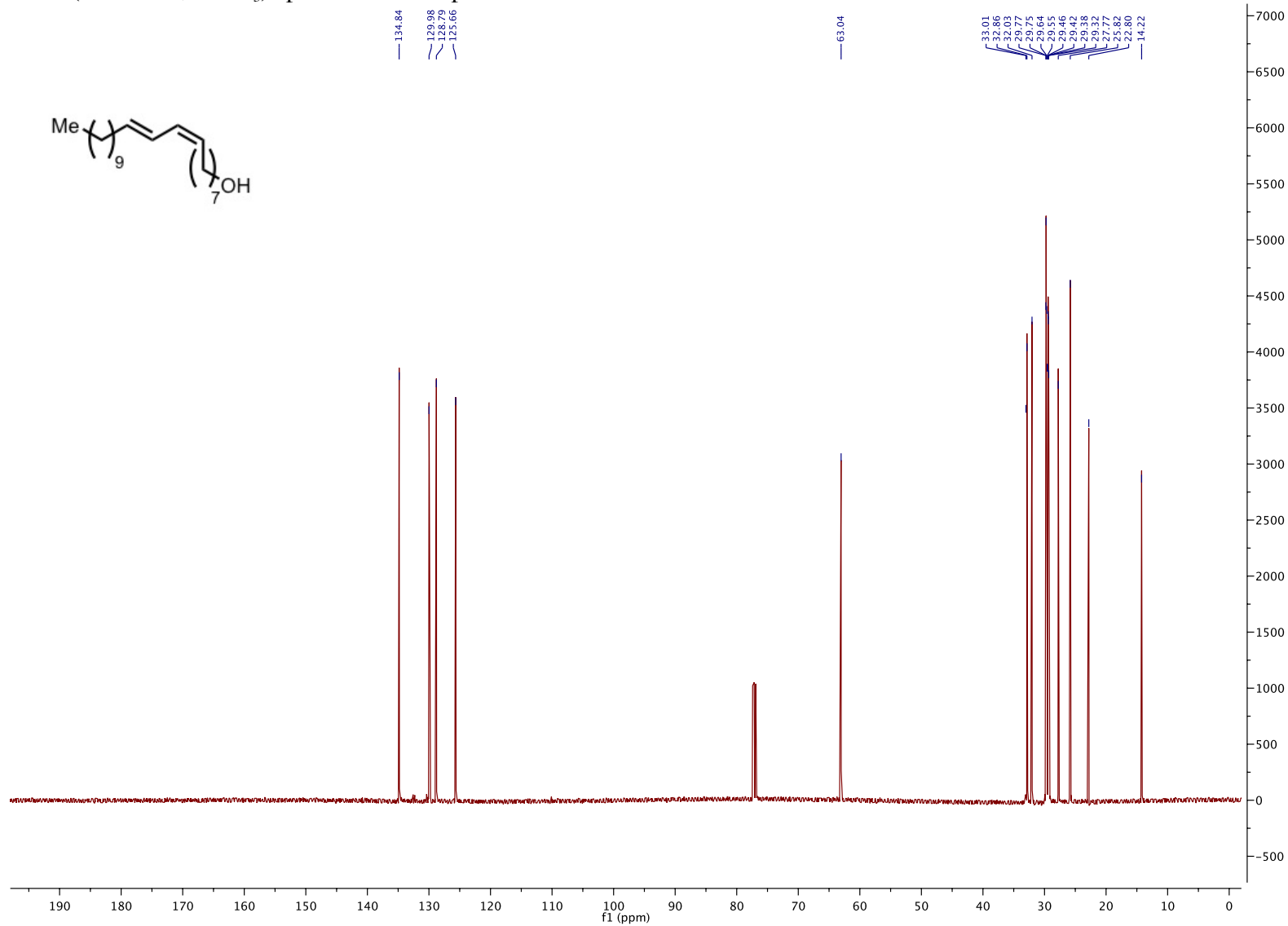


S136

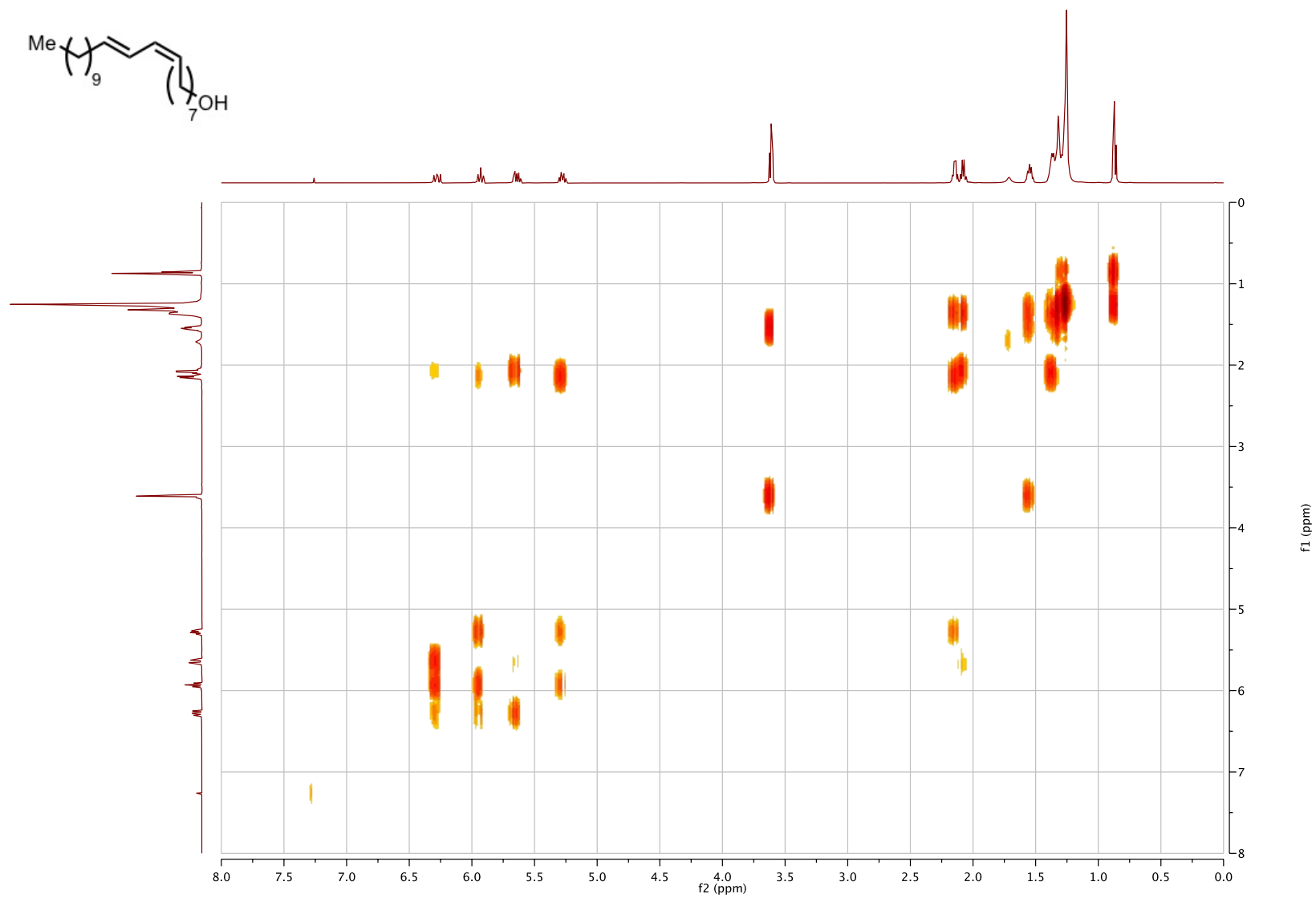
^1H NMR (500 MHz, CDCl_3) spectrum of compound **9a**.



^{13}C NMR (126 MHz, CDCl_3) spectrum of compound **9a**.

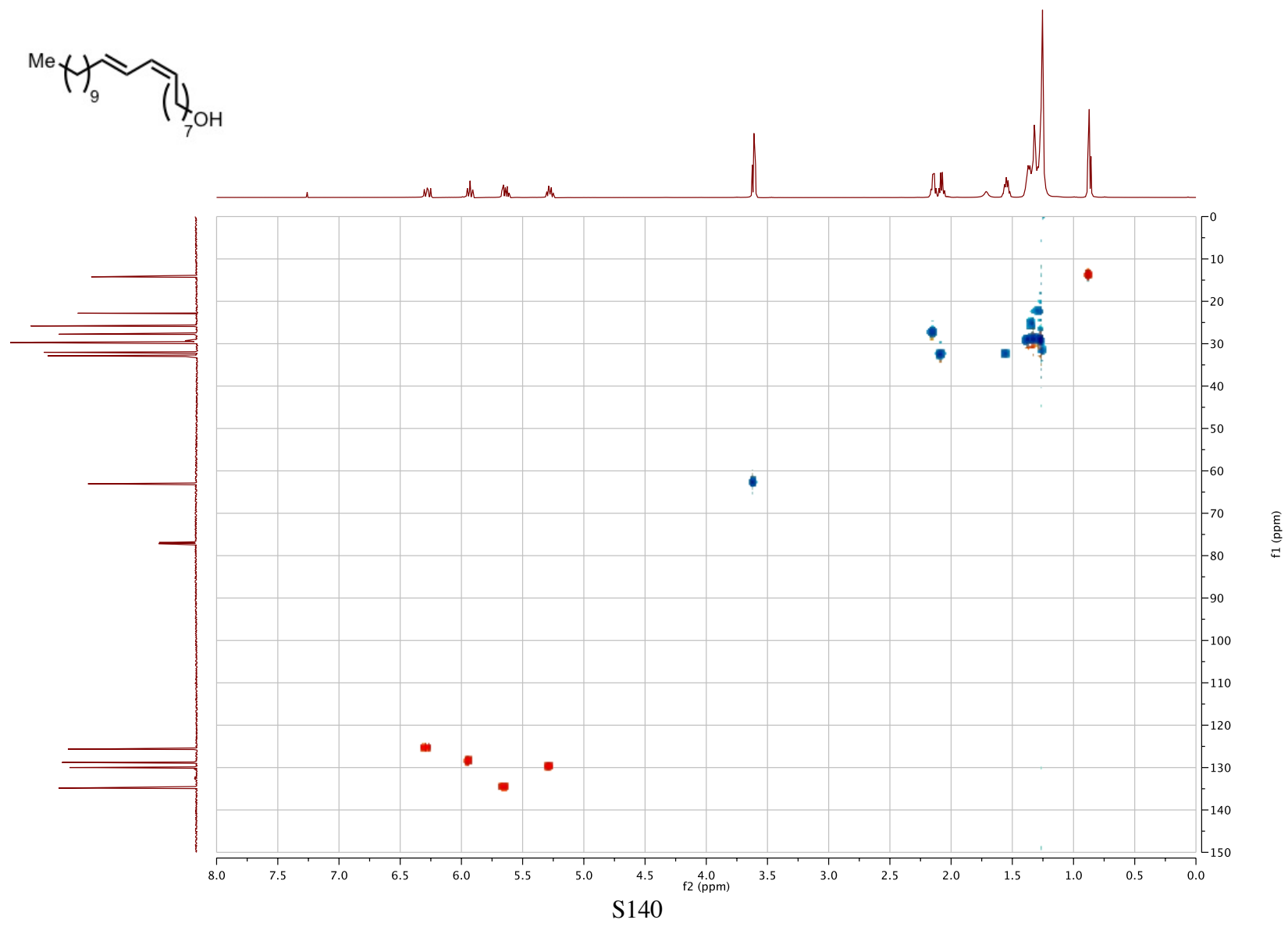


gCOSY spectrum of compound **9a**.

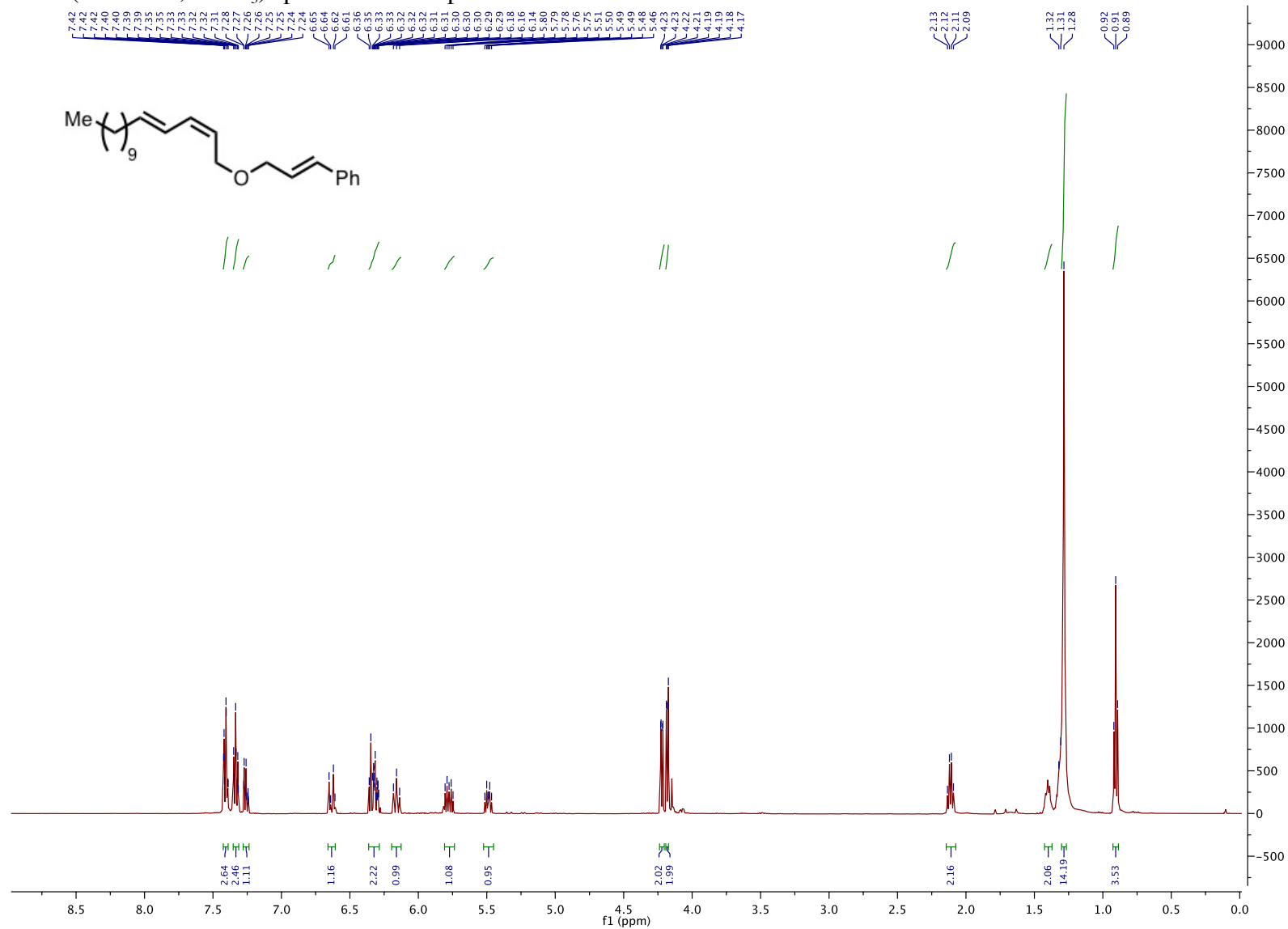


S139

HSQC spectrum of compound **9a**.

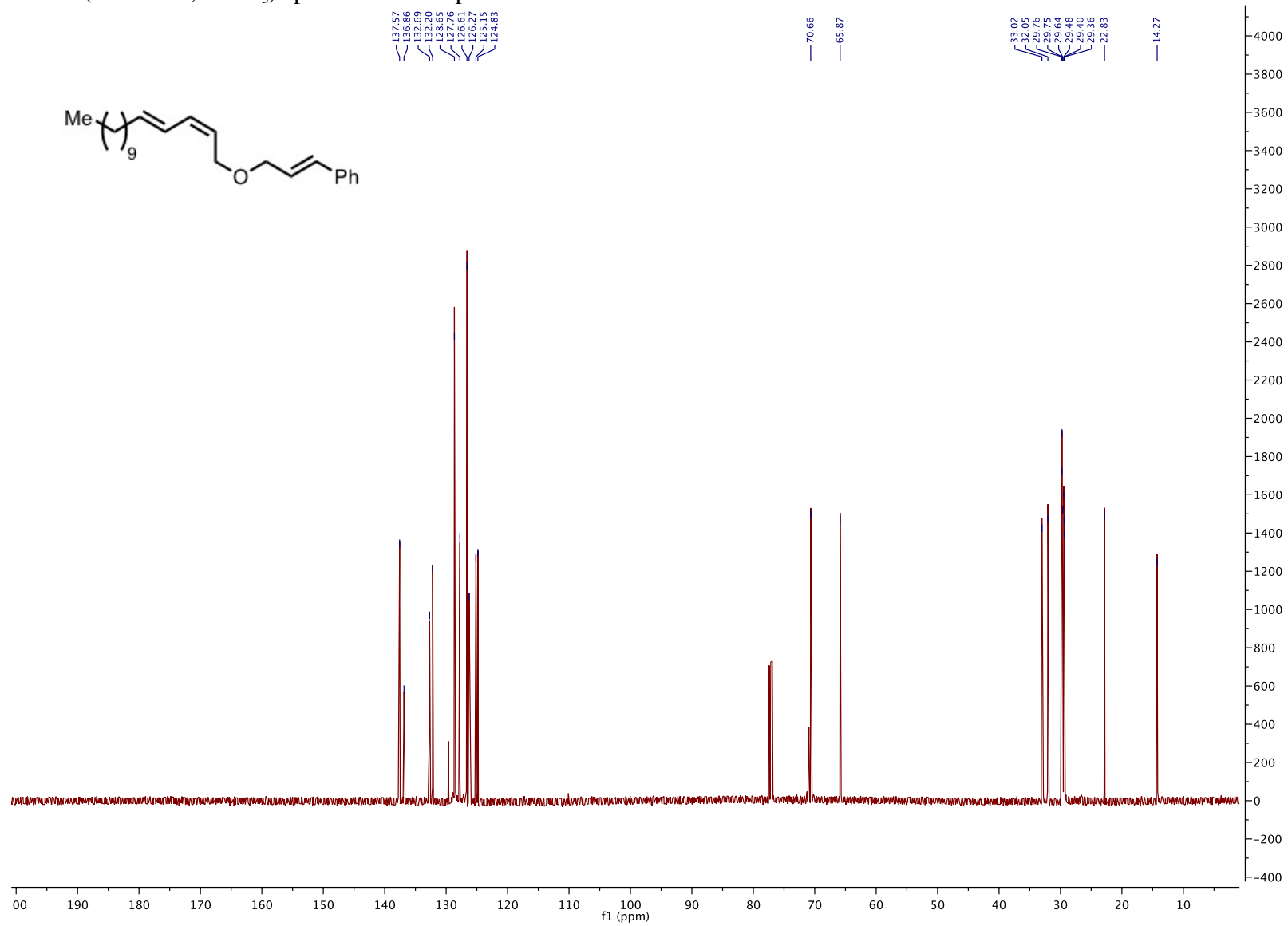


^1H NMR (500 MHz, CDCl_3) spectrum of compound **9b**.



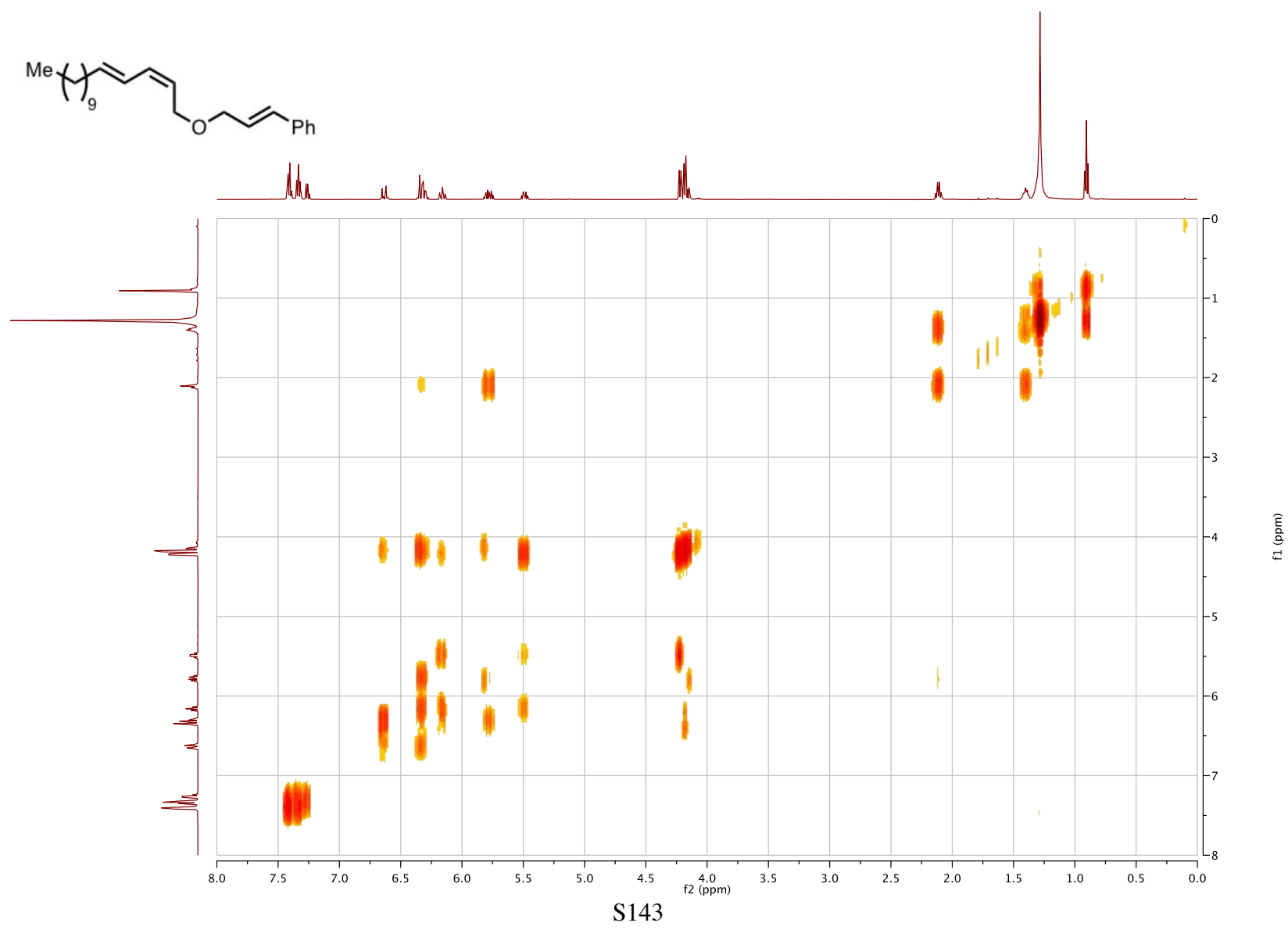
S141

^{13}C NMR (126 MHz, CDCl_3) spectrum of compound **9b**.

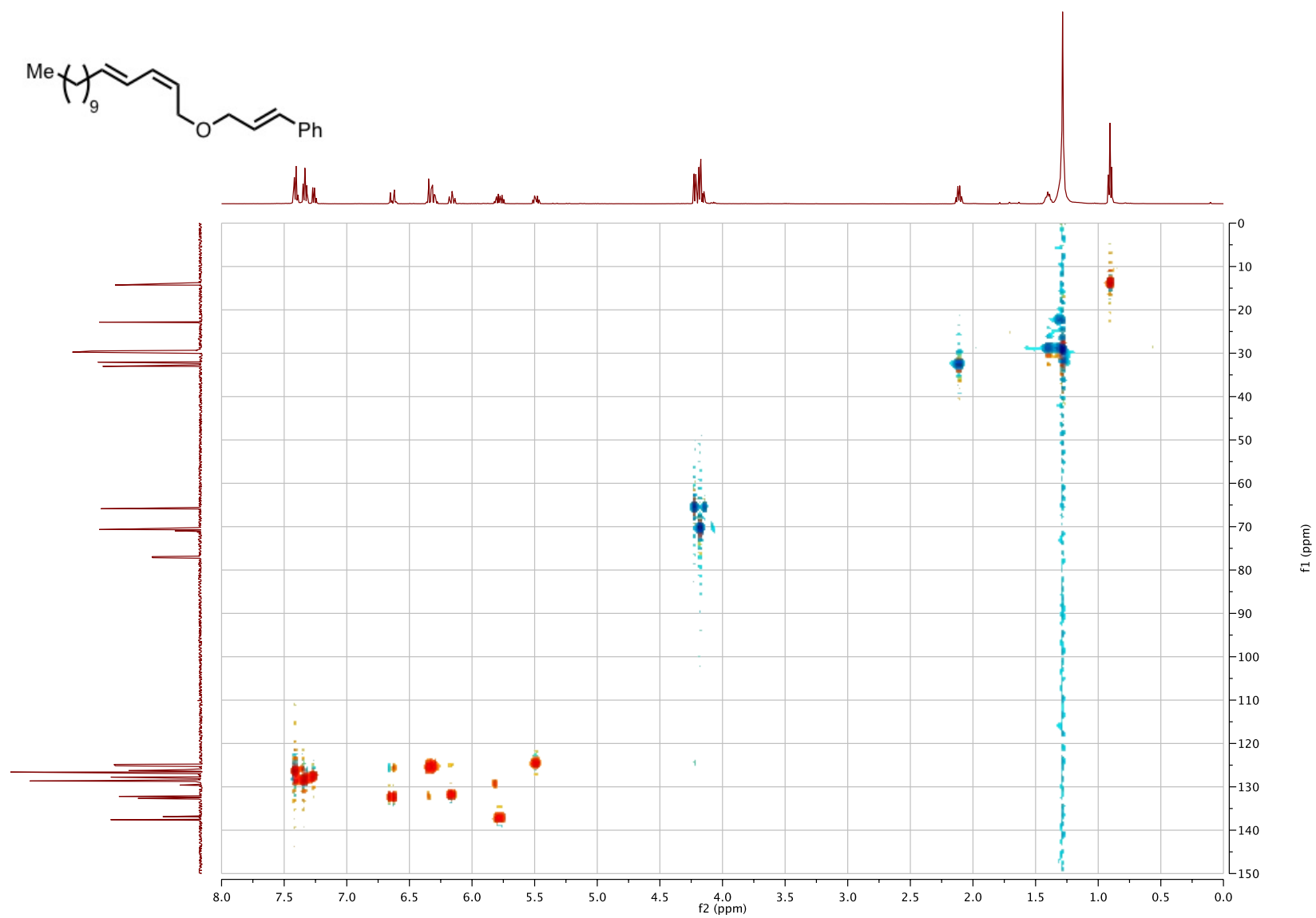


S142

gCOSY spectrum of compound **9b**.

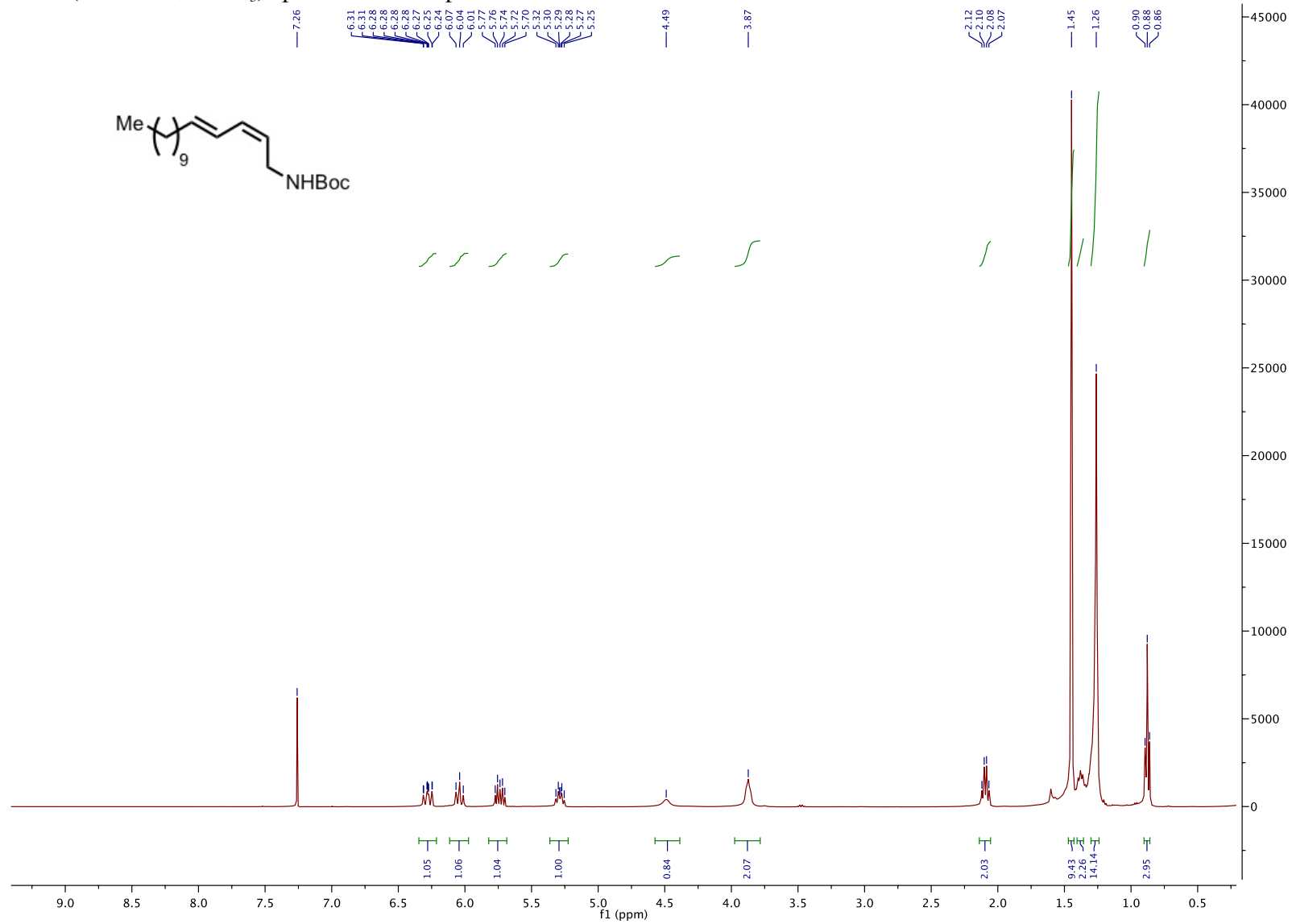


HSQC spectrum of compound **9b**.



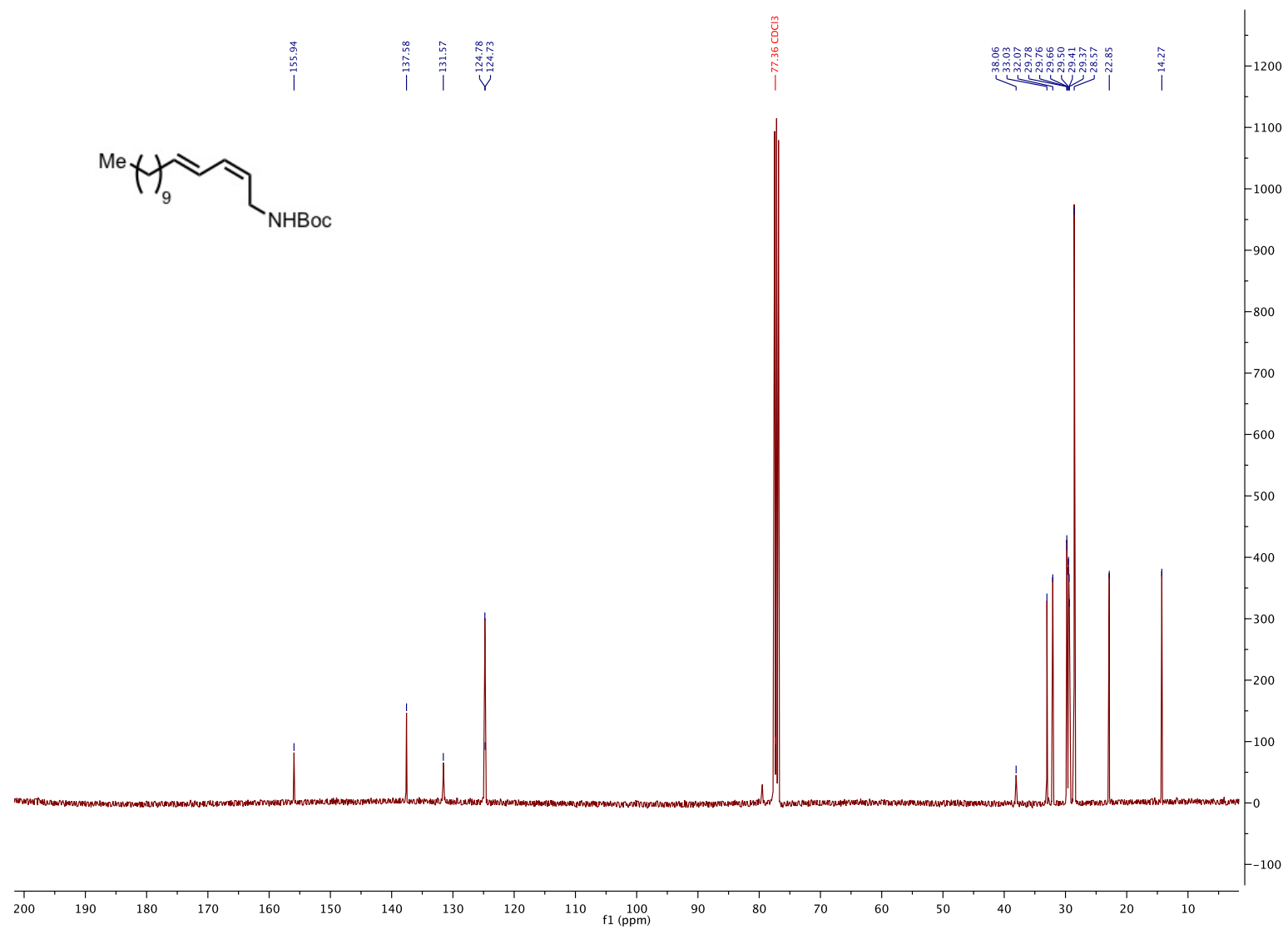
S144

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9c**.



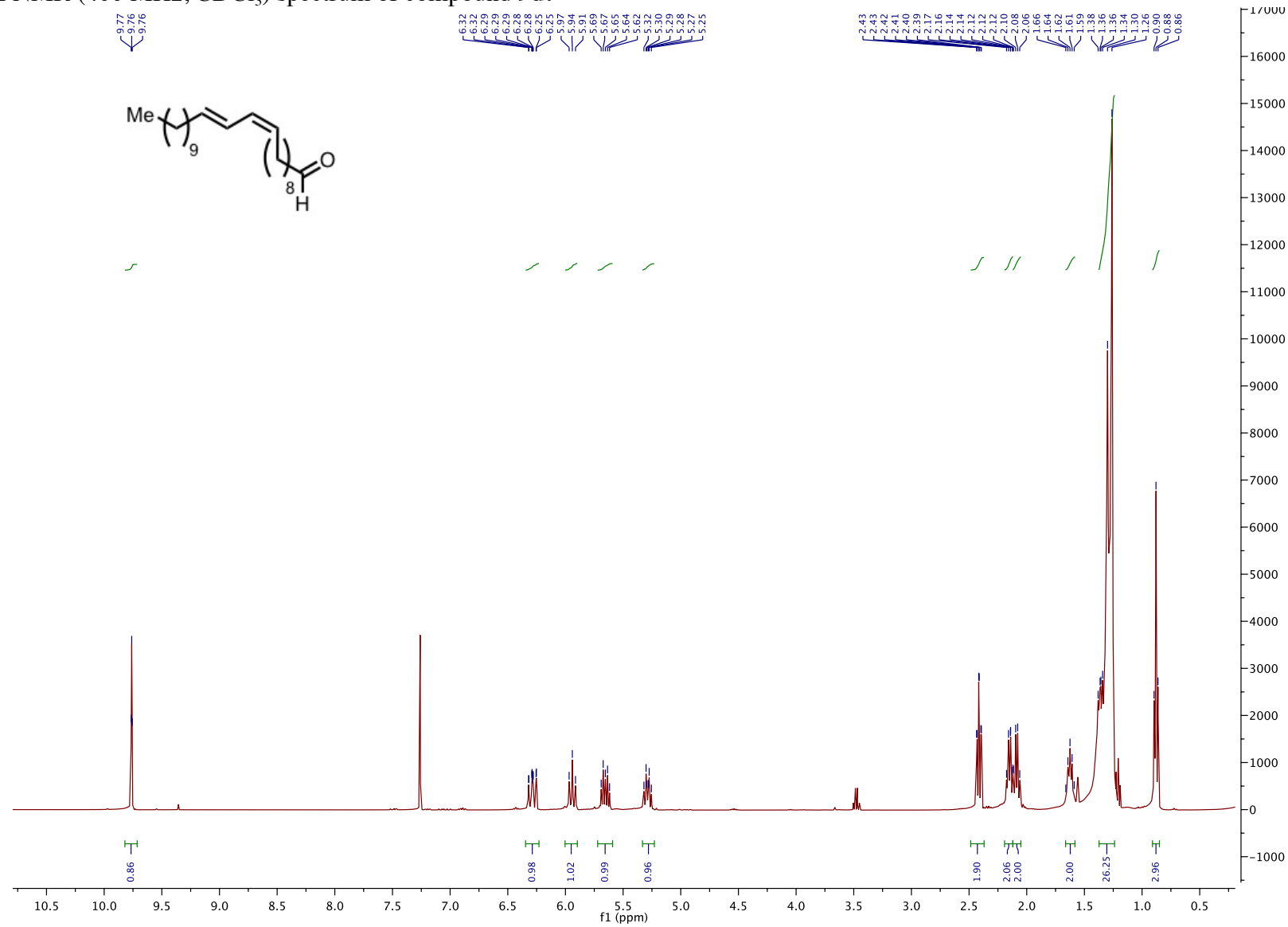
S145

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9c**.



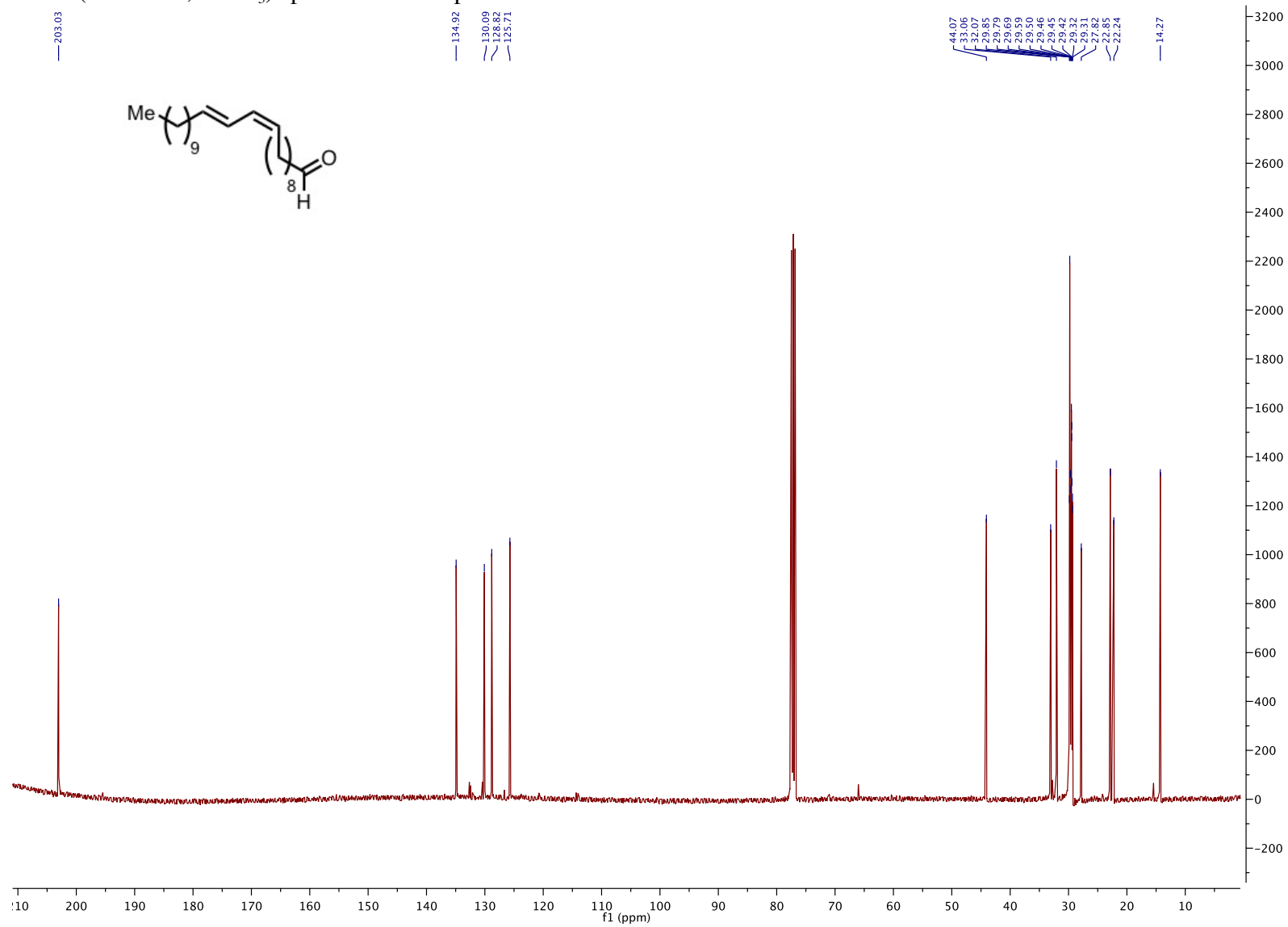
S146

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9d**.



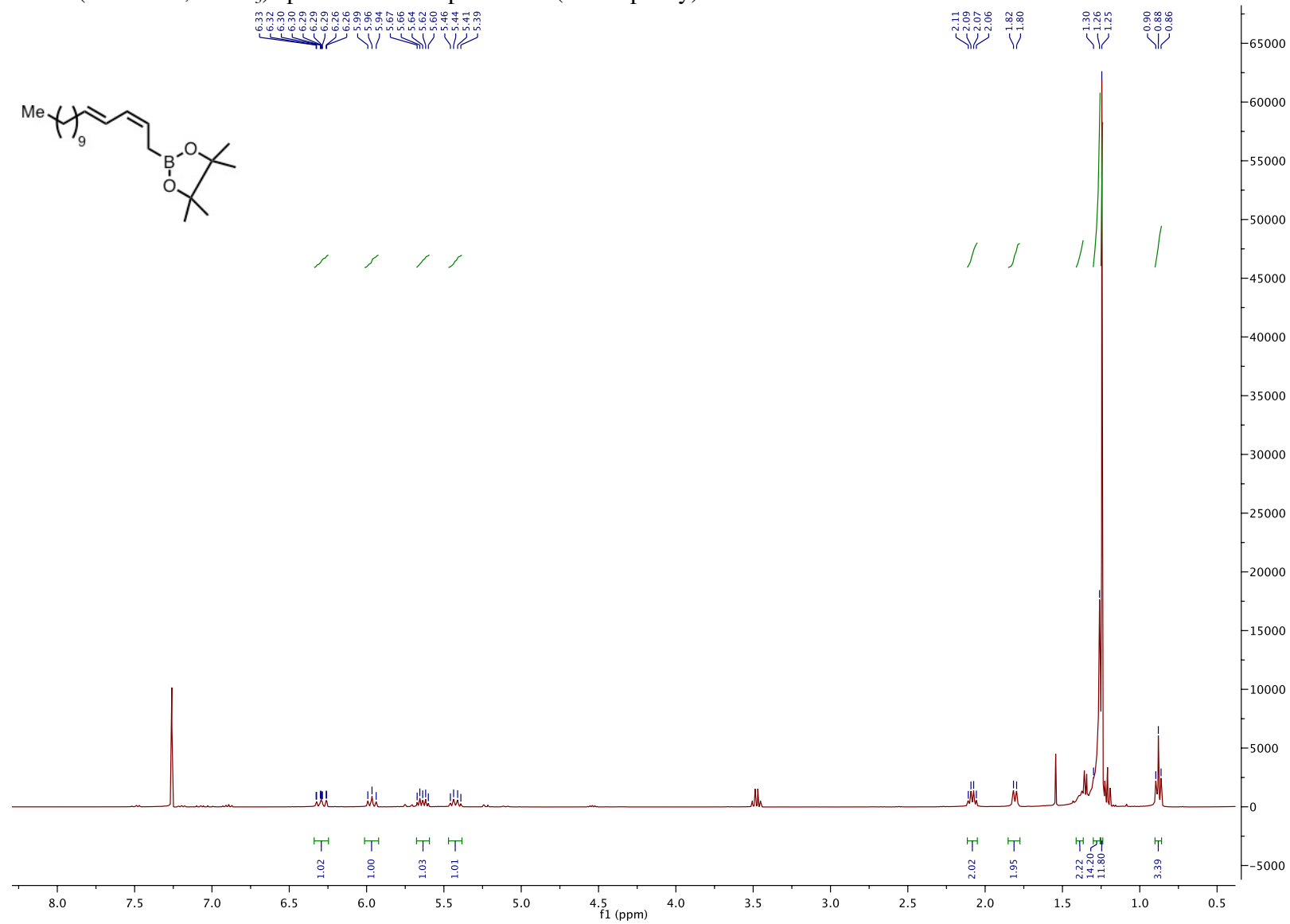
S147

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9d**.



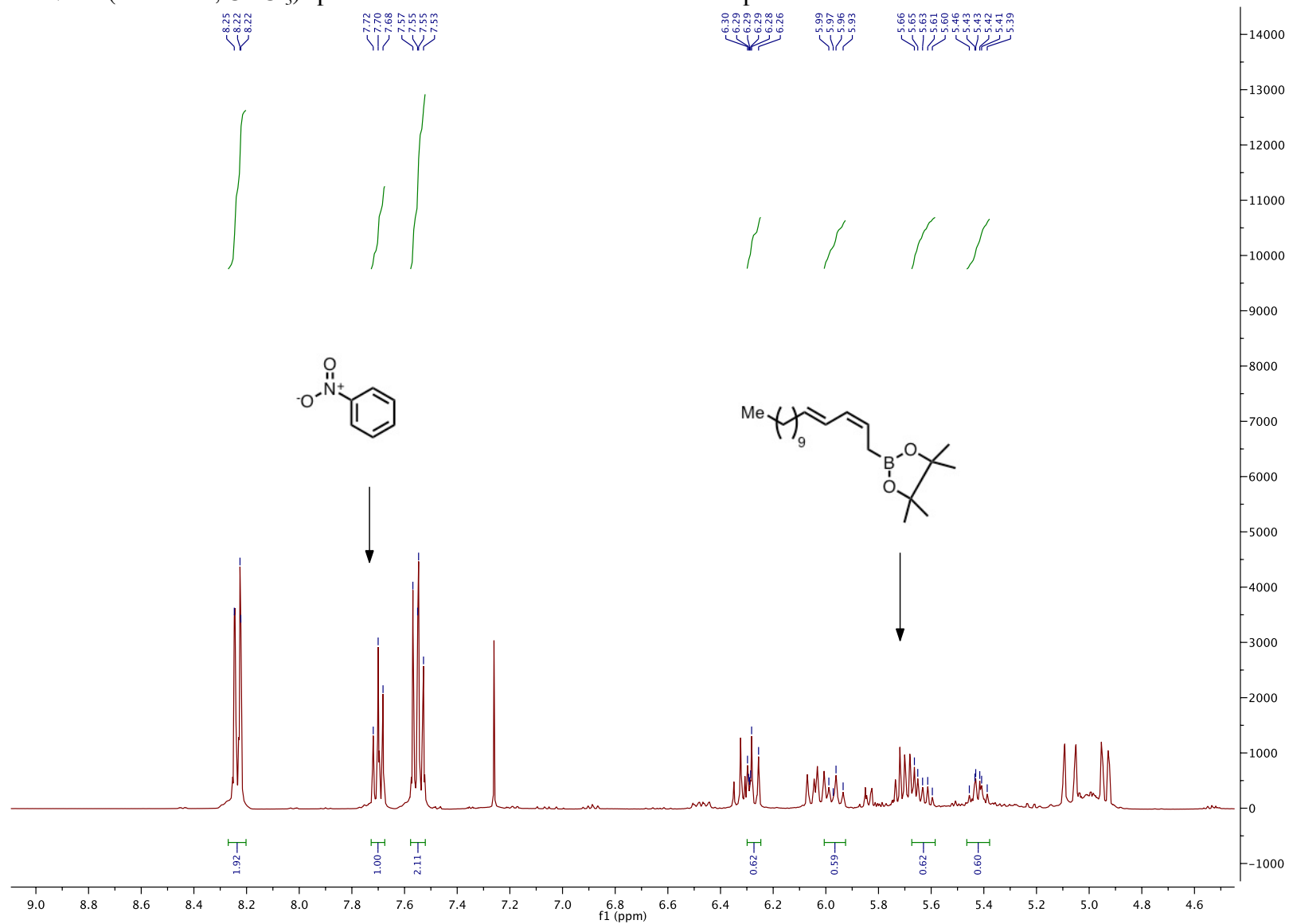
S148

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9e**. (~94% purity)



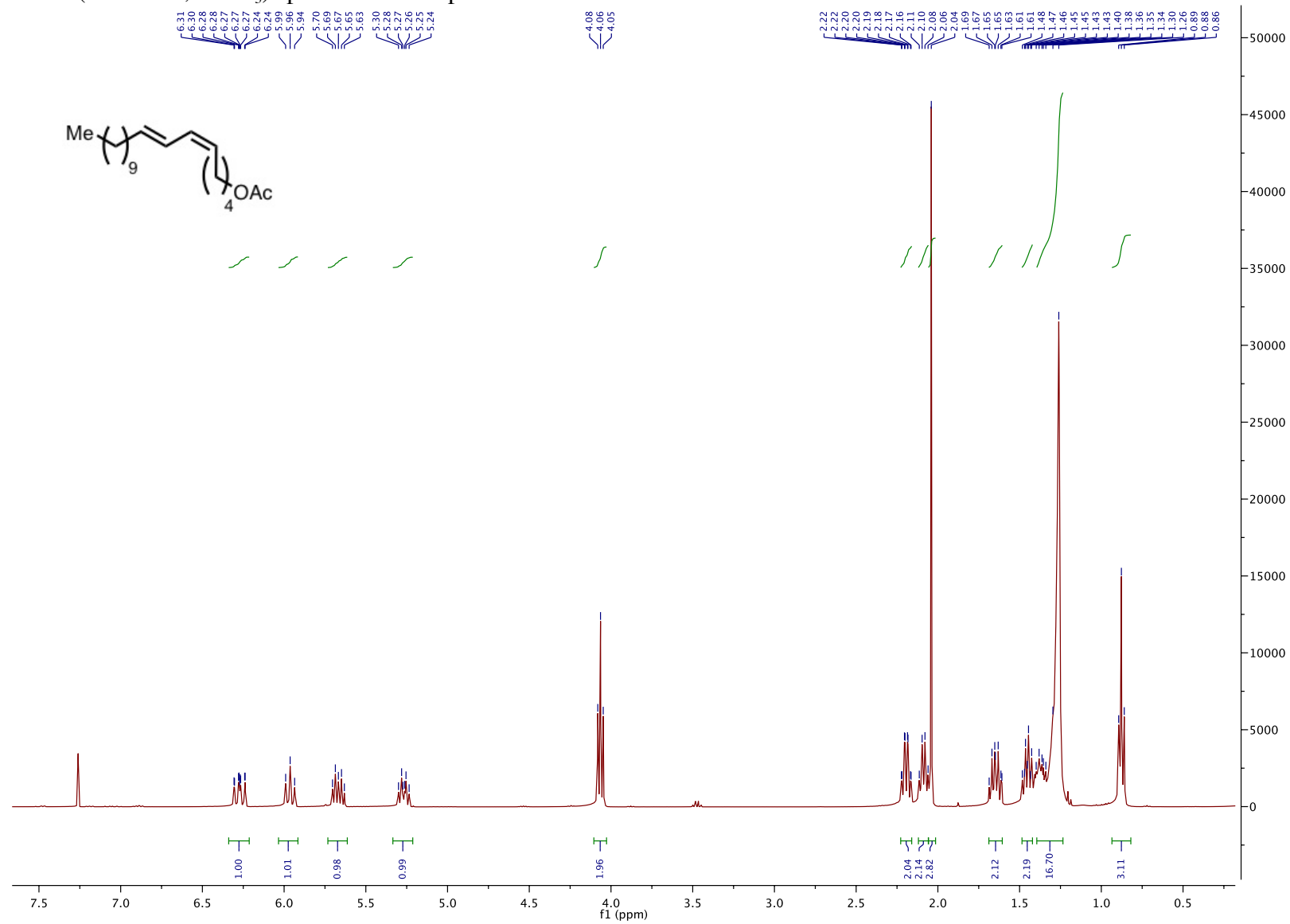
S149

¹H NMR (400 MHz, CDCl₃) spectrum of crude reaction mixture of compound **9e** with nitrobenzene internal standard.



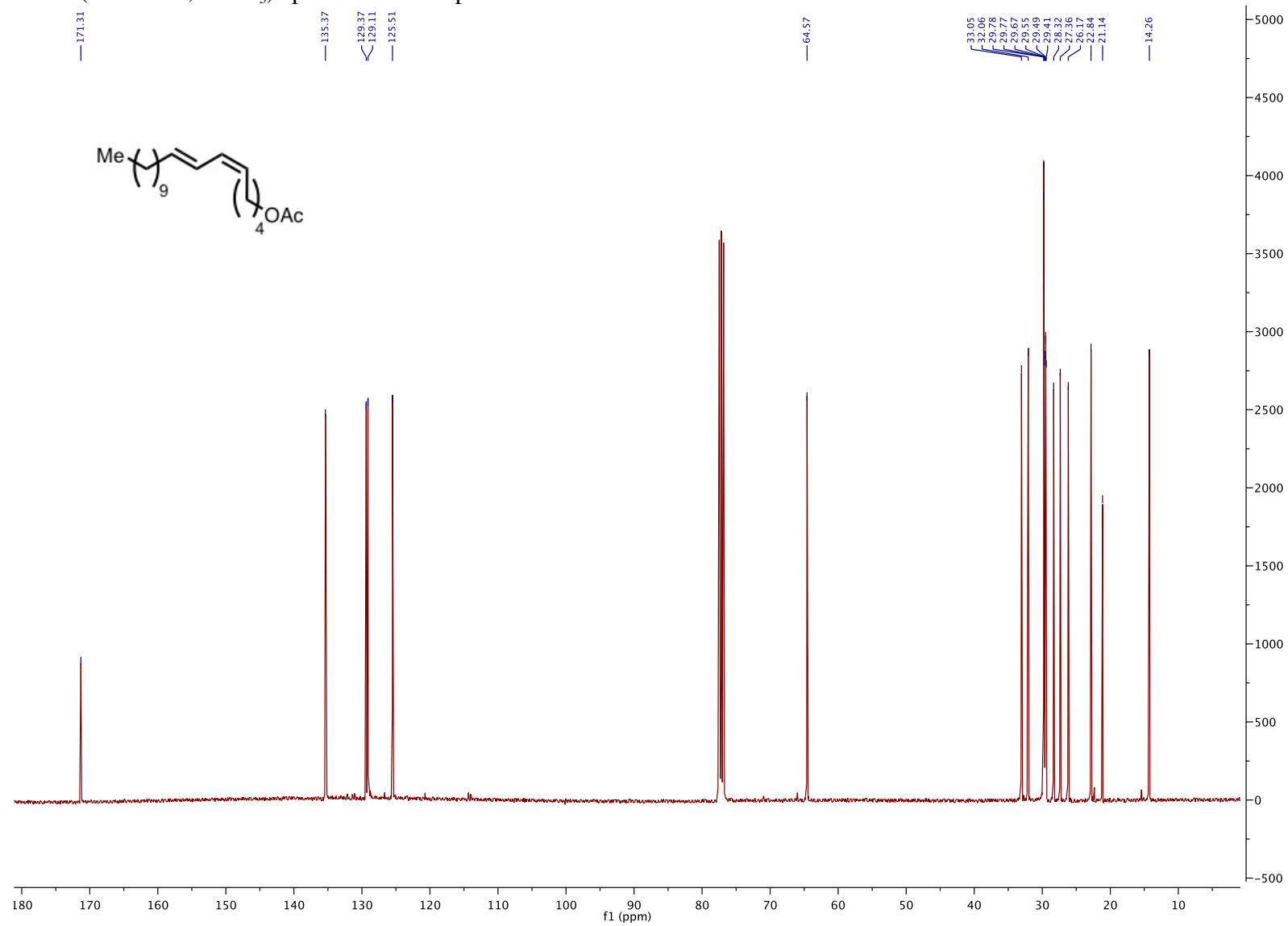
S150

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9f**.

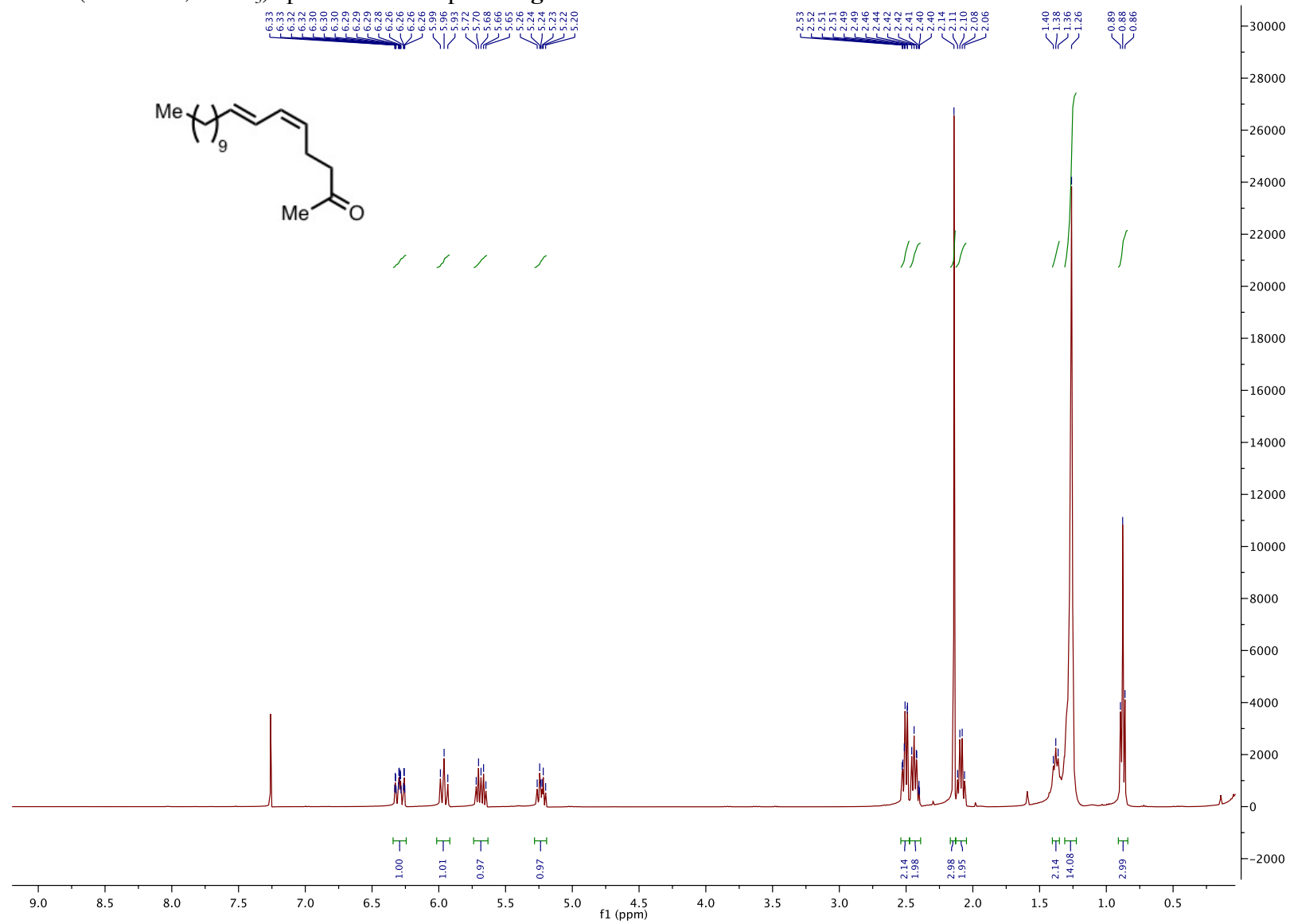


S151

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9f**.

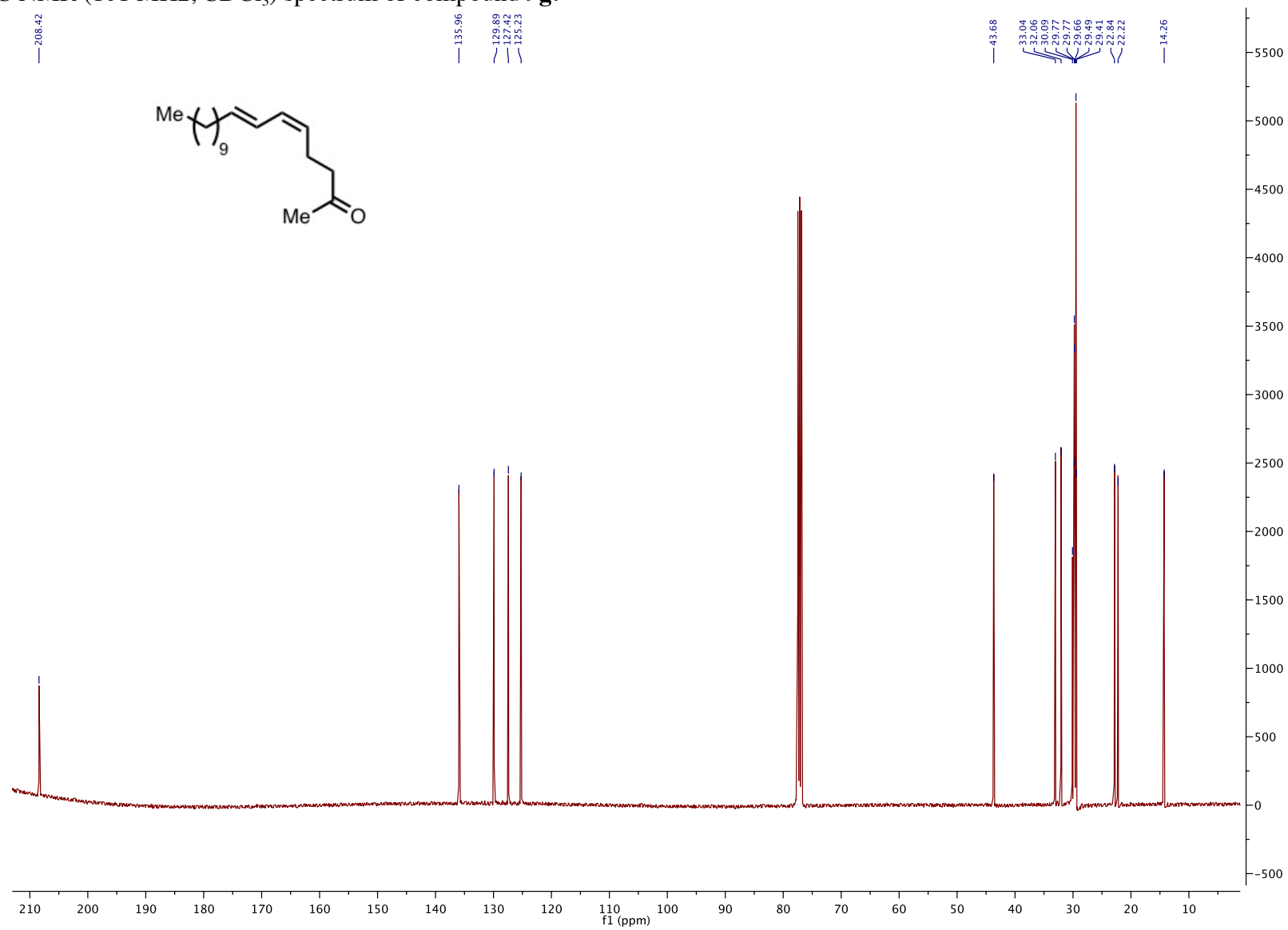


^1H NMR (400 MHz, CDCl_3) spectrum of compound **9g**.



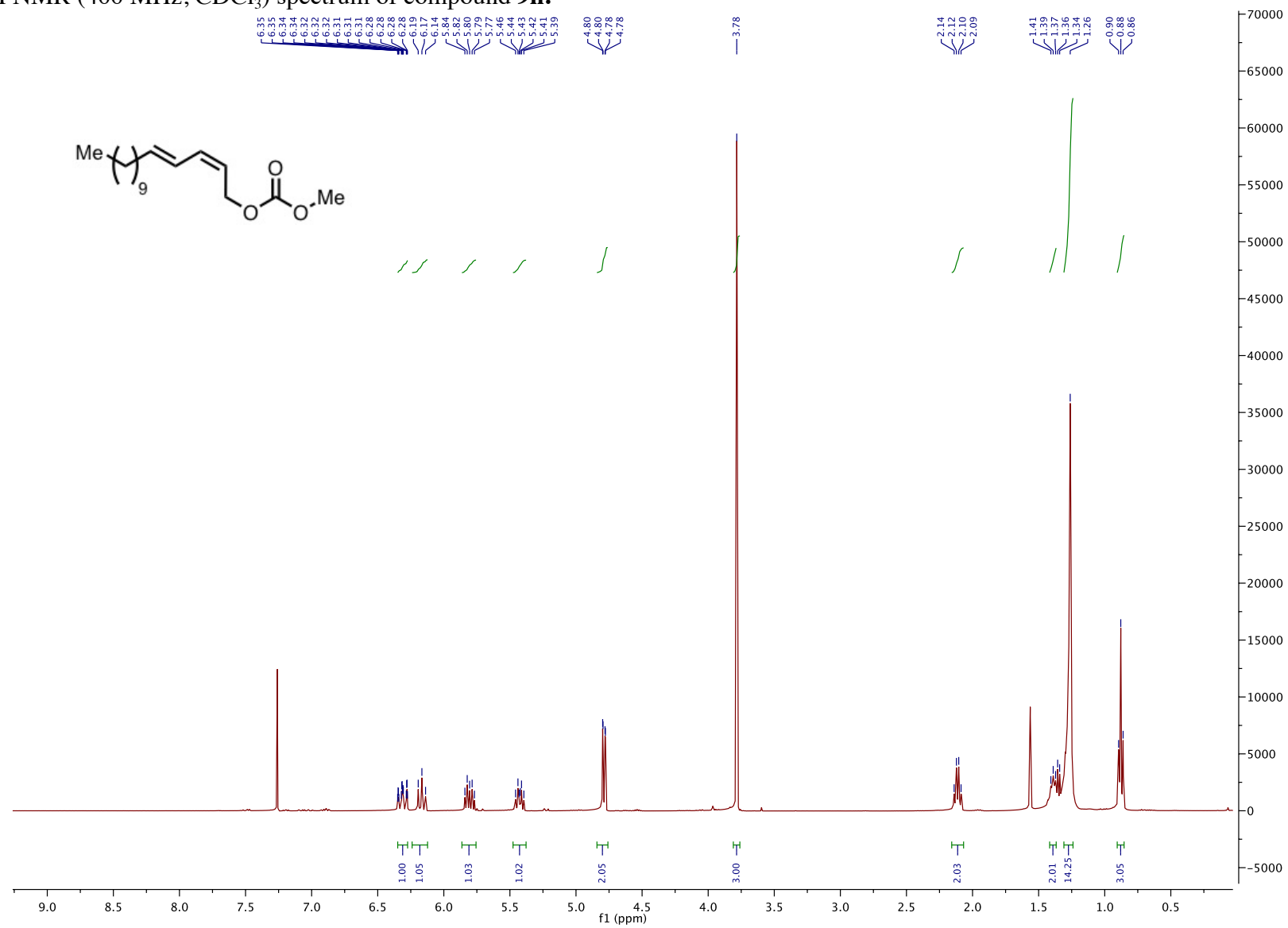
S153

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9g**.



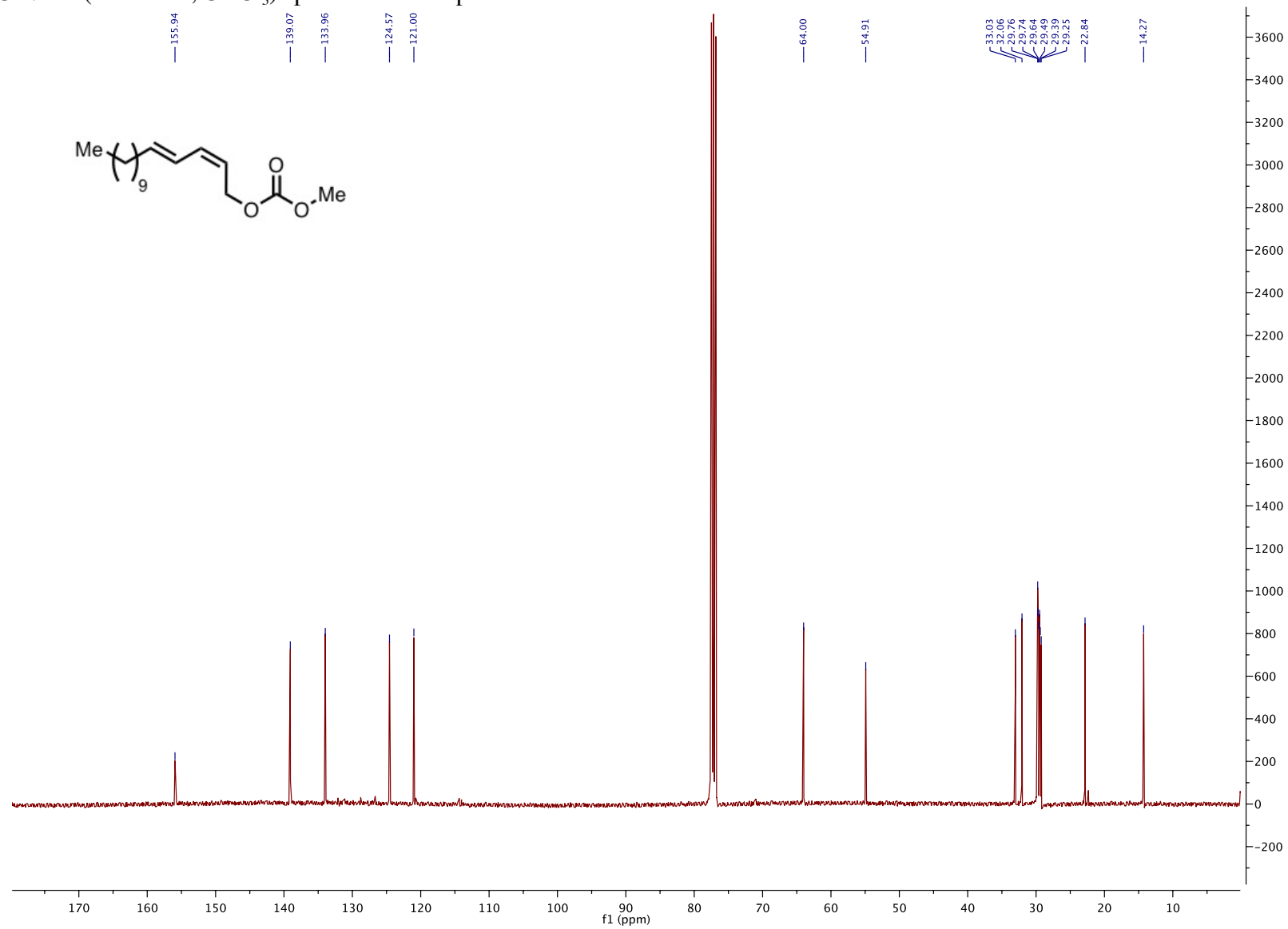
S154

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9h**.



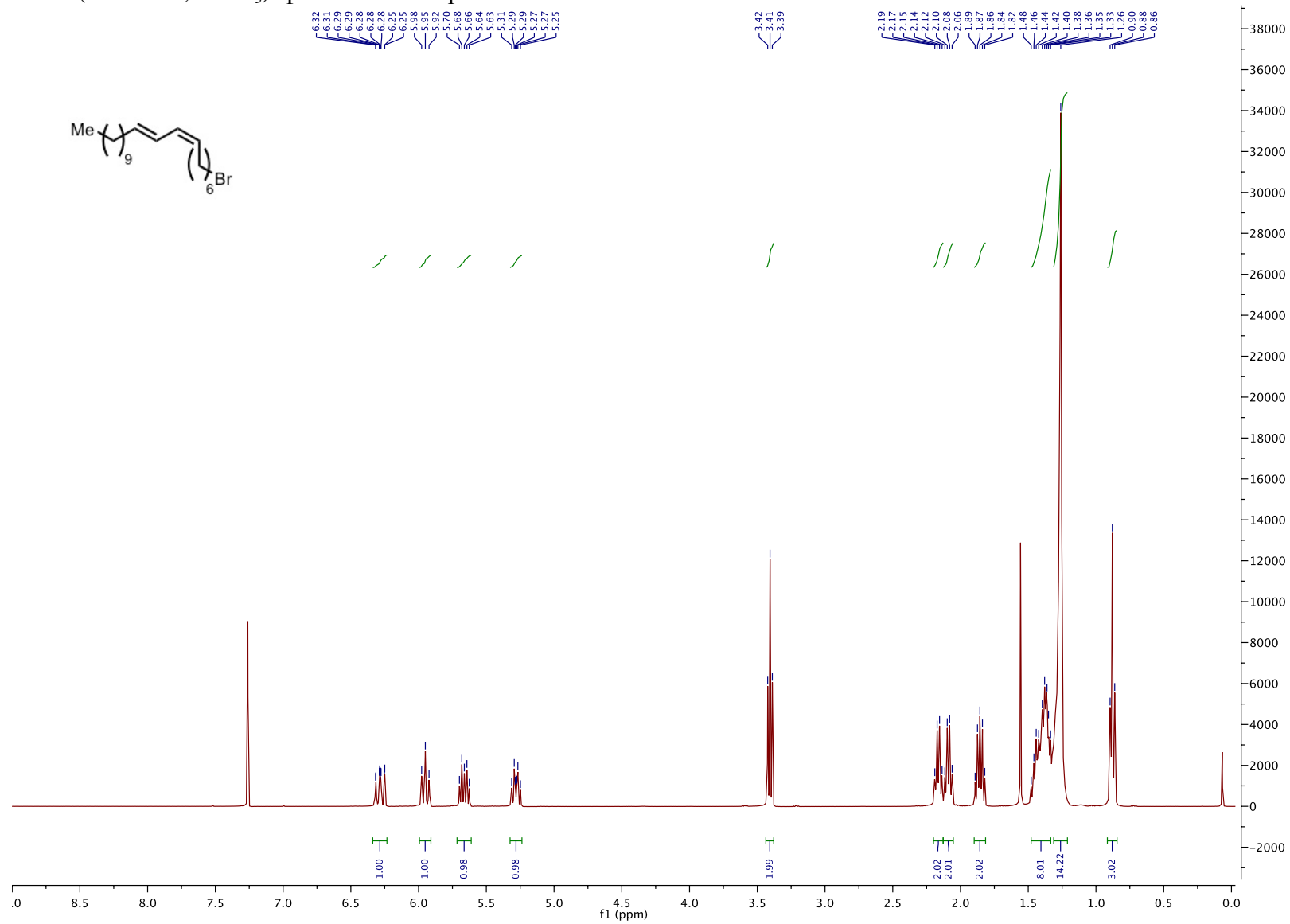
S155

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9h**.



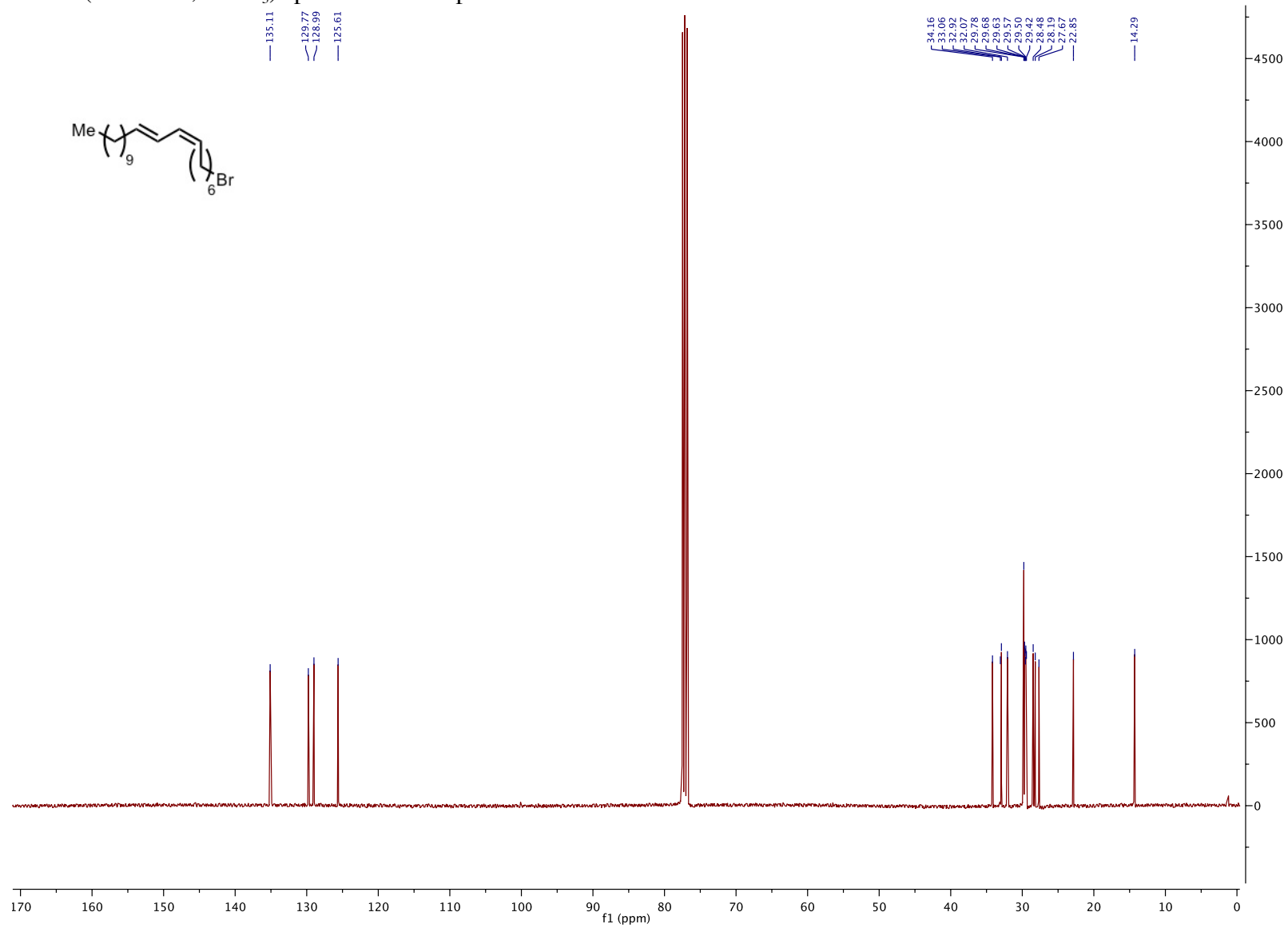
S156

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9i**.



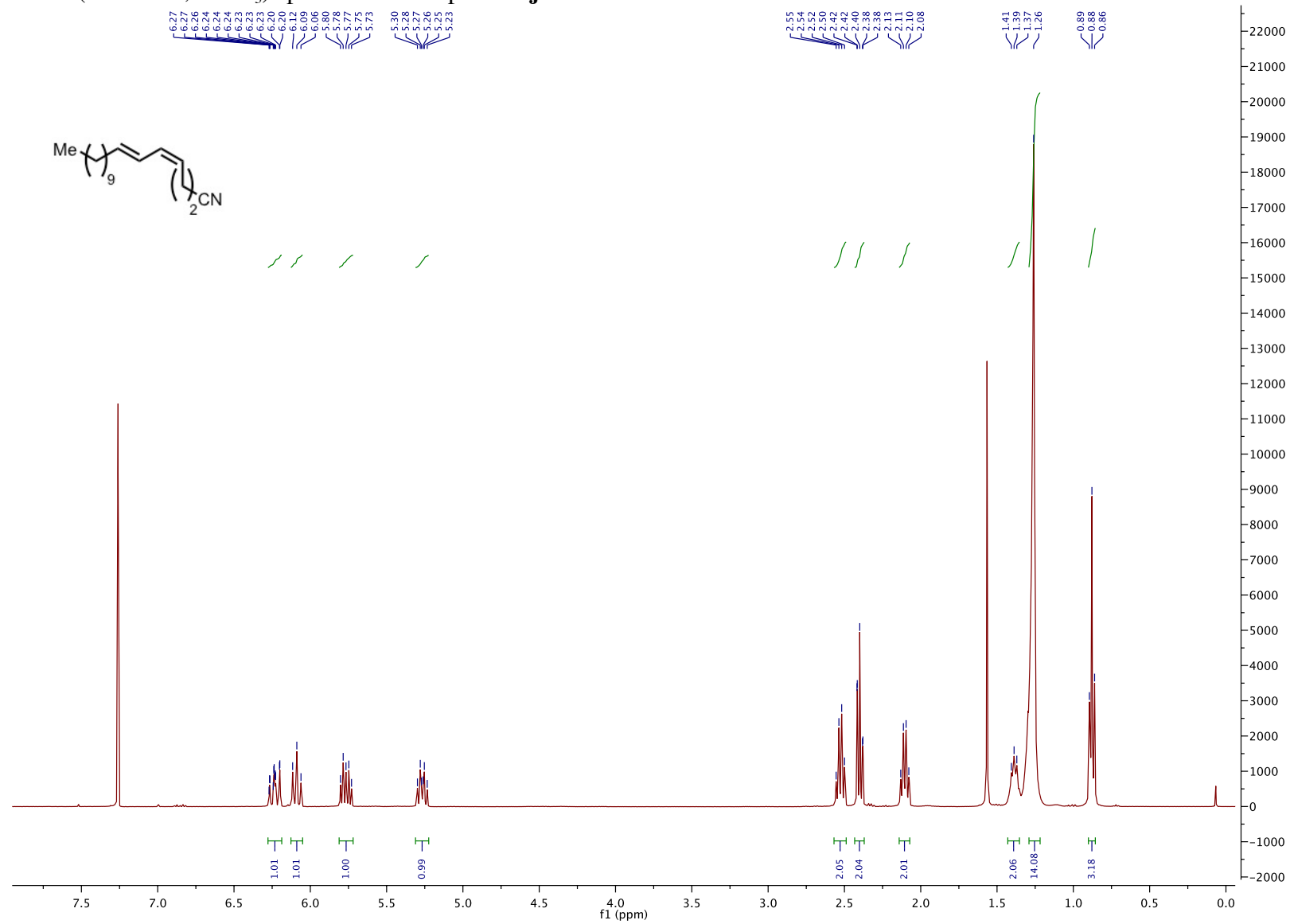
S157

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9i**.



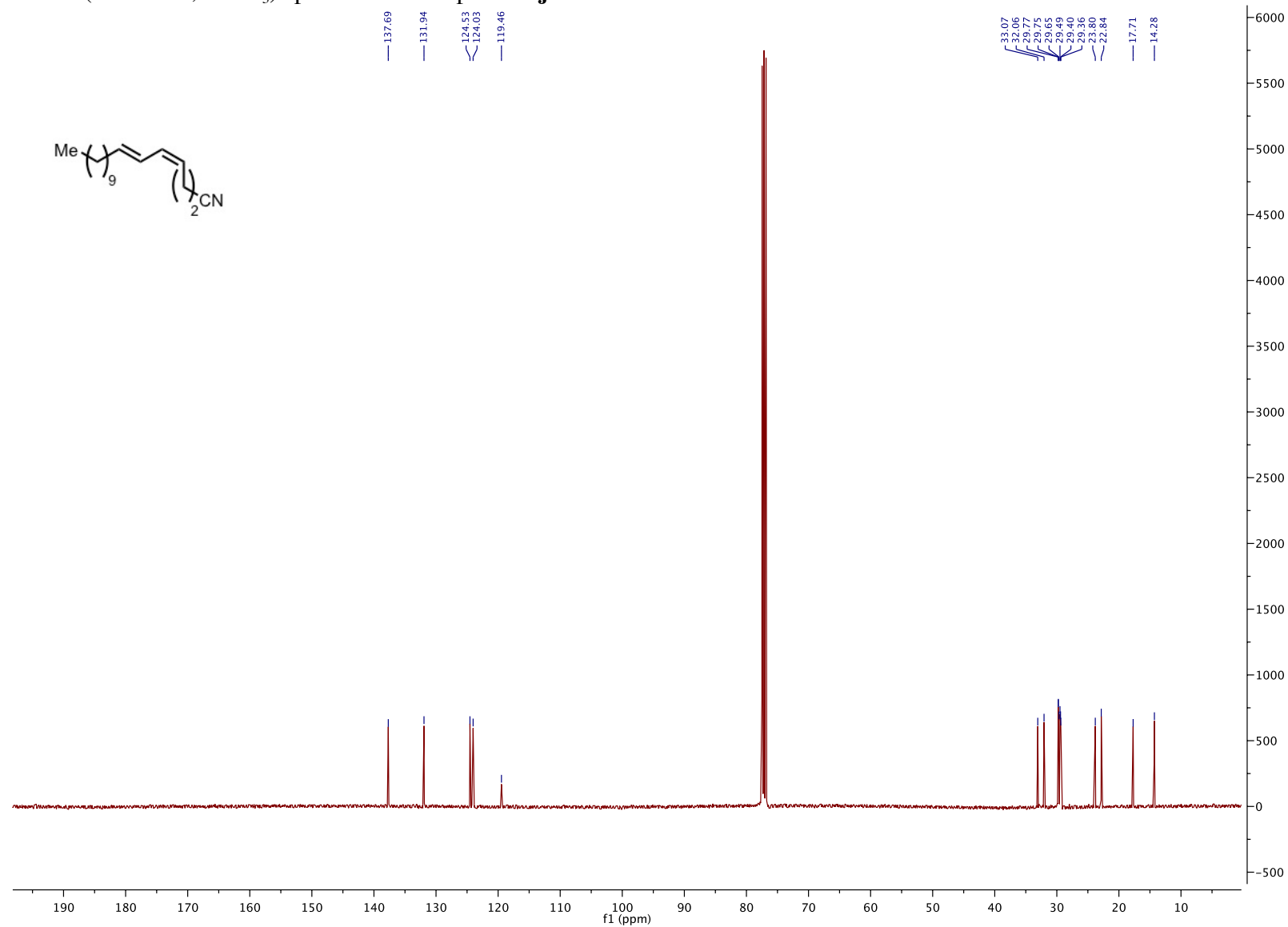
S158

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9j**.



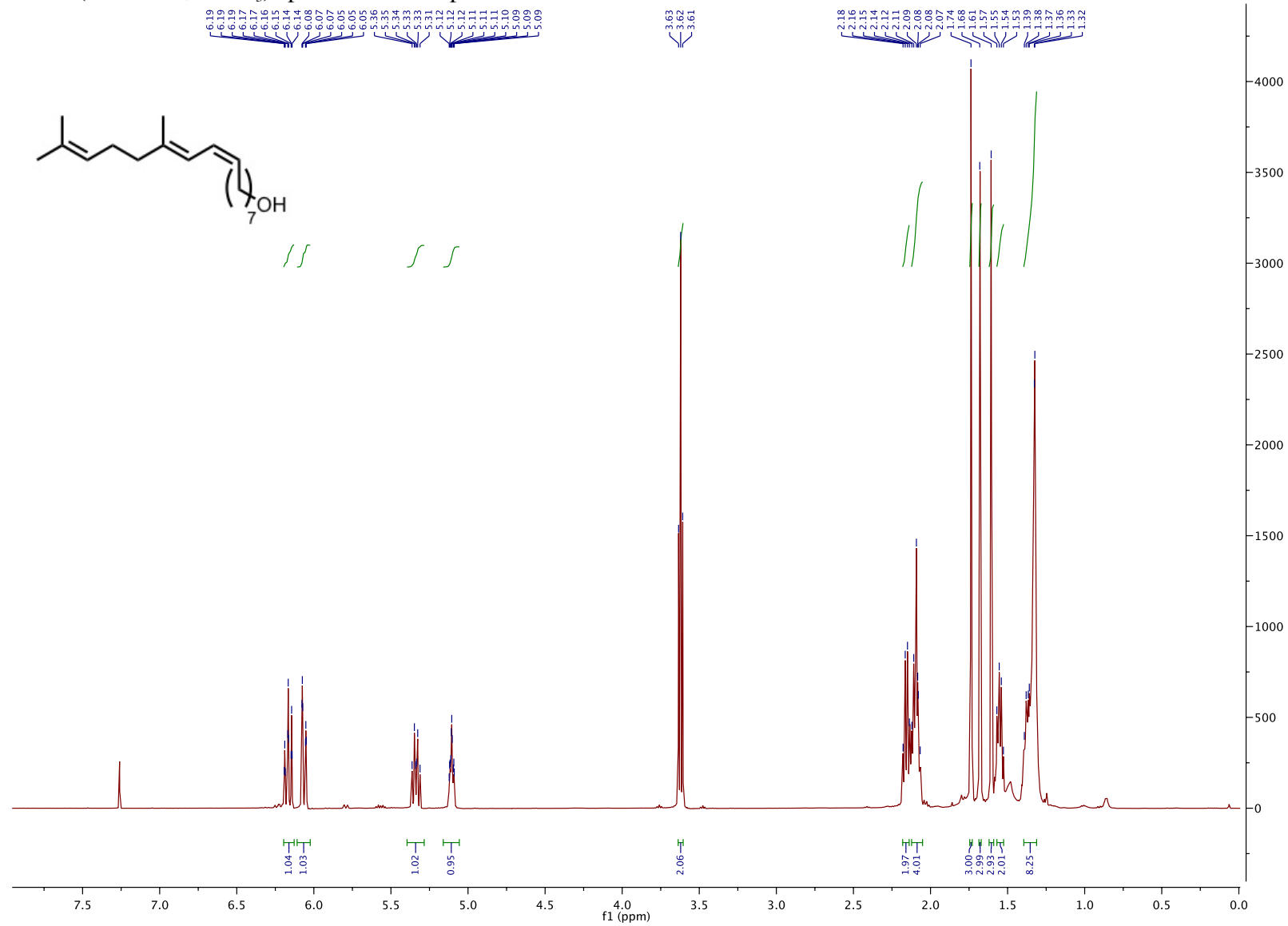
S159

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9j**.

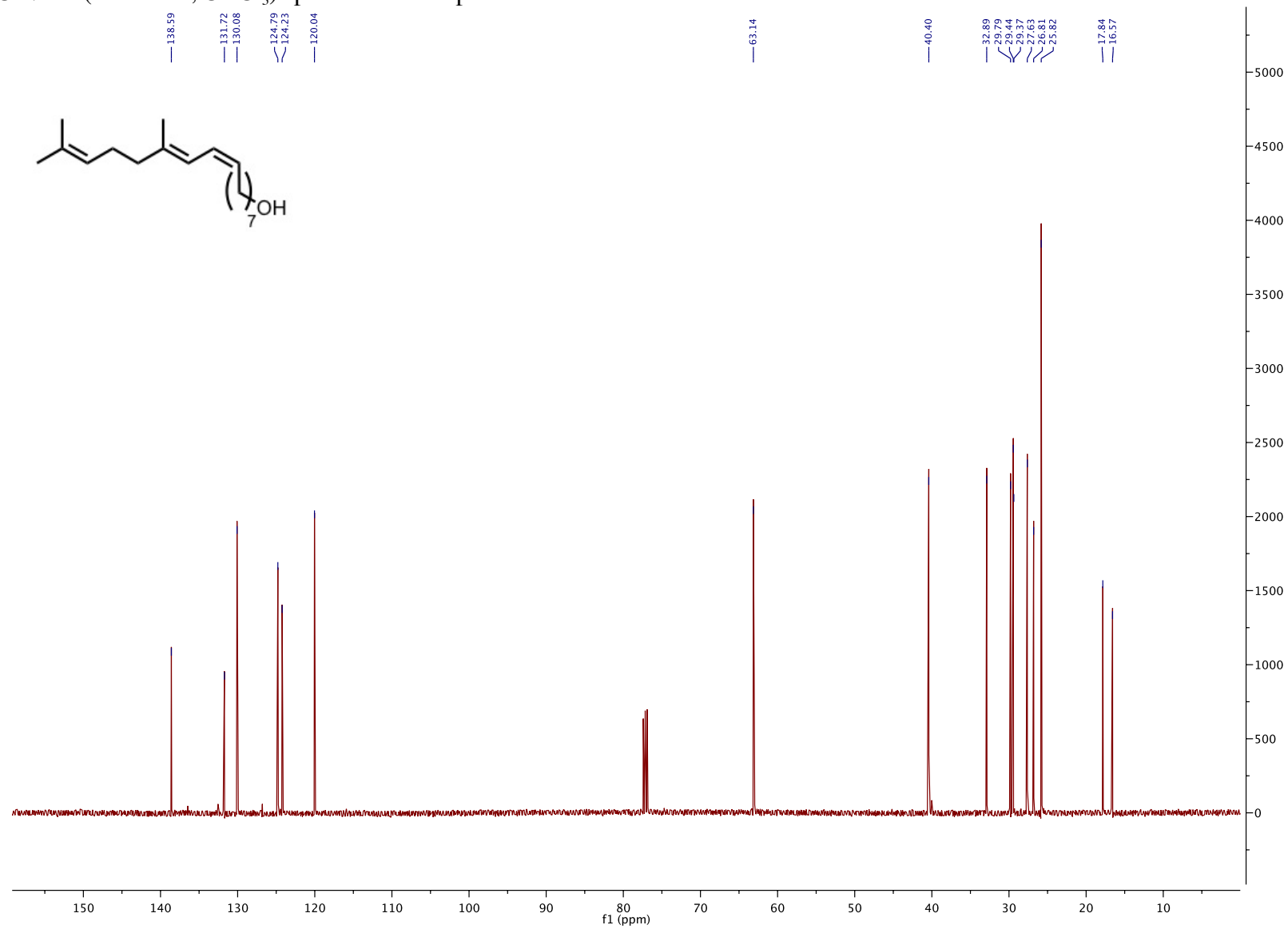


S160

^1H NMR (500 MHz, CDCl_3) spectrum of compound **9k**.

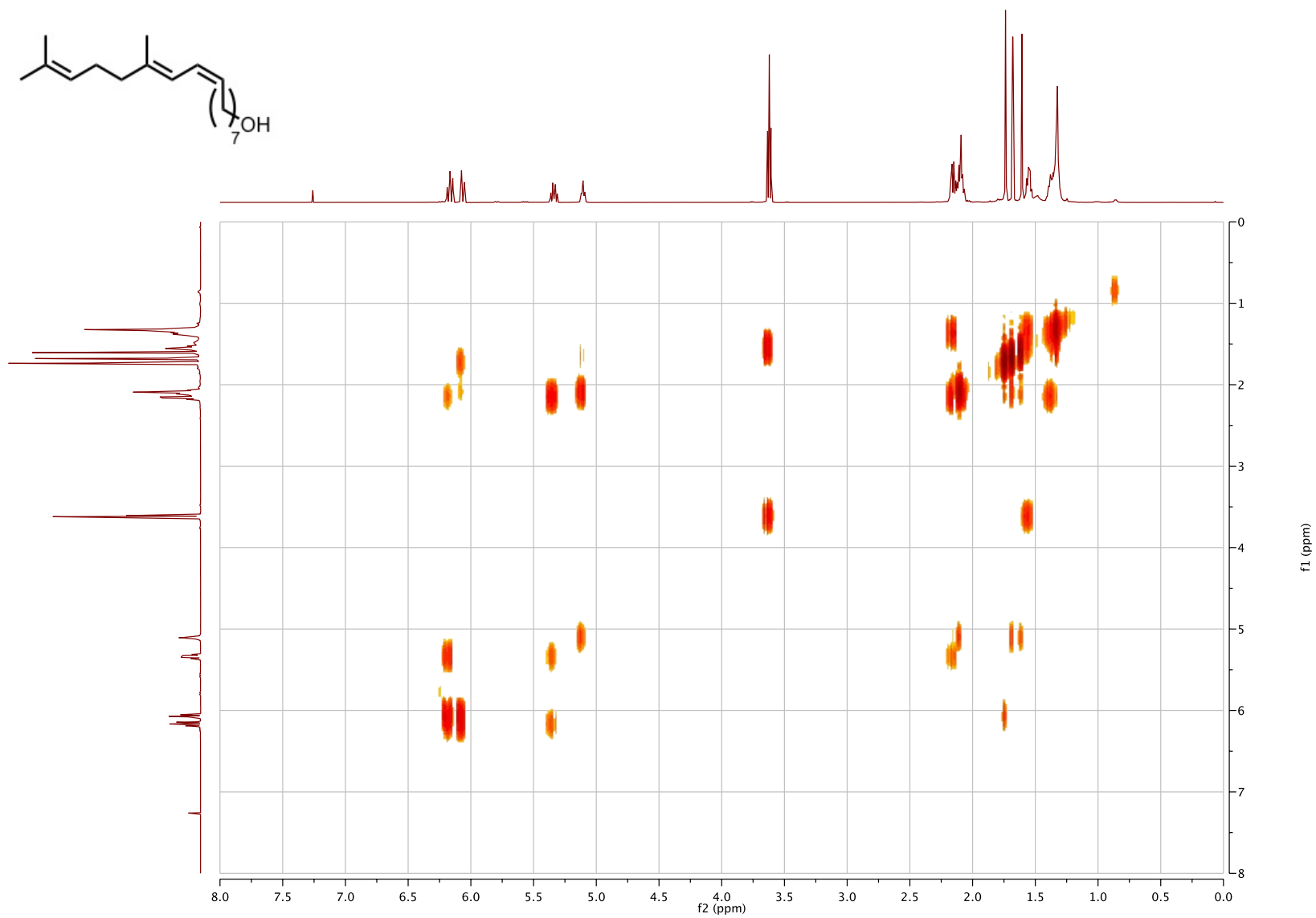


^{13}C NMR (126 MHz, CDCl_3) spectrum of compound **9k**.



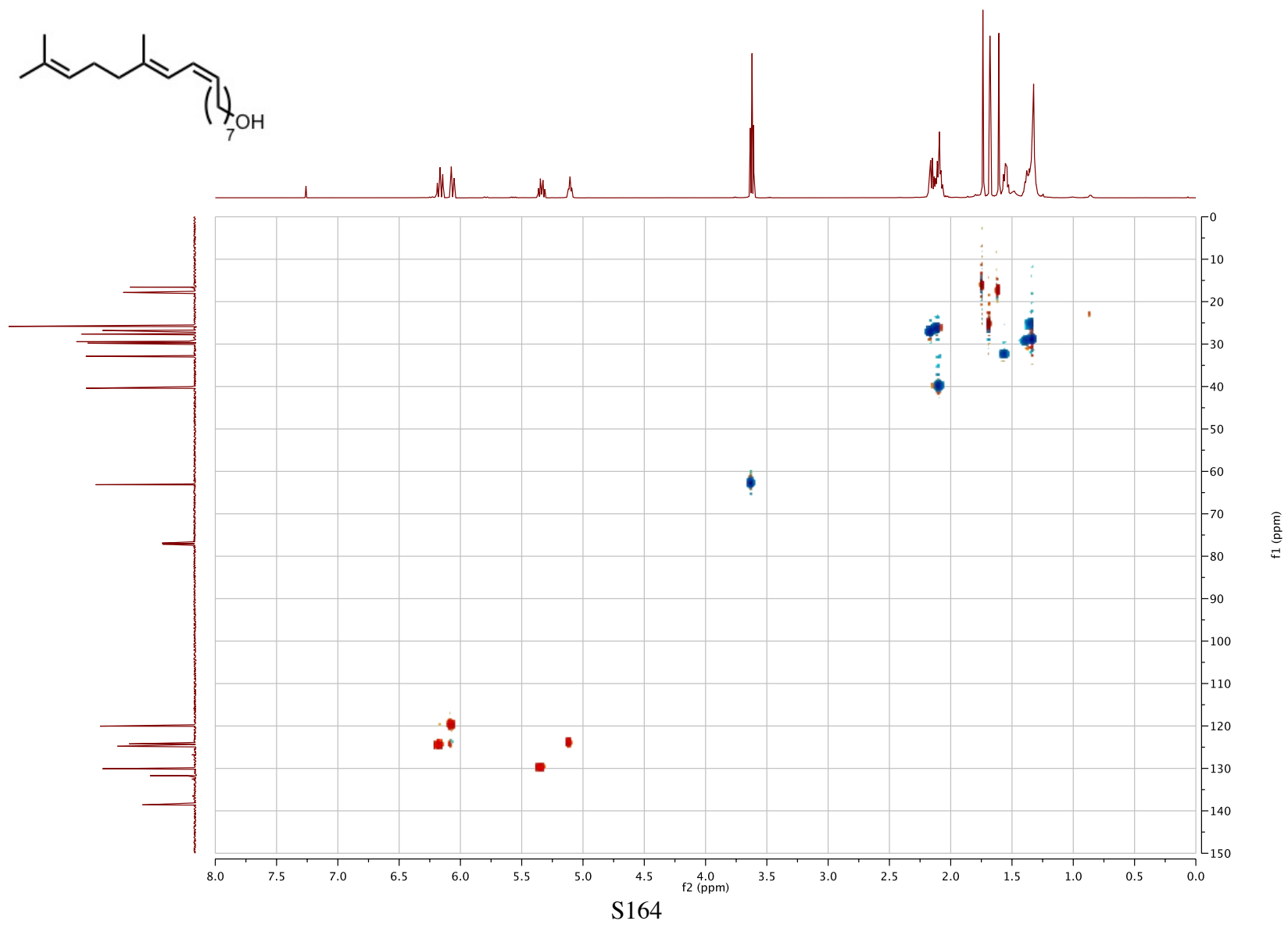
S162

gCOSY spectrum of compound **9k**.

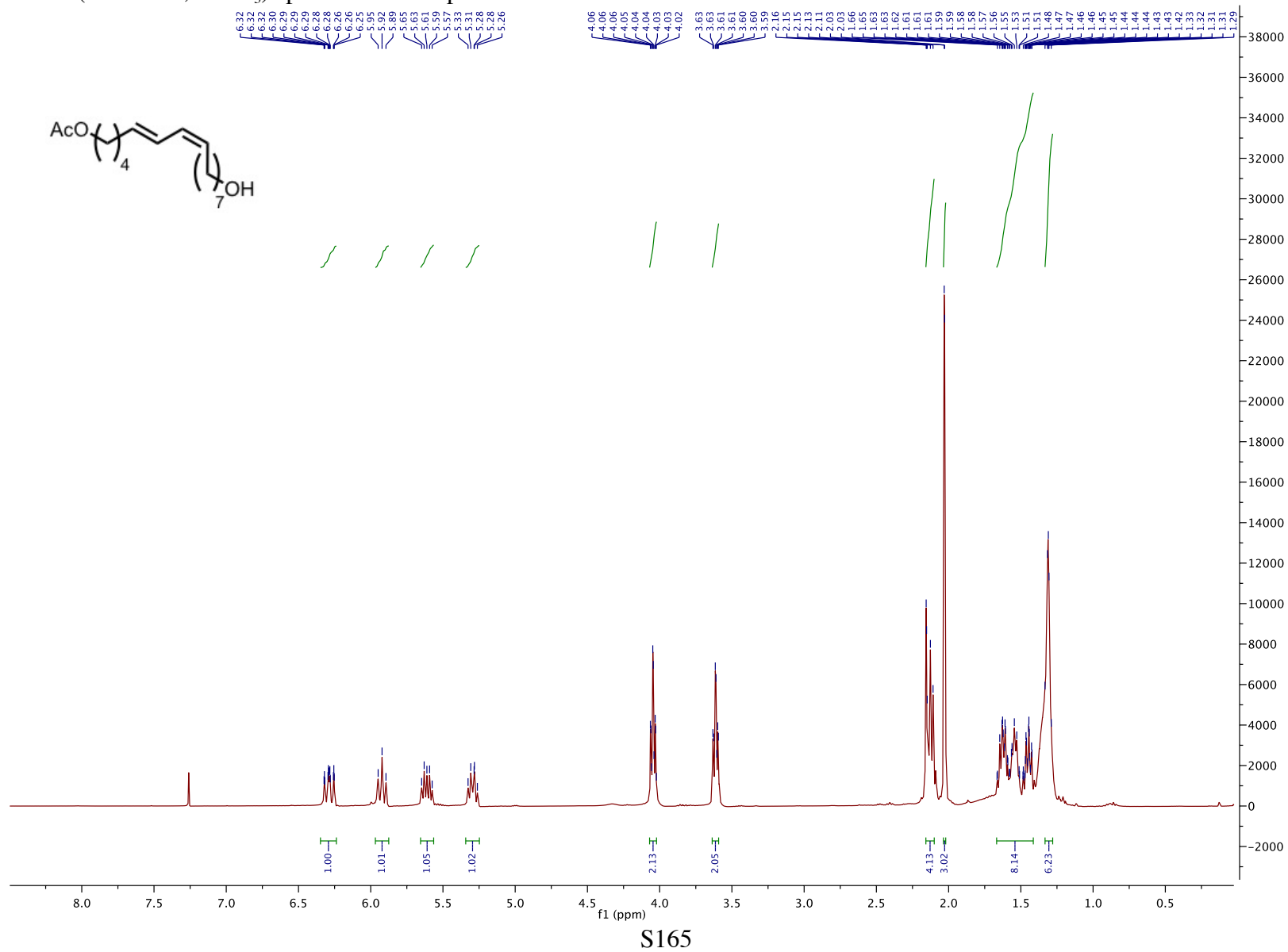


S163

HSQC spectrum of compound **9k**.



^1H NMR (400 MHz, CDCl_3) spectrum of compound **9l**.



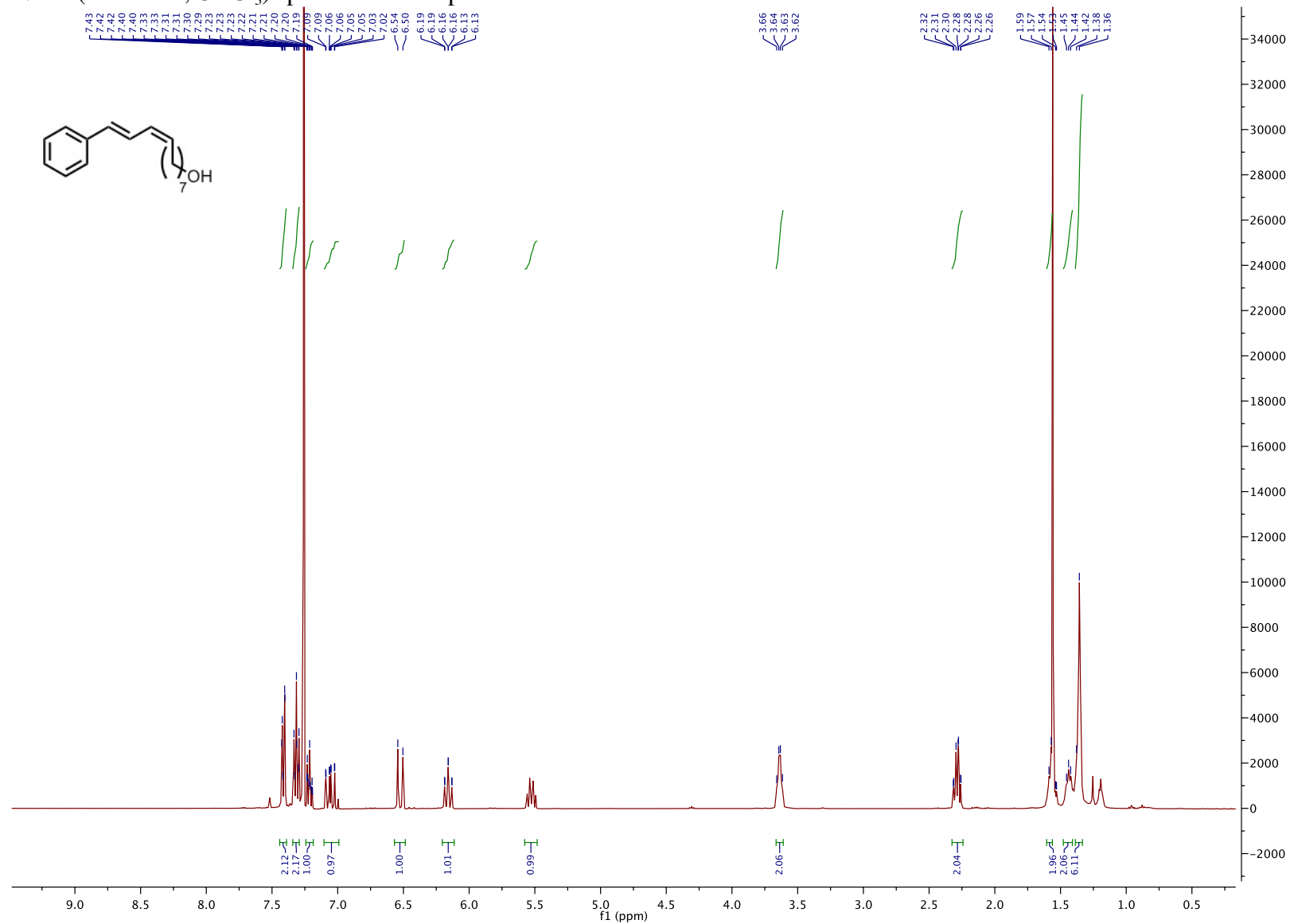
The figure displays the ¹³C NMR spectrum of poly(4-vinylpyridine). The x-axis represents the chemical shift in ppm, ranging from 180 to 20. The y-axis represents the intensity, ranging from -500 to 5000. The spectrum shows several distinct peaks corresponding to the different carbon environments in the polymer chain. A chemical structure of poly(4-vinylpyridine) is shown in the top left corner, with the repeating unit labeled with a subscript 4. The peaks are labeled with their chemical shift values in ppm: 171.41, 133.76, 130.51, 128.54, 126.56, 64.53, 63.07, 32.85, 32.48, 28.71, 28.38, 28.00, 27.75, 25.80, 25.78, and 21.12.

Chemical structure of poly(4-vinylpyridine) is shown in the top left corner, with the repeating unit labeled with a subscript 4.

Chemical shift values (ppm) are listed on the right side of the spectrum:

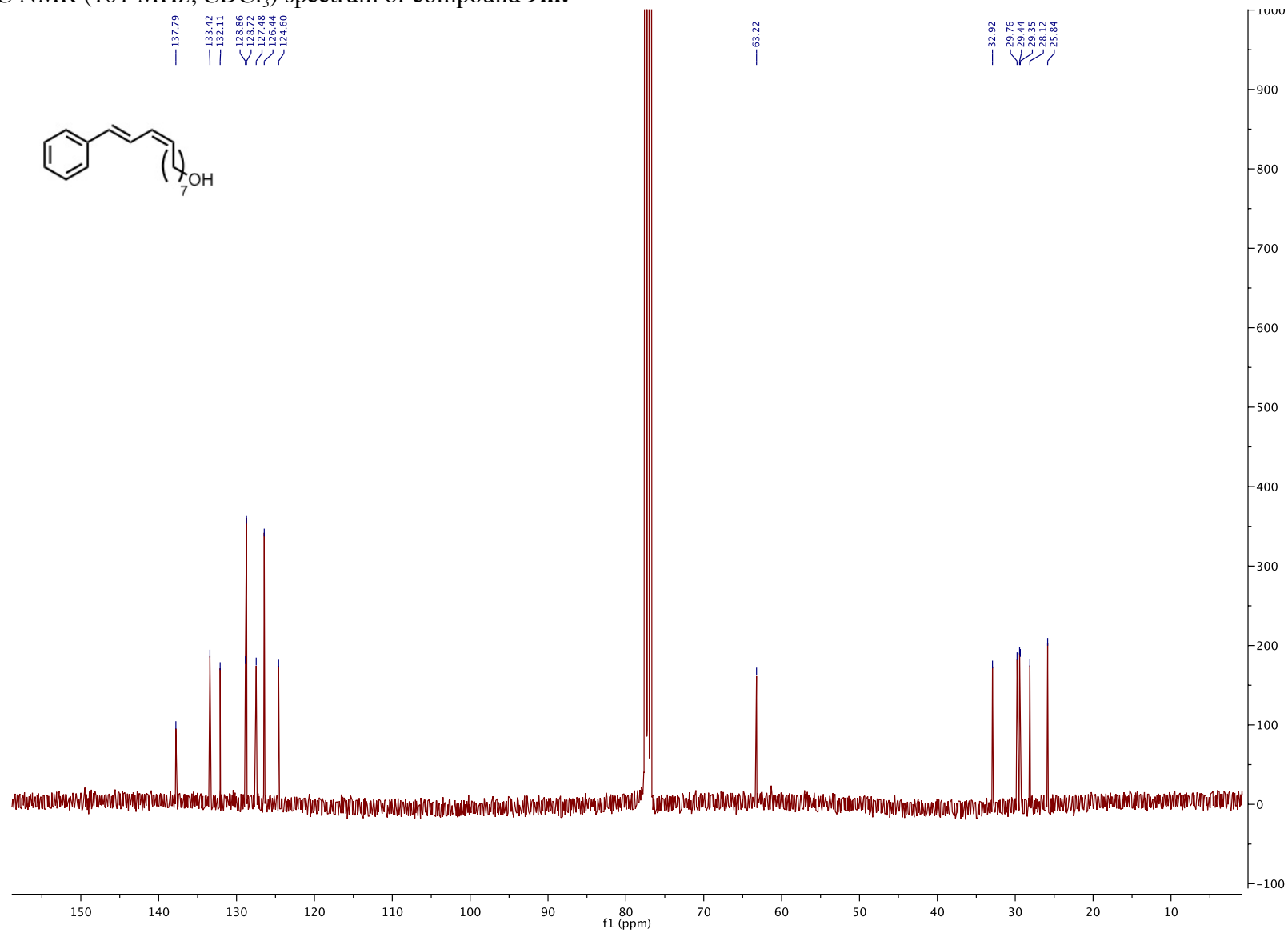
- 171.41
- 133.76
- 130.51
- 128.54
- 126.56
- 64.53
- 63.07
- 32.85
- 32.48
- 28.71
- 28.38
- 28.00
- 27.75
- 25.80
- 25.78
- 21.12

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9m**.



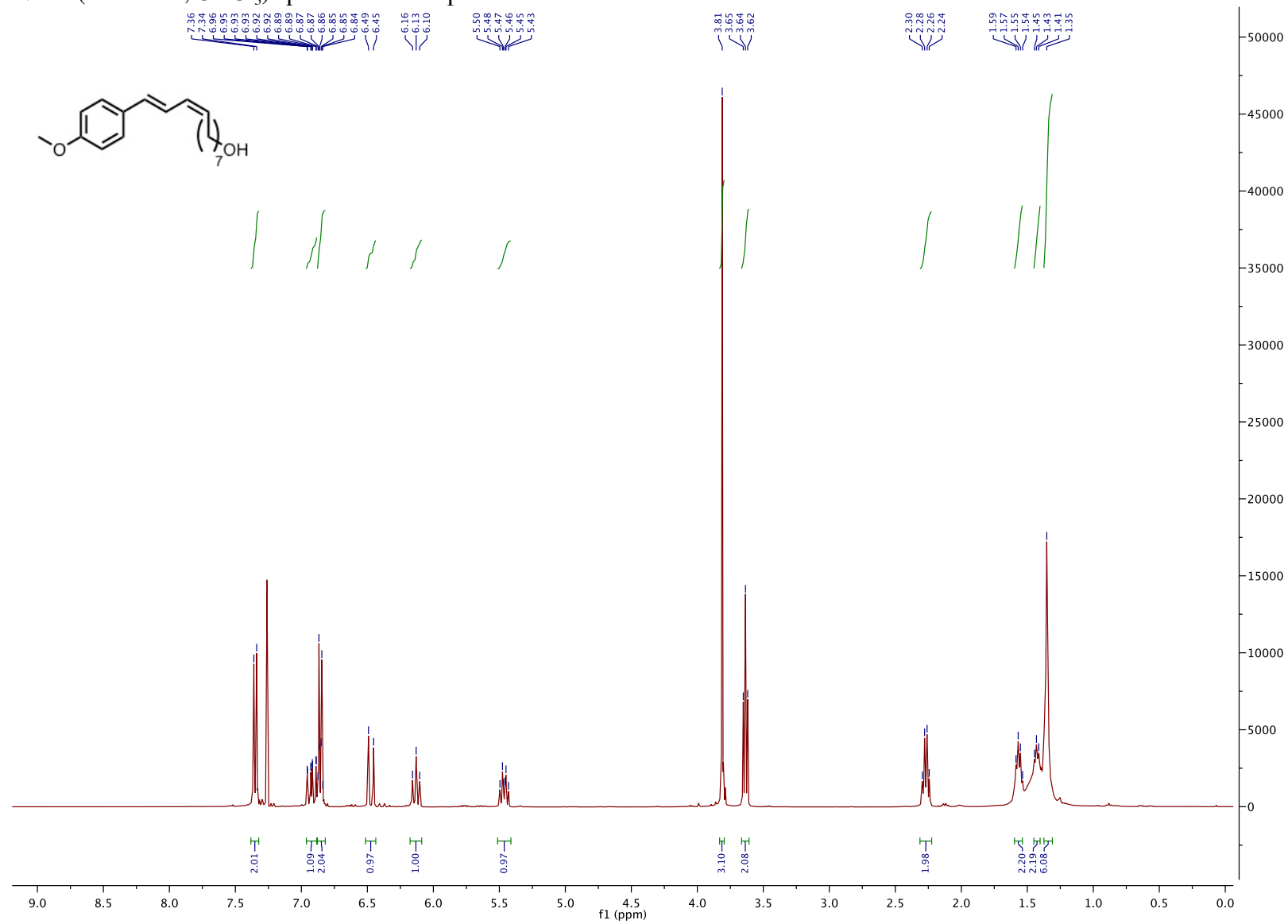
S167

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9m**.



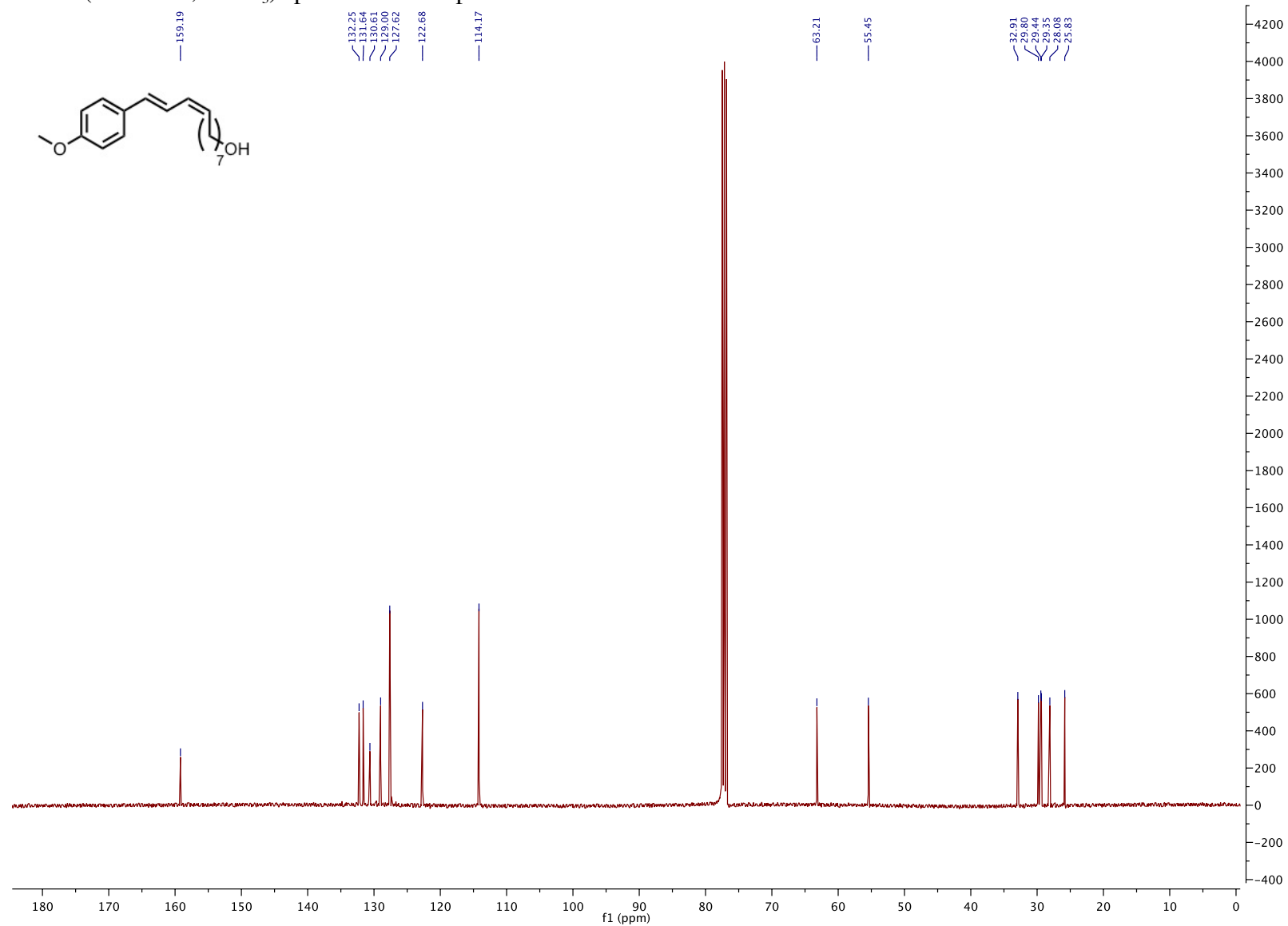
S168

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9n**.



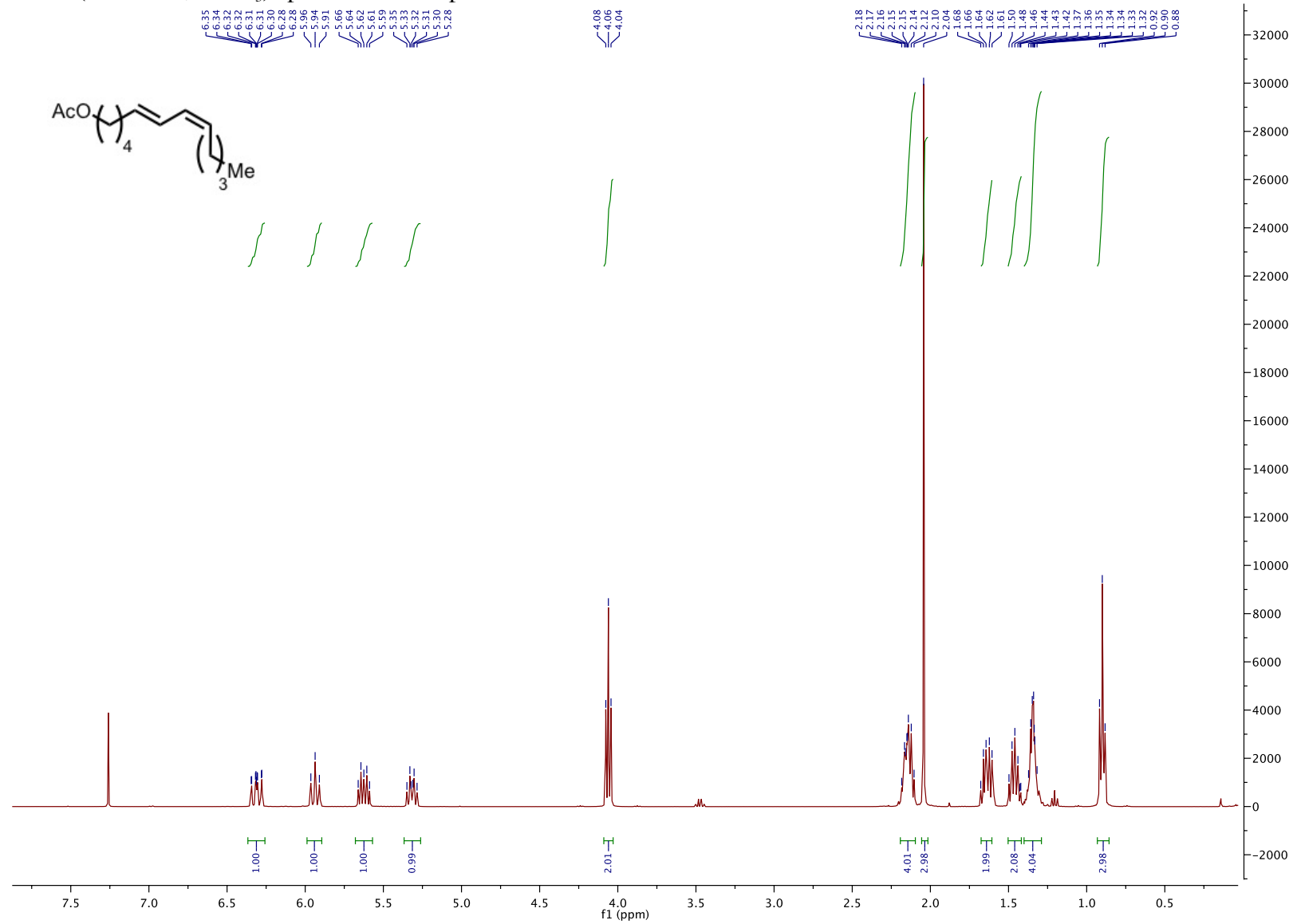
S169

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9n**.



S170

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9o**.



S171

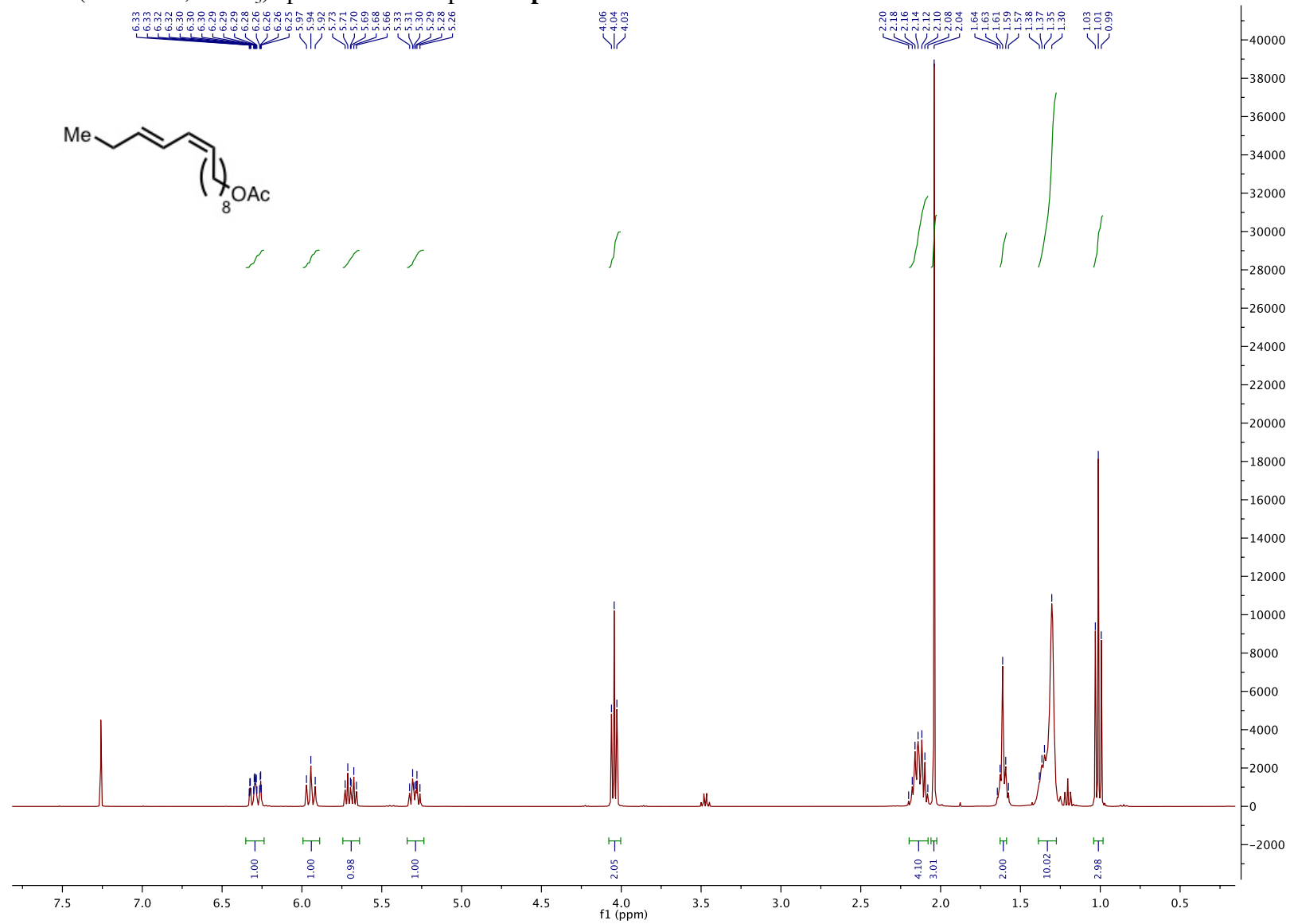
Chemical structure of poly(4-vinylstyrene): CC(=C)C=C(C)C(=O)OC

Peak assignments (ppm):

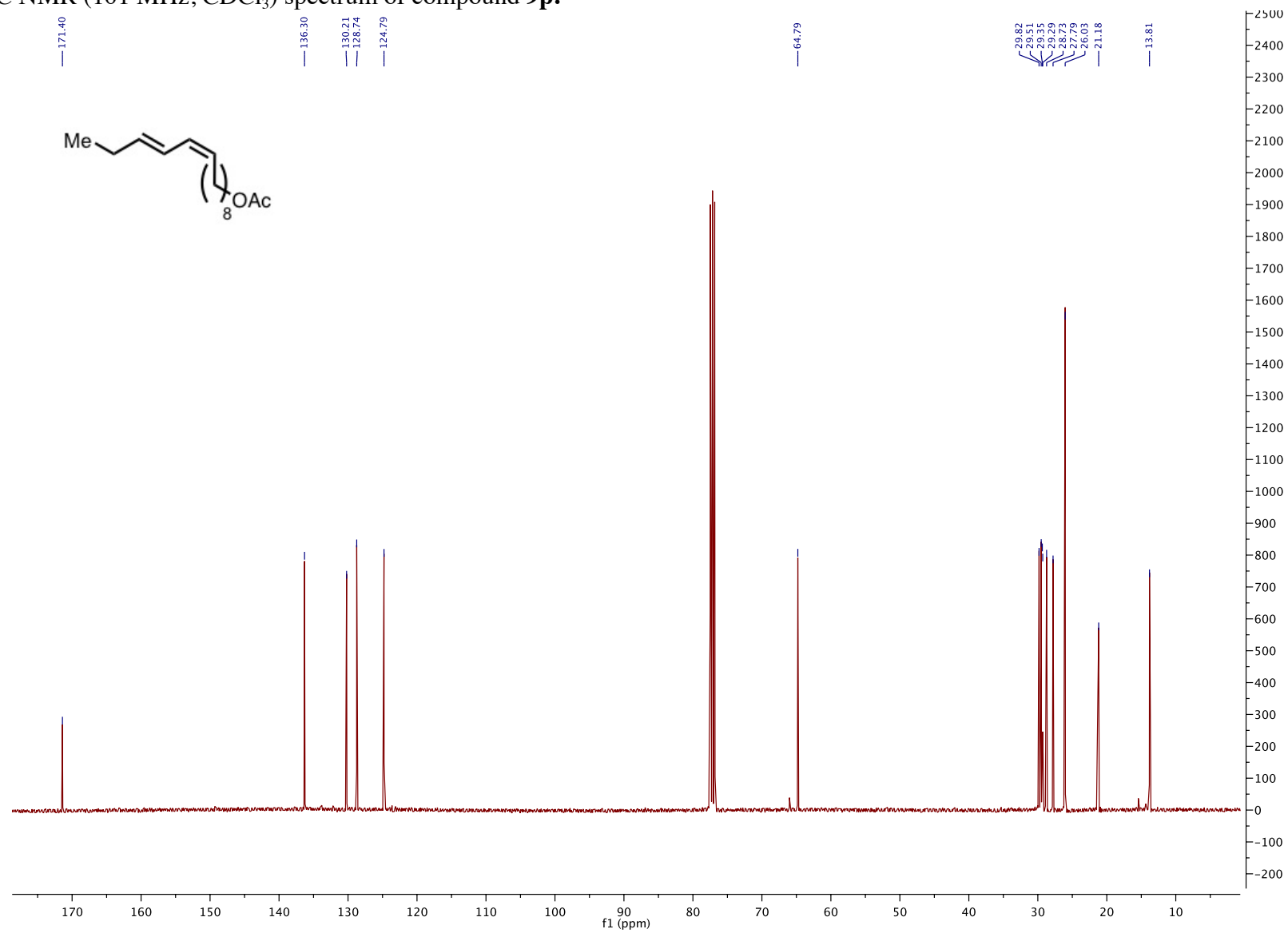
- 171.37
- 133.73
- 130.67
- 128.50
- 126.32
- 77.48
- 77.16
- 64.56
- 32.53
- 32.02
- 28.25
- 27.55
- 25.84
- 22.47
- 21.16
- 14.12

S172

^1H NMR (400 MHz, CDCl_3) spectrum of compound **9p**.

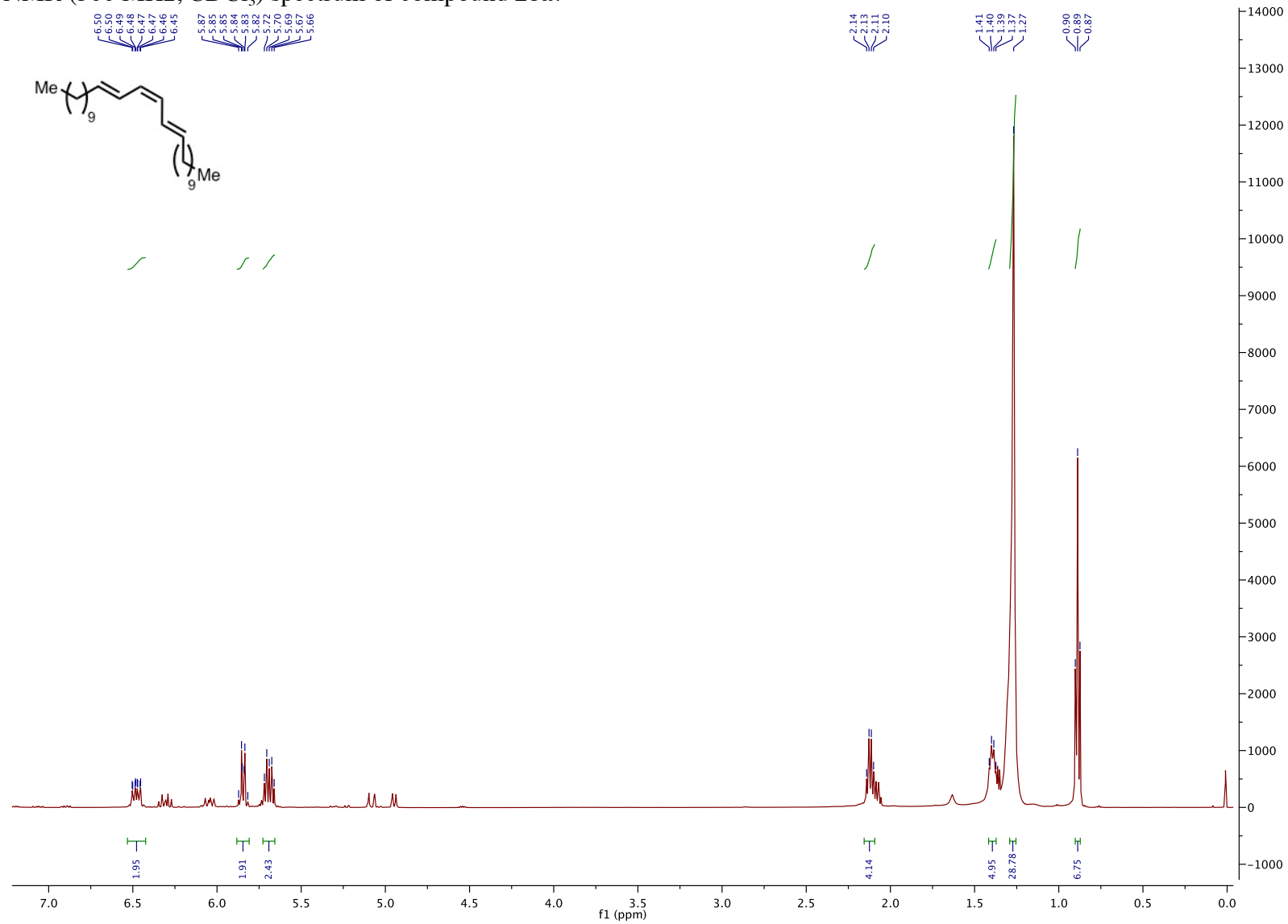


^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **9p**.



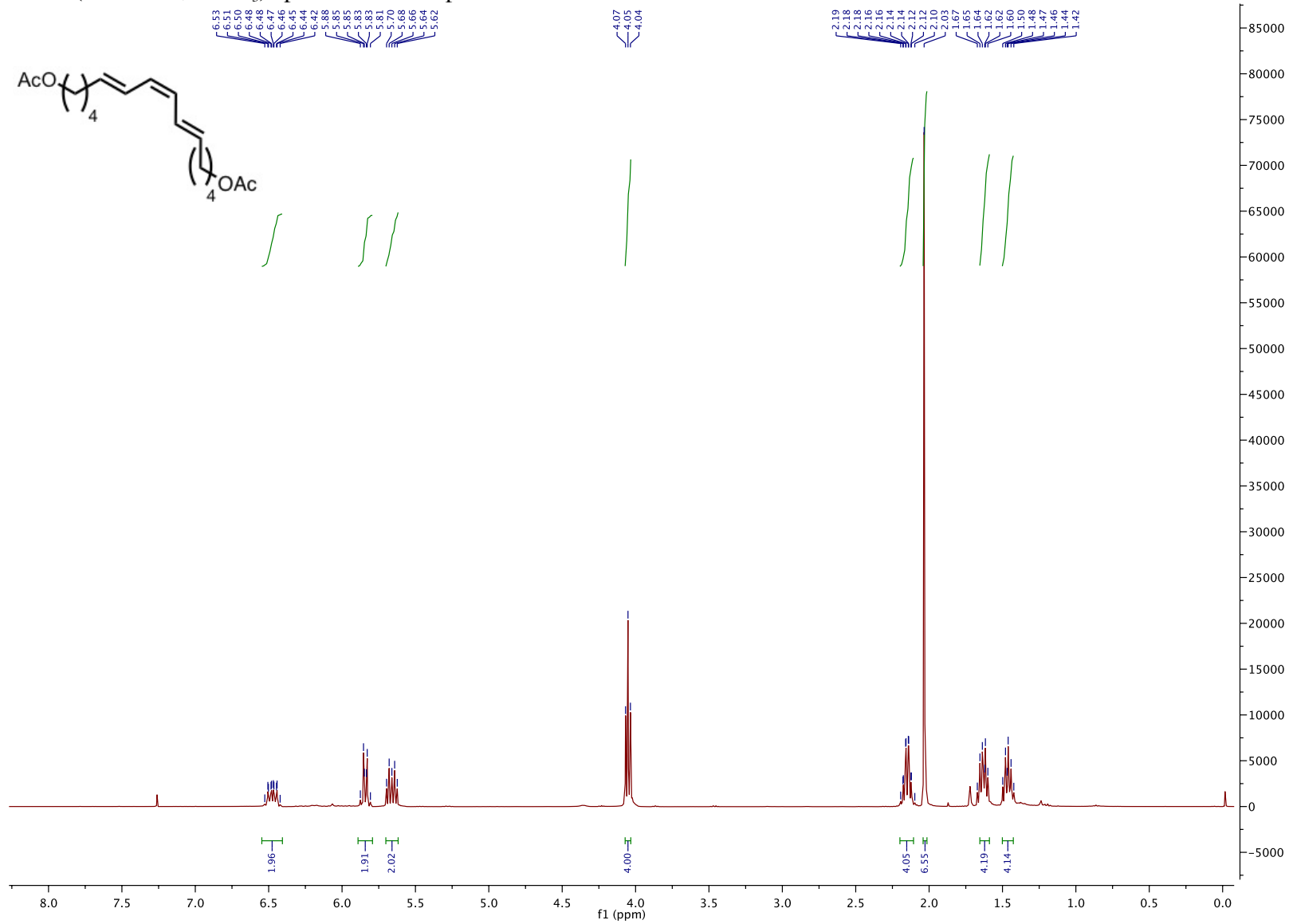
S174

^1H NMR (500 MHz, CDCl_3) spectrum of compound **28a**.



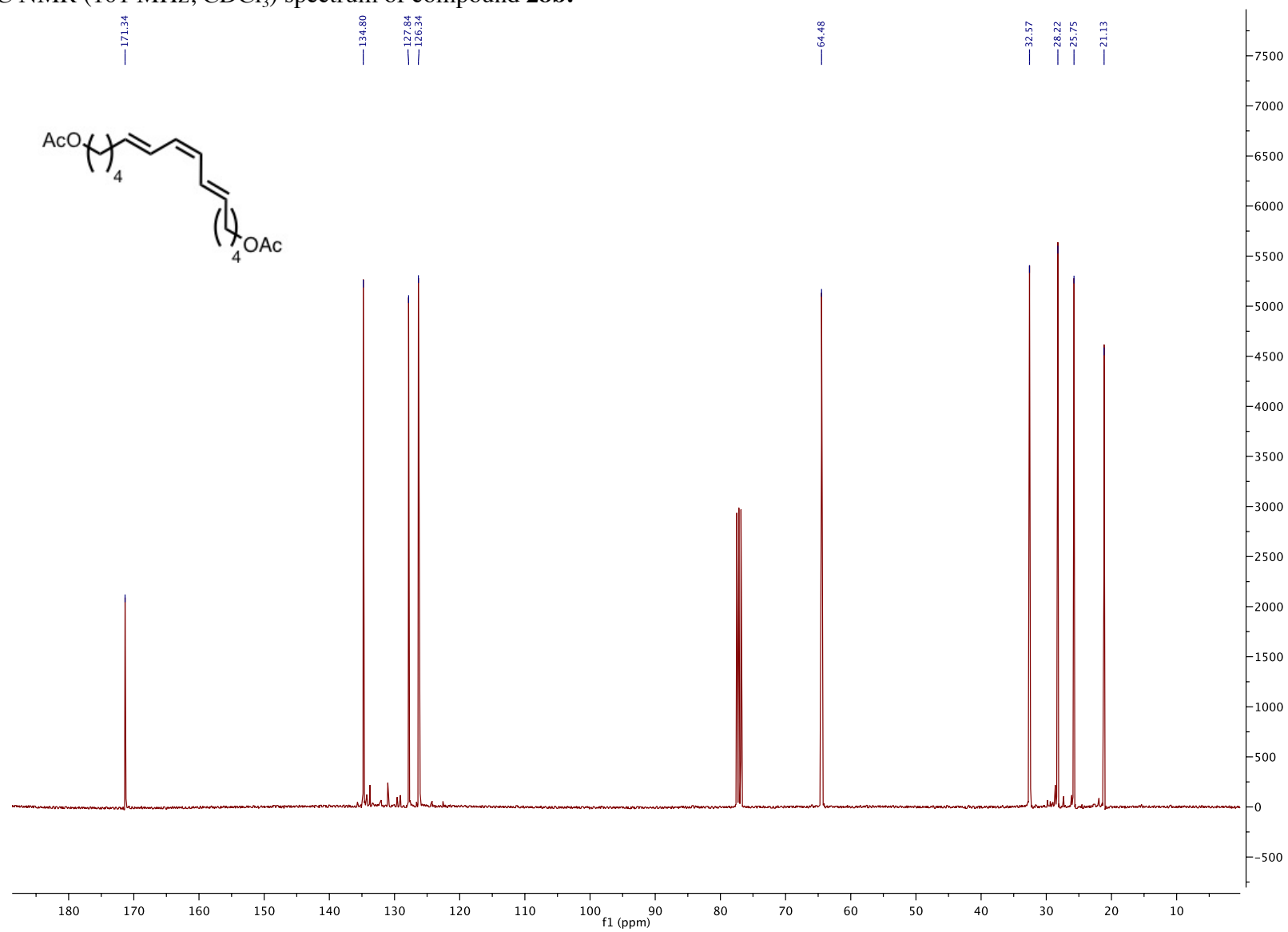
S175

^1H NMR (400 MHz, CDCl_3) spectrum of compound **28b**.



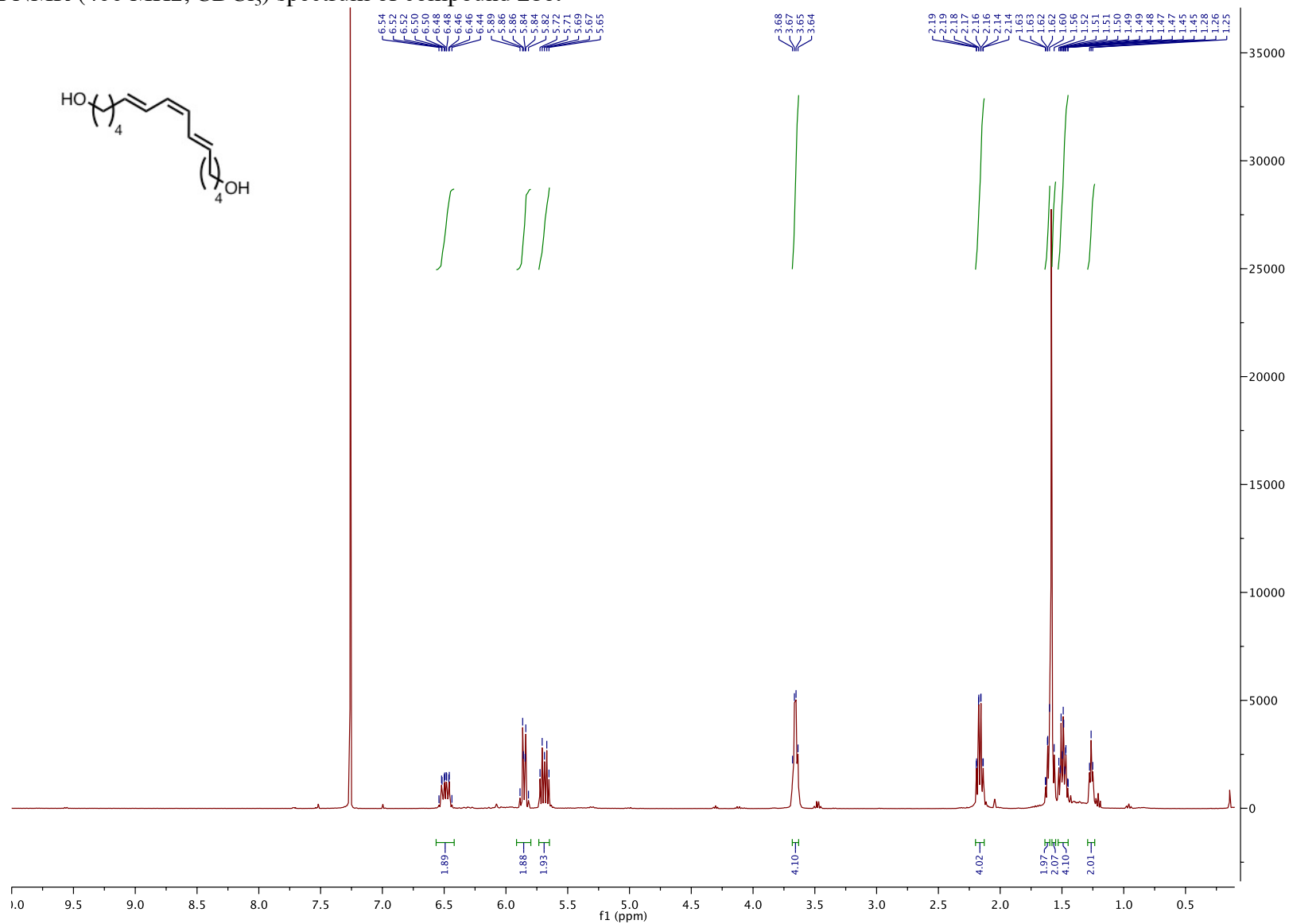
S176

^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **28b**.

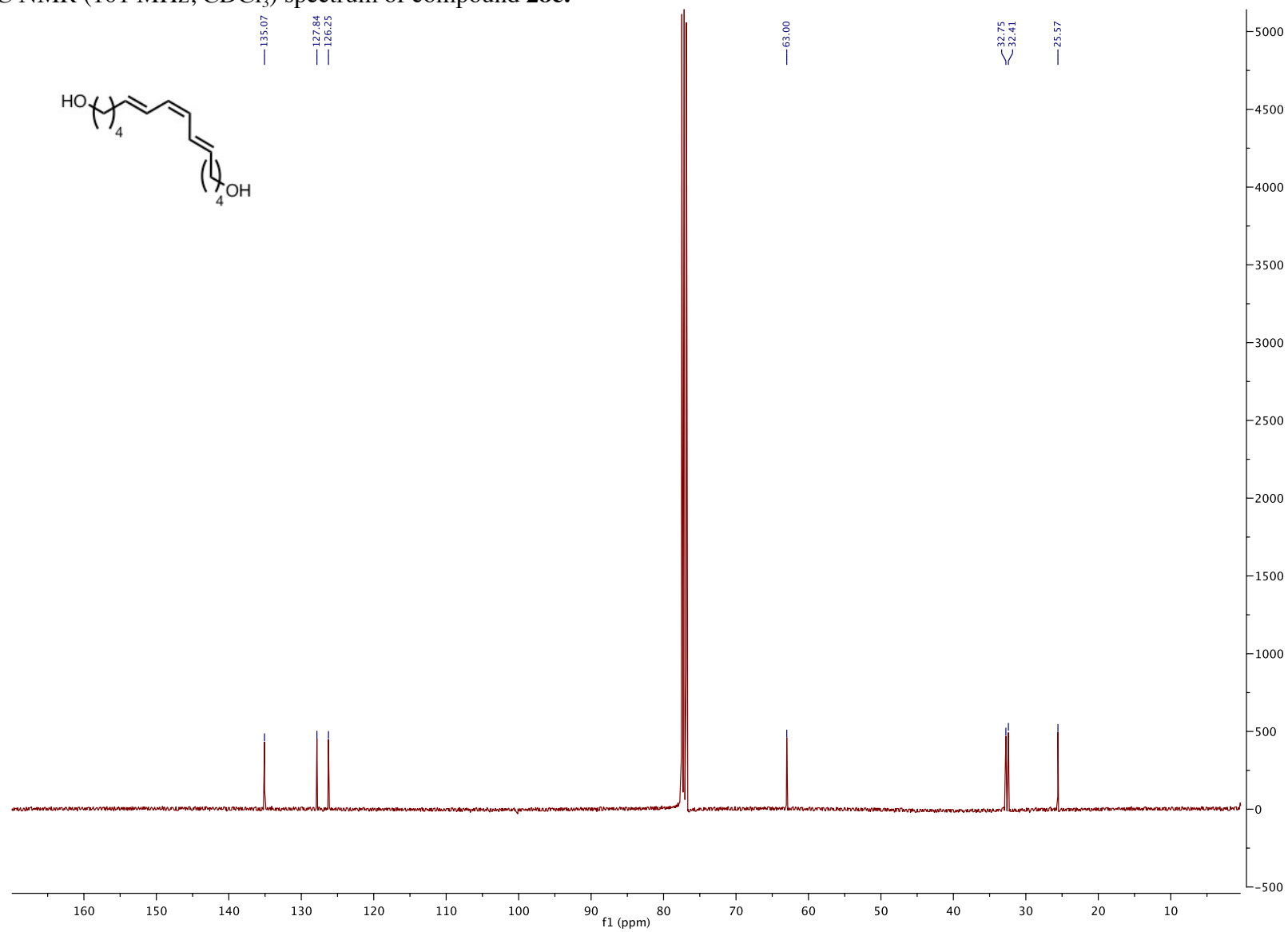


S177

^1H NMR (400 MHz, CDCl_3) spectrum of compound **28c**.

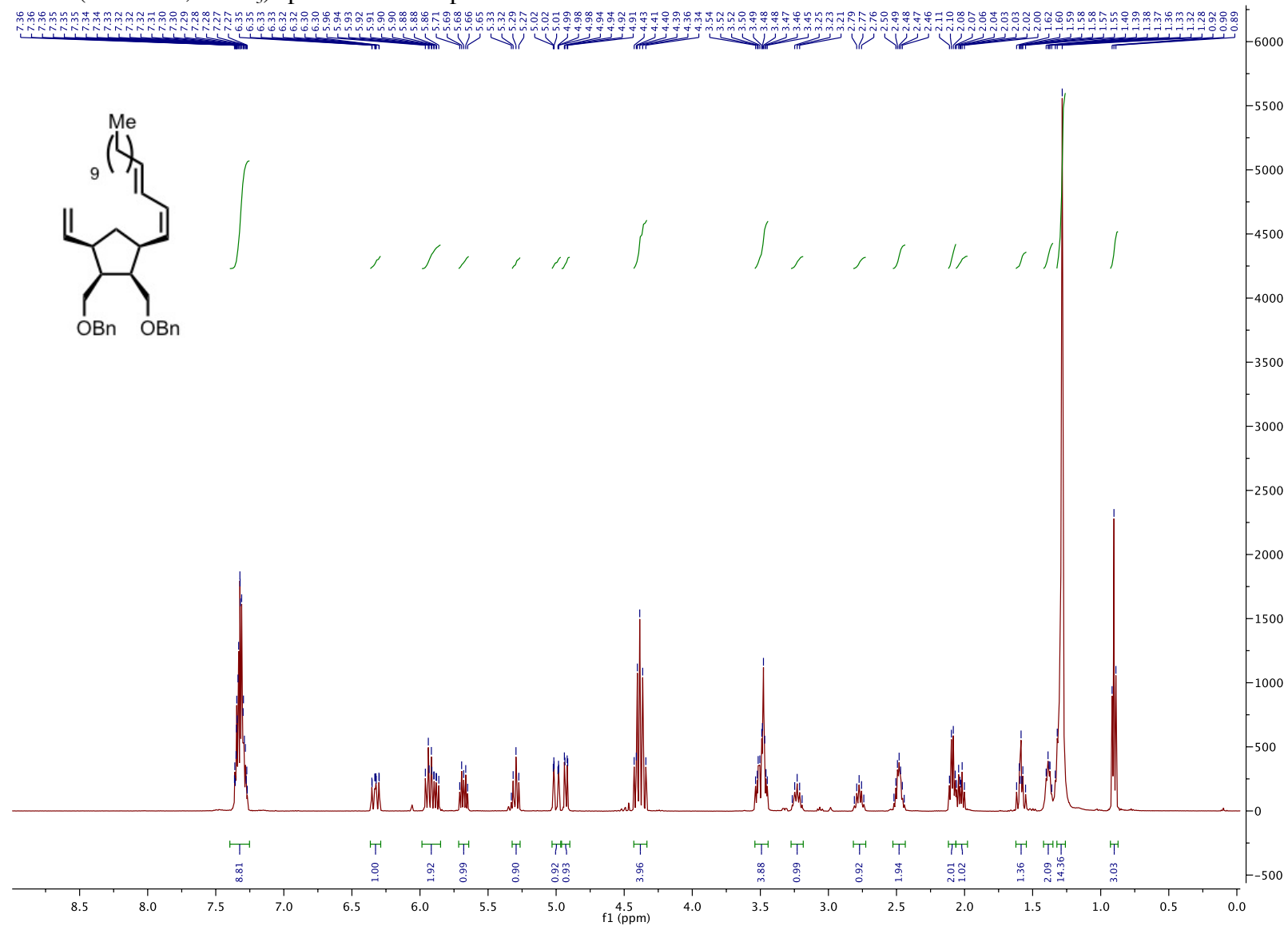


^{13}C NMR (101 MHz, CDCl_3) spectrum of compound **28c**.



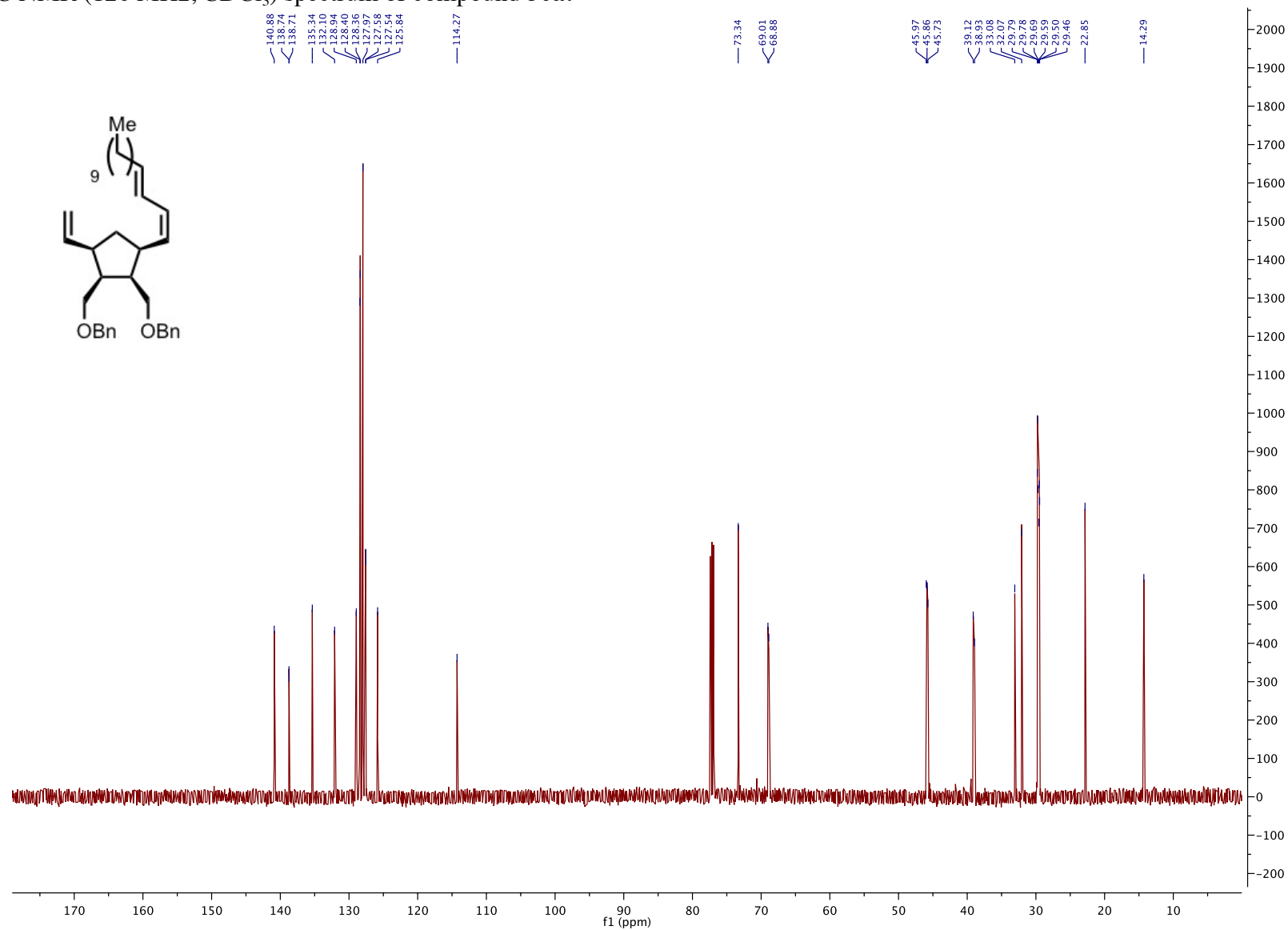
S179

^1H NMR (500 MHz, CDCl_3) spectrum of compound **30a**.



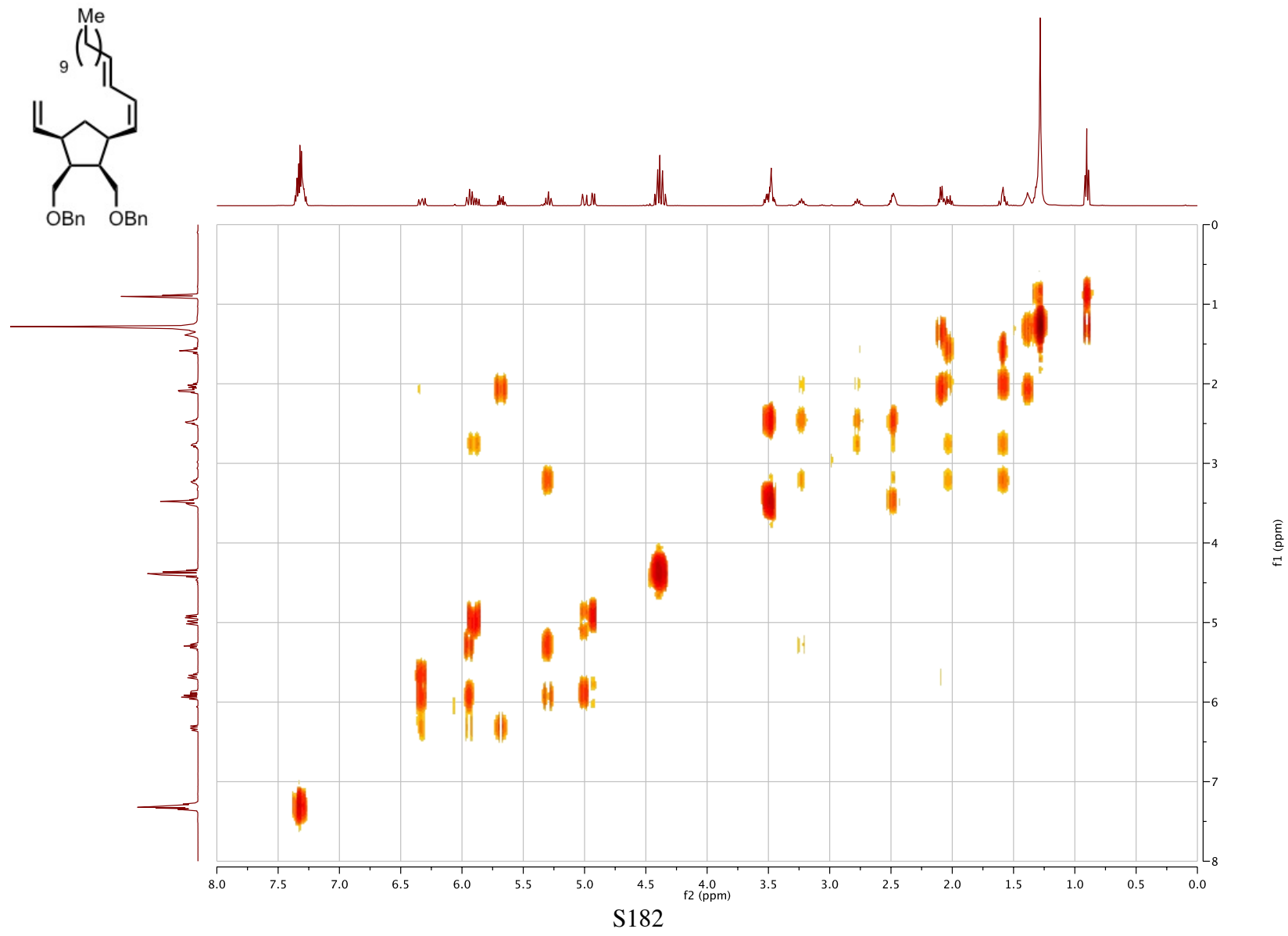
S180

^{13}C NMR (126 MHz, CDCl_3) spectrum of compound **30a**.

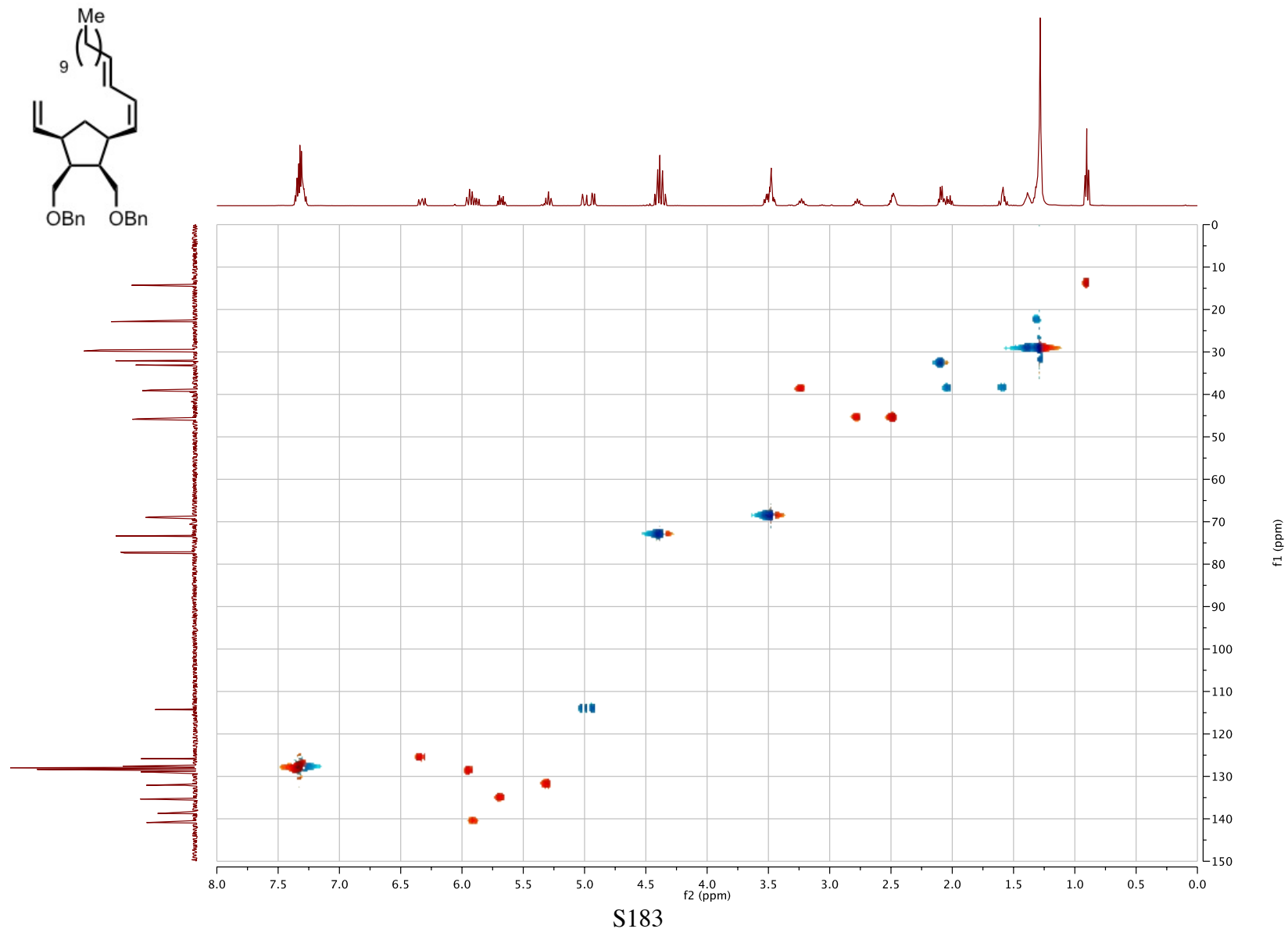


S181

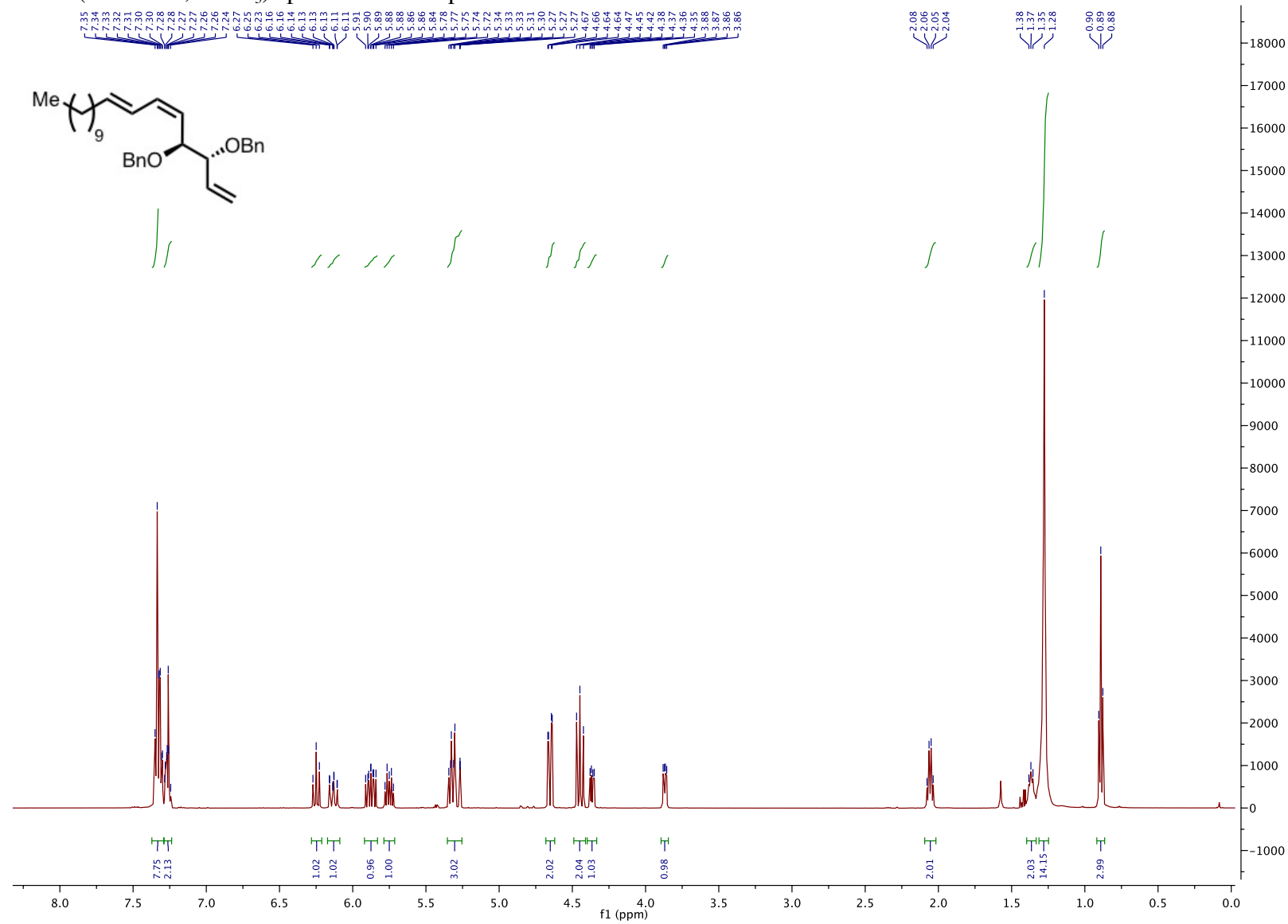
gCOSY spectrum of compound **30a**.



HSQC spectrum of compound **30a**.

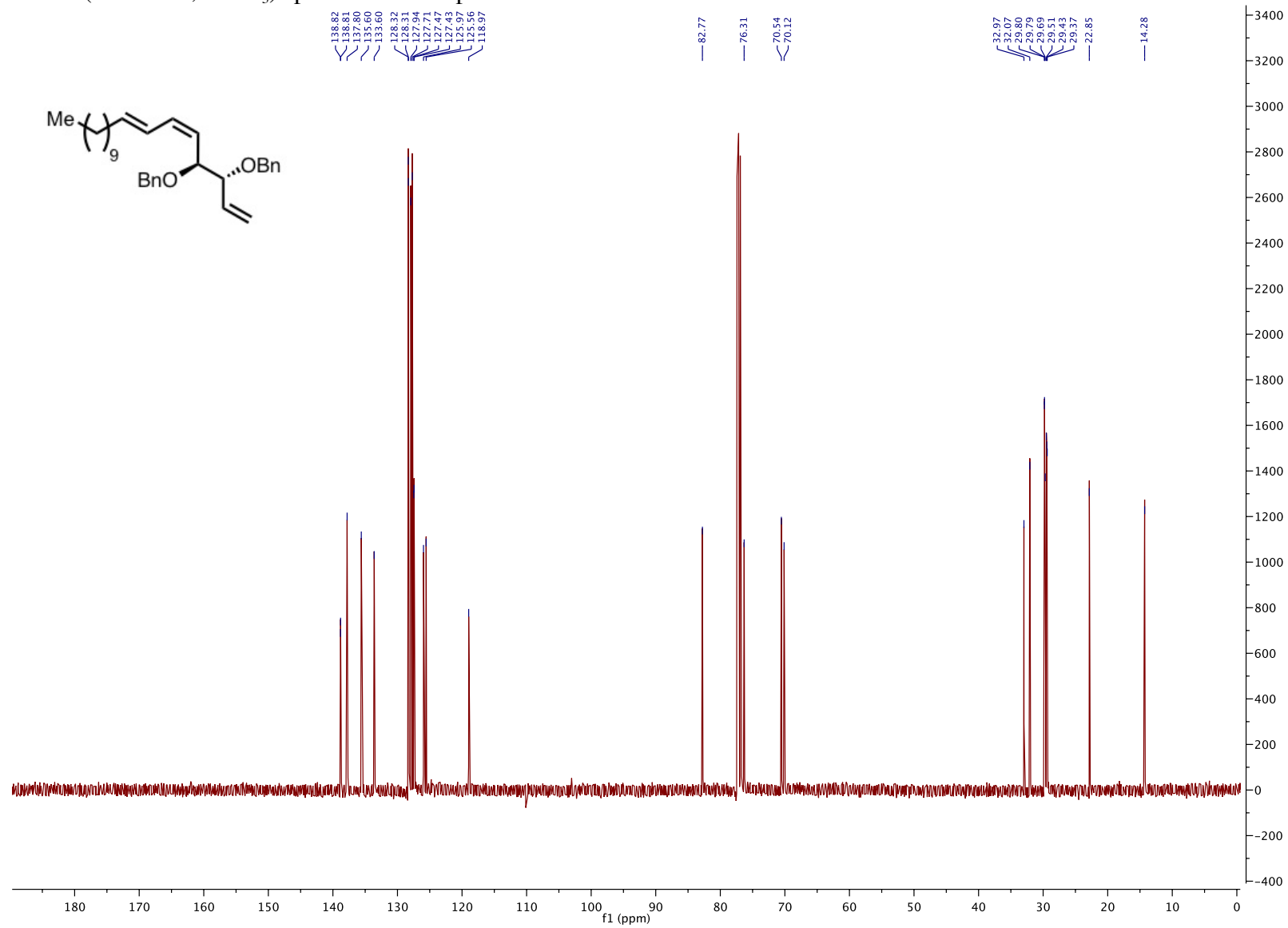


^1H NMR (500 MHz, CDCl_3) spectrum of compound **30b**.



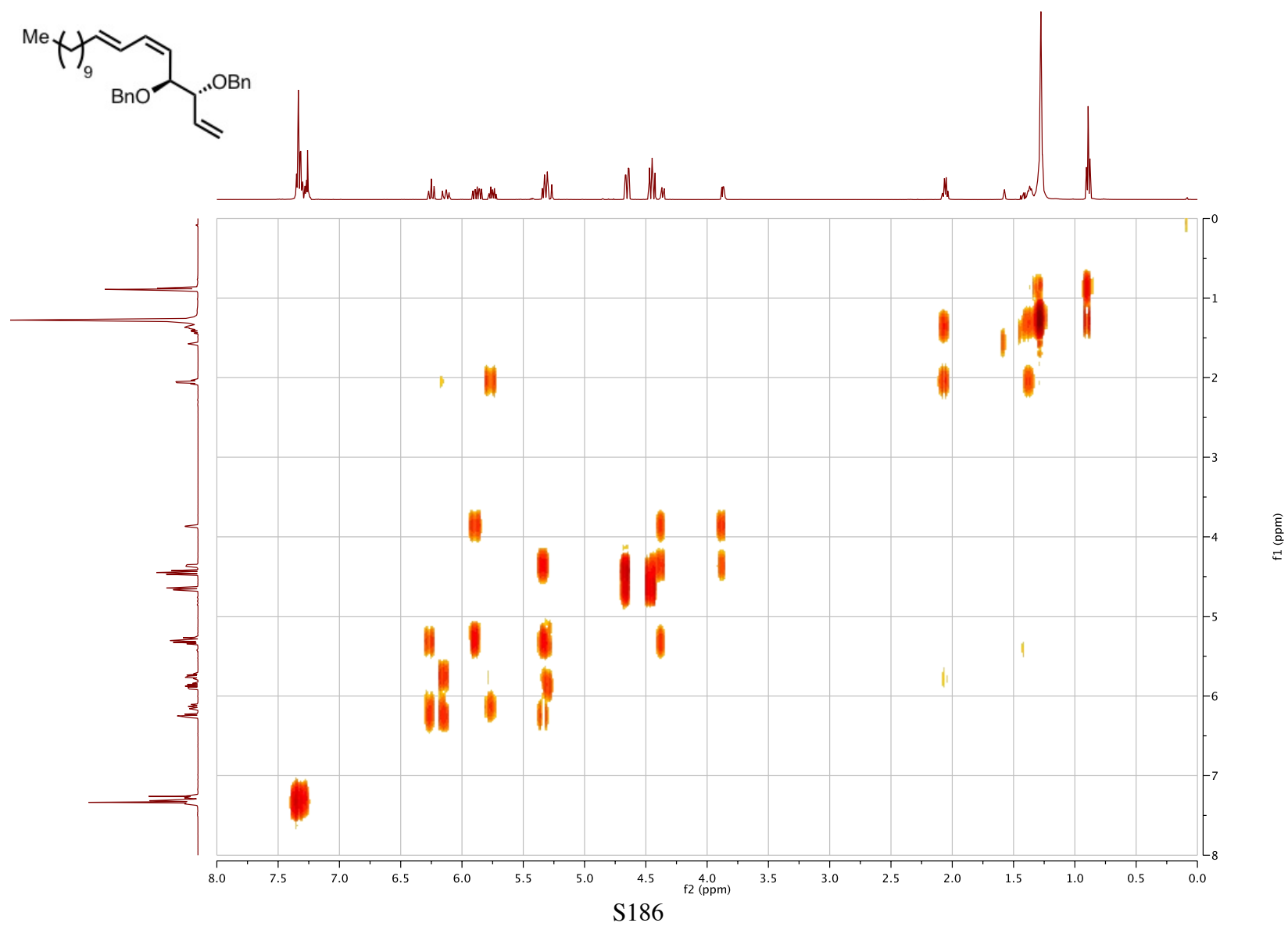
S184

^{13}C NMR (126 MHz, CDCl_3) spectrum of compound **30b**.

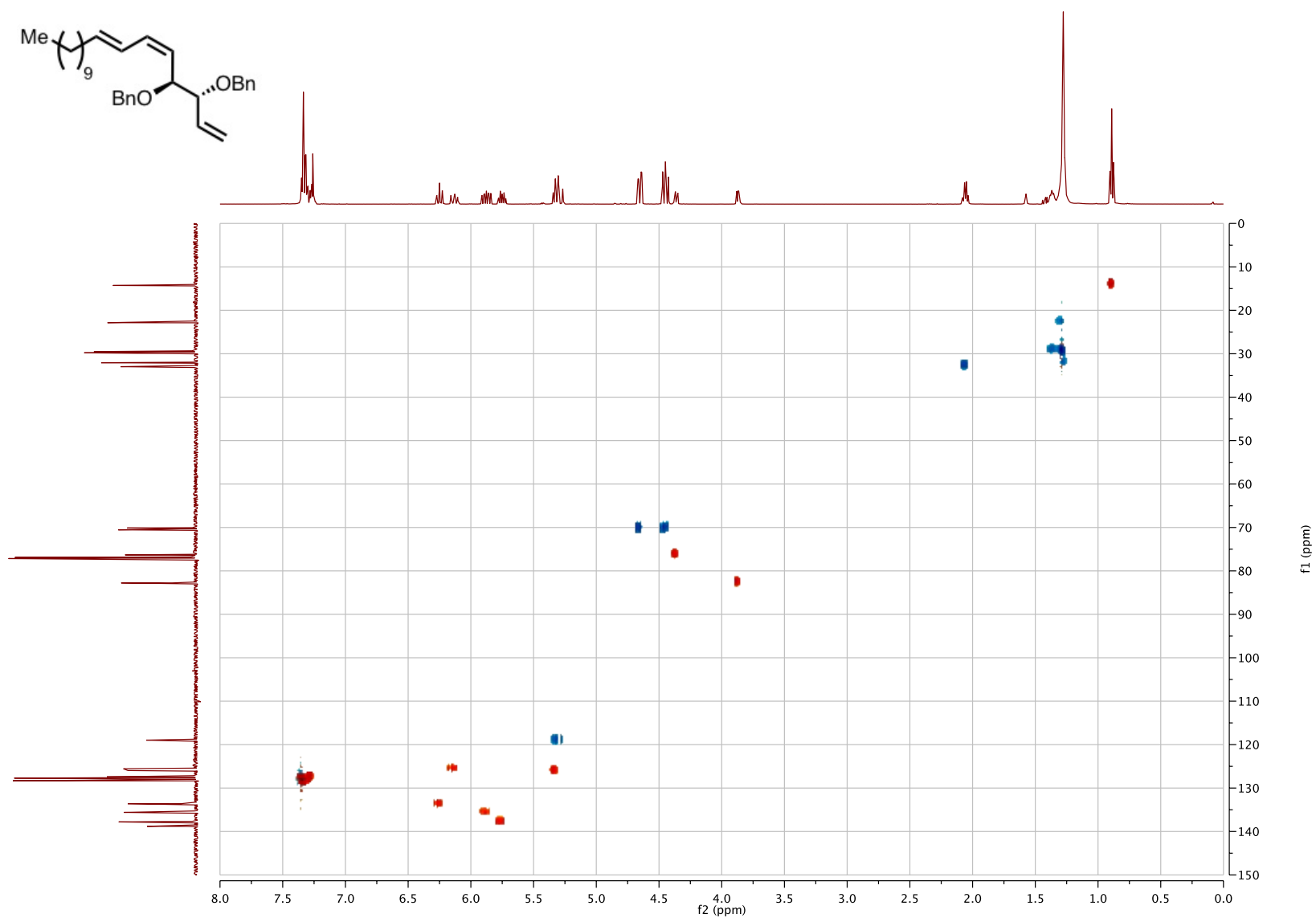


S185

gCOSY spectrum of compound **30b**.



HSQC spectrum of compound **30b**.



S187